Full wwPDB EM Validation Report ⓘ

Aug 6, 2026 – 08:02 PM JST

PDB ID	:	8XNO / pdb_00008xno
EMDB ID	:	EMD-38509
Title	:	Respiratory complex Peripheral Arm of CI, close form A, focus-refined map of type IA, Wild type mouse under Cold Acclimation
Authors	:	Shin, Y.-C.; Liao, M.
Deposited on	:	2023-12-30
Resolution	:	3.40 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

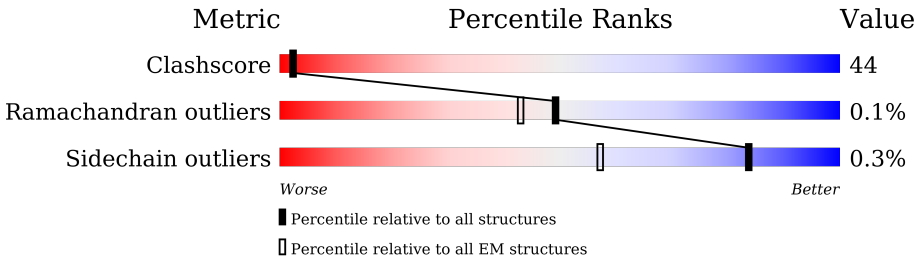
EMDB validation analysis	:	0.0.1.dev133
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

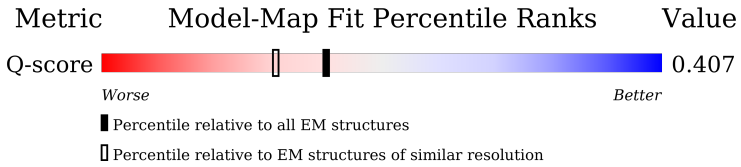
1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.





Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14717 (2.90 - 3.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	115	23% 23% 51% 5% 20%
2	B	224	• 29% 34% 7% 30%
3	C	263	6% 37% 36% • 25%
4	D	463	7% 34% 46% • 17%

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Mol	Chain	Length	Quality of chain
5	E	248	45% 27% 54% 15%
6	F	464	38% 34% 52% 5% 8%
7	G	727	8% 38% 50% 6% 6%
8	H	318	10% 29% 59% 10%
9	I	212	39% 38% 5% 18%
10	P	377	45% 33% 53% 5% 10%
11	Q	175	15% 38% 26% 33%
12	R	116	46% 26% 41% 5% 28%
13	S	99	11% 31% 44% 8% 16%
14	T	156	29% 12% 30% 6% 52%
15	V	116	5% 51% 40% 6%
16	W	131	23% 36% 46% 5% 13%
17	X	172	12% 34% 44% 5% 17%
18	Z	144	12% 40% 55%
19	a	70	6% 34% 57%
20	b	84	21% 27% 67% 5%
21	q	145	71% 37% 39% 7% 17%
22	r	113	28% 22% 17% 6% 55%
23	s	104	12% 7% 6% 88%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	SF4	B	301	-	-	X	-
25	SF4	F	502	-	-	X	-
25	SF4	G	802	-	-	X	-
25	SF4	I	303	-	-	X	-
25	SF4	I	304	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
27	UQ1	D	501	-	-	X	-
28	FES	E	301	-	-	X	-
28	FES	G	803	-	-	X	-

2 Entry composition (i)

There are 34 unique types of molecules in this entry. The entry contains 33909 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called NADH-ubiquinone oxidoreductase chain 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	92	754	523	107	119	5	0	0

- Molecule 2 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	157	1258	802	227	215	14	0	0

- Molecule 3 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	198	1641	1060	279	299	3	0	0

- Molecule 4 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	384	3079	1965	531	560	23	0	0

- Molecule 5 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	210	1635	1039	275	310	11	0	0

- Molecule 6 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	426	Total 3288	C 2073	N 588	O 605	S 22	0	0

- Molecule 7 is a protein called NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	687	Total 5287	C 3316	N 918	O 1012	S 41	0	0

- Molecule 8 is a protein called NADH-ubiquinone oxidoreductase chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	313	Total 2500	C 1680	N 379	O 419	S 22	0	0

- Molecule 9 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	174	Total 1398	C 880	N 240	O 266	S 12	0	0

- Molecule 10 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	340	Total 2730	C 1765	N 479	O 479	S 7	0	0

- Molecule 11 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Q	118	Total 957	C 608	N 165	O 180	S 4	0	0

- Molecule 12 is a protein called NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	R	83	Total 660	C 411	N 120	O 126	S 3	0	0

- Molecule 13 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	S	83	Total	C	N	O	S	0	0
			667	419	126	119	3		

- Molecule 14 is a protein called Acyl carrier protein, mitochondrial.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	T	75	Total	C	N	O	S	0	0
			604	388	89	122	5		

- Molecule 15 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	V	112	Total	C	N	O	S	0	0
			915	596	152	164	3		

- Molecule 16 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	W	114	Total	C	N	O	S	0	0
			970	619	180	165	6		

- Molecule 17 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	X	142	Total	C	N	O	S	0	0
			1164	736	209	209	10		

- Molecule 18 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Z	139	Total	C	N	O	S	0	0
			1152	741	204	199	8		

- Molecule 19 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	a	67	Total	C	N	O	S	0	0
			548	356	97	91	4		

- Molecule 20 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	b	80	Total	C	N	O	S	0	0
			628	414	99	111	4		

- Molecule 21 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	q	120	Total	C	N	O	S	0	0
			1004	645	178	177	4		

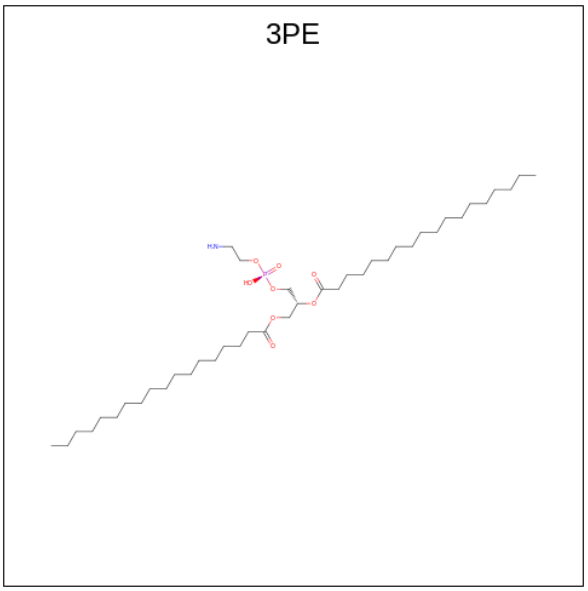
- Molecule 22 is a protein called NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	r	51	Total	C	N	O	S	0	0
			418	266	78	73	1		

- Molecule 23 is a protein called NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial.

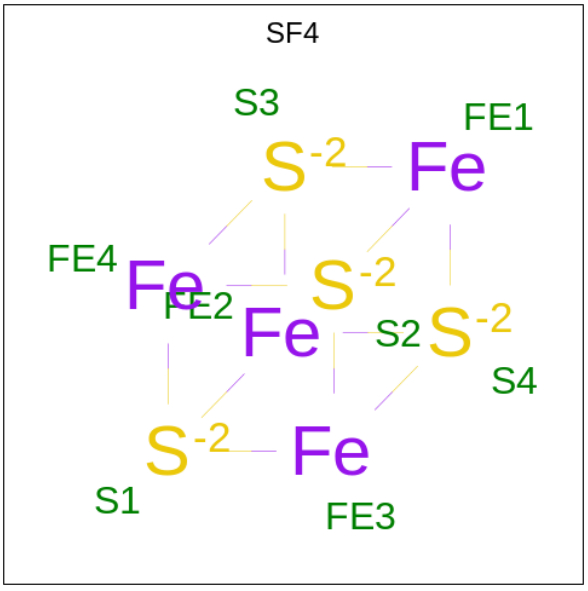
Mol	Chain	Residues	Atoms				AltConf	Trace
23	s	13	Total	C	N	O	0	0
			107	69	15	23		

- Molecule 24 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (CCD ID: 3PE) (formula: $C_{41}H_{82}NO_8P$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
24	A	1	Total	C	N	O	P	0
			46	36	1	8	1	
24	I	1	Total	C	N	O	P	0
			51	41	1	8	1	
24	b	1	Total	C	N	O	P	0
			46	36	1	8	1	

- Molecule 25 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe_4S_4).



Mol	Chain	Residues	Atoms			AltConf
25	B	1	Total	Fe	S	0
			8	4	4	

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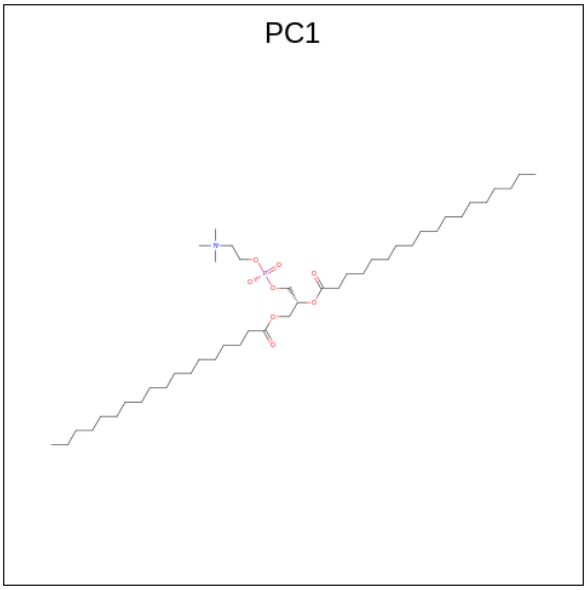
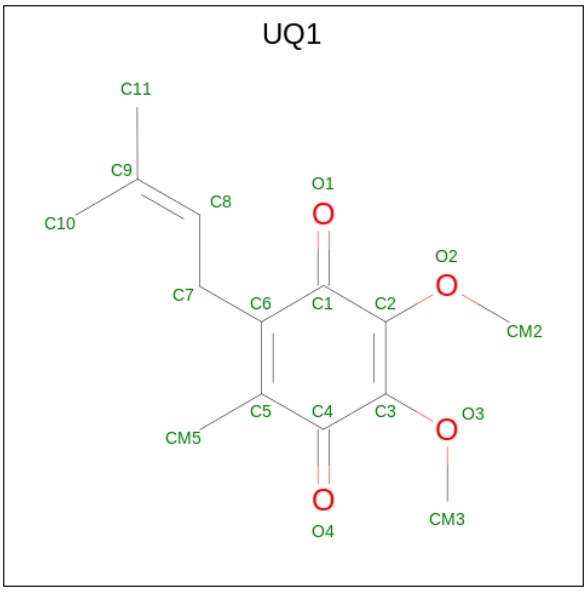
Mol	Chain	Residues	Atoms	AltConf
25	F	1	Total Fe S 8 4 4	0
25	G	1	Total Fe S 8 4 4	0
25	G	1	Total Fe S 8 4 4	0
25	I	1	Total Fe S 8 4 4	0
25	I	1	Total Fe S 8 4 4	0

- Molecule 26 is 1,2-DIACYL-SN-GLYCERO-3-PHOSPHOCHOLINE (CCD ID: PC1) (formula: $C_{44}H_{88}NO_8P$) (labeled as "Ligand of Interest" by depositor).



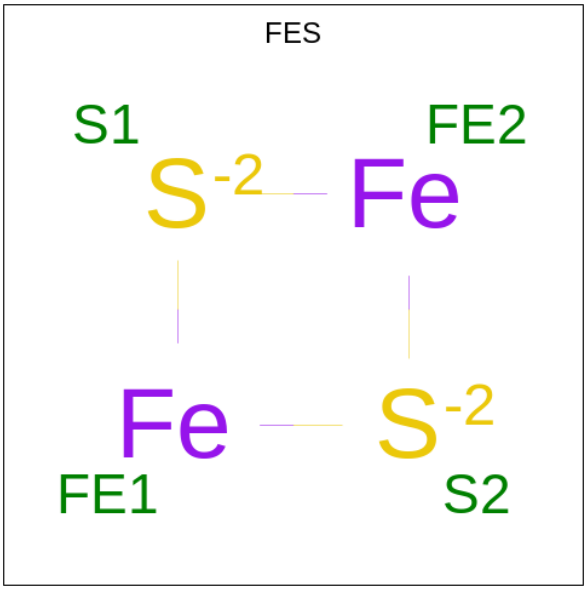
Mol	Chain	Residues	Atoms	AltConf
26	B	1	Total C N O P 35 25 1 8 1	0
26	H	1	Total C N O P 42 32 1 8 1	0
26	I	1	Total C N O P 47 37 1 8 1	0

- Molecule 27 is UBIQUINONE-1 (CCD ID: UQ1) (formula: $C_{14}H_{18}O_4$).



Mol	Chain	Residues	Atoms			AltConf
27	D	1	Total	C	O	0
			18	14	4	

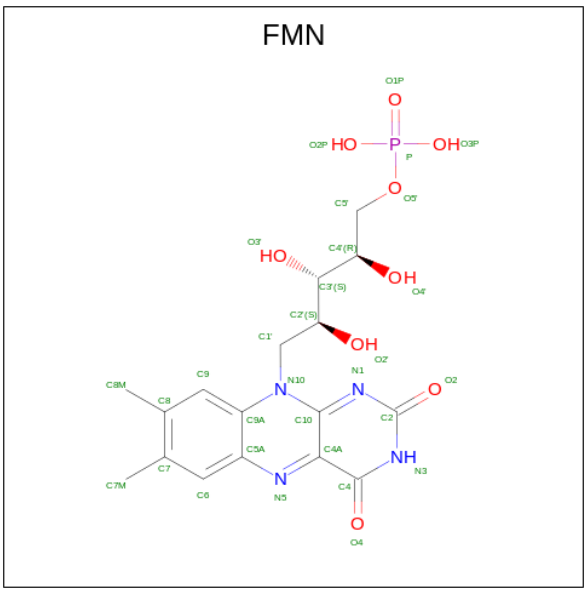
- Molecule 28 is FE2/S2 (INORGANIC) CLUSTER (CCD ID: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms			AltConf
28	E	1	Total	Fe	S	0
			4	2	2	
28	G	1	Total	Fe	S	0
			4	2	2	

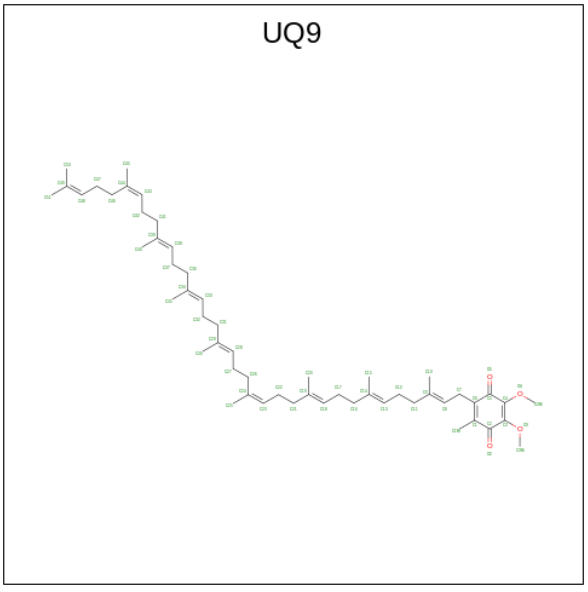
- Molecule 29 is FLAVIN MONONUCLEOTIDE (CCD ID: FMN) (formula: $C_{17}H_{21}N_4O_9P$)

(labeled as "Ligand of Interest" by depositor).



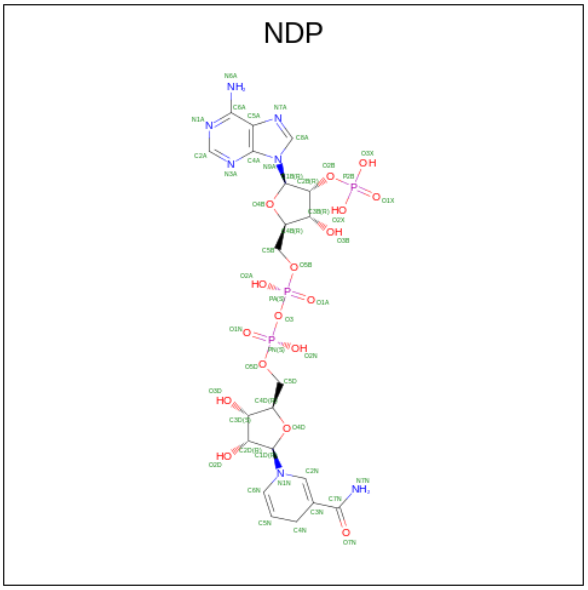
Mol	Chain	Residues	Atoms					AltConf
29	F	1	Total	C	N	O	P	0
			31	17	4	9	1	

- Molecule 30 is Ubiquinone-9 (CCD ID: UQ9) (formula: $C_{54}H_{82}O_4$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			AltConf
30	H	1	Total	C	O	0
			35	31	4	

- Molecule 31 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (CCD ID: NDP) (formula: $C_{21}H_{30}N_7O_{17}P_3$) (labeled as "Ligand of Interest" by depositor).

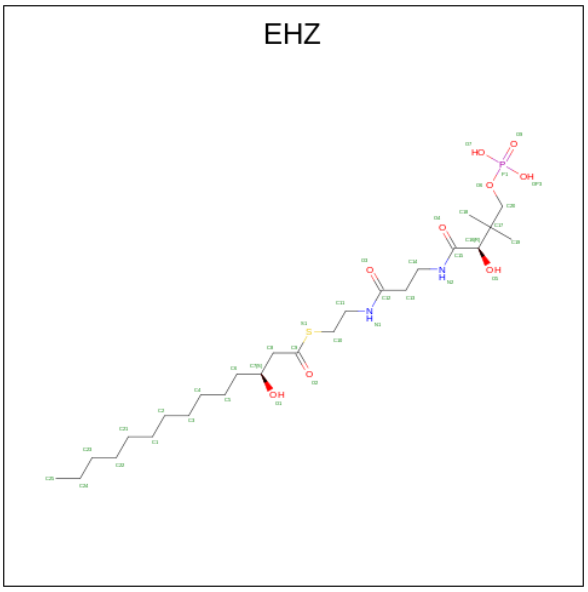


Mol	Chain	Residues	Atoms					AltConf
31	P	1	Total	C	N	O	P	0
			48	21	7	17	3	

- Molecule 32 is ZINC ION (CCD ID: ZN) (formula: Zn).

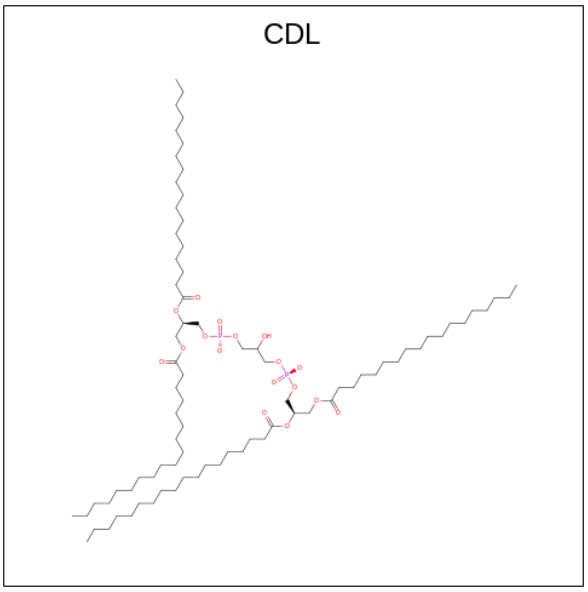
Mol	Chain	Residues	Atoms		AltConf
32	R	1	Total	Zn	0
			1	1	

- Molecule 33 is {S}-[2-[3-[[(2 {R})-3,3-dimethyl-2-oxidanyl-4-phosphonooxy-butanoyl]amino]propanoylamino]ethyl] (3 {S})-3-oxidanyltetradecanethioate (CCD ID: EHZ) (formula: $C_{25}H_{49}N_2O_9PS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						AltConf
33	W	1	Total	C	N	O	P	S	0
			32	19	2	9	1	1	

- Molecule 34 is CARDIOLIPIN (CCD ID: CDL) (formula: $C_{81}H_{156}O_{17}P_2$) (labeled as "Ligand of Interest" by depositor).

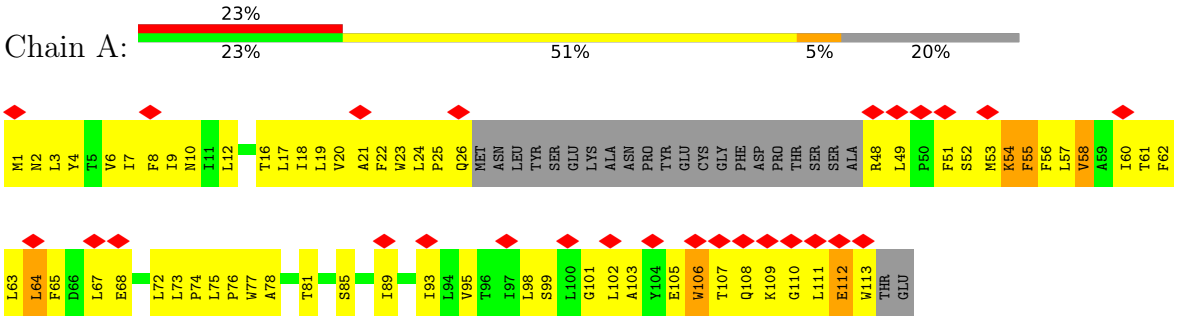


Mol	Chain	Residues	Atoms				AltConf
34	q	1	Total	C	O	P	0
			57	38	17	2	

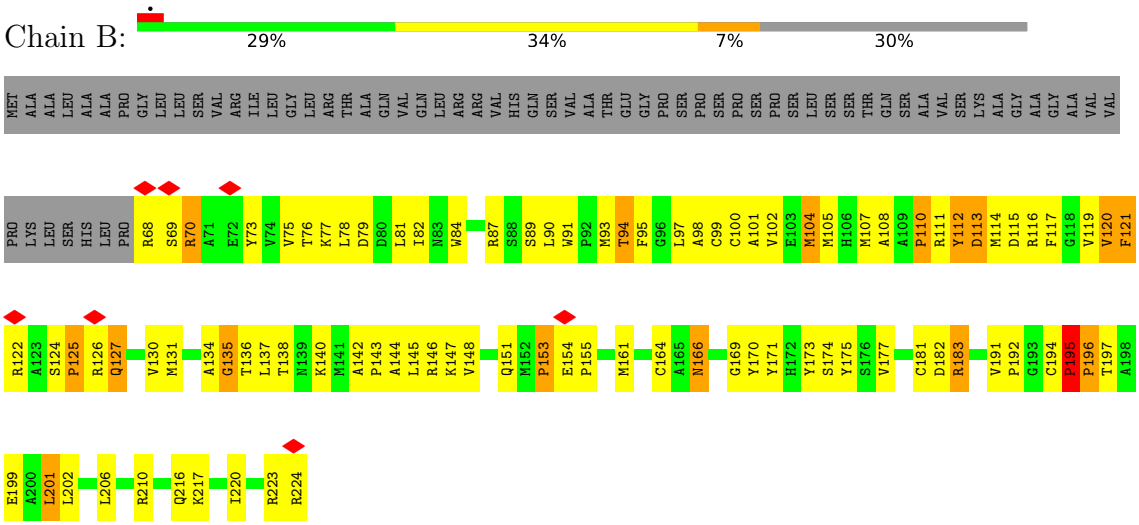
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

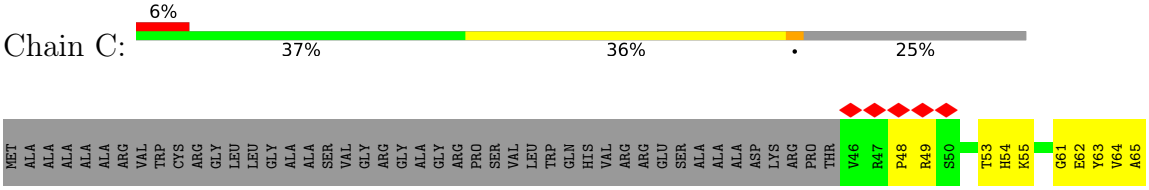
• Molecule 1: NADH-ubiquinone oxidoreductase chain 3

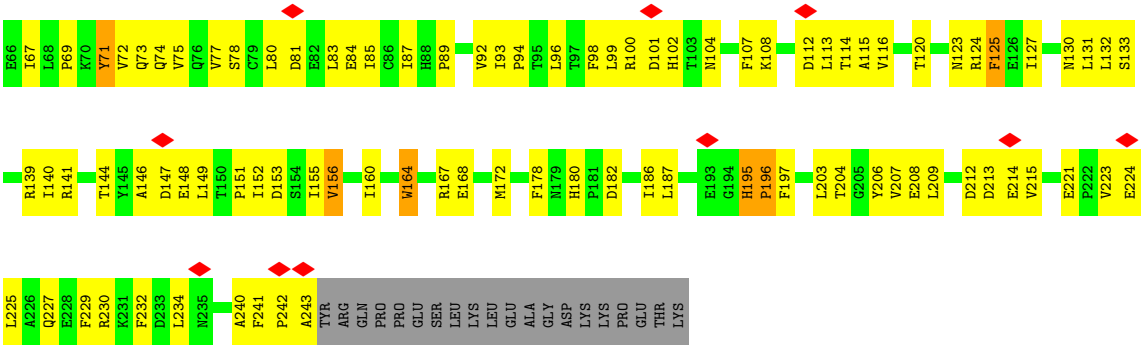


• Molecule 2: NADH dehydrogenase [ubiquinone] iron-sulfur protein 7, mitochondrial



• Molecule 3: NADH dehydrogenase [ubiquinone] iron-sulfur protein 3, mitochondrial

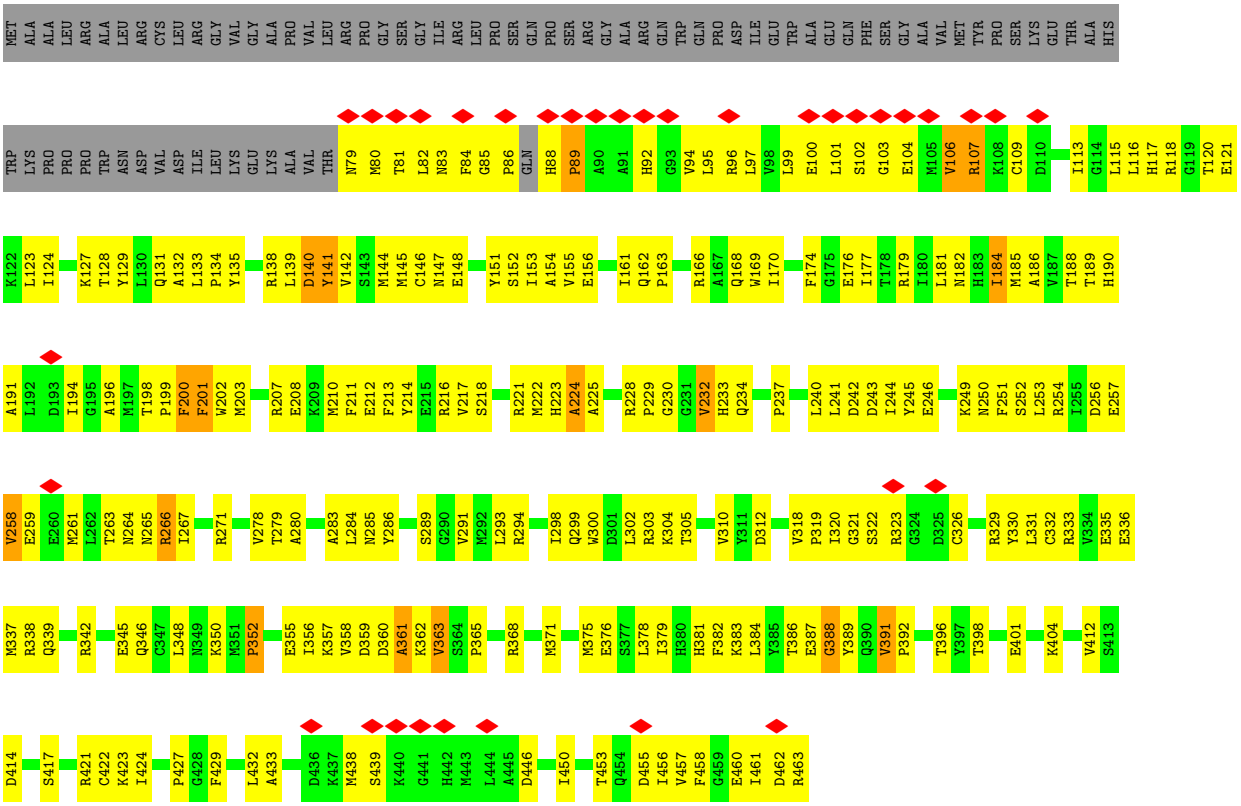




• Molecule 4: NADH dehydrogenase [ubiquinone] iron-sulfur protein 2, mitochondrial

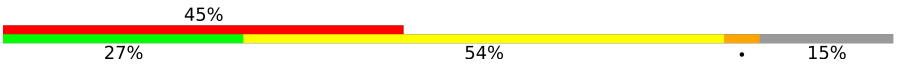
Chain D:

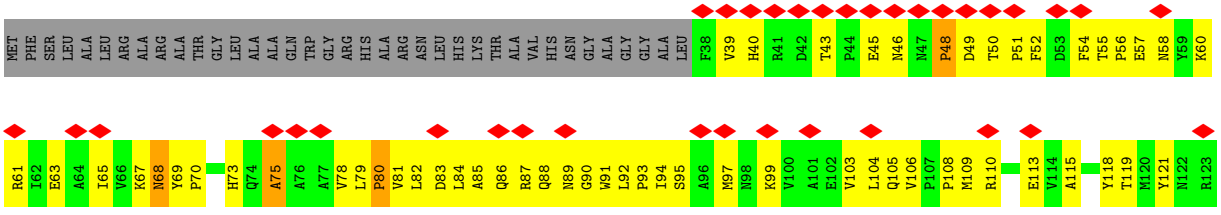


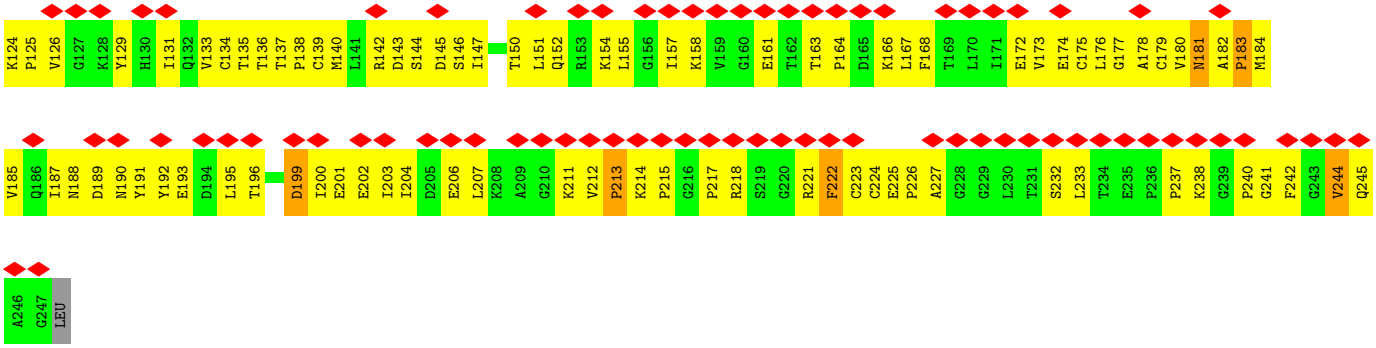


• Molecule 5: NADH dehydrogenase [ubiquinone] flavoprotein 2, mitochondrial

Chain E:



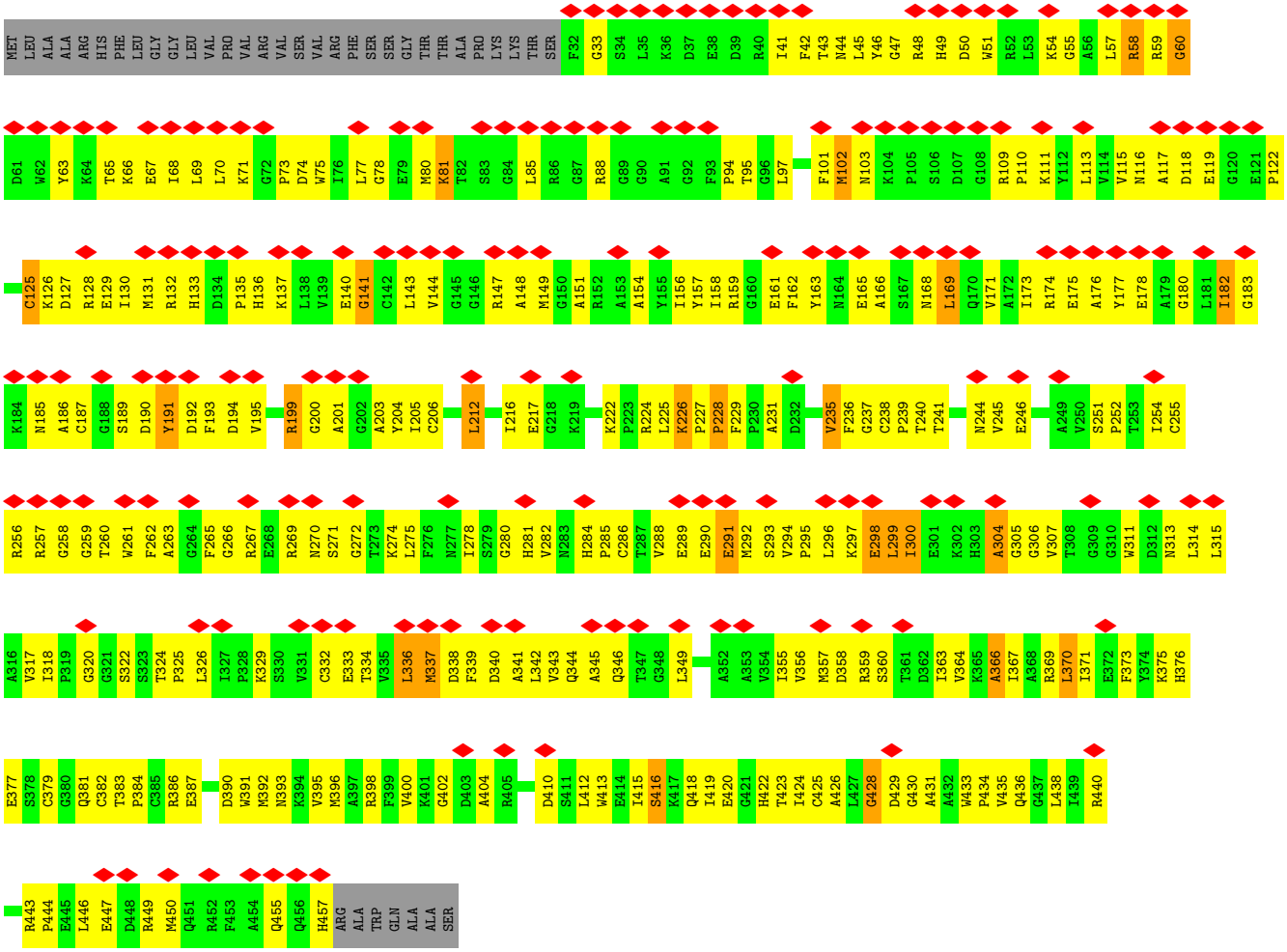




• Molecule 6: NADH dehydrogenase [ubiquinone] flavoprotein 1, mitochondrial

Chain F:

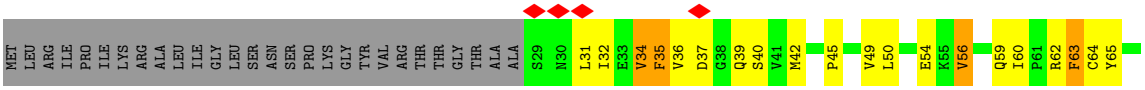


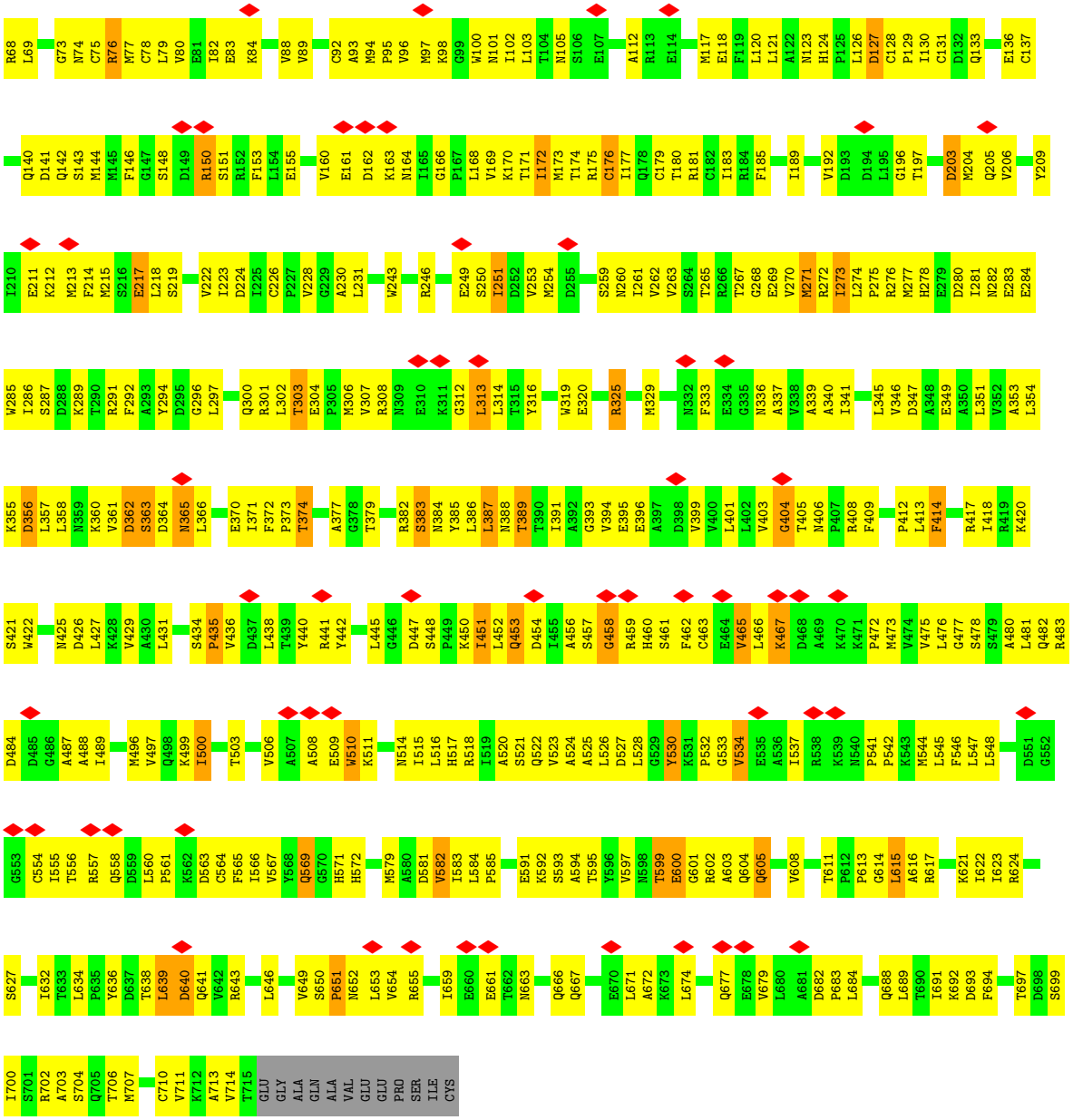


• Molecule 7: NADH-ubiquinone oxidoreductase 75 kDa subunit, mitochondrial

Chain G:



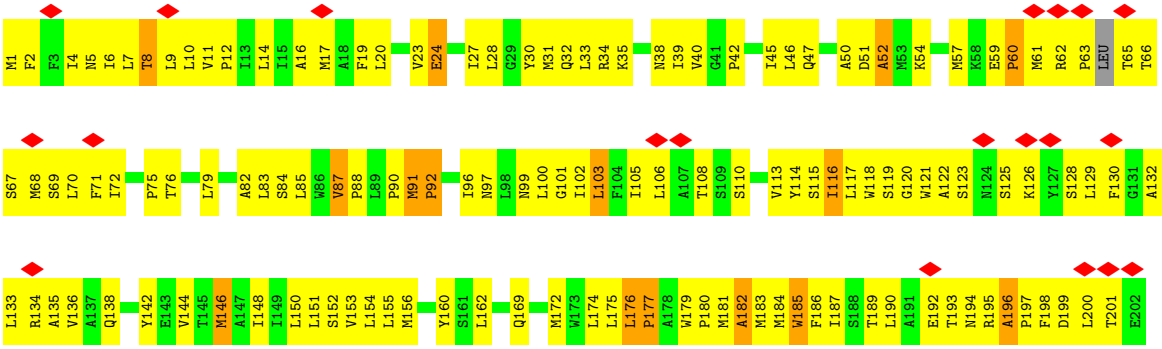


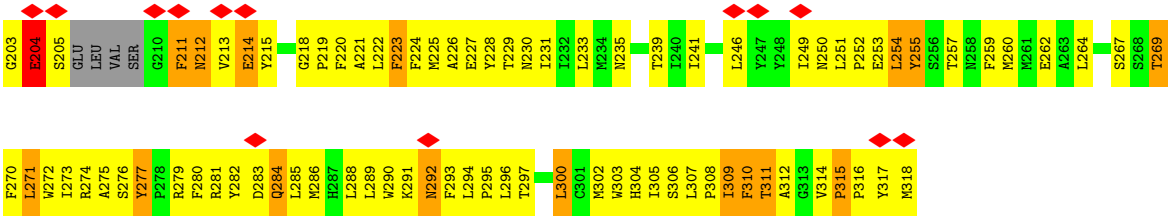


• Molecule 8: NADH-ubiquinone oxidoreductase chain 1

Chain H:



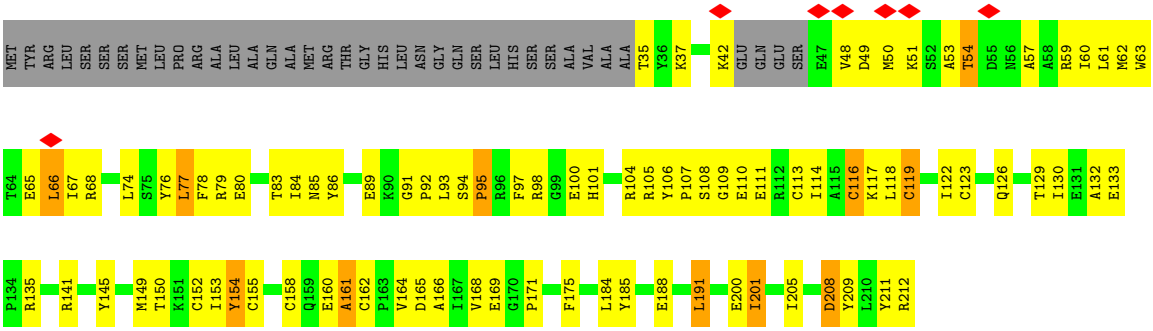




• Molecule 9: NADH dehydrogenase [ubiquinone] iron-sulfur protein 8, mitochondrial

Chain I:

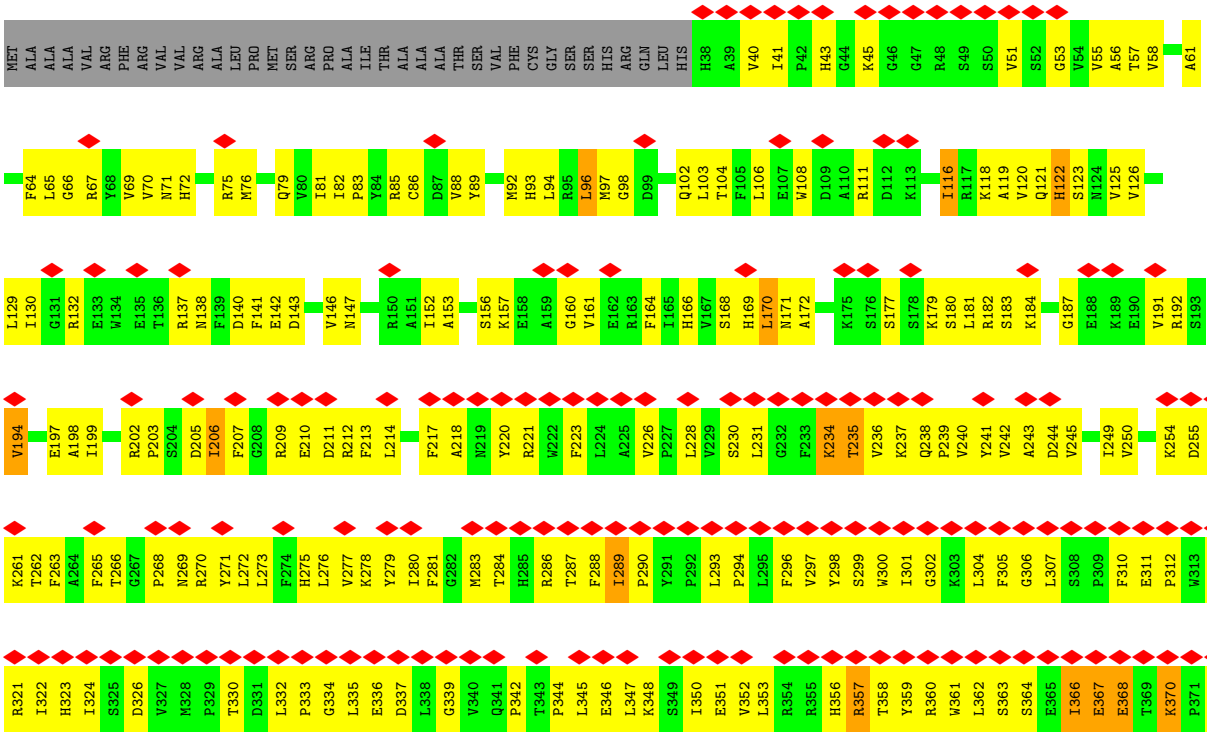




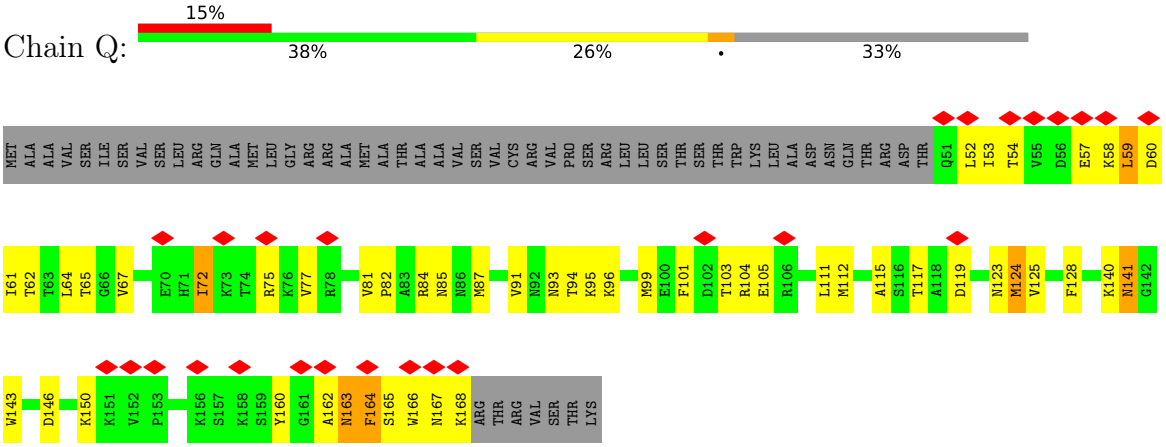
• Molecule 10: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 9, mitochondrial

Chain P:

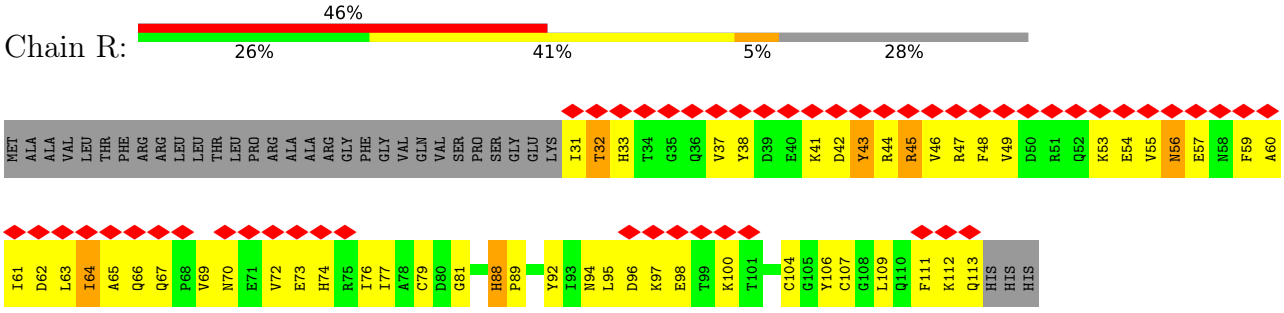




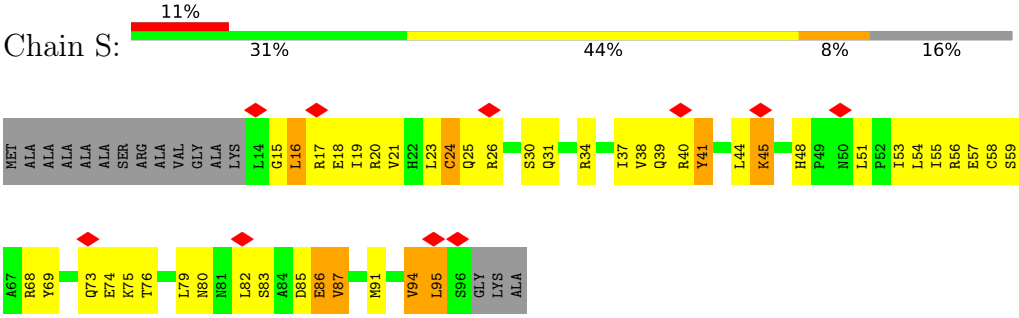
• Molecule 11: NADH dehydrogenase [ubiquinone] iron-sulfur protein 4, mitochondrial



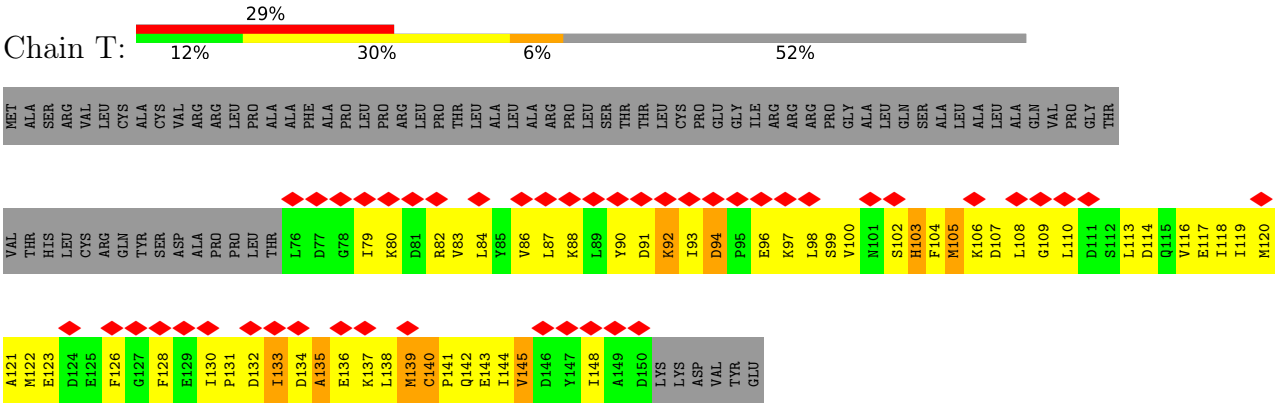
• Molecule 12: NADH dehydrogenase [ubiquinone] iron-sulfur protein 6, mitochondrial



• Molecule 13: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 2

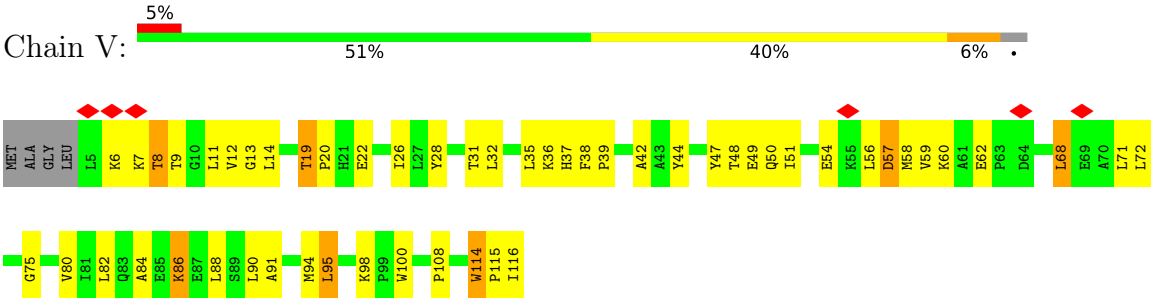


• Molecule 14: Acyl carrier protein, mitochondrial



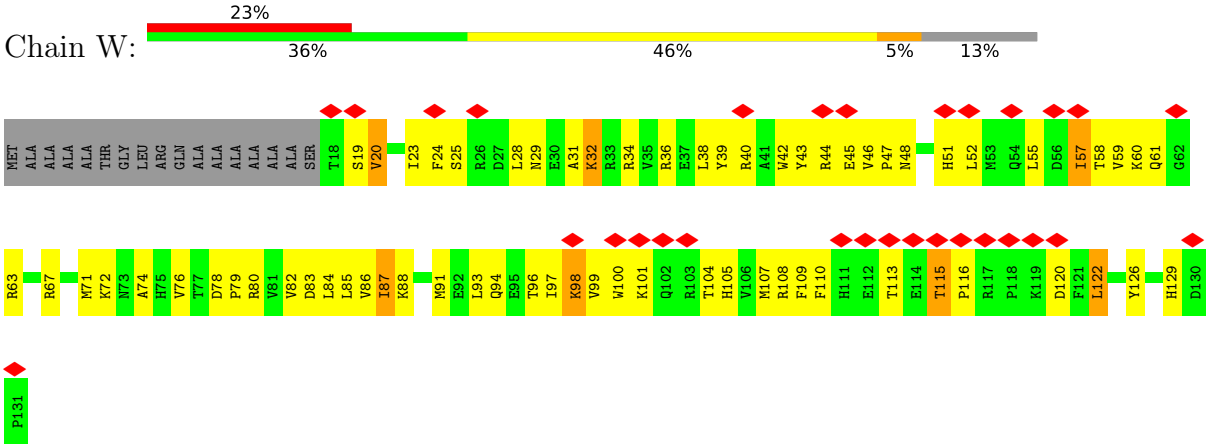
• Molecule 15: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 5

Chain V:



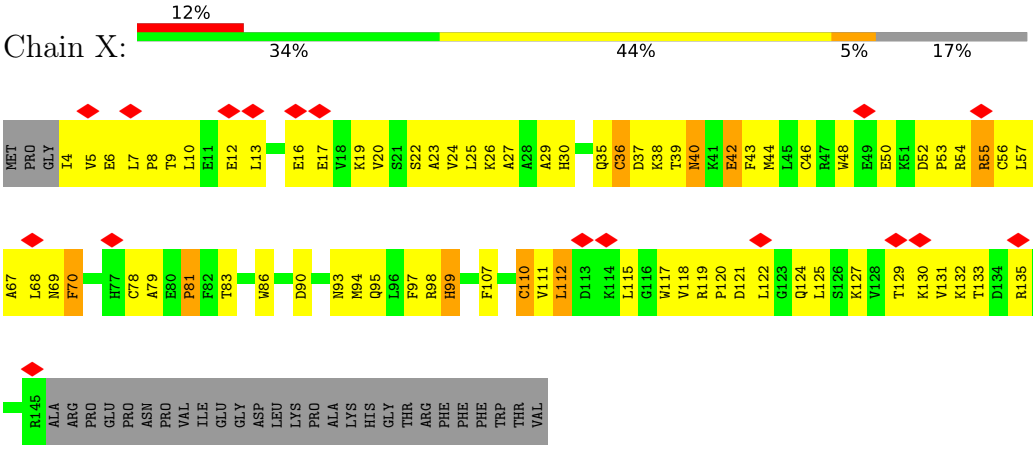
• Molecule 16: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 6

Chain W:



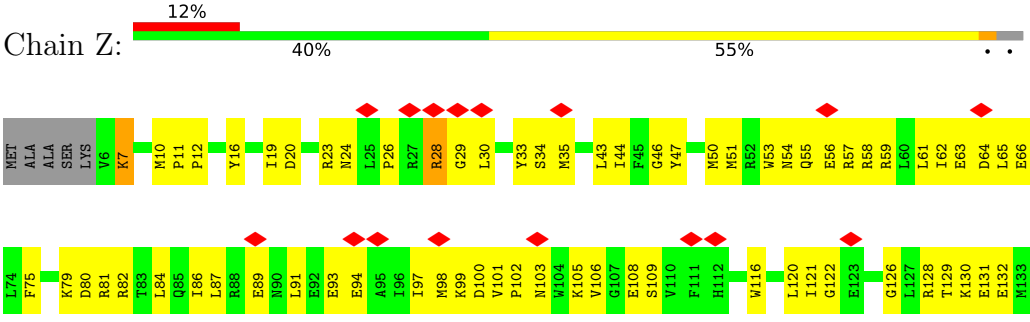
• Molecule 17: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 8

Chain X:



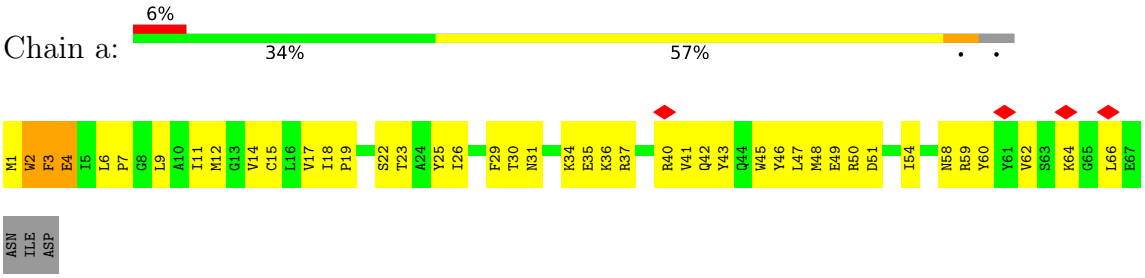
• Molecule 18: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 13

Chain Z:

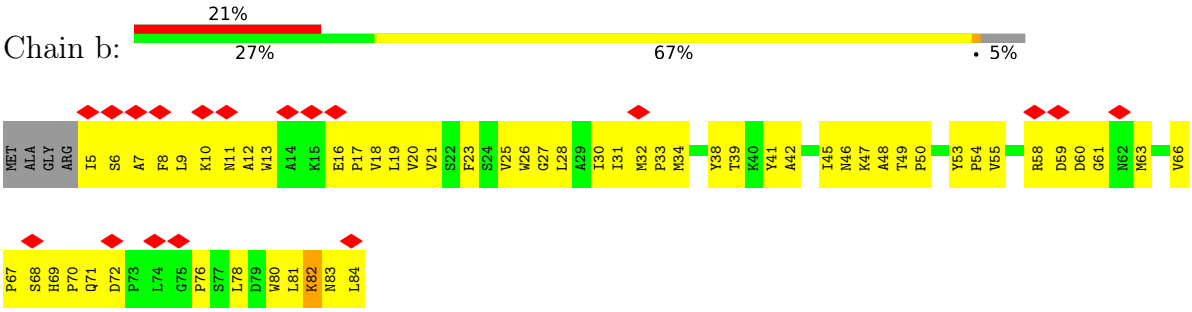




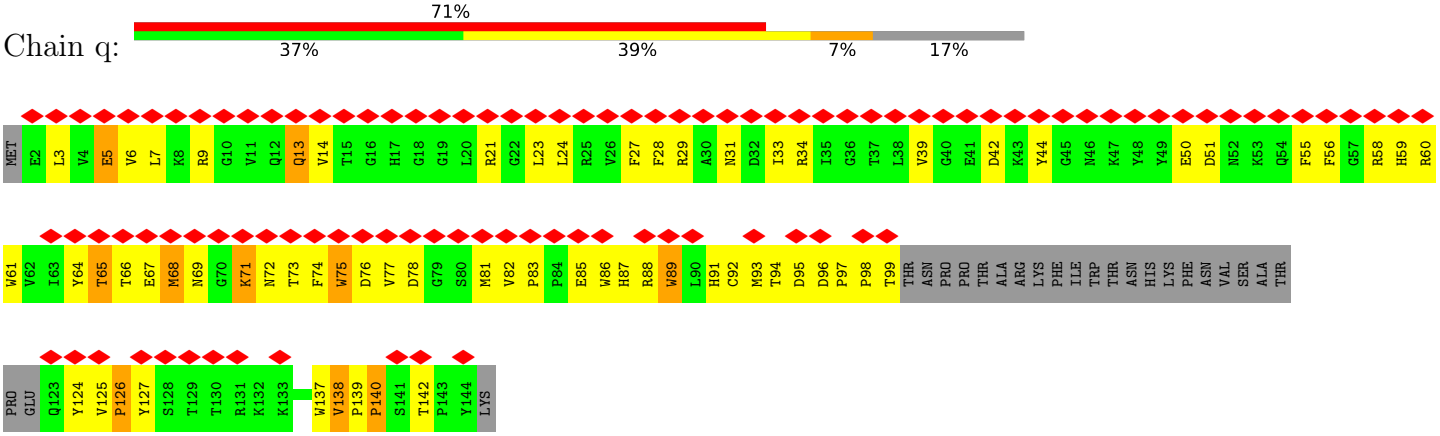
• Molecule 19: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 1



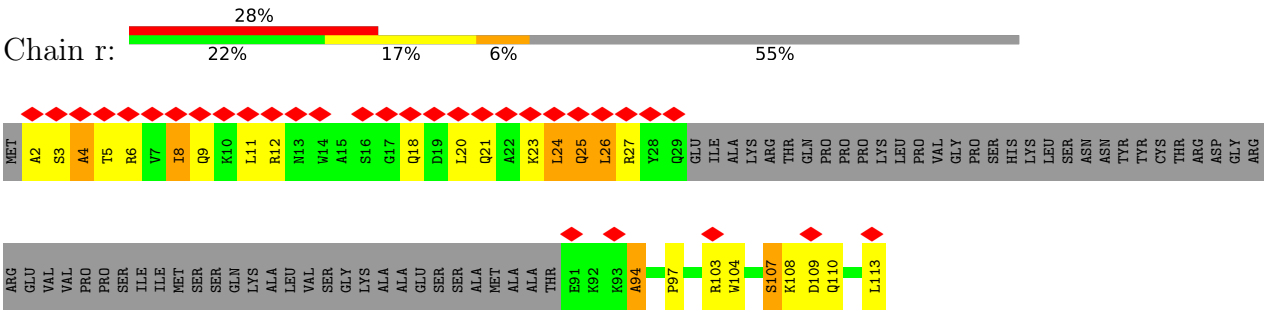
• Molecule 20: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 3



• Molecule 21: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 12



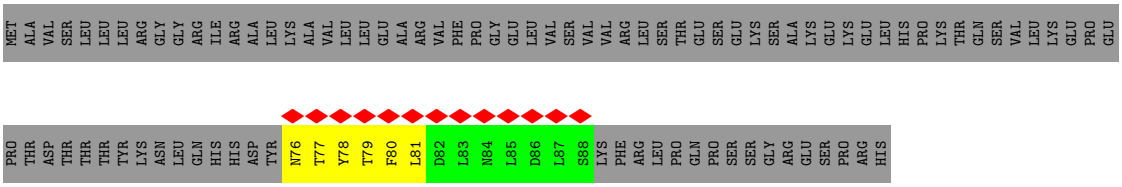
• Molecule 22: NADH dehydrogenase [ubiquinone] 1 alpha subcomplex subunit 7



• Molecule 23: NADH dehydrogenase [ubiquinone] flavoprotein 3, mitochondrial

Chain s:


12%
7%
6%
88%


MET ALA VAL SER LEU LEU LEU ARG GLY GLY ARG ILE ARG ALA LEU LYS ALA VAL LEU LEU GLU ALA ARG VAL PHE PRO GLY GLU LEU VAL SER VAL VAL ARG LEU SER THR GLU SER GLU LYS SER ALA LYS GLU LYS GLU LEU HIS PRO LYS THR GLN SER VAL LEU LYS GLU PRO GLU
PRO THR ASP THR THR THR TYR LYS ASN LEU GLN HIS HIS ASP TYR N76 T77 Y78 T79 F80 L81 D82 L83 N84 L85 D86 L87 S88 LYS PHE ARG LEU PRO GLN PRO SER SER GLY ARG GLU SER PRO ARG HIS

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	47191	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	46.1, 45.9	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k), GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.315	Depositor
Minimum map value	-1.329	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.084	Depositor
Recommended contour level	0.55	Depositor
Map size (Å)	422.40002, 422.40002, 422.40002	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.1, 1.1, 1.1	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CDL, PC1, UQ9, 3PE, UQ1, NDP, EHZ, FES, SF4, ZN, FMN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.83	0/774	1.33	10/1056 (0.9%)
2	B	0.98	1/1289 (0.1%)	1.44	18/1744 (1.0%)
3	C	0.87	1/1687 (0.1%)	1.31	14/2297 (0.6%)
4	D	0.95	5/3152 (0.2%)	1.34	25/4261 (0.6%)
5	E	0.81	2/1675 (0.1%)	1.25	15/2282 (0.7%)
6	F	0.88	1/3363 (0.0%)	1.44	54/4543 (1.2%)
7	G	0.89	6/5374 (0.1%)	1.59	104/7281 (1.4%)
8	H	0.94	2/2575 (0.1%)	1.48	55/3516 (1.6%)
9	I	0.90	0/1427	1.54	19/1927 (1.0%)
10	P	0.79	1/2804 (0.0%)	1.26	34/3802 (0.9%)
11	Q	0.87	1/980 (0.1%)	1.29	12/1324 (0.9%)
12	R	0.63	0/671	1.19	9/903 (1.0%)
13	S	0.93	1/678 (0.1%)	1.65	17/915 (1.9%)
14	T	0.91	0/613	1.51	9/826 (1.1%)
15	V	0.87	0/937	1.47	14/1270 (1.1%)
16	W	0.80	0/993	1.32	15/1335 (1.1%)
17	X	0.84	1/1191 (0.1%)	1.45	22/1605 (1.4%)
18	Z	0.76	0/1183	1.10	7/1597 (0.4%)
19	a	0.82	0/561	1.36	5/755 (0.7%)
20	b	0.70	0/651	0.91	1/895 (0.1%)
21	q	0.96	1/1037 (0.1%)	1.45	15/1408 (1.1%)
22	r	0.98	1/426 (0.2%)	1.57	9/573 (1.6%)
23	s	0.75	0/108	1.08	0/147
All	All	0.87	24/34149 (0.1%)	1.41	483/46262 (1.0%)

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	235	VAL	N-CA	-9.32	1.34	1.46
11	Q	53	ILE	C-O	7.76	1.33	1.24
7	G	203	ASP	CA-C	6.74	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	106	VAL	C-N	-6.54	1.24	1.33
7	G	600	GLU	CA-C	6.46	1.61	1.52
2	B	110	PRO	C-O	-6.30	1.16	1.24
7	G	127	ASP	CA-C	6.26	1.62	1.52
4	D	266	ARG	C-O	-6.24	1.16	1.24
7	G	76	ARG	CA-C	6.16	1.61	1.53
5	E	93	PRO	N-CD	-5.92	1.39	1.47
17	X	54	ARG	CA-C	5.92	1.60	1.52
7	G	361	VAL	CA-C	5.88	1.60	1.52
22	r	25	GLN	CA-C	5.79	1.60	1.52
5	E	80	PRO	N-CD	5.67	1.55	1.47
4	D	392	PRO	C-O	-5.57	1.20	1.24
13	S	95	LEU	CA-C	5.53	1.59	1.52
4	D	107	ARG	C-N	5.52	1.40	1.33
7	G	683	PRO	N-CD	-5.43	1.40	1.47
8	H	211	PHE	CA-C	5.40	1.59	1.52
21	q	126	PRO	N-CD	5.37	1.55	1.47
10	P	235	THR	CA-C	5.30	1.59	1.53
4	D	266	ARG	CA-C	-5.25	1.45	1.52
3	C	61	GLY	C-N	-5.05	1.27	1.33
8	H	310	PHE	CA-C	5.05	1.59	1.52

All (483) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	174	THR	N-CA-C	-16.80	89.10	114.64
4	D	142	VAL	N-CA-C	-14.34	96.91	110.82
7	G	251	ILE	N-CA-C	13.32	126.82	108.17
7	G	77	MET	N-CA-C	-13.07	97.31	113.38
9	I	164	VAL	N-CA-C	-12.88	100.08	112.83
7	G	500	ILE	N-CA-C	-12.52	98.76	110.53
6	F	171	VAL	N-CA-C	-11.80	99.44	110.53
7	G	204	MET	N-CA-C	-11.64	91.45	109.25
6	F	449	ARG	N-CA-C	-11.60	98.72	111.36
7	G	599	THR	N-CA-C	11.37	126.25	112.38
11	Q	60	ASP	N-CA-C	-11.34	90.30	109.24
13	S	39	GLN	N-CA-C	11.16	125.42	111.69
16	W	87	ILE	N-CA-C	-11.09	99.77	110.42
15	V	57	ASP	N-CA-C	-11.04	99.26	111.07
1	A	54	LYS	N-CA-C	-10.99	98.17	111.69
8	H	259	PHE	N-CA-C	-10.94	99.43	111.36
17	X	70	PHE	N-CA-C	-10.61	99.71	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	77	LEU	N-CA-C	-10.45	99.69	111.71
14	T	139	MET	N-CA-C	-10.43	97.42	113.89
5	E	68	ASN	N-CA-C	-10.36	99.98	111.07
2	B	195	PRO	N-CA-C	-10.34	98.08	110.70
8	H	284	GLN	N-CA-C	-10.32	100.02	111.07
16	W	59	VAL	N-CA-C	-10.31	100.53	110.42
7	G	280	ASP	N-CA-C	10.30	122.51	111.28
4	D	337	MET	N-CA-C	-10.26	100.09	111.07
4	D	140	ASP	CB-CA-C	-10.24	98.00	111.42
19	a	4	GLU	N-CA-C	10.23	124.86	112.38
10	P	366	ILE	N-CA-C	10.22	121.05	110.62
9	I	161	ALA	N-CA-C	10.07	122.26	111.28
7	G	414	PHE	N-CA-C	-10.06	101.50	113.88
14	T	135	ALA	N-CA-C	-10.05	100.33	111.28
7	G	325	ARG	N-CA-C	-9.88	100.20	110.97
9	I	166	ALA	N-CA-C	-9.87	100.78	113.12
6	F	178	GLU	N-CA-C	-9.87	99.27	111.11
6	F	103	ASN	N-CA-C	-9.82	100.98	113.16
6	F	141	GLY	N-CA-C	-9.77	101.17	112.50
6	F	144	VAL	N-CA-C	-9.77	101.35	110.53
7	G	654	VAL	N-CA-C	9.75	123.27	111.09
7	G	35	PHE	N-CA-C	9.67	124.34	108.96
7	G	337	ALA	N-CA-C	-9.59	100.79	114.12
6	F	418	GLN	N-CA-C	-9.58	100.80	111.14
8	H	52	ALA	N-CA-C	-9.53	100.88	111.07
19	a	2	TRP	N-CA-C	-9.46	101.66	113.01
14	T	133	ILE	N-CA-C	9.35	119.89	110.82
7	G	694	PHE	N-CA-C	9.33	121.45	111.28
7	G	692	LYS	N-CA-C	-9.33	100.48	112.23
10	P	367	GLU	N-CA-C	9.24	122.54	111.82
7	G	640	ASP	N-CA-C	-9.23	101.30	111.36
5	E	85	ALA	N-CA-C	-9.15	101.39	111.36
7	G	389	THR	N-CA-C	-9.12	96.29	109.96
10	P	157	LYS	N-CA-C	-9.12	101.42	111.36
8	H	91	MET	N-CA-C	-9.05	98.44	109.57
17	X	55	ARG	N-CA-C	9.02	130.01	110.80
2	B	121	PHE	CB-CA-C	8.91	124.68	110.96
7	G	133	GLN	N-CA-CB	8.75	121.47	110.45
7	G	365	ASN	N-CA-C	-8.75	102.16	112.92
7	G	212	LYS	N-CA-C	-8.71	94.70	108.90
9	I	154	TYR	N-CA-CB	-8.71	99.17	111.62
16	W	20	VAL	N-CA-C	8.66	120.74	108.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	212	ASN	N-CA-C	-8.64	101.86	114.39
10	P	96	LEU	N-CA-C	8.63	121.64	111.71
13	S	86	GLU	N-CA-C	-8.53	102.06	111.36
12	R	57	GLU	N-CA-C	-8.49	98.28	110.59
10	P	373	LYS	N-CA-C	8.48	121.89	110.35
13	S	18	GLU	N-CA-C	8.46	123.19	109.40
16	W	100	TRP	N-CA-C	-8.44	99.89	112.04
17	X	99	HIS	N-CA-C	-8.39	102.22	111.36
3	C	108	LYS	N-CA-C	8.39	120.05	111.07
16	W	57	ILE	N-CA-C	8.35	122.03	109.17
7	G	452	LEU	N-CA-C	-8.35	102.18	111.28
11	Q	54	THR	N-CA-C	8.35	123.31	109.46
7	G	558	GLN	N-CA-C	-8.26	102.23	111.07
1	A	55	PHE	N-CA-C	-8.25	102.25	111.07
8	H	196	ALA	N-CA-C	8.24	128.03	109.81
8	H	311	THR	N-CA-C	-8.23	102.54	112.59
3	C	196	PRO	N-CA-C	8.16	124.87	113.53
7	G	691	ILE	N-CA-C	8.15	123.62	111.89
16	W	96	THR	N-CA-C	-8.15	102.34	111.14
15	V	86	LYS	N-CA-C	-8.14	102.35	111.14
6	F	298	GLU	N-CA-C	8.14	120.15	111.28
7	G	484	ASP	N-CA-C	8.12	121.05	111.71
6	F	191	TYR	N-CA-C	8.10	121.66	110.24
2	B	110	PRO	N-CA-C	8.09	124.58	113.65
1	A	64	LEU	N-CA-C	-8.06	102.45	111.07
7	G	500	ILE	N-CA-CB	8.04	120.86	110.57
13	S	76	THR	N-CA-C	8.00	121.93	108.90
17	X	43	PHE	N-CA-C	-7.98	102.52	111.14
7	G	534	VAL	N-CA-C	-7.98	104.81	111.91
16	W	98	LYS	N-CA-C	-7.98	101.59	113.72
8	H	271	LEU	N-CA-C	-7.97	102.53	111.14
17	X	112	LEU	N-CA-C	-7.97	102.53	111.14
9	I	201	ILE	N-CA-C	-7.97	102.67	110.72
1	A	9	ILE	N-CA-C	-7.96	102.50	110.62
10	P	206	ILE	N-CA-C	7.94	120.94	108.87
21	q	67	GLU	CB-CA-C	-7.94	99.60	112.06
7	G	651	PRO	CB-CA-C	-7.92	98.49	111.56
17	X	46	CYS	N-CA-C	-7.92	102.72	111.36
8	H	311	THR	N-CA-CB	7.91	123.57	110.92
15	V	6	LYS	N-CA-C	-7.88	100.12	110.53
2	B	121	PHE	CA-CB-CG	-7.88	105.92	113.80
17	X	55	ARG	N-CA-CB	-7.85	97.23	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	270	VAL	N-CA-CB	-7.84	100.66	110.31
9	I	160	GLU	N-CA-C	7.81	124.18	111.37
7	G	389	THR	N-CA-CB	7.79	121.46	109.85
10	P	235	THR	CB-CA-C	-7.79	100.07	112.07
1	A	53	MET	N-CA-C	-7.78	103.93	113.19
17	X	58	LYS	N-CA-C	-7.77	102.76	111.07
9	I	74	LEU	N-CA-C	-7.75	102.83	111.28
4	D	361	ALA	N-CA-C	-7.71	102.97	112.38
8	H	253	GLU	N-CA-C	7.71	121.94	112.54
21	q	44	TYR	N-CA-C	-7.67	98.93	110.28
6	F	58	ARG	N-CA-C	-7.67	103.00	111.36
6	F	171	VAL	N-CA-CB	7.64	120.34	110.57
21	q	89	TRP	N-CA-C	-7.63	102.90	111.14
2	B	153	PRO	CB-CA-C	-7.63	98.97	111.56
12	R	32	THR	N-CA-C	7.63	119.65	110.19
7	G	569	GLN	N-CA-C	7.62	122.03	108.24
7	G	56	VAL	N-CA-C	-7.61	103.03	110.72
8	H	223	PHE	CB-CA-C	-7.59	98.97	110.88
5	E	68	ASN	N-CA-CB	7.58	121.00	110.01
9	I	119	CYS	N-CA-C	-7.54	103.15	111.36
12	R	74	HIS	N-CA-C	7.53	121.11	110.50
7	G	467	LYS	N-CA-C	-7.50	102.26	111.33
7	G	277	MET	N-CA-C	7.48	120.59	109.59
7	G	303	THR	N-CA-C	7.46	123.10	113.18
9	I	158	CYS	N-CA-C	-7.45	103.16	111.28
6	F	430	GLY	N-CA-C	7.42	121.64	112.73
7	G	510	TRP	N-CA-CB	7.42	120.91	109.85
15	V	57	ASP	N-CA-CB	7.39	120.72	110.01
2	B	183	ARG	N-CA-C	-7.37	104.53	113.97
4	D	350	LYS	CB-CA-C	-7.33	101.07	111.85
21	q	24	LEU	N-CA-C	-7.32	103.31	111.28
13	S	94	VAL	N-CA-C	7.29	117.42	110.42
7	G	374	THR	CB-CA-C	-7.25	99.82	111.28
7	G	384	ASN	N-CA-C	-7.25	103.41	111.82
8	H	309	ILE	N-CA-C	7.24	117.33	110.30
14	T	105	MET	N-CA-C	7.24	119.25	111.36
7	G	497	VAL	N-CA-C	-7.24	103.24	110.62
8	H	212	ASN	N-CA-CB	7.23	120.52	110.98
3	C	195	HIS	CB-CA-C	7.22	117.32	110.17
15	V	68	LEU	N-CA-C	-7.22	103.41	111.28
8	H	50	ALA	N-CA-C	7.21	118.78	111.07
10	P	370	LYS	N-CA-C	7.20	119.25	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	465	VAL	N-CA-CB	7.19	118.49	110.51
7	G	661	GLU	N-CA-C	7.18	118.79	110.97
6	F	73	PRO	N-CA-C	-7.17	103.79	113.40
6	F	81	LYS	N-CA-C	-7.17	103.55	111.36
7	G	217	GLU	N-CA-C	-7.15	101.62	110.41
8	H	214	GLU	N-CA-CB	-7.14	98.86	110.42
7	G	461	SER	N-CA-C	7.09	119.91	111.33
15	V	95	LEU	N-CA-C	-7.08	103.56	111.28
6	F	78	GLY	N-CA-C	-7.08	104.24	112.73
8	H	254	LEU	N-CA-C	-7.07	103.62	111.82
11	Q	162	ALA	N-CA-C	7.04	118.96	111.28
7	G	148	SER	N-CA-C	7.03	120.86	109.40
21	q	77	VAL	N-CA-C	-7.00	99.68	109.21
7	G	150	ARG	N-CA-C	7.00	119.57	109.14
7	G	294	TYR	N-CA-C	-6.98	104.58	113.23
8	H	176	LEU	CA-C-N	-6.98	113.61	120.52
8	H	176	LEU	C-N-CA	-6.98	113.61	120.52
6	F	418	GLN	N-CA-CB	6.97	120.18	110.07
6	F	455	GLN	N-CA-C	6.97	118.53	111.07
6	F	428	GLY	N-CA-C	-6.96	103.85	112.77
6	F	246	GLU	N-CA-C	-6.96	103.69	111.28
6	F	169	LEU	N-CA-C	6.96	118.87	111.28
2	B	166	ASN	N-CA-C	-6.96	103.39	110.97
8	H	292	ASN	N-CA-C	6.95	118.94	111.36
6	F	103	ASN	N-CA-CB	6.95	121.07	110.44
7	G	582	VAL	N-CA-C	6.95	118.49	108.48
10	P	235	THR	CA-C-O	6.95	128.13	121.67
3	C	69	PRO	N-CA-C	-6.93	104.30	113.65
5	E	152	GLN	N-CA-C	-6.92	103.66	111.07
7	G	300	GLN	N-CA-CB	6.92	122.53	112.08
6	F	148	ALA	N-CA-C	-6.91	103.83	111.36
16	W	87	ILE	N-CA-CB	6.91	118.63	110.55
8	H	300	LEU	N-CA-C	-6.89	104.14	112.54
7	G	362	ASP	N-CA-C	6.87	125.44	110.80
14	T	145	VAL	N-CA-C	-6.87	103.78	110.72
8	H	87	VAL	CA-C-N	-6.87	113.12	120.47
8	H	87	VAL	C-N-CA	-6.87	113.12	120.47
18	Z	34	SER	N-CA-C	-6.86	103.73	111.07
18	Z	28	ARG	N-CA-C	6.85	119.69	108.52
12	R	56	ASN	N-CA-C	6.81	120.00	108.90
7	G	133	GLN	N-CA-C	-6.81	101.22	110.68
7	G	268	GLY	N-CA-C	6.80	124.76	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	244	ASN	N-CA-C	-6.80	100.91	110.50
8	H	305	ILE	N-CA-C	-6.77	103.43	113.39
1	A	112	GLU	N-CA-C	-6.75	102.36	111.87
7	G	434	SER	N-CA-C	-6.73	101.00	110.29
22	r	11	LEU	N-CA-C	-6.72	104.04	111.36
9	I	208	ASP	N-CA-C	6.69	121.60	113.17
15	V	8	THR	N-CA-C	6.69	119.03	108.79
8	H	8	THR	N-CA-C	-6.68	101.26	110.35
5	E	199	ASP	N-CA-C	-6.68	103.69	110.97
16	W	105	HIS	N-CA-C	-6.67	104.95	113.23
7	G	601	GLY	N-CA-C	6.67	124.91	115.30
8	H	60	PRO	N-CA-C	-6.67	98.72	112.47
17	X	97	PHE	N-CA-C	6.67	118.63	111.36
17	X	129	THR	N-CA-C	6.64	120.87	110.17
8	H	204	GLU	N-CA-C	-6.64	96.65	110.80
7	G	640	ASP	N-CA-CB	6.64	119.99	110.16
10	P	116	ILE	N-CA-C	-6.64	104.01	110.72
15	V	114	TRP	N-CA-CB	6.64	120.19	110.30
3	C	125	PHE	N-CA-CB	-6.63	100.62	110.17
6	F	344	GLN	N-CA-C	-6.63	103.98	111.07
7	G	287	SER	N-CA-C	6.62	119.27	110.53
15	V	86	LYS	N-CA-CB	6.61	119.66	110.07
6	F	228	PRO	N-CA-C	-6.61	98.86	112.47
8	H	182	ALA	N-CA-C	-6.59	104.02	111.07
6	F	336	LEU	N-CA-CB	-6.58	100.97	111.43
13	S	40	ARG	N-CA-C	6.56	122.80	113.02
4	D	184	ILE	N-CA-C	-6.56	103.93	110.62
7	G	435	PRO	N-CA-C	-6.55	100.22	110.50
11	Q	141	ASN	N-CA-CB	6.53	120.72	110.46
7	G	605	GLN	N-CA-C	6.52	119.15	108.52
8	H	223	PHE	N-CA-C	-6.51	104.11	111.07
8	H	203	GLY	N-CA-C	-6.50	104.93	112.73
13	S	16	LEU	N-CA-C	-6.49	98.32	108.90
17	X	81	PRO	N-CA-C	-6.48	104.20	113.47
17	X	98	ARG	N-CA-C	6.47	120.43	112.54
4	D	388	GLY	N-CA-C	6.47	119.56	110.38
12	R	81	GLY	N-CA-C	-6.46	106.81	115.21
15	V	49	GLU	N-CA-C	-6.46	104.24	111.28
22	r	24	LEU	N-CA-C	6.46	119.61	110.50
21	q	75	TRP	N-CA-C	6.45	121.41	112.45
3	C	125	PHE	N-CA-C	6.44	119.58	110.50
8	H	267	SER	N-CA-C	-6.44	104.34	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	250	SER	N-CA-C	6.43	116.77	108.34
6	F	178	GLU	N-CA-CB	6.43	119.52	109.94
8	H	255	TYR	N-CA-CB	6.42	119.32	110.01
8	H	177	PRO	N-CA-C	-6.42	101.57	111.13
12	R	43	TYR	N-CA-C	-6.40	99.81	109.79
7	G	273	ILE	N-CA-C	-6.40	98.30	107.77
6	F	125	CYS	N-CA-C	-6.39	105.47	113.20
9	I	205	ILE	N-CA-C	-6.38	104.27	110.72
8	H	271	LEU	N-CA-CB	6.37	119.31	110.07
9	I	66	LEU	N-CA-C	-6.37	104.41	111.36
7	G	95	PRO	N-CA-C	-6.37	101.19	110.80
6	F	370	LEU	N-CA-C	-6.36	104.42	111.36
11	Q	59	LEU	N-CA-C	-6.36	100.76	110.30
4	D	140	ASP	N-CA-C	-6.36	96.61	107.23
4	D	96	ARG	N-CA-C	-6.32	96.11	107.98
6	F	144	VAL	N-CA-CB	6.32	118.65	110.57
22	r	8	ILE	N-CA-C	-6.32	104.34	110.72
1	A	101	GLY	N-CA-C	-6.31	105.18	112.50
4	D	141	TYR	N-CA-C	6.31	120.98	113.16
15	V	91	ALA	N-CA-C	-6.31	104.41	111.28
7	G	176	CYS	N-CA-C	6.30	119.61	110.42
21	q	28	PHE	N-CA-C	6.29	117.80	111.07
6	F	415	ILE	N-CA-C	-6.28	104.38	110.72
6	F	255	CYS	N-CA-C	-6.28	104.52	111.36
19	a	26	ILE	N-CA-C	-6.27	104.54	113.07
15	V	71	LEU	N-CA-C	6.27	118.11	111.28
7	G	356	ASP	N-CA-CB	6.27	119.33	110.12
2	B	113	ASP	N-CA-CB	6.25	119.53	109.28
17	X	99	HIS	N-CA-CB	6.25	119.41	110.16
6	F	101	PHE	N-CA-C	6.25	118.89	111.33
7	G	383	SER	N-CA-C	-6.24	106.88	114.75
21	q	69	ASN	N-CA-CB	6.23	121.38	111.66
8	H	52	ALA	N-CA-CB	6.22	119.03	110.01
5	E	50	THR	N-CA-CB	6.22	121.44	110.37
11	Q	141	ASN	N-CA-C	-6.22	105.69	113.28
6	F	192	ASP	N-CA-C	6.20	119.05	109.07
7	G	451	ILE	N-CA-C	-6.20	104.94	113.00
10	P	118	LYS	N-CA-C	6.20	119.01	111.82
17	X	36	CYS	CB-CA-C	-6.20	97.25	110.76
8	H	269	THR	N-CA-C	6.19	118.03	111.28
10	P	368	GLU	N-CA-CB	6.19	119.83	110.30
6	F	212	LEU	N-CA-C	-6.18	104.55	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	r	26	LEU	N-CA-CB	-6.17	101.15	110.35
8	H	76	THR	N-CA-C	-6.17	104.56	111.28
7	G	420	LYS	N-CA-C	6.16	118.78	111.33
7	G	418	ILE	N-CA-C	-6.14	103.44	112.04
8	H	276	SER	N-CA-C	6.14	118.94	111.82
4	D	427	PRO	N-CA-C	-6.13	99.84	112.47
13	S	40	ARG	N-CA-CB	-6.12	101.11	111.27
4	D	291	VAL	N-CA-C	-6.12	103.44	111.09
7	G	325	ARG	N-CA-CB	6.09	118.80	109.91
7	G	508	ALA	N-CA-C	6.08	117.91	111.28
8	H	185	TRP	N-CA-C	-6.08	104.00	112.45
2	B	70	ARG	N-CA-C	-6.07	101.32	110.24
13	S	87	VAL	N-CA-C	-6.05	104.44	110.62
8	H	7	LEU	N-CA-C	-6.04	104.33	111.03
7	G	353	ALA	N-CA-C	-6.03	104.64	112.23
8	H	24	GLU	N-CA-C	-6.02	104.08	112.45
13	S	61	VAL	N-CA-C	-6.01	99.58	107.88
22	r	108	LYS	N-CA-C	6.00	117.90	111.36
8	H	315	PRO	O-C-N	5.99	123.96	121.15
7	G	638	THR	N-CA-C	-5.98	100.20	109.24
2	B	196	PRO	N-CA-C	-5.98	101.82	111.03
17	X	40	ASN	N-CA-C	-5.98	104.67	111.07
8	H	103	LEU	N-CA-C	-5.97	104.85	111.36
9	I	116	CYS	N-CA-C	-5.94	105.52	112.89
6	F	291	GLU	N-CA-C	5.94	118.21	110.43
7	G	387	LEU	CB-CA-C	-5.92	101.73	111.68
13	S	30	SER	N-CA-C	-5.91	106.11	113.38
4	D	352	PRO	N-CA-C	5.90	117.90	110.70
18	Z	44	ILE	N-CA-C	-5.89	104.76	110.42
21	q	5	GLU	N-CA-C	-5.89	104.94	111.36
14	T	94	ASP	N-CA-CB	-5.89	105.12	111.66
1	A	58	VAL	CB-CA-C	-5.88	104.18	111.70
3	C	71	TYR	N-CA-C	5.86	120.24	113.38
4	D	258	VAL	N-CA-C	-5.85	103.95	110.62
21	q	65	THR	N-CA-C	5.85	119.20	110.14
3	C	209	LEU	N-CA-CB	-5.84	100.67	110.83
7	G	480	ALA	N-CA-C	-5.83	105.00	111.36
13	S	86	GLU	N-CA-CB	5.82	118.77	110.16
7	G	639	LEU	N-CA-C	5.81	118.56	111.82
7	G	672	ALA	N-CA-C	-5.81	104.95	111.28
6	F	226	LYS	CA-C-N	-5.81	114.40	120.38
6	F	226	LYS	C-N-CA	-5.81	114.40	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	P	367	GLU	CB-CA-C	-5.80	99.53	110.67
7	G	289	LYS	N-CA-C	5.80	117.60	111.28
8	H	116	ILE	N-CA-C	-5.80	104.85	110.42
10	P	157	LYS	N-CA-CB	5.80	118.74	110.16
15	V	19	THR	N-CA-CB	5.80	120.69	110.37
12	R	45	ARG	N-CA-C	-5.79	104.92	113.61
2	B	135	GLY	CA-C-O	-5.78	117.95	122.52
10	P	122	HIS	N-CA-C	5.78	120.03	112.92
7	G	34	VAL	N-CA-C	5.78	116.20	108.11
6	F	299	LEU	N-CA-C	5.78	118.52	111.82
10	P	234	LYS	CB-CA-C	-5.76	103.39	111.80
6	F	102	MET	CB-CA-C	-5.75	101.45	110.94
4	D	414	ASP	N-CA-C	-5.75	101.45	110.36
8	H	211	PHE	CA-C-O	5.74	126.90	119.95
11	Q	164	PHE	N-CA-CB	5.74	119.72	110.42
10	P	272	LEU	N-CA-C	-5.74	101.79	110.28
13	S	73	GLN	N-CA-C	-5.72	100.38	109.59
17	X	79	ALA	N-CA-C	5.72	117.19	111.07
18	Z	72	MET	CA-C-N	-5.72	113.30	119.24
18	Z	72	MET	C-N-CA	-5.72	113.30	119.24
1	A	55	PHE	N-CA-CB	5.71	118.29	110.01
21	q	140	PRO	N-CA-C	-5.71	102.18	110.80
8	H	252	PRO	N-CA-CB	-5.70	98.03	103.51
6	F	393	ASN	N-CA-C	-5.69	104.98	111.07
6	F	41	ILE	N-CA-C	5.69	115.77	110.42
5	E	119	THR	N-CA-C	-5.69	105.84	112.89
10	P	119	ALA	N-CA-C	-5.68	105.00	111.14
6	F	457	HIS	N-CA-CB	-5.67	100.87	110.50
17	X	65	GLY	N-CA-C	-5.67	105.93	112.50
2	B	112	TYR	N-CA-C	5.65	122.83	110.80
11	Q	124	MET	CA-C-N	-5.64	114.97	122.98
11	Q	124	MET	C-N-CA	-5.64	114.97	122.98
7	G	599	THR	CA-C-N	-5.64	114.15	122.83
7	G	599	THR	C-N-CA	-5.64	114.15	122.83
7	G	59	GLN	N-CA-C	5.63	117.95	107.99
6	F	304	ALA	CB-CA-C	-5.62	110.07	116.54
17	X	56	CYS	N-CA-C	5.62	119.83	112.92
7	G	530	TYR	N-CA-C	-5.61	101.98	110.28
6	F	416	SER	N-CA-C	5.60	117.83	111.11
9	I	191	LEU	N-CA-C	-5.60	105.25	111.36
6	F	176	ALA	N-CA-C	5.58	118.08	111.33
7	G	615	LEU	N-CA-C	-5.58	106.24	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	q	142	THR	N-CA-CB	5.58	119.88	109.68
5	E	183	PRO	N-CA-C	-5.57	102.18	111.26
21	q	68	MET	N-CA-C	5.55	119.31	112.54
6	F	294	VAL	CA-C-N	-5.55	114.04	119.76
6	F	294	VAL	C-N-CA	-5.55	114.04	119.76
14	T	135	ALA	N-CA-CB	5.54	118.27	110.12
7	G	127	ASP	CA-C-O	5.54	129.03	121.89
10	P	130	ILE	N-CA-C	5.54	115.23	107.37
17	X	54	ARG	CB-CA-C	5.54	119.48	110.96
21	q	71	LYS	N-CA-C	5.53	120.01	113.16
5	E	222	PHE	CB-CA-C	-5.51	100.65	109.75
7	G	363	SER	N-CA-C	-5.50	100.21	109.07
2	B	120	VAL	CA-C-N	-5.49	113.40	120.65
2	B	120	VAL	C-N-CA	-5.49	113.40	120.65
2	B	201	LEU	N-CA-C	-5.49	105.19	111.07
6	F	118	ASP	N-CA-C	-5.49	102.15	110.28
3	C	71	TYR	CB-CA-C	-5.49	102.28	111.23
22	r	94	ALA	N-CA-C	-5.48	101.74	109.96
10	P	86	CYS	N-CA-C	-5.48	103.15	110.55
7	G	313	LEU	N-CA-C	5.48	118.48	109.72
4	D	132	ALA	N-CA-C	-5.46	106.62	113.72
19	a	25	TYR	N-CA-C	-5.46	107.86	114.75
4	D	200	PHE	CA-CB-CG	5.44	119.24	113.80
7	G	682	ASP	CA-C-N	-5.44	114.16	119.76
7	G	682	ASP	C-N-CA	-5.44	114.16	119.76
7	G	404	GLY	N-CA-C	5.43	121.41	113.48
17	X	27	ALA	N-CA-C	-5.42	105.03	111.69
3	C	81	ASP	N-CA-C	-5.41	104.43	111.74
12	R	88	HIS	CB-CA-C	5.41	117.36	109.08
4	D	391	VAL	CA-C-N	-5.41	115.76	119.66
4	D	391	VAL	C-N-CA	-5.41	115.76	119.66
7	G	150	ARG	N-CA-CB	-5.41	102.85	111.62
14	T	92	LYS	N-CA-C	-5.41	106.27	112.92
10	P	357	ARG	N-CA-C	5.40	117.50	110.43
7	G	420	LYS	N-CA-CB	-5.40	101.96	110.06
5	E	48	PRO	N-CA-C	5.40	120.86	113.84
13	S	41	TYR	N-CA-C	-5.39	105.49	111.36
10	P	374	THR	N-CA-C	5.39	117.51	108.73
6	F	199	ARG	N-CA-C	5.37	117.48	109.59
13	S	24	CYS	N-CA-C	-5.36	103.32	110.55
18	Z	50	MET	N-CA-C	-5.35	105.45	111.28
4	D	201	PHE	N-CA-C	-5.35	105.53	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	P	339	GLY	N-CA-C	5.34	122.69	115.00
11	Q	163	ASN	CB-CA-C	-5.34	99.32	109.95
18	Z	55	GLN	N-CA-C	-5.34	105.46	111.28
7	G	510	TRP	N-CA-C	-5.33	101.96	109.96
11	Q	164	PHE	N-CA-C	-5.33	106.75	113.20
16	W	32	LYS	N-CA-C	-5.33	104.88	111.33
7	G	356	ASP	N-CA-C	-5.32	105.48	111.28
5	E	222	PHE	N-CA-C	5.32	117.90	109.24
8	H	146	MET	N-CA-C	-5.29	105.42	111.07
10	P	137	ARG	N-CA-C	5.28	122.05	110.80
8	H	252	PRO	CA-N-CD	5.28	119.39	112.00
4	D	141	TYR	N-CA-CB	-5.28	102.37	110.44
5	E	48	PRO	CB-CA-C	-5.28	104.36	111.85
11	Q	72	ILE	N-CA-C	-5.28	108.36	113.53
8	H	46	LEU	N-CA-C	-5.27	106.62	113.16
10	P	330	THR	N-CA-C	-5.27	106.75	114.39
7	G	362	ASP	CA-CB-CG	5.26	117.86	112.60
9	I	54	THR	N-CA-C	-5.26	104.96	111.33
9	I	160	GLU	N-CA-CB	-5.26	100.77	109.72
7	G	435	PRO	CB-CA-C	-5.26	105.83	111.56
4	D	363	VAL	N-CA-C	5.25	116.33	111.81
16	W	122	LEU	N-CA-C	-5.25	105.56	111.28
6	F	300	ILE	N-CA-CB	5.24	119.32	110.56
10	P	260	GLY	N-CA-C	-5.24	108.39	115.36
7	G	277	MET	N-CA-CB	-5.24	101.65	109.71
16	W	120	ASP	N-CA-C	-5.22	102.55	110.28
2	B	125	PRO	CB-CA-C	-5.21	104.73	112.55
7	G	600	GLU	CB-CA-C	-5.21	102.98	111.06
7	G	713	ALA	N-CA-C	-5.21	105.50	111.07
3	C	164	TRP	N-CA-C	5.20	117.02	111.36
8	H	310	PHE	N-CA-C	5.20	119.25	113.01
10	P	192	ARG	N-CA-C	-5.19	105.62	111.28
1	A	106	TRP	CB-CA-C	-5.19	102.38	110.94
22	r	107	SER	N-CA-C	-5.19	102.18	109.96
10	P	194	VAL	N-CA-CB	5.18	118.35	110.58
7	G	556	THR	N-CA-C	-5.18	101.54	109.41
22	r	25	GLN	N-CA-C	5.17	118.85	112.54
13	S	85	ASP	N-CA-C	5.17	117.82	111.82
7	G	172	ILE	N-CA-C	-5.16	98.60	109.34
10	P	198	ALA	N-CA-C	-5.16	100.11	108.52
6	F	337	MET	CB-CA-C	-5.16	103.02	111.68
7	G	63	PHE	CA-C-O	-5.15	115.08	121.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	H	277	TYR	N-CA-C	5.15	117.98	110.10
4	D	391	VAL	N-CA-C	5.14	113.80	109.02
7	G	569	GLN	CB-CA-C	-5.14	104.23	112.05
7	G	387	LEU	N-CA-C	-5.14	98.32	107.98
16	W	115	THR	CA-C-N	-5.12	113.44	119.84
16	W	115	THR	C-N-CA	-5.12	113.44	119.84
19	a	3	PHE	CB-CA-C	-5.12	102.61	110.81
2	B	94	THR	N-CA-CB	-5.12	102.24	110.69
4	D	106	VAL	O-C-N	-5.12	116.70	122.94
6	F	60	GLY	N-CA-C	-5.12	105.99	114.48
7	G	458	GLY	N-CA-C	-5.11	108.27	115.32
15	V	84	ALA	N-CA-C	5.11	116.54	111.07
20	b	82	LYS	N-CA-C	-5.11	103.79	110.53
4	D	224	ALA	CA-C-O	-5.09	115.45	120.90
9	I	95	PRO	N-CA-C	5.09	121.19	113.81
8	H	196	ALA	CA-C-N	-5.09	113.57	119.47
8	H	196	ALA	C-N-CA	-5.09	113.57	119.47
5	E	181	ASN	N-CA-C	-5.09	99.50	108.20
10	P	356	HIS	N-CA-C	-5.08	105.86	111.71
16	W	91	MET	N-CA-C	-5.08	105.93	111.82
17	X	42	GLU	N-CA-C	-5.07	105.83	111.36
3	C	156	VAL	N-CA-C	-5.07	104.17	111.17
8	H	101	GLY	N-CA-C	5.07	118.38	112.50
13	S	45	LYS	N-CA-C	-5.06	105.84	111.36
3	C	208	GLU	CA-C-O	-5.06	115.68	121.40
7	G	203	ASP	CA-C-O	5.06	127.19	121.32
10	P	170	LEU	N-CA-C	5.06	117.06	110.43
8	H	214	GLU	N-CA-C	5.05	119.32	113.20
10	P	376	ASN	CB-CA-C	-5.05	102.26	110.85
22	r	4	ALA	N-CA-C	-5.05	105.87	112.23
7	G	280	ASP	N-CA-CB	-5.05	102.70	110.12
12	R	65	ALA	N-CA-C	-5.04	105.91	111.71
14	T	140	CYS	CB-CA-C	-5.04	104.10	109.85
10	P	289	ILE	CA-C-N	-5.04	114.39	119.83
10	P	289	ILE	C-N-CA	-5.04	114.39	119.83
3	C	221	GLU	N-CA-C	-5.04	102.41	108.25
21	q	13	GLN	N-CA-C	-5.04	105.68	111.07
2	B	127	GLN	N-CA-CB	-5.03	103.18	110.47
7	G	393	GLY	N-CA-C	-5.03	107.81	115.66
6	F	366	ALA	N-CA-C	-5.03	105.49	110.97
7	G	453	GLN	N-CA-C	-5.02	105.88	111.36
17	X	110	CYS	CB-CA-C	-5.02	103.22	110.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	75	ALA	N-CA-C	5.02	117.41	111.33
5	E	213	PRO	CB-CA-C	-5.02	106.32	112.89
8	H	254	LEU	N-CA-CB	5.01	118.05	110.28
9	I	160	GLU	CB-CA-C	5.00	119.15	110.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	754	0	814	114	0
2	B	1258	0	1270	161	0
3	C	1641	0	1596	132	0
4	D	3079	0	3050	296	0
5	E	1635	0	1626	188	0
6	F	3288	0	3243	344	0
7	G	5287	0	5323	550	0
8	H	2500	0	2583	384	0
9	I	1398	0	1359	149	0
10	P	2730	0	2747	235	0
11	Q	957	0	949	71	0
12	R	660	0	639	75	0
13	S	667	0	685	67	0
14	T	604	0	596	90	0
15	V	915	0	954	80	0
16	W	970	0	991	78	0
17	X	1164	0	1150	85	0
18	Z	1152	0	1148	98	0
19	a	548	0	562	65	0
20	b	628	0	628	94	0
21	q	1004	0	962	82	0
22	r	418	0	434	44	0
23	s	107	0	100	10	0
24	A	46	0	69	5	0
24	I	51	0	82	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
24	b	46	0	69	16	0
25	B	8	0	0	6	0
25	F	8	0	0	10	0
25	G	16	0	0	5	0
25	I	16	0	0	16	0
26	B	35	0	44	6	0
26	H	42	0	58	7	0
26	I	47	0	71	10	0
27	D	18	0	18	24	0
28	E	4	0	0	5	0
28	G	4	0	0	4	0
29	F	31	0	19	1	0
30	H	35	0	43	3	0
31	P	48	0	26	7	0
32	R	1	0	0	0	0
33	W	32	0	0	7	0
34	q	57	0	58	18	0
All	All	33909	0	33966	3005	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 44.

All (3005) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:571:HIS:HD2	7:G:572:HIS:ND1	1.32	1.27
10:P:93:HIS:CD2	10:P:94:LEU:HD12	1.75	1.22
8:H:251:LEU:HD12	8:H:251:LEU:O	1.42	1.19
7:G:126:LEU:HD12	7:G:126:LEU:O	1.38	1.19
2:B:112:TYR:OH	9:I:91:GLY:HA3	1.38	1.19
7:G:63:PHE:O	7:G:64:CYS:SG	2.01	1.19
15:V:44:TYR:CE1	15:V:48:THR:HG21	1.77	1.18
10:P:156:SER:HB2	10:P:161:VAL:CG2	1.75	1.16
6:F:392:MET:CE	6:F:419:ILE:HD12	1.76	1.14
4:D:185:MET:CE	27:D:501:UQ1:HM21	1.77	1.13
7:G:126:LEU:CD1	12:R:89:PRO:HB2	1.77	1.13
6:F:382:CYS:SG	25:F:502:SF4:FE3	1.38	1.12
3:C:149:LEU:HD11	16:W:80:ARG:NH2	1.64	1.12
6:F:392:MET:HE3	6:F:419:ILE:CD1	1.78	1.12
13:S:51:LEU:HD13	13:S:95:LEU:HD21	1.23	1.12
2:B:126:ARG:HH22	8:H:63:PRO:HD3	1.13	1.11

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:123:CYS:SG	25:I:303:SF4:FE1	1.40	1.11
10:P:40:VAL:HG22	12:R:43:TYR:CE2	1.86	1.10
1:A:48:ARG:HH22	8:H:126:LYS:HA	0.98	1.09
9:I:101:HIS:HB2	9:I:149:MET:HE1	1.33	1.09
6:F:379:CYS:SG	25:F:502:SF4:FE4	1.43	1.09
6:F:33:GLY:HA2	6:F:291:GLU:HB3	1.27	1.09
6:F:392:MET:HE3	6:F:419:ILE:HD12	1.10	1.08
5:E:48:PRO:HA	5:E:95:SER:HB2	1.30	1.08
9:I:85:ASN:HB2	9:I:89:GLU:OE1	1.53	1.08
7:G:571:HIS:CD2	7:G:572:HIS:ND1	2.22	1.07
7:G:389:THR:HG22	7:G:514:ASN:HD22	1.16	1.07
3:C:168:GLU:HB2	3:C:186:ILE:HD11	1.33	1.07
7:G:399:VAL:HG21	7:G:462:PHE:CZ	1.88	1.07
8:H:172:MET:HE2	8:H:177:PRO:HD3	1.33	1.07
14:T:138:LEU:HD12	14:T:138:LEU:O	1.55	1.07
7:G:355:LYS:HA	7:G:366:LEU:HD21	1.18	1.06
9:I:152:CYS:SG	25:I:303:SF4:FE2	1.46	1.06
10:P:299:SER:HB3	10:P:316:LYS:HE3	1.37	1.06
2:B:100:CYS:SG	25:B:301:SF4:FE4	1.48	1.05
4:D:279:THR:HG23	15:V:13:GLY:HA3	1.36	1.05
8:H:106:LEU:HD21	8:H:150:LEU:HD12	1.35	1.05
8:H:142:TYR:HA	8:H:289:LEU:CD1	1.85	1.05
15:V:44:TYR:CE1	15:V:48:THR:CG2	2.39	1.05
2:B:112:TYR:CE1	9:I:84:ILE:HD11	1.92	1.05
3:C:98:PHE:HA	15:V:90:LEU:HD11	1.36	1.05
8:H:24:GLU:HA	8:H:271:LEU:HD23	1.39	1.05
13:S:79:LEU:HA	13:S:82:LEU:HD12	1.37	1.04
22:r:2:ALA:N	22:r:26:LEU:HD12	1.69	1.04
6:F:266:GLY:CA	6:F:271:SER:HA	1.86	1.04
10:P:156:SER:HB2	10:P:161:VAL:HG22	1.34	1.04
3:C:102:HIS:HE1	15:V:48:THR:HG22	1.20	1.03
4:D:359:ASP:HB3	7:G:150:ARG:HH22	1.23	1.03
7:G:387:LEU:HA	7:G:514:ASN:HB2	1.38	1.03
2:B:105:MET:HE1	27:D:501:UQ1:HM23	1.07	1.03
8:H:142:TYR:CD1	8:H:289:LEU:HD12	1.94	1.03
2:B:82:ILE:HG23	8:H:57:MET:SD	1.99	1.02
9:I:208:ASP:O	9:I:208:ASP:OD1	1.76	1.02
6:F:300:ILE:HG23	6:F:305:GLY:O	1.59	1.02
7:G:579:MET:O	7:G:579:MET:HG3	1.58	1.02
7:G:611:THR:HG21	11:Q:105:GLU:HA	1.42	1.02
3:C:203:LEU:HD11	4:D:123:LEU:HD13	1.41	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:199:ARG:HD3	23:s:80:PHE:CE2	1.95	1.02
2:B:202:LEU:HD12	9:I:86:TYR:CD2	1.95	1.02
8:H:186:PHE:CE1	8:H:270:PHE:CE1	2.48	1.02
5:E:179:CYS:SG	28:E:301:FES:FE2	1.50	1.01
21:q:66:THR:HG22	21:q:74:PHE:HB2	1.39	1.01
3:C:124:ARG:NH1	3:C:125:PHE:CZ	2.30	1.00
7:G:387:LEU:HD12	7:G:514:ASN:CG	1.87	1.00
9:I:155:CYS:SG	25:I:303:SF4:FE4	1.51	1.00
15:V:72:LEU:HD11	15:V:80:VAL:HG21	1.40	1.00
15:V:44:TYR:CZ	15:V:48:THR:HG21	1.97	1.00
2:B:122:ARG:HH12	27:D:501:UQ1:HM53	1.27	0.99
6:F:266:GLY:HA3	6:F:271:SER:CA	1.90	0.99
7:G:450:LYS:HD2	7:G:453:GLN:HG3	1.43	0.99
4:D:185:MET:CE	27:D:501:UQ1:CM2	2.39	0.99
4:D:185:MET:O	4:D:189:THR:HG22	1.63	0.99
7:G:360:LYS:HB2	7:G:632:ILE:HD12	1.43	0.99
6:F:154:ALA:HB3	6:F:193:PHE:HZ	1.25	0.99
7:G:646:LEU:HD22	7:G:653:LEU:HD13	1.45	0.99
8:H:186:PHE:CE1	8:H:270:PHE:HE1	1.81	0.99
7:G:389:THR:HG22	7:G:514:ASN:ND2	1.76	0.98
7:G:126:LEU:HD11	12:R:89:PRO:HB2	1.44	0.98
3:C:168:GLU:CB	3:C:186:ILE:HD11	1.92	0.98
7:G:213:MET:HE2	7:G:215:MET:HB2	1.40	0.98
7:G:355:LYS:CA	7:G:366:LEU:HD21	1.93	0.98
2:B:82:ILE:HG12	8:H:57:MET:CE	1.94	0.97
6:F:299:LEU:HD12	6:F:300:ILE:N	1.80	0.97
6:F:379:CYS:HG	25:F:502:SF4:FE4	0.74	0.97
7:G:467:LYS:HE3	7:G:503:THR:HG21	1.47	0.97
3:C:227:GLN:NE2	3:C:230:ARG:HH12	1.63	0.96
7:G:399:VAL:HG21	7:G:462:PHE:HZ	1.30	0.96
7:G:92:CYS:SG	28:G:803:FES:S1	2.63	0.96
7:G:597:VAL:HG12	7:G:603:ALA:HA	1.48	0.96
7:G:557:ARG:HG3	7:G:579:MET:HE3	1.48	0.96
2:B:82:ILE:HG12	8:H:57:MET:HE1	1.43	0.96
10:P:376:ASN:OD1	10:P:377:TYR:N	1.98	0.96
10:P:40:VAL:HG22	12:R:43:TYR:CD2	1.99	0.96
3:C:227:GLN:HE21	3:C:230:ARG:NH1	1.64	0.95
4:D:79:ASN:HB2	4:D:100:GLU:HB3	1.45	0.95
8:H:251:LEU:HD13	8:H:254:LEU:HG	1.46	0.95
5:E:57:GLU:HA	5:E:60:LYS:HE2	1.45	0.95
6:F:345:ALA:O	6:F:346:GLN:HG2	1.66	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:382:CYS:HG	25:F:502:SF4:FE3	0.66	0.95
9:I:152:CYS:HG	25:I:303:SF4:FE2	0.70	0.95
6:F:278:ILE:CD1	6:F:282:VAL:HG21	1.97	0.95
13:S:16:LEU:HD11	13:S:51:LEU:HD11	1.46	0.95
13:S:19:ILE:HG13	13:S:95:LEU:HD11	1.49	0.95
19:a:64:LYS:HE2	19:a:66:LEU:HD12	1.43	0.95
7:G:445:LEU:HD22	7:G:460:HIS:CE1	2.02	0.94
7:G:569:GLN:HE22	7:G:622:ILE:HG21	1.30	0.94
9:I:94:SER:HB2	9:I:95:PRO:HD2	1.48	0.94
6:F:300:ILE:HG22	6:F:306:GLY:HA2	1.47	0.94
6:F:113:LEU:HD13	6:F:149:MET:CE	1.96	0.94
7:G:76:ARG:HH21	7:G:79:LEU:HD21	1.31	0.94
4:D:198:THR:HG22	8:H:32:GLN:HE21	1.32	0.94
7:G:355:LYS:HA	7:G:366:LEU:CD2	1.97	0.94
8:H:142:TYR:HA	8:H:289:LEU:HD11	1.48	0.94
9:I:113:CYS:SG	25:I:304:SF4:FE3	1.59	0.94
4:D:302:LEU:HB2	4:D:401:GLU:HG2	1.48	0.94
6:F:128:ARG:HA	6:F:131:MET:HE2	1.50	0.93
1:A:48:ARG:NH2	8:H:126:LYS:HA	1.84	0.93
3:C:80:LEU:HD13	4:D:396:THR:HG22	1.51	0.92
5:E:179:CYS:HG	28:E:301:FES:FE2	0.66	0.92
5:E:240:PRO:HA	6:F:60:GLY:HA3	1.49	0.92
10:P:93:HIS:CD2	10:P:94:LEU:CD1	2.52	0.92
5:E:158:LYS:HE2	5:E:161:GLU:HG3	1.51	0.92
7:G:545:LEU:HB3	7:G:566:ILE:HG22	1.52	0.92
7:G:399:VAL:CG2	7:G:462:PHE:HZ	1.82	0.92
2:B:126:ARG:HH21	8:H:61:MET:HB2	1.33	0.91
21:q:3:LEU:HD13	34:q:201:CDL:HB4	1.49	0.91
8:H:181:MET:HE1	8:H:304:HIS:ND1	1.86	0.91
21:q:85:GLU:HG2	21:q:98:PRO:HB3	1.53	0.91
2:B:81:LEU:HG	26:B:302:PC1:H261	1.52	0.90
7:G:262:VAL:HG23	7:G:276:ARG:HB3	1.51	0.90
6:F:425:CYS:HG	25:F:502:SF4:FE1	0.63	0.90
7:G:283:GLU:O	7:G:283:GLU:HG2	1.71	0.90
15:V:75:GLY:HA2	22:r:103:ARG:HD2	1.52	0.90
4:D:185:MET:HE3	27:D:501:UQ1:HM21	1.52	0.90
10:P:93:HIS:NE2	10:P:94:LEU:CD1	2.35	0.90
7:G:62:ARG:HD2	7:G:65:TYR:HD2	1.36	0.90
2:B:105:MET:HE1	27:D:501:UQ1:CM2	2.00	0.89
4:D:232:VAL:HG12	4:D:356:ILE:HD13	1.53	0.89
2:B:95:PHE:HZ	2:B:148:VAL:HB	1.35	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:V:72:LEU:HD12	15:V:72:LEU:O	1.73	0.89
21:q:76:ASP:OD1	21:q:76:ASP:O	1.90	0.89
7:G:176:CYS:HG	25:G:802:SF4:FE4	0.62	0.89
7:G:399:VAL:CG2	7:G:462:PHE:CZ	2.55	0.89
7:G:431:LEU:HD22	7:G:438:LEU:HD11	1.53	0.89
6:F:296:LEU:HD13	6:F:337:MET:HE3	1.53	0.89
6:F:404:ALA:O	6:F:450:MET:SD	2.32	0.88
19:a:37:ARG:HB2	19:a:48:MET:HE2	1.54	0.88
6:F:266:GLY:HA3	6:F:271:SER:HA	0.94	0.88
6:F:257:ARG:HG2	6:F:261:TRP:CD2	2.08	0.88
4:D:185:MET:HE3	27:D:501:UQ1:CM2	2.02	0.88
3:C:186:ILE:HD12	4:D:429:PHE:HZ	1.36	0.88
8:H:181:MET:HE3	8:H:304:HIS:CE1	2.09	0.88
10:P:96:LEU:HD12	10:P:97:MET:N	1.88	0.88
10:P:344:PRO:HB2	10:P:347:LEU:HD13	1.56	0.88
4:D:101:LEU:HD11	4:D:106:VAL:HG22	1.56	0.88
9:I:61:LEU:HD21	20:b:17:PRO:O	1.74	0.88
13:S:16:LEU:HD22	13:S:19:ILE:HD11	1.53	0.88
20:b:60:ASP:OD1	20:b:61:GLY:N	2.07	0.87
22:r:2:ALA:N	22:r:26:LEU:CD1	2.37	0.87
7:G:97:MET:HB2	7:G:100:TRP:CD1	2.09	0.87
7:G:546:PHE:HZ	7:G:569:GLN:HE21	1.16	0.87
8:H:79:LEU:HD11	8:H:83:LEU:HD11	1.54	0.87
5:E:204:ILE:HA	5:E:207:LEU:HD12	1.56	0.87
6:F:338:ASP:OD1	6:F:341:ALA:HB3	1.75	0.87
8:H:24:GLU:HA	8:H:271:LEU:CD2	2.04	0.86
1:A:48:ARG:HH22	8:H:126:LYS:CA	1.86	0.86
14:T:138:LEU:HD13	14:T:144:ILE:HG12	1.56	0.86
7:G:404:GLY:HA3	7:G:684:LEU:HD13	1.57	0.86
13:S:16:LEU:HD12	13:S:16:LEU:O	1.76	0.86
14:T:79:ILE:HB	14:T:145:VAL:HG13	1.55	0.86
8:H:92:PRO:HD3	8:H:255:TYR:CD1	2.10	0.86
2:B:105:MET:CE	27:D:501:UQ1:HM23	2.01	0.86
10:P:156:SER:HB2	10:P:161:VAL:HG21	1.55	0.86
5:E:174:GLU:OE1	6:F:376:HIS:HB2	1.76	0.86
8:H:92:PRO:HD3	8:H:255:TYR:HD1	1.38	0.86
7:G:64:CYS:SG	7:G:75:CYS:SG	2.73	0.86
7:G:78:CYS:SG	28:G:803:FES:FE2	1.68	0.86
3:C:168:GLU:HB2	3:C:186:ILE:CD1	2.04	0.85
9:I:162:CYS:SG	25:I:304:SF4:FE4	1.68	0.85
6:F:154:ALA:HB3	6:F:193:PHE:CZ	2.11	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:ARG:NH1	27:D:501:UQ1:HM53	1.90	0.85
21:q:42:ASP:OD2	21:q:83:PRO:HG2	1.77	0.85
4:D:359:ASP:HB3	7:G:150:ARG:NH2	1.90	0.85
6:F:278:ILE:HD12	6:F:282:VAL:HG21	1.56	0.85
7:G:36:VAL:HB	7:G:56:VAL:HG21	1.58	0.85
7:G:253:VAL:HG12	7:G:345:LEU:HG	1.58	0.85
10:P:132:ARG:HG2	31:P:401:NDP:H8A	1.56	0.85
3:C:80:LEU:CD1	4:D:396:THR:HG22	2.07	0.85
8:H:102:ILE:CG2	8:H:150:LEU:HD13	2.07	0.84
14:T:110:LEU:HG	14:T:114:ASP:HB2	1.59	0.84
2:B:93:MET:HE1	2:B:148:VAL:HG11	1.59	0.84
8:H:251:LEU:CD1	8:H:254:LEU:HG	2.07	0.84
7:G:404:GLY:CA	7:G:684:LEU:HD13	2.08	0.84
7:G:571:HIS:HD2	7:G:572:HIS:CE1	1.96	0.84
15:V:56:LEU:HD12	15:V:57:ASP:N	1.92	0.84
3:C:80:LEU:HD13	4:D:396:THR:CG2	2.08	0.84
6:F:116:ASN:OD1	6:F:116:ASN:O	1.94	0.84
20:b:23:PHE:HB3	24:b:201:3PE:H2D2	1.58	0.84
10:P:275:HIS:HA	10:P:278:LYS:HE2	1.60	0.84
4:D:271:ARG:HD2	8:H:279:ARG:O	1.78	0.84
8:H:172:MET:CE	8:H:176:LEU:HB2	2.07	0.84
7:G:304:GLU:HG2	7:G:615:LEU:HD12	1.60	0.83
3:C:172:MET:CE	3:C:187:LEU:HB2	2.08	0.83
1:A:108:GLN:HG2	1:A:109:LYS:H	1.43	0.83
4:D:88:HIS:CE1	27:D:501:UQ1:H71	2.12	0.83
5:E:174:GLU:HG2	6:F:369:ARG:HH12	1.42	0.83
7:G:456:ALA:O	7:G:499:LYS:HE2	1.77	0.83
17:X:122:LEU:HD23	20:b:82:LYS:HG2	1.59	0.83
2:B:126:ARG:NH2	8:H:61:MET:HB2	1.93	0.83
3:C:172:MET:HE1	3:C:187:LEU:HB2	1.60	0.82
8:H:181:MET:CE	8:H:304:HIS:CE1	2.61	0.82
3:C:186:ILE:CD1	4:D:429:PHE:HZ	1.93	0.82
7:G:357:LEU:HD12	7:G:632:ILE:HD11	1.62	0.82
7:G:130:ILE:HG22	7:G:175:ARG:HH22	1.43	0.82
8:H:1:MET:HG3	19:a:30:THR:CG2	2.08	0.82
4:D:329:ARG:HD2	4:D:453:THR:HB	1.61	0.82
4:D:383:LYS:HD3	7:G:140:GLN:NE2	1.94	0.82
8:H:1:MET:HG3	19:a:30:THR:HG22	1.58	0.82
6:F:117:ALA:HB1	6:F:131:MET:SD	2.19	0.82
6:F:113:LEU:HD13	6:F:149:MET:HE1	1.60	0.82
11:Q:146:ASP:OD1	11:Q:146:ASP:O	1.97	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:422:HIS:HD2	7:G:79:LEU:HD12	1.45	0.82
7:G:425:ASN:OD1	7:G:426:ASP:N	2.12	0.81
22:r:4:ALA:HB1	22:r:9:GLN:HB2	1.60	0.81
7:G:404:GLY:HA2	7:G:684:LEU:CD1	2.09	0.81
4:D:79:ASN:HB2	4:D:100:GLU:CB	2.10	0.81
6:F:162:PHE:HB3	6:F:165:GLU:HB2	1.61	0.81
8:H:246:LEU:HD12	8:H:246:LEU:O	1.81	0.81
21:q:71:LYS:O	21:q:72:ASN:OD1	1.99	0.81
7:G:78:CYS:HG	28:G:803:FES:FE2	0.51	0.81
8:H:1:MET:HE3	19:a:29:PHE:CE2	2.15	0.81
9:I:123:CYS:HG	25:I:303:SF4:FE1	0.52	0.81
7:G:652:ASN:OD1	7:G:653:LEU:N	2.14	0.81
8:H:172:MET:CE	8:H:177:PRO:HD3	2.09	0.81
5:E:158:LYS:HE2	5:E:161:GLU:CG	2.10	0.81
6:F:422:HIS:NE2	7:G:112:ALA:HA	1.95	0.80
8:H:67:SER:HA	26:H:402:PC1:H121	1.63	0.80
6:F:278:ILE:CD1	6:F:285:PRO:HA	2.11	0.80
7:G:73:GLY:HA2	28:G:803:FES:S1	2.21	0.80
9:I:171:PRO:HB3	21:q:93:MET:HE1	1.61	0.80
3:C:102:HIS:CE1	15:V:48:THR:HG22	2.11	0.80
8:H:51:ASP:OD1	8:H:52:ALA:N	2.15	0.80
14:T:87:LEU:HD21	14:T:104:PHE:HZ	1.47	0.80
6:F:422:HIS:HD2	7:G:79:LEU:CD1	1.94	0.80
8:H:181:MET:CE	8:H:304:HIS:ND1	2.45	0.80
8:H:116:ILE:HG21	8:H:135:ALA:HB3	1.64	0.80
9:I:162:CYS:HG	25:I:304:SF4:FE4	0.52	0.80
4:D:92:HIS:HB2	4:D:458:PHE:HD2	1.47	0.80
15:V:95:LEU:HA	15:V:100:TRP:HH2	1.46	0.80
2:B:89:SER:O	8:H:54:LYS:HD3	1.82	0.79
6:F:154:ALA:CB	6:F:193:PHE:HZ	1.94	0.79
7:G:340:ALA:HB1	7:G:354:LEU:HD21	1.63	0.79
8:H:235:ASN:ND2	8:H:270:PHE:CE2	2.50	0.79
4:D:127:LYS:HB3	4:D:131:GLN:HG3	1.65	0.79
6:F:392:MET:CE	6:F:416:SER:HA	2.12	0.79
6:F:338:ASP:OD1	6:F:341:ALA:CB	2.30	0.79
7:G:385:TYR:HA	7:G:515:ILE:HD11	1.63	0.79
8:H:17:MET:SD	8:H:229:THR:OG1	2.41	0.79
8:H:251:LEU:O	8:H:251:LEU:CD1	2.28	0.79
8:H:306:SER:OG	8:H:310:PHE:CE2	2.36	0.79
21:q:3:LEU:CD1	34:q:201:CDL:HB4	2.11	0.79
7:G:213:MET:HE2	7:G:215:MET:CB	2.13	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:120:PRO:CB	17:X:125:LEU:HD11	2.13	0.79
4:D:271:ARG:HG2	8:H:281:ARG:HG3	1.62	0.79
7:G:617:ARG:NH1	16:W:129:HIS:HA	1.97	0.79
8:H:142:TYR:OH	8:H:288:LEU:HD22	1.82	0.79
14:T:93:ILE:HG21	14:T:110:LEU:HD22	1.63	0.79
6:F:109:ARG:HD2	6:F:237:GLY:O	1.83	0.79
7:G:404:GLY:CA	7:G:684:LEU:CD1	2.60	0.79
17:X:4:ILE:HG22	17:X:5:VAL:H	1.48	0.79
3:C:227:GLN:NE2	3:C:230:ARG:NH1	2.25	0.79
8:H:97:ASN:OD1	8:H:97:ASN:O	1.98	0.78
9:I:113:CYS:HG	25:I:304:SF4:FE3	0.49	0.78
7:G:463:CYS:SG	7:G:467:LYS:NZ	2.56	0.78
8:H:200:LEU:HD22	8:H:282:TYR:HB2	1.65	0.78
5:E:180:VAL:HG11	5:E:224:CYS:SG	2.24	0.78
7:G:169:VAL:HG22	7:G:223:ILE:HD11	1.64	0.78
10:P:40:VAL:CG2	12:R:43:TYR:CE2	2.66	0.78
8:H:27:ILE:HG23	8:H:31:MET:HE3	1.66	0.78
8:H:20:LEU:HD22	8:H:228:TYR:HD2	1.48	0.78
14:T:87:LEU:HD22	14:T:104:PHE:CE1	2.19	0.78
13:S:20:ARG:HG3	13:S:54:LEU:HB2	1.65	0.78
14:T:83:VAL:CG2	14:T:126:PHE:HZ	1.97	0.78
6:F:422:HIS:CD2	7:G:79:LEU:CD1	2.66	0.78
8:H:151:LEU:HA	8:H:154:LEU:HD12	1.66	0.78
13:S:51:LEU:HD13	13:S:95:LEU:CD2	2.11	0.78
5:E:227:ALA:HB3	6:F:284:HIS:ND1	1.99	0.78
20:b:66:VAL:HG13	20:b:72:ASP:HB2	1.65	0.77
2:B:89:SER:O	8:H:54:LYS:CD	2.32	0.77
4:D:128:THR:H	4:D:131:GLN:HE21	1.33	0.77
7:G:117:MET:HE3	7:G:143:SER:N	1.99	0.77
7:G:126:LEU:O	7:G:126:LEU:CD1	2.26	0.77
7:G:462:PHE:CE2	7:G:466:LEU:HD21	2.19	0.77
7:G:600:GLU:HG3	7:G:659:ILE:HD12	1.66	0.77
8:H:306:SER:OG	8:H:310:PHE:HE2	1.67	0.77
16:W:47:PRO:HG3	16:W:63:ARG:HH21	1.49	0.77
12:R:95:LEU:HD21	12:R:111:PHE:HB3	1.66	0.77
17:X:124:GLN:O	17:X:125:LEU:HD12	1.85	0.77
1:A:61:THR:CG2	8:H:290:TRP:CH2	2.67	0.77
7:G:506:VAL:HG21	7:G:510:TRP:CD1	2.20	0.77
17:X:20:VAL:HG22	17:X:24:VAL:HG21	1.66	0.77
1:A:112:GLU:O	1:A:112:GLU:CD	2.28	0.77
6:F:424:ILE:HD11	7:G:73:GLY:O	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:377:ALA:HB2	7:G:671:LEU:HD22	1.67	0.77
11:Q:81:VAL:HG21	11:Q:150:LYS:HG3	1.66	0.77
11:Q:112:MET:SD	21:q:126:PRO:HB2	2.24	0.77
10:P:142:GLU:O	10:P:146:VAL:HG12	1.84	0.77
14:T:93:ILE:HG23	14:T:110:LEU:HD13	1.66	0.77
1:A:61:THR:HG21	8:H:290:TRP:CZ3	2.20	0.76
6:F:423:THR:HG21	6:F:428:GLY:HA3	1.67	0.76
7:G:632:ILE:HG13	7:G:632:ILE:O	1.85	0.76
8:H:196:ALA:HB2	8:H:274:ARG:HG3	1.66	0.76
21:q:56:PHE:HA	21:q:59:HIS:HD2	1.50	0.76
3:C:80:LEU:CD1	4:D:396:THR:CG2	2.63	0.76
5:E:183:PRO:HB2	5:E:195:LEU:H	1.50	0.76
8:H:183:MET:HE2	26:I:302:PC1:H2A1	1.68	0.76
14:T:119:ILE:HD12	14:T:138:LEU:HD11	1.67	0.76
8:H:228:TYR:HA	8:H:231:ILE:HD12	1.68	0.76
7:G:406:ASN:ND2	7:G:436:VAL:HG21	2.01	0.76
6:F:163:TYR:HA	6:F:199:ARG:HH12	1.51	0.76
6:F:314:LEU:HB3	6:F:329:LYS:HD3	1.68	0.76
8:H:91:MET:O	8:H:92:PRO:C	2.27	0.76
6:F:225:LEU:H	11:Q:160:TYR:HE2	1.31	0.76
2:B:112:TYR:OH	9:I:91:GLY:CA	2.27	0.76
4:D:456:ILE:HG23	4:D:461:ILE:HD11	1.68	0.76
9:I:80:GLU:HG3	19:a:1:MET:SD	2.26	0.76
6:F:392:MET:HE1	6:F:416:SER:HA	1.66	0.75
7:G:462:PHE:CE2	7:G:466:LEU:HG	2.21	0.75
3:C:98:PHE:HA	15:V:90:LEU:CD1	2.16	0.75
21:q:96:ASP:OD1	21:q:97:PRO:HD2	1.85	0.75
4:D:371:MET:SD	4:D:381:HIS:CD2	2.80	0.75
7:G:506:VAL:HG21	7:G:510:TRP:HD1	1.50	0.75
10:P:348:LYS:O	10:P:351:GLU:HG2	1.86	0.75
8:H:251:LEU:HD11	8:H:254:LEU:HD12	1.69	0.75
6:F:154:ALA:CB	6:F:193:PHE:CZ	2.69	0.75
8:H:35:LYS:HG3	9:I:83:THR:HG22	1.69	0.75
21:q:55:PHE:CD1	22:r:26:LEU:HD22	2.21	0.75
4:D:174:PHE:CZ	4:D:217:VAL:HG11	2.21	0.75
7:G:608:VAL:HG23	11:Q:103:THR:OG1	1.87	0.75
11:Q:167:ASN:O	11:Q:168:LYS:CD	2.35	0.75
5:E:139:CYS:SG	28:E:301:FES:FE1	1.78	0.75
12:R:104:CYS:SG	12:R:107:CYS:HB2	2.27	0.75
6:F:94:PRO:HG2	6:F:97:LEU:HD12	1.67	0.75
7:G:261:ILE:HG22	7:G:286:ILE:HG21	1.68	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:214:LEU:HG	10:P:353:LEU:HD21	1.68	0.74
14:T:117:GLU:HA	14:T:120:MET:HE3	1.68	0.74
5:E:138:PRO:HG2	6:F:122:PRO:HB3	1.67	0.74
7:G:399:VAL:HG11	7:G:466:LEU:HD23	1.68	0.74
11:Q:61:ILE:O	11:Q:61:ILE:HD12	1.86	0.74
6:F:203:ALA:HB3	6:F:206:CYS:SG	2.28	0.74
7:G:347:ASP:HB2	7:G:594:ALA:HB1	1.69	0.74
9:I:57:ALA:HB2	20:b:13:TRP:O	1.87	0.74
2:B:89:SER:O	8:H:54:LYS:HE2	1.87	0.74
6:F:293:SER:HA	6:F:336:LEU:HD13	1.68	0.74
7:G:76:ARG:NH2	7:G:79:LEU:HD21	2.02	0.74
8:H:123:SER:HB3	8:H:214:GLU:HG3	1.68	0.74
4:D:253:LEU:HB2	22:r:23:LYS:HD2	1.67	0.74
2:B:98:ALA:HB3	2:B:135:GLY:HA3	1.70	0.74
3:C:99:LEU:HD13	3:C:140:ILE:HD11	1.70	0.74
7:G:173:MET:HG3	7:G:176:CYS:HB2	1.70	0.74
7:G:283:GLU:O	7:G:285:TRP:CE3	2.41	0.74
1:A:61:THR:HG21	8:H:290:TRP:CH2	2.23	0.74
4:D:88:HIS:NE2	27:D:501:UQ1:H71	2.03	0.74
17:X:23:ALA:HB2	17:X:95:GLN:NE2	2.03	0.74
20:b:31:ILE:HA	20:b:34:MET:HE2	1.69	0.74
21:q:56:PHE:HD1	21:q:59:HIS:HE2	1.35	0.74
6:F:80:MET:HE1	6:F:85:LEU:HD23	1.70	0.74
7:G:399:VAL:HG21	7:G:462:PHE:CE1	2.22	0.74
8:H:272:TRP:HH2	26:I:302:PC1:H381	1.52	0.74
14:T:94:ASP:HB3	14:T:98:LEU:HB2	1.69	0.74
6:F:425:CYS:SG	25:F:502:SF4:FE1	1.78	0.74
8:H:316:PRO:HA	18:Z:58:ARG:HH11	1.52	0.74
6:F:117:ALA:HB3	6:F:158:ILE:HA	1.68	0.73
6:F:296:LEU:HD12	6:F:299:LEU:HD21	1.69	0.73
10:P:203:PRO:HG2	31:P:401:NDP:H6N	1.69	0.73
10:P:336:GLU:HG3	10:P:342:PRO:HD3	1.67	0.73
21:q:68:MET:SD	21:q:81:MET:HB3	2.28	0.73
3:C:186:ILE:HD12	4:D:429:PHE:CZ	2.19	0.73
5:E:192:TYR:CE1	5:E:215:PRO:HA	2.23	0.73
9:I:110:GLU:OE2	12:R:64:ILE:HB	1.88	0.73
15:V:54:GLU:HG2	15:V:58:MET:HE2	1.70	0.73
5:E:43:THR:HG23	5:E:46:ASN:H	1.51	0.73
6:F:225:LEU:HB3	6:F:227:PRO:HD2	1.70	0.73
3:C:149:LEU:CD1	16:W:80:ARG:NH2	2.48	0.73
4:D:280:ALA:CB	15:V:11:LEU:HG	2.19	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:183:ILE:HD11	7:G:206:VAL:HG13	1.69	0.73
10:P:350:ILE:HB	10:P:366:ILE:HG23	1.70	0.73
14:T:88:LYS:HG3	14:T:98:LEU:HD22	1.70	0.73
14:T:103:HIS:CG	14:T:106:LYS:HD2	2.23	0.73
1:A:25:PRO:HG3	8:H:60:PRO:HD3	1.70	0.73
7:G:617:ARG:HH11	16:W:129:HIS:HA	1.52	0.73
8:H:172:MET:HE3	8:H:176:LEU:HB2	1.71	0.73
15:V:12:VAL:HG13	15:V:13:GLY:N	2.04	0.73
16:W:110:PHE:HZ	33:W:201:EHZ:C2	2.00	0.73
20:b:69:HIS:HD2	20:b:70:PRO:HD2	1.54	0.73
7:G:226:CYS:HG	25:G:802:SF4:FE1	1.05	0.73
8:H:292:ASN:O	20:b:18:VAL:HG11	1.88	0.73
6:F:193:PHE:HE2	6:F:195:VAL:HB	1.52	0.73
7:G:126:LEU:HD13	12:R:89:PRO:HB2	1.68	0.73
9:I:68:ARG:NH2	18:Z:26:PRO:HD2	2.04	0.73
5:E:163:THR:CG2	5:E:168:PHE:HB2	2.19	0.72
6:F:278:ILE:HD13	6:F:282:VAL:HG21	1.70	0.72
9:I:184:LEU:HD23	11:Q:112:MET:HG3	1.71	0.72
13:S:69:TYR:CE2	13:S:75:LYS:HG3	2.24	0.72
7:G:462:PHE:CE2	7:G:466:LEU:CD2	2.72	0.72
21:q:56:PHE:HA	21:q:59:HIS:CD2	2.24	0.72
3:C:93:ILE:HB	3:C:94:PRO:HD3	1.71	0.72
26:I:302:PC1:H112	18:Z:29:GLY:HA3	1.71	0.72
10:P:40:VAL:CG2	12:R:43:TYR:CD2	2.71	0.72
21:q:13:GLN:HE22	34:q:201:CDL:HA32	1.53	0.72
1:A:49:LEU:HD23	4:D:80:MET:HB2	1.72	0.72
7:G:254:MET:CE	7:G:345:LEU:HD21	2.19	0.72
17:X:90:ASP:OD2	19:a:62:VAL:HG11	1.90	0.72
7:G:89:VAL:HB	7:G:94:MET:HG3	1.71	0.72
10:P:262:THR:H	10:P:332:LEU:HD12	1.54	0.72
11:Q:167:ASN:O	11:Q:168:LYS:HD2	1.88	0.72
7:G:394:VAL:HB	7:G:417:ARG:CG	2.20	0.72
18:Z:98:MET:HE3	18:Z:101:VAL:HG21	1.70	0.72
5:E:158:LYS:CE	5:E:161:GLU:HG3	2.20	0.72
7:G:75:CYS:SG	7:G:76:ARG:N	2.63	0.72
1:A:21:ALA:O	1:A:25:PRO:HD3	1.88	0.72
5:E:232:SER:HB3	6:F:288:VAL:HG23	1.71	0.72
8:H:35:LYS:HG3	9:I:83:THR:CG2	2.20	0.72
2:B:95:PHE:HE1	2:B:131:MET:HE2	1.54	0.71
5:E:133:VAL:HG22	5:E:185:VAL:HG12	1.71	0.71
1:A:3:LEU:HA	8:H:96:ILE:HD13	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:ARG:HH12	27:D:501:UQ1:H8	1.55	0.71
2:B:108:ALA:HA	2:B:114:MET:HG2	1.71	0.71
7:G:254:MET:HE1	7:G:345:LEU:HD21	1.73	0.71
1:A:17:LEU:HB3	8:H:222:LEU:HD11	1.73	0.71
2:B:194:CYS:HB3	2:B:195:PRO:HD3	1.73	0.71
6:F:236:PHE:HA	11:Q:166:TRP:CD1	2.25	0.71
7:G:362:ASP:OD1	7:G:362:ASP:O	2.08	0.71
13:S:48:HIS:ND1	13:S:95:LEU:HD23	2.05	0.71
17:X:93:ASN:OD1	17:X:94:MET:N	2.24	0.71
3:C:67:ILE:HG21	3:C:98:PHE:CZ	2.26	0.71
3:C:172:MET:HE3	3:C:187:LEU:HD12	1.72	0.71
6:F:329:LYS:HA	6:F:332:CYS:SG	2.31	0.71
6:F:422:HIS:CD2	7:G:79:LEU:HD13	2.25	0.71
7:G:283:GLU:HG2	7:G:285:TRP:CZ3	2.25	0.71
8:H:187:ILE:HD12	24:I:301:3PE:H242	1.72	0.71
4:D:439:SER:HB3	4:D:450:ILE:HD12	1.72	0.71
6:F:278:ILE:HD11	6:F:285:PRO:HA	1.72	0.71
7:G:275:PRO:HG3	7:G:286:ILE:HG12	1.70	0.71
8:H:172:MET:HE3	8:H:176:LEU:HD12	1.73	0.71
8:H:215:TYR:CD2	8:H:219:PRO:HB2	2.26	0.71
4:D:140:ASP:HB3	4:D:147:ASN:HD21	1.56	0.71
8:H:113:VAL:HG22	8:H:136:VAL:HG23	1.71	0.71
10:P:170:LEU:O	10:P:171:ASN:OD1	2.09	0.71
2:B:93:MET:HE1	2:B:148:VAL:CG1	2.21	0.71
4:D:266:ARG:HB2	9:I:65:GLU:OE2	1.91	0.71
7:G:286:ILE:HA	7:G:413:LEU:HD11	1.73	0.71
8:H:312:ALA:HB2	20:b:38:TYR:HB3	1.73	0.71
13:S:63:PRO:HB2	13:S:79:LEU:HB2	1.72	0.71
4:D:86:PRO:HA	4:D:89:PRO:HD3	1.72	0.71
4:D:141:TYR:O	4:D:144:MET:SD	2.49	0.71
26:I:302:PC1:H2D1	26:I:302:PC1:H291	1.73	0.71
13:S:51:LEU:CD1	13:S:95:LEU:HD21	2.12	0.71
3:C:102:HIS:HE1	15:V:48:THR:CG2	2.01	0.70
3:C:124:ARG:NH1	3:C:125:PHE:CE1	2.59	0.70
5:E:78:VAL:HA	5:E:104:LEU:HD13	1.73	0.70
6:F:371:ILE:HD11	6:F:435:VAL:HG22	1.71	0.70
7:G:597:VAL:HG12	7:G:603:ALA:CA	2.19	0.70
9:I:153:ILE:HD11	9:I:155:CYS:HB3	1.72	0.70
12:R:67:GLN:HG2	12:R:109:LEU:CD2	2.21	0.70
1:A:65:PHE:CE2	8:H:294:LEU:HD21	2.26	0.70
8:H:61:MET:O	8:H:62:ARG:C	2.34	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
16:W:42:TRP:CD2	16:W:93:LEU:HD12	2.26	0.70
2:B:202:LEU:CD1	9:I:86:TYR:CD2	2.72	0.70
8:H:169:GLN:HE21	8:H:174:LEU:H	1.38	0.70
19:a:37:ARG:CB	19:a:48:MET:HE2	2.22	0.70
2:B:136:THR:HG21	2:B:177:VAL:HG22	1.73	0.70
5:E:46:ASN:HB2	5:E:91:TRP:HZ2	1.57	0.70
5:E:192:TYR:HB3	5:E:195:LEU:HD11	1.72	0.70
12:R:70:ASN:HB2	12:R:111:PHE:HD1	1.55	0.70
14:T:100:VAL:HB	14:T:142:GLN:HB2	1.74	0.70
8:H:318:MET:HG2	19:a:40:ARG:NH2	2.06	0.70
16:W:110:PHE:CZ	33:W:201:EHZ:C2	2.75	0.70
15:V:12:VAL:HG13	15:V:13:GLY:H	1.56	0.70
16:W:58:THR:HB	16:W:61:GLN:CB	2.22	0.70
6:F:51:TRP:HE3	6:F:135:PRO:HG3	1.55	0.69
15:V:56:LEU:HD12	15:V:56:LEU:C	2.16	0.69
18:Z:12:PRO:HD3	18:Z:16:TYR:CZ	2.25	0.69
3:C:84:GLU:HG2	3:C:141:ARG:HH11	1.56	0.69
6:F:113:LEU:CD1	6:F:149:MET:HE1	2.21	0.69
6:F:329:LYS:HE3	6:F:359:ARG:HH11	1.57	0.69
15:V:35:LEU:HA	15:V:38:PHE:CD1	2.27	0.69
7:G:127:ASP:HA	12:R:106:TYR:OH	1.90	0.69
6:F:345:ALA:O	6:F:346:GLN:CG	2.40	0.69
4:D:174:PHE:HZ	4:D:217:VAL:HG11	1.58	0.69
6:F:113:LEU:HD23	6:F:154:ALA:HB2	1.73	0.69
7:G:462:PHE:HE2	7:G:466:LEU:HD21	1.56	0.69
5:E:49:ASP:O	5:E:51:PRO:HD3	1.93	0.69
6:F:68:ILE:HG23	6:F:75:TRP:HZ3	1.58	0.69
6:F:300:ILE:HG22	6:F:306:GLY:CA	2.23	0.69
7:G:476:LEU:HB3	7:G:515:ILE:HG22	1.75	0.69
8:H:196:ALA:HB3	8:H:274:ARG:HA	1.75	0.69
10:P:171:ASN:OD1	10:P:171:ASN:O	2.11	0.69
13:S:19:ILE:HG13	13:S:95:LEU:CD1	2.22	0.69
13:S:23:LEU:HD12	13:S:23:LEU:O	1.93	0.69
14:T:87:LEU:HD22	14:T:104:PHE:HE1	1.58	0.69
3:C:186:ILE:HB	4:D:113:ILE:HD11	1.75	0.69
4:D:185:MET:HE1	27:D:501:UQ1:CM2	2.21	0.69
8:H:85:LEU:HD21	8:H:108:THR:HB	1.74	0.69
9:I:93:LEU:O	21:q:93:MET:HG2	1.93	0.69
9:I:155:CYS:HG	25:I:303:SF4:FE4	1.09	0.69
34:q:201:CDL:H341	34:q:201:CDL:H171	1.74	0.69
6:F:126:LYS:O	6:F:129:GLU:HG2	1.93	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:204:TYR:HB3	6:F:377:GLU:HG3	1.74	0.69
10:P:191:VAL:HA	10:P:194:VAL:HG22	1.73	0.69
14:T:138:LEU:HD13	14:T:144:ILE:CG1	2.23	0.69
4:D:92:HIS:HB2	4:D:458:PHE:CD2	2.27	0.68
9:I:200:GLU:OE2	21:q:93:MET:SD	2.51	0.68
5:E:190:ASN:HB3	5:E:192:TYR:CE2	2.28	0.68
6:F:383:THR:HG21	7:G:120:LEU:CD2	2.23	0.68
7:G:387:LEU:CA	7:G:514:ASN:HB2	2.20	0.68
8:H:79:LEU:CD1	8:H:83:LEU:HD11	2.24	0.68
8:H:283:ASP:OD1	8:H:284:GLN:N	2.26	0.68
4:D:194:ILE:HG23	4:D:271:ARG:HE	1.57	0.68
8:H:33:LEU:HD23	22:r:25:GLN:HG2	1.76	0.68
2:B:217:LYS:O	2:B:220:ILE:HG12	1.94	0.68
7:G:355:LYS:CA	7:G:366:LEU:CD2	2.66	0.68
8:H:186:PHE:CZ	8:H:270:PHE:CE1	2.81	0.68
10:P:344:PRO:HD2	10:P:347:LEU:HD22	1.74	0.68
14:T:116:VAL:HG12	14:T:120:MET:HE2	1.75	0.68
15:V:72:LEU:HD11	15:V:80:VAL:CG2	2.19	0.68
7:G:171:THR:HG22	7:G:231:LEU:HB3	1.75	0.68
13:S:19:ILE:HD12	13:S:94:VAL:HG11	1.76	0.68
5:E:150:THR:O	5:E:154:LYS:HG2	1.93	0.68
8:H:175:LEU:O	8:H:179:TRP:HB3	1.93	0.68
15:V:116:ILE:HG23	15:V:116:ILE:O	1.92	0.68
22:r:20:LEU:C	22:r:20:LEU:HD12	2.18	0.68
1:A:61:THR:HG22	8:H:290:TRP:CH2	2.29	0.68
5:E:137:THR:HG22	5:E:138:PRO:HD3	1.75	0.68
7:G:272:ARG:HE	7:G:274:LEU:HD23	1.58	0.68
7:G:283:GLU:HG2	7:G:285:TRP:HZ3	1.56	0.68
8:H:62:ARG:O	8:H:63:PRO:C	2.37	0.68
8:H:102:ILE:HG21	8:H:150:LEU:HD13	1.74	0.68
6:F:88:ARG:HD2	6:F:274:LYS:HG3	1.75	0.68
7:G:387:LEU:CD2	7:G:391:ILE:HD13	2.22	0.68
5:E:78:VAL:HG12	5:E:104:LEU:HD13	1.76	0.68
16:W:84:LEU:HD21	16:W:88:LYS:HE3	1.74	0.68
18:Z:121:ILE:HD11	18:Z:136:ALA:CB	2.24	0.68
7:G:301:ARG:NH2	7:G:591:GLU:OE1	2.27	0.67
7:G:357:LEU:HD13	7:G:627:SER:OG	1.94	0.67
9:I:188:GLU:OE2	12:R:56:ASN:HB2	1.94	0.67
17:X:78:CYS:SG	17:X:111:VAL:HG13	2.35	0.67
1:A:61:THR:HG22	8:H:290:TRP:HH2	1.59	0.67
1:A:112:GLU:O	1:A:112:GLU:OE1	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:341:ILE:HD12	7:G:555:ILE:HG12	1.76	0.67
3:C:149:LEU:HD11	16:W:80:ARG:HH21	1.57	0.67
4:D:94:VAL:HB	4:D:115:LEU:HB2	1.77	0.67
9:I:188:GLU:CD	12:R:56:ASN:HB2	2.19	0.67
13:S:16:LEU:HB3	13:S:69:TYR:HD1	1.58	0.67
2:B:89:SER:O	8:H:54:LYS:CE	2.42	0.67
6:F:426:ALA:O	6:F:429:ASP:HB2	1.95	0.67
7:G:175:ARG:HB2	7:G:230:ALA:HA	1.74	0.67
7:G:371:ILE:HG12	7:G:533:GLY:HA2	1.74	0.67
17:X:64:ASN:O	17:X:68:LEU:HG	1.94	0.67
2:B:95:PHE:HZ	2:B:148:VAL:CB	2.05	0.67
7:G:557:ARG:HD2	7:G:579:MET:HB2	1.76	0.67
8:H:224:PHE:CZ	30:H:401:UQ9:H12A	2.29	0.67
10:P:180:SER:O	10:P:184:LYS:HG3	1.95	0.67
10:P:156:SER:CB	10:P:161:VAL:HG22	2.20	0.67
10:P:197:GLU:HB3	10:P:259:VAL:CG2	2.24	0.67
10:P:302:GLY:HA2	10:P:314:THR:HG23	1.77	0.67
15:V:72:LEU:O	15:V:72:LEU:CD1	2.42	0.67
19:a:60:TYR:O	19:a:62:VAL:HG13	1.95	0.67
2:B:68:ARG:HD2	2:B:73:TYR:CB	2.25	0.67
5:E:46:ASN:HB2	5:E:91:TRP:CZ2	2.30	0.67
5:E:147:ILE:HG23	5:E:151:LEU:HD13	1.77	0.67
6:F:278:ILE:HD12	6:F:285:PRO:HA	1.77	0.67
6:F:375:LYS:HD2	6:F:390:ASP:OD1	1.95	0.67
4:D:375:MET:HE3	7:G:124:HIS:HB3	1.75	0.67
6:F:156:ILE:HD12	6:F:169:LEU:HD21	1.77	0.67
8:H:1:MET:CE	19:a:29:PHE:HE2	2.08	0.67
18:Z:121:ILE:HD11	18:Z:136:ALA:HB1	1.77	0.67
2:B:82:ILE:HA	8:H:57:MET:HE1	1.77	0.67
3:C:160:ILE:HD12	4:D:286:TYR:HE1	1.60	0.67
8:H:196:ALA:O	8:H:197:PRO:C	2.37	0.67
2:B:126:ARG:NH2	8:H:63:PRO:HD3	1.98	0.67
3:C:114:THR:HG22	4:D:421:ARG:NH1	2.10	0.67
5:E:240:PRO:CA	6:F:60:GLY:HA3	2.25	0.67
5:E:240:PRO:HG3	6:F:57:LEU:O	1.94	0.67
9:I:67:ILE:HG13	26:I:302:PC1:H251	1.77	0.67
7:G:569:GLN:OE1	7:G:622:ILE:HD13	1.96	0.66
14:T:87:LEU:CD2	14:T:104:PHE:CZ	2.78	0.66
2:B:170:TYR:HB2	9:I:153:ILE:HG21	1.77	0.66
3:C:98:PHE:CA	15:V:90:LEU:HD11	2.21	0.66
4:D:169:TRP:CD1	4:D:352:PRO:HD3	2.30	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:141:GLY:HA2	6:F:252:PRO:HD3	1.77	0.66
6:F:300:ILE:HD11	6:F:356:VAL:HG21	1.78	0.66
10:P:94:LEU:HA	10:P:97:MET:HE3	1.77	0.66
10:P:320:GLU:O	10:P:324:ILE:HG12	1.95	0.66
4:D:253:LEU:HB2	22:r:23:LYS:CD	2.26	0.66
14:T:130:ILE:HG23	14:T:131:PRO:HD2	1.77	0.66
23:s:78:TYR:HA	23:s:81:LEU:HD12	1.76	0.66
3:C:172:MET:CE	3:C:187:LEU:HD12	2.26	0.66
4:D:207:ARG:HA	4:D:210:MET:HE3	1.78	0.66
6:F:300:ILE:CG2	6:F:307:VAL:N	2.59	0.66
6:F:383:THR:N	6:F:384:PRO:HD2	2.10	0.66
7:G:308:ARG:HG3	7:G:581:ASP:HA	1.78	0.66
8:H:310:PHE:HB3	20:b:33:PRO:HA	1.77	0.66
9:I:92:PRO:HA	21:q:91:HIS:O	1.96	0.66
7:G:634:LEU:HD13	7:G:636:TYR:OH	1.96	0.66
8:H:1:MET:HE3	19:a:29:PHE:HE2	1.58	0.66
9:I:35:THR:CG2	22:r:107:SER:HA	2.26	0.66
9:I:80:GLU:OE2	22:r:26:LEU:CD1	2.44	0.66
10:P:268:PRO:HG2	10:P:344:PRO:HA	1.76	0.66
6:F:300:ILE:HG21	6:F:307:VAL:N	2.11	0.66
7:G:301:ARG:HE	7:G:613:PRO:HG3	1.59	0.66
7:G:374:THR:O	7:G:374:THR:OG1	2.08	0.66
10:P:156:SER:CB	10:P:161:VAL:CG2	2.66	0.66
15:V:44:TYR:CE1	15:V:48:THR:HG23	2.30	0.66
16:W:24:PHE:HB2	16:W:83:ASP:CG	2.20	0.66
3:C:197:PHE:CE2	4:D:121:GLU:OE1	2.49	0.66
4:D:101:LEU:CD1	4:D:106:VAL:HA	2.26	0.66
6:F:110:PRO:O	6:F:238:CYS:HB3	1.96	0.66
8:H:251:LEU:CD1	8:H:254:LEU:CG	2.73	0.66
8:H:311:THR:HB	18:Z:51:MET:SD	2.36	0.66
10:P:263:PHE:HD2	10:P:333:PRO:O	1.79	0.66
14:T:83:VAL:HG22	14:T:126:PHE:CZ	2.31	0.66
15:V:72:LEU:HD12	15:V:72:LEU:C	2.19	0.66
2:B:154:GLU:HB2	8:H:59:GLU:HB2	1.77	0.66
12:R:76:ILE:HD11	12:R:92:TYR:HB3	1.77	0.66
5:E:139:CYS:HA	5:E:182:ALA:HB1	1.77	0.65
5:E:203:ILE:HG12	5:E:218:ARG:NH1	2.11	0.65
7:G:339:ALA:HB1	7:G:537:ILE:CD1	2.26	0.65
7:G:462:PHE:CE2	7:G:466:LEU:CG	2.78	0.65
4:D:230:GLY:O	4:D:358:VAL:HG23	1.96	0.65
12:R:97:LYS:HE3	12:R:100:LYS:HD3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:97:ILE:HG13	18:Z:98:MET:H	1.61	0.65
1:A:6:VAL:HG11	8:H:87:VAL:CG2	2.27	0.65
1:A:54:LYS:O	1:A:58:VAL:HG23	1.95	0.65
2:B:146:ARG:O	2:B:147:LYS:C	2.39	0.65
4:D:359:ASP:CB	7:G:150:ARG:HH22	2.06	0.65
7:G:218:LEU:HD21	7:G:413:LEU:HD23	1.77	0.65
7:G:639:LEU:HD21	7:G:643:ARG:NE	2.11	0.65
7:G:671:LEU:HD21	13:S:45:LYS:HG2	1.77	0.65
13:S:24:CYS:HA	13:S:58:CYS:O	1.97	0.65
7:G:421:SER:HB2	7:G:427:LEU:CD1	2.26	0.65
10:P:199:ILE:HD11	10:P:258:ALA:O	1.96	0.65
10:P:236:VAL:CG1	10:P:270:ARG:HH21	2.10	0.65
12:R:70:ASN:HB2	12:R:111:PHE:CD1	2.31	0.65
13:S:16:LEU:HB3	13:S:69:TYR:CD1	2.32	0.65
15:V:38:PHE:CD1	15:V:95:LEU:HD21	2.31	0.65
8:H:303:TRP:CZ3	20:b:28:LEU:HG	2.31	0.65
18:Z:98:MET:CE	18:Z:101:VAL:HG21	2.27	0.65
1:A:85:SER:O	1:A:89:ILE:HG12	1.97	0.65
3:C:114:THR:HG22	4:D:421:ARG:HH12	1.62	0.65
4:D:237:PRO:HG2	4:D:240:LEU:HB2	1.78	0.65
14:T:118:ILE:HG23	14:T:122:MET:HE3	1.78	0.65
10:P:169:HIS:H	10:P:184:LYS:HE3	1.61	0.65
10:P:363:SER:HB3	16:W:51:HIS:CD2	2.32	0.65
10:P:226:VAL:HG21	10:P:281:PHE:CZ	2.32	0.65
18:Z:69:ILE:HD12	20:b:53:TYR:HA	1.78	0.65
6:F:339:PHE:CD1	6:F:349:LEU:HB3	2.32	0.65
10:P:88:VAL:HG12	10:P:92:MET:HE2	1.79	0.65
18:Z:75:PHE:CD1	19:a:46:TYR:HE2	2.15	0.65
4:D:217:VAL:HG12	4:D:240:LEU:HD22	1.78	0.64
7:G:458:GLY:HA2	7:G:463:CYS:SG	2.37	0.64
7:G:651:PRO:HG3	13:S:57:GLU:H	1.61	0.64
8:H:180:PRO:HD3	18:Z:43:LEU:HD21	1.79	0.64
7:G:360:LYS:HE3	7:G:632:ILE:HB	1.78	0.64
8:H:63:PRO:HB2	8:H:65:THR:HA	1.79	0.64
8:H:142:TYR:HA	8:H:289:LEU:HD13	1.79	0.64
9:I:93:LEU:HD13	9:I:97:PHE:CD2	2.33	0.64
12:R:38:TYR:HB2	12:R:45:ARG:HD3	1.79	0.64
3:C:99:LEU:HD13	3:C:140:ILE:CD1	2.27	0.64
5:E:70:PRO:HB2	5:E:73:HIS:HD2	1.62	0.64
7:G:388:ASN:HD22	7:G:511:LYS:HD2	1.61	0.64
11:Q:163:ASN:OD1	11:Q:164:PHE:N	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:76:ARG:HH21	7:G:79:LEU:CD2	2.07	0.64
12:R:112:LYS:O	12:R:113:GLN:C	2.40	0.64
13:S:69:TYR:CD2	13:S:75:LYS:HG3	2.33	0.64
3:C:67:ILE:HG21	3:C:98:PHE:CE1	2.33	0.64
6:F:102:MET:SD	6:F:149:MET:HB2	2.37	0.64
6:F:299:LEU:HD12	6:F:299:LEU:C	2.23	0.64
7:G:358:LEU:HB2	7:G:366:LEU:HD11	1.79	0.64
16:W:115:THR:O	16:W:116:PRO:C	2.39	0.64
19:a:1:MET:HG3	34:q:201:CDL:HB21	1.80	0.64
8:H:33:LEU:CD2	22:r:25:GLN:HG2	2.26	0.64
8:H:69:SER:O	8:H:72:ILE:HG13	1.98	0.64
5:E:163:THR:HG21	5:E:168:PHE:HB2	1.79	0.64
6:F:147:ARG:NH1	6:F:191:TYR:HB2	2.12	0.64
1:A:106:TRP:CZ2	8:H:291:LYS:HA	2.32	0.64
2:B:82:ILE:HG12	8:H:57:MET:HE2	1.77	0.64
2:B:136:THR:CG2	2:B:177:VAL:HG22	2.28	0.64
3:C:125:PHE:HE2	3:C:148:GLU:HA	1.62	0.64
4:D:185:MET:HE2	27:D:501:UQ1:HM21	1.72	0.64
5:E:87:ARG:HD2	23:s:77:THR:HG22	1.79	0.64
7:G:394:VAL:HB	7:G:417:ARG:HG3	1.80	0.64
7:G:579:MET:O	7:G:579:MET:CG	2.35	0.64
8:H:35:LYS:HE3	8:H:38:ASN:ND2	2.12	0.64
8:H:172:MET:HE1	18:Z:46:GLY:CA	2.28	0.64
13:S:15:GLY:HA3	13:S:17:ARG:HH22	1.62	0.64
18:Z:62:ILE:HG12	20:b:49:THR:HG22	1.79	0.64
1:A:54:LYS:HD2	1:A:113:TRP:HB2	1.79	0.64
5:E:176:LEU:HB2	5:E:184:MET:CE	2.28	0.64
6:F:80:MET:HE1	6:F:85:LEU:CD2	2.27	0.64
13:S:19:ILE:CG1	13:S:95:LEU:HD11	2.26	0.64
5:E:81:VAL:HB	5:E:104:LEU:HD11	1.79	0.64
7:G:370:GLU:OE2	7:G:478:SER:HB3	1.97	0.64
8:H:20:LEU:HD22	8:H:228:TYR:CD2	2.33	0.64
14:T:83:VAL:HG23	14:T:126:PHE:HZ	1.62	0.64
15:V:38:PHE:CE1	15:V:95:LEU:HD21	2.33	0.64
2:B:122:ARG:NH1	27:D:501:UQ1:H8	2.12	0.63
2:B:202:LEU:HD12	9:I:86:TYR:CG	2.34	0.63
6:F:326:LEU:HD23	6:F:367:ILE:HD11	1.80	0.63
8:H:195:ARG:O	8:H:199:ASP:HB2	1.97	0.63
8:H:196:ALA:CB	8:H:274:ARG:HA	2.28	0.63
9:I:105:ARG:HG2	9:I:111:GLU:HA	1.79	0.63
13:S:16:LEU:HA	13:S:69:TYR:HA	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:T:93:ILE:CG2	14:T:110:LEU:HD13	2.28	0.63
4:D:280:ALA:HB1	15:V:11:LEU:HG	1.79	0.63
5:E:40:HIS:CD2	5:E:94:ILE:HB	2.34	0.63
7:G:541:PRO:HB2	7:G:561:PRO:HG3	1.79	0.63
14:T:87:LEU:HD21	14:T:104:PHE:CZ	2.32	0.63
14:T:138:LEU:O	14:T:138:LEU:CD1	2.40	0.63
1:A:99:SER:HB3	24:b:201:3PE:H392	1.81	0.63
8:H:172:MET:HE1	18:Z:46:GLY:HA2	1.80	0.63
1:A:25:PRO:HG3	8:H:60:PRO:CD	2.28	0.63
4:D:348:LEU:O	18:Z:11:PRO:HB3	1.98	0.63
6:F:424:ILE:HA	7:G:76:ARG:NH1	2.13	0.63
8:H:85:LEU:HB3	8:H:233:LEU:HD21	1.79	0.63
8:H:110:SER:O	8:H:113:VAL:HG12	1.99	0.63
10:P:93:HIS:NE2	10:P:94:LEU:HD11	2.14	0.63
10:P:299:SER:CB	10:P:316:LYS:HE3	2.23	0.63
10:P:333:PRO:HB2	10:P:337:ASP:HB2	1.80	0.63
22:r:109:ASP:O	22:r:110:GLN:HG2	1.99	0.63
3:C:212:ASP:HB3	3:C:215:VAL:HG22	1.80	0.63
7:G:388:ASN:ND2	7:G:511:LYS:HD2	2.13	0.63
8:H:88:PRO:HG2	8:H:105:ILE:HD11	1.79	0.63
13:S:16:LEU:HD12	13:S:16:LEU:C	2.22	0.63
1:A:4:TYR:CE2	24:A:401:3PE:H231	2.34	0.63
4:D:106:VAL:HG11	4:D:109:CYS:SG	2.39	0.63
4:D:257:GLU:O	4:D:258:VAL:C	2.40	0.63
4:D:375:MET:HE1	7:G:126:LEU:HA	1.80	0.63
6:F:116:ASN:HB3	6:F:212:LEU:HD22	1.80	0.63
6:F:173:ILE:HD13	6:F:195:VAL:HG13	1.80	0.63
7:G:475:VAL:HG21	7:G:516:LEU:HD23	1.78	0.63
10:P:132:ARG:HG2	31:P:401:NDP:C8A	2.29	0.63
21:q:137:TRP:CZ2	21:q:140:PRO:HD3	2.34	0.63
6:F:222:LYS:HB3	6:F:381:GLN:OE1	1.98	0.63
8:H:307:LEU:HB3	8:H:308:PRO:HD3	1.79	0.63
10:P:66:GLY:O	10:P:67:ARG:C	2.42	0.63
14:T:103:HIS:CD2	14:T:106:LYS:HD2	2.34	0.63
17:X:83:THR:HA	17:X:86:TRP:CD1	2.34	0.63
1:A:95:VAL:HG11	8:H:302:MET:HG3	1.81	0.63
2:B:98:ALA:HB3	2:B:135:GLY:CA	2.28	0.63
4:D:181:LEU:HD22	4:D:207:ARG:HG3	1.81	0.63
7:G:340:ALA:CB	7:G:354:LEU:HD21	2.29	0.63
8:H:251:LEU:HD11	8:H:254:LEU:CG	2.28	0.63
6:F:346:GLN:HE22	6:F:440:ARG:HD3	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:66:THR:HG21	8:H:123:SER:HA	1.81	0.62
6:F:48:ARG:HH11	6:F:48:ARG:HA	1.64	0.62
7:G:68:ARG:HD3	7:G:285:TRP:CZ3	2.34	0.62
9:I:188:GLU:HG3	12:R:55:VAL:HA	1.80	0.62
5:E:176:LEU:HB2	5:E:184:MET:HE3	1.80	0.62
14:T:103:HIS:ND1	14:T:140:CYS:SG	2.73	0.62
16:W:83:ASP:O	16:W:86:VAL:HG22	1.99	0.62
18:Z:65:LEU:HB3	20:b:50:PRO:O	1.99	0.62
1:A:3:LEU:HD23	24:A:401:3PE:H251	1.80	0.62
8:H:102:ILE:HD12	8:H:154:LEU:HD21	1.80	0.62
10:P:240:VAL:HB	10:P:266:THR:O	2.00	0.62
34:q:201:CDL:H1	22:r:3:SER:HB2	1.82	0.62
4:D:188:THR:HB	4:D:200:PHE:HA	1.81	0.62
8:H:1:MET:HE3	19:a:29:PHE:CD2	2.33	0.62
10:P:297:VAL:O	10:P:300:TRP:HB3	1.98	0.62
2:B:82:ILE:CG1	8:H:57:MET:HE1	2.26	0.62
2:B:112:TYR:HH	9:I:91:GLY:HA3	1.60	0.62
3:C:160:ILE:HB	4:D:286:TYR:CD1	2.35	0.62
3:C:206:TYR:C	3:C:223:VAL:HG23	2.24	0.62
6:F:33:GLY:HA2	6:F:291:GLU:CB	2.16	0.62
7:G:222:VAL:HG12	7:G:231:LEU:HD11	1.81	0.62
7:G:476:LEU:HD21	7:G:481:LEU:HD21	1.82	0.62
8:H:153:VAL:O	8:H:156:MET:HG2	2.00	0.62
17:X:53:PRO:O	17:X:57:LEU:HG	1.99	0.62
22:r:20:LEU:HD12	22:r:21:GLN:N	2.14	0.62
3:C:168:GLU:CA	3:C:186:ILE:HD11	2.30	0.62
4:D:283:ALA:HB1	4:D:293:LEU:HD23	1.81	0.62
6:F:299:LEU:CD1	6:F:300:ILE:HG13	2.30	0.62
7:G:176:CYS:SG	25:G:802:SF4:FE4	1.78	0.62
7:G:394:VAL:HB	7:G:417:ARG:HG2	1.82	0.62
10:P:179:LYS:HA	10:P:182:ARG:HG2	1.82	0.62
13:S:16:LEU:CD2	13:S:19:ILE:HD11	2.28	0.62
4:D:333:ARG:NH1	4:D:455:ASP:OD1	2.33	0.62
5:E:151:LEU:HD11	5:E:200:ILE:HG21	1.81	0.62
6:F:426:ALA:HB3	29:F:501:FMN:HM81	1.81	0.62
7:G:347:ASP:CB	7:G:594:ALA:HB1	2.28	0.62
7:G:488:ALA:HB2	7:G:677:GLN:HB3	1.80	0.62
9:I:78:PHE:HD1	19:a:2:TRP:CD1	2.17	0.62
9:I:135:ARG:HE	9:I:141:ARG:HG3	1.64	0.62
14:T:138:LEU:HD12	14:T:138:LEU:C	2.24	0.62
17:X:115:LEU:HD13	17:X:117:TRP:CH2	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:421:SER:CB	7:G:427:LEU:CD1	2.78	0.62
8:H:33:LEU:HD11	9:I:76:TYR:CD1	2.35	0.62
10:P:43:HIS:H	10:P:51:VAL:HG13	1.64	0.62
10:P:318:LYS:HA	10:P:321:ARG:NH1	2.15	0.62
14:T:79:ILE:CB	14:T:145:VAL:HG13	2.28	0.62
18:Z:58:ARG:NH2	20:b:49:THR:HG21	2.15	0.62
7:G:373:PRO:HG2	7:G:481:LEU:HD22	1.81	0.61
10:P:169:HIS:H	10:P:184:LYS:CE	2.13	0.61
14:T:87:LEU:CD2	14:T:104:PHE:HZ	2.12	0.61
4:D:379:ILE:HD13	7:G:140:GLN:HA	1.82	0.61
6:F:50:ASP:HB3	6:F:55:GLY:HA3	1.83	0.61
6:F:226:LYS:O	6:F:227:PRO:C	2.42	0.61
6:F:392:MET:HE1	6:F:419:ILE:HD12	1.80	0.61
6:F:424:ILE:HA	7:G:76:ARG:HH12	1.65	0.61
7:G:260:ASN:H	7:G:281:ILE:HD11	1.65	0.61
7:G:515:ILE:O	7:G:515:ILE:HG13	1.98	0.61
7:G:545:LEU:HB3	7:G:566:ILE:CG2	2.29	0.61
8:H:142:TYR:CD1	8:H:289:LEU:CD1	2.80	0.61
8:H:251:LEU:HD11	8:H:254:LEU:CD1	2.29	0.61
20:b:8:PHE:C	20:b:9:LEU:HD12	2.25	0.61
4:D:141:TYR:HB3	4:D:223:HIS:HE1	1.66	0.61
5:E:139:CYS:HB3	5:E:144:SER:HB3	1.82	0.61
7:G:172:ILE:N	7:G:230:ALA:O	2.31	0.61
7:G:306:MET:HG2	7:G:316:TYR:HA	1.82	0.61
8:H:181:MET:HE3	8:H:304:HIS:HE1	1.62	0.61
12:R:98:GLU:CD	12:R:98:GLU:H	2.06	0.61
1:A:51:PHE:CD1	4:D:102:SER:HB2	2.36	0.61
5:E:39:VAL:HG23	7:G:205:GLN:HE22	1.66	0.61
7:G:557:ARG:HA	7:G:560:LEU:HD12	1.81	0.61
7:G:666:GLN:HE21	7:G:667:GLN:NE2	1.99	0.61
8:H:183:MET:HE2	26:I:302:PC1:H271	1.83	0.61
9:I:209:TYR:HA	9:I:212:ARG:HG2	1.82	0.61
10:P:41:ILE:HB	10:P:43:HIS:CE1	2.35	0.61
11:Q:167:ASN:O	11:Q:168:LYS:CG	2.49	0.61
21:q:74:PHE:CD2	21:q:75:TRP:CD1	2.89	0.61
1:A:113:TRP:CE2	8:H:283:ASP:HB2	2.35	0.61
2:B:122:ARG:HH12	27:D:501:UQ1:CM5	2.08	0.61
3:C:147:ASP:OD1	3:C:148:GLU:N	2.29	0.61
5:E:226:PRO:HA	6:F:286:CYS:HB3	1.82	0.61
6:F:357:MET:HE1	6:F:363:ILE:HG13	1.82	0.61
7:G:370:GLU:HB3	7:G:522:GLN:OE1	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:71:LYS:O	21:q:72:ASN:CG	2.43	0.61
5:E:135:THR:HG21	5:E:172:GLU:HG3	1.81	0.61
7:G:117:MET:HE3	7:G:143:SER:CA	2.31	0.61
7:G:421:SER:CB	7:G:427:LEU:HD11	2.30	0.61
8:H:251:LEU:HD12	8:H:251:LEU:C	2.23	0.61
16:W:32:LYS:NZ	33:W:201:EHZ:C19	2.63	0.61
18:Z:28:ARG:HG3	18:Z:28:ARG:O	1.99	0.61
3:C:100:ARG:HH12	15:V:86:LYS:NZ	1.99	0.61
4:D:104:GLU:HG3	4:D:104:GLU:O	1.99	0.61
21:q:7:LEU:HD23	34:q:201:CDL:H311	1.82	0.61
1:A:21:ALA:CB	8:H:218:GLY:HA3	2.30	0.61
3:C:186:ILE:HG13	3:C:187:LEU:HG	1.83	0.61
5:E:182:ALA:O	5:E:183:PRO:C	2.43	0.61
6:F:375:LYS:CD	6:F:390:ASP:OD1	2.48	0.61
7:G:82:ILE:CG2	7:G:100:TRP:HB3	2.30	0.61
7:G:246:ARG:NH2	11:Q:123:ASN:OD1	2.33	0.61
7:G:339:ALA:HB1	7:G:537:ILE:HD12	1.83	0.61
13:S:31:GLN:HA	13:S:34:ARG:HE	1.65	0.61
16:W:25:SER:HB2	16:W:31:ALA:HB2	1.83	0.61
4:D:456:ILE:HG23	4:D:461:ILE:CD1	2.31	0.61
7:G:569:GLN:NE2	7:G:622:ILE:HG21	2.11	0.61
10:P:169:HIS:HD2	10:P:181:LEU:HD11	1.65	0.61
14:T:103:HIS:HB2	14:T:106:LYS:HB2	1.83	0.61
2:B:112:TYR:CE1	2:B:199:GLU:HG2	2.36	0.61
5:E:191:TYR:OH	6:F:161:GLU:HB3	2.01	0.61
5:E:233:LEU:HD22	6:F:43:THR:HA	1.83	0.61
15:V:82:LEU:O	15:V:86:LYS:HG3	2.00	0.61
2:B:100:CYS:SG	25:B:301:SF4:S2	2.99	0.60
4:D:186:ALA:HB1	4:D:455:ASP:OD1	2.02	0.60
4:D:404:LYS:HZ2	4:D:455:ASP:HB3	1.66	0.60
7:G:339:ALA:CB	7:G:537:ILE:HD12	2.31	0.60
9:I:78:PHE:HB3	22:r:8:ILE:CG2	2.31	0.60
10:P:146:VAL:HG23	10:P:187:GLY:HA2	1.82	0.60
16:W:24:PHE:HB2	16:W:83:ASP:HB3	1.82	0.60
21:q:34:ARG:NE	21:q:58:ARG:NH2	2.48	0.60
5:E:39:VAL:HG11	7:G:163:LYS:NZ	2.15	0.60
7:G:63:PHE:C	7:G:64:CYS:SG	2.84	0.60
7:G:68:ARG:CD	7:G:285:TRP:CZ3	2.84	0.60
10:P:268:PRO:CG	10:P:344:PRO:HA	2.30	0.60
3:C:242:PRO:O	3:C:243:ALA:C	2.43	0.60
8:H:311:THR:O	18:Z:51:MET:HG3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:TRP:O	1:A:113:TRP:CD1	2.54	0.60
3:C:63:TYR:OH	3:C:102:HIS:NE2	2.32	0.60
7:G:339:ALA:O	7:G:545:LEU:HD12	2.01	0.60
16:W:58:THR:HB	16:W:61:GLN:HB2	1.83	0.60
1:A:54:LYS:HE3	1:A:55:PHE:CE1	2.37	0.60
4:D:378:LEU:HD22	7:G:126:LEU:HD13	1.83	0.60
7:G:421:SER:HB2	7:G:427:LEU:HD12	1.83	0.60
9:I:80:GLU:OE2	22:r:26:LEU:HD11	2.01	0.60
10:P:217:PHE:HA	10:P:220:TYR:CD2	2.37	0.60
17:X:53:PRO:HD3	18:Z:116:TRP:CD1	2.36	0.60
18:Z:143:TYR:O	18:Z:144:THR:C	2.45	0.60
2:B:75:VAL:O	2:B:76:THR:C	2.43	0.60
2:B:144:ALA:O	2:B:145:LEU:C	2.45	0.60
4:D:339:GLN:NE2	9:I:37:LYS:NZ	2.49	0.60
5:E:147:ILE:HG23	5:E:151:LEU:CD1	2.31	0.60
6:F:193:PHE:CE2	6:F:195:VAL:HB	2.35	0.60
7:G:197:THR:HG22	7:G:206:VAL:HG22	1.82	0.60
21:q:86:TRP:HA	21:q:98:PRO:HG2	1.84	0.60
1:A:3:LEU:HA	8:H:96:ILE:CD1	2.32	0.60
6:F:447:GLU:O	6:F:450:MET:HB2	2.01	0.60
7:G:130:ILE:HG22	7:G:175:ARG:NH2	2.15	0.60
7:G:395:GLU:HA	7:G:421:SER:OG	2.01	0.60
16:W:97:ILE:HG23	16:W:98:LYS:HG3	1.82	0.60
22:r:12:ARG:HB3	22:r:20:LEU:HD21	1.84	0.60
8:H:306:SER:HG	8:H:310:PHE:HE2	1.34	0.60
13:S:16:LEU:CB	13:S:69:TYR:HD1	2.15	0.60
24:A:401:3PE:H2E1	24:A:401:3PE:H2I2	1.84	0.60
7:G:281:ILE:CG2	7:G:602:ARG:NH1	2.65	0.60
7:G:373:PRO:HB3	7:G:487:ALA:HA	1.84	0.60
15:V:35:LEU:HA	15:V:38:PHE:HD1	1.65	0.60
4:D:156:GLU:HG3	4:D:229:PRO:O	2.01	0.60
8:H:17:MET:HE1	8:H:225:MET:HB3	1.84	0.60
8:H:306:SER:C	8:H:310:PHE:CE2	2.80	0.60
4:D:345:GLU:HB2	18:Z:19:ILE:HD12	1.82	0.59
5:E:190:ASN:HB3	5:E:192:TYR:CD2	2.37	0.59
6:F:297:LYS:HB2	6:F:333:GLU:CB	2.32	0.59
7:G:366:LEU:HD23	7:G:530:TYR:CZ	2.37	0.59
17:X:16:GLU:CD	17:X:68:LEU:HD13	2.27	0.59
19:a:2:TRP:HH2	34:q:201:CDL:H522	1.67	0.59
19:a:36:LYS:HA	19:a:59:ARG:HH22	1.67	0.59
7:G:131:CYS:HA	7:G:175:ARG:NH1	2.18	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:239:THR:O	8:H:239:THR:HG22	2.01	0.59
14:T:83:VAL:HG22	14:T:126:PHE:HZ	1.66	0.59
17:X:20:VAL:HG12	17:X:25:LEU:HD21	1.84	0.59
3:C:124:ARG:HD2	11:Q:140:LYS:NZ	2.17	0.59
3:C:224:GLU:OE2	10:P:45:LYS:HB3	2.02	0.59
4:D:256:ASP:O	4:D:259:GLU:HB2	2.02	0.59
5:E:185:VAL:HG22	5:E:195:LEU:HD12	1.83	0.59
9:I:63:TRP:CZ2	24:I:301:3PE:H331	2.37	0.59
16:W:122:LEU:HD11	16:W:126:TYR:CZ	2.37	0.59
18:Z:61:LEU:HA	18:Z:64:ASP:OD2	2.02	0.59
21:q:6:VAL:HG13	34:q:201:CDL:HA21	1.82	0.59
6:F:398:ARG:NH2	7:G:155:GLU:HG3	2.17	0.59
7:G:304:GLU:OE2	10:P:41:ILE:HG12	2.01	0.59
7:G:555:ILE:HD13	7:G:560:LEU:HD21	1.85	0.59
15:V:90:LEU:HD21	15:V:94:MET:CE	2.33	0.59
18:Z:54:ASN:O	18:Z:58:ARG:HG2	2.02	0.59
21:q:96:ASP:OD1	21:q:97:PRO:CD	2.50	0.59
5:E:222:PHE:H	5:E:225:GLU:CD	2.10	0.59
6:F:157:TYR:CZ	6:F:200:GLY:HA2	2.37	0.59
7:G:267:THR:HB	11:Q:115:ALA:HB2	1.84	0.59
8:H:318:MET:HG2	19:a:40:ARG:HH22	1.67	0.59
16:W:43:TYR:CE1	16:W:63:ARG:HD3	2.37	0.59
17:X:124:GLN:HA	17:X:127:LYS:HE3	1.83	0.59
6:F:235:VAL:HG22	6:F:236:PHE:CD2	2.37	0.59
7:G:312:GLY:C	7:G:313:LEU:HD12	2.28	0.59
7:G:651:PRO:HD3	13:S:56:ARG:HB3	1.82	0.59
8:H:142:TYR:CG	8:H:289:LEU:HD12	2.38	0.59
10:P:350:ILE:HB	10:P:366:ILE:CG2	2.32	0.59
1:A:68:GLU:CD	1:A:98:LEU:HG	2.28	0.59
3:C:65:ALA:HA	3:C:72:VAL:HG21	1.83	0.59
5:E:237:PRO:HG3	6:F:49:HIS:CD2	2.38	0.59
6:F:296:LEU:CD1	6:F:299:LEU:HD21	2.33	0.59
8:H:175:LEU:HD21	26:I:302:PC1:H2C1	1.84	0.59
8:H:246:LEU:HD12	8:H:246:LEU:C	2.28	0.59
9:I:114:ILE:HG22	9:I:141:ARG:HH12	1.66	0.59
18:Z:105:LYS:O	18:Z:106:VAL:C	2.46	0.59
1:A:6:VAL:HG11	8:H:87:VAL:HG22	1.85	0.59
4:D:388:GLY:HA3	4:D:417:SER:OG	2.03	0.59
7:G:259:SER:HA	7:G:281:ILE:CD1	2.32	0.59
10:P:96:LEU:HD12	10:P:96:LEU:C	2.28	0.59
4:D:233:HIS:CE1	4:D:234:GLN:HE21	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:192:TYR:CB	5:E:195:LEU:HD11	2.32	0.59
7:G:68:ARG:HD3	7:G:285:TRP:HZ3	1.66	0.59
13:S:25:GLN:HG3	13:S:26:ARG:N	2.17	0.59
17:X:120:PRO:HB2	17:X:125:LEU:HD11	1.85	0.59
21:q:51:ASP:O	21:q:59:HIS:HB2	2.03	0.59
3:C:160:ILE:HD12	4:D:286:TYR:CE1	2.37	0.58
4:D:404:LYS:NZ	4:D:455:ASP:HB3	2.18	0.58
7:G:253:VAL:CG1	7:G:345:LEU:HG	2.33	0.58
8:H:1:MET:CE	19:a:29:PHE:CE2	2.85	0.58
10:P:318:LYS:HG2	10:P:322:ILE:HD11	1.84	0.58
15:V:31:THR:HG22	15:V:88:LEU:HD13	1.85	0.58
1:A:108:GLN:HG2	1:A:109:LYS:N	2.16	0.58
4:D:191:ALA:HB1	4:D:196:ALA:HB3	1.85	0.58
4:D:249:LYS:HA	18:Z:19:ILE:HG23	1.86	0.58
4:D:266:ARG:NH2	9:I:63:TRP:HA	2.18	0.58
7:G:346:VAL:HG21	7:G:548:LEU:HD21	1.85	0.58
7:G:517:HIS:H	7:G:599:THR:HG21	1.68	0.58
8:H:30:TYR:OH	19:a:4:GLU:OE1	2.21	0.58
10:P:57:THR:HG23	10:P:123:SER:CB	2.33	0.58
16:W:67:ARG:HD3	16:W:71:MET:HG2	1.85	0.58
4:D:79:ASN:HD22	4:D:107:ARG:HD3	1.69	0.58
6:F:199:ARG:CD	23:s:80:PHE:CE2	2.80	0.58
6:F:227:PRO:HB2	6:F:228:PRO:HD3	1.84	0.58
6:F:326:LEU:C	6:F:326:LEU:HD12	2.28	0.58
6:F:387:GLU:HG3	7:G:123:ASN:OD1	2.03	0.58
9:I:93:LEU:HD13	9:I:97:PHE:CE2	2.38	0.58
18:Z:82:ARG:O	18:Z:86:ILE:HG13	2.03	0.58
6:F:382:CYS:SG	25:F:502:SF4:S1	3.02	0.58
8:H:11:VAL:HB	8:H:12:PRO:HD3	1.85	0.58
2:B:124:SER:HB3	2:B:125:PRO:HD2	1.84	0.58
3:C:130:ASN:HD21	3:C:141:ARG:HE	1.51	0.58
4:D:266:ARG:CB	9:I:65:GLU:OE2	2.52	0.58
5:E:150:THR:HG23	5:E:154:LYS:HE2	1.84	0.58
6:F:217:GLU:CD	11:Q:166:TRP:HE1	2.10	0.58
6:F:346:GLN:HE22	6:F:440:ARG:CD	2.17	0.58
17:X:124:GLN:O	20:b:70:PRO:HB2	2.04	0.58
2:B:68:ARG:HD2	2:B:73:TYR:HB2	1.86	0.58
2:B:115:ASP:O	2:B:116:ARG:C	2.44	0.58
7:G:387:LEU:HD23	7:G:391:ILE:HD13	1.84	0.58
7:G:592:LYS:CA	7:G:608:VAL:HG12	2.34	0.58
9:I:208:ASP:O	9:I:208:ASP:CG	2.44	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:57:THR:HG23	10:P:123:SER:HB2	1.86	0.58
20:b:27:GLY:O	20:b:30:ILE:HG22	2.02	0.58
4:D:185:MET:HE1	27:D:501:UQ1:HM23	1.85	0.58
5:E:233:LEU:HD11	6:F:289:GLU:OE2	2.02	0.58
7:G:548:LEU:HA	7:G:569:GLN:HB3	1.86	0.58
11:Q:77:VAL:HG12	11:Q:101:PHE:HA	1.86	0.58
16:W:104:THR:O	16:W:108:ARG:HG3	2.02	0.58
18:Z:135:ASN:O	18:Z:139:GLY:HA3	2.04	0.58
1:A:58:VAL:HG21	8:H:286:MET:HE1	1.85	0.58
1:A:112:GLU:O	1:A:113:TRP:C	2.47	0.58
2:B:154:GLU:O	10:P:89:TYR:OH	2.20	0.58
6:F:326:LEU:HD21	6:F:363:ILE:HD11	1.85	0.58
10:P:81:ILE:CD1	12:R:46:VAL:HG11	2.34	0.58
13:S:16:LEU:O	13:S:16:LEU:CD1	2.52	0.58
4:D:128:THR:H	4:D:131:GLN:NE2	2.01	0.58
5:E:163:THR:HG23	5:E:168:PHE:HB2	1.84	0.58
6:F:424:ILE:CG1	7:G:76:ARG:HH11	2.16	0.58
7:G:171:THR:HA	7:G:231:LEU:HA	1.86	0.58
7:G:445:LEU:CD2	7:G:460:HIS:CE1	2.83	0.58
8:H:85:LEU:CD2	8:H:108:THR:HB	2.34	0.58
10:P:275:HIS:HB3	10:P:372:ALA:HB1	1.86	0.58
12:R:48:PHE:CD2	21:q:125:VAL:HG21	2.39	0.58
20:b:69:HIS:CD2	20:b:70:PRO:HD2	2.36	0.58
1:A:2:ASN:HB2	18:Z:143:TYR:HE1	1.69	0.58
4:D:198:THR:N	4:D:199:PRO:HD2	2.19	0.58
6:F:391:TRP:CH2	7:G:118:GLU:OE2	2.57	0.58
7:G:171:THR:HG22	7:G:231:LEU:CB	2.34	0.58
10:P:220:TYR:HA	10:P:223:PHE:HD2	1.67	0.58
13:S:16:LEU:HD11	13:S:51:LEU:CD1	2.29	0.58
13:S:65:LEU:HB2	13:S:79:LEU:HD11	1.84	0.58
6:F:113:LEU:HD23	6:F:154:ALA:CB	2.33	0.57
7:G:275:PRO:HB3	7:G:286:ILE:HG23	1.85	0.57
7:G:528:LEU:HD22	7:G:649:VAL:HG21	1.86	0.57
7:G:572:HIS:HB2	7:G:699:SER:OG	2.03	0.57
8:H:102:ILE:HG13	8:H:162:LEU:HD12	1.85	0.57
8:H:197:PRO:HD3	8:H:273:ILE:HG22	1.85	0.57
14:T:90:TYR:CE2	14:T:92:LYS:CB	2.87	0.57
16:W:25:SER:CB	16:W:31:ALA:HB2	2.34	0.57
16:W:42:TRP:CZ2	33:W:201:EHZ:O1	2.56	0.57
1:A:78:ALA:HA	1:A:81:THR:HG23	1.86	0.57
7:G:466:LEU:HD13	7:G:500:ILE:HG12	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:567:VAL:HG12	7:G:582:VAL:HB	1.86	0.57
10:P:106:LEU:HD21	12:R:49:VAL:HG11	1.85	0.57
10:P:245:VAL:O	10:P:249:ILE:HG13	2.04	0.57
4:D:326:CYS:SG	4:D:453:THR:HG21	2.44	0.57
6:F:422:HIS:CD2	7:G:79:LEU:HD12	2.31	0.57
7:G:546:PHE:CD1	7:G:567:VAL:HG23	2.40	0.57
8:H:19:PHE:CE1	19:a:11:ILE:HD12	2.40	0.57
8:H:87:VAL:HG11	8:H:96:ILE:HD12	1.85	0.57
14:T:90:TYR:CE2	14:T:92:LYS:HB3	2.39	0.57
17:X:122:LEU:HD21	20:b:81:LEU:HD23	1.86	0.57
17:X:130:LYS:HE3	20:b:67:PRO:HB3	1.86	0.57
19:a:50:ARG:NH1	19:a:54:ILE:HD11	2.20	0.57
4:D:148:GLU:OE2	4:D:225:ALA:HA	2.04	0.57
6:F:346:GLN:NE2	6:F:440:ARG:CD	2.67	0.57
7:G:126:LEU:HD11	12:R:89:PRO:CB	2.29	0.57
8:H:42:PRO:HD2	8:H:45:ILE:HG12	1.86	0.57
8:H:152:SER:HB3	8:H:181:MET:HE1	1.87	0.57
8:H:227:GLU:O	8:H:231:ILE:HG13	2.04	0.57
2:B:99:CYS:C	2:B:101:ALA:N	2.59	0.57
6:F:74:ASP:OD1	6:F:75:TRP:N	2.37	0.57
10:P:55:VAL:HA	10:P:79:GLN:HB3	1.86	0.57
15:V:28:TYR:HE2	15:V:59:VAL:HG21	1.69	0.57
2:B:95:PHE:CZ	2:B:148:VAL:HB	2.27	0.57
2:B:194:CYS:HB2	9:I:153:ILE:O	2.05	0.57
26:B:302:PC1:H131	8:H:39:ILE:HD11	1.87	0.57
7:G:137:CYS:HB3	7:G:140:GLN:HG2	1.87	0.57
8:H:142:TYR:CE1	8:H:289:LEU:HD12	2.39	0.57
8:H:183:MET:HB3	9:I:63:TRP:CH2	2.38	0.57
10:P:214:LEU:HD23	10:P:352:VAL:CG1	2.34	0.57
19:a:36:LYS:HA	19:a:59:ARG:NH2	2.19	0.57
2:B:161:MET:SD	2:B:201:LEU:HD22	2.45	0.57
15:V:31:THR:O	15:V:35:LEU:HG	2.05	0.57
18:Z:122:GLY:O	18:Z:126:GLY:N	2.36	0.57
19:a:43:TYR:CZ	19:a:47:LEU:HD11	2.40	0.57
21:q:65:THR:HG22	21:q:66:THR:N	2.20	0.57
2:B:202:LEU:HD13	2:B:202:LEU:C	2.29	0.57
6:F:336:LEU:C	6:F:336:LEU:HD12	2.30	0.57
7:G:422:TRP:CZ2	7:G:441:ARG:HB3	2.40	0.57
7:G:571:HIS:CD2	7:G:572:HIS:CE1	2.82	0.57
21:q:14:VAL:HG13	21:q:23:LEU:CD2	2.35	0.57
4:D:259:GLU:O	4:D:263:THR:HG22	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:363:VAL:O	4:D:389:TYR:CE1	2.57	0.57
7:G:136:GLU:CD	11:Q:87:MET:HG3	2.30	0.57
11:Q:125:VAL:HG23	11:Q:125:VAL:O	2.05	0.57
18:Z:70:ALA:O	18:Z:73:PRO:HD2	2.04	0.57
1:A:52:SER:C	1:A:54:LYS:H	2.11	0.57
4:D:212:GLU:O	4:D:216:ARG:HG2	2.05	0.57
5:E:52:PHE:HE1	5:E:88:GLN:HG2	1.70	0.57
7:G:425:ASN:CG	7:G:426:ASP:H	2.11	0.57
8:H:142:TYR:CG	8:H:289:LEU:CD1	2.88	0.57
16:W:83:ASP:O	16:W:87:ILE:HG12	2.04	0.57
1:A:1:MET:O	1:A:4:TYR:N	2.38	0.56
2:B:110:PRO:HB3	8:H:33:LEU:O	2.04	0.56
2:B:153:PRO:HB2	2:B:155:PRO:HD2	1.85	0.56
5:E:56:PRO:O	5:E:60:LYS:HG3	2.04	0.56
7:G:399:VAL:HG22	7:G:462:PHE:HZ	1.68	0.56
7:G:569:GLN:HE22	7:G:622:ILE:CG2	2.10	0.56
8:H:66:THR:HB	8:H:122:ALA:O	2.05	0.56
9:I:168:VAL:HG21	9:I:201:ILE:HG21	1.87	0.56
17:X:5:VAL:HG13	17:X:7:LEU:HG	1.87	0.56
18:Z:131:GLU:O	18:Z:132:GLU:C	2.48	0.56
21:q:55:PHE:CG	22:r:26:LEU:HD22	2.40	0.56
2:B:79:ASP:OD2	2:B:216:GLN:HA	2.05	0.56
4:D:379:ILE:HG23	7:G:140:GLN:HB2	1.86	0.56
6:F:51:TRP:CE3	6:F:135:PRO:HG3	2.37	0.56
8:H:8:THR:O	8:H:9:LEU:HB3	2.06	0.56
10:P:156:SER:CB	10:P:161:VAL:HG21	2.30	0.56
10:P:315:THR:HG22	10:P:317:ASP:H	1.69	0.56
2:B:173:TYR:O	3:C:203:LEU:HD22	2.05	0.56
3:C:167:ARG:HB3	3:C:186:ILE:HG23	1.86	0.56
6:F:392:MET:HG2	6:F:412:LEU:HD11	1.87	0.56
7:G:161:GLU:OE1	12:R:97:LYS:HE2	2.06	0.56
7:G:372:PHE:H	7:G:532:PRO:HB2	1.70	0.56
12:R:62:ASP:O	12:R:66:GLN:HG3	2.06	0.56
13:S:23:LEU:HD12	13:S:23:LEU:C	2.29	0.56
14:T:134:ASP:OD1	14:T:134:ASP:O	2.23	0.56
16:W:101:LYS:HZ1	16:W:109:PHE:HE2	1.53	0.56
2:B:115:ASP:HA	2:B:119:VAL:O	2.05	0.56
7:G:253:VAL:HG13	7:G:520:ALA:CB	2.35	0.56
7:G:546:PHE:CZ	7:G:569:GLN:HB2	2.40	0.56
9:I:54:THR:HG21	18:Z:33:TYR:CZ	2.40	0.56
17:X:48:TRP:NE1	20:b:55:VAL:HG22	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:PHE:O	1:A:25:PRO:HD2	2.05	0.56
1:A:77:TRP:HZ2	8:H:100:LEU:HD21	1.71	0.56
2:B:81:LEU:HD22	26:B:302:PC1:H352	1.87	0.56
7:G:572:HIS:CE1	7:G:700:ILE:HG12	2.41	0.56
10:P:323:HIS:ND1	10:P:323:HIS:O	2.39	0.56
10:P:358:THR:HG22	10:P:359:TYR:CD1	2.41	0.56
14:T:130:ILE:HD11	14:T:148:ILE:HD11	1.86	0.56
17:X:48:TRP:CD1	20:b:55:VAL:HG13	2.39	0.56
8:H:134:ARG:HE	8:H:200:LEU:HD21	1.71	0.56
18:Z:7:LYS:HB2	18:Z:7:LYS:NZ	2.20	0.56
7:G:387:LEU:HD12	7:G:514:ASN:ND2	2.21	0.56
7:G:639:LEU:O	7:G:643:ARG:HG2	2.06	0.56
10:P:64:PHE:HE1	10:P:209:ARG:O	1.88	0.56
5:E:178:ALA:HA	6:F:125:CYS:SG	2.46	0.56
6:F:190:ASP:OD1	6:F:191:TYR:N	2.38	0.56
7:G:160:VAL:HG12	7:G:161:GLU:N	2.21	0.56
7:G:600:GLU:OE1	7:G:600:GLU:N	2.39	0.56
7:G:655:ARG:HH12	13:S:59:SER:N	2.03	0.56
8:H:190:LEU:HD21	8:H:270:PHE:CD1	2.41	0.56
11:Q:165:SER:HB3	11:Q:168:LYS:O	2.06	0.56
12:R:38:TYR:OH	21:q:127:TYR:HB2	2.06	0.56
14:T:90:TYR:HE2	14:T:92:LYS:CB	2.19	0.56
19:a:14:VAL:O	19:a:18:ILE:HG13	2.06	0.56
20:b:11:ASN:OD1	20:b:12:ALA:N	2.39	0.56
2:B:171:TYR:HE1	4:D:120:THR:HG22	1.70	0.56
4:D:375:MET:HG2	7:G:121:LEU:HD22	1.88	0.56
6:F:140:GLU:HG3	6:F:252:PRO:HG3	1.86	0.56
7:G:172:ILE:O	7:G:172:ILE:HG22	2.06	0.56
9:I:119:CYS:SG	9:I:130:ILE:HD11	2.46	0.56
7:G:215:MET:SD	7:G:714:VAL:HG22	2.46	0.55
7:G:346:VAL:HG21	7:G:548:LEU:CD2	2.35	0.55
7:G:483:ARG:HH21	7:G:489:ILE:HD11	1.70	0.55
12:R:77:ILE:HD11	12:R:111:PHE:CG	2.41	0.55
21:q:68:MET:SD	21:q:81:MET:CB	2.95	0.55
24:A:401:3PE:H322	24:A:401:3PE:H262	1.88	0.55
2:B:136:THR:HG21	4:D:118:ARG:HG2	1.87	0.55
3:C:160:ILE:HB	4:D:286:TYR:HD1	1.71	0.55
7:G:206:VAL:O	7:G:206:VAL:HG12	2.05	0.55
7:G:472:PRO:O	7:G:510:TRP:NE1	2.32	0.55
16:W:32:LYS:HZ3	33:W:201:EHZ:C19	2.19	0.55
17:X:124:GLN:C	17:X:125:LEU:HD12	2.31	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:85:GLU:HG2	21:q:98:PRO:CB	2.31	0.55
1:A:52:SER:C	1:A:54:LYS:N	2.62	0.55
1:A:106:TRP:HZ3	20:b:19:LEU:HD21	1.72	0.55
8:H:42:PRO:HD2	8:H:45:ILE:CG1	2.37	0.55
10:P:104:THR:HG22	10:P:106:LEU:CD1	2.36	0.55
16:W:24:PHE:HB2	16:W:83:ASP:CB	2.37	0.55
16:W:58:THR:HG22	16:W:60:LYS:N	2.21	0.55
3:C:124:ARG:HD2	11:Q:140:LYS:HZ2	1.72	0.55
5:E:139:CYS:CB	5:E:144:SER:HB3	2.35	0.55
5:E:182:ALA:HB3	5:E:183:PRO:HD3	1.88	0.55
7:G:707:MET:O	7:G:711:VAL:HG23	2.05	0.55
8:H:102:ILE:HG23	8:H:150:LEU:HD13	1.89	0.55
11:Q:167:ASN:O	11:Q:168:LYS:HG2	2.05	0.55
21:q:68:MET:HE1	21:q:81:MET:O	2.06	0.55
1:A:52:SER:HB3	1:A:54:LYS:HG2	1.88	0.55
9:I:106:TYR:O	9:I:107:PRO:C	2.49	0.55
10:P:61:ALA:HB3	10:P:82:ILE:HG23	1.88	0.55
18:Z:56:GLU:HA	18:Z:59:ARG:HH11	1.72	0.55
1:A:18:ILE:HG12	8:H:222:LEU:HD22	1.87	0.55
1:A:54:LYS:HG3	1:A:55:PHE:N	2.20	0.55
2:B:95:PHE:CE1	2:B:131:MET:HE2	2.40	0.55
4:D:355:GLU:HG2	4:D:357:LYS:H	1.71	0.55
6:F:67:GLU:O	6:F:71:LYS:HG2	2.06	0.55
7:G:218:LEU:HD21	7:G:413:LEU:CD2	2.37	0.55
10:P:98:GLY:HA3	10:P:103:LEU:HG	1.87	0.55
10:P:236:VAL:HG13	10:P:270:ARG:HH21	1.71	0.55
10:P:376:ASN:OD1	10:P:376:ASN:C	2.50	0.55
17:X:20:VAL:HG13	17:X:24:VAL:HB	1.87	0.55
18:Z:53:TRP:O	18:Z:57:ARG:HG3	2.06	0.55
18:Z:62:ILE:HD12	20:b:81:LEU:HD22	1.88	0.55
1:A:49:LEU:CD2	4:D:80:MET:HB2	2.35	0.55
2:B:107:MET:HE3	2:B:114:MET:HE2	1.88	0.55
4:D:329:ARG:CD	4:D:453:THR:HB	2.36	0.55
7:G:141:ASP:O	7:G:144:MET:N	2.39	0.55
7:G:525:ALA:O	7:G:530:TYR:HB2	2.07	0.55
7:G:634:LEU:HB3	7:G:636:TYR:CZ	2.42	0.55
8:H:4:ILE:H	8:H:4:ILE:HD12	1.72	0.55
8:H:133:LEU:HA	8:H:136:VAL:HG12	1.88	0.55
10:P:217:PHE:HA	10:P:220:TYR:HD2	1.71	0.55
10:P:357:ARG:HB2	10:P:362:LEU:HD23	1.89	0.55
11:Q:163:ASN:OD1	11:Q:163:ASN:C	2.49	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:q:64:TYR:CE2	21:q:82:VAL:HG13	2.42	0.55
3:C:120:THR:OG1	11:Q:128:PHE:HA	2.07	0.55
4:D:278:VAL:CG1	4:D:438:MET:HG2	2.37	0.55
6:F:382:CYS:SG	25:F:502:SF4:S4	3.05	0.55
17:X:22:SER:HB2	19:a:47:LEU:HD23	1.89	0.55
2:B:113:ASP:CG	8:H:34:ARG:HD2	2.31	0.55
3:C:64:VAL:HG11	3:C:85:ILE:HD13	1.88	0.55
4:D:322:SER:O	4:D:323:ARG:C	2.47	0.55
7:G:192:VAL:HG11	7:G:214:PHE:CE1	2.42	0.55
7:G:274:LEU:C	7:G:274:LEU:HD12	2.32	0.55
8:H:70:LEU:HG	8:H:118:TRP:HB3	1.88	0.55
14:T:128:PHE:CE2	14:T:130:ILE:HG13	2.42	0.55
3:C:124:ARG:NH1	3:C:125:PHE:HZ	1.99	0.55
5:E:78:VAL:HA	5:E:104:LEU:CD1	2.36	0.55
5:E:187:ILE:O	5:E:188:ASN:C	2.48	0.55
6:F:77:LEU:O	6:F:81:LYS:HG2	2.07	0.55
6:F:336:LEU:HD11	6:F:338:ASP:CG	2.32	0.55
6:F:386:ARG:HB3	6:F:387:GLU:OE1	2.07	0.55
7:G:399:VAL:CG2	7:G:462:PHE:CE1	2.87	0.55
10:P:71:ASN:HA	10:P:97:MET:SD	2.47	0.55
10:P:237:LYS:HE3	10:P:322:ILE:O	2.07	0.55
12:R:48:PHE:CD2	12:R:53:LYS:HB2	2.42	0.55
17:X:121:ASP:O	17:X:122:LEU:C	2.50	0.55
6:F:116:ASN:HB3	6:F:212:LEU:CD2	2.37	0.54
7:G:655:ARG:HH12	13:S:59:SER:H	1.56	0.54
8:H:90:PRO:O	8:H:91:MET:C	2.50	0.54
14:T:83:VAL:CG2	14:T:126:PHE:CZ	2.83	0.54
2:B:90:LEU:HD22	2:B:130:VAL:HG23	1.88	0.54
3:C:172:MET:HE3	3:C:187:LEU:CD1	2.37	0.54
6:F:424:ILE:HG12	7:G:76:ARG:HH11	1.72	0.54
10:P:273:LEU:O	10:P:277:VAL:HG23	2.06	0.54
20:b:38:TYR:HA	20:b:41:TYR:CD2	2.42	0.54
2:B:171:TYR:CE1	4:D:120:THR:HG22	2.41	0.54
3:C:186:ILE:O	4:D:113:ILE:HG13	2.07	0.54
4:D:253:LEU:HD11	22:r:18:GLN:HG3	1.90	0.54
7:G:68:ARG:HE	7:G:283:GLU:HG3	1.72	0.54
7:G:357:LEU:HD12	7:G:632:ILE:CD1	2.36	0.54
7:G:688:GLN:HA	7:G:693:ASP:HB3	1.89	0.54
8:H:11:VAL:O	8:H:12:PRO:C	2.49	0.54
9:I:98:ARG:O	9:I:169:GLU:HB3	2.07	0.54
12:R:41:LYS:H	12:R:41:LYS:HD2	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2:ASN:HB2	18:Z:143:TYR:CE1	2.41	0.54
2:B:113:ASP:OD1	8:H:34:ARG:HD2	2.08	0.54
6:F:339:PHE:O	6:F:343:VAL:HG23	2.08	0.54
6:F:382:CYS:C	6:F:384:PRO:HD2	2.32	0.54
7:G:467:LYS:HE3	7:G:503:THR:CG2	2.31	0.54
7:G:639:LEU:HD21	7:G:643:ARG:CZ	2.36	0.54
9:I:123:CYS:SG	25:I:303:SF4:S3	3.06	0.54
9:I:208:ASP:OD1	9:I:211:TYR:HB2	2.08	0.54
17:X:55:ARG:HB3	17:X:135:ARG:HH22	1.72	0.54
18:Z:24:ASN:OD1	18:Z:24:ASN:O	2.24	0.54
21:q:3:LEU:HD13	34:q:201:CDL:OB7	2.06	0.54
1:A:95:VAL:HG11	8:H:302:MET:CG	2.38	0.54
4:D:145:MET:O	4:D:148:GLU:N	2.40	0.54
7:G:336:ASN:H	7:G:363:SER:HB2	1.72	0.54
8:H:116:ILE:HG21	8:H:135:ALA:CB	2.38	0.54
13:S:41:TYR:HE1	13:S:53:ILE:HG23	1.73	0.54
16:W:23:ILE:HG22	16:W:24:PHE:CD1	2.42	0.54
16:W:58:THR:HG22	16:W:60:LYS:H	1.72	0.54
18:Z:62:ILE:HG23	20:b:50:PRO:HD3	1.89	0.54
1:A:54:LYS:CG	1:A:55:PHE:N	2.71	0.54
4:D:154:ALA:HB2	4:D:398:THR:CG2	2.37	0.54
7:G:547:LEU:HD11	7:G:566:ILE:HD12	1.90	0.54
7:G:566:ILE:HD11	7:G:579:MET:O	2.07	0.54
8:H:306:SER:O	8:H:310:PHE:CD2	2.59	0.54
11:Q:59:LEU:HD21	16:W:80:ARG:HH12	1.72	0.54
11:Q:160:TYR:CZ	11:Q:164:PHE:HZ	2.26	0.54
13:S:79:LEU:HA	13:S:82:LEU:CD1	2.24	0.54
2:B:93:MET:HE2	2:B:95:PHE:CE1	2.42	0.54
2:B:166:ASN:HB3	9:I:150:THR:HG22	1.90	0.54
3:C:116:VAL:HG21	4:D:412:VAL:HG21	1.89	0.54
7:G:395:GLU:OE2	7:G:417:ARG:NH1	2.41	0.54
7:G:684:LEU:HD12	7:G:684:LEU:O	2.08	0.54
8:H:5:ASN:HD21	19:a:23:THR:HG23	1.73	0.54
8:H:9:LEU:HD23	8:H:91:MET:HE1	1.88	0.54
9:I:130:ILE:HG12	9:I:145:TYR:CD1	2.42	0.54
9:I:132:ALA:O	9:I:133:GLU:HG3	2.07	0.54
10:P:239:PRO:HG2	10:P:345:LEU:HD12	1.90	0.54
14:T:87:LEU:HD22	14:T:104:PHE:CZ	2.41	0.54
17:X:130:LYS:CE	20:b:67:PRO:HB3	2.38	0.54
4:D:166:ARG:O	4:D:170:ILE:HG12	2.07	0.54
6:F:269:ARG:HD2	6:F:340:ASP:HB2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:68:ARG:NE	7:G:283:GLU:HG3	2.23	0.54
7:G:278:HIS:HB3	7:G:281:ILE:HG13	1.89	0.54
7:G:307:VAL:HG21	7:G:325:ARG:HG3	1.89	0.54
7:G:346:VAL:O	7:G:521:SER:HB3	2.08	0.54
7:G:608:VAL:HG23	11:Q:103:THR:HG1	1.73	0.54
8:H:102:ILE:HD12	8:H:154:LEU:CD2	2.37	0.54
8:H:116:ILE:HD13	8:H:135:ALA:HB1	1.88	0.54
8:H:172:MET:HE2	8:H:177:PRO:CD	2.22	0.54
10:P:207:PHE:CE1	10:P:214:LEU:HD22	2.43	0.54
10:P:300:TRP:O	10:P:304:LEU:HG	2.08	0.54
1:A:72:LEU:HB3	8:H:151:LEU:HD21	1.90	0.54
1:A:75:LEU:HB3	8:H:155:LEU:HD21	1.90	0.54
3:C:197:PHE:HE2	4:D:121:GLU:OE1	1.90	0.54
5:E:179:CYS:O	5:E:180:VAL:C	2.51	0.54
5:E:180:VAL:CG1	5:E:224:CYS:SG	2.96	0.54
6:F:278:ILE:CD1	6:F:282:VAL:CG2	2.80	0.54
7:G:189:ILE:HG13	7:G:285:TRP:CZ2	2.43	0.54
7:G:357:LEU:CD1	7:G:632:ILE:HD11	2.36	0.54
7:G:534:VAL:HG21	7:G:554:CYS:HB3	1.90	0.54
9:I:80:GLU:CB	22:r:26:LEU:HD11	2.38	0.54
13:S:44:LEU:HD13	13:S:91:MET:HG2	1.88	0.54
14:T:97:LYS:HG3	14:T:97:LYS:O	2.08	0.54
2:B:99:CYS:HB3	4:D:141:TYR:CG	2.43	0.54
5:E:226:PRO:HG3	6:F:286:CYS:SG	2.48	0.54
6:F:159:ARG:HB3	6:F:162:PHE:CD2	2.43	0.54
6:F:284:HIS:H	6:F:305:GLY:HA3	1.72	0.54
7:G:163:LYS:HB3	7:G:211:GLU:OE1	2.08	0.54
7:G:482:GLN:HG3	7:G:518:ARG:HH21	1.73	0.54
8:H:40:VAL:CG1	8:H:47:GLN:NE2	2.71	0.54
8:H:71:PHE:CE2	8:H:219:PRO:HG3	2.43	0.54
9:I:109:GLY:O	12:R:63:LEU:HD12	2.08	0.54
11:Q:117:THR:HG22	11:Q:119:ASP:H	1.73	0.54
12:R:32:THR:OG1	12:R:33:HIS:N	2.39	0.54
14:T:140:CYS:HB2	14:T:143:GLU:HG2	1.90	0.54
18:Z:53:TRP:NE1	18:Z:57:ARG:HD2	2.23	0.54
21:q:88:ARG:HD2	21:q:94:THR:OG1	2.08	0.54
6:F:42:PHE:CD1	6:F:130:ILE:HD12	2.44	0.53
6:F:300:ILE:CG2	6:F:305:GLY:O	2.45	0.53
7:G:170:LYS:O	7:G:231:LEU:HA	2.08	0.53
7:G:341:ILE:CD1	7:G:555:ILE:HG12	2.38	0.53
7:G:466:LEU:HD13	7:G:500:ILE:CD1	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:40:VAL:HG11	8:H:47:GLN:NE2	2.24	0.53
26:H:402:PC1:H281	26:H:402:PC1:H3B1	1.90	0.53
13:S:16:LEU:HD13	13:S:19:ILE:CD1	2.38	0.53
2:B:137:LEU:HD22	2:B:145:LEU:HD22	1.90	0.53
5:E:139:CYS:C	5:E:144:SER:HB3	2.33	0.53
6:F:325:PRO:HG3	6:F:433:TRP:HB3	1.88	0.53
7:G:35:PHE:HB2	7:G:101:ASN:HA	1.90	0.53
7:G:68:ARG:NH2	7:G:283:GLU:HB2	2.23	0.53
8:H:51:ASP:OD1	8:H:51:ASP:C	2.52	0.53
10:P:58:VAL:O	10:P:83:PRO:HD2	2.09	0.53
12:R:94:ASN:OD1	12:R:96:ASP:HB2	2.08	0.53
1:A:1:MET:O	1:A:2:ASN:C	2.48	0.53
4:D:319:PRO:HG3	4:D:336:GLU:HG3	1.89	0.53
7:G:557:ARG:CD	7:G:579:MET:HB2	2.38	0.53
8:H:1:MET:HA	8:H:4:ILE:HD13	1.89	0.53
11:Q:82:PRO:O	11:Q:94:THR:HG23	2.08	0.53
14:T:87:LEU:HD23	14:T:122:MET:HE1	1.91	0.53
20:b:28:LEU:HA	20:b:31:ILE:HG22	1.90	0.53
4:D:368:ARG:HA	4:D:371:MET:HG2	1.89	0.53
5:E:131:ILE:HG13	5:E:187:ILE:HG12	1.89	0.53
6:F:68:ILE:HG23	6:F:75:TRP:CZ3	2.42	0.53
6:F:262:PHE:CZ	6:F:272:GLY:HA3	2.43	0.53
7:G:36:VAL:O	7:G:39:GLN:HG2	2.07	0.53
7:G:370:GLU:OE2	7:G:478:SER:CB	2.56	0.53
21:q:95:ASP:OD1	21:q:96:ASP:N	2.41	0.53
3:C:100:ARG:HH12	15:V:86:LYS:HZ1	1.56	0.53
6:F:80:MET:HE2	6:F:95:THR:HG21	1.90	0.53
6:F:147:ARG:HH11	6:F:191:TYR:HB2	1.72	0.53
6:F:422:HIS:NE2	7:G:112:ALA:CA	2.68	0.53
8:H:23:VAL:O	8:H:23:VAL:HG12	2.07	0.53
8:H:251:LEU:HD21	8:H:254:LEU:CD1	2.38	0.53
9:I:54:THR:HA	20:b:13:TRP:HE1	1.73	0.53
10:P:206:ILE:HG13	31:P:401:NDP:H42N	1.89	0.53
10:P:262:THR:N	10:P:332:LEU:HD12	2.24	0.53
11:Q:58:LYS:O	11:Q:59:LEU:C	2.49	0.53
12:R:98:GLU:HA	12:R:113:GLN:CD	2.33	0.53
15:V:114:TRP:O	15:V:115:PRO:C	2.52	0.53
18:Z:12:PRO:HD3	18:Z:16:TYR:CE1	2.43	0.53
20:b:59:ASP:HA	20:b:63:MET:HE2	1.89	0.53
3:C:123:ASN:ND2	15:V:108:PRO:HG2	2.24	0.53
3:C:234:LEU:O	4:D:387:GLU:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:101:LEU:HD12	4:D:106:VAL:HA	1.91	0.53
4:D:210:MET:O	4:D:211:PHE:C	2.50	0.53
4:D:217:VAL:CG1	4:D:240:LEU:HD22	2.38	0.53
5:E:203:ILE:HA	5:E:206:GLU:OE1	2.09	0.53
5:E:206:GLU:CB	5:E:213:PRO:HB3	2.39	0.53
6:F:85:LEU:HD13	6:F:262:PHE:CE2	2.44	0.53
7:G:600:GLU:OE2	7:G:602:ARG:NH1	2.42	0.53
8:H:87:VAL:CG1	8:H:96:ILE:HD12	2.38	0.53
10:P:370:LYS:HG3	10:P:370:LYS:O	2.08	0.53
14:T:118:ILE:HG23	14:T:122:MET:CE	2.37	0.53
4:D:141:TYR:CB	4:D:223:HIS:HE1	2.21	0.53
4:D:170:ILE:HG21	4:D:232:VAL:HG21	1.90	0.53
5:E:81:VAL:CB	5:E:104:LEU:HD11	2.38	0.53
9:I:80:GLU:OE2	22:r:26:LEU:HD13	2.08	0.53
9:I:80:GLU:HB3	22:r:26:LEU:HD11	1.90	0.53
10:P:122:HIS:CB	12:R:46:VAL:HG22	2.39	0.53
10:P:275:HIS:HA	10:P:278:LYS:HG2	1.91	0.53
2:B:199:GLU:HB3	9:I:86:TYR:HE1	1.74	0.53
5:E:226:PRO:HD3	6:F:46:TYR:CZ	2.44	0.53
7:G:462:PHE:CZ	7:G:466:LEU:CD2	2.92	0.53
7:G:546:PHE:HD1	7:G:567:VAL:CG2	2.22	0.53
7:G:640:ASP:OD1	7:G:641:GLN:N	2.42	0.53
8:H:146:MET:HE1	8:H:192:GLU:HB2	1.90	0.53
10:P:164:PHE:CE2	10:P:166:HIS:HB2	2.44	0.53
2:B:116:ARG:O	8:H:39:ILE:HG22	2.08	0.53
4:D:129:TYR:OH	4:D:391:VAL:HG21	2.08	0.53
7:G:364:ASP:C	7:G:364:ASP:OD1	2.51	0.53
7:G:435:PRO:O	7:G:435:PRO:HG2	2.08	0.53
8:H:179:TRP:CG	8:H:180:PRO:HD3	2.43	0.53
1:A:54:LYS:HD2	1:A:113:TRP:CB	2.38	0.53
2:B:122:ARG:NH1	27:D:501:UQ1:CM5	2.68	0.53
4:D:141:TYR:HB3	4:D:223:HIS:CE1	2.44	0.53
4:D:166:ARG:HH22	18:Z:10:MET:HG2	1.74	0.53
7:G:563:ASP:O	7:G:564:CYS:C	2.51	0.53
8:H:42:PRO:HB3	21:q:27:PHE:CE2	2.43	0.53
8:H:296:LEU:HD11	8:H:300:LEU:HD11	1.91	0.53
9:I:209:TYR:HA	9:I:212:ARG:CG	2.38	0.53
10:P:336:GLU:CG	10:P:342:PRO:HD3	2.38	0.53
12:R:45:ARG:HD2	12:R:48:PHE:CD1	2.44	0.53
12:R:69:VAL:HG12	12:R:112:LYS:N	2.25	0.53
12:R:95:LEU:HD21	12:R:111:PHE:CB	2.37	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:S:82:LEU:HD13	13:S:86:GLU:OE1	2.08	0.53
19:a:6:LEU:O	19:a:7:PRO:C	2.52	0.53
19:a:51:ASP:HA	19:a:54:ILE:HD12	1.91	0.53
9:I:100:GLU:HB2	9:I:175:PHE:CE2	2.43	0.52
10:P:153:ALA:CB	10:P:191:VAL:HG23	2.39	0.52
10:P:265:PHE:HD1	10:P:334:GLY:HA3	1.74	0.52
11:Q:72:ILE:HD13	11:Q:143:TRP:NE1	2.24	0.52
21:q:29:ARG:HD3	21:q:74:PHE:CE1	2.44	0.52
3:C:96:LEU:HD12	3:C:155:ILE:HG21	1.91	0.52
4:D:383:LYS:HD3	7:G:140:GLN:CD	2.34	0.52
6:F:54:LYS:HG3	6:F:58:ARG:NH2	2.23	0.52
6:F:238:CYS:O	6:F:239:PRO:C	2.51	0.52
7:G:260:ASN:H	7:G:281:ILE:CD1	2.21	0.52
7:G:679:VAL:HG23	7:G:679:VAL:O	2.09	0.52
9:I:62:MET:SD	18:Z:35:MET:HG2	2.49	0.52
10:P:305:PHE:CG	10:P:314:THR:HG22	2.45	0.52
18:Z:65:LEU:O	18:Z:69:ILE:HG12	2.09	0.52
4:D:99:LEU:HD13	4:D:101:LEU:HD13	1.91	0.52
4:D:128:THR:N	4:D:131:GLN:HE21	2.04	0.52
6:F:199:ARG:HD3	23:s:80:PHE:CD2	2.41	0.52
6:F:383:THR:HG21	7:G:120:LEU:HD21	1.91	0.52
7:G:203:ASP:C	7:G:203:ASP:OD1	2.52	0.52
7:G:261:ILE:HD13	7:G:273:ILE:HG23	1.92	0.52
9:I:118:LEU:CD1	9:I:161:ALA:HB1	2.39	0.52
9:I:153:ILE:O	9:I:153:ILE:HD12	2.09	0.52
18:Z:94:GLU:HA	18:Z:97:ILE:CG1	2.39	0.52
1:A:8:PHE:O	1:A:12:LEU:HG	2.09	0.52
1:A:19:LEU:O	1:A:20:VAL:C	2.51	0.52
5:E:63:GLU:O	5:E:67:LYS:HD3	2.09	0.52
6:F:270:ASN:HD21	6:F:340:ASP:HB3	1.75	0.52
6:F:346:GLN:NE2	6:F:440:ARG:HD2	2.24	0.52
6:F:422:HIS:NE2	7:G:112:ALA:CB	2.72	0.52
7:G:438:LEU:HD12	7:G:442:TYR:CD1	2.44	0.52
8:H:135:ALA:HB2	8:H:201:THR:HG21	1.90	0.52
10:P:179:LYS:O	10:P:182:ARG:HG2	2.10	0.52
12:R:113:GLN:CD	12:R:113:GLN:N	2.66	0.52
14:T:103:HIS:HD1	14:T:140:CYS:HG	1.51	0.52
15:V:48:THR:HA	15:V:51:ILE:HD12	1.90	0.52
21:q:125:VAL:HG23	21:q:125:VAL:O	2.08	0.52
1:A:105:GLU:HG2	1:A:111:LEU:HG	1.90	0.52
2:B:138:THR:HG21	4:D:116:LEU:HA	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:363:VAL:O	4:D:389:TYR:HE1	1.92	0.52
5:E:87:ARG:HD2	23:s:77:THR:CG2	2.40	0.52
6:F:66:LYS:C	6:F:66:LYS:HD3	2.35	0.52
8:H:307:LEU:HD11	18:Z:47:TYR:CG	2.45	0.52
14:T:130:ILE:CG2	14:T:131:PRO:HD2	2.40	0.52
17:X:35:GLN:HB2	17:X:70:PHE:CE1	2.44	0.52
18:Z:68:ARG:O	18:Z:69:ILE:C	2.49	0.52
19:a:1:MET:HB2	19:a:3:PHE:CE2	2.43	0.52
19:a:64:LYS:HG3	19:a:66:LEU:H	1.75	0.52
20:b:66:VAL:HG11	20:b:70:PRO:HA	1.92	0.52
2:B:69:SER:O	2:B:70:ARG:C	2.50	0.52
2:B:197:THR:HG23	4:D:221:ARG:HD2	1.91	0.52
4:D:198:THR:OG1	4:D:261:MET:HE1	2.10	0.52
6:F:159:ARG:HG2	6:F:161:GLU:HB2	1.91	0.52
7:G:34:VAL:HG11	7:G:96:VAL:HG22	1.92	0.52
8:H:174:LEU:C	8:H:177:PRO:HD2	2.34	0.52
10:P:283:MET:HE2	10:P:366:ILE:HG22	1.92	0.52
2:B:194:CYS:O	25:B:301:SF4:S2	2.67	0.52
6:F:326:LEU:CD2	6:F:363:ILE:HD11	2.40	0.52
7:G:35:PHE:CE1	7:G:40:SER:HB2	2.45	0.52
7:G:388:ASN:HD21	7:G:511:LYS:HB3	1.75	0.52
8:H:250:ASN:OD1	8:H:251:LEU:N	2.42	0.52
9:I:155:CYS:SG	25:I:303:SF4:S2	3.08	0.52
10:P:85:ARG:HE	31:P:401:NDP:C2A	2.22	0.52
16:W:94:GLN:HA	16:W:97:ILE:HG22	1.92	0.52
19:a:7:PRO:HD3	34:q:201:CDL:H181	1.91	0.52
21:q:56:PHE:HD1	21:q:59:HIS:NE2	2.06	0.52
6:F:299:LEU:HD12	6:F:300:ILE:HG13	1.91	0.52
7:G:177:ILE:HG12	7:G:228:VAL:HG21	1.92	0.52
7:G:371:ILE:HG12	7:G:533:GLY:CA	2.38	0.52
7:G:388:ASN:ND2	7:G:511:LYS:HB3	2.24	0.52
10:P:203:PRO:HG2	31:P:401:NDP:C6N	2.37	0.52
1:A:54:LYS:CD	1:A:113:TRP:HB2	2.40	0.52
7:G:164:ASN:ND2	7:G:166:GLY:H	2.08	0.52
7:G:231:LEU:HD12	7:G:231:LEU:O	2.09	0.52
8:H:230:ASN:O	8:H:231:ILE:C	2.53	0.52
10:P:236:VAL:HG11	10:P:270:ARG:HH21	1.75	0.52
14:T:79:ILE:CG2	14:T:145:VAL:HG13	2.40	0.52
14:T:100:VAL:O	14:T:141:PRO:HD2	2.10	0.52
20:b:82:LYS:O	20:b:83:ASN:C	2.52	0.52
3:C:104:ASN:O	22:r:97:PRO:HD3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:339:GLN:NE2	9:I:37:LYS:HZ1	2.07	0.52
5:E:196:THR:O	5:E:200:ILE:HD12	2.10	0.52
6:F:396:MET:HE2	6:F:438:LEU:HD13	1.91	0.52
8:H:33:LEU:HD11	9:I:76:TYR:HD1	1.74	0.52
9:I:94:SER:CB	9:I:95:PRO:HD2	2.29	0.52
16:W:71:MET:O	16:W:72:LYS:C	2.51	0.52
21:q:65:THR:CG2	21:q:66:THR:N	2.72	0.52
21:q:137:TRP:CH2	21:q:140:PRO:HD3	2.44	0.52
3:C:203:LEU:HD11	4:D:123:LEU:CD1	2.28	0.51
6:F:177:TYR:CZ	6:F:182:ILE:HD12	2.45	0.51
6:F:227:PRO:HG3	7:G:94:MET:SD	2.50	0.51
7:G:31:LEU:HB3	7:G:42:MET:HE2	1.93	0.51
7:G:136:GLU:HB3	11:Q:87:MET:HB3	1.92	0.51
7:G:528:LEU:HD21	7:G:653:LEU:CD1	2.39	0.51
8:H:23:VAL:HG11	19:a:9:LEU:HD21	1.91	0.51
8:H:186:PHE:CZ	8:H:270:PHE:CD1	2.99	0.51
8:H:280:PHE:HD2	8:H:284:GLN:CG	2.23	0.51
21:q:29:ARG:HD3	21:q:74:PHE:CD1	2.45	0.51
1:A:106:TRP:CZ3	20:b:19:LEU:HD21	2.45	0.51
4:D:218:SER:CB	4:D:224:ALA:HB1	2.40	0.51
4:D:382:PHE:O	4:D:386:THR:HG23	2.10	0.51
5:E:147:ILE:HG12	5:E:200:ILE:HD11	1.91	0.51
7:G:128:CYS:N	7:G:129:PRO:HD2	2.25	0.51
8:H:223:PHE:O	8:H:224:PHE:C	2.53	0.51
8:H:309:ILE:HD13	8:H:314:VAL:HG12	1.92	0.51
14:T:140:CYS:HB2	14:T:143:GLU:CG	2.40	0.51
18:Z:99:LYS:HG3	18:Z:100:ASP:N	2.25	0.51
3:C:227:GLN:NE2	9:I:129:THR:OG1	2.43	0.51
8:H:2:PHE:CE2	8:H:6:ILE:HD11	2.46	0.51
8:H:142:TYR:CA	8:H:289:LEU:CD1	2.75	0.51
9:I:89:GLU:HG3	21:q:61:TRP:HB3	1.92	0.51
21:q:88:ARG:HB2	21:q:93:MET:HB2	1.91	0.51
2:B:122:ARG:NH2	27:D:501:UQ1:H102	2.25	0.51
6:F:259:GLY:O	6:F:263:ALA:N	2.40	0.51
6:F:296:LEU:HD22	6:F:337:MET:CE	2.39	0.51
7:G:457:SER:HB2	7:G:459:ARG:HG3	1.92	0.51
8:H:212:ASN:HA	8:H:215:TYR:HB2	1.93	0.51
8:H:273:ILE:HG23	8:H:277:TYR:CD2	2.45	0.51
15:V:62:GLU:HB3	15:V:68:LEU:HD13	1.93	0.51
15:V:95:LEU:HA	15:V:100:TRP:CH2	2.35	0.51
17:X:25:LEU:O	17:X:29:ALA:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:87:ARG:HH11	26:B:302:PC1:P	2.34	0.51
4:D:462:ASP:O	4:D:463:ARG:C	2.53	0.51
6:F:177:TYR:O	6:F:180:GLY:N	2.43	0.51
7:G:127:ASP:HA	12:R:106:TYR:HH	1.75	0.51
7:G:621:LYS:O	7:G:622:ILE:C	2.54	0.51
7:G:704:SER:HB2	7:G:707:MET:HB2	1.92	0.51
9:I:149:MET:CE	9:I:185:TYR:CD2	2.94	0.51
15:V:44:TYR:CD1	15:V:48:THR:HG23	2.46	0.51
18:Z:62:ILE:HG23	20:b:50:PRO:CD	2.41	0.51
20:b:7:ALA:C	20:b:9:LEU:N	2.68	0.51
21:q:88:ARG:HG3	21:q:89:TRP:N	2.26	0.51
4:D:156:GLU:OE1	4:D:163:PRO:HD3	2.10	0.51
6:F:42:PHE:CD1	6:F:137:LYS:HD2	2.46	0.51
7:G:379:THR:HG23	7:G:526:LEU:O	2.11	0.51
7:G:389:THR:CG2	7:G:514:ASN:ND2	2.62	0.51
7:G:421:SER:HB3	7:G:427:LEU:CD1	2.41	0.51
7:G:546:PHE:HD1	7:G:567:VAL:HG23	1.73	0.51
8:H:63:PRO:HB2	8:H:65:THR:CA	2.41	0.51
8:H:186:PHE:CZ	8:H:270:PHE:HE1	2.19	0.51
8:H:222:LEU:O	8:H:223:PHE:C	2.50	0.51
20:b:23:PHE:CB	24:b:201:3PE:H2D2	2.37	0.51
3:C:232:PHE:CD1	7:G:243:TRP:HD1	2.29	0.51
6:F:117:ALA:CB	6:F:158:ILE:HG22	2.40	0.51
7:G:253:VAL:HG12	7:G:253:VAL:O	2.11	0.51
7:G:355:LYS:CB	7:G:366:LEU:CD2	2.89	0.51
7:G:445:LEU:HD22	7:G:460:HIS:HE1	1.68	0.51
7:G:448:SER:O	7:G:451:ILE:HG12	2.09	0.51
8:H:176:LEU:HB2	8:H:177:PRO:HD3	1.93	0.51
11:Q:91:VAL:HG13	11:Q:95:LYS:NZ	2.26	0.51
14:T:87:LEU:HD23	14:T:122:MET:CE	2.40	0.51
1:A:6:VAL:HG11	8:H:87:VAL:HG21	1.92	0.51
1:A:24:LEU:N	1:A:25:PRO:CD	2.73	0.51
1:A:57:LEU:O	1:A:58:VAL:C	2.54	0.51
3:C:115:ALA:HB2	3:C:127:ILE:HD13	1.91	0.51
5:E:39:VAL:HG11	7:G:163:LYS:HZ2	1.76	0.51
7:G:403:VAL:CG1	7:G:476:LEU:HA	2.41	0.51
10:P:234:LYS:HG2	10:P:234:LYS:O	2.10	0.51
10:P:305:PHE:HB2	10:P:314:THR:HG22	1.92	0.51
13:S:54:LEU:HD22	13:S:56:ARG:NH1	2.25	0.51
15:V:12:VAL:CG1	15:V:13:GLY:N	2.72	0.51
17:X:78:CYS:C	17:X:81:PRO:HD2	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:80:ASP:O	18:Z:84:LEU:HG	2.11	0.51
2:B:169:GLY:O	2:B:170:TYR:C	2.53	0.51
5:E:75:ALA:O	5:E:78:VAL:HG22	2.11	0.51
5:E:135:THR:CG2	5:E:172:GLU:HG3	2.41	0.51
6:F:278:ILE:HD12	6:F:282:VAL:CG2	2.36	0.51
9:I:48:VAL:O	20:b:10:LYS:NZ	2.42	0.51
9:I:130:ILE:HD11	9:I:145:TYR:CE1	2.46	0.51
10:P:315:THR:HB	10:P:318:LYS:HB2	1.92	0.51
10:P:374:THR:HG23	10:P:374:THR:O	2.11	0.51
4:D:279:THR:HA	15:V:12:VAL:HG13	1.93	0.51
6:F:132:ARG:NH1	6:F:133:HIS:HE2	2.09	0.51
7:G:183:ILE:CD1	7:G:206:VAL:HG13	2.40	0.51
7:G:421:SER:HB3	7:G:427:LEU:HD11	1.91	0.51
7:G:488:ALA:HB2	7:G:677:GLN:CB	2.41	0.51
7:G:639:LEU:HD23	7:G:639:LEU:C	2.35	0.51
9:I:149:MET:HE3	9:I:185:TYR:CD2	2.46	0.51
10:P:69:VAL:HG21	10:P:129:LEU:HD11	1.91	0.51
10:P:172:ALA:H	10:P:202:ARG:NH2	2.08	0.51
13:S:16:LEU:HD21	13:S:95:LEU:CD1	2.41	0.51
1:A:108:GLN:CG	1:A:109:LYS:H	2.19	0.50
3:C:84:GLU:CG	3:C:141:ARG:HH11	2.23	0.50
7:G:82:ILE:CD1	7:G:102:ILE:HG13	2.41	0.50
8:H:152:SER:CB	8:H:181:MET:HE1	2.41	0.50
8:H:228:TYR:HA	8:H:231:ILE:CD1	2.40	0.50
9:I:149:MET:HE3	9:I:185:TYR:CE2	2.46	0.50
10:P:348:LYS:HB3	10:P:351:GLU:OE2	2.12	0.50
11:Q:77:VAL:HG12	11:Q:101:PHE:CG	2.46	0.50
14:T:130:ILE:HG23	14:T:131:PRO:CD	2.40	0.50
16:W:28:LEU:HG	16:W:32:LYS:HE2	1.93	0.50
1:A:21:ALA:HB2	8:H:218:GLY:HA3	1.91	0.50
6:F:345:ALA:C	6:F:346:GLN:HG2	2.34	0.50
7:G:463:CYS:O	7:G:467:LYS:HG2	2.11	0.50
7:G:517:HIS:H	7:G:599:THR:CG2	2.23	0.50
11:Q:167:ASN:C	11:Q:168:LYS:HG2	2.36	0.50
17:X:44:MET:SD	18:Z:73:PRO:HA	2.51	0.50
17:X:48:TRP:CD1	20:b:55:VAL:HG22	2.46	0.50
18:Z:121:ILE:HG23	18:Z:122:GLY:N	2.25	0.50
19:a:31:ASN:ND2	19:a:36:LYS:HB2	2.27	0.50
1:A:22:PHE:HA	8:H:60:PRO:HG2	1.92	0.50
4:D:189:THR:OG1	27:D:501:UQ1:CM3	2.59	0.50
6:F:296:LEU:CD1	6:F:337:MET:HE3	2.34	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:60:ILE:HG21	7:G:78:CYS:HB2	1.94	0.50
7:G:541:PRO:HB2	7:G:561:PRO:HD3	1.93	0.50
26:H:402:PC1:H151	10:P:359:TYR:CD1	2.46	0.50
10:P:65:LEU:HD23	10:P:129:LEU:HD22	1.93	0.50
10:P:209:ARG:N	10:P:352:VAL:HG22	2.26	0.50
11:Q:75:ARG:HH12	11:Q:104:ARG:HG2	1.76	0.50
12:R:72:VAL:HG12	12:R:73:GLU:N	2.26	0.50
14:T:90:TYR:CE2	14:T:92:LYS:HB2	2.46	0.50
15:V:90:LEU:HD21	15:V:94:MET:HE3	1.94	0.50
17:X:9:THR:HG23	17:X:12:GLU:H	1.77	0.50
18:Z:81:ARG:HG3	18:Z:82:ARG:N	2.25	0.50
18:Z:102:PRO:O	18:Z:103:ASN:C	2.53	0.50
1:A:109:LYS:O	1:A:109:LYS:HG2	2.12	0.50
2:B:99:CYS:C	2:B:101:ALA:H	2.19	0.50
2:B:224:ARG:HG3	10:P:85:ARG:HH22	1.76	0.50
5:E:199:ASP:O	5:E:202:GLU:HB3	2.11	0.50
6:F:392:MET:HE2	6:F:416:SER:HA	1.94	0.50
7:G:254:MET:HE2	7:G:345:LEU:HD21	1.93	0.50
7:G:306:MET:HG2	7:G:316:TYR:CA	2.40	0.50
7:G:429:VAL:HG11	7:G:440:TYR:CE1	2.46	0.50
13:S:21:VAL:CG2	13:S:91:MET:HE1	2.41	0.50
14:T:105:MET:HB2	14:T:139:MET:SD	2.51	0.50
18:Z:93:GLU:O	18:Z:97:ILE:HG12	2.11	0.50
3:C:149:LEU:CD1	16:W:80:ARG:HH21	2.19	0.50
3:C:186:ILE:HG13	3:C:187:LEU:N	2.27	0.50
6:F:126:LYS:CD	6:F:275:LEU:HB2	2.42	0.50
9:I:118:LEU:C	9:I:118:LEU:HD12	2.37	0.50
12:R:55:VAL:HG22	12:R:56:ASN:H	1.77	0.50
15:V:31:THR:HA	15:V:88:LEU:HD13	1.92	0.50
19:a:37:ARG:CB	19:a:48:MET:CE	2.90	0.50
4:D:176:GLU:O	4:D:177:ILE:C	2.53	0.50
5:E:82:LEU:HD21	5:E:115:ALA:HB2	1.93	0.50
5:E:214:LYS:HG3	5:E:214:LYS:O	2.12	0.50
7:G:68:ARG:CD	7:G:285:TRP:HZ3	2.24	0.50
7:G:339:ALA:HB1	7:G:537:ILE:HD11	1.93	0.50
7:G:382:ARG:NH1	7:G:652:ASN:HD22	2.09	0.50
8:H:113:VAL:CG2	8:H:136:VAL:HG23	2.39	0.50
14:T:140:CYS:O	14:T:144:ILE:HG13	2.12	0.50
15:V:7:LYS:O	15:V:8:THR:OG1	2.29	0.50
15:V:12:VAL:CG1	15:V:13:GLY:H	2.22	0.50
17:X:141:PRO:HG2	17:X:142:TYR:HD1	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:20:VAL:HG22	24:b:201:3PE:H282	1.92	0.50
6:F:225:LEU:HB2	11:Q:160:TYR:CE2	2.47	0.50
7:G:68:ARG:HD2	7:G:285:TRP:CZ3	2.47	0.50
7:G:283:GLU:O	7:G:285:TRP:CZ3	2.65	0.50
8:H:273:ILE:HD11	24:I:301:3PE:H2A1	1.93	0.50
10:P:205:ASP:OD1	10:P:205:ASP:O	2.30	0.50
17:X:119:ARG:HD2	17:X:120:PRO:HD2	1.94	0.50
18:Z:130:LYS:O	18:Z:131:GLU:C	2.52	0.50
1:A:21:ALA:HB1	8:H:218:GLY:HA3	1.93	0.50
4:D:81:THR:HA	4:D:99:LEU:O	2.12	0.50
4:D:182:ASN:HD21	4:D:404:LYS:NZ	2.10	0.50
4:D:266:ARG:NH1	9:I:60:ILE:HA	2.27	0.50
6:F:371:ILE:HD11	6:F:435:VAL:CG2	2.41	0.50
7:G:272:ARG:HH11	7:G:274:LEU:HD23	1.77	0.50
10:P:70:VAL:HG12	10:P:97:MET:SD	2.52	0.50
16:W:97:ILE:C	16:W:99:VAL:H	2.18	0.50
20:b:28:LEU:HA	20:b:31:ILE:CG2	2.42	0.50
22:r:6:ARG:HG2	22:r:6:ARG:O	2.11	0.50
2:B:191:VAL:HG21	2:B:201:LEU:HD12	1.94	0.50
4:D:207:ARG:O	4:D:208:GLU:C	2.53	0.50
4:D:289:SER:N	4:D:293:LEU:HG	2.27	0.50
4:D:304:LYS:HE2	9:I:35:THR:N	2.26	0.50
5:E:78:VAL:CG1	5:E:104:LEU:HD13	2.42	0.50
6:F:136:HIS:O	6:F:137:LYS:C	2.55	0.50
6:F:225:LEU:N	11:Q:160:TYR:HE2	2.07	0.50
7:G:401:LEU:HD23	7:G:496:MET:HE1	1.92	0.50
7:G:611:THR:HG21	11:Q:105:GLU:CA	2.27	0.50
10:P:122:HIS:HB2	12:R:46:VAL:HG22	1.94	0.50
2:B:84:TRP:HA	2:B:87:ARG:HG2	1.93	0.49
2:B:94:THR:CG2	2:B:104:MET:SD	3.00	0.49
2:B:192:PRO:HG2	9:I:175:PHE:CD1	2.46	0.49
3:C:112:ASP:OD1	3:C:113:LEU:N	2.45	0.49
4:D:198:THR:HA	8:H:32:GLN:HG2	1.94	0.49
4:D:271:ARG:CD	8:H:279:ARG:O	2.56	0.49
4:D:460:GLU:O	4:D:463:ARG:HG2	2.11	0.49
5:E:55:THR:O	5:E:56:PRO:C	2.53	0.49
6:F:391:TRP:HZ3	7:G:118:GLU:HG2	1.76	0.49
7:G:79:LEU:HD22	7:G:88:VAL:HG23	1.93	0.49
8:H:155:LEU:O	8:H:315:PRO:HG3	2.12	0.49
8:H:269:THR:O	8:H:273:ILE:HG12	2.11	0.49
10:P:346:GLU:H	10:P:346:GLU:CD	2.20	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:LEU:HD11	1:A:106:TRP:HE1	1.77	0.49
2:B:99:CYS:O	2:B:101:ALA:N	2.44	0.49
6:F:113:LEU:HD13	6:F:149:MET:HE3	1.90	0.49
6:F:185:ASN:HA	6:F:189:SER:O	2.12	0.49
7:G:403:VAL:HG13	7:G:476:LEU:HD12	1.94	0.49
8:H:17:MET:CE	8:H:225:MET:HB3	2.42	0.49
8:H:184:MET:SD	8:H:296:LEU:HD23	2.52	0.49
10:P:40:VAL:HB	10:P:53:GLY:HA2	1.93	0.49
12:R:70:ASN:HD22	12:R:111:PHE:HE1	1.60	0.49
19:a:4:GLU:O	19:a:7:PRO:HD2	2.11	0.49
20:b:38:TYR:HA	20:b:41:TYR:HD2	1.76	0.49
1:A:61:THR:CG2	8:H:290:TRP:CZ3	2.91	0.49
2:B:90:LEU:HD22	2:B:130:VAL:CG2	2.42	0.49
2:B:116:ARG:NH2	2:B:117:PHE:CZ	2.79	0.49
2:B:164:CYS:SG	25:B:301:SF4:S4	3.10	0.49
3:C:146:ALA:HB2	3:C:152:ILE:HD11	1.93	0.49
3:C:172:MET:SD	3:C:196:PRO:HG2	2.52	0.49
5:E:97:MET:HE2	5:E:115:ALA:CB	2.42	0.49
5:E:211:LYS:HG3	5:E:212:VAL:HG23	1.93	0.49
7:G:386:LEU:HD22	7:G:599:THR:O	2.11	0.49
8:H:185:TRP:O	8:H:189:THR:HG23	2.12	0.49
10:P:367:GLU:HG2	10:P:368:GLU:N	2.26	0.49
12:R:32:THR:HA	12:R:59:PHE:CZ	2.46	0.49
12:R:67:GLN:HG2	12:R:109:LEU:HD21	1.95	0.49
13:S:25:GLN:O	13:S:26:ARG:C	2.55	0.49
18:Z:140:PHE:O	18:Z:141:THR:C	2.55	0.49
1:A:103:ALA:O	1:A:107:THR:HG23	2.12	0.49
4:D:250:ASN:O	4:D:251:PHE:C	2.53	0.49
7:G:340:ALA:HB2	7:G:358:LEU:HD11	1.94	0.49
7:G:405:THR:HB	7:G:477:GLY:HA3	1.94	0.49
10:P:207:PHE:HE1	10:P:214:LEU:HD22	1.76	0.49
11:Q:72:ILE:HD13	11:Q:143:TRP:HE1	1.76	0.49
14:T:138:LEU:HD13	14:T:144:ILE:CD1	2.43	0.49
19:a:51:ASP:O	19:a:54:ILE:HB	2.11	0.49
3:C:241:PHE:H	7:G:146:PHE:HE1	1.59	0.49
4:D:128:THR:HG22	4:D:131:GLN:CD	2.38	0.49
4:D:145:MET:O	4:D:146:CYS:C	2.54	0.49
4:D:259:GLU:OE1	4:D:263:THR:HB	2.13	0.49
5:E:78:VAL:HG23	5:E:79:LEU:HD12	1.93	0.49
5:E:129:TYR:CE2	5:E:167:LEU:HG	2.47	0.49
5:E:147:ILE:CG2	5:E:151:LEU:HD13	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:157:TYR:CD2	6:F:212:LEU:HD11	2.48	0.49
7:G:355:LYS:HG3	7:G:366:LEU:HD22	1.94	0.49
7:G:360:LYS:CB	7:G:632:ILE:HD12	2.31	0.49
7:G:447:ASP:OD1	7:G:447:ASP:O	2.29	0.49
8:H:148:ILE:HG22	8:H:297:THR:HG22	1.95	0.49
10:P:64:PHE:CZ	10:P:211:ASP:HB3	2.48	0.49
15:V:39:PRO:HB2	15:V:42:ALA:HB2	1.94	0.49
3:C:53:THR:O	3:C:54:HIS:C	2.55	0.49
4:D:94:VAL:HB	4:D:115:LEU:CB	2.43	0.49
4:D:152:SER:O	4:D:153:ILE:C	2.56	0.49
4:D:329:ARG:O	4:D:330:TYR:C	2.53	0.49
4:D:365:PRO:HA	4:D:384:LEU:HD12	1.95	0.49
5:E:57:GLU:CA	5:E:60:LYS:HE2	2.31	0.49
5:E:129:TYR:HD2	5:E:167:LEU:O	1.94	0.49
6:F:212:LEU:O	6:F:216:ILE:HG12	2.13	0.49
7:G:162:ASP:O	7:G:163:LYS:HD3	2.13	0.49
7:G:371:ILE:N	7:G:482:GLN:OE1	2.46	0.49
8:H:179:TRP:N	8:H:180:PRO:CD	2.76	0.49
10:P:315:THR:HB	10:P:318:LYS:H	1.78	0.49
17:X:48:TRP:HD1	20:b:55:VAL:HG13	1.77	0.49
20:b:48:ALA:O	20:b:49:THR:C	2.53	0.49
2:B:117:PHE:HA	8:H:39:ILE:HG21	1.94	0.49
4:D:383:LYS:CD	7:G:140:GLN:NE2	2.73	0.49
6:F:333:GLU:OE2	6:F:334:THR:HG23	2.13	0.49
7:G:565:PHE:HA	7:G:581:ASP:OD2	2.12	0.49
7:G:593:SER:OG	7:G:639:LEU:HD13	2.12	0.49
10:P:238:GLN:HB2	10:P:270:ARG:HG2	1.94	0.49
10:P:360:ARG:O	10:P:361:TRP:HB2	2.13	0.49
15:V:56:LEU:HA	15:V:59:VAL:HB	1.94	0.49
2:B:175:TYR:OH	4:D:117:HIS:HE1	1.96	0.49
5:E:164:PRO:C	5:E:166:LYS:H	2.21	0.49
9:I:49:ASP:O	9:I:50:MET:C	2.55	0.49
10:P:235:THR:O	10:P:236:VAL:C	2.56	0.49
10:P:318:LYS:O	10:P:322:ILE:HG13	2.13	0.49
1:A:51:PHE:CD2	4:D:103:GLY:HA3	2.47	0.49
4:D:266:ARG:HG2	4:D:266:ARG:O	2.13	0.49
5:E:137:THR:HG22	6:F:370:LEU:HD21	1.95	0.49
6:F:299:LEU:HD11	6:F:300:ILE:HG13	1.93	0.49
6:F:379:CYS:SG	25:F:502:SF4:S1	3.11	0.49
7:G:557:ARG:CG	7:G:579:MET:HE3	2.33	0.49
9:I:114:ILE:HD13	12:R:106:TYR:CD1	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:116:CYS:O	9:I:117:LYS:HB2	2.12	0.49
11:Q:64:LEU:HG	16:W:84:LEU:HD22	1.93	0.49
14:T:88:LYS:NZ	14:T:96:GLU:H	2.11	0.49
1:A:18:ILE:O	1:A:21:ALA:HB3	2.13	0.49
6:F:51:TRP:HZ3	6:F:168:ASN:O	1.96	0.49
7:G:160:VAL:HG12	7:G:161:GLU:H	1.77	0.49
7:G:175:ARG:HB2	7:G:230:ALA:CA	2.43	0.49
7:G:179:CYS:HG	25:G:802:SF4:FE3	1.28	0.49
7:G:262:VAL:CG2	7:G:276:ARG:HB3	2.34	0.49
7:G:421:SER:HB2	7:G:427:LEU:HD11	1.92	0.49
8:H:16:ALA:HB2	19:a:15:CYS:HB2	1.94	0.49
8:H:187:ILE:CD1	24:I:301:3PE:H242	2.41	0.49
8:H:198:PHE:HB3	8:H:285:LEU:HD11	1.95	0.49
8:H:239:THR:CG2	8:H:262:GLU:HB2	2.43	0.49
8:H:300:LEU:HD23	20:b:25:VAL:HG11	1.95	0.49
10:P:111:ARG:NH1	10:P:138:ASN:O	2.44	0.49
16:W:42:TRP:O	16:W:43:TYR:C	2.55	0.49
1:A:106:TRP:CE3	24:b:201:3PE:H331	2.48	0.48
2:B:99:CYS:HB3	4:D:141:TYR:CD2	2.47	0.48
2:B:192:PRO:HG2	9:I:175:PHE:CE1	2.48	0.48
3:C:131:LEU:O	3:C:139:ARG:HG3	2.12	0.48
3:C:227:GLN:HE21	3:C:230:ARG:HH11	1.52	0.48
4:D:279:THR:HG22	4:D:280:ALA:N	2.28	0.48
5:E:81:VAL:HG21	5:E:104:LEU:HD21	1.94	0.48
5:E:97:MET:HE2	5:E:115:ALA:HB1	1.95	0.48
6:F:163:TYR:CE1	23:s:80:PHE:HB3	2.48	0.48
6:F:183:GLY:O	6:F:186:ALA:HB2	2.13	0.48
7:G:387:LEU:CD1	7:G:514:ASN:CG	2.74	0.48
15:V:90:LEU:HD23	15:V:94:MET:HG2	1.94	0.48
19:a:2:TRP:O	19:a:3:PHE:C	2.56	0.48
3:C:151:PRO:HB2	3:C:178:PHE:CE2	2.47	0.48
6:F:443:ARG:N	6:F:444:PRO:HD2	2.28	0.48
10:P:298:TYR:HA	10:P:301:ILE:HG12	1.95	0.48
14:T:119:ILE:HG13	14:T:135:ALA:HB1	1.95	0.48
17:X:115:LEU:HD13	17:X:117:TRP:CZ3	2.48	0.48
22:r:12:ARG:HE	22:r:20:LEU:HD21	1.78	0.48
4:D:375:MET:HE1	7:G:126:LEU:CA	2.43	0.48
5:E:129:TYR:CD2	5:E:167:LEU:O	2.66	0.48
6:F:314:LEU:HD13	6:F:356:VAL:HG13	1.95	0.48
10:P:197:GLU:HB3	10:P:259:VAL:HG23	1.93	0.48
12:R:31:ILE:HD11	12:R:37:VAL:HG23	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:19:LEU:HD21	24:b:201:3PE:H332	1.95	0.48
3:C:107:PHE:CE2	3:C:140:ILE:HD13	2.48	0.48
4:D:79:ASN:OD1	4:D:79:ASN:N	2.46	0.48
5:E:137:THR:CG2	5:E:138:PRO:HD3	2.42	0.48
6:F:46:TYR:O	6:F:48:ARG:HG2	2.13	0.48
6:F:339:PHE:CE1	6:F:349:LEU:HB3	2.48	0.48
7:G:261:ILE:HD13	7:G:273:ILE:CG2	2.44	0.48
7:G:496:MET:HG2	7:G:500:ILE:CD1	2.43	0.48
8:H:102:ILE:HG13	8:H:162:LEU:CD1	2.43	0.48
10:P:228:LEU:HD11	10:P:288:PHE:HZ	1.78	0.48
11:Q:99:MET:SD	11:Q:128:PHE:HE2	2.36	0.48
16:W:32:LYS:HG2	33:W:201:EHZ:C19	2.44	0.48
18:Z:89:GLU:HG2	18:Z:128:ARG:NH1	2.27	0.48
21:q:14:VAL:HG13	21:q:23:LEU:HD22	1.95	0.48
3:C:48:PRO:HD3	4:D:162:GLN:OE1	2.13	0.48
3:C:75:VAL:HG22	3:C:85:ILE:HG23	1.94	0.48
4:D:184:ILE:HD11	4:D:251:PHE:CZ	2.48	0.48
5:E:45:GLU:CD	5:E:45:GLU:H	2.21	0.48
6:F:290:GLU:HG2	6:F:291:GLU:N	2.27	0.48
9:I:154:TYR:N	9:I:154:TYR:CD1	2.81	0.48
12:R:43:TYR:CD1	12:R:44:ARG:HB2	2.49	0.48
14:T:90:TYR:HE2	14:T:92:LYS:HB3	1.78	0.48
2:B:121:PHE:CD1	2:B:121:PHE:C	2.89	0.48
3:C:127:ILE:HB	3:C:144:THR:CG2	2.43	0.48
4:D:213:PHE:O	4:D:217:VAL:HG13	2.13	0.48
5:E:138:PRO:CG	6:F:122:PRO:HB3	2.38	0.48
7:G:68:ARG:NE	7:G:283:GLU:CG	2.76	0.48
7:G:183:ILE:CD1	7:G:197:THR:HG23	2.43	0.48
7:G:349:GLU:OE2	7:G:595:THR:HG23	2.14	0.48
7:G:566:ILE:CD1	7:G:579:MET:HE2	2.43	0.48
8:H:85:LEU:CB	8:H:233:LEU:HD21	2.43	0.48
8:H:113:VAL:HG23	8:H:136:VAL:HA	1.95	0.48
8:H:296:LEU:HD21	24:I:301:3PE:H351	1.94	0.48
10:P:221:ARG:CD	10:P:286:ARG:HD3	2.43	0.48
10:P:318:LYS:HA	10:P:321:ARG:HH12	1.78	0.48
11:Q:82:PRO:HG2	11:Q:93:ASN:O	2.14	0.48
16:W:122:LEU:HD11	16:W:126:TYR:CE2	2.48	0.48
17:X:17:GLU:HB3	17:X:19:LYS:HG3	1.96	0.48
5:E:118:TYR:CD2	6:F:201:ALA:HB3	2.49	0.48
7:G:435:PRO:O	7:G:435:PRO:CG	2.61	0.48
8:H:130:PHE:CE2	8:H:134:ARG:HD3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:79:GLN:NE2	10:P:102:GLN:O	2.47	0.48
17:X:5:VAL:O	17:X:6:GLU:C	2.54	0.48
20:b:78:LEU:HA	20:b:80:TRP:CD1	2.49	0.48
3:C:89:PRO:O	3:C:92:VAL:HG23	2.13	0.48
4:D:82:LEU:O	4:D:83:ASN:C	2.56	0.48
4:D:198:THR:CG2	8:H:275:ALA:HB1	2.44	0.48
4:D:360:ASP:C	4:D:362:LYS:N	2.71	0.48
5:E:46:ASN:CG	5:E:91:TRP:HE1	2.21	0.48
5:E:143:ASP:O	5:E:144:SER:C	2.55	0.48
6:F:257:ARG:HG2	6:F:261:TRP:CG	2.48	0.48
6:F:326:LEU:HD12	6:F:326:LEU:O	2.13	0.48
12:R:32:THR:HA	12:R:59:PHE:HZ	1.78	0.48
12:R:79:CYS:O	12:R:88:HIS:CE1	2.67	0.48
14:T:132:ASP:HB3	16:W:40:ARG:HH12	1.78	0.48
20:b:26:TRP:CZ3	24:b:201:3PE:H2G2	2.48	0.48
21:q:60:ARG:HH12	21:q:95:ASP:HA	1.78	0.48
2:B:170:TYR:CE1	4:D:135:TYR:CZ	3.01	0.48
4:D:266:ARG:NH2	9:I:65:GLU:HG2	2.28	0.48
7:G:403:VAL:HG13	7:G:476:LEU:HA	1.96	0.48
7:G:541:PRO:HB2	7:G:561:PRO:CG	2.44	0.48
8:H:235:ASN:CG	8:H:270:PHE:CE2	2.92	0.48
12:R:88:HIS:HB2	12:R:89:PRO:HD2	1.95	0.48
15:V:11:LEU:HD23	15:V:14:LEU:HD13	1.96	0.48
20:b:23:PHE:HD1	24:b:201:3PE:H3B2	1.77	0.48
2:B:75:VAL:O	2:B:78:LEU:N	2.47	0.48
3:C:114:THR:CG2	4:D:421:ARG:NH1	2.76	0.48
4:D:79:ASN:O	4:D:100:GLU:HB3	2.14	0.48
7:G:265:THR:HG23	7:G:265:THR:O	2.14	0.48
7:G:454:ASP:OD1	7:G:459:ARG:NH1	2.47	0.48
10:P:294:PRO:HB3	10:P:296:PHE:HD1	1.79	0.48
13:S:79:LEU:CA	13:S:82:LEU:HD12	2.26	0.48
2:B:107:MET:HE3	2:B:114:MET:CE	2.44	0.47
3:C:73:GLN:O	3:C:74:GLN:C	2.57	0.47
6:F:387:GLU:OE1	6:F:387:GLU:N	2.47	0.47
6:F:410:ASP:O	6:F:413:TRP:HB3	2.14	0.47
7:G:297:LEU:O	7:G:297:LEU:HD23	2.14	0.47
7:G:383:SER:HB3	7:G:663:ASN:HB2	1.95	0.47
9:I:98:ARG:HA	9:I:169:GLU:HB3	1.95	0.47
14:T:104:PHE:CZ	14:T:118:ILE:HG21	2.48	0.47
19:a:18:ILE:N	19:a:19:PRO:CD	2.76	0.47
4:D:456:ILE:HD12	4:D:461:ILE:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:281:HIS:HB3	6:F:358:ASP:OD1	2.14	0.47
6:F:364:VAL:HG12	6:F:400:VAL:HG22	1.97	0.47
7:G:401:LEU:HD23	7:G:496:MET:CE	2.43	0.47
8:H:172:MET:HE1	18:Z:46:GLY:HA3	1.94	0.47
9:I:171:PRO:HG2	9:I:200:GLU:CD	2.39	0.47
10:P:311:GLU:O	10:P:312:PRO:C	2.57	0.47
14:T:82:ARG:NH1	14:T:126:PHE:HA	2.29	0.47
17:X:132:LYS:HB3	20:b:59:ASP:HB3	1.96	0.47
23:s:76:ASN:HB3	23:s:79:THR:HB	1.96	0.47
2:B:127:GLN:NE2	8:H:215:TYR:O	2.47	0.47
4:D:303:ARG:HG3	4:D:401:GLU:HG3	1.96	0.47
5:E:145:ASP:O	5:E:146:SER:C	2.56	0.47
6:F:369:ARG:O	6:F:373:PHE:N	2.47	0.47
7:G:496:MET:HG2	7:G:500:ILE:HD12	1.95	0.47
7:G:688:GLN:HA	7:G:693:ASP:CB	2.43	0.47
8:H:154:LEU:HD13	8:H:160:TYR:CE1	2.49	0.47
10:P:335:LEU:O	10:P:336:GLU:HB2	2.15	0.47
10:P:358:THR:HG22	10:P:359:TYR:H	1.79	0.47
14:T:117:GLU:HG2	16:W:43:TYR:CZ	2.48	0.47
17:X:69:ASN:OD1	17:X:70:PHE:N	2.47	0.47
5:E:40:HIS:HB2	7:G:209:TYR:CE2	2.49	0.47
5:E:142:ARG:O	5:E:143:ASP:HB2	2.13	0.47
6:F:257:ARG:HG2	6:F:261:TRP:CE2	2.48	0.47
7:G:373:PRO:HD3	7:G:481:LEU:HB3	1.96	0.47
8:H:154:LEU:HD22	8:H:160:TYR:HA	1.97	0.47
15:V:116:ILE:O	15:V:116:ILE:CG2	2.61	0.47
21:q:6:VAL:CG1	34:q:201:CDL:HA21	2.45	0.47
21:q:76:ASP:OD1	21:q:76:ASP:C	2.57	0.47
4:D:303:ARG:HG3	4:D:401:GLU:HB2	1.96	0.47
6:F:156:ILE:CD1	6:F:169:LEU:HD21	2.45	0.47
7:G:37:ASP:OD1	7:G:103:LEU:HA	2.14	0.47
7:G:117:MET:HE3	7:G:142:GLN:C	2.39	0.47
7:G:217:GLU:C	7:G:219:SER:H	2.21	0.47
7:G:605:GLN:NE2	7:G:643:ARG:HH22	2.13	0.47
10:P:170:LEU:HG	10:P:171:ASN:N	2.28	0.47
19:a:43:TYR:CE1	19:a:47:LEU:HD11	2.50	0.47
20:b:46:ASN:OD1	20:b:47:LYS:N	2.48	0.47
20:b:68:SER:O	20:b:69:HIS:C	2.56	0.47
21:q:68:MET:SD	21:q:81:MET:HG2	2.55	0.47
22:r:12:ARG:HB3	22:r:20:LEU:CD2	2.44	0.47
4:D:329:ARG:O	4:D:332:CYS:HB2	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:70:PRO:HG2	6:F:236:PHE:CE2	2.50	0.47
6:F:174:ARG:HH21	6:F:175:GLU:CD	2.23	0.47
6:F:254:ILE:O	6:F:258:GLY:N	2.48	0.47
7:G:517:HIS:CD2	7:G:523:VAL:HG22	2.49	0.47
8:H:9:LEU:O	8:H:9:LEU:HD13	2.14	0.47
10:P:237:LYS:HZ2	10:P:322:ILE:HG23	1.79	0.47
10:P:304:LEU:O	10:P:307:LEU:HB3	2.14	0.47
17:X:20:VAL:CG2	17:X:24:VAL:HG21	2.40	0.47
21:q:23:LEU:HD11	21:q:33:ILE:HG12	1.96	0.47
2:B:135:GLY:HA2	25:B:301:SF4:S3	2.54	0.47
2:B:182:ASP:C	2:B:182:ASP:OD1	2.55	0.47
3:C:195:HIS:HE1	16:W:88:LYS:NZ	2.12	0.47
4:D:254:ARG:HH11	22:r:25:GLN:HB2	1.80	0.47
4:D:381:HIS:HE1	9:I:161:ALA:O	1.98	0.47
5:E:83:ASP:O	5:E:87:ARG:HG2	2.14	0.47
6:F:336:LEU:HD11	6:F:338:ASP:OD2	2.14	0.47
6:F:338:ASP:OD1	6:F:338:ASP:O	2.33	0.47
6:F:425:CYS:SG	25:F:502:SF4:S4	3.13	0.47
7:G:697:THR:O	7:G:702:ARG:NH1	2.48	0.47
9:I:49:ASP:O	9:I:53:ALA:N	2.41	0.47
10:P:55:VAL:HG12	10:P:123:SER:HA	1.96	0.47
10:P:108:TRP:CZ2	31:P:401:NDP:H2A	2.49	0.47
11:Q:99:MET:SD	11:Q:128:PHE:CE2	3.08	0.47
12:R:32:THR:O	12:R:33:HIS:C	2.57	0.47
17:X:8:PRO:HB3	17:X:12:GLU:CD	2.39	0.47
17:X:36:CYS:O	17:X:39:THR:HG22	2.15	0.47
17:X:139:GLU:CD	17:X:139:GLU:H	2.22	0.47
19:a:22:SER:O	19:a:23:THR:C	2.57	0.47
20:b:23:PHE:CD1	24:b:201:3PE:H3B2	2.50	0.47
20:b:69:HIS:CD2	20:b:71:GLN:H	2.33	0.47
21:q:55:PHE:CZ	21:q:58:ARG:HG3	2.50	0.47
1:A:63:LEU:O	1:A:67:LEU:HG	2.14	0.47
2:B:99:CYS:O	2:B:102:VAL:N	2.45	0.47
3:C:132:LEU:HD11	4:D:300:TRP:CZ2	2.50	0.47
5:E:179:CYS:H	6:F:125:CYS:HB2	1.79	0.47
6:F:154:ALA:HB2	6:F:193:PHE:CZ	2.49	0.47
6:F:187:CYS:O	6:F:187:CYS:SG	2.71	0.47
6:F:370:LEU:O	6:F:373:PHE:HB3	2.15	0.47
7:G:329:MET:HE3	7:G:333:PHE:CE2	2.49	0.47
9:I:188:GLU:OE1	12:R:56:ASN:CB	2.63	0.47
10:P:76:MET:HE1	10:P:254:LYS:CE	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:221:ARG:HD3	10:P:286:ARG:HD3	1.97	0.47
11:Q:85:ASN:N	11:Q:85:ASN:OD1	2.48	0.47
16:W:29:ASN:O	16:W:29:ASN:OD1	2.33	0.47
19:a:3:PHE:O	19:a:6:LEU:HG	2.15	0.47
20:b:16:GLU:CD	24:b:201:3PE:H12	2.39	0.47
1:A:58:VAL:CG2	8:H:286:MET:HE1	2.45	0.47
4:D:299:GLN:HB3	22:r:104:TRP:CE3	2.49	0.47
6:F:159:ARG:HB3	6:F:162:PHE:CE2	2.50	0.47
6:F:217:GLU:CD	6:F:224:ARG:HH22	2.23	0.47
6:F:296:LEU:HD13	6:F:337:MET:CE	2.34	0.47
6:F:311:TRP:CZ2	6:F:333:GLU:HB3	2.50	0.47
8:H:71:PHE:CD1	8:H:215:TYR:CE1	3.03	0.47
9:I:68:ARG:HH22	18:Z:26:PRO:HD2	1.77	0.47
9:I:119:CYS:SG	9:I:130:ILE:CD1	3.03	0.47
10:P:207:PHE:CD2	10:P:241:TYR:HD1	2.33	0.47
13:S:16:LEU:HD21	13:S:95:LEU:HD12	1.97	0.47
3:C:67:ILE:HD11	15:V:47:TYR:CD2	2.50	0.47
6:F:166:ALA:HB1	23:s:80:PHE:CD1	2.50	0.47
6:F:281:HIS:HB3	6:F:358:ASP:CG	2.40	0.47
6:F:446:LEU:O	6:F:450:MET:HG2	2.15	0.47
7:G:82:ILE:HG21	7:G:100:TRP:HB3	1.96	0.47
7:G:429:VAL:HG11	7:G:440:TYR:HE1	1.80	0.47
8:H:1:MET:CB	19:a:30:THR:HG21	2.45	0.47
8:H:310:PHE:O	20:b:38:TYR:HB2	2.15	0.47
10:P:287:THR:HG23	10:P:289:ILE:HD11	1.97	0.47
12:R:47:ARG:HG3	12:R:48:PHE:CD1	2.50	0.47
17:X:120:PRO:HB2	17:X:125:LEU:CD1	2.44	0.47
4:D:117:HIS:HD2	4:D:462:ASP:O	1.97	0.46
4:D:359:ASP:O	7:G:150:ARG:NH2	2.48	0.46
5:E:78:VAL:HG12	5:E:104:LEU:CD1	2.44	0.46
5:E:173:VAL:HG22	5:E:174:GLU:N	2.30	0.46
6:F:115:VAL:HG12	6:F:245:VAL:HG12	1.97	0.46
6:F:127:ASP:O	6:F:131:MET:HG3	2.14	0.46
6:F:395:VAL:HG22	7:G:155:GLU:OE2	2.15	0.46
7:G:64:CYS:CA	7:G:181:ARG:HE	2.28	0.46
8:H:150:LEU:HD23	8:H:150:LEU:HA	1.80	0.46
8:H:306:SER:OG	20:b:33:PRO:HG3	2.15	0.46
10:P:318:LYS:O	10:P:319:VAL:C	2.58	0.46
12:R:54:GLU:HB2	21:q:124:TYR:CD1	2.51	0.46
13:S:25:GLN:HG3	13:S:26:ARG:H	1.80	0.46
4:D:151:TYR:CZ	4:D:155:VAL:HG21	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:212:ARG:O	10:P:213:PHE:C	2.55	0.46
10:P:245:VAL:HA	10:P:265:PHE:CD2	2.49	0.46
12:R:72:VAL:HG21	12:R:77:ILE:HG21	1.97	0.46
16:W:58:THR:HB	16:W:61:GLN:HB3	1.94	0.46
16:W:113:THR:O	16:W:113:THR:HG22	2.15	0.46
22:r:109:ASP:O	22:r:110:GLN:OE1	2.32	0.46
5:E:52:PHE:CE1	5:E:88:GLN:HG2	2.49	0.46
5:E:92:LEU:HG	5:E:92:LEU:O	2.14	0.46
5:E:109:MET:HE3	5:E:113:GLU:HG2	1.98	0.46
7:G:462:PHE:CD1	7:G:465:VAL:HB	2.50	0.46
15:V:22:GLU:O	15:V:26:ILE:HG12	2.16	0.46
17:X:94:MET:O	17:X:95:GLN:C	2.59	0.46
17:X:107:PHE:O	17:X:110:CYS:SG	2.73	0.46
17:X:115:LEU:HD13	17:X:117:TRP:CZ2	2.51	0.46
1:A:54:LYS:O	1:A:55:PHE:C	2.58	0.46
2:B:174:SER:HA	3:C:203:LEU:CD2	2.46	0.46
4:D:82:LEU:C	4:D:84:PHE:N	2.70	0.46
4:D:82:LEU:HB2	4:D:99:LEU:CD1	2.46	0.46
5:E:191:TYR:O	5:E:192:TYR:C	2.58	0.46
6:F:358:ASP:C	6:F:360:SER:H	2.23	0.46
8:H:224:PHE:CE2	30:H:401:UQ9:H12A	2.50	0.46
10:P:153:ALA:HB3	10:P:194:VAL:CG2	2.46	0.46
13:S:19:ILE:HD12	13:S:94:VAL:CG1	2.44	0.46
14:T:119:ILE:CD1	14:T:138:LEU:HD11	2.43	0.46
15:V:50:GLN:HE22	22:r:94:ALA:H	1.63	0.46
15:V:56:LEU:HD12	15:V:57:ASP:CA	2.45	0.46
17:X:35:GLN:O	17:X:36:CYS:CB	2.64	0.46
1:A:106:TRP:CH2	8:H:291:LYS:HA	2.51	0.46
2:B:107:MET:O	2:B:112:TYR:O	2.32	0.46
4:D:161:ILE:HD12	4:D:161:ILE:HA	1.82	0.46
6:F:45:LEU:HG	6:F:46:TYR:CD1	2.51	0.46
8:H:249:ILE:HG21	17:X:99:HIS:CE1	2.50	0.46
8:H:307:LEU:HD11	18:Z:47:TYR:CD1	2.50	0.46
9:I:53:ALA:O	9:I:54:THR:C	2.56	0.46
10:P:209:ARG:O	10:P:210:GLU:HB2	2.15	0.46
10:P:276:LEU:O	10:P:280:ILE:HG13	2.15	0.46
13:S:34:ARG:O	13:S:38:VAL:HG23	2.16	0.46
15:V:72:LEU:CD1	15:V:72:LEU:C	2.89	0.46
20:b:28:LEU:O	20:b:32:MET:HG2	2.15	0.46
2:B:140:LYS:O	2:B:143:PRO:HD2	2.15	0.46
3:C:49:ARG:NH2	3:C:54:HIS:CD2	2.84	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:216:ARG:HG3	4:D:240:LEU:HD13	1.97	0.46
4:D:338:ARG:NH1	18:Z:23:ARG:HA	2.31	0.46
4:D:432:LEU:O	4:D:433:ALA:C	2.58	0.46
5:E:238:LYS:HE2	5:E:242:PHE:CE1	2.50	0.46
6:F:224:ARG:HD3	11:Q:164:PHE:CE1	2.51	0.46
6:F:225:LEU:O	6:F:228:PRO:HD2	2.16	0.46
6:F:296:LEU:HD21	6:F:317:VAL:HG11	1.98	0.46
6:F:420:GLU:O	6:F:429:ASP:OD1	2.32	0.46
8:H:1:MET:O	8:H:2:PHE:C	2.58	0.46
8:H:187:ILE:HG23	8:H:198:PHE:CE2	2.50	0.46
8:H:249:ILE:HD13	17:X:99:HIS:CG	2.50	0.46
10:P:142:GLU:O	10:P:146:VAL:CG1	2.61	0.46
20:b:19:LEU:CD2	24:b:201:3PE:H332	2.46	0.46
21:q:14:VAL:HA	21:q:23:LEU:HD22	1.98	0.46
3:C:62:GLU:O	3:C:63:TYR:C	2.58	0.46
5:E:143:ASP:O	5:E:146:SER:N	2.49	0.46
6:F:177:TYR:CE2	6:F:182:ILE:HD12	2.51	0.46
7:G:35:PHE:O	7:G:101:ASN:HA	2.16	0.46
7:G:301:ARG:HE	7:G:613:PRO:CG	2.26	0.46
7:G:544:MET:HA	7:G:565:PHE:O	2.16	0.46
7:G:655:ARG:NH1	13:S:59:SER:H	2.14	0.46
7:G:689:LEU:HD12	7:G:689:LEU:HA	1.79	0.46
8:H:28:LEU:HD11	8:H:274:ARG:HH11	1.81	0.46
10:P:55:VAL:HG22	10:P:79:GLN:HB3	1.97	0.46
14:T:87:LEU:CD2	14:T:122:MET:HE1	2.46	0.46
17:X:133:THR:HG23	20:b:58:ARG:HH12	1.81	0.46
2:B:107:MET:HE1	2:B:201:LEU:HD23	1.96	0.46
4:D:211:PHE:O	4:D:214:TYR:HB2	2.16	0.46
4:D:289:SER:HA	4:D:293:LEU:CD1	2.46	0.46
6:F:300:ILE:HD13	6:F:307:VAL:HG22	1.96	0.46
6:F:318:ILE:HB	6:F:355:ILE:HB	1.98	0.46
7:G:32:ILE:HD11	7:G:45:PRO:HG3	1.98	0.46
7:G:251:ILE:HG13	7:G:604:GLN:HB3	1.98	0.46
10:P:261:LYS:HB2	10:P:263:PHE:CE1	2.51	0.46
15:V:32:LEU:O	15:V:36:LYS:HG2	2.16	0.46
17:X:120:PRO:HB3	17:X:125:LEU:HD11	1.94	0.46
24:A:401:3PE:H262	24:A:401:3PE:C32	2.45	0.46
7:G:269:GLU:HG2	7:G:271:MET:HE3	1.98	0.46
7:G:339:ALA:C	7:G:545:LEU:HD12	2.40	0.46
7:G:456:ALA:O	7:G:499:LYS:CE	2.57	0.46
7:G:545:LEU:O	7:G:566:ILE:HA	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:88:PRO:CG	8:H:105:ILE:HD11	2.46	0.46
26:H:402:PC1:C21	26:H:402:PC1:H252	2.46	0.46
13:S:65:LEU:HD23	13:S:65:LEU:O	2.16	0.46
16:W:42:TRP:CZ2	16:W:93:LEU:HB2	2.51	0.46
17:X:7:LEU:CD1	18:Z:87:LEU:HB3	2.46	0.46
19:a:45:TRP:O	19:a:46:TYR:C	2.58	0.46
21:q:71:LYS:HB2	21:q:73:THR:HG23	1.98	0.46
2:B:99:CYS:O	2:B:100:CYS:C	2.57	0.46
2:B:174:SER:HB2	4:D:123:LEU:HD21	1.98	0.46
5:E:118:TYR:HE2	6:F:206:CYS:SG	2.39	0.46
5:E:136:THR:HB	28:E:301:FES:S2	2.56	0.46
6:F:117:ALA:HB3	6:F:158:ILE:HG22	1.98	0.46
6:F:342:LEU:HD12	6:F:349:LEU:HA	1.97	0.46
7:G:35:PHE:CE1	7:G:40:SER:CB	2.99	0.46
7:G:176:CYS:SG	25:G:802:SF4:S1	3.14	0.46
7:G:406:ASN:ND2	7:G:436:VAL:CG2	2.76	0.46
8:H:150:LEU:HD21	8:H:241:ILE:HD13	1.97	0.46
16:W:97:ILE:C	16:W:99:VAL:N	2.73	0.46
16:W:99:VAL:HG13	16:W:99:VAL:O	2.15	0.46
17:X:37:ASP:OD2	20:b:70:PRO:HD3	2.16	0.46
20:b:45:ILE:N	20:b:80:TRP:HH2	2.14	0.46
1:A:77:TRP:CZ2	8:H:100:LEU:HD21	2.50	0.45
4:D:86:PRO:HD3	4:D:95:LEU:O	2.16	0.45
4:D:302:LEU:HB2	4:D:401:GLU:CG	2.33	0.45
4:D:376:GLU:HG3	7:G:151:SER:HB2	1.97	0.45
6:F:51:TRP:CB	6:F:133:HIS:O	2.64	0.45
7:G:260:ASN:N	7:G:281:ILE:HD11	2.30	0.45
8:H:239:THR:O	8:H:239:THR:CG2	2.63	0.45
9:I:188:GLU:OE1	12:R:56:ASN:HB2	2.16	0.45
12:R:54:GLU:HB2	21:q:124:TYR:HD1	1.81	0.45
14:T:133:ILE:O	14:T:136:GLU:N	2.46	0.45
15:V:56:LEU:HD13	15:V:60:LYS:HE2	1.98	0.45
17:X:5:VAL:CG1	17:X:7:LEU:HG	2.46	0.45
2:B:107:MET:CE	2:B:201:LEU:HD23	2.46	0.45
3:C:100:ARG:NH1	15:V:86:LYS:NZ	2.64	0.45
4:D:241:LEU:HD22	4:D:348:LEU:HD23	1.98	0.45
4:D:279:THR:CG2	15:V:13:GLY:HA3	2.26	0.45
5:E:244:VAL:HG23	6:F:256:ARG:HG3	1.98	0.45
7:G:168:LEU:HD21	7:G:710:CYS:SG	2.56	0.45
7:G:652:ASN:OD1	7:G:653:LEU:HG	2.16	0.45
8:H:125:SER:HB2	8:H:128:SER:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:251:LEU:HD21	8:H:254:LEU:HD12	1.97	0.45
8:H:316:PRO:HG3	18:Z:57:ARG:HB3	1.98	0.45
9:I:60:ILE:CG2	24:I:301:3PE:H111	2.46	0.45
10:P:66:GLY:O	10:P:69:VAL:N	2.48	0.45
13:S:37:ILE:HD12	13:S:55:ILE:HD12	1.98	0.45
20:b:38:TYR:O	20:b:39:THR:C	2.59	0.45
4:D:134:PRO:O	4:D:138:ARG:NH1	2.48	0.45
4:D:202:TRP:CZ2	9:I:76:TYR:CE2	3.05	0.45
4:D:214:TYR:O	4:D:217:VAL:HG22	2.16	0.45
4:D:279:THR:HG23	15:V:13:GLY:CA	2.27	0.45
4:D:342:ARG:O	4:D:346:GLN:HG3	2.17	0.45
5:E:69:TYR:HE2	5:E:80:PRO:HG2	1.81	0.45
5:E:134:CYS:SG	5:E:139:CYS:SG	3.06	0.45
7:G:35:PHE:CD1	7:G:40:SER:HB2	2.51	0.45
7:G:82:ILE:HG23	7:G:100:TRP:HB3	1.96	0.45
7:G:97:MET:HB2	7:G:100:TRP:NE1	2.30	0.45
7:G:387:LEU:HD23	7:G:391:ILE:CD1	2.47	0.45
8:H:10:LEU:O	8:H:11:VAL:C	2.59	0.45
8:H:79:LEU:HG	8:H:83:LEU:HD12	1.98	0.45
8:H:312:ALA:CB	20:b:38:TYR:HB3	2.44	0.45
9:I:107:PRO:O	9:I:108:SER:C	2.57	0.45
10:P:170:LEU:HD12	10:P:171:ASN:H	1.81	0.45
10:P:220:TYR:HA	10:P:223:PHE:CD2	2.51	0.45
13:S:44:LEU:CD1	13:S:91:MET:HG2	2.45	0.45
34:q:201:CDL:H141	34:q:201:CDL:H321	1.97	0.45
2:B:199:GLU:HB3	9:I:86:TYR:CE1	2.51	0.45
4:D:252:SER:O	4:D:253:LEU:C	2.59	0.45
6:F:154:ALA:HB2	6:F:193:PHE:CE1	2.51	0.45
6:F:299:LEU:CD1	6:F:300:ILE:N	2.67	0.45
7:G:34:VAL:HG11	7:G:96:VAL:CG2	2.47	0.45
7:G:385:TYR:HA	7:G:515:ILE:CD1	2.39	0.45
7:G:592:LYS:HA	7:G:608:VAL:HG12	1.98	0.45
8:H:120:GLY:HA3	8:H:132:ALA:HB2	1.98	0.45
8:H:148:ILE:CG2	8:H:297:THR:HG22	2.45	0.45
9:I:123:CYS:SG	25:I:303:SF4:S4	3.13	0.45
11:Q:77:VAL:HG21	11:Q:99:MET:HE3	1.97	0.45
20:b:45:ILE:CA	20:b:80:TRP:HH2	2.28	0.45
21:q:74:PHE:HD2	21:q:75:TRP:CD1	2.33	0.45
1:A:7:ILE:HA	1:A:10:ASN:ND2	2.31	0.45
2:B:147:LYS:HE3	2:B:151:GLN:NE2	2.32	0.45
3:C:204:THR:CB	3:C:225:LEU:HD11	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:124:ILE:HG21	4:D:422:CYS:SG	2.56	0.45
4:D:243:ASP:C	4:D:245:TYR:N	2.72	0.45
4:D:266:ARG:NH2	9:I:59:ARG:O	2.50	0.45
5:E:39:VAL:HG21	7:G:163:LYS:NZ	2.31	0.45
5:E:73:HIS:ND1	11:Q:166:TRP:CE3	2.84	0.45
5:E:245:GLN:HB3	6:F:256:ARG:O	2.16	0.45
6:F:240:THR:HG22	6:F:241:THR:N	2.30	0.45
7:G:127:ASP:HB2	7:G:130:ILE:HD12	1.98	0.45
7:G:217:GLU:HG3	7:G:412:PRO:HB3	1.97	0.45
9:I:61:LEU:O	24:I:301:3PE:H332	2.15	0.45
9:I:76:TYR:O	9:I:77:LEU:C	2.59	0.45
10:P:259:VAL:H	10:P:261:LYS:HG2	1.82	0.45
17:X:4:ILE:HG22	17:X:5:VAL:N	2.25	0.45
19:a:45:TRP:O	19:a:48:MET:N	2.50	0.45
21:q:85:GLU:CG	21:q:98:PRO:HB3	2.37	0.45
34:q:201:CDL:H321	34:q:201:CDL:C14	2.47	0.45
4:D:251:PHE:O	4:D:252:SER:C	2.56	0.45
6:F:300:ILE:CG2	6:F:306:GLY:C	2.90	0.45
6:F:392:MET:CE	6:F:419:ILE:CD1	2.60	0.45
7:G:163:LYS:HE2	12:R:97:LYS:NZ	2.31	0.45
7:G:263:VAL:HG22	7:G:273:ILE:HG12	1.98	0.45
7:G:447:ASP:O	7:G:447:ASP:CG	2.59	0.45
8:H:4:ILE:HD12	8:H:4:ILE:N	2.31	0.45
8:H:67:SER:CA	26:H:402:PC1:H121	2.42	0.45
8:H:288:LEU:HD21	8:H:293:PHE:CE2	2.52	0.45
8:H:302:MET:SD	20:b:26:TRP:CD1	3.09	0.45
11:Q:77:VAL:CG1	11:Q:101:PHE:CD2	3.00	0.45
21:q:98:PRO:O	21:q:99:THR:C	2.59	0.45
2:B:91:TRP:HA	2:B:120:VAL:HG12	1.99	0.45
2:B:94:THR:HG21	2:B:104:MET:SD	2.57	0.45
4:D:154:ALA:HB2	4:D:398:THR:HG22	1.97	0.45
4:D:163:PRO:HG2	4:D:168:GLN:CG	2.46	0.45
4:D:198:THR:HG21	8:H:275:ALA:HB1	1.99	0.45
4:D:294:ARG:HD2	4:D:318:VAL:CG1	2.47	0.45
7:G:259:SER:HA	7:G:281:ILE:HD13	1.99	0.45
7:G:282:ASN:HB2	7:G:285:TRP:O	2.17	0.45
7:G:301:ARG:NE	7:G:613:PRO:HG3	2.30	0.45
8:H:2:PHE:O	8:H:6:ILE:HG13	2.17	0.45
8:H:27:ILE:O	8:H:31:MET:HG3	2.15	0.45
10:P:218:ALA:HB2	10:P:280:ILE:CG2	2.47	0.45
15:V:56:LEU:HD11	15:V:57:ASP:OD1	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:38:LYS:HZ1	17:X:131:VAL:HA	1.81	0.45
17:X:137:LEU:HA	17:X:138:PRO:HD3	1.85	0.45
4:D:94:VAL:CG1	4:D:115:LEU:HB3	2.47	0.45
5:E:52:PHE:O	5:E:99:LYS:HG3	2.17	0.45
6:F:177:TYR:C	6:F:180:GLY:H	2.24	0.45
7:G:117:MET:HE3	7:G:143:SER:HA	1.98	0.45
7:G:358:LEU:HD12	7:G:366:LEU:HD11	1.98	0.45
7:G:624:ARG:HA	7:G:634:LEU:HD12	1.99	0.45
8:H:79:LEU:CD1	8:H:83:LEU:CD1	2.92	0.45
8:H:181:MET:O	8:H:185:TRP:N	2.49	0.45
11:Q:99:MET:HG2	11:Q:128:PHE:HE2	1.82	0.45
17:X:115:LEU:HB3	17:X:117:TRP:CE2	2.52	0.45
18:Z:94:GLU:HA	18:Z:97:ILE:HG12	1.99	0.45
1:A:49:LEU:HD21	4:D:80:MET:HE2	1.99	0.45
3:C:98:PHE:HE1	15:V:44:TYR:CE1	2.35	0.45
4:D:300:TRP:CE3	4:D:305:THR:HG21	2.52	0.45
5:E:90:GLY:HA3	5:E:126:VAL:HG12	1.99	0.45
5:E:173:VAL:HG11	5:E:176:LEU:HD11	1.99	0.45
6:F:88:ARG:HA	6:F:274:LYS:HE2	1.98	0.45
6:F:251:SER:N	6:F:252:PRO:HD2	2.32	0.45
7:G:128:CYS:N	7:G:129:PRO:CD	2.80	0.45
7:G:169:VAL:HG22	7:G:223:ILE:CD1	2.40	0.45
7:G:296:GLY:HA2	7:G:703:ALA:O	2.16	0.45
8:H:179:TRP:CD1	18:Z:43:LEU:HD21	2.52	0.45
10:P:55:VAL:HA	10:P:79:GLN:O	2.17	0.45
10:P:116:ILE:HG21	10:P:152:ILE:HA	1.99	0.45
10:P:209:ARG:CA	10:P:352:VAL:HG22	2.47	0.45
14:T:83:VAL:HG21	14:T:145:VAL:HG22	1.99	0.45
14:T:87:LEU:CD2	14:T:104:PHE:CE1	2.94	0.45
14:T:130:ILE:CG2	14:T:131:PRO:CD	2.95	0.45
15:V:8:THR:CG2	15:V:9:THR:N	2.79	0.45
16:W:32:LYS:HZ2	33:W:201:EHZ:C19	2.28	0.45
17:X:7:LEU:HD13	18:Z:87:LEU:HB3	1.99	0.45
18:Z:62:ILE:O	18:Z:66:GLU:HG3	2.16	0.45
22:r:109:ASP:O	22:r:110:GLN:CG	2.64	0.45
2:B:136:THR:HG21	2:B:177:VAL:CG2	2.45	0.45
2:B:170:TYR:CE2	4:D:134:PRO:HB2	2.52	0.45
5:E:54:PHE:HE2	5:E:103:VAL:HG21	1.82	0.45
5:E:55:THR:O	5:E:58:ASN:N	2.50	0.45
5:E:158:LYS:HE2	5:E:161:GLU:HG2	1.96	0.45
6:F:346:GLN:NE2	6:F:440:ARG:HD3	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:391:TRP:CZ3	7:G:118:GLU:HG2	2.51	0.45
7:G:32:ILE:CG2	7:G:98:LYS:HD2	2.47	0.45
7:G:185:PHE:CE2	7:G:285:TRP:NE1	2.85	0.45
7:G:341:ILE:HD12	7:G:555:ILE:CG1	2.47	0.45
7:G:358:LEU:HD12	7:G:366:LEU:CD1	2.47	0.45
8:H:71:PHE:CZ	8:H:219:PRO:HG3	2.52	0.45
8:H:146:MET:HE1	8:H:192:GLU:CB	2.47	0.45
8:H:204:GLU:O	8:H:205:SER:C	2.57	0.45
8:H:293:PHE:CE1	24:I:301:3PE:H32	2.52	0.45
9:I:50:MET:O	9:I:51:LYS:C	2.60	0.45
9:I:60:ILE:HG23	24:I:301:3PE:H111	1.99	0.45
10:P:238:GLN:HB3	10:P:326:ASP:OD2	2.17	0.45
12:R:97:LYS:CE	12:R:100:LYS:HD3	2.45	0.45
13:S:62:GLN:HB2	13:S:80:ASN:CG	2.42	0.45
13:S:74:GLU:OE1	13:S:74:GLU:N	2.49	0.45
14:T:90:TYR:O	14:T:91:ASP:HB2	2.17	0.45
17:X:9:THR:O	17:X:12:GLU:HB3	2.17	0.45
2:B:94:THR:O	2:B:94:THR:OG1	2.36	0.44
2:B:126:ARG:HG3	8:H:213:VAL:O	2.17	0.44
4:D:92:HIS:H	4:D:458:PHE:HE2	1.65	0.44
5:E:177:GLY:O	28:E:301:FES:S1	2.75	0.44
6:F:382:CYS:HA	7:G:74:ASN:O	2.17	0.44
7:G:136:GLU:OE1	11:Q:87:MET:HG3	2.17	0.44
7:G:509:GLU:HG2	7:G:510:TRP:N	2.32	0.44
11:Q:65:THR:HG23	11:Q:67:VAL:HG23	1.99	0.44
16:W:47:PRO:HG3	16:W:63:ARG:NH2	2.26	0.44
2:B:126:ARG:NH1	8:H:214:GLU:OE1	2.50	0.44
3:C:130:ASN:ND2	3:C:141:ARG:HE	2.13	0.44
3:C:164:TRP:CZ3	4:D:113:ILE:HD13	2.52	0.44
3:C:207:VAL:N	3:C:223:VAL:HG23	2.32	0.44
4:D:174:PHE:HZ	4:D:240:LEU:HD21	1.83	0.44
4:D:243:ASP:C	4:D:245:TYR:H	2.24	0.44
5:E:55:THR:N	5:E:58:ASN:HB2	2.32	0.44
5:E:104:LEU:O	5:E:106:VAL:HG13	2.17	0.44
6:F:383:THR:CG2	7:G:120:LEU:HD23	2.47	0.44
8:H:133:LEU:HA	8:H:136:VAL:CG1	2.48	0.44
8:H:174:LEU:O	8:H:177:PRO:O	2.35	0.44
8:H:186:PHE:CE2	24:I:301:3PE:H2B1	2.52	0.44
8:H:223:PHE:O	8:H:226:ALA:N	2.50	0.44
10:P:245:VAL:HA	10:P:265:PHE:HD2	1.82	0.44
4:D:95:LEU:HG	4:D:97:LEU:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:245:TYR:O	4:D:246:GLU:C	2.60	0.44
4:D:284:LEU:HD21	4:D:298:ILE:HG21	1.99	0.44
5:E:164:PRO:C	5:E:166:LYS:N	2.72	0.44
6:F:44:ASN:ND2	6:F:51:TRP:HA	2.32	0.44
6:F:119:GLU:HG3	6:F:127:ASP:HB2	1.98	0.44
7:G:127:ASP:C	7:G:127:ASP:OD1	2.59	0.44
7:G:169:VAL:HG11	7:G:231:LEU:HD13	1.99	0.44
7:G:259:SER:HB2	7:G:282:ASN:HB3	1.99	0.44
8:H:291:LYS:HE2	8:H:291:LYS:HB2	1.61	0.44
9:I:48:VAL:HG12	20:b:10:LYS:HZ2	1.82	0.44
10:P:361:TRP:O	10:P:364:SER:HB3	2.18	0.44
11:Q:62:THR:HG22	11:Q:141:ASN:O	2.18	0.44
12:R:89:PRO:HG2	12:R:106:TYR:CZ	2.51	0.44
14:T:79:ILE:O	14:T:83:VAL:HG23	2.18	0.44
14:T:133:ILE:HG23	14:T:134:ASP:N	2.32	0.44
18:Z:131:GLU:O	18:Z:134:SER:N	2.51	0.44
20:b:20:VAL:HA	24:b:201:3PE:H282	2.00	0.44
1:A:48:ARG:C	1:A:49:LEU:HD22	2.43	0.44
1:A:99:SER:O	1:A:102:LEU:HB3	2.17	0.44
3:C:107:PHE:CE1	3:C:133:SER:HB3	2.53	0.44
3:C:149:LEU:O	16:W:23:ILE:HD11	2.17	0.44
3:C:168:GLU:HA	3:C:186:ILE:HD11	2.00	0.44
4:D:189:THR:OG1	27:D:501:UQ1:HM33	2.18	0.44
4:D:244:ILE:HG22	4:D:244:ILE:O	2.17	0.44
4:D:376:GLU:HG2	7:G:121:LEU:HD12	1.99	0.44
5:E:192:TYR:CZ	5:E:215:PRO:HA	2.51	0.44
6:F:297:LYS:HB2	6:F:333:GLU:HB2	2.00	0.44
7:G:284:GLU:OE2	11:Q:84:ARG:NH2	2.51	0.44
7:G:387:LEU:CD2	7:G:391:ILE:CD1	2.94	0.44
7:G:473:MET:HE3	7:G:514:ASN:HD21	1.83	0.44
8:H:72:ILE:C	8:H:72:ILE:HD12	2.42	0.44
26:I:302:PC1:H112	18:Z:29:GLY:CA	2.45	0.44
24:b:201:3PE:H281	24:b:201:3PE:H252	1.85	0.44
22:r:109:ASP:OD1	22:r:110:GLN:N	2.51	0.44
2:B:90:LEU:O	2:B:119:VAL:HA	2.17	0.44
3:C:101:ASP:OD1	15:V:86:LYS:HE3	2.16	0.44
3:C:197:PHE:CZ	4:D:121:GLU:HB2	2.53	0.44
4:D:375:MET:HE2	4:D:375:MET:HB2	1.66	0.44
4:D:376:GLU:HG2	7:G:121:LEU:CD1	2.47	0.44
5:E:54:PHE:CE2	5:E:103:VAL:HG21	2.53	0.44
5:E:221:ARG:HB2	5:E:225:GLU:HG2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:49:VAL:HG11	7:G:80:VAL:HG21	1.99	0.44
7:G:278:HIS:CG	7:G:281:ILE:HG13	2.52	0.44
7:G:319:TRP:CZ3	7:G:584:LEU:HD22	2.52	0.44
7:G:365:ASN:HB3	7:G:537:ILE:HD11	1.99	0.44
8:H:288:LEU:HD21	8:H:293:PHE:CZ	2.52	0.44
9:I:42:LYS:HD3	9:I:42:LYS:HA	1.84	0.44
10:P:298:TYR:O	10:P:299:SER:C	2.60	0.44
10:P:305:PHE:CB	10:P:314:THR:HG22	2.47	0.44
16:W:71:MET:O	16:W:74:ALA:N	2.43	0.44
17:X:30:HIS:CE1	18:Z:63:GLU:HG3	2.51	0.44
22:r:5:THR:HG22	22:r:5:THR:O	2.18	0.44
2:B:127:GLN:OE1	2:B:127:GLN:N	2.51	0.44
4:D:128:THR:HG22	4:D:131:GLN:HG2	2.00	0.44
4:D:446:ASP:O	4:D:450:ILE:HG13	2.16	0.44
5:E:155:LEU:HB3	5:E:157:ILE:HG22	2.00	0.44
6:F:286:CYS:SG	6:F:304:ALA:HA	2.57	0.44
7:G:259:SER:HA	7:G:281:ILE:HD12	1.98	0.44
7:G:281:ILE:HD12	7:G:282:ASN:H	1.83	0.44
7:G:671:LEU:HA	7:G:674:LEU:HD12	1.99	0.44
8:H:11:VAL:O	8:H:14:LEU:N	2.51	0.44
8:H:114:TYR:O	8:H:115:SER:C	2.59	0.44
8:H:196:ALA:C	8:H:198:PHE:N	2.76	0.44
8:H:215:TYR:HD2	8:H:219:PRO:HB2	1.77	0.44
8:H:277:TYR:CE2	24:I:301:3PE:H271	2.53	0.44
10:P:168:SER:O	10:P:202:ARG:HA	2.17	0.44
10:P:345:LEU:C	10:P:345:LEU:HD23	2.43	0.44
11:Q:91:VAL:HG22	11:Q:91:VAL:O	2.18	0.44
14:T:117:GLU:HA	14:T:120:MET:CE	2.41	0.44
15:V:56:LEU:C	15:V:56:LEU:CD1	2.85	0.44
18:Z:72:MET:O	18:Z:73:PRO:C	2.56	0.44
3:C:133:SER:O	3:C:133:SER:OG	2.32	0.44
4:D:141:TYR:CB	4:D:223:HIS:CE1	3.01	0.44
4:D:339:GLN:NE2	9:I:37:LYS:HZ2	2.14	0.44
4:D:361:ALA:O	4:D:384:LEU:HD11	2.18	0.44
6:F:260:THR:O	6:F:261:TRP:C	2.60	0.44
7:G:68:ARG:CB	7:G:285:TRP:HH2	2.31	0.44
7:G:450:LYS:O	7:G:450:LYS:HG3	2.18	0.44
8:H:142:TYR:CA	8:H:289:LEU:HD13	2.45	0.44
8:H:280:PHE:HD2	8:H:284:GLN:HG3	1.81	0.44
10:P:231:LEU:HD11	10:P:290:PRO:HB2	2.00	0.44
10:P:298:TYR:C	10:P:300:TRP:N	2.71	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:315:THR:O	10:P:316:LYS:C	2.57	0.44
16:W:20:VAL:HG21	16:W:80:ARG:CZ	2.48	0.44
16:W:58:THR:HB	16:W:61:GLN:H	1.82	0.44
19:a:62:VAL:HG23	19:a:62:VAL:O	2.18	0.44
2:B:121:PHE:HZ	2:B:122:ARG:HH21	1.65	0.44
2:B:202:LEU:HD12	9:I:86:TYR:CE2	2.46	0.44
3:C:114:THR:HG22	3:C:115:ALA:N	2.33	0.44
5:E:206:GLU:HB2	5:E:213:PRO:HB3	1.99	0.44
7:G:362:ASP:O	7:G:362:ASP:CG	2.61	0.44
10:P:72:HIS:HB2	10:P:250:VAL:HG21	2.00	0.44
10:P:81:ILE:HG23	10:P:106:LEU:HD13	2.00	0.44
10:P:357:ARG:NH2	10:P:364:SER:O	2.47	0.44
13:S:83:SER:O	13:S:87:VAL:HG23	2.17	0.44
16:W:23:ILE:HG22	16:W:24:PHE:HD1	1.81	0.44
18:Z:28:ARG:O	18:Z:28:ARG:CG	2.64	0.44
19:a:43:TYR:O	19:a:47:LEU:HD13	2.18	0.44
2:B:97:LEU:HB2	2:B:134:ALA:O	2.18	0.44
3:C:78:SER:C	3:C:80:LEU:H	2.24	0.44
6:F:375:LYS:HD3	6:F:390:ASP:OD1	2.17	0.44
7:G:131:CYS:HA	7:G:175:ARG:HH12	1.83	0.44
7:G:303:THR:HB	7:G:614:GLY:HA3	1.98	0.44
24:I:301:3PE:H241	24:I:301:3PE:H272	1.60	0.44
10:P:164:PHE:HE2	10:P:166:HIS:HB2	1.82	0.44
11:Q:77:VAL:HG21	11:Q:99:MET:CE	2.48	0.44
14:T:113:LEU:O	14:T:116:VAL:HB	2.17	0.44
21:q:6:VAL:HG13	34:q:201:CDL:CA2	2.47	0.44
2:B:117:PHE:HA	8:H:39:ILE:CG2	2.48	0.43
4:D:330:TYR:O	4:D:331:LEU:C	2.60	0.43
4:D:335:GLU:OE2	9:I:37:LYS:NZ	2.51	0.43
5:E:39:VAL:HG21	7:G:163:LYS:HZ1	1.83	0.43
5:E:60:LYS:O	5:E:61:ARG:C	2.57	0.43
5:E:176:LEU:HB2	5:E:184:MET:HE1	2.00	0.43
6:F:44:ASN:HB2	6:F:59:ARG:HD3	1.99	0.43
6:F:50:ASP:HB3	6:F:55:GLY:CA	2.47	0.43
6:F:102:MET:CE	6:F:111:LYS:HB3	2.48	0.43
6:F:149:MET:HG3	6:F:151:ALA:HB2	2.00	0.43
6:F:383:THR:N	6:F:384:PRO:CD	2.79	0.43
7:G:185:PHE:HE2	7:G:285:TRP:CD1	2.36	0.43
7:G:346:VAL:HG11	7:G:351:LEU:HD21	1.99	0.43
7:G:387:LEU:HD12	7:G:514:ASN:CB	2.45	0.43
8:H:85:LEU:CB	8:H:233:LEU:CD2	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:101:PHE:CE1	11:Q:124:MET:HE3	2.53	0.43
13:S:16:LEU:HD21	13:S:95:LEU:HG	2.00	0.43
13:S:20:ARG:HG3	13:S:54:LEU:CB	2.43	0.43
14:T:118:ILE:HD13	14:T:118:ILE:HA	1.83	0.43
21:q:55:PHE:CD1	22:r:26:LEU:CD2	2.96	0.43
1:A:105:GLU:OE2	1:A:110:GLY:HA3	2.18	0.43
2:B:105:MET:CE	27:D:501:UQ1:C1	2.96	0.43
6:F:174:ARG:NH2	6:F:175:GLU:HG2	2.32	0.43
6:F:431:ALA:O	6:F:434:PRO:HD2	2.18	0.43
7:G:82:ILE:HG22	7:G:100:TRP:HE3	1.83	0.43
7:G:185:PHE:HE2	7:G:285:TRP:NE1	2.16	0.43
7:G:466:LEU:HD13	7:G:500:ILE:CG1	2.48	0.43
8:H:85:LEU:HB2	8:H:233:LEU:CD2	2.47	0.43
10:P:140:ASP:O	10:P:141:PHE:C	2.61	0.43
10:P:170:LEU:O	10:P:171:ASN:CG	2.61	0.43
16:W:36:ARG:O	16:W:39:TYR:N	2.51	0.43
18:Z:97:ILE:HG13	18:Z:98:MET:N	2.30	0.43
1:A:63:LEU:O	1:A:64:LEU:C	2.61	0.43
1:A:106:TRP:CH2	8:H:295:PRO:HG2	2.53	0.43
2:B:114:MET:SD	2:B:121:PHE:HA	2.58	0.43
3:C:155:ILE:O	3:C:156:VAL:C	2.61	0.43
5:E:124:LYS:HB3	5:E:125:PRO:HD2	2.01	0.43
5:E:140:MET:HE1	6:F:366:ALA:HA	2.00	0.43
6:F:80:MET:CE	6:F:85:LEU:HD23	2.44	0.43
6:F:231:ALA:O	6:F:239:PRO:HA	2.18	0.43
6:F:320:GLY:HA3	6:F:324:THR:HG21	1.99	0.43
8:H:71:PHE:CE1	8:H:215:TYR:CE1	3.06	0.43
8:H:277:TYR:OH	9:I:66:LEU:HB3	2.17	0.43
10:P:269:ASN:ND2	10:P:271:TYR:OH	2.51	0.43
11:Q:59:LEU:O	11:Q:140:LYS:HA	2.18	0.43
15:V:19:THR:N	15:V:20:PRO:CD	2.81	0.43
21:q:7:LEU:CD2	34:q:201:CDL:H311	2.49	0.43
1:A:52:SER:O	1:A:55:PHE:N	2.51	0.43
4:D:194:ILE:HG23	4:D:271:ARG:NE	2.29	0.43
4:D:217:VAL:HG23	4:D:218:SER:N	2.31	0.43
4:D:256:ASP:OD1	4:D:338:ARG:NH2	2.42	0.43
7:G:281:ILE:HG23	7:G:602:ARG:NH1	2.32	0.43
7:G:364:ASP:OD1	7:G:364:ASP:O	2.37	0.43
7:G:462:PHE:CZ	7:G:466:LEU:HD21	2.54	0.43
8:H:113:VAL:CG2	8:H:136:VAL:HA	2.49	0.43
9:I:76:TYR:HA	9:I:79:ARG:HD2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:P:81:ILE:HD13	12:R:46:VAL:HG11	2.00	0.43
10:P:126:VAL:HG23	10:P:161:VAL:HG11	2.00	0.43
18:Z:53:TRP:CE2	18:Z:57:ARG:HD2	2.53	0.43
18:Z:68:ARG:HG3	18:Z:69:ILE:N	2.33	0.43
1:A:23:TRP:O	1:A:26:GLN:HG3	2.19	0.43
3:C:55:LYS:HE2	3:C:55:LYS:HB3	1.84	0.43
3:C:167:ARG:CZ	3:C:186:ILE:HG22	2.49	0.43
4:D:133:LEU:HB3	4:D:134:PRO:HD3	2.00	0.43
4:D:264:ASN:O	4:D:265:ASN:C	2.57	0.43
6:F:333:GLU:H	6:F:333:GLU:CD	2.25	0.43
8:H:85:LEU:HD23	8:H:105:ILE:HA	2.00	0.43
8:H:154:LEU:CD2	8:H:160:TYR:HA	2.49	0.43
8:H:220:PHE:O	8:H:224:PHE:HB2	2.19	0.43
10:P:197:GLU:HB3	10:P:259:VAL:HG22	1.99	0.43
16:W:57:ILE:HG23	16:W:107:MET:HE1	2.00	0.43
17:X:66:CYS:O	17:X:67:ALA:C	2.62	0.43
19:a:50:ARG:O	19:a:54:ILE:HG13	2.18	0.43
5:E:94:ILE:HD13	7:G:209:TYR:HE2	1.84	0.43
5:E:214:LYS:N	5:E:215:PRO:HD3	2.33	0.43
6:F:177:TYR:OH	6:F:194:ASP:OD1	2.23	0.43
8:H:125:SER:O	8:H:126:LYS:C	2.61	0.43
8:H:294:LEU:HB3	8:H:295:PRO:HD3	2.00	0.43
8:H:303:TRP:HB2	20:b:25:VAL:CG1	2.49	0.43
10:P:64:PHE:CE1	10:P:209:ARG:O	2.69	0.43
10:P:104:THR:HG22	10:P:106:LEU:HD12	2.00	0.43
10:P:169:HIS:CD2	10:P:181:LEU:HD11	2.49	0.43
14:T:92:LYS:O	14:T:92:LYS:HG2	2.16	0.43
15:V:56:LEU:CD1	15:V:57:ASP:OD1	2.67	0.43
17:X:35:GLN:HB2	17:X:70:PHE:CD1	2.54	0.43
19:a:37:ARG:H	19:a:59:ARG:NH2	2.17	0.43
1:A:49:LEU:CD2	4:D:80:MET:HE2	2.49	0.43
3:C:149:LEU:HD21	11:Q:59:LEU:HD22	2.00	0.43
3:C:180:HIS:CD2	3:C:182:ASP:H	2.37	0.43
4:D:141:TYR:O	4:D:222:MET:HE3	2.18	0.43
4:D:259:GLU:C	4:D:261:MET:N	2.75	0.43
7:G:349:GLU:HG3	7:G:646:LEU:HD11	2.00	0.43
26:H:402:PC1:H371	26:H:402:PC1:H342	1.85	0.43
14:T:93:ILE:HD11	14:T:118:ILE:HD11	2.00	0.43
17:X:50:GLU:OE1	17:X:55:ARG:HB3	2.18	0.43
17:X:52:ASP:HA	18:Z:116:TRP:CD1	2.54	0.43
20:b:42:ALA:HA	20:b:45:ILE:HG22	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:116:ARG:NH2	9:I:86:TYR:H	2.17	0.43
3:C:93:ILE:HD11	3:C:153:ASP:HB3	2.00	0.43
4:D:151:TYR:O	4:D:152:SER:C	2.59	0.43
4:D:184:ILE:HD12	4:D:210:MET:HE1	1.99	0.43
5:E:185:VAL:HG23	5:E:185:VAL:O	2.19	0.43
6:F:226:LYS:HD2	6:F:229:PHE:CD1	2.53	0.43
7:G:283:GLU:OE1	7:G:283:GLU:N	2.48	0.43
8:H:200:LEU:CD2	8:H:282:TYR:HB2	2.44	0.43
26:H:402:PC1:H342	26:H:402:PC1:H251	1.99	0.43
9:I:191:LEU:HD23	9:I:191:LEU:HA	1.91	0.43
10:P:76:MET:HE1	10:P:254:LYS:HE2	2.01	0.43
10:P:280:ILE:HG23	10:P:353:LEU:HD22	2.00	0.43
11:Q:99:MET:O	11:Q:99:MET:HG3	2.18	0.43
12:R:72:VAL:HG11	12:R:77:ILE:HG22	2.01	0.43
15:V:8:THR:HG22	15:V:9:THR:N	2.34	0.43
17:X:39:THR:HG23	17:X:40:ASN:N	2.33	0.43
18:Z:121:ILE:HD11	18:Z:136:ALA:HB3	1.98	0.43
22:r:113:LEU:HD12	22:r:113:LEU:HA	1.77	0.43
1:A:98:LEU:HD13	1:A:98:LEU:HA	1.86	0.43
4:D:326:CYS:CB	4:D:453:THR:HG21	2.49	0.43
5:E:88:GLN:HG3	5:E:89:ASN:CG	2.44	0.43
5:E:233:LEU:CD2	6:F:43:THR:HA	2.48	0.43
6:F:127:ASP:HB3	6:F:245:VAL:HG21	2.00	0.43
6:F:338:ASP:OD1	6:F:338:ASP:C	2.61	0.43
7:G:68:ARG:CD	7:G:285:TRP:CH2	3.02	0.43
7:G:651:PRO:HB3	13:S:58:CYS:HA	2.01	0.43
8:H:257:THR:O	8:H:260:MET:HB3	2.19	0.43
9:I:101:HIS:CE1	9:I:169:GLU:CD	2.97	0.43
9:I:152:CYS:SG	25:I:303:SF4:S3	3.17	0.43
9:I:162:CYS:SG	25:I:304:SF4:S2	3.17	0.43
10:P:306:GLY:HA2	10:P:312:PRO:HB3	2.01	0.43
10:P:310:PHE:O	10:P:311:GLU:C	2.59	0.43
12:R:72:VAL:HG11	12:R:77:ILE:CG2	2.49	0.43
15:V:36:LYS:HA	15:V:36:LYS:HD3	1.89	0.43
1:A:73:LEU:N	1:A:74:PRO:HD2	2.34	0.43
4:D:133:LEU:CD2	4:D:228:ARG:HG2	2.49	0.43
5:E:189:ASP:CG	6:F:163:TYR:HB3	2.44	0.43
6:F:113:LEU:O	6:F:154:ALA:HA	2.19	0.43
7:G:302:LEU:HB3	7:G:585:PRO:HB3	2.01	0.43
7:G:356:ASP:O	7:G:360:LYS:HG3	2.18	0.43
7:G:597:VAL:HG12	7:G:603:ALA:CB	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:35:THR:HG22	22:r:107:SER:HA	1.97	0.43
10:P:153:ALA:HB2	10:P:191:VAL:HG23	2.01	0.43
13:S:75:LYS:HE2	13:S:75:LYS:HA	2.01	0.43
16:W:25:SER:OG	16:W:34:ARG:NH2	2.52	0.43
19:a:17:VAL:O	19:a:18:ILE:C	2.62	0.43
20:b:82:LYS:HB3	20:b:82:LYS:HE2	1.81	0.43
2:B:82:ILE:CG1	8:H:57:MET:CE	2.83	0.42
5:E:43:THR:CG2	5:E:46:ASN:HB3	2.49	0.42
5:E:109:MET:O	5:E:110:ARG:C	2.62	0.42
7:G:69:LEU:HD23	7:G:69:LEU:HA	1.84	0.42
7:G:292:PHE:HB3	7:G:706:THR:HG21	2.01	0.42
7:G:422:TRP:HZ2	7:G:441:ARG:HB3	1.82	0.42
8:H:1:MET:O	8:H:4:ILE:N	2.52	0.42
8:H:33:LEU:HD21	22:r:25:GLN:HG2	2.01	0.42
10:P:259:VAL:N	10:P:261:LYS:HG2	2.33	0.42
10:P:358:THR:O	10:P:362:LEU:HG	2.19	0.42
18:Z:62:ILE:CG1	20:b:49:THR:HG22	2.48	0.42
18:Z:129:THR:O	18:Z:130:LYS:C	2.62	0.42
20:b:53:TYR:HA	20:b:54:PRO:HD3	1.92	0.42
21:q:21:ARG:HD2	21:q:21:ARG:HA	1.80	0.42
21:q:138:VAL:O	21:q:139:PRO:C	2.62	0.42
3:C:78:SER:C	3:C:80:LEU:N	2.76	0.42
3:C:213:ASP:O	3:C:214:GLU:C	2.61	0.42
4:D:279:THR:HA	15:V:12:VAL:CG1	2.49	0.42
5:E:109:MET:HE2	7:G:196:GLY:CA	2.49	0.42
6:F:126:LYS:HG3	6:F:275:LEU:HD22	2.01	0.42
6:F:143:LEU:HD12	6:F:191:TYR:HE2	1.84	0.42
7:G:281:ILE:HD12	7:G:282:ASN:N	2.33	0.42
7:G:545:LEU:CD2	7:G:555:ILE:HD11	2.49	0.42
9:I:104:ARG:HD2	9:I:201:ILE:HG21	2.01	0.42
10:P:235:THR:HG21	10:P:323:HIS:CD2	2.55	0.42
11:Q:64:LEU:HD12	16:W:85:LEU:HD21	2.01	0.42
13:S:58:CYS:SG	13:S:59:SER:N	2.92	0.42
14:T:113:LEU:HD22	16:W:71:MET:HE2	2.01	0.42
15:V:37:HIS:O	15:V:38:PHE:C	2.63	0.42
16:W:83:ASP:O	16:W:86:VAL:CG2	2.66	0.42
17:X:26:LYS:HD3	17:X:95:GLN:OE1	2.19	0.42
19:a:4:GLU:C	19:a:7:PRO:HD2	2.44	0.42
20:b:6:SER:OG	20:b:10:LYS:HD2	2.18	0.42
1:A:99:SER:HB3	24:b:201:3PE:C38	2.49	0.42
2:B:105:MET:CE	27:D:501:UQ1:O1	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:78:VAL:O	5:E:82:LEU:HB2	2.20	0.42
6:F:296:LEU:O	6:F:299:LEU:HG	2.19	0.42
7:G:117:MET:SD	7:G:143:SER:HB2	2.59	0.42
7:G:283:GLU:CG	7:G:285:TRP:HZ3	2.26	0.42
7:G:329:MET:HG3	7:G:565:PHE:CZ	2.54	0.42
7:G:567:VAL:HG23	7:G:567:VAL:O	2.19	0.42
8:H:8:THR:O	8:H:9:LEU:CB	2.67	0.42
8:H:17:MET:HE1	8:H:225:MET:HE3	2.01	0.42
8:H:39:ILE:HG13	21:q:31:ASN:ND2	2.35	0.42
8:H:97:ASN:OD1	8:H:97:ASN:C	2.61	0.42
8:H:182:ALA:O	8:H:183:MET:C	2.60	0.42
9:I:76:TYR:CD1	9:I:79:ARG:HD2	2.54	0.42
10:P:316:LYS:O	10:P:320:GLU:HG2	2.19	0.42
15:V:35:LEU:HA	15:V:38:PHE:CE1	2.54	0.42
20:b:5:ILE:HD12	20:b:6:SER:N	2.34	0.42
1:A:81:THR:O	20:b:46:ASN:ND2	2.52	0.42
2:B:114:MET:O	2:B:115:ASP:C	2.62	0.42
5:E:65:ILE:HG21	5:E:80:PRO:HB2	2.01	0.42
5:E:70:PRO:HG2	6:F:236:PHE:CD2	2.54	0.42
5:E:179:CYS:C	5:E:181:ASN:N	2.78	0.42
5:E:200:ILE:O	5:E:201:GLU:C	2.61	0.42
6:F:291:GLU:OE2	6:F:292:MET:N	2.53	0.42
7:G:83:GLU:C	7:G:84:LYS:HG2	2.44	0.42
7:G:639:LEU:HD23	7:G:643:ARG:HG2	2.01	0.42
7:G:651:PRO:O	7:G:652:ASN:C	2.62	0.42
8:H:1:MET:HG3	19:a:30:THR:HG21	1.98	0.42
8:H:75:PRO:HA	8:H:223:PHE:CE1	2.55	0.42
9:I:78:PHE:HB3	22:r:8:ILE:HG22	1.99	0.42
10:P:183:SER:O	10:P:184:LYS:C	2.63	0.42
10:P:376:ASN:O	10:P:377:TYR:C	2.61	0.42
13:S:16:LEU:CB	13:S:69:TYR:CD1	2.97	0.42
16:W:42:TRP:CE2	16:W:93:LEU:HB2	2.54	0.42
16:W:78:ASP:HA	16:W:79:PRO:HD3	1.94	0.42
1:A:60:ILE:O	1:A:61:THR:C	2.62	0.42
1:A:73:LEU:O	1:A:76:PRO:HD2	2.18	0.42
5:E:104:LEU:O	5:E:105:GLN:C	2.62	0.42
6:F:50:ASP:O	6:F:55:GLY:HA3	2.19	0.42
6:F:314:LEU:HD11	6:F:317:VAL:HG23	2.02	0.42
7:G:404:GLY:CA	7:G:684:LEU:HD11	2.44	0.42
7:G:445:LEU:CD2	7:G:460:HIS:HE1	2.27	0.42
7:G:527:ASP:OD2	7:G:650:SER:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:592:LYS:N	7:G:608:VAL:HG12	2.34	0.42
10:P:300:TRP:NE1	10:P:304:LEU:HD21	2.35	0.42
13:S:64:LYS:HE2	13:S:66:TRP:CZ2	2.55	0.42
16:W:38:LEU:O	16:W:39:TYR:C	2.62	0.42
17:X:10:LEU:HD12	17:X:13:LEU:HD12	2.01	0.42
17:X:130:LYS:HG2	20:b:67:PRO:CA	2.50	0.42
17:X:130:LYS:HG2	20:b:67:PRO:HA	2.02	0.42
20:b:31:ILE:HG23	20:b:32:MET:N	2.34	0.42
1:A:7:ILE:O	1:A:10:ASN:HB2	2.19	0.42
6:F:257:ARG:CG	6:F:261:TRP:CG	3.03	0.42
6:F:296:LEU:HD22	6:F:337:MET:HE1	2.01	0.42
7:G:613:PRO:O	7:G:616:ALA:HB3	2.19	0.42
8:H:24:GLU:CA	8:H:271:LEU:CD2	2.88	0.42
10:P:81:ILE:HD11	12:R:46:VAL:HG11	2.00	0.42
10:P:207:PHE:O	10:P:241:TYR:HA	2.20	0.42
10:P:220:TYR:CG	10:P:226:VAL:HG13	2.55	0.42
11:Q:59:LEU:HD23	11:Q:59:LEU:HA	1.84	0.42
13:S:19:ILE:O	13:S:53:ILE:HD12	2.20	0.42
14:T:87:LEU:CD2	14:T:122:MET:CE	2.97	0.42
14:T:90:TYR:CD2	14:T:92:LYS:HB3	2.54	0.42
14:T:109:GLY:O	14:T:110:LEU:C	2.61	0.42
15:V:32:LEU:HD23	15:V:32:LEU:HA	1.90	0.42
17:X:132:LYS:HB3	17:X:132:LYS:HE2	1.84	0.42
18:Z:64:ASP:OD1	18:Z:65:LEU:N	2.52	0.42
18:Z:120:LEU:HD12	18:Z:121:ILE:H	1.85	0.42
20:b:69:HIS:HD2	20:b:70:PRO:CD	2.26	0.42
7:G:414:PHE:CE2	7:G:516:LEU:CD2	3.03	0.42
8:H:221:ALA:O	8:H:224:PHE:HB3	2.20	0.42
10:P:242:VAL:HG13	10:P:243:ALA:N	2.35	0.42
10:P:283:MET:HE3	10:P:357:ARG:HH11	1.85	0.42
13:S:16:LEU:HD13	13:S:19:ILE:HD11	2.02	0.42
18:Z:94:GLU:HA	18:Z:97:ILE:HD11	2.01	0.42
18:Z:108:GLU:O	18:Z:109:SER:C	2.61	0.42
21:q:74:PHE:HE2	21:q:75:TRP:HE1	1.68	0.42
1:A:73:LEU:O	8:H:160:TYR:OH	2.30	0.42
3:C:102:HIS:CE1	15:V:44:TYR:HE1	2.37	0.42
4:D:368:ARG:NH2	9:I:165:ASP:HB2	2.35	0.42
5:E:173:VAL:HG22	5:E:174:GLU:H	1.84	0.42
5:E:196:THR:O	5:E:199:ASP:HB2	2.19	0.42
6:F:80:MET:HE2	6:F:95:THR:CG2	2.50	0.42
6:F:261:TRP:CE2	6:F:265:PHE:CZ	3.08	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:297:LYS:HB2	6:F:333:GLU:HB3	2.00	0.42
7:G:643:ARG:HA	7:G:646:LEU:HD12	2.02	0.42
8:H:196:ALA:HB2	8:H:274:ARG:CG	2.42	0.42
10:P:172:ALA:H	10:P:202:ARG:HH21	1.67	0.42
11:Q:85:ASN:C	11:Q:87:MET:N	2.76	0.42
17:X:38:LYS:O	17:X:42:GLU:HG3	2.20	0.42
21:q:13:GLN:HE22	34:q:201:CDL:CA3	2.28	0.42
21:q:39:VAL:HG21	21:q:89:TRP:CZ2	2.55	0.42
22:r:18:GLN:OE1	22:r:18:GLN:N	2.53	0.42
1:A:20:VAL:O	1:A:21:ALA:C	2.63	0.42
2:B:81:LEU:CD2	26:B:302:PC1:H352	2.48	0.42
2:B:194:CYS:O	2:B:196:PRO:HD3	2.20	0.42
2:B:223:ARG:HG2	2:B:223:ARG:O	2.20	0.42
4:D:339:GLN:HE21	9:I:37:LYS:HZ2	1.67	0.42
5:E:58:ASN:HB3	5:E:84:LEU:HD21	2.01	0.42
6:F:199:ARG:HD3	23:s:80:PHE:CZ	2.48	0.42
6:F:383:THR:CG2	7:G:120:LEU:CD2	2.95	0.42
7:G:462:PHE:HA	7:G:465:VAL:HG23	2.02	0.42
8:H:42:PRO:HD2	8:H:45:ILE:HD11	2.02	0.42
8:H:179:TRP:CE3	8:H:183:MET:HE3	2.55	0.42
10:P:279:TYR:O	10:P:280:ILE:C	2.62	0.42
11:Q:58:LYS:O	11:Q:58:LYS:HG3	2.20	0.42
14:T:132:ASP:O	16:W:40:ARG:NH2	2.53	0.42
16:W:55:LEU:HB3	16:W:57:ILE:HG12	2.01	0.42
17:X:127:LYS:HB2	20:b:76:PRO:HD2	2.02	0.42
20:b:32:MET:N	20:b:33:PRO:CD	2.82	0.42
2:B:202:LEU:HD13	2:B:202:LEU:O	2.19	0.42
3:C:241:PHE:O	3:C:242:PRO:C	2.62	0.42
4:D:154:ALA:HB2	4:D:398:THR:HG21	2.01	0.42
4:D:198:THR:N	4:D:199:PRO:CD	2.83	0.42
4:D:320:ILE:HG22	4:D:321:GLY:N	2.33	0.42
6:F:44:ASN:HA	6:F:49:HIS:ND1	2.35	0.42
6:F:329:LYS:HE3	6:F:359:ARG:NH1	2.28	0.42
6:F:364:VAL:HA	6:F:438:LEU:HD11	2.01	0.42
7:G:83:GLU:O	7:G:84:LYS:C	2.63	0.42
7:G:155:GLU:CD	7:G:155:GLU:N	2.78	0.42
7:G:189:ILE:HG21	7:G:285:TRP:CE2	2.55	0.42
7:G:537:ILE:HG23	7:G:542:PRO:HD3	2.02	0.42
8:H:12:PRO:O	19:a:15:CYS:HB3	2.20	0.42
8:H:66:THR:O	8:H:67:SER:C	2.59	0.42
8:H:84:SER:O	8:H:87:VAL:HG23	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:121:TRP:HA	8:H:129:LEU:HD13	2.01	0.42
9:I:122:ILE:HG13	9:I:122:ILE:O	2.19	0.42
10:P:156:SER:O	10:P:160:GLY:N	2.45	0.42
10:P:177:SER:O	10:P:182:ARG:NH2	2.53	0.42
14:T:123:GLU:HG2	14:T:130:ILE:HD12	2.02	0.42
16:W:93:LEU:HD23	16:W:93:LEU:C	2.45	0.42
19:a:34:LYS:O	19:a:35:GLU:C	2.63	0.42
20:b:59:ASP:HA	20:b:63:MET:CE	2.50	0.42
21:q:5:GLU:HG2	21:q:9:ARG:HE	1.85	0.42
1:A:99:SER:HB3	24:b:201:3PE:C39	2.48	0.41
1:A:102:LEU:HD23	24:b:201:3PE:H371	2.02	0.41
2:B:68:ARG:NH1	2:B:73:TYR:CD1	2.88	0.41
2:B:170:TYR:CG	4:D:135:TYR:CE1	3.08	0.41
4:D:264:ASN:O	9:I:65:GLU:OE1	2.38	0.41
6:F:267:ARG:N	6:F:270:ASN:O	2.52	0.41
6:F:295:PRO:HB2	6:F:298:GLU:HB2	2.01	0.41
7:G:213:MET:HE2	7:G:215:MET:CG	2.50	0.41
7:G:249:GLU:HG2	7:G:262:VAL:HG22	2.01	0.41
7:G:404:GLY:HA2	7:G:684:LEU:HD11	2.00	0.41
8:H:193:THR:O	8:H:194:ASN:C	2.61	0.41
9:I:76:TYR:C	9:I:78:PHE:N	2.74	0.41
10:P:140:ASP:O	10:P:143:ASP:N	2.51	0.41
10:P:179:LYS:O	10:P:180:SER:C	2.63	0.41
10:P:284:THR:HG22	10:P:286:ARG:HG3	2.02	0.41
12:R:72:VAL:HG12	12:R:73:GLU:H	1.85	0.41
18:Z:72:MET:N	18:Z:73:PRO:CD	2.83	0.41
18:Z:79:LYS:HE2	18:Z:79:LYS:HB3	1.82	0.41
18:Z:91:LEU:HD13	18:Z:91:LEU:C	2.45	0.41
20:b:31:ILE:O	20:b:32:MET:C	2.63	0.41
2:B:111:ARG:NH1	4:D:212:GLU:OE2	2.53	0.41
4:D:144:MET:HG2	4:D:223:HIS:H	1.85	0.41
4:D:181:LEU:HD21	4:D:210:MET:HB2	2.02	0.41
4:D:208:GLU:OE1	4:D:221:ARG:NH2	2.51	0.41
5:E:134:CYS:SG	5:E:175:CYS:HA	2.60	0.41
6:F:315:LEU:O	6:F:315:LEU:HD23	2.20	0.41
6:F:391:TRP:O	6:F:395:VAL:HG23	2.20	0.41
7:G:36:VAL:O	7:G:37:ASP:C	2.63	0.41
7:G:272:ARG:HH11	7:G:274:LEU:CD2	2.33	0.41
7:G:314:LEU:HD23	7:G:583:ILE:CG1	2.50	0.41
7:G:408:ARG:HD3	7:G:409:PHE:CZ	2.54	0.41
8:H:68:MET:O	8:H:69:SER:C	2.62	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:239:THR:HG23	8:H:262:GLU:HB2	2.02	0.41
8:H:306:SER:O	8:H:310:PHE:CE2	2.73	0.41
9:I:152:CYS:SG	25:I:303:SF4:S1	3.17	0.41
10:P:231:LEU:CD1	10:P:290:PRO:HB2	2.49	0.41
10:P:255:ASP:OD1	10:P:256:PRO:HD2	2.21	0.41
11:Q:75:ARG:NH1	11:Q:104:ARG:HG2	2.34	0.41
11:Q:104:ARG:HA	11:Q:104:ARG:HD3	1.88	0.41
14:T:80:LYS:O	14:T:84:LEU:HG	2.20	0.41
1:A:56:PHE:CZ	1:A:60:ILE:HD11	2.55	0.41
2:B:68:ARG:HG2	2:B:69:SER:N	2.35	0.41
2:B:194:CYS:SG	4:D:138:ARG:NE	2.91	0.41
5:E:136:THR:HG21	6:F:122:PRO:HG3	2.01	0.41
5:E:180:VAL:HG13	5:E:181:ASN:N	2.34	0.41
5:E:181:ASN:HB3	5:E:193:GLU:HB2	2.01	0.41
5:E:225:GLU:O	5:E:226:PRO:C	2.60	0.41
6:F:131:MET:HE3	6:F:131:MET:HB2	1.91	0.41
6:F:225:LEU:HD22	7:G:93:ALA:CB	2.51	0.41
6:F:413:TRP:CH2	6:F:436:GLN:HG2	2.56	0.41
7:G:224:ASP:OD2	7:G:291:ARG:NH2	2.50	0.41
7:G:253:VAL:CG1	7:G:253:VAL:O	2.68	0.41
7:G:354:LEU:HB2	7:G:623:ILE:HD13	2.03	0.41
8:H:16:ALA:HB2	19:a:15:CYS:CB	2.50	0.41
8:H:135:ALA:O	8:H:138:GLN:HG2	2.19	0.41
8:H:172:MET:HE3	8:H:176:LEU:CB	2.47	0.41
9:I:92:PRO:HB3	21:q:92:CYS:HB2	2.01	0.41
10:P:228:LEU:HD11	10:P:288:PHE:CZ	2.54	0.41
10:P:230:SER:O	10:P:231:LEU:C	2.63	0.41
10:P:265:PHE:N	10:P:265:PHE:CD1	2.87	0.41
16:W:76:VAL:HG13	16:W:82:VAL:HG22	2.02	0.41
21:q:56:PHE:HD2	22:r:27:ARG:HH22	1.68	0.41
22:r:24:LEU:HD23	22:r:24:LEU:HA	1.85	0.41
1:A:24:LEU:HD13	1:A:24:LEU:O	2.20	0.41
5:E:167:LEU:HD23	5:E:168:PHE:HE1	1.86	0.41
5:E:241:GLY:HA3	6:F:63:TYR:CZ	2.56	0.41
6:F:391:TRP:HH2	7:G:118:GLU:OE2	2.02	0.41
7:G:50:LEU:HD22	7:G:65:TYR:CE2	2.55	0.41
7:G:319:TRP:O	7:G:320:GLU:C	2.63	0.41
7:G:319:TRP:HZ3	7:G:584:LEU:HD22	1.86	0.41
8:H:251:LEU:HD21	8:H:254:LEU:HD11	2.03	0.41
16:W:44:ARG:O	16:W:47:PRO:HG2	2.20	0.41
20:b:45:ILE:HG23	20:b:46:ASN:N	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:b:78:LEU:O	20:b:81:LEU:N	2.53	0.41
21:q:6:VAL:O	34:q:201:CDL:HA62	2.20	0.41
22:r:12:ARG:HH21	22:r:20:LEU:CD1	2.33	0.41
1:A:93:ILE:HD13	1:A:93:ILE:HA	1.90	0.41
2:B:100:CYS:SG	25:B:301:SF4:S3	3.19	0.41
2:B:147:LYS:HD2	2:B:147:LYS:HA	1.75	0.41
3:C:152:ILE:HG22	3:C:153:ASP:N	2.35	0.41
4:D:140:ASP:O	4:D:147:ASN:ND2	2.53	0.41
5:E:45:GLU:HB3	5:E:91:TRP:CH2	2.55	0.41
5:E:108:PRO:O	5:E:109:MET:C	2.63	0.41
7:G:160:VAL:CG1	7:G:161:GLU:N	2.84	0.41
7:G:517:HIS:CD2	7:G:523:VAL:CG2	3.03	0.41
7:G:524:ALA:HB2	7:G:597:VAL:HG22	2.01	0.41
7:G:639:LEU:O	7:G:639:LEU:HD23	2.21	0.41
8:H:23:VAL:HG11	19:a:9:LEU:CD2	2.50	0.41
8:H:225:MET:SD	30:H:401:UQ9:H20B	2.61	0.41
26:I:302:PC1:H122	18:Z:35:MET:HE1	2.01	0.41
10:P:214:LEU:HD23	10:P:352:VAL:HG12	2.01	0.41
13:S:21:VAL:HG23	13:S:91:MET:HE1	2.02	0.41
20:b:61:GLY:O	20:b:63:MET:HG3	2.20	0.41
3:C:229:PHE:O	11:Q:123:ASN:ND2	2.54	0.41
4:D:82:LEU:HB2	4:D:99:LEU:HD12	2.03	0.41
4:D:101:LEU:HD11	4:D:106:VAL:CG2	2.39	0.41
4:D:151:TYR:O	4:D:155:VAL:HG23	2.20	0.41
4:D:188:THR:HG21	4:D:203:MET:HB2	2.02	0.41
4:D:280:ALA:CB	15:V:11:LEU:CG	2.95	0.41
4:D:423:LYS:HD3	4:D:424:ILE:N	2.35	0.41
5:E:142:ARG:HB3	5:E:182:ALA:HB3	2.03	0.41
5:E:193:GLU:HG3	5:E:217:PRO:HG3	2.02	0.41
6:F:70:LEU:O	6:F:71:LYS:C	2.62	0.41
6:F:300:ILE:HD13	6:F:307:VAL:CG2	2.51	0.41
6:F:313:ASN:O	6:F:358:ASP:HA	2.20	0.41
7:G:64:CYS:H	7:G:181:ARG:NE	2.18	0.41
7:G:282:ASN:O	7:G:282:ASN:CG	2.63	0.41
7:G:541:PRO:HB2	7:G:561:PRO:CD	2.51	0.41
8:H:10:LEU:HD23	8:H:10:LEU:HA	1.89	0.41
8:H:99:ASN:OD1	19:a:40:ARG:HG3	2.21	0.41
8:H:296:LEU:CD1	8:H:300:LEU:HD11	2.50	0.41
11:Q:52:LEU:HD23	16:W:19:SER:O	2.20	0.41
21:q:87:HIS:O	21:q:91:HIS:HD2	2.04	0.41
2:B:191:VAL:HG12	2:B:196:PRO:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:ARG:HG3	10:P:85:ARG:HH12	1.84	0.41
4:D:121:GLU:HG2	4:D:424:ILE:HD12	2.03	0.41
5:E:48:PRO:HD3	5:E:94:ILE:CG2	2.51	0.41
5:E:78:VAL:CA	5:E:104:LEU:HD13	2.46	0.41
5:E:145:ASP:OD1	5:E:145:ASP:N	2.54	0.41
6:F:65:THR:O	6:F:69:LEU:HG	2.21	0.41
6:F:391:TRP:CE2	7:G:153:PHE:HD1	2.39	0.41
8:H:100:LEU:HD13	8:H:103:LEU:HD12	2.02	0.41
8:H:174:LEU:HD23	8:H:174:LEU:HA	1.80	0.41
9:I:149:MET:HE2	9:I:185:TYR:CD2	2.56	0.41
10:P:75:ARG:HH21	16:W:113:THR:HG23	1.86	0.41
12:R:42:ASP:C	12:R:43:TYR:O	2.61	0.41
15:V:98:LYS:HG2	15:V:100:TRP:CZ2	2.55	0.41
16:W:45:GLU:O	16:W:46:VAL:C	2.62	0.41
17:X:70:PHE:CE1	17:X:117:TRP:CZ3	3.08	0.41
17:X:112:LEU:HD13	17:X:118:VAL:HG22	2.03	0.41
18:Z:19:ILE:HG22	18:Z:20:ASP:N	2.36	0.41
21:q:50:GLU:HA	21:q:59:HIS:O	2.20	0.41
1:A:52:SER:O	1:A:55:PHE:HB2	2.21	0.41
1:A:60:ILE:HD13	1:A:60:ILE:HA	1.83	0.41
1:A:111:LEU:HD13	8:H:290:TRP:HB3	2.02	0.41
2:B:137:LEU:HD11	2:B:142:ALA:HA	2.03	0.41
3:C:77:VAL:HG22	3:C:83:LEU:HD13	2.03	0.41
4:D:99:LEU:O	4:D:99:LEU:HD12	2.21	0.41
4:D:189:THR:OG1	27:D:501:UQ1:HM32	2.21	0.41
4:D:198:THR:OG1	4:D:261:MET:SD	2.78	0.41
5:E:190:ASN:O	5:E:191:TYR:C	2.63	0.41
5:E:200:ILE:O	5:E:204:ILE:HG13	2.21	0.41
5:E:223:CYS:CB	6:F:133:HIS:CE1	3.04	0.41
6:F:88:ARG:HA	6:F:88:ARG:HD3	1.85	0.41
6:F:280:GLY:O	6:F:356:VAL:HB	2.20	0.41
7:G:50:LEU:HD11	7:G:62:ARG:HD3	2.02	0.41
7:G:373:PRO:CG	7:G:481:LEU:HD22	2.47	0.41
8:H:71:PHE:CD1	8:H:215:TYR:CZ	3.09	0.41
8:H:283:ASP:OD1	8:H:283:ASP:C	2.63	0.41
8:H:317:TYR:CZ	19:a:40:ARG:NH1	2.79	0.41
9:I:54:THR:HG21	18:Z:33:TYR:CE2	2.56	0.41
10:P:243:ALA:O	10:P:244:ASP:C	2.63	0.41
11:Q:111:LEU:HD11	21:q:126:PRO:HG2	2.03	0.41
12:R:48:PHE:CE2	12:R:53:LYS:HB2	2.56	0.41
14:T:134:ASP:HA	14:T:137:LYS:NZ	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:X:38:LYS:HD2	17:X:131:VAL:HG12	2.02	0.41
18:Z:59:ARG:HH21	20:b:84:LEU:H	1.68	0.41
1:A:61:THR:O	1:A:62:PHE:C	2.64	0.41
2:B:81:LEU:HD23	2:B:81:LEU:HA	1.88	0.41
2:B:84:TRP:CZ3	26:B:302:PC1:H351	2.56	0.41
2:B:117:PHE:CD2	2:B:206:LEU:HD21	2.55	0.41
2:B:145:LEU:O	2:B:146:ARG:C	2.64	0.41
2:B:170:TYR:CD1	4:D:135:TYR:CE1	3.09	0.41
2:B:173:TYR:HE2	9:I:126:GLN:HB2	1.84	0.41
2:B:181:CYS:C	2:B:183:ARG:H	2.27	0.41
2:B:210:ARG:NE	21:q:78:ASP:OD1	2.53	0.41
3:C:107:PHE:CD1	3:C:133:SER:HB3	2.56	0.41
4:D:141:TYR:CZ	4:D:457:VAL:HG13	2.56	0.41
4:D:240:LEU:O	4:D:241:LEU:C	2.62	0.41
4:D:242:ASP:O	4:D:245:TYR:HB3	2.20	0.41
4:D:323:ARG:HG2	4:D:323:ARG:O	2.20	0.41
5:E:67:LYS:O	5:E:68:ASN:C	2.64	0.41
5:E:129:TYR:HE2	5:E:167:LEU:HG	1.86	0.41
6:F:45:LEU:O	6:F:46:TYR:HB2	2.21	0.41
6:F:113:LEU:HD13	6:F:149:MET:SD	2.60	0.41
6:F:217:GLU:OE2	6:F:224:ARG:NH2	2.53	0.41
6:F:296:LEU:HD22	6:F:337:MET:HE3	2.01	0.41
7:G:50:LEU:O	7:G:54:GLU:HG2	2.21	0.41
7:G:213:MET:CE	7:G:215:MET:HB2	2.29	0.41
7:G:217:GLU:C	7:G:219:SER:N	2.79	0.41
7:G:528:LEU:CD2	7:G:649:VAL:HG21	2.50	0.41
8:H:251:LEU:HD11	8:H:254:LEU:HB2	2.02	0.41
8:H:296:LEU:CD2	24:I:301:3PE:H351	2.50	0.41
9:I:149:MET:HB3	9:I:154:TYR:OH	2.20	0.41
9:I:162:CYS:HB3	9:I:165:ASP:HA	2.02	0.41
10:P:143:ASP:OD1	10:P:147:ASN:ND2	2.54	0.41
10:P:293:LEU:HD12	10:P:294:PRO:HD2	2.01	0.41
12:R:38:TYR:HE2	12:R:44:ARG:NE	2.19	0.41
12:R:55:VAL:HG22	12:R:56:ASN:N	2.35	0.41
12:R:60:ALA:O	12:R:61:ILE:C	2.63	0.41
14:T:82:ARG:O	14:T:86:VAL:HG23	2.20	0.41
14:T:99:SER:HB2	14:T:102:SER:HB2	2.03	0.41
14:T:107:ASP:OD1	14:T:108:LEU:N	2.54	0.41
14:T:120:MET:O	14:T:121:ALA:C	2.63	0.41
16:W:24:PHE:HB2	16:W:83:ASP:OD2	2.20	0.41
18:Z:99:LYS:HB2	18:Z:99:LYS:HE3	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:Z:140:PHE:C	18:Z:142:TRP:N	2.77	0.41
19:a:12:MET:HE2	19:a:12:MET:HB3	1.90	0.41
20:b:7:ALA:C	20:b:9:LEU:H	2.27	0.41
3:C:71:TYR:O	3:C:87:ILE:HA	2.21	0.41
5:E:238:LYS:HB3	5:E:242:PHE:CG	2.56	0.41
6:F:306:GLY:O	6:F:307:VAL:C	2.64	0.41
6:F:412:LEU:HD12	6:F:412:LEU:HA	1.85	0.41
7:G:74:ASN:ND2	7:G:180:THR:OG1	2.54	0.41
7:G:466:LEU:O	7:G:467:LYS:C	2.64	0.41
7:G:517:HIS:CD2	7:G:599:THR:HG22	2.56	0.41
8:H:27:ILE:CG2	8:H:31:MET:HE3	2.43	0.41
10:P:132:ARG:HD3	10:P:132:ARG:HA	1.92	0.41
17:X:26:LYS:HE2	17:X:26:LYS:HB3	1.85	0.41
19:a:45:TRP:NE1	19:a:49:GLU:HG3	2.36	0.41
4:D:85:GLY:O	4:D:89:PRO:HB3	2.21	0.40
4:D:139:LEU:HD13	4:D:424:ILE:HG12	2.02	0.40
5:E:86:GLN:NE2	5:E:121:TYR:HA	2.36	0.40
6:F:47:GLY:O	6:F:48:ARG:HB2	2.21	0.40
7:G:185:PHE:CD2	7:G:189:ILE:HB	2.56	0.40
7:G:396:GLU:O	7:G:396:GLU:HG2	2.21	0.40
8:H:28:LEU:CD1	8:H:274:ARG:HH11	2.34	0.40
8:H:306:SER:CB	8:H:310:PHE:HE2	2.34	0.40
10:P:96:LEU:HD12	10:P:97:MET:CA	2.51	0.40
12:R:64:ILE:HD12	12:R:64:ILE:HA	1.95	0.40
17:X:23:ALA:HB2	17:X:95:GLN:HE22	1.82	0.40
1:A:3:LEU:CA	8:H:96:ILE:HD13	2.45	0.40
1:A:108:GLN:CG	1:A:109:LYS:N	2.80	0.40
3:C:92:VAL:HG21	3:C:152:ILE:CG2	2.51	0.40
3:C:160:ILE:HG13	4:D:285:ASN:ND2	2.36	0.40
4:D:176:GLU:OE2	4:D:179:ARG:NH1	2.54	0.40
4:D:190:HIS:O	4:D:194:ILE:HG12	2.20	0.40
4:D:299:GLN:OE1	22:r:104:TRP:HB2	2.20	0.40
4:D:310:VAL:C	4:D:312:ASP:H	2.29	0.40
7:G:64:CYS:SG	7:G:75:CYS:CB	3.09	0.40
8:H:82:ALA:HA	8:H:85:LEU:HD12	2.02	0.40
8:H:153:VAL:HG11	8:H:241:ILE:HG23	2.03	0.40
8:H:264:LEU:HD21	19:a:12:MET:HE2	2.03	0.40
9:I:94:SER:HB2	9:I:95:PRO:CD	2.34	0.40
10:P:180:SER:HB2	10:P:321:ARG:HH21	1.87	0.40
21:q:89:TRP:HB2	21:q:98:PRO:HD3	2.03	0.40
1:A:16:THR:O	1:A:20:VAL:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:201:PHE:HB2	8:H:32:GLN:HB3	2.04	0.40
6:F:205:ILE:O	6:F:206:CYS:C	2.63	0.40
6:F:257:ARG:HG2	6:F:261:TRP:CE3	2.55	0.40
6:F:322:SER:HB2	6:F:370:LEU:HD22	2.02	0.40
7:G:314:LEU:HD23	7:G:583:ILE:HG13	2.02	0.40
10:P:181:LEU:CD1	10:P:321:ARG:HE	2.35	0.40
18:Z:10:MET:HE2	18:Z:10:MET:HB3	1.72	0.40
19:a:41:VAL:O	19:a:42:GLN:C	2.64	0.40
3:C:240:ALA:O	3:C:241:PHE:C	2.62	0.40
5:E:109:MET:HE2	7:G:196:GLY:HA3	2.04	0.40
6:F:257:ARG:CG	6:F:261:TRP:CD2	2.93	0.40
7:G:49:VAL:HG13	7:G:102:ILE:HG12	2.03	0.40
8:H:114:TYR:O	8:H:117:LEU:N	2.55	0.40
8:H:303:TRP:HZ3	20:b:28:LEU:HG	1.85	0.40
10:P:56:ALA:HA	10:P:125:VAL:O	2.20	0.40
10:P:96:LEU:C	10:P:96:LEU:CD1	2.94	0.40
14:T:140:CYS:HB2	14:T:143:GLU:HB2	2.02	0.40
16:W:48:ASN:O	16:W:52:LEU:HG	2.22	0.40
17:X:117:TRP:CD1	17:X:117:TRP:N	2.87	0.40
20:b:49:THR:HA	20:b:50:PRO:HD3	1.89	0.40
1:A:62:PHE:HD1	8:H:144:VAL:CG2	2.35	0.40
1:A:75:LEU:HD23	1:A:75:LEU:HA	1.86	0.40
2:B:76:THR:O	2:B:77:LYS:C	2.62	0.40
3:C:243:ALA:C	7:G:105:ASN:ND2	2.79	0.40
4:D:181:LEU:HD21	4:D:210:MET:CB	2.51	0.40
4:D:265:ASN:C	4:D:267:ILE:H	2.29	0.40
6:F:402:GLY:HA2	6:F:450:MET:HE2	2.04	0.40
7:G:173:MET:HE1	7:G:206:VAL:O	2.22	0.40
7:G:355:LYS:HB2	7:G:366:LEU:CD2	2.52	0.40
8:H:119:SER:OG	8:H:211:PHE:HB2	2.21	0.40
24:I:301:3PE:H392	20:b:21:VAL:HG11	2.03	0.40
26:I:302:PC1:H152	18:Z:30:LEU:O	2.22	0.40
10:P:120:VAL:O	10:P:121:GLN:C	2.64	0.40
10:P:153:ALA:HB3	10:P:194:VAL:HG21	2.03	0.40
10:P:300:TRP:CE2	10:P:304:LEU:HD21	2.57	0.40
11:Q:57:GLU:O	11:Q:58:LYS:C	2.65	0.40
19:a:58:ASN:ND2	19:a:60:TYR:OH	2.55	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	88/115 (76%)	79 (90%)	9 (10%)	0	100	100
2	B	155/224 (69%)	145 (94%)	9 (6%)	1 (1%)	21	50
3	C	196/263 (74%)	185 (94%)	11 (6%)	0	100	100
4	D	380/463 (82%)	351 (92%)	28 (7%)	1 (0%)	36	65
5	E	208/248 (84%)	188 (90%)	20 (10%)	0	100	100
6	F	424/464 (91%)	404 (95%)	20 (5%)	0	100	100
7	G	685/727 (94%)	627 (92%)	58 (8%)	0	100	100
8	H	307/318 (96%)	288 (94%)	17 (6%)	2 (1%)	18	47
9	I	170/212 (80%)	169 (99%)	1 (1%)	0	100	100
10	P	338/377 (90%)	315 (93%)	23 (7%)	0	100	100
11	Q	116/175 (66%)	114 (98%)	2 (2%)	0	100	100
12	R	81/116 (70%)	76 (94%)	5 (6%)	0	100	100
13	S	81/99 (82%)	78 (96%)	3 (4%)	0	100	100
14	T	73/156 (47%)	72 (99%)	1 (1%)	0	100	100
15	V	110/116 (95%)	107 (97%)	3 (3%)	0	100	100
16	W	112/131 (86%)	106 (95%)	6 (5%)	0	100	100
17	X	140/172 (81%)	129 (92%)	11 (8%)	0	100	100
18	Z	137/144 (95%)	129 (94%)	8 (6%)	0	100	100
19	a	65/70 (93%)	57 (88%)	8 (12%)	0	100	100
20	b	78/84 (93%)	68 (87%)	10 (13%)	0	100	100
21	q	116/145 (80%)	114 (98%)	2 (2%)	0	100	100
22	r	47/113 (42%)	43 (92%)	4 (8%)	0	100	100
23	s	11/104 (11%)	11 (100%)	0	0	100	100
All	All	4118/5036 (82%)	3855 (94%)	259 (6%)	4 (0%)	49	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
8	H	92	PRO
4	D	89	PRO
8	H	204	GLU
2	B	195	PRO

5.3.2 Protein sidechains (i)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	84/104 (81%)	84 (100%)	0	100	100
2	B	133/185 (72%)	132 (99%)	1 (1%)	73	77
3	C	180/227 (79%)	180 (100%)	0	100	100
4	D	331/395 (84%)	330 (100%)	1 (0%)	86	84
5	E	182/206 (88%)	181 (100%)	1 (0%)	81	81
6	F	341/370 (92%)	340 (100%)	1 (0%)	86	84
7	G	579/610 (95%)	578 (100%)	1 (0%)	87	85
8	H	275/280 (98%)	275 (100%)	0	100	100
9	I	148/178 (83%)	148 (100%)	0	100	100
10	P	297/325 (91%)	296 (100%)	1 (0%)	86	84
11	Q	105/153 (69%)	104 (99%)	1 (1%)	68	75
12	R	70/96 (73%)	69 (99%)	1 (1%)	59	70
13	S	74/80 (92%)	73 (99%)	1 (1%)	59	70
14	T	69/135 (51%)	68 (99%)	1 (1%)	59	70
15	V	100/102 (98%)	100 (100%)	0	100	100
16	W	108/114 (95%)	108 (100%)	0	100	100
17	X	129/154 (84%)	129 (100%)	0	100	100
18	Z	120/123 (98%)	119 (99%)	1 (1%)	73	77
19	a	57/60 (95%)	57 (100%)	0	100	100
20	b	71/73 (97%)	71 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
21	q	108/131 (82%)	107 (99%)	1 (1%)	70 76
22	r	44/96 (46%)	44 (100%)	0	100 100
23	s	13/95 (14%)	13 (100%)	0	100 100
All	All	3618/4292 (84%)	3606 (100%)	12 (0%)	84 84

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	104	MET
4	D	232	VAL
5	E	244	VAL
6	F	182	ILE
7	G	271	MET
10	P	316	LYS
11	Q	96	LYS
12	R	64	ILE
13	S	68	ARG
14	T	103	HIS
18	Z	7	LYS
21	q	138	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
2	B	151	GLN
2	B	172	HIS
2	B	209	GLN
3	C	54	HIS
3	C	88	HIS
3	C	123	ASN
3	C	130	ASN
3	C	179	ASN
3	C	180	HIS
3	C	195	HIS
3	C	227	GLN
3	C	235	ASN
4	D	79	ASN
4	D	92	HIS
4	D	117	HIS

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Mol	Chain	Res	Type
4	D	131	GLN
4	D	147	ASN
4	D	182	ASN
4	D	234	GLN
4	D	313	GLN
4	D	339	GLN
4	D	346	GLN
4	D	381	HIS
4	D	454	GLN
5	E	132	GLN
5	E	152	GLN
5	E	190	ASN
5	E	245	GLN
6	F	44	ASN
6	F	168	ASN
6	F	170	GLN
6	F	244	ASN
6	F	270	ASN
6	F	277	ASN
6	F	346	GLN
7	G	59	GLN
7	G	74	ASN
7	G	101	ASN
7	G	105	ASN
7	G	140	GLN
7	G	164	ASN
7	G	205	GLN
7	G	444	HIS
7	G	495	ASN
7	G	498	GLN
7	G	569	GLN
7	G	571	HIS
7	G	605	GLN
7	G	666	GLN
7	G	677	GLN
7	G	705	GLN
8	H	5	ASN
8	H	32	GLN
8	H	47	GLN
8	H	93	HIS
8	H	97	ASN
8	H	169	GLN

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Mol	Chain	Res	Type
8	H	171	HIS
8	H	212	ASN
8	H	258	ASN
8	H	292	ASN
9	I	126	GLN
9	I	186	ASN
10	P	43	HIS
10	P	71	ASN
10	P	169	HIS
10	P	216	HIS
10	P	251	ASN
10	P	269	ASN
10	P	275	HIS
10	P	323	HIS
10	P	341	GLN
11	Q	51	GLN
11	Q	88	GLN
15	V	50	GLN
16	W	29	ASN
16	W	54	GLN
17	X	30	HIS
19	a	27	HIS
19	a	58	ASN
20	b	69	HIS
20	b	83	ASN
21	q	13	GLN
21	q	31	ASN
21	q	52	ASN
21	q	54	GLN
21	q	87	HIS
21	q	91	HIS
22	r	21	GLN
22	r	110	GLN
23	s	84	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 21 ligands modelled in this entry, 1 is monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
24	3PE	b	201	-	45,45,50	0.95	2 (4%)	48,50,55	1.10	3 (6%)
26	PC1	B	302	-	34,34,53	1.15	2 (5%)	40,42,61	1.15	3 (7%)
25	SF4	F	502	6	0,12,12	-	-	-		
25	SF4	I	303	9	0,12,12	-	-	-		
25	SF4	G	802	7	0,12,12	-	-	-		
28	FES	E	301	5	0,4,4	-	-	-		
26	PC1	I	302	-	46,46,53	0.99	2 (4%)	52,54,61	1.08	3 (5%)
25	SF4	G	801	7	0,12,12	-	-	-		
29	FMN	F	501	-	33,33,33	1.40	5 (15%)	48,50,50	1.22	7 (14%)
25	SF4	B	301	2	0,12,12	-	-	-		
25	SF4	I	304	9	0,12,12	-	-	-		
24	3PE	I	301	-	50,50,50	0.89	2 (4%)	53,55,55	1.03	4 (7%)
27	UQ1	D	501	-	18,18,18	2.41	4 (22%)	22,25,25	1.77	3 (13%)
26	PC1	H	402	-	41,41,53	1.05	2 (4%)	47,49,61	1.06	4 (8%)
31	NDP	P	401	-	49,52,52	1.20	5 (10%)	66,80,80	1.68	11 (16%)
34	CDL	q	201	-	56,56,99	1.19	4 (7%)	62,68,111	1.29	6 (9%)
30	UQ9	H	401	-	35,35,58	0.81	2 (5%)	42,45,73	0.49	0
28	FES	G	803	7	0,4,4	-	-	-		
33	EHZ	W	201	-	27,31,37	1.89	7 (25%)	37,41,47	1.86	11 (29%)
24	3PE	A	401	-	45,45,50	0.93	2 (4%)	48,50,55	1.01	2 (4%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.

'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	3PE	b	201	-	-	8/49/49/54	-
26	PC1	B	302	-	-	11/38/38/57	-
25	SF4	F	502	6	-	-	0/6/5/5
25	SF4	I	303	9	-	-	0/6/5/5
25	SF4	G	802	7	-	-	0/6/5/5
28	FES	E	301	5	-	-	0/1/1/1
26	PC1	I	302	-	-	13/50/50/57	-
25	SF4	G	801	7	-	-	0/6/5/5
29	FMN	F	501	-	-	4/18/18/18	0/3/3/3
25	SF4	B	301	2	-	-	0/6/5/5
25	SF4	I	304	9	-	-	0/6/5/5
24	3PE	I	301	-	-	17/54/54/54	-
27	UQ1	D	501	-	-	0/9/33/33	0/1/1/1
26	PC1	H	402	-	-	15/45/45/57	-
31	NDP	P	401	-	-	6/34/77/77	0/5/5/5
34	CDL	q	201	-	-	14/67/67/110	-
30	UQ9	H	401	-	-	16/30/54/81	0/1/1/1
28	FES	G	803	7	-	-	0/1/1/1
33	EHZ	W	201	-	-	22/39/39/45	-
24	3PE	A	401	-	-	14/49/49/54	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	D	501	UQ1	C6-C5	7.68	1.49	1.35
33	W	201	EHZ	C15-N2	5.37	1.45	1.33
33	W	201	EHZ	C12-N1	5.13	1.45	1.33
29	F	501	FMN	C9A-C5A	4.75	1.49	1.41
27	D	501	UQ1	O2-CM2	-4.49	1.34	1.45
31	P	401	NDP	C5A-C4A	4.26	1.47	1.39
26	I	302	PC1	O31-C31	4.19	1.45	1.33
26	B	302	PC1	O31-C31	4.17	1.45	1.33
34	q	201	CDL	OB8-CB7	4.16	1.45	1.33
26	H	402	PC1	O31-C31	4.15	1.45	1.33
24	b	201	3PE	O31-C31	4.12	1.45	1.33
34	q	201	CDL	OA8-CA7	4.10	1.45	1.33
26	I	302	PC1	O21-C21	4.09	1.45	1.34
24	I	301	3PE	O31-C31	4.08	1.45	1.33
34	q	201	CDL	OA6-CA5	4.08	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	A	401	3PE	O31-C31	4.08	1.45	1.33
34	q	201	CDL	OB6-CB5	4.07	1.45	1.34
24	b	201	3PE	O21-C21	4.06	1.45	1.34
26	B	302	PC1	O21-C21	4.03	1.45	1.34
26	H	402	PC1	O21-C21	4.03	1.45	1.34
24	I	301	3PE	O21-C21	3.99	1.45	1.34
24	A	401	3PE	O21-C21	3.94	1.45	1.34
27	D	501	UQ1	O3-CM3	3.65	1.53	1.45
31	P	401	NDP	C6N-C5N	3.22	1.39	1.33
29	F	501	FMN	C8-C7	3.18	1.48	1.40
27	D	501	UQ1	C3-C2	3.10	1.49	1.36
29	F	501	FMN	C4-N3	-2.75	1.33	1.38
30	H	401	UQ9	C4-C5	-2.67	1.41	1.48
30	H	401	UQ9	C3-C2	-2.58	1.41	1.48
33	W	201	EHZ	P1-O7	2.55	1.64	1.54
31	P	401	NDP	C5A-C6A	2.52	1.48	1.41
33	W	201	EHZ	O4-C15	-2.47	1.18	1.23
33	W	201	EHZ	C9-S1	2.39	1.81	1.76
29	F	501	FMN	C5A-N5	-2.38	1.34	1.39
33	W	201	EHZ	O3-C12	-2.37	1.18	1.23
31	P	401	NDP	C8A-N7A	2.37	1.36	1.31
31	P	401	NDP	C5A-N7A	-2.34	1.34	1.39
33	W	201	EHZ	P1-OP3	-2.21	1.46	1.54
29	F	501	FMN	C4A-N5	2.05	1.34	1.30

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	D	501	UQ1	CM3-O3-C3	6.63	139.97	116.47
33	W	201	EHZ	C8-C9-S1	6.28	121.39	113.63
31	P	401	NDP	C5A-C4A-N3A	-6.06	118.84	126.75
31	P	401	NDP	N3A-C4A-N9A	4.75	134.91	127.08
34	q	201	CDL	OA6-CA5-C11	4.35	120.87	111.50
26	I	302	PC1	O21-C21-C22	4.24	120.64	111.50
34	q	201	CDL	OB6-CB5-C51	4.12	120.37	111.50
31	P	401	NDP	C2A-N3A-C4A	3.79	120.69	111.75
26	B	302	PC1	O21-C21-C22	3.77	119.62	111.50
24	A	401	3PE	O21-C21-C22	3.76	119.60	111.50
26	H	402	PC1	O21-C21-C22	3.72	119.53	111.50
24	I	301	3PE	O21-C21-C22	3.67	119.40	111.50
31	P	401	NDP	PN-O3-PA	-3.56	120.61	132.83
24	b	201	3PE	O21-C21-C22	3.48	119.01	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	b	201	3PE	C2-O21-C21	-3.48	109.23	117.79
31	P	401	NDP	C4A-C5A-N7A	-3.31	106.58	110.62
33	W	201	EHZ	C13-C12-N1	3.08	121.61	116.42
31	P	401	NDP	N3A-C2A-N1A	-3.06	123.81	128.60
33	W	201	EHZ	C14-C13-C12	-3.04	107.30	112.36
33	W	201	EHZ	OP3-P1-O9	-2.90	99.32	110.68
33	W	201	EHZ	C7-C8-C9	-2.90	107.28	113.89
31	P	401	NDP	C4A-N9A-C8A	2.84	108.81	105.73
26	I	302	PC1	C2-O21-C21	-2.84	110.81	117.79
31	P	401	NDP	C5A-N7A-C8A	2.80	107.48	103.51
26	B	302	PC1	O31-C31-C32	2.78	120.64	111.91
34	q	201	CDL	OA8-CA7-C31	2.75	120.53	111.91
34	q	201	CDL	CA4-OA6-CA5	-2.74	111.05	117.79
26	B	302	PC1	C2-O21-C21	-2.70	111.15	117.79
24	I	301	3PE	O31-C31-C32	2.66	120.25	111.91
29	F	501	FMN	C4A-C10-N1	-2.63	118.64	124.73
26	H	402	PC1	O31-C31-C32	2.61	120.11	111.91
26	I	302	PC1	O31-C31-C32	2.58	120.00	111.91
24	A	401	3PE	O31-C31-C32	2.57	119.96	111.91
29	F	501	FMN	O4-C4-C4A	-2.53	119.89	126.60
24	b	201	3PE	O31-C31-C32	2.50	119.76	111.91
31	P	401	NDP	C3D-C2D-C1D	2.47	106.11	101.43
34	q	201	CDL	OB8-CB7-C71	2.43	119.53	111.91
33	W	201	EHZ	C5-C6-C7	-2.40	107.96	114.85
27	D	501	UQ1	C7-C8-C9	-2.39	119.77	127.26
33	W	201	EHZ	C10-S1-C9	2.25	108.89	101.87
34	q	201	CDL	CB4-OB6-CB5	-2.23	112.30	117.79
27	D	501	UQ1	C11-C9-C10	2.22	119.52	114.60
31	P	401	NDP	N9A-C8A-N7A	-2.22	110.88	113.91
31	P	401	NDP	C6A-C5A-N7A	2.21	136.14	132.02
33	W	201	EHZ	C11-N1-C12	-2.21	118.74	122.84
29	F	501	FMN	C4-C4A-N5	2.19	121.34	118.23
26	H	402	PC1	C2-O21-C21	-2.18	112.42	117.79
33	W	201	EHZ	O6-P1-O9	2.10	112.37	106.47
29	F	501	FMN	C4A-C10-N10	2.09	119.54	116.48
33	W	201	EHZ	O2-C9-S1	-2.09	119.90	122.61
29	F	501	FMN	O2-C2-N1	-2.06	118.41	121.83
33	W	201	EHZ	O3-C12-N1	-2.06	119.13	123.01
26	H	402	PC1	C11-C12-N	-2.04	108.95	115.78
29	F	501	FMN	C10-N1-C2	2.04	120.99	116.90
24	I	301	3PE	O31-C31-O32	-2.02	118.50	123.59
29	F	501	FMN	C4A-C4-N3	2.01	118.29	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	I	301	3PE	C2-O21-C21	-2.00	112.86	117.79

There are no chirality outliers.

All (140) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	A	401	3PE	C12-C11-O13-P
24	A	401	3PE	O32-C31-O31-C3
24	A	401	3PE	C32-C31-O31-C3
24	I	301	3PE	C11-O13-P-O12
24	b	201	3PE	O22-C21-O21-C2
24	b	201	3PE	C22-C21-O21-C2
26	B	302	PC1	C1-O11-P-O12
26	B	302	PC1	C1-O11-P-O14
26	B	302	PC1	C1-O11-P-O13
26	B	302	PC1	C22-C21-O21-C2
26	H	402	PC1	C11-O13-P-O12
26	H	402	PC1	C11-O13-P-O14
26	H	402	PC1	C11-O13-P-O11
26	H	402	PC1	C12-C11-O13-P
26	H	402	PC1	O32-C31-O31-C3
26	I	302	PC1	C11-O13-P-O12
26	I	302	PC1	C11-O13-P-O14
26	I	302	PC1	C11-O13-P-O11
26	I	302	PC1	C1-O11-P-O12
29	F	501	FMN	N10-C1'-C2'-O2'
29	F	501	FMN	C5'-O5'-P-O1P
29	F	501	FMN	C5'-O5'-P-O3P
30	H	401	UQ9	C7-C8-C9-C11
30	H	401	UQ9	C7-C8-C9-C10
31	P	401	NDP	C2N-C3N-C7N-N7N
33	W	201	EHZ	O1-C7-C8-C9
33	W	201	EHZ	C6-C7-C8-C9
33	W	201	EHZ	C7-C8-C9-S1
33	W	201	EHZ	S1-C10-C11-N1
33	W	201	EHZ	C11-C10-S1-C9
33	W	201	EHZ	C16-C17-C20-O6
33	W	201	EHZ	C20-O6-P1-O7
33	W	201	EHZ	C20-O6-P1-O9
33	W	201	EHZ	C20-O6-P1-OP3
34	q	201	CDL	CA3-OA5-PA1-OA2
34	q	201	CDL	CA3-OA5-PA1-OA3

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Mol	Chain	Res	Type	Atoms
34	q	201	CDL	CA3-OA5-PA1-OA4
26	I	302	PC1	O32-C31-O31-C3
26	I	302	PC1	C32-C31-O31-C3
26	B	302	PC1	O22-C21-O21-C2
26	H	402	PC1	C32-C31-O31-C3
30	H	401	UQ9	C25-C24-C26-C27
30	H	401	UQ9	C20-C19-C21-C22
30	H	401	UQ9	C15-C14-C16-C17
30	H	401	UQ9	C23-C24-C26-C27
30	H	401	UQ9	C18-C19-C21-C22
30	H	401	UQ9	C13-C14-C16-C17
30	H	401	UQ9	C9-C11-C12-C13
24	A	401	3PE	C22-C21-O21-C2
24	I	301	3PE	C32-C31-O31-C3
24	b	201	3PE	C32-C31-O31-C3
34	q	201	CDL	C12-C13-C14-C15
26	I	302	PC1	C11-C12-N-C15
24	I	301	3PE	O32-C31-O31-C3
24	b	201	3PE	O32-C31-O31-C3
24	A	401	3PE	O22-C21-O21-C2
24	A	401	3PE	C11-O13-P-O11
24	I	301	3PE	C1-O11-P-O13
24	I	301	3PE	C11-O13-P-O11
26	I	302	PC1	C1-O11-P-O13
34	q	201	CDL	C31-CA7-OA8-CA6
26	H	402	PC1	C24-C25-C26-C27
34	q	201	CDL	OA9-CA7-OA8-CA6
26	I	302	PC1	C11-C12-N-C13
24	A	401	3PE	C31-C32-C33-C34
34	q	201	CDL	C51-CB5-OB6-CB4
34	q	201	CDL	OB7-CB5-OB6-CB4
26	I	302	PC1	C11-C12-N-C14
24	I	301	3PE	C22-C21-O21-C2
24	I	301	3PE	C24-C25-C26-C27
24	b	201	3PE	C2A-C2B-C2C-C2D
24	I	301	3PE	O22-C21-O21-C2
26	B	302	PC1	C2-C1-O11-P
26	B	302	PC1	C32-C33-C34-C35
33	W	201	EHZ	N2-C15-C16-C17
33	W	201	EHZ	C3-C4-C5-C6
33	W	201	EHZ	C5-C6-C7-O1
26	B	302	PC1	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
33	W	201	EHZ	O2-C9-S1-C10
24	A	401	3PE	C3-C2-O21-C21
26	H	402	PC1	C22-C23-C24-C25
26	B	302	PC1	O32-C31-O31-C3
31	P	401	NDP	C2B-O2B-P2B-O2X
26	H	402	PC1	O22-C21-O21-C2
24	A	401	3PE	C2E-C2F-C2G-C2H
24	A	401	3PE	C2-C1-O11-P
34	q	201	CDL	CA4-CA3-OA5-PA1
24	A	401	3PE	C11-O13-P-O14
24	I	301	3PE	C1-O11-P-O12
24	I	301	3PE	C1-O11-P-O14
24	I	301	3PE	C11-O13-P-O14
24	A	401	3PE	O11-C1-C2-C3
30	H	401	UQ9	C5-C4-O4-C4M
24	A	401	3PE	O11-C1-C2-O21
26	H	402	PC1	C22-C21-O21-C2
26	B	302	PC1	O13-C11-C12-N
26	H	402	PC1	O13-C11-C12-N
26	H	402	PC1	C27-C28-C29-C2A
24	I	301	3PE	O21-C2-C3-O31
33	W	201	EHZ	O4-C15-C16-O5
33	W	201	EHZ	C19-C17-C20-O6
24	b	201	3PE	C2B-C2C-C2D-C2E
34	q	201	CDL	CB2-OB2-PB2-OB5
30	H	401	UQ9	C12-C11-C9-C10
31	P	401	NDP	O4D-C1D-N1N-C6N
33	W	201	EHZ	C2-C3-C4-C5
26	B	302	PC1	C34-C35-C36-C37
34	q	201	CDL	C1-CB2-OB2-PB2
31	P	401	NDP	C2D-C1D-N1N-C6N
24	I	301	3PE	C37-C38-C39-C3A
24	b	201	3PE	C24-C25-C26-C27
26	I	302	PC1	C2E-C2F-C2G-C2H
31	P	401	NDP	PN-O3-PA-O2A
30	H	401	UQ9	C12-C11-C9-C8
24	I	301	3PE	C35-C36-C37-C38
24	I	301	3PE	C33-C34-C35-C36
29	F	501	FMN	C5'-O5'-P-O2P
33	W	201	EHZ	N2-C15-C16-O5
33	W	201	EHZ	C18-C17-C20-O6
33	W	201	EHZ	C8-C9-S1-C10

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Mol	Chain	Res	Type	Atoms
26	H	402	PC1	C11-C12-N-C13
33	W	201	EHZ	C15-C16-C17-C18
31	P	401	NDP	C2B-O2B-P2B-O3X
33	W	201	EHZ	O5-C16-C17-C18
34	q	201	CDL	C32-C31-CA7-OA8
30	H	401	UQ9	C21-C22-C23-C24
30	H	401	UQ9	C16-C17-C18-C19
30	H	401	UQ9	C11-C12-C13-C14
24	I	301	3PE	C1-C2-C3-O31
26	H	402	PC1	C1-O11-P-O14
26	H	402	PC1	C35-C36-C37-C38
24	A	401	3PE	O13-C11-C12-N
26	I	302	PC1	C12-C11-O13-P
33	W	201	EHZ	O4-C15-C16-C17
34	q	201	CDL	OA7-CA5-OA6-CA4
24	I	301	3PE	C2-C1-O11-P
30	H	401	UQ9	C3-C4-O4-C4M
34	q	201	CDL	C32-C31-CA7-OA9
26	I	302	PC1	C2C-C2D-C2E-C2F
24	b	201	3PE	C39-C3A-C3B-C3C

There are no ring outliers.

19 monomers are involved in 164 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
24	b	201	3PE	16	0
26	B	302	PC1	6	0
25	F	502	SF4	10	0
25	I	303	SF4	11	0
25	G	802	SF4	5	0
28	E	301	FES	5	0
26	I	302	PC1	10	0
29	F	501	FMN	1	0
25	B	301	SF4	6	0
25	I	304	SF4	5	0
24	I	301	3PE	14	0
27	D	501	UQ1	24	0
26	H	402	PC1	7	0
31	P	401	NDP	7	0
34	q	201	CDL	18	0
30	H	401	UQ9	3	0
28	G	803	FES	4	0

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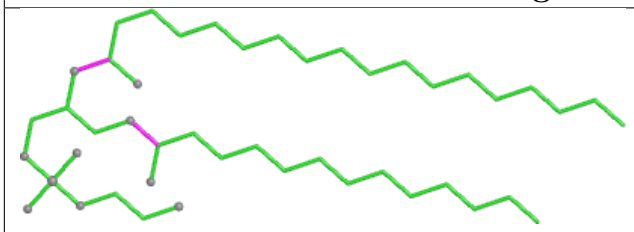
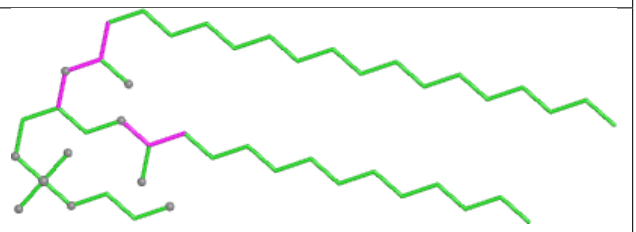
Mol	Chain	Res	Type	Clashes	Symm-Clashes
33	W	201	EHZ	7	0
24	A	401	3PE	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

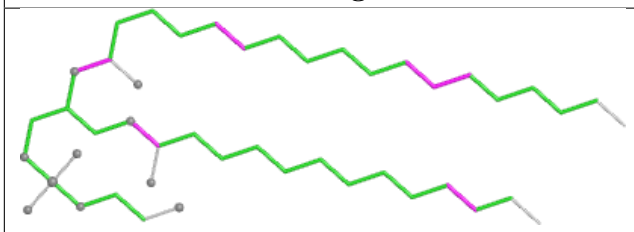
Ligand 3PE b 201



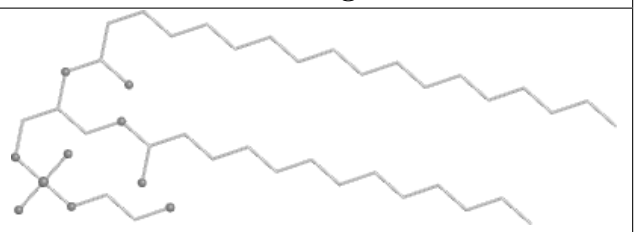
Bond lengths



Bond angles

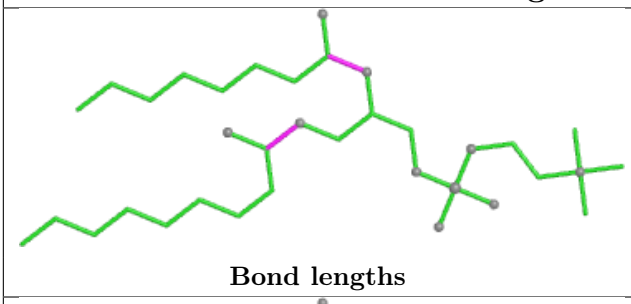


Torsions



Rings

Ligand PC1 B 302



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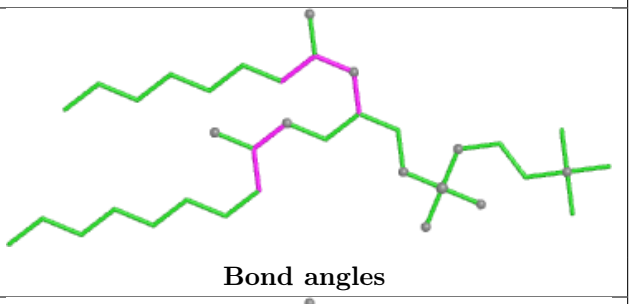
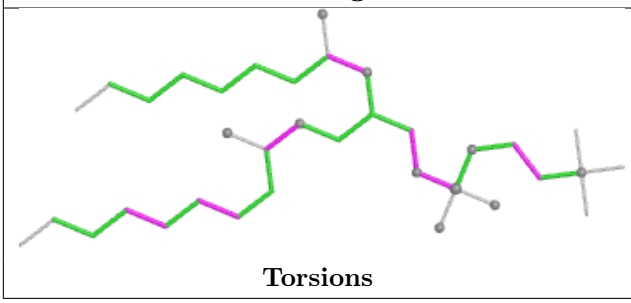


Bond angles



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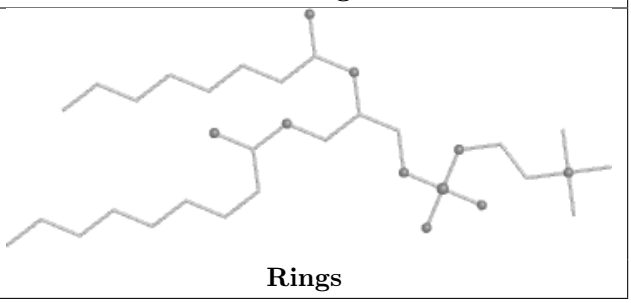
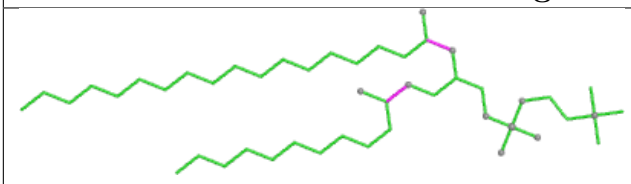


Rings

Ligand PC1 I 302



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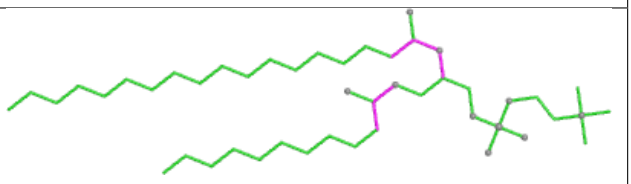
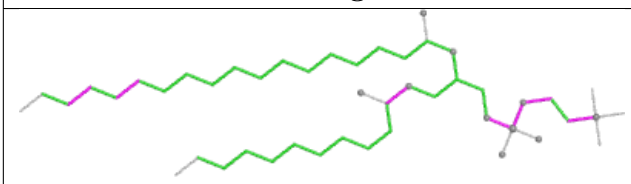


Bond angles



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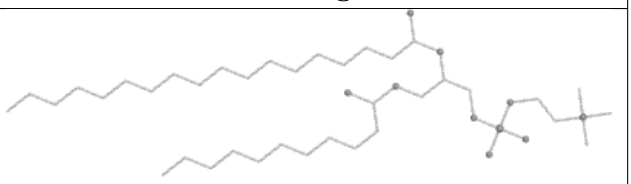
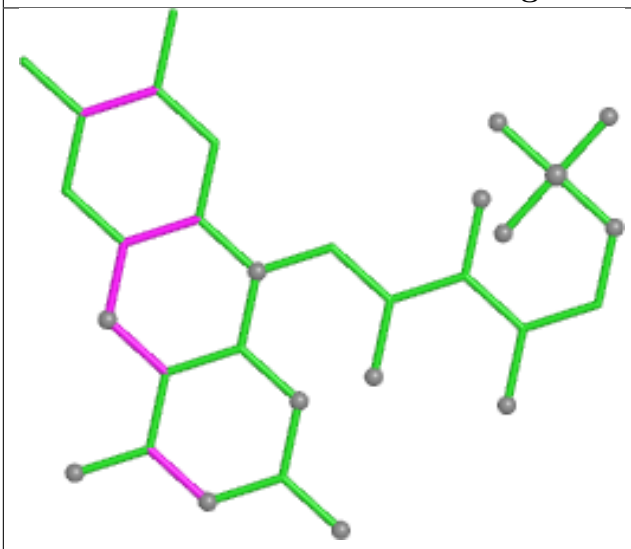


Rings

Ligand FMN F 501



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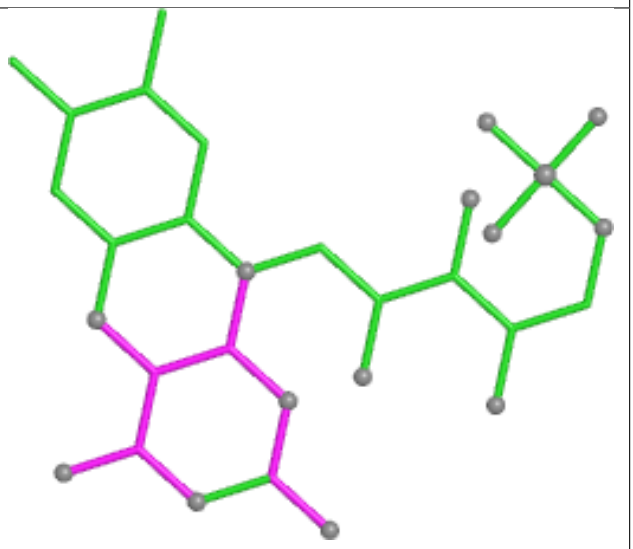
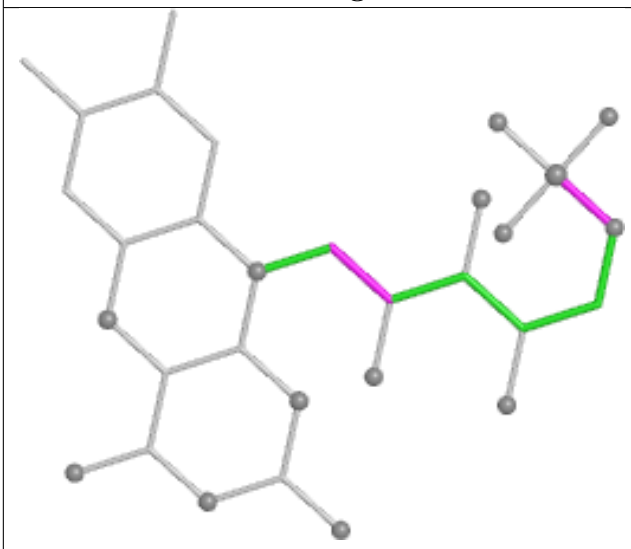


Bond angles



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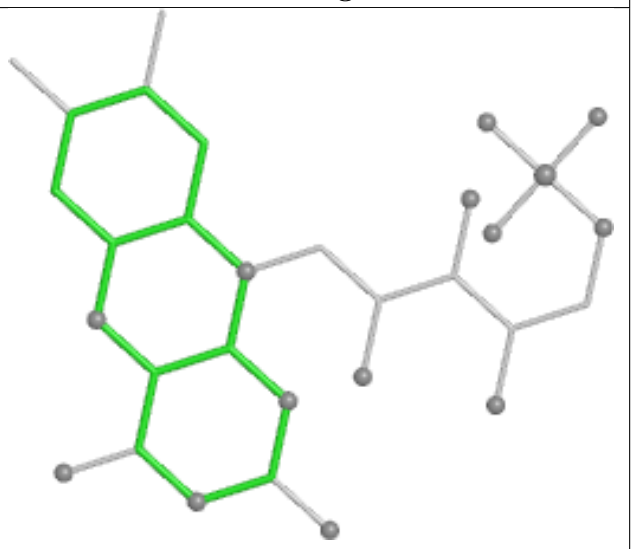
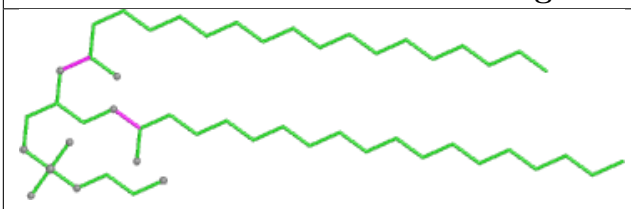


Rings

Ligand 3PE I 301



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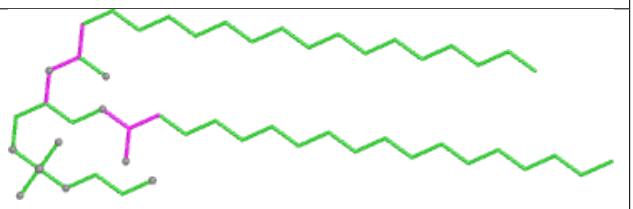
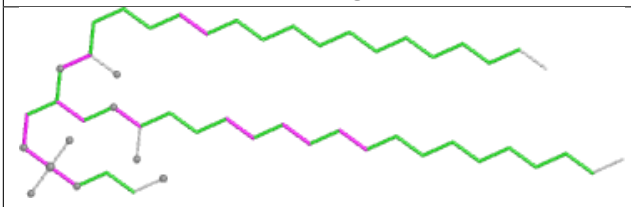


Bond angles



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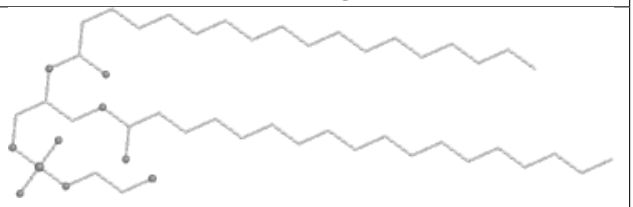
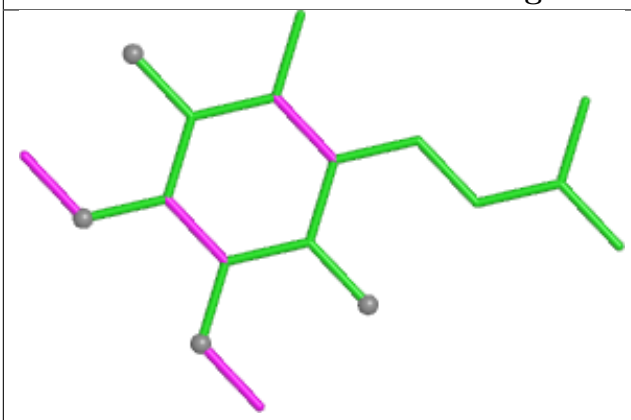


Rings

Ligand UQ1 D 501



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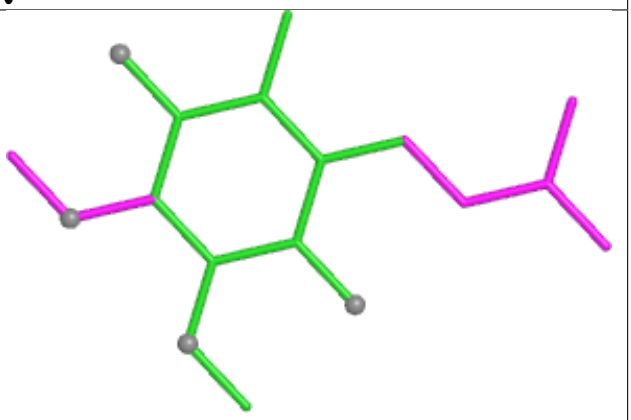
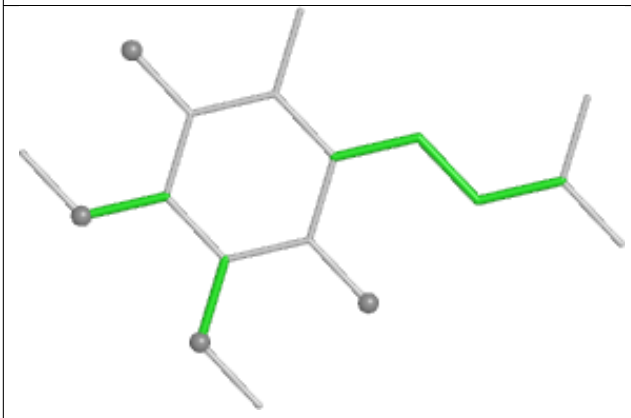


Bond angles



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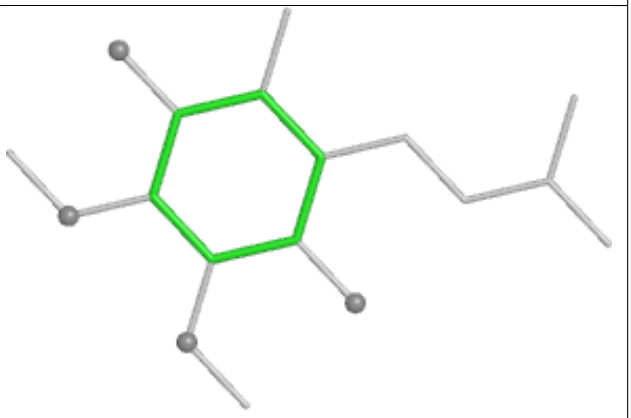
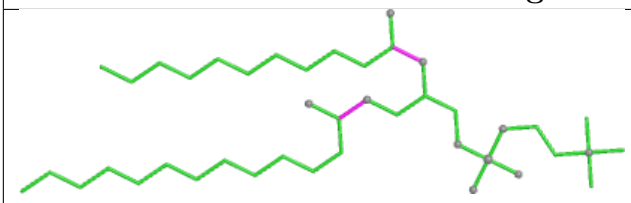


Rings

Ligand PC1 H 402



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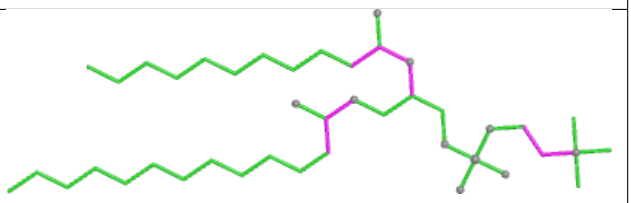
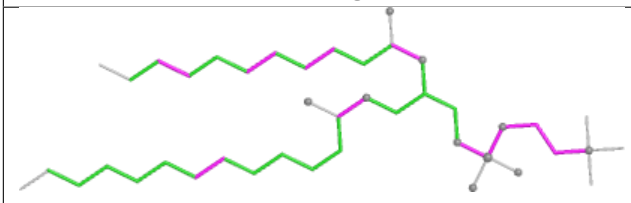


Bond angles



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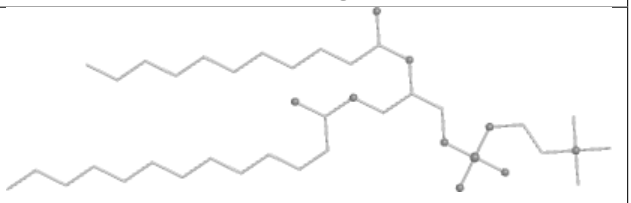
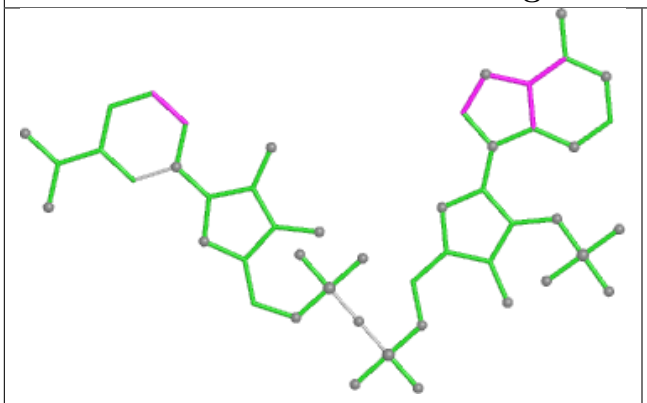


Rings

Ligand NDP P 401



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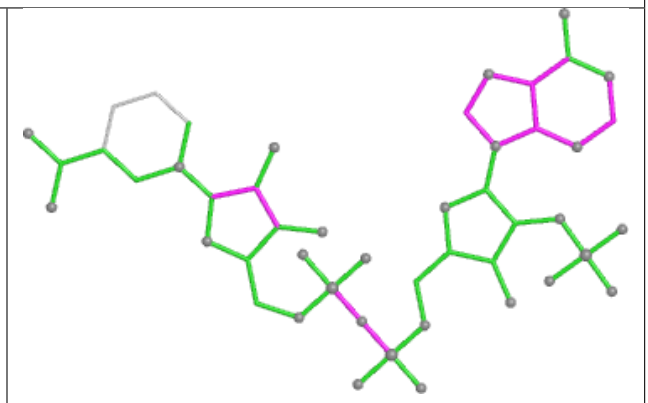
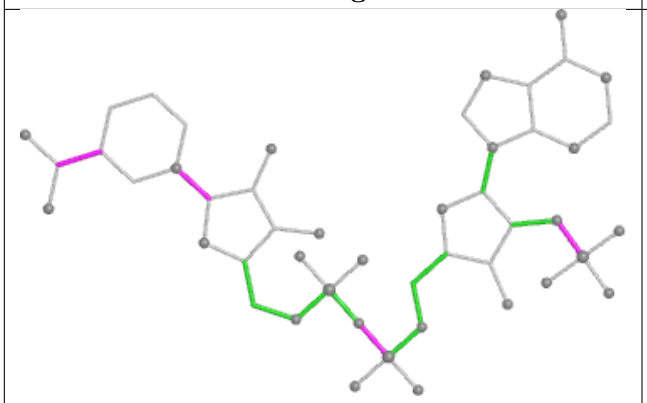


Bond angles



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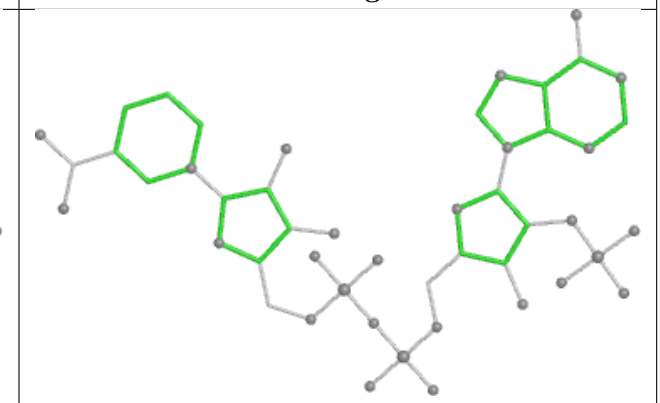
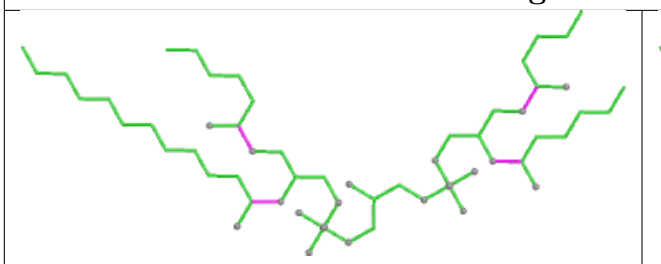


Rings

Ligand CDL q 201



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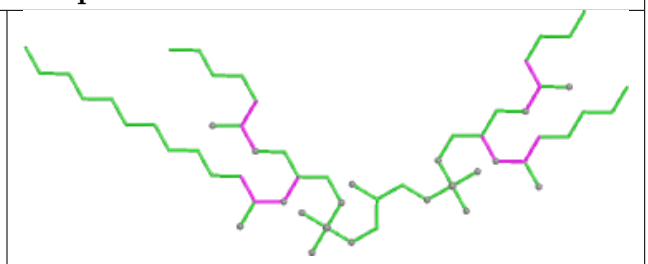
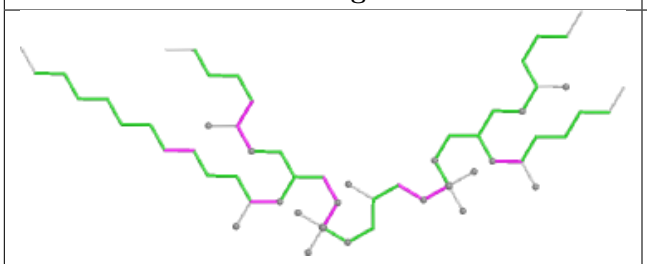


Bond angles



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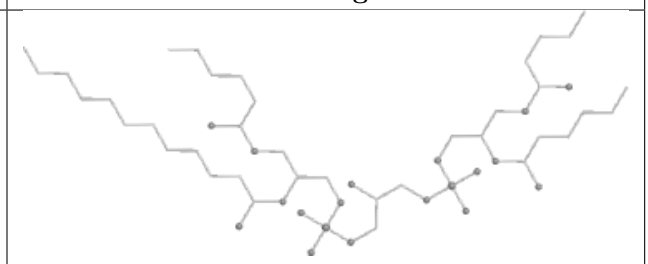
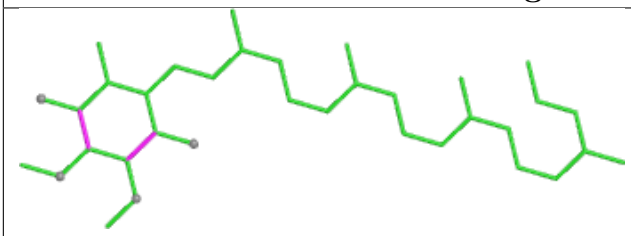


Rings

Ligand UQ9 H 401



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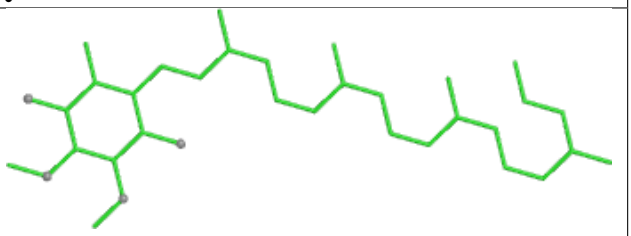
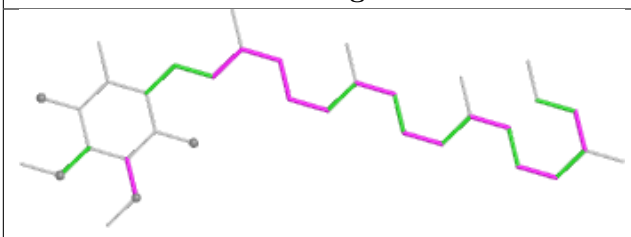


Bond angles



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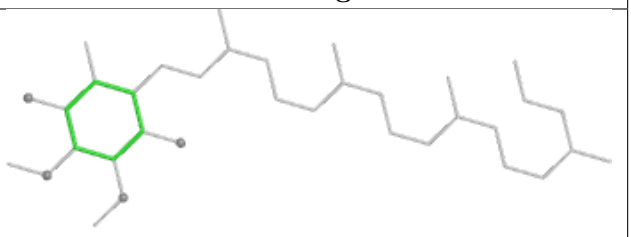
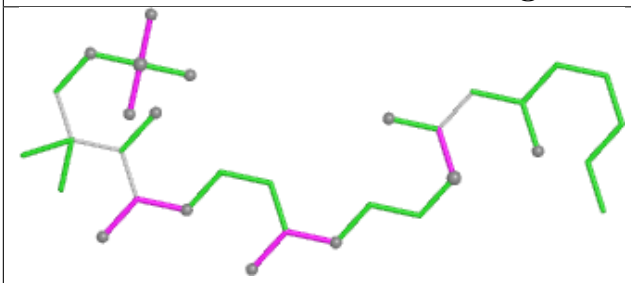


Rings

Ligand EHZ W 201



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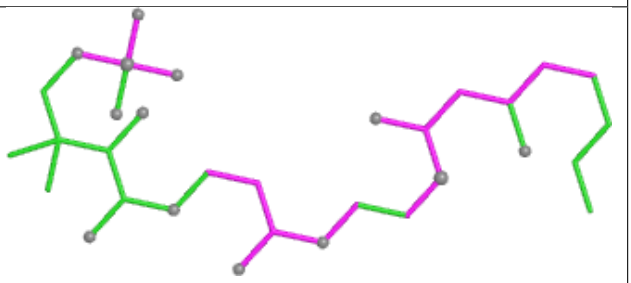
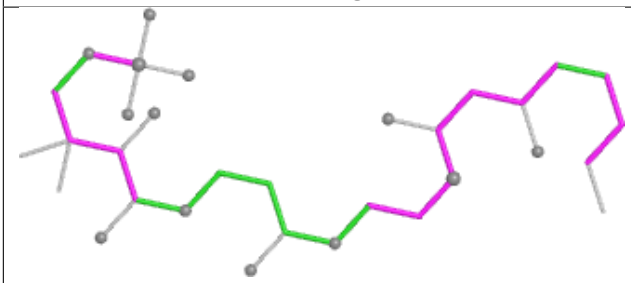


Bond angles



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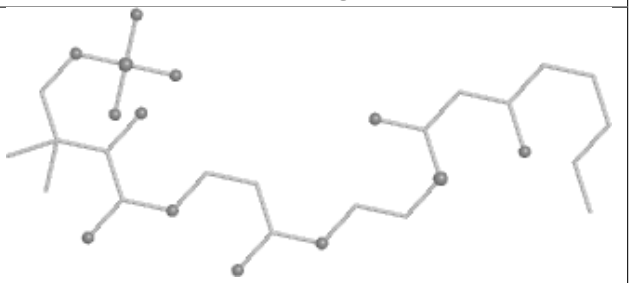
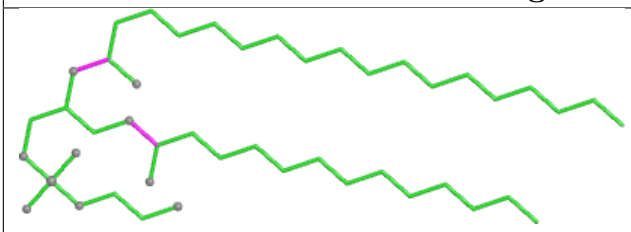


Rings

Ligand 3PE A 401



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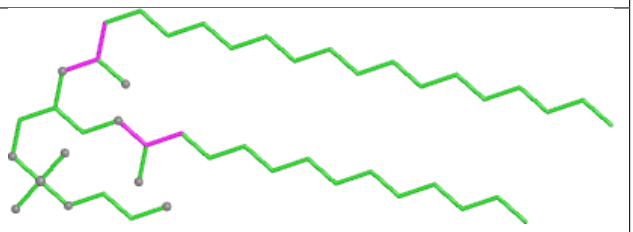
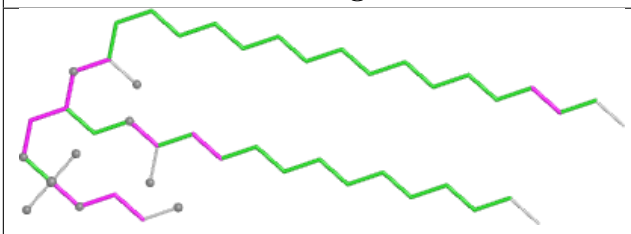
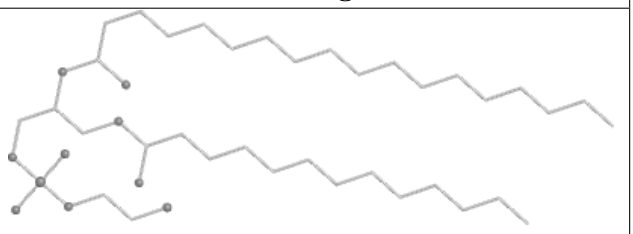


Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

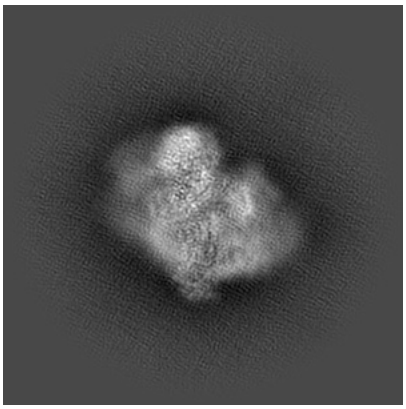
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-38509. These allow visual inspection of the internal detail of the map and identification of artifacts.

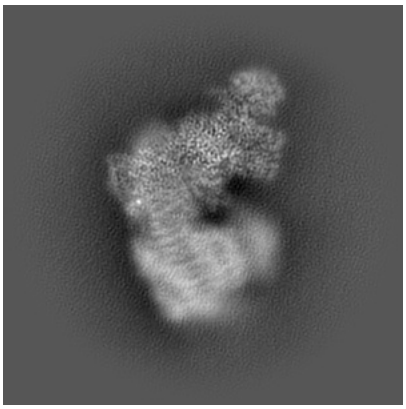
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

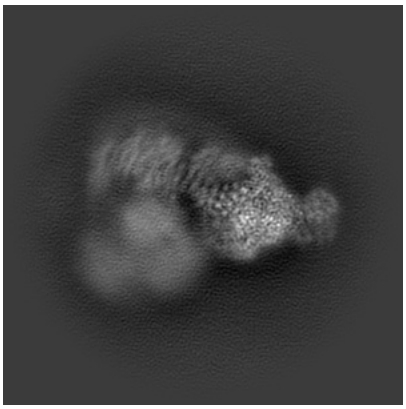
6.1.1 Primary map



X

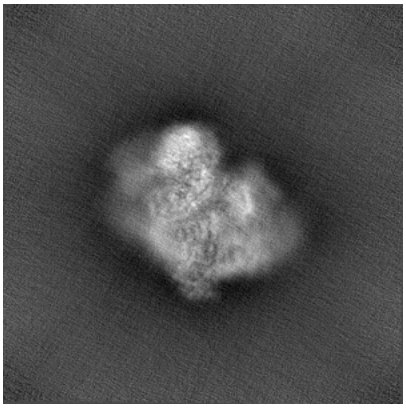


Y

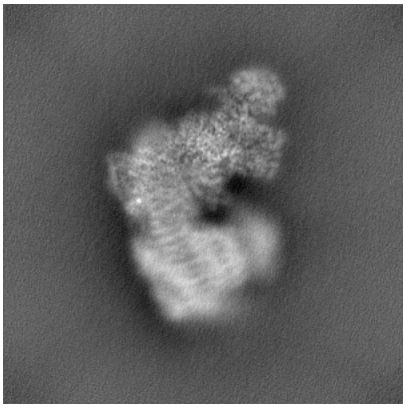


Z

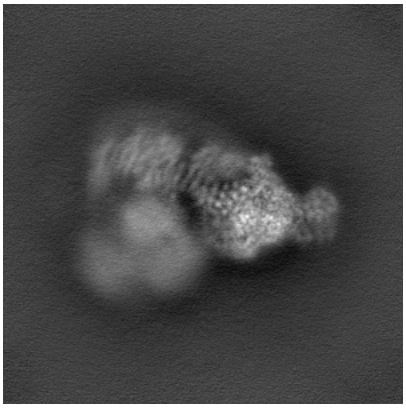
6.1.2 Raw map



X



Y

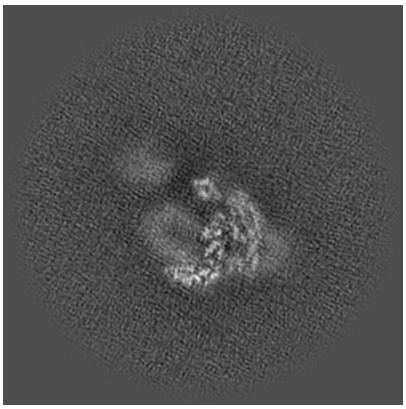


Z

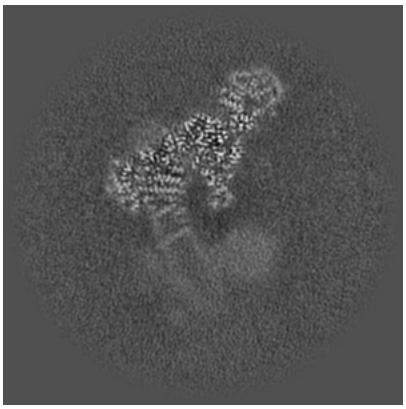
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

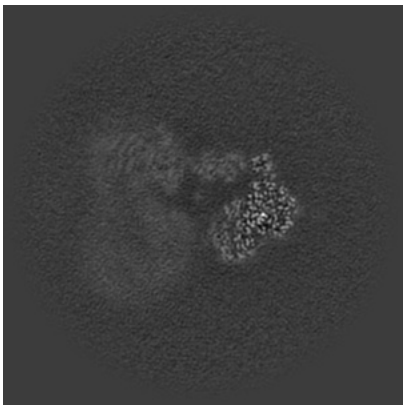
6.2.1 Primary map



X Index: 192

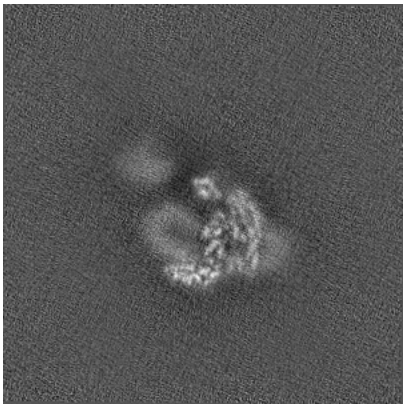


Y Index: 192

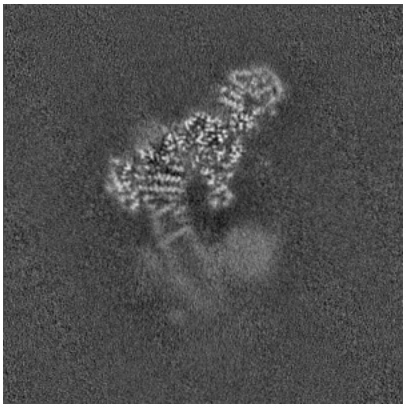


Z Index: 192

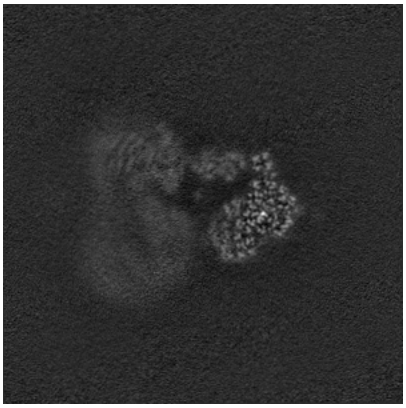
6.2.2 Raw map



X Index: 192



Y Index: 192

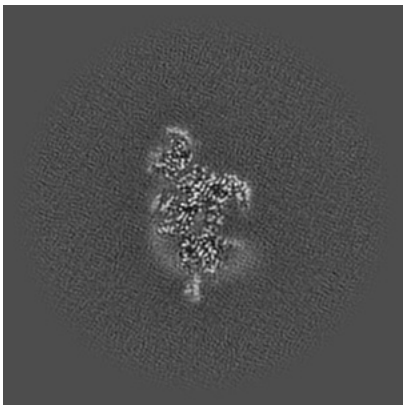


Z Index: 192

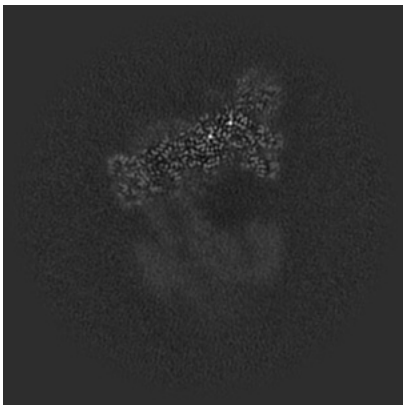
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

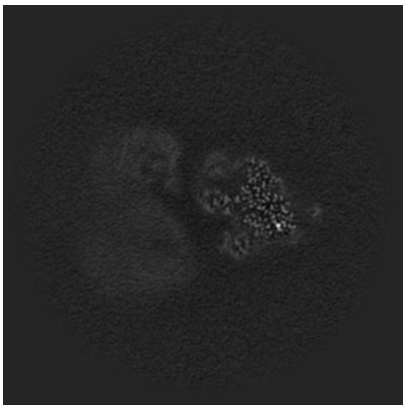
6.3.1 Primary map



X Index: 239

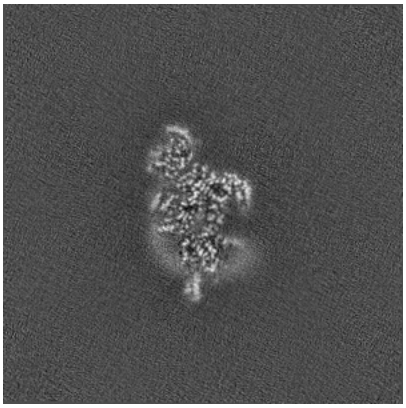


Y Index: 177

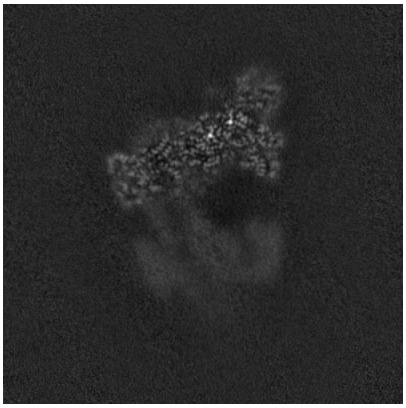


Z Index: 205

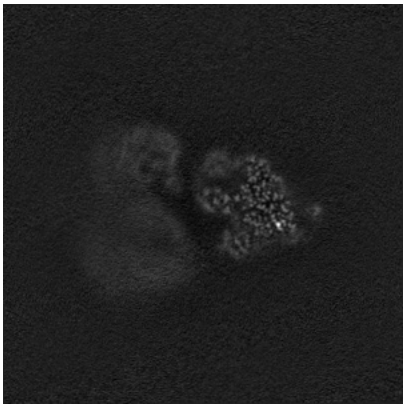
6.3.2 Raw map



X Index: 239



Y Index: 177

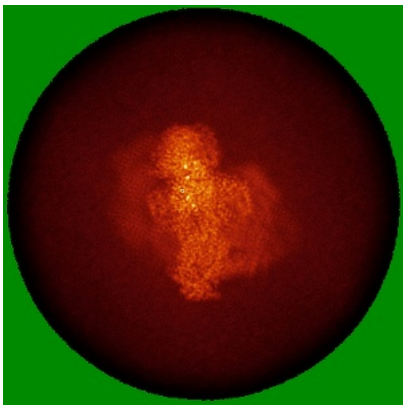


Z Index: 205

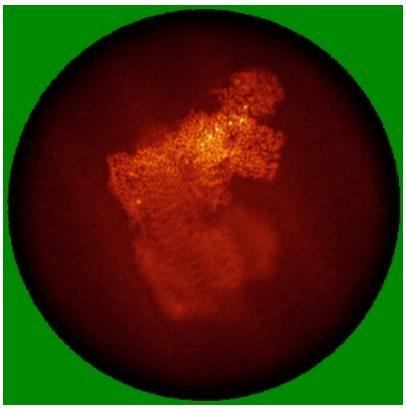
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

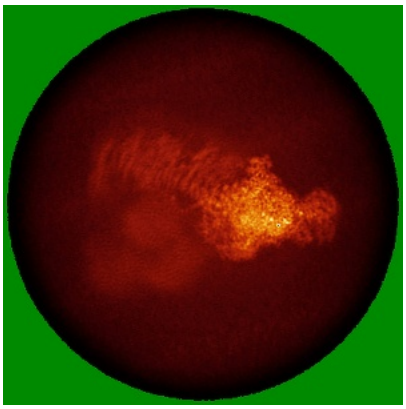
6.4.1 Primary map



X

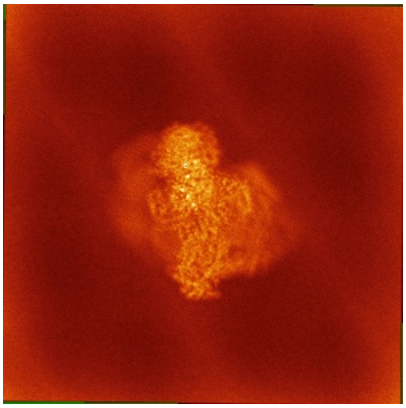


Y

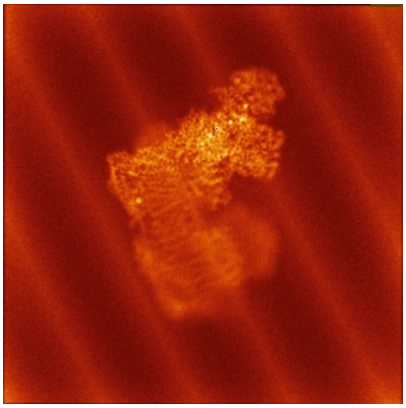


Z

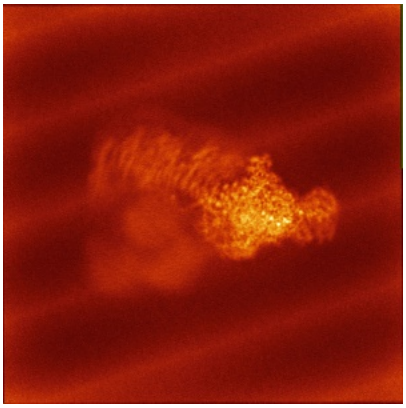
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

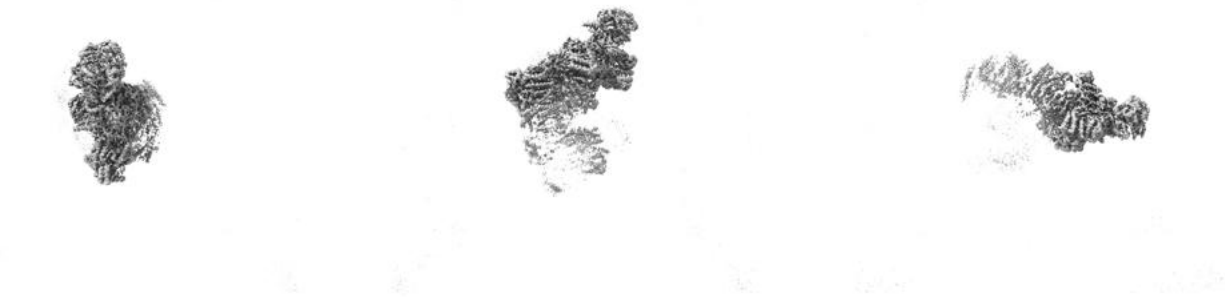
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.55. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

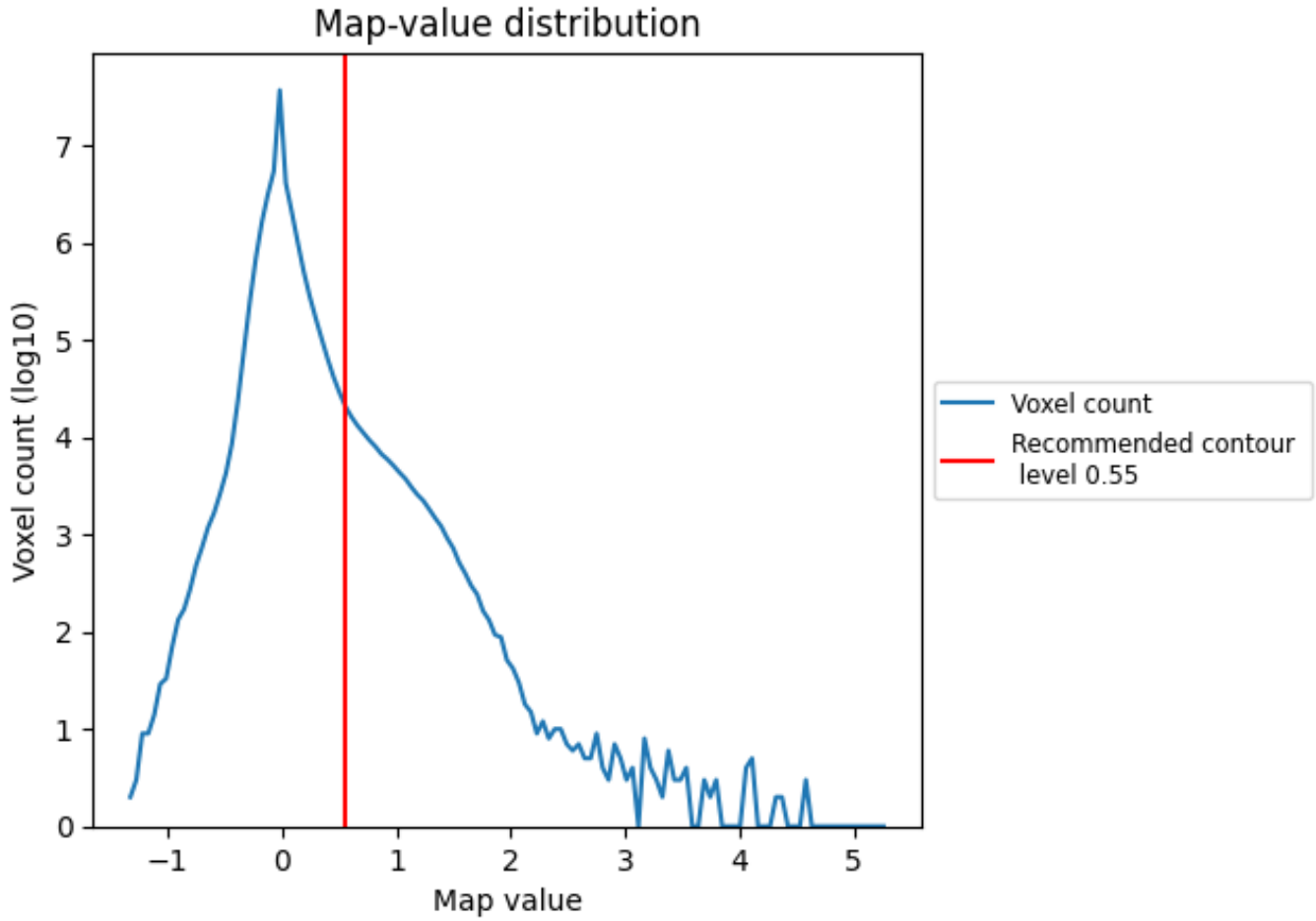
6.6 Mask visualisation (i)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis

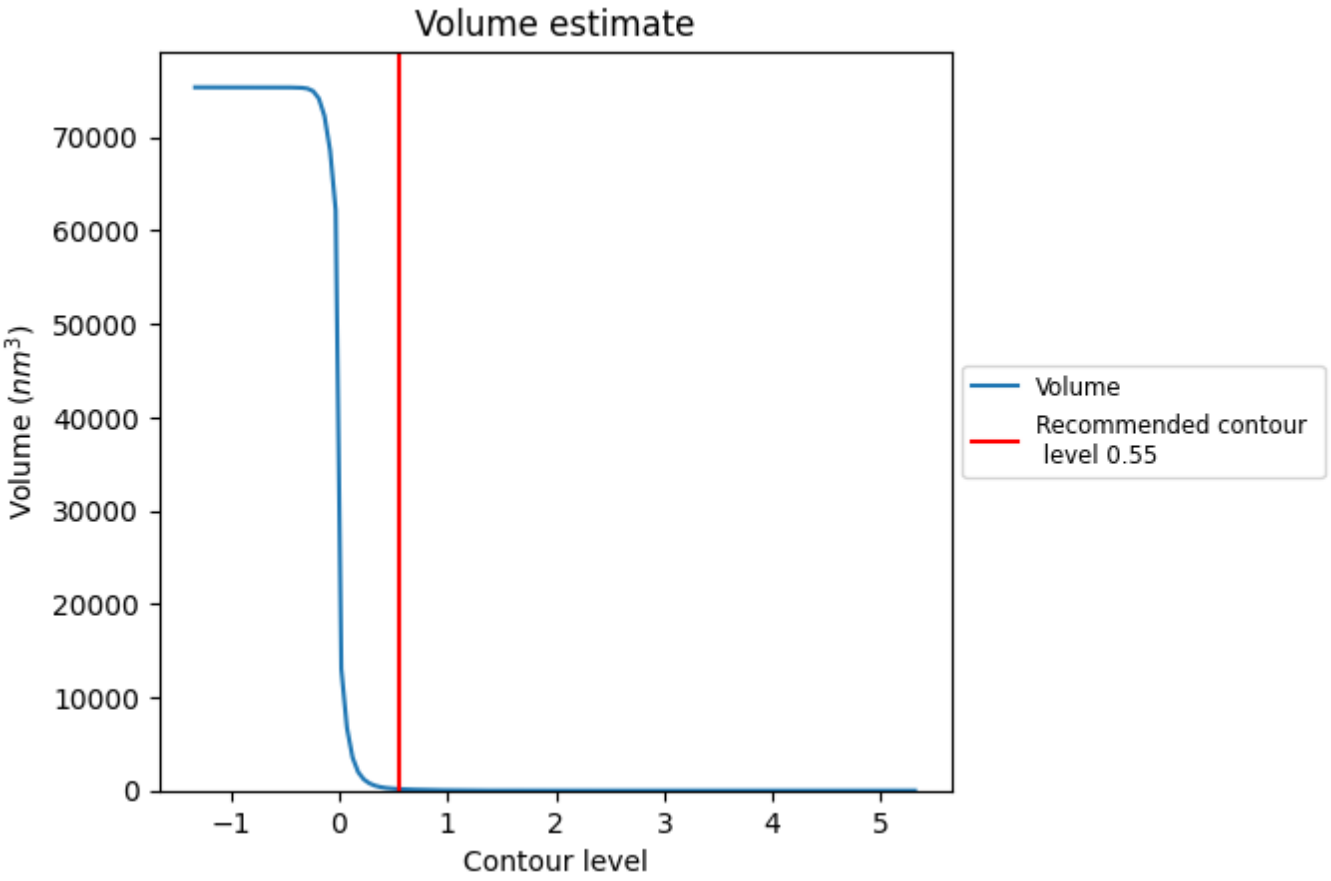
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

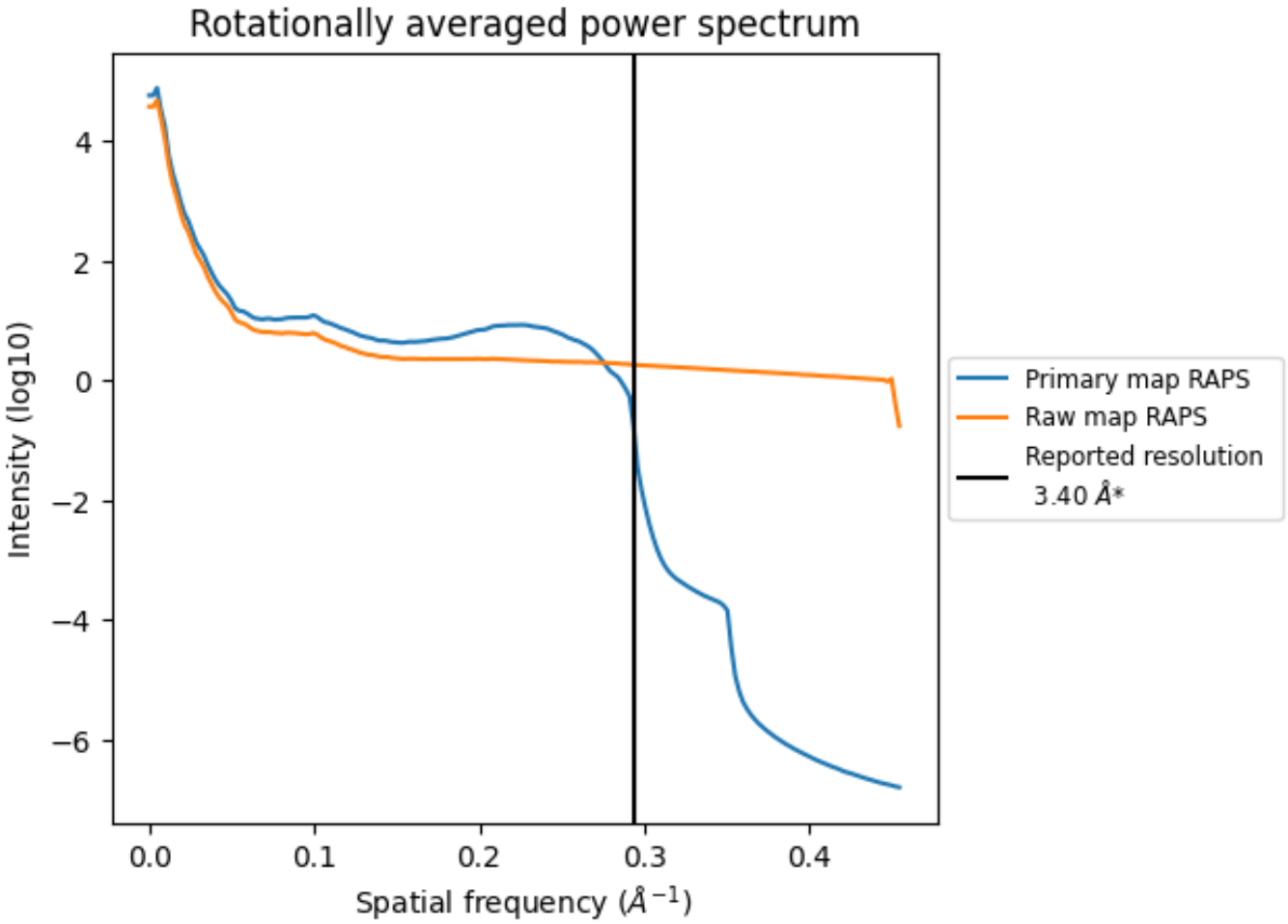
7.2 Volume estimate



The volume at the recommended contour level is 164 nm^3; this corresponds to an approximate mass of 148 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)

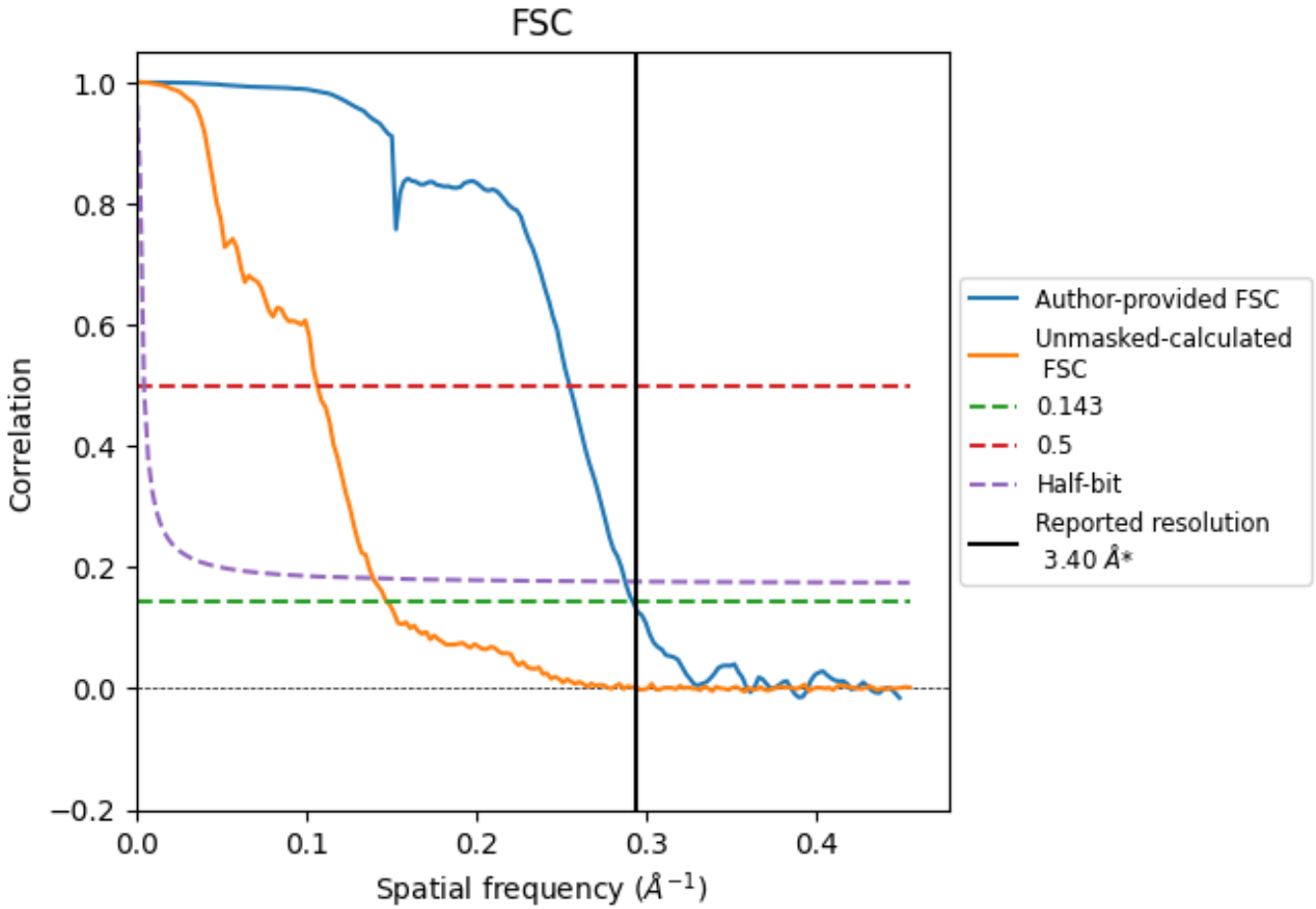


*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.294 Å^{-1}

8.2 Resolution estimates (i)

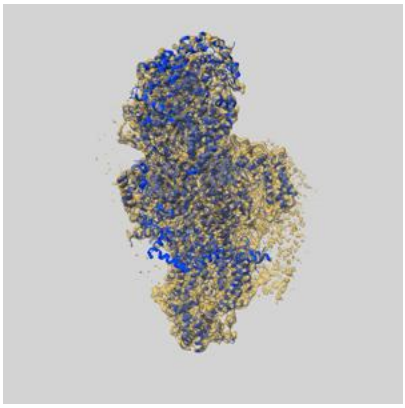
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.43	3.93	3.48
Unmasked-calculated*	6.79	9.39	7.18

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 6.79 differs from the reported value 3.4 by more than 10 %

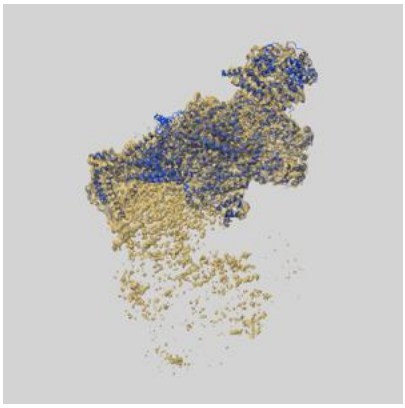
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-38509 and PDB model 8XNO. Per-residue inclusion information can be found in section 3 on page 15.

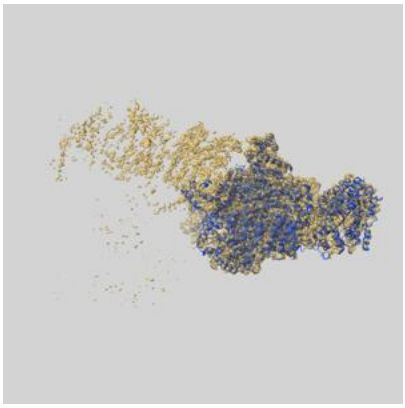
9.1 Map-model overlay



X



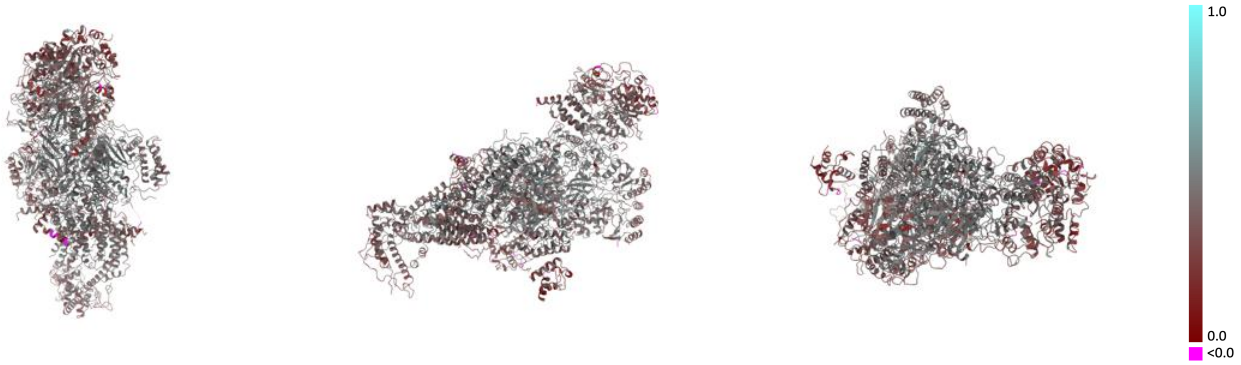
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.55 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

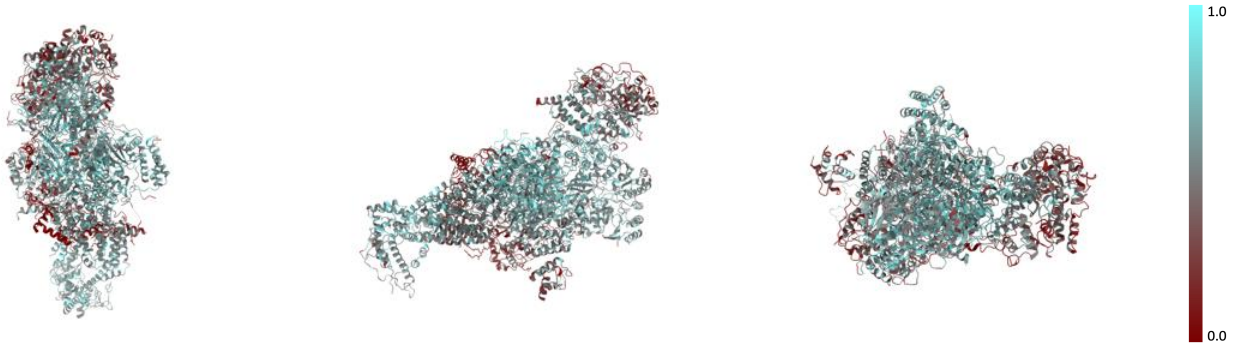
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

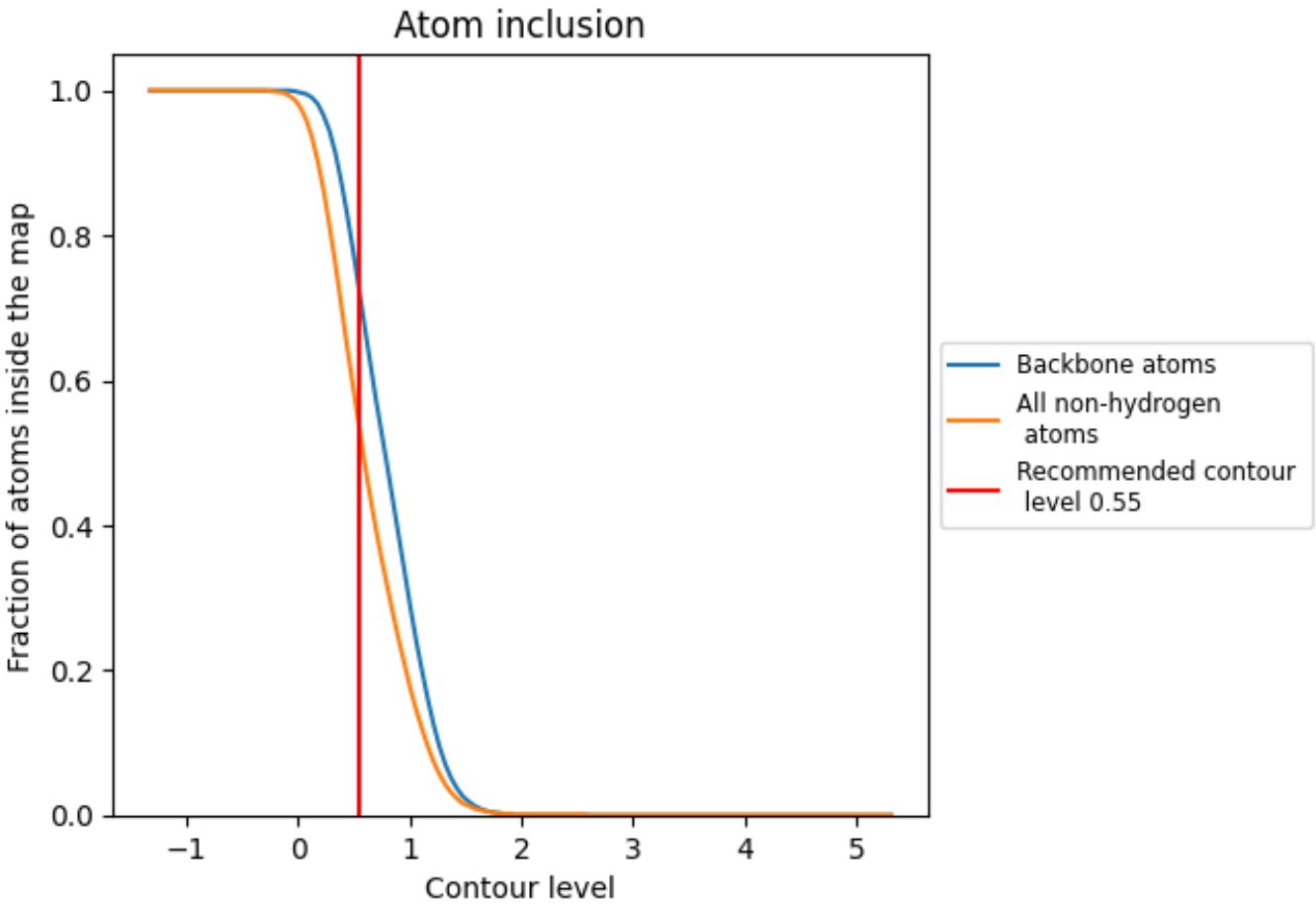
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.55).

9.4 Atom inclusion (i)



At the recommended contour level, 72% of all backbone atoms, 53% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.55) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5300	0.4070
A	0.4590	0.3800
B	0.6490	0.4670
C	0.6570	0.4900
D	0.6540	0.4750
E	0.3650	0.3530
F	0.4530	0.3580
G	0.6340	0.4360
H	0.5730	0.4360
I	0.6680	0.4670
P	0.3780	0.3530
Q	0.5080	0.4400
R	0.2470	0.3250
S	0.5710	0.3680
T	0.3490	0.2460
V	0.6220	0.4150
W	0.4990	0.4120
X	0.5890	0.3660
Z	0.5950	0.3850
a	0.6630	0.4330
b	0.4980	0.3580
q	0.1530	0.3390
r	0.2540	0.3460
s	0.0750	0.2640

