Full wwPDB EM Validation Report (i)

Feb 11, 2024 – 09:35 PM EST

PDB ID	:	3EDL
EMDB ID	:	EMD-5027
Title	:	Kinesin13-Microtubule Ring complex
Authors	:	Tan, D.; Rice, W.J.; Sosa, H.
Deposited on	:	2008-09-03
Resolution	:	28.00 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 (i) 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 (1)) were used in the production of this report:

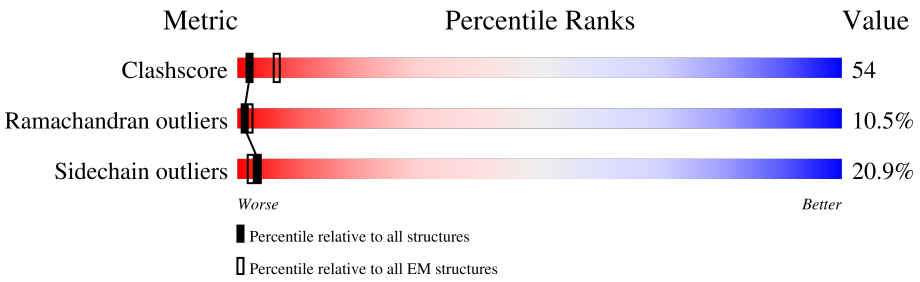
EMDB validation analysis	:	0.0.1.dev70
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 28.00 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)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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	451	22%; 16%; 57%; 17%; • ; 9%
2	B	445	19%; 20%; 55%; 18%; • ; •
2	G	445	12%; 37%; 35%; 19%; • ; 6%
3	D	331	7%; 55%; 32%; • ; 9%
4	F	451	8%; 38%; 37%; 16%; • ; 7%

2 Entry composition (i)

There are 12 unique types of molecules in this entry. The entry contains 15757 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 Tubulin alpha-1A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	412	3227	2043	551	613	20	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	265	GLY	ALA	conflict	UNP P02550

- Molecule 2 is a protein called Beta tubulin.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	426	3351	2105	575	646	25	0	0
2	G	419	3237	2037	544	631	25	0	0

- Molecule 3 is a protein called Kinesin-like protein KIF2C.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	D	301	2368	1496	416	438	18	0	0

- Molecule 4 is a protein called Tubulin alpha-1A chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	F	421	3220	2043	544	612	21	0	0

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	265	ILE	ALA	conflict	UNP P02550

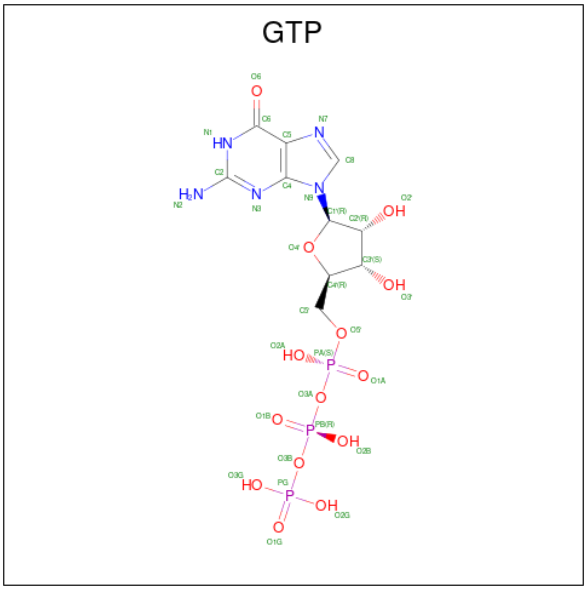
- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
			Total	Zn	
5	A	1	1	1	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

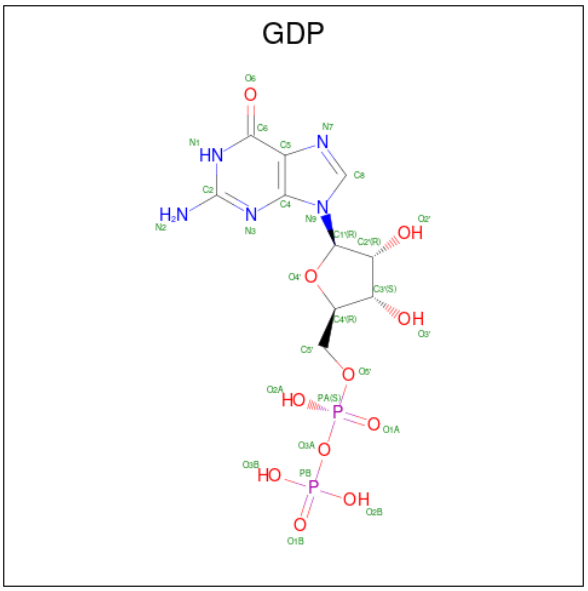
Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
6	A	1	1	1	0
6	D	1	1	1	0
6	F	1	1	1	0

- Molecule 7 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



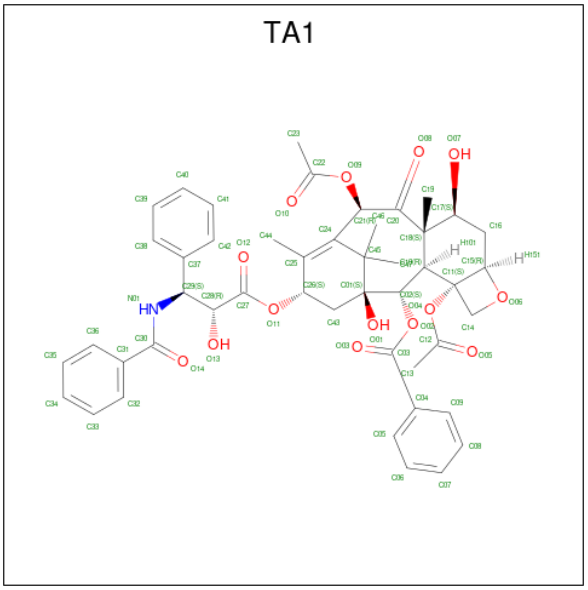
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
7	B	1	32	10	5	14	3	0
7	F	1	32	10	5	14	3	0

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
8	B	1	28	10	5	11	2	0
			Total	C	N	O	P	
8	F	1	28	10	5	11	2	0

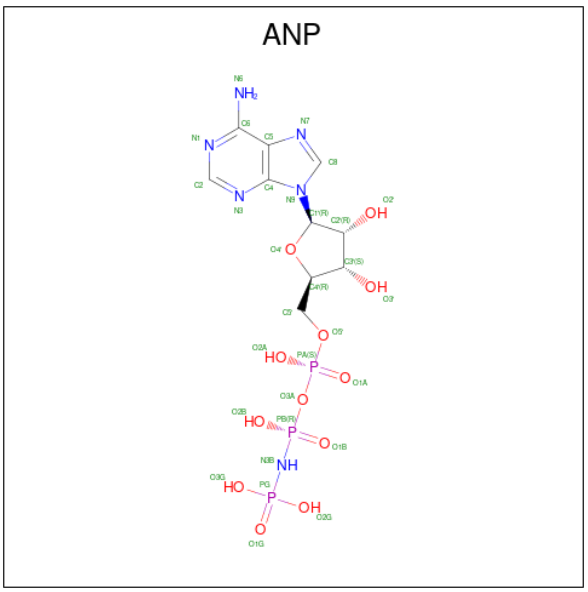
- Molecule 9 is TAXOL (three-letter code: TA1) (formula: $C_{47}H_{51}NO_{14}$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
9	B	1	62	47	1	14	0

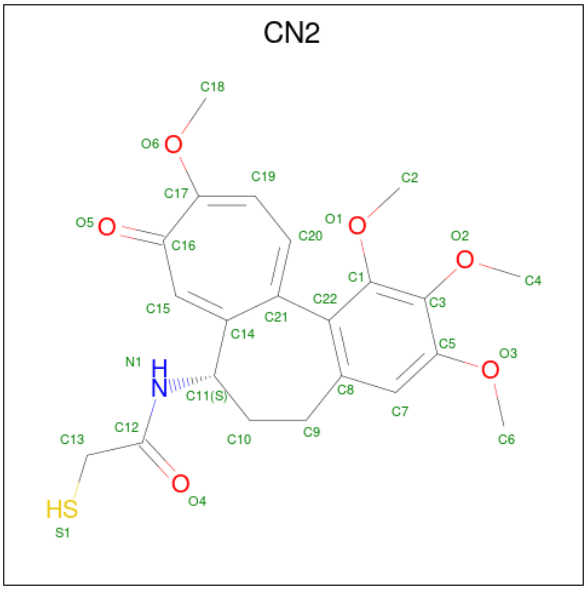
- Molecule 10 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-

letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
10	D	1	31	10	6	12	3	0

- Molecule 11 is 2-MERCAPTO-N-[1,2,3,10-TETRAMETHOXY-9-OXO-5,6,7,9-TETRA HYDRO-BENZO[A]HEPTALEN-7-YL]ACETAMIDE (three-letter code: CN2) (formula: $C_{22}H_{25}NO_6S$).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
11	G	1	30	22	1	6	1	0

- Molecule 12 is water.

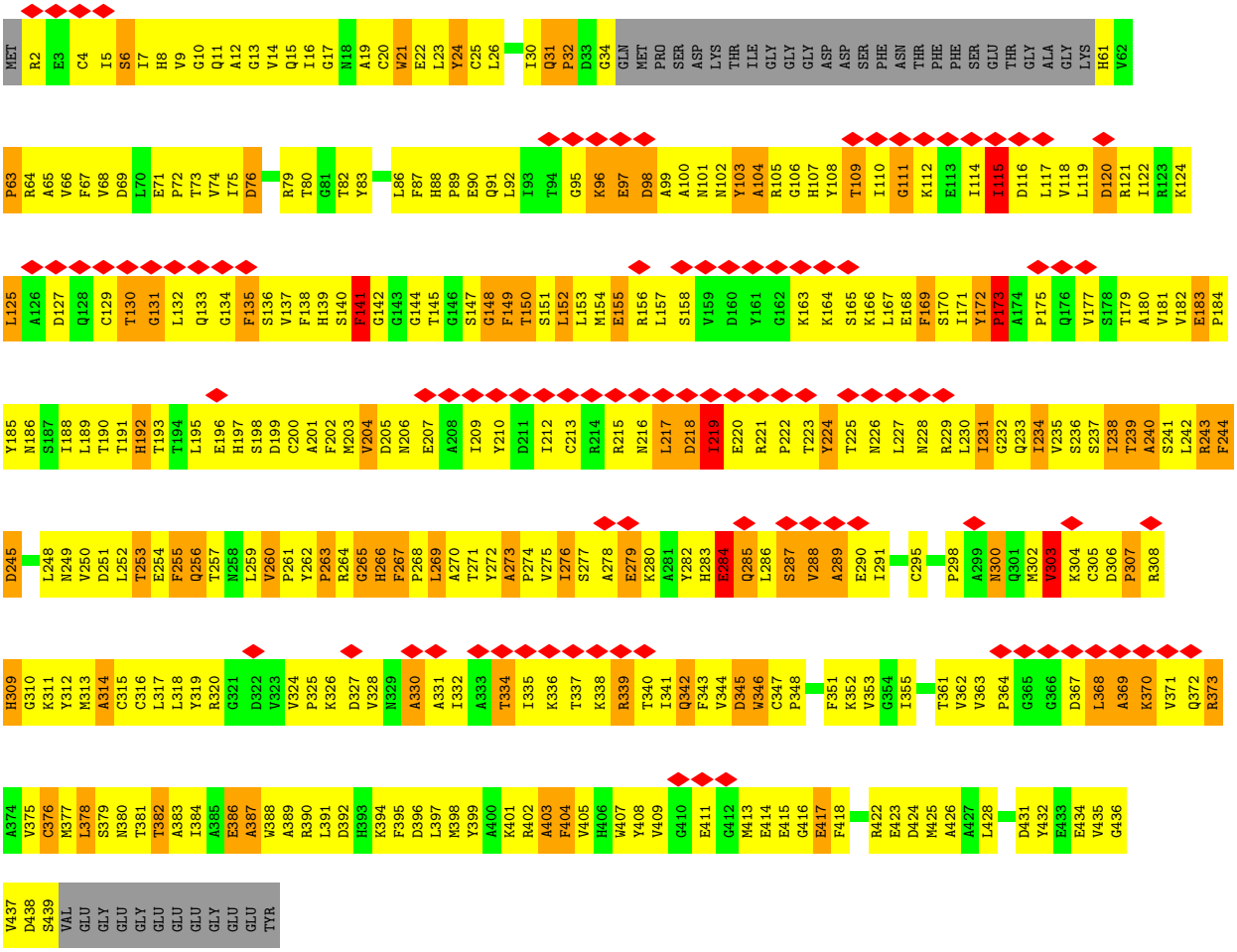
Mol	Chain	Residues	Atoms		AltConf
			Total	O	
12	D	98	98	98	0
			Total	O	
12	F	9	9	9	0

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.

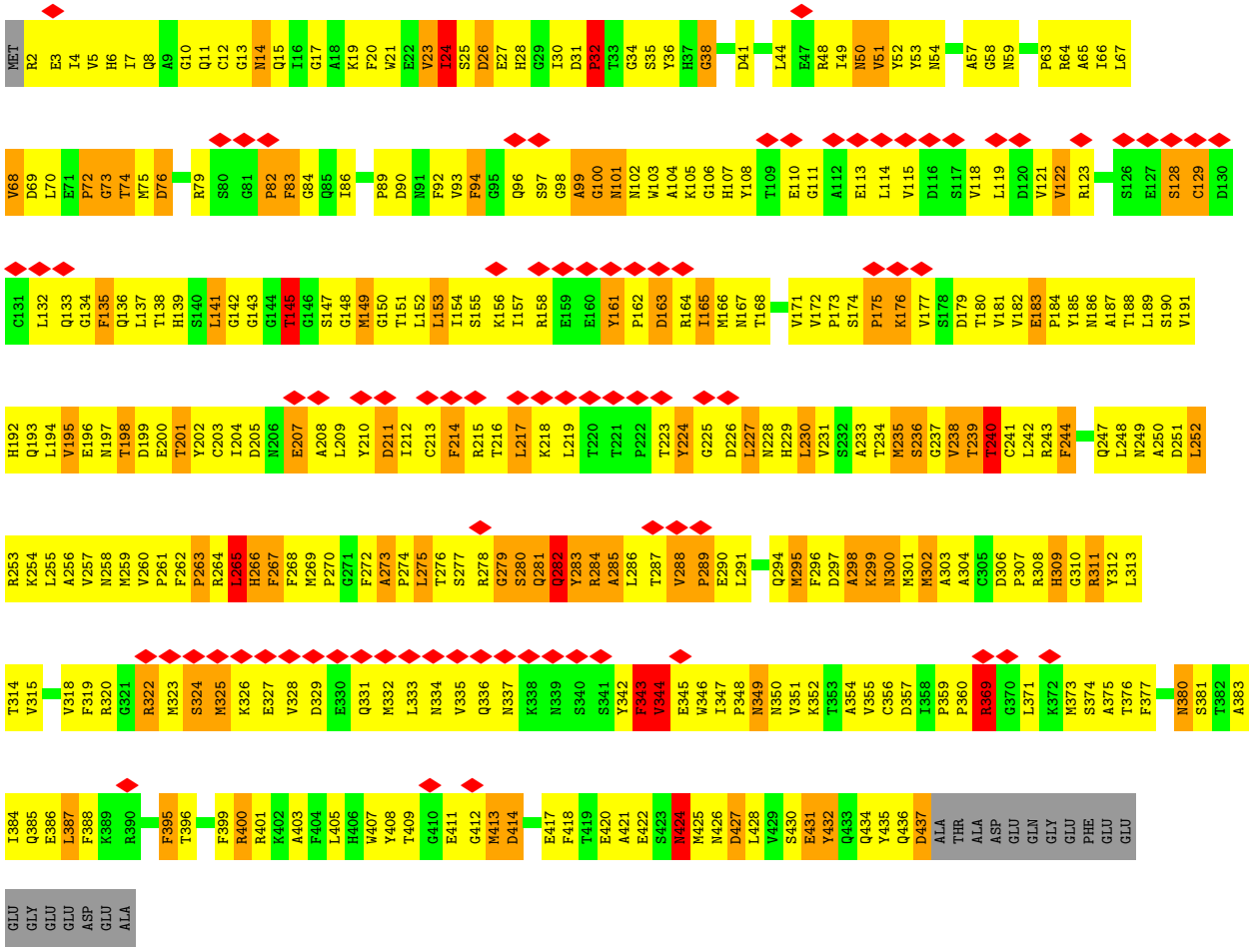
- Molecule 1: Tubulin alpha-1A chain

Chain A: 22% 16% 57% 17% • 9%



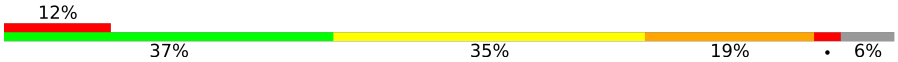
- Molecule 2: Beta tubulin

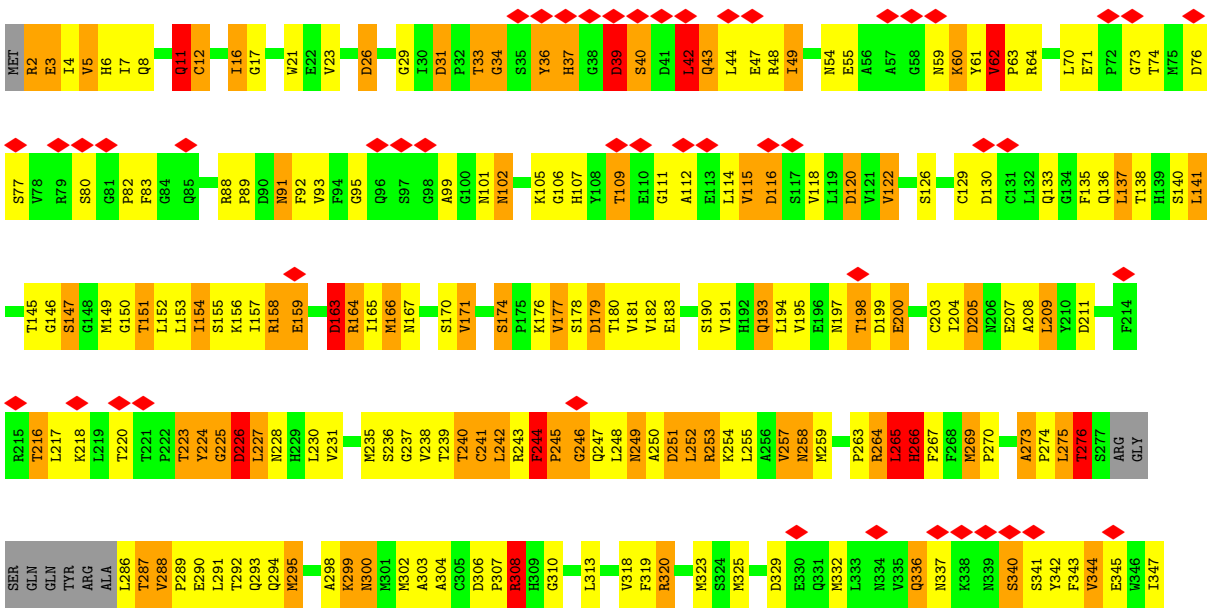
Chain B: 19% 20% 55% 18% • •

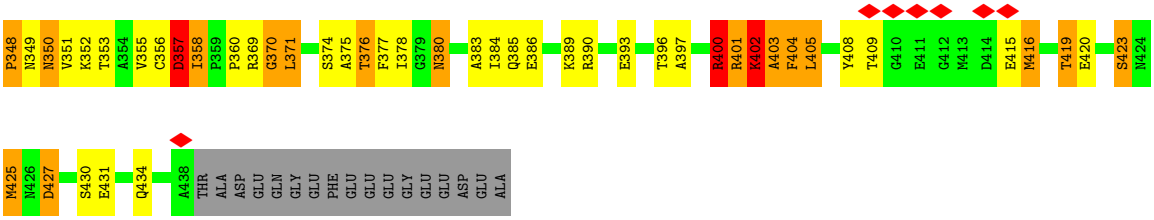


- Molecule 2: Beta tubulin

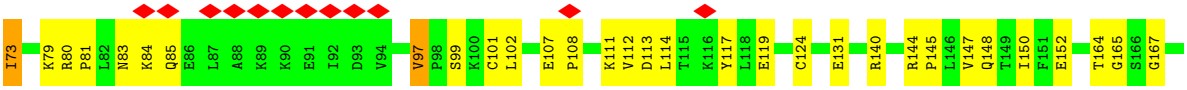
Chain G:

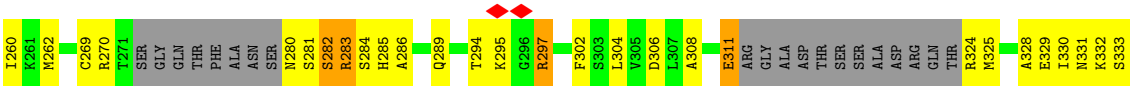


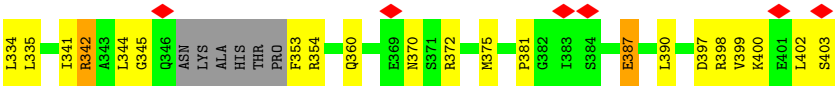




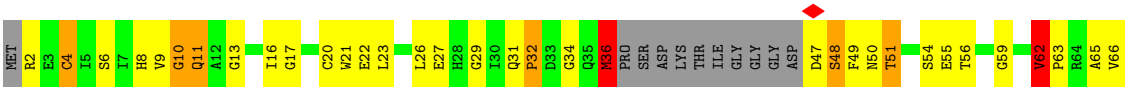
• Molecule 3: Kinesin-like protein KIF2C

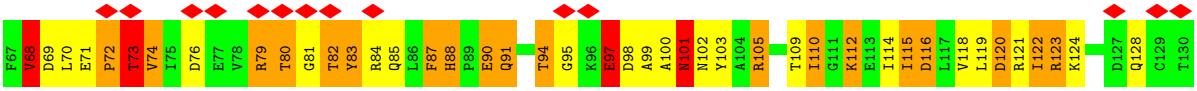


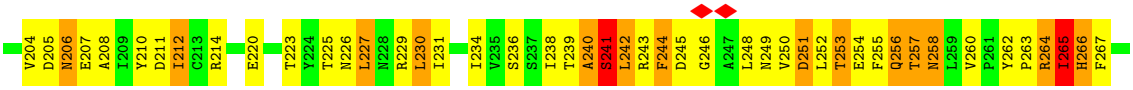


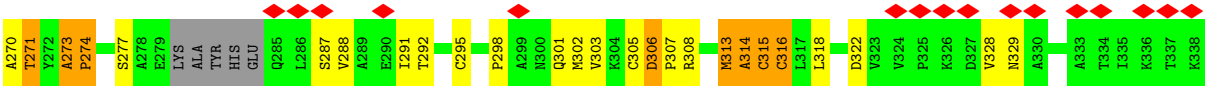


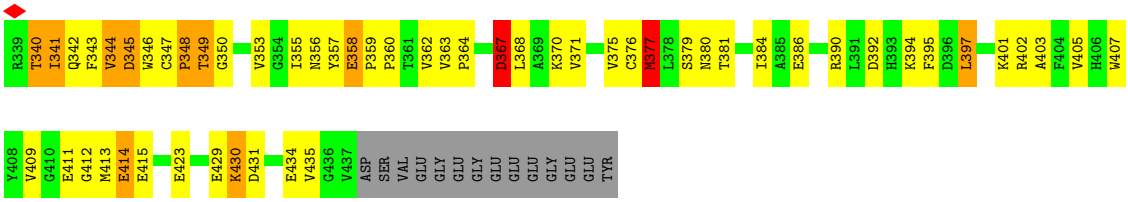
• Molecule 4: Tubulin alpha-1A chain










R339
T340
I341
Q342
F343
V344
D345
W346
C347
P348
T349
G350
V353
G354
I355
N356
Y357
E358
P359
P360
T361
V362
V363
P364
D367
L368
A369
K370
V371
V375
C376
W377
L378
S379
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I384
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4 Experimental information (i)

Property	Value	Source
EM reconstruction method	HELICAL	Depositor
Imposed symmetry	HELICAL, twist=Not provided°, rise=Not provided Å, axial sym=Not provided	Depositor
Number of segments used	Not provided	
Resolution determination method	Not provided	
CTF correction method	Each particle	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/Å^2$)	Not provided	
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	50000	Depositor
Image detector	KODAK SO-163 FILM	Depositor
Maximum map value	55.000	Depositor
Minimum map value	-48.000	Depositor
Average map value	0.563	Depositor
Map value standard deviation	12.837	Depositor
Recommended contour level	11.1	Depositor
Map size (Å)	606.0, 606.0, 246.0	wwPDB
Map dimensions	101, 101, 41	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	6.0, 6.0, 6.0	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, GTP, CN2, GDP, TA1, ANP

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	0.51	0/3300	0.73	0/4482
2	B	0.51	0/3426	0.76	2/4642 (0.0%)
2	G	0.61	0/3309	1.00	20/4494 (0.4%)
3	D	0.46	0/2398	0.71	2/3217 (0.1%)
4	F	0.66	2/3292 (0.1%)	0.95	15/4479 (0.3%)
All	All	0.56	2/15725 (0.0%)	0.84	39/21314 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	97	GLU	CD-OE1	-6.53	1.18	1.25
4	F	97	GLU	CD-OE2	-5.40	1.19	1.25

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	160	ASP	CB-CG-OD2	6.88	124.49	118.30
2	G	205	ASP	CB-CG-OD2	6.84	124.45	118.30
2	G	163	ASP	CB-CG-OD2	6.73	124.36	118.30
4	F	244	PHE	N-CA-C	6.73	129.17	111.00
2	G	116	ASP	CB-CG-OD2	6.32	123.99	118.30
2	G	179	ASP	CB-CG-OD2	6.29	123.97	118.30
2	G	244	PHE	N-CA-C	6.19	127.70	111.00
4	F	397	LEU	CA-CB-CG	6.14	129.43	115.30
2	G	242	LEU	CA-CB-CG	6.13	129.40	115.30
2	B	235	MET	CG-SD-CE	6.09	109.95	100.20
2	G	26	ASP	CB-CG-OD2	5.95	123.65	118.30
4	F	116	ASP	CB-CG-OD2	5.93	123.63	118.30
3	D	241	GLN	C-N-CA	-5.91	106.93	121.70
2	G	357	ASP	CB-CG-OD2	5.90	123.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	F	120	ASP	CB-CG-OD2	5.83	123.54	118.30
2	G	266	HIS	CB-CA-C	5.76	121.91	110.40
4	F	142	GLY	N-CA-C	-5.71	98.84	113.10
4	F	95	GLY	N-CA-C	5.70	127.35	113.10
4	F	76	ASP	CB-CG-OD2	5.62	123.35	118.30
2	G	427	ASP	CB-CG-OD2	5.52	123.27	118.30
3	D	241	GLN	O-C-N	-5.41	114.05	122.70
4	F	97	GLU	OE1-CD-OE2	-5.38	116.84	123.30
4	F	322	ASP	CB-CG-OD2	5.37	123.13	118.30
2	B	217	LEU	N-CA-C	-5.36	96.52	111.00
4	F	36	MET	CG-SD-CE	5.34	108.74	100.20
2	G	211	ASP	CB-CG-OD2	5.33	123.10	118.30
2	G	39	ASP	CB-CG-OD2	5.31	123.08	118.30
2	G	226	ASP	CB-CG-OD2	5.30	123.07	118.30
2	G	199	ASP	CB-CG-OD2	5.28	123.05	118.30
2	G	308	ARG	N-CA-C	-5.27	96.78	111.00
4	F	68	VAL	CB-CA-C	-5.25	101.43	111.40
4	F	199	ASP	CB-CG-OD2	5.23	123.00	118.30
4	F	367	ASP	CB-CG-OD2	5.21	122.99	118.30
2	G	306	ASP	CB-CG-OD2	5.13	122.92	118.30
2	G	31	ASP	CB-CG-OD2	5.08	122.87	118.30
2	G	246	GLY	N-CA-C	-5.07	100.43	113.10
4	F	345	ASP	CB-CG-OD2	5.05	122.85	118.30
2	G	163	ASP	N-CA-CB	-5.03	101.54	110.60
2	G	329	ASP	CB-CG-OD2	5.03	122.82	118.30

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	3227	0	3143	548	0
2	B	3351	0	3229	545	0
2	G	3237	0	3060	269	0
3	D	2368	0	2410	219	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	3220	0	3074	232	0
5	A	1	0	0	0	0
6	A	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	B	32	0	12	4	0
7	F	32	0	12	2	0
8	B	28	0	12	1	0
8	F	28	0	12	1	0
9	B	62	0	51	6	0
10	D	31	0	13	3	0
11	G	30	0	23	8	0
12	D	98	0	0	4	0
12	F	9	0	0	10	0
All	All	15757	0	15051	1665	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 54.

All (1665) 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)
3:D:238:ASP:CA	2:G:419:THR:HB	1.24	1.61
3:D:236:LEU:CD2	2:G:416:MET:CE	2.11	1.28
3:D:237:GLU:O	2:G:420:GLU:HA	1.30	1.28
3:D:238:ASP:CB	2:G:419:THR:HB	1.63	1.27
3:D:112:VAL:HG11	4:F:435:VAL:CG2	1.62	1.27
3:D:236:LEU:CD2	2:G:416:MET:SD	2.25	1.24
3:D:238:ASP:HA	2:G:419:THR:CB	1.67	1.24
3:D:113:ASP:HA	4:F:262:TYR:CD2	1.75	1.22
3:D:238:ASP:HB2	2:G:419:THR:CG2	1.70	1.21
2:B:234:THR:HG21	2:B:270:PRO:HB2	1.23	1.19
3:D:236:LEU:HD21	2:G:416:MET:CE	1.73	1.18
3:D:236:LEU:HD23	2:G:416:MET:SD	1.87	1.14
1:A:243:ARG:NH2	1:A:252:LEU:H	1.45	1.14
2:G:273:ALA:HB3	2:G:274:PRO:HD3	1.22	1.14
3:D:112:VAL:HB	4:F:431:ASP:HB3	1.19	1.14
3:D:237:GLU:HG2	2:G:423:SER:CB	1.78	1.13
3:D:237:GLU:CG	2:G:423:SER:HB3	1.77	1.13
3:D:113:ASP:HB2	4:F:262:TYR:CE2	1.84	1.13
3:D:238:ASP:CA	2:G:419:THR:CB	2.21	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:198:SER:CB	4:F:265:ILE:HD11	1.78	1.12
3:D:353:PHE:N	2:G:434:GLN:HE22	1.45	1.12
4:F:99:ALA:HB2	4:F:145:THR:HG22	1.21	1.11
3:D:176:LEU:HG	3:D:181:GLN:HG3	1.32	1.10
3:D:236:LEU:HD23	2:G:416:MET:CE	1.76	1.10
3:D:238:ASP:CB	2:G:419:THR:CB	2.28	1.10
3:D:353:PHE:N	2:G:434:GLN:NE2	1.97	1.10
3:D:342:ARG:HG2	3:D:342:ARG:HH11	1.11	1.09
3:D:236:LEU:HD21	2:G:416:MET:HE1	1.22	1.08
3:D:237:GLU:HG2	2:G:423:SER:HB3	1.30	1.08
4:F:79:ARG:NH2	4:F:94:THR:HG21	1.68	1.08
2:B:93:VAL:HG11	2:B:118:VAL:HG22	1.30	1.08
4:F:88:HIS:HB2	4:F:91:GLN:HE21	1.15	1.08
4:F:434:GLU:CB	12:F:606:HOH:O	2.01	1.08
4:F:198:SER:HB3	4:F:265:ILE:CD1	1.85	1.06
3:D:114:LEU:HD11	4:F:263:PRO:HG3	1.32	1.06
4:F:273:ALA:CB	4:F:274:PRO:HD3	1.86	1.05
3:D:176:LEU:HG	3:D:181:GLN:CG	1.87	1.03
3:D:112:VAL:HG11	4:F:435:VAL:HG23	1.04	1.03
1:A:243:ARG:HH21	1:A:252:LEU:N	1.57	1.03
2:B:172:VAL:HG11	2:B:387:LEU:HD21	1.37	1.02
3:D:237:GLU:CG	2:G:423:SER:CB	2.36	1.02
3:D:238:ASP:HB2	2:G:419:THR:HG21	1.38	1.01
3:D:237:GLU:H	2:G:420:GLU:HG3	1.20	1.01
1:A:11:GLN:HG3	1:A:74:VAL:HG11	1.43	1.01
4:F:79:ARG:HH22	4:F:94:THR:CG2	1.74	1.01
3:D:112:VAL:CB	4:F:431:ASP:HB3	1.90	1.01
2:G:48:ARG:HH12	2:G:245:PRO:HD2	1.22	1.01
3:D:239:SER:H	2:G:419:THR:HG22	1.24	1.00
1:A:109:THR:HG22	1:A:110:ILE:N	1.70	1.00
4:F:434:GLU:HB2	12:F:606:HOH:O	1.57	1.00
2:B:236:SER:O	2:B:240:THR:HG23	1.61	1.00
3:D:238:ASP:O	2:G:423:SER:HB2	1.60	1.00
4:F:79:ARG:HH22	4:F:94:THR:HG21	0.84	1.00
2:G:273:ALA:CB	2:G:274:PRO:HD3	1.92	0.99
2:B:299:LYS:H	2:B:299:LYS:HD3	1.24	0.99
3:D:402:LEU:HD13	3:D:402:LEU:O	1.61	0.99
3:D:113:ASP:CB	4:F:262:TYR:CE2	2.45	0.98
4:F:99:ALA:CB	4:F:145:THR:HG22	1.94	0.97
3:D:114:LEU:HD21	4:F:263:PRO:CG	1.95	0.96
1:A:98:ASP:HB2	1:A:105:ARG:HH21	1.31	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:238:ASP:O	2:G:423:SER:CB	2.14	0.95
1:A:316:CYS:HB3	1:A:378:LEU:HD11	1.48	0.95
2:G:291:LEU:HD21	2:G:375:ALA:HB2	1.49	0.94
3:D:286:ALA:HB3	3:D:306:ASP:HB3	1.49	0.94
2:B:281:GLN:O	2:B:283:TYR:N	2.00	0.94
2:B:132:LEU:HD23	2:B:164:ARG:HG3	1.50	0.94
1:A:259:LEU:HD11	1:A:378:LEU:HD13	1.47	0.94
1:A:237:SER:HB2	1:A:376:CYS:SG	2.08	0.94
1:A:251:ASP:N	1:A:254:GLU:HG3	1.82	0.93
2:B:70:LEU:H	2:B:145:THR:HG21	1.33	0.93
2:B:273:ALA:HB3	2:B:274:PRO:HD3	1.48	0.93
2:G:291:LEU:HD21	2:G:375:ALA:CB	1.96	0.93
1:A:251:ASP:H	1:A:254:GLU:HG3	1.33	0.93
3:D:114:LEU:HD21	4:F:263:PRO:HG2	1.51	0.93
3:D:237:GLU:O	2:G:420:GLU:CA	2.17	0.93
3:D:241:GLN:HA	2:G:423:SER:OG	1.69	0.92
4:F:273:ALA:CB	4:F:375:VAL:H	1.82	0.92
4:F:431:ASP:N	12:F:706:HOH:O	2.01	0.92
2:B:264:ARG:O	2:B:265:LEU:HB3	1.69	0.92
3:D:112:VAL:CG1	4:F:435:VAL:CG2	2.47	0.91
3:D:113:ASP:HA	4:F:262:TYR:CE2	2.05	0.91
3:D:236:LEU:HD23	2:G:416:MET:HE3	1.52	0.91
1:A:151:SER:HB3	1:A:193:THR:HG21	1.51	0.91
1:A:31:GLN:HB3	1:A:32:PRO:HD2	1.51	0.91
2:B:147:SER:O	2:B:151:THR:HB	1.71	0.91
3:D:238:ASP:HB2	2:G:419:THR:CB	1.95	0.90
4:F:273:ALA:HB3	4:F:274:PRO:HD3	1.53	0.90
2:B:101:ASN:HD21	2:B:143:GLY:HA2	1.38	0.89
3:D:237:GLU:H	2:G:420:GLU:CG	1.85	0.89
1:A:110:ILE:HG23	1:A:111:GLY:H	1.38	0.89
2:B:93:VAL:HG11	2:B:118:VAL:CG2	2.03	0.88
2:B:102:ASN:HD21	2:B:408:TYR:HA	1.38	0.88
2:B:8:GLN:OE1	2:B:67:LEU:HD22	1.72	0.88
1:A:119:LEU:HD23	1:A:122:ILE:HD11	1.53	0.88
1:A:343:PHE:CZ	1:A:351:PHE:CE1	2.61	0.88
1:A:407:TRP:HE1	2:B:260:VAL:HG23	1.38	0.88
1:A:147:SER:HB2	1:A:190:THR:OG1	1.73	0.88
2:B:276:THR:HB	2:B:281:GLN:HG3	1.56	0.88
2:B:311:ARG:HD3	2:B:342:TYR:HA	1.56	0.88
2:G:247:GLN:HG2	2:G:248:LEU:H	1.37	0.88
3:D:111:LYS:HE2	4:F:434:GLU:OE2	1.72	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:264:ARG:HB2	2:B:266:HIS:CD2	2.08	0.87
2:B:360:PRO:HG2	2:B:371:LEU:HB3	1.56	0.87
1:A:122:ILE:HD12	1:A:157:LEU:HD21	1.54	0.87
2:B:10:GLY:HA2	2:B:145:THR:HB	1.55	0.86
3:D:112:VAL:CG1	4:F:435:VAL:HG23	1.98	0.86
3:D:282:SER:OG	3:D:283:ARG:N	2.07	0.86
4:F:273:ALA:HB2	4:F:375:VAL:H	1.38	0.86
2:B:6:HIS:CE1	2:B:8:GLN:HG2	2.10	0.86
2:G:308:ARG:HG3	2:G:308:ARG:HH11	1.39	0.86
2:B:153:LEU:O	2:B:157:ILE:HG12	1.76	0.86
1:A:109:THR:HG22	1:A:110:ILE:H	1.33	0.85
2:B:195:VAL:HG13	2:B:196:GLU:HG2	1.57	0.85
3:D:112:VAL:HB	4:F:431:ASP:CB	2.03	0.85
1:A:184:PRO:HG2	1:A:398:MET:HE1	1.57	0.85
2:B:234:THR:HG21	2:B:270:PRO:CB	2.06	0.85
2:G:332:MET:HG3	2:G:353:THR:HG21	1.55	0.85
3:D:311:GLU:O	4:F:414:GLU:CG	2.25	0.85
2:G:336:GLN:OE1	2:G:351:VAL:HG11	1.75	0.85
2:G:287:THR:HG23	2:G:289:PRO:HD2	1.56	0.85
1:A:264:ARG:O	1:A:266:HIS:N	2.09	0.85
3:D:238:ASP:HA	2:G:419:THR:HB	0.87	0.85
2:B:242:LEU:HD22	2:B:250:ALA:H	1.42	0.85
3:D:342:ARG:HH11	3:D:402:LEU:HB2	1.40	0.85
3:D:353:PHE:CD1	2:G:434:GLN:NE2	2.45	0.85
4:F:178:SER:HB3	11:G:701:CN2:S1	2.17	0.85
3:D:114:LEU:CD1	4:F:263:PRO:HG3	2.07	0.84
1:A:234:ILE:HG13	1:A:270:ALA:HB1	1.59	0.84
4:F:273:ALA:HB1	4:F:274:PRO:HD3	1.57	0.84
4:F:431:ASP:HA	12:F:706:HOH:O	1.77	0.84
1:A:204:VAL:HG11	1:A:231:ILE:HD12	1.59	0.84
3:D:113:ASP:CA	4:F:262:TYR:CE2	2.60	0.84
2:B:19:LYS:HG3	2:B:228:ASN:HB3	1.57	0.84
2:B:20:PHE:CD2	2:B:235:MET:SD	2.71	0.84
2:B:324:SER:HB3	2:B:327:GLU:HG2	1.60	0.84
3:D:282:SER:C	3:D:283:ARG:HG2	1.98	0.84
4:F:341:ILE:HG12	4:F:342:GLN:H	1.43	0.83
4:F:273:ALA:CB	4:F:274:PRO:CD	2.57	0.83
3:D:353:PHE:N	2:G:434:GLN:CD	2.31	0.83
2:B:101:ASN:ND2	2:B:143:GLY:HA2	1.94	0.83
2:B:156:LYS:HE2	2:B:156:LYS:HA	1.61	0.83
2:B:209:LEU:HB3	2:B:227:LEU:HD22	1.59	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:GLU:O	2:B:133:GLN:HB3	1.78	0.83
2:B:148:GLY:O	2:B:151:THR:HG22	1.79	0.83
1:A:316:CYS:HB3	1:A:378:LEU:CD1	2.08	0.83
1:A:106:GLY:O	1:A:111:GLY:HA3	1.78	0.83
2:G:265:LEU:HD12	2:G:265:LEU:O	1.79	0.83
1:A:264:ARG:HB2	1:A:266:HIS:CD2	2.13	0.82
2:B:4:ILE:HD13	2:B:136:GLN:HE21	1.42	0.82
2:B:150:GLY:HA2	2:B:153:LEU:HD22	1.59	0.82
2:B:287:THR:O	2:B:288:VAL:HG23	1.78	0.82
4:F:386:GLU:O	4:F:390:ARG:HG3	1.79	0.82
3:D:237:GLU:CD	2:G:423:SER:HB3	1.99	0.82
2:G:48:ARG:NH1	2:G:245:PRO:HD2	1.93	0.82
1:A:23:LEU:HD23	1:A:236:SER:HB2	1.60	0.82
1:A:151:SER:CB	1:A:193:THR:HG21	2.09	0.82
4:F:341:ILE:HG12	4:F:342:GLN:N	1.95	0.82
2:B:147:SER:HB2	2:B:190:SER:HB3	1.60	0.81
4:F:198:SER:HB3	4:F:265:ILE:HD11	0.89	0.81
1:A:248:LEU:HD23	1:A:353:VAL:O	1.80	0.81
4:F:98:ASP:HB3	2:G:251:ASP:OD2	1.81	0.81
2:B:191:VAL:HG11	2:B:425:MET:HG3	1.60	0.81
1:A:313:MET:HB3	1:A:344:VAL:HG21	1.63	0.81
4:F:105:ARG:NH1	2:G:253:ARG:HH21	1.78	0.81
1:A:109:THR:CG2	1:A:110:ILE:N	2.44	0.80
2:B:20:PHE:CZ	2:B:24:ILE:HD12	2.15	0.80
2:B:110:GLU:O	2:B:113:GLU:HG2	1.79	0.80
3:D:342:ARG:HG2	3:D:342:ARG:NH1	1.87	0.80
1:A:220:GLU:C	1:A:222:PRO:HD3	2.02	0.80
3:D:237:GLU:N	2:G:420:GLU:HG3	1.96	0.80
2:G:205:ASP:OD1	2:G:207:GLU:HB3	1.81	0.80
2:B:236:SER:O	2:B:240:THR:CG2	2.29	0.80
3:D:353:PHE:HD1	2:G:434:GLN:NE2	1.80	0.80
4:F:316:CYS:O	4:F:377:MET:HA	1.81	0.80
1:A:7:ILE:HG22	1:A:66:VAL:HG22	1.63	0.80
3:D:164:THR:HG23	10:D:500:ANP:O1G	1.81	0.80
1:A:234:ILE:HD13	1:A:234:ILE:O	1.81	0.79
2:G:70:LEU:HA	2:G:95:GLY:HA3	1.64	0.79
1:A:267:PHE:N	1:A:267:PHE:CD1	2.49	0.79
2:B:54:ASN:HD21	2:B:64:ARG:HD3	1.46	0.79
2:B:68:VAL:HG12	2:B:149:MET:SD	2.22	0.79
2:B:259:MET:HA	2:B:314:THR:HG21	1.65	0.79
4:F:229:ARG:HH11	4:F:229:ARG:HG2	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:6:SER:HB3	1:A:136:SER:OG	1.81	0.79
1:A:132:LEU:HD23	1:A:132:LEU:H	1.46	0.79
4:F:100:ALA:O	4:F:101:ASN:HB2	1.81	0.79
2:B:413:MET:HG3	2:B:414:ASP:H	1.47	0.78
3:D:113:ASP:HB2	4:F:262:TYR:HE2	1.43	0.78
1:A:199:ASP:HB3	1:A:256:GLN:NE2	1.98	0.78
1:A:204:VAL:HG13	1:A:209:ILE:HD11	1.66	0.78
2:B:264:ARG:HB2	2:B:266:HIS:HD2	1.45	0.78
2:B:265:LEU:HD12	2:B:265:LEU:O	1.83	0.78
1:A:241:SER:O	1:A:244:PHE:HB3	1.82	0.78
2:B:234:THR:CG2	2:B:270:PRO:HB2	2.11	0.78
3:D:84:LYS:HB2	3:D:85:GLN:HE22	1.48	0.78
3:D:84:LYS:HB2	3:D:85:GLN:NE2	1.97	0.78
3:D:282:SER:O	3:D:283:ARG:CG	2.32	0.78
1:A:69:ASP:HA	1:A:145:THR:HG21	1.66	0.78
1:A:155:GLU:HA	1:A:197:HIS:ND1	1.99	0.78
3:D:239:SER:N	2:G:419:THR:HG22	1.99	0.78
2:G:273:ALA:HB3	2:G:274:PRO:CD	2.07	0.77
1:A:172:TYR:C	1:A:172:TYR:HD1	1.87	0.77
2:B:396:THR:HG23	2:B:422:GLU:OE2	1.83	0.77
1:A:243:ARG:HH21	1:A:252:LEU:H	0.79	0.77
3:D:204:TYR:HA	3:D:207:LEU:HD23	1.64	0.77
1:A:11:GLN:HG3	1:A:74:VAL:CG1	2.13	0.77
2:B:35:SER:HB3	2:B:59:ASN:HA	1.65	0.77
2:B:205:ASP:OD1	2:B:304:ALA:HB2	1.84	0.77
3:D:328:ALA:HA	4:F:409:VAL:HG11	1.65	0.77
1:A:110:ILE:HG23	1:A:111:GLY:N	1.99	0.77
1:A:225:THR:O	1:A:229:ARG:HG3	1.85	0.77
2:B:192:HIS:ND1	2:B:424:ASN:OD1	2.18	0.76
2:G:247:GLN:CG	2:G:248:LEU:H	1.97	0.76
2:B:250:ALA:HA	2:B:254:LYS:HE2	1.67	0.76
2:B:259:MET:HG2	2:B:314:THR:HG21	1.67	0.76
2:B:198:THR:O	2:B:265:LEU:HD22	1.85	0.76
1:A:231:ILE:HA	1:A:234:ILE:HG22	1.66	0.76
3:D:282:SER:O	3:D:283:ARG:HG3	1.85	0.76
4:F:133:GLN:HE21	4:F:252:LEU:HG	1.49	0.76
1:A:344:VAL:HG11	1:A:346:TRP:CE2	2.21	0.76
1:A:221:ARG:O	1:A:221:ARG:HD3	1.85	0.76
1:A:163:LYS:O	1:A:164:LYS:HG2	1.86	0.76
1:A:223:THR:HB	1:A:225:THR:HG22	1.67	0.76
3:D:239:SER:H	2:G:419:THR:CG2	1.98	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:167:LEU:HG	1:A:200:CYS:HB3	1.69	0.76
2:B:176:LYS:HE3	2:B:207:GLU:HG3	1.68	0.76
1:A:331:ALA:O	1:A:335:ILE:HG12	1.86	0.75
3:D:238:ASP:CB	2:G:419:THR:CG2	2.55	0.75
4:F:142:GLY:HA3	4:F:183:GLU:HG3	1.68	0.75
1:A:172:TYR:OH	1:A:387:ALA:HB1	1.87	0.75
1:A:205:ASP:CB	1:A:303:VAL:HA	2.17	0.75
3:D:114:LEU:HD21	4:F:263:PRO:HG3	1.66	0.75
3:D:311:GLU:O	4:F:414:GLU:HG3	1.87	0.75
2:B:209:LEU:HG	2:B:230:LEU:HD22	1.69	0.75
3:D:111:LYS:HG2	4:F:434:GLU:OE2	1.86	0.75
2:G:21:TRP:CZ3	2:G:63:PRO:HB3	2.22	0.75
1:A:4:CYS:SG	1:A:252:LEU:HD11	2.27	0.75
1:A:101:ASN:ND2	2:B:254:LYS:HD2	2.02	0.75
1:A:306:ASP:O	1:A:308:ARG:N	2.20	0.75
2:B:19:LYS:HG3	2:B:228:ASN:CB	2.17	0.75
2:G:36:TYR:OH	2:G:40:SER:O	2.03	0.75
1:A:276:ILE:HG23	1:A:369:ALA:CB	2.16	0.74
3:D:342:ARG:NH1	3:D:402:LEU:HB2	2.03	0.74
1:A:7:ILE:HD12	1:A:153:LEU:HD21	1.68	0.74
3:D:342:ARG:HG2	3:D:402:LEU:HB2	1.68	0.74
2:B:168:THR:HB	2:B:201:THR:HG23	1.68	0.74
2:B:217:LEU:C	2:B:219:LEU:H	1.90	0.74
2:B:274:PRO:HG2	2:B:371:LEU:HD21	1.69	0.74
1:A:264:ARG:C	1:A:266:HIS:H	1.91	0.74
3:D:85:GLN:CD	3:D:85:GLN:H	1.90	0.74
3:D:353:PHE:N	2:G:434:GLN:OE1	2.20	0.74
1:A:317:LEU:HB3	1:A:319:TYR:HE1	1.52	0.74
4:F:70:LEU:HD23	4:F:110:ILE:HG23	1.69	0.74
1:A:362:VAL:HG13	1:A:368:LEU:HD12	1.68	0.74
2:B:242:LEU:HD13	2:B:250:ALA:C	2.08	0.74
3:D:117:TYR:OH	4:F:430:LYS:HE3	1.88	0.74
2:G:265:LEU:O	2:G:266:HIS:O	2.05	0.74
3:D:345:GLY:O	3:D:402:LEU:HD11	1.87	0.74
4:F:101:ASN:HD22	2:G:254:LYS:HG2	1.53	0.74
2:B:103:TRP:CZ3	2:B:108:TYR:HE1	2.05	0.73
3:D:236:LEU:HD21	2:G:416:MET:SD	2.23	0.73
1:A:31:GLN:HB3	1:A:32:PRO:CD	2.18	0.73
1:A:104:ALA:HB2	1:A:413:MET:HG3	1.71	0.73
1:A:242:LEU:HG	1:A:250:VAL:O	1.88	0.73
2:B:217:LEU:O	2:B:219:LEU:N	2.22	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:325:MET:HE3	2:B:325:MET:HA	1.70	0.73
3:D:237:GLU:HG2	2:G:423:SER:HB2	1.67	0.73
1:A:104:ALA:CB	1:A:413:MET:HG3	2.18	0.73
3:D:176:LEU:HG	3:D:181:GLN:HG2	1.71	0.73
1:A:7:ILE:HD11	1:A:137:VAL:HG22	1.71	0.73
2:B:8:GLN:CD	2:B:67:LEU:HD22	2.08	0.73
2:B:76:ASP:HA	2:B:79:ARG:HG2	1.71	0.73
1:A:63:PRO:O	1:A:64:ARG:HG2	1.88	0.73
1:A:112:LYS:O	1:A:115:ILE:HG22	1.89	0.73
1:A:103:TYR:CD2	1:A:189:LEU:HD13	2.24	0.73
2:B:191:VAL:CG1	2:B:425:MET:HG3	2.19	0.72
1:A:172:TYR:C	1:A:172:TYR:CD1	2.61	0.72
2:B:356:CYS:SG	2:B:357:ASP:N	2.62	0.72
2:G:247:GLN:HG3	2:G:248:LEU:HG	1.71	0.72
2:G:273:ALA:CB	2:G:274:PRO:CD	2.67	0.72
1:A:105:ARG:O	1:A:110:ILE:HG22	1.89	0.72
2:B:243:ARG:NH2	2:B:252:LEU:HG	2.05	0.72
1:A:7:ILE:CG1	1:A:137:VAL:HG22	2.20	0.72
1:A:312:TYR:O	1:A:344:VAL:HG23	1.90	0.72
2:B:70:LEU:HG	2:B:145:THR:CG2	2.20	0.72
3:D:238:ASP:O	2:G:423:SER:OG	2.07	0.72
3:D:282:SER:C	3:D:283:ARG:CG	2.58	0.72
1:A:425:MET:HE2	1:A:428:LEU:HD23	1.72	0.72
4:F:181:VAL:HB	2:G:258:ASN:ND2	2.05	0.72
4:F:273:ALA:HB3	4:F:274:PRO:CD	2.17	0.72
1:A:166:LYS:HE3	1:A:199:ASP:OD1	1.90	0.72
2:B:48:ARG:HG2	2:B:243:ARG:O	1.90	0.72
2:B:237:GLY:O	2:B:241:CYS:HB3	1.90	0.72
1:A:259:LEU:HD11	1:A:378:LEU:CD1	2.20	0.71
1:A:343:PHE:CZ	1:A:351:PHE:HE1	2.08	0.71
3:D:80:ARG:O	3:D:381:PRO:HG3	1.90	0.71
2:B:111:GLY:O	2:B:115:VAL:HG23	1.89	0.71
2:B:201:THR:OG1	2:B:265:LEU:HD11	1.90	0.71
3:D:238:ASP:C	2:G:419:THR:O	2.28	0.71
3:D:114:LEU:HD11	4:F:263:PRO:CG	2.17	0.71
2:G:251:ASP:C	2:G:253:ARG:H	1.94	0.71
4:F:88:HIS:HB2	4:F:91:GLN:NE2	1.98	0.71
2:G:347:ILE:HG22	2:G:350:ASN:HB3	1.72	0.71
3:D:175:ASP:O	3:D:176:LEU:HB2	1.89	0.71
2:B:431:GLU:OE1	2:B:432:TYR:HA	1.91	0.71
3:D:238:ASP:HA	2:G:419:THR:C	2.11	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:319:PHE:HB2	2:G:355:VAL:HG12	1.73	0.71
3:D:111:LYS:HG2	4:F:434:GLU:CD	2.11	0.71
1:A:12:ALA:HB3	1:A:140:SER:OG	1.91	0.71
2:B:10:GLY:O	2:B:14:ASN:HB2	1.90	0.71
2:G:12:CYS:SG	2:G:171:VAL:HG21	2.30	0.71
1:A:25:CYS:HB2	1:A:30:ILE:O	1.89	0.70
1:A:317:LEU:HD12	1:A:351:PHE:HD2	1.55	0.70
2:B:70:LEU:HG	2:B:145:THR:HG23	1.74	0.70
1:A:242:LEU:HD21	1:A:250:VAL:HB	1.71	0.70
2:B:175:PRO:HD2	2:B:207:GLU:OE2	1.91	0.70
1:A:63:PRO:C	1:A:64:ARG:HG2	2.12	0.70
3:D:147:VAL:O	3:D:150:ILE:HG12	1.92	0.70
2:G:140:SER:HA	2:G:171:VAL:HG23	1.74	0.70
1:A:88:HIS:C	1:A:90:GLU:H	1.95	0.70
2:B:8:GLN:NE2	2:B:17:GLY:HA3	2.06	0.70
2:B:6:HIS:HE1	2:B:8:GLN:HG2	1.52	0.70
2:B:255:LEU:O	2:B:259:MET:HG3	1.91	0.70
2:B:291:LEU:O	2:B:295:MET:HG3	1.91	0.70
1:A:5:ILE:HG22	1:A:6:SER:N	2.07	0.69
1:A:234:ILE:HG21	1:A:302:MET:HE3	1.73	0.69
2:B:24:ILE:HD11	2:B:52:TYR:CE1	2.28	0.69
1:A:244:PHE:HD2	1:A:245:ASP:N	1.89	0.69
2:B:180:THR:HG22	2:B:181:VAL:N	2.07	0.69
2:B:234:THR:O	2:B:238:VAL:HG23	1.92	0.69
2:B:332:MET:HE3	2:B:351:VAL:HG11	1.73	0.69
3:D:113:ASP:CA	4:F:262:TYR:CD2	2.66	0.69
2:G:164:ARG:HE	2:G:164:ARG:HA	1.57	0.69
1:A:148:GLY:O	1:A:151:SER:HB2	1.91	0.69
3:D:342:ARG:HH12	3:D:402:LEU:HD23	1.58	0.69
1:A:222:PRO:HD2	2:B:326:LYS:HB3	1.74	0.69
3:D:236:LEU:CD2	2:G:416:MET:HE3	2.10	0.69
3:D:311:GLU:O	4:F:414:GLU:HG2	1.91	0.69
1:A:298:PRO:HB3	1:A:307:PRO:HD2	1.74	0.69
2:B:251:ASP:O	2:B:253:ARG:N	2.26	0.69
2:B:359:PRO:HB2	2:B:360:PRO:HD2	1.74	0.69
1:A:394:LYS:HG2	2:B:348:PRO:HG3	1.75	0.69
3:D:236:LEU:CD2	2:G:416:MET:HE1	1.96	0.69
4:F:70:LEU:N	4:F:70:LEU:HD12	2.07	0.69
1:A:343:PHE:HZ	1:A:351:PHE:CE1	2.10	0.69
2:G:307:PRO:O	2:G:308:ARG:CD	2.41	0.69
2:G:307:PRO:O	2:G:308:ARG:HD3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:SER:CB	1:A:376:CYS:SG	2.80	0.68
2:B:209:LEU:HD23	2:B:227:LEU:HB3	1.75	0.68
2:B:257:VAL:O	2:B:257:VAL:HG12	1.93	0.68
4:F:431:ASP:CA	12:F:706:HOH:O	2.28	0.68
2:G:54:ASN:HB2	2:G:64:ARG:HD3	1.76	0.68
2:G:337:ASN:HA	2:G:340:SER:HB3	1.76	0.68
1:A:141:PHE:O	1:A:147:SER:HB3	1.93	0.68
1:A:205:ASP:HB3	1:A:303:VAL:HA	1.73	0.68
1:A:217:LEU:HD12	1:A:277:SER:HB3	1.75	0.68
1:A:221:ARG:N	1:A:222:PRO:HD3	2.09	0.68
2:B:242:LEU:CD2	2:B:250:ALA:H	2.07	0.68
3:D:111:LYS:CE	4:F:434:GLU:OE2	2.40	0.68
2:G:352:LYS:HG3	11:G:701:CN2:O5	1.94	0.68
2:B:204:ILE:HD13	2:B:231:VAL:HG22	1.76	0.68
1:A:381:THR:C	1:A:383:ALA:H	1.95	0.68
4:F:423:GLU:OE1	12:F:698:HOH:O	2.12	0.68
2:G:241:CYS:CB	2:G:248:LEU:HD12	2.24	0.68
1:A:7:ILE:HD12	1:A:153:LEU:CD2	2.24	0.68
1:A:115:ILE:CD1	1:A:119:LEU:HG	2.23	0.68
1:A:407:TRP:HE1	2:B:260:VAL:CG2	2.07	0.68
3:D:175:ASP:N	3:D:175:ASP:OD1	2.27	0.68
1:A:95:GLY:O	1:A:97:GLU:N	2.27	0.68
1:A:102:ASN:HB2	1:A:408:TYR:CE2	2.29	0.67
1:A:71:GLU:HG3	2:B:2:ARG:HH21	1.58	0.67
2:B:44:LEU:HD12	2:B:49:ILE:HD13	1.76	0.67
1:A:133:GLN:HG2	1:A:243:ARG:HH22	1.57	0.67
1:A:371:VAL:HG12	1:A:372:GLN:H	1.57	0.67
2:B:66:ILE:C	2:B:67:LEU:HD23	2.15	0.67
2:B:107:HIS:CD2	2:B:151:THR:CG2	2.78	0.67
2:B:108:TYR:CD1	2:B:413:MET:HE1	2.29	0.67
2:B:310:GLY:HA3	2:B:436:GLN:HE21	1.59	0.67
3:D:111:LYS:HG2	4:F:434:GLU:OE1	1.95	0.67
3:D:236:LEU:HD22	2:G:416:MET:SD	2.31	0.67
2:G:133:GLN:HE21	2:G:252:LEU:HB3	1.59	0.67
2:B:299:LYS:HD3	2:B:299:LYS:N	2.04	0.67
2:B:325:MET:CE	2:B:355:VAL:HG21	2.24	0.67
2:B:328:VAL:O	2:B:332:MET:HG2	1.94	0.67
2:G:238:VAL:HG13	2:G:378:ILE:HD11	1.76	0.67
1:A:251:ASP:O	1:A:254:GLU:HB2	1.94	0.67
3:D:112:VAL:CA	4:F:431:ASP:HB3	2.25	0.67
3:D:240:ARG:C	3:D:241:GLN:CG	2.62	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:350:ASN:H	2:G:350:ASN:HD22	1.43	0.67
1:A:100:ALA:CB	1:A:105:ARG:HD3	2.25	0.67
1:A:199:ASP:HB3	1:A:256:GLN:HE21	1.57	0.67
2:B:276:THR:HB	2:B:281:GLN:CG	2.25	0.67
2:B:250:ALA:HB1	2:B:254:LYS:HB2	1.75	0.67
2:B:256:ALA:O	2:B:260:VAL:HG22	1.94	0.67
2:G:247:GLN:CG	2:G:248:LEU:N	2.56	0.67
1:A:152:LEU:HA	1:A:155:GLU:HB2	1.77	0.66
2:B:4:ILE:HG21	2:B:136:GLN:HG2	1.76	0.66
2:B:243:ARG:HH22	2:B:252:LEU:HG	1.59	0.66
3:D:113:ASP:HB2	4:F:262:TYR:CZ	2.31	0.66
1:A:276:ILE:O	1:A:369:ALA:HB2	1.95	0.66
3:D:240:ARG:O	3:D:241:GLN:HG3	1.95	0.66
4:F:123:ARG:HD3	4:F:161:TYR:OH	1.94	0.66
2:G:308:ARG:HG3	2:G:308:ARG:NH1	2.11	0.66
2:G:42:LEU:O	2:G:44:LEU:N	2.29	0.66
2:G:289:PRO:O	2:G:293:GLN:HG3	1.96	0.66
1:A:172:TYR:HD1	1:A:173:PRO:N	1.93	0.66
1:A:341:ILE:HG12	1:A:341:ILE:O	1.95	0.66
2:B:230:LEU:HD23	2:B:231:VAL:N	2.10	0.66
4:F:430:LYS:C	12:F:706:HOH:O	2.32	0.66
3:D:176:LEU:CG	3:D:181:GLN:CG	2.68	0.66
3:D:238:ASP:HA	2:G:419:THR:CA	2.26	0.66
2:G:88:ARG:O	2:G:91:ASN:HB2	1.96	0.66
2:B:265:LEU:HD12	2:B:265:LEU:C	2.16	0.66
3:D:238:ASP:C	2:G:419:THR:HB	2.13	0.66
1:A:68:VAL:HG11	1:A:149:PHE:CZ	2.31	0.65
1:A:217:LEU:HD11	1:A:367:ASP:O	1.96	0.65
1:A:372:GLN:O	1:A:373:ARG:HB3	1.96	0.65
4:F:273:ALA:HB2	4:F:375:VAL:N	2.11	0.65
1:A:305:CYS:SG	1:A:384:ILE:HD13	2.37	0.65
4:F:249:ASN:HB3	4:F:255:PHE:CD2	2.32	0.65
2:B:242:LEU:CD1	2:B:255:LEU:HD11	2.26	0.65
1:A:175:PRO:HG3	1:A:304:LYS:HG2	1.76	0.65
3:D:324:ARG:O	3:D:324:ARG:HG3	1.97	0.65
2:B:182:VAL:HG23	2:B:186:ASN:HD21	1.60	0.65
3:D:193:ARG:O	3:D:197:LEU:HD13	1.95	0.65
1:A:313:MET:HB3	1:A:344:VAL:CG2	2.26	0.65
2:B:66:ILE:CD1	2:B:122:VAL:HG12	2.26	0.65
2:B:431:GLU:O	2:B:434:GLN:HG2	1.97	0.65
1:A:115:ILE:HG23	1:A:116:ASP:N	2.12	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.79	0.65
2:B:242:LEU:HD12	2:B:255:LEU:HD11	1.78	0.65
2:G:241:CYS:HB2	2:G:248:LEU:HD12	1.76	0.65
2:B:267:PHE:N	2:B:267:PHE:CD1	2.62	0.65
1:A:271:THR:HG23	1:A:300:ASN:O	1.97	0.64
1:A:344:VAL:HG12	1:A:345:ASP:N	2.12	0.64
2:B:172:VAL:HG11	2:B:387:LEU:CD2	2.22	0.64
2:B:281:GLN:O	2:B:283:TYR:HB2	1.96	0.64
2:B:284:ARG:O	2:B:286:LEU:N	2.31	0.64
2:B:422:GLU:O	2:B:426:ASN:HB2	1.97	0.64
1:A:206:ASN:OD1	1:A:227:LEU:HD13	1.96	0.64
1:A:224:TYR:CD1	2:B:325:MET:HG2	2.33	0.64
2:B:241:CYS:O	2:B:244:PHE:HB2	1.97	0.64
2:B:325:MET:HE1	2:B:355:VAL:HG11	1.79	0.64
1:A:317:LEU:HD12	1:A:351:PHE:CD2	2.32	0.64
2:B:103:TRP:HZ3	2:B:108:TYR:HE1	1.42	0.64
3:D:202:PRO:HA	3:D:205:ARG:HD2	1.80	0.64
1:A:151:SER:O	1:A:155:GLU:HB2	1.98	0.64
2:B:35:SER:HB3	2:B:59:ASN:CA	2.26	0.64
2:B:66:ILE:HD13	2:B:122:VAL:HG12	1.79	0.64
2:B:243:ARG:HH21	2:B:252:LEU:H	1.45	0.64
2:B:299:LYS:O	2:B:300:ASN:HB2	1.97	0.64
2:B:413:MET:HG2	2:B:418:PHE:HE1	1.61	0.64
1:A:386:GLU:O	1:A:389:ALA:N	2.31	0.64
4:F:208:ALA:O	4:F:212:ILE:HD12	1.98	0.64
2:B:114:LEU:O	2:B:118:VAL:HG23	1.98	0.64
2:B:158:ARG:NE	2:B:197:ASN:O	2.30	0.64
2:G:369:ARG:O	2:G:370:GLY:C	2.34	0.64
1:A:315:CYS:HB3	1:A:377:MET:HE2	1.78	0.64
2:B:105:LYS:O	2:B:110:GLU:HB2	1.97	0.64
2:B:192:HIS:O	2:B:195:VAL:HG12	1.98	0.64
2:B:427:ASP:O	2:B:430:SER:HB3	1.97	0.64
2:B:180:THR:CG2	2:B:181:VAL:N	2.61	0.64
4:F:133:GLN:NE2	4:F:252:LEU:HG	2.13	0.64
1:A:7:ILE:HG22	1:A:66:VAL:CG2	2.28	0.63
1:A:269:LEU:O	1:A:378:LEU:HA	1.99	0.63
1:A:273:ALA:HB3	1:A:274:PRO:HD3	1.81	0.63
1:A:276:ILE:HG23	1:A:369:ALA:HB2	1.80	0.63
3:D:324:ARG:O	3:D:324:ARG:CG	2.46	0.63
4:F:98:ASP:OD1	4:F:99:ALA:N	2.32	0.63
2:G:59:ASN:O	2:G:60:LYS:O	2.16	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:234:ILE:HD13	1:A:234:ILE:C	2.18	0.63
2:B:137:LEU:HD22	2:B:154:ILE:CG2	2.28	0.63
2:B:107:HIS:HD2	2:B:151:THR:CG2	2.12	0.63
2:G:401:ARG:HG3	2:G:401:ARG:HH11	1.63	0.63
4:F:100:ALA:O	4:F:101:ASN:CB	2.46	0.63
4:F:434:GLU:HB3	12:F:606:HOH:O	1.79	0.63
2:G:396:THR:HG22	2:G:400:ARG:HH21	1.63	0.63
11:G:701:CN2:H43	11:G:701:CN2:H62	1.80	0.63
2:B:63:PRO:HD2	2:B:86:ILE:HG12	1.80	0.63
3:D:238:ASP:O	2:G:419:THR:O	2.16	0.63
1:A:175:PRO:HG2	1:A:207:GLU:OE1	1.98	0.63
2:B:133:GLN:HG3	2:B:165:ILE:HD11	1.80	0.63
2:B:205:ASP:OD1	2:B:304:ALA:N	2.32	0.63
2:B:282:GLN:O	2:B:282:GLN:HG2	1.97	0.63
1:A:23:LEU:HD22	1:A:232:GLY:O	1.99	0.63
3:D:144:ARG:HB3	3:D:145:PRO:HD3	1.81	0.63
1:A:7:ILE:CD1	1:A:137:VAL:HG22	2.29	0.62
2:B:315:VAL:HG13	2:B:377:PHE:CE1	2.34	0.62
1:A:152:LEU:HD12	1:A:153:LEU:N	2.14	0.62
4:F:99:ALA:HB2	4:F:145:THR:CG2	2.14	0.62
2:B:115:VAL:HG21	2:B:152:LEU:CD2	2.30	0.62
2:B:253:ARG:O	2:B:256:ALA:N	2.33	0.62
1:A:236:SER:O	1:A:240:ALA:HB3	1.99	0.62
1:A:288:VAL:O	1:A:290:GLU:N	2.33	0.62
2:B:4:ILE:HA	2:B:134:GLY:O	1.99	0.62
4:F:206:ASN:HD21	7:F:601:GTP:HN22	1.47	0.62
1:A:278:ALA:HA	1:A:282:TYR:OH	1.99	0.62
1:A:315:CYS:HB3	1:A:377:MET:CE	2.29	0.62
2:B:318:VAL:HA	2:B:354:ALA:HB3	1.81	0.62
3:D:176:LEU:CG	3:D:181:GLN:HG2	2.28	0.62
2:G:266:HIS:H	2:G:266:HIS:CD2	2.17	0.62
1:A:166:LYS:H	1:A:199:ASP:CG	2.03	0.62
1:A:243:ARG:NH2	1:A:252:LEU:N	2.28	0.62
1:A:402:ARG:O	1:A:403:ALA:C	2.36	0.62
3:D:111:LYS:CD	4:F:434:GLU:OE2	2.47	0.62
1:A:118:VAL:HG11	1:A:149:PHE:HZ	1.65	0.62
1:A:317:LEU:HB3	1:A:319:TYR:CE1	2.33	0.62
2:G:158:ARG:O	2:G:159:GLU:HB2	2.00	0.62
2:G:263:PRO:O	2:G:265:LEU:N	2.31	0.62
2:B:204:ILE:CD1	2:B:231:VAL:HG13	2.30	0.62
3:D:148:GLN:O	3:D:152:GLU:HG3	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:HIS:O	1:A:90:GLU:N	2.33	0.62
2:B:230:LEU:O	2:B:233:ALA:HB3	2.00	0.62
4:F:176:GLN:H	4:F:176:GLN:NE2	1.98	0.62
2:G:237:GLY:HA3	2:G:376:THR:HG21	1.82	0.62
2:G:287:THR:HG22	2:G:290:GLU:HG3	1.82	0.62
2:B:4:ILE:HG23	2:B:134:GLY:O	2.00	0.61
9:B:601:TA1:H463	9:B:601:TA1:H261	1.80	0.61
1:A:168:GLU:OE1	1:A:198:SER:HB2	2.01	0.61
1:A:179:THR:HG21	2:B:248:LEU:HD21	1.82	0.61
2:B:70:LEU:CG	2:B:145:THR:HG23	2.30	0.61
2:B:211:ASP:OD1	2:B:212:ILE:N	2.33	0.61
4:F:229:ARG:HH11	4:F:229:ARG:CG	2.14	0.61
4:F:249:ASN:HB3	4:F:255:PHE:HD2	1.65	0.61
1:A:177:VAL:HG11	2:B:329:ASP:HB3	1.83	0.61
1:A:179:THR:HG22	2:B:352:LYS:NZ	2.15	0.61
2:G:223:THR:HB	2:G:225:GLY:H	1.65	0.61
1:A:179:THR:HG21	2:B:248:LEU:CD2	2.30	0.61
1:A:407:TRP:NE1	2:B:260:VAL:HG23	2.14	0.61
2:B:172:VAL:CG1	2:B:387:LEU:HD21	2.24	0.61
1:A:102:ASN:OD1	1:A:105:ARG:HB3	2.00	0.61
1:A:317:LEU:HD11	1:A:351:PHE:HE2	1.63	0.61
2:B:114:LEU:HD23	2:B:149:MET:CE	2.30	0.61
3:D:210:GLU:HG3	3:D:252:LEU:HD11	1.82	0.61
2:G:403:ALA:C	2:G:405:LEU:H	2.03	0.61
1:A:115:ILE:HG13	1:A:152:LEU:HD13	1.81	0.61
3:D:335:LEU:HD11	4:F:402:ARG:HG3	1.82	0.61
2:G:287:THR:CG2	2:G:290:GLU:HG3	2.30	0.61
1:A:167:LEU:HA	1:A:200:CYS:O	2.01	0.61
1:A:205:ASP:HB2	1:A:303:VAL:HA	1.82	0.61
3:D:230:LYS:HE3	3:D:269:CYS:O	2.01	0.61
1:A:11:GLN:HE21	1:A:74:VAL:HG22	1.66	0.60
1:A:362:VAL:HG13	1:A:368:LEU:HB2	1.83	0.60
3:D:112:VAL:HG11	4:F:435:VAL:HG22	1.78	0.60
3:D:239:SER:HB2	2:G:419:THR:HG22	1.82	0.60
2:G:6:HIS:HE1	2:G:8:GLN:HE21	1.48	0.60
1:A:311:LYS:HE3	1:A:342:GLN:CD	2.22	0.60
2:B:54:ASN:ND2	2:B:64:ARG:HD3	2.15	0.60
3:D:112:VAL:CG1	4:F:435:VAL:HG22	2.32	0.60
1:A:345:ASP:C	1:A:347:CYS:H	2.04	0.60
3:D:79:LYS:HE3	3:D:381:PRO:HB3	1.82	0.60
1:A:177:VAL:CG1	2:B:329:ASP:HB3	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:204:ILE:HG21	2:B:231:VAL:HG22	1.84	0.60
2:B:324:SER:O	2:B:328:VAL:HG23	2.01	0.60
2:B:332:MET:CE	2:B:351:VAL:HG11	2.31	0.60
1:A:181:VAL:HG21	2:B:258:ASN:O	2.01	0.60
2:G:126:SER:O	2:G:129:CYS:HB2	2.01	0.60
1:A:267:PHE:HD1	1:A:267:PHE:H	1.47	0.60
2:B:324:SER:CB	2:B:327:GLU:HG2	2.30	0.60
3:D:114:LEU:CD2	4:F:263:PRO:HG3	2.31	0.60
2:G:136:GLN:HA	2:G:167:ASN:O	2.02	0.60
2:G:151:THR:HB	2:G:193:GLN:HG2	1.83	0.60
2:G:158:ARG:O	2:G:159:GLU:CB	2.49	0.60
1:A:119:LEU:O	1:A:122:ILE:HG12	2.02	0.60
2:B:49:ILE:O	2:B:51:VAL:N	2.35	0.60
4:F:105:ARG:CZ	2:G:253:ARG:HH21	2.14	0.60
4:F:115:ILE:CD1	4:F:119:LEU:HD13	2.32	0.60
1:A:229:ARG:NH1	1:A:363:VAL:HG21	2.16	0.60
1:A:248:LEU:CD2	1:A:353:VAL:O	2.49	0.60
2:B:324:SER:C	2:B:326:LYS:H	2.03	0.60
2:G:205:ASP:OD2	2:G:390:ARG:NH1	2.34	0.60
1:A:284:GLU:O	1:A:286:LEU:N	2.35	0.60
3:D:207:LEU:HB3	3:D:209:LEU:HG	1.83	0.60
3:D:329:GLU:HA	3:D:332:LYS:HE3	1.83	0.60
1:A:169:PHE:CE1	1:A:235:VAL:HG22	2.36	0.59
1:A:191:THR:HG21	1:A:425:MET:SD	2.41	0.59
2:B:205:ASP:OD1	2:B:304:ALA:CB	2.50	0.59
2:B:279:GLY:O	2:B:282:GLN:HB3	2.01	0.59
2:B:408:TYR:CG	2:B:418:PHE:HZ	2.20	0.59
1:A:435:VAL:HG12	1:A:435:VAL:O	2.01	0.59
2:G:164:ARG:HE	2:G:164:ARG:CA	2.14	0.59
2:G:247:GLN:HG2	2:G:248:LEU:N	2.13	0.59
2:B:70:LEU:N	2:B:145:THR:HG21	2.11	0.59
2:B:285:ALA:HB1	2:B:290:GLU:HG2	1.82	0.59
1:A:6:SER:HA	1:A:136:SER:O	2.03	0.59
1:A:344:VAL:HG11	1:A:346:TRP:NE1	2.16	0.59
2:B:141:LEU:CD1	2:B:141:LEU:N	2.65	0.59
1:A:115:ILE:HD13	1:A:115:ILE:O	2.02	0.59
2:B:102:ASN:ND2	2:B:407:TRP:O	2.35	0.59
1:A:371:VAL:HG12	1:A:372:GLN:N	2.17	0.59
2:B:30:ILE:HD13	2:B:53:TYR:CE2	2.38	0.59
2:B:68:VAL:CG1	2:B:149:MET:SD	2.90	0.59
2:B:115:VAL:HG21	2:B:152:LEU:HD23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:299:LYS:O	2:B:300:ASN:CB	2.51	0.59
3:D:97:VAL:O	3:D:97:VAL:HG22	2.02	0.59
2:G:275:LEU:O	2:G:276:THR:HB	2.03	0.59
1:A:278:ALA:HB2	1:A:369:ALA:HA	1.85	0.59
2:B:161:TYR:C	2:B:163:ASP:H	2.05	0.59
2:B:89:PRO:HA	2:B:92:PHE:CD1	2.38	0.58
2:B:299:LYS:H	2:B:299:LYS:CD	2.07	0.58
3:D:294:THR:HG23	3:D:295:LYS:H	1.68	0.58
4:F:66:VAL:HG11	4:F:122:ILE:HG22	1.85	0.58
4:F:70:LEU:N	4:F:70:LEU:CD1	2.65	0.58
4:F:264:ARG:O	4:F:266:HIS:CD2	2.56	0.58
1:A:413:MET:O	1:A:414:GLU:HG3	2.03	0.58
2:B:198:THR:HG22	2:B:265:LEU:HD22	1.85	0.58
2:G:348:PRO:O	2:G:350:ASN:N	2.36	0.58
1:A:407:TRP:O	1:A:411:GLU:HG2	2.02	0.58
2:B:349:ASN:C	2:B:349:ASN:HD22	2.06	0.58
4:F:265:ILE:CG2	4:F:267:PHE:CZ	2.86	0.58
2:B:70:LEU:H	2:B:145:THR:CG2	2.10	0.58
2:B:270:PRO:HA	2:B:377:PHE:O	2.04	0.58
1:A:2:ARG:N	1:A:131:GLY:O	2.36	0.58
1:A:381:THR:C	1:A:383:ALA:N	2.56	0.58
2:B:151:THR:OG1	2:B:193:GLN:HB3	2.03	0.58
3:D:304:LEU:N	3:D:304:LEU:HD22	2.18	0.58
4:F:181:VAL:HB	2:G:258:ASN:HD22	1.69	0.58
1:A:166:LYS:HD2	1:A:197:HIS:O	2.04	0.58
2:B:180:THR:CG2	2:B:181:VAL:H	2.17	0.58
4:F:168:GLU:HG2	4:F:201:ALA:HB2	1.85	0.58
1:A:88:HIS:C	1:A:90:GLU:N	2.57	0.58
1:A:268:PRO:HA	1:A:379:SER:O	2.04	0.58
2:B:320:ARG:O	2:B:359:PRO:HA	2.04	0.58
3:D:328:ALA:CA	4:F:409:VAL:HG11	2.31	0.58
2:B:183:GLU:HB3	2:B:184:PRO:CD	2.33	0.58
2:B:253:ARG:O	2:B:254:LYS:C	2.42	0.58
2:B:307:PRO:HB3	2:B:312:TYR:OH	2.04	0.58
1:A:119:LEU:CD2	1:A:122:ILE:HD11	2.28	0.58
1:A:218:ASP:O	1:A:219:ILE:HG23	2.04	0.58
2:B:70:LEU:C	2:B:99:ALA:HB2	2.24	0.58
1:A:63:PRO:HD3	1:A:86:LEU:O	2.04	0.58
2:B:93:VAL:CG1	2:B:118:VAL:HG22	2.19	0.58
4:F:298:PRO:HA	4:F:301:GLN:NE2	2.19	0.58
1:A:317:LEU:HD11	1:A:351:PHE:CE2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:114:LEU:CD2	4:F:263:PRO:CG	2.79	0.57
1:A:264:ARG:HB2	1:A:266:HIS:HD2	1.67	0.57
3:D:111:LYS:CG	4:F:434:GLU:OE2	2.51	0.57
4:F:313:MET:O	4:F:314:ALA:HB2	2.04	0.57
2:B:19:LYS:CG	2:B:228:ASN:HB3	2.31	0.57
3:D:387:GLU:CD	3:D:387:GLU:H	2.07	0.57
4:F:301:GLN:HE22	4:F:307:PRO:HD3	1.70	0.57
1:A:117:LEU:HD11	1:A:121:ARG:HH22	1.69	0.57
1:A:202:PHE:CE2	1:A:378:LEU:HD22	2.38	0.57
1:A:362:VAL:HG11	1:A:368:LEU:O	2.04	0.57
2:B:5:VAL:CG2	2:B:135:PHE:HD2	2.18	0.57
4:F:8:HIS:CD2	4:F:17:GLY:HA3	2.39	0.57
2:G:135:PHE:HB2	2:G:166:MET:CE	2.34	0.57
1:A:338:LYS:O	1:A:340:THR:N	2.34	0.57
2:B:132:LEU:CD2	2:B:164:ARG:HG3	2.32	0.57
2:B:217:LEU:C	2:B:219:LEU:N	2.55	0.57
2:B:301:MET:CE	2:B:377:PHE:HE2	2.17	0.57
2:B:319:PHE:HA	2:B:375:ALA:HA	1.86	0.57
3:D:237:GLU:HG3	2:G:423:SER:CB	2.32	0.57
8:F:603:GDP:O3B	2:G:145:THR:HG23	2.05	0.57
2:G:357:ASP:OD2	2:G:357:ASP:N	2.38	0.57
4:F:11:GLN:HB3	7:F:601:GTP:O2A	2.04	0.57
4:F:69:ASP:C	4:F:70:LEU:HD12	2.25	0.57
4:F:249:ASN:CB	4:F:255:PHE:CD2	2.87	0.57
2:G:358:ILE:O	2:G:358:ILE:HG23	2.04	0.57
1:A:152:LEU:HA	1:A:155:GLU:CB	2.35	0.57
1:A:369:ALA:O	1:A:370:LYS:HB3	2.03	0.57
4:F:346:TRP:CE3	4:F:347:CYS:HB2	2.40	0.57
2:G:240:THR:HG21	2:G:320:ARG:CZ	2.34	0.57
2:G:266:HIS:HB3	2:G:380:ASN:HD21	1.70	0.57
1:A:286:LEU:HD12	1:A:290:GLU:HG2	1.87	0.57
1:A:345:ASP:O	1:A:347:CYS:N	2.38	0.57
2:B:274:PRO:CG	2:B:371:LEU:HD21	2.34	0.57
2:B:319:PHE:CD2	2:B:375:ALA:HB2	2.40	0.57
1:A:362:VAL:CG1	1:A:368:LEU:HB2	2.35	0.57
4:F:29:GLY:O	4:F:36:MET:HB3	2.05	0.57
1:A:19:ALA:CB	1:A:228:ASN:HB3	2.35	0.57
1:A:209:ILE:CG2	1:A:227:LEU:HD22	2.35	0.57
2:B:50:ASN:O	2:B:64:ARG:NH2	2.38	0.57
3:D:238:ASP:CB	2:G:419:THR:HG21	2.23	0.57
4:F:328:VAL:HG11	4:F:353:VAL:HG11	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:SER:HA	1:A:199:ASP:OD2	2.04	0.56
1:A:313:MET:O	1:A:314:ALA:HB2	2.04	0.56
2:B:30:ILE:HA	2:B:35:SER:O	2.04	0.56
2:B:259:MET:CA	2:B:314:THR:HG21	2.35	0.56
4:F:265:ILE:HG22	4:F:267:PHE:CZ	2.40	0.56
1:A:331:ALA:O	1:A:334:THR:HG22	2.05	0.56
1:A:409:VAL:C	1:A:411:GLU:H	2.09	0.56
2:B:6:HIS:HB3	2:B:65:ALA:HB2	1.87	0.56
2:B:283:TYR:C	2:B:284:ARG:HG2	2.25	0.56
4:F:187:SER:O	4:F:191:THR:HG22	2.05	0.56
1:A:175:PRO:HG3	1:A:304:LYS:CG	2.35	0.56
2:B:4:ILE:HD13	2:B:136:GLN:NE2	2.18	0.56
2:B:14:ASN:OD1	2:B:75:MET:HG2	2.05	0.56
2:B:182:VAL:HG23	2:B:186:ASN:ND2	2.20	0.56
2:B:216:THR:O	2:B:217:LEU:HD12	2.05	0.56
3:D:240:ARG:O	3:D:241:GLN:CG	2.54	0.56
4:F:23:LEU:HD23	4:F:236:SER:HB2	1.87	0.56
4:F:308:ARG:HA	4:F:340:THR:HG21	1.85	0.56
1:A:16:ILE:HD12	1:A:171:ILE:HD11	1.87	0.56
1:A:388:TRP:CE3	1:A:388:TRP:HA	2.41	0.56
2:B:149:MET:O	2:B:153:LEU:HD13	2.05	0.56
3:D:342:ARG:NH1	3:D:342:ARG:CG	2.65	0.56
4:F:180:ALA:O	4:F:183:GLU:HB2	2.05	0.56
2:G:203:CYS:SG	2:G:267:PHE:HB3	2.45	0.56
2:G:287:THR:CG2	2:G:289:PRO:HD2	2.32	0.56
2:G:403:ALA:O	2:G:405:LEU:N	2.38	0.56
1:A:210:TYR:CE2	1:A:227:LEU:HD11	2.40	0.56
2:B:139:HIS:HE1	2:B:168:THR:HG23	1.71	0.56
2:B:312:TYR:O	2:B:344:VAL:HB	2.05	0.56
2:G:135:PHE:HB2	2:G:166:MET:HE1	1.86	0.56
1:A:71:GLU:HG3	2:B:2:ARG:NH2	2.18	0.56
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.88	0.56
2:B:147:SER:O	2:B:151:THR:CB	2.51	0.56
1:A:11:GLN:HE22	2:B:249:ASN:ND2	2.03	0.56
1:A:110:ILE:CG2	1:A:111:GLY:H	2.15	0.56
1:A:139:HIS:CE1	1:A:170:SER:HB3	2.40	0.56
2:B:31:ASP:O	2:B:32:PRO:C	2.44	0.56
3:D:329:GLU:O	3:D:332:LYS:HG2	2.06	0.56
2:G:226:ASP:OD1	2:G:226:ASP:N	2.37	0.56
1:A:242:LEU:C	1:A:244:PHE:H	2.09	0.56
1:A:394:LYS:HG2	2:B:348:PRO:CG	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:THR:OG1	2:B:193:GLN:CB	2.54	0.56
2:B:166:MET:HB3	2:B:198:THR:OG1	2.06	0.56
2:G:247:GLN:CG	2:G:248:LEU:HG	2.36	0.56
1:A:216:ASN:O	1:A:217:LEU:HB2	2.05	0.56
1:A:231:ILE:HA	1:A:234:ILE:CG2	2.36	0.56
1:A:253:THR:O	1:A:256:GLN:HG2	2.06	0.56
2:B:70:LEU:CD1	2:B:145:THR:HG23	2.35	0.56
2:B:190:SER:O	2:B:194:LEU:HG	2.06	0.56
3:D:165:GLY:H	10:D:500:ANP:HNB1	1.52	0.56
2:B:191:VAL:HA	2:B:194:LEU:HD12	1.87	0.55
2:B:204:ILE:HG21	2:B:231:VAL:CG2	2.36	0.55
2:B:210:TYR:HD2	2:B:227:LEU:HD21	1.71	0.55
2:B:311:ARG:HD2	2:B:344:VAL:H	1.71	0.55
1:A:436:GLY:C	1:A:438:ASP:H	2.08	0.55
2:B:119:LEU:O	2:B:123:ARG:HG3	2.06	0.55
2:B:310:GLY:CA	2:B:436:GLN:HE21	2.19	0.55
2:B:422:GLU:O	2:B:426:ASN:N	2.37	0.55
1:A:408:TYR:CD1	1:A:418:PHE:HZ	2.24	0.55
2:B:239:THR:HG22	2:B:240:THR:N	2.22	0.55
2:G:177:VAL:HG12	2:G:177:VAL:O	2.07	0.55
2:G:191:VAL:HG11	2:G:425:MET:CE	2.37	0.55
2:B:19:LYS:O	2:B:23:VAL:HG23	2.06	0.55
2:B:325:MET:HE2	2:B:355:VAL:HG21	1.87	0.55
3:D:81:PRO:HB3	3:D:131:GLU:HB2	1.89	0.55
3:D:227:LEU:HD22	3:D:262:MET:HE3	1.87	0.55
2:G:209:LEU:HB3	2:G:227:LEU:HD11	1.88	0.55
2:B:223:THR:HG22	2:B:224:TYR:N	2.21	0.55
2:B:272:PHE:HB3	2:B:275:LEU:HD22	1.88	0.55
3:D:240:ARG:C	3:D:241:GLN:HG2	2.27	0.55
4:F:256:GLN:C	4:F:258:ASN:N	2.59	0.55
4:F:265:ILE:O	4:F:266:HIS:O	2.24	0.55
2:G:5:VAL:HG22	2:G:135:PHE:CD2	2.41	0.55
2:G:180:THR:HG21	2:G:182:VAL:HG22	1.89	0.55
1:A:5:ILE:CG2	1:A:6:SER:N	2.70	0.55
1:A:150:THR:O	1:A:153:LEU:N	2.40	0.55
1:A:381:THR:OG1	1:A:383:ALA:HB3	2.07	0.55
2:B:424:ASN:C	2:B:424:ASN:HD22	2.09	0.55
3:D:294:THR:HG23	3:D:295:LYS:N	2.22	0.55
2:B:5:VAL:HG22	2:B:135:PHE:CD2	2.42	0.55
2:B:250:ALA:CA	2:B:254:LYS:HE2	2.35	0.55
1:A:118:VAL:HG21	1:A:149:PHE:CZ	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:LEU:O	2:B:49:ILE:HG12	2.07	0.54
2:B:239:THR:O	2:B:241:CYS:N	2.41	0.54
2:G:171:VAL:HA	2:G:204:ILE:O	2.07	0.54
4:F:252:LEU:O	4:F:253:THR:C	2.45	0.54
2:B:324:SER:C	2:B:326:LYS:N	2.59	0.54
2:G:2:ARG:HH11	2:G:133:GLN:HA	1.72	0.54
1:A:101:ASN:CG	2:B:254:LYS:HD2	2.27	0.54
1:A:172:TYR:OH	1:A:387:ALA:O	2.24	0.54
2:B:67:LEU:HD23	2:B:67:LEU:N	2.22	0.54
3:D:210:GLU:HG3	3:D:252:LEU:CD1	2.36	0.54
2:G:342:TYR:N	2:G:342:TYR:CD2	2.75	0.54
1:A:9:VAL:CG1	1:A:139:HIS:HB3	2.38	0.54
1:A:115:ILE:HD13	1:A:115:ILE:C	2.28	0.54
2:B:165:ILE:HD13	2:B:165:ILE:H	1.71	0.54
2:G:408:TYR:O	2:G:409:THR:C	2.45	0.54
1:A:6:SER:O	1:A:65:ALA:HB1	2.07	0.54
1:A:98:ASP:CB	1:A:105:ARG:HH21	2.14	0.54
2:B:20:PHE:CE2	2:B:24:ILE:HD12	2.43	0.54
2:B:194:LEU:C	2:B:196:GLU:H	2.11	0.54
3:D:237:GLU:HG3	2:G:423:SER:OG	2.08	0.54
2:G:223:THR:HB	2:G:225:GLY:N	2.23	0.54
1:A:17:GLY:O	1:A:21:TRP:HB2	2.08	0.54
4:F:256:GLN:C	4:F:258:ASN:H	2.11	0.54
2:G:194:LEU:O	2:G:265:LEU:CD2	2.56	0.54
1:A:382:THR:O	1:A:382:THR:HG22	2.05	0.54
2:B:27:GLU:O	2:B:27:GLU:HG2	2.08	0.54
2:B:424:ASN:C	2:B:424:ASN:ND2	2.62	0.54
2:B:427:ASP:OD1	2:B:428:LEU:N	2.41	0.54
2:G:401:ARG:HG3	2:G:401:ARG:NH1	2.23	0.54
1:A:173:PRO:HB2	1:A:391:LEU:CD1	2.38	0.54
1:A:408:TYR:O	1:A:411:GLU:N	2.39	0.54
2:B:323:MET:HG3	2:B:328:VAL:HG21	1.90	0.54
2:B:343:PHE:O	2:B:344:VAL:O	2.26	0.54
1:A:110:ILE:O	1:A:112:LYS:N	2.41	0.53
1:A:248:LEU:HB3	1:A:355:ILE:H	1.73	0.53
1:A:339:ARG:C	1:A:341:ILE:H	2.11	0.53
2:B:31:ASP:HB3	2:B:32:PRO:HD2	1.90	0.53
2:B:133:GLN:HE21	2:B:252:LEU:HB2	1.73	0.53
2:B:213:CYS:SG	2:B:219:LEU:HD23	2.48	0.53
1:A:163:LYS:O	1:A:163:LYS:HG2	2.08	0.53
1:A:324:VAL:O	1:A:327:ASP:HB2	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:259:MET:CG	2:B:314:THR:HG21	2.36	0.53
3:D:255:CYS:SG	3:D:257:ASP:HB2	2.47	0.53
3:D:331:ASN:O	3:D:335:LEU:HG	2.07	0.53
2:B:21:TRP:CZ2	2:B:65:ALA:HB2	2.44	0.53
2:B:36:TYR:CZ	2:B:38:GLY:HA3	2.43	0.53
2:B:325:MET:CE	2:B:355:VAL:HG11	2.38	0.53
1:A:5:ILE:O	1:A:135:PHE:HA	2.09	0.53
1:A:98:ASP:O	1:A:110:ILE:HD13	2.08	0.53
1:A:179:THR:HG22	2:B:352:LYS:HZ1	1.73	0.53
1:A:243:ARG:CZ	1:A:252:LEU:HG	2.39	0.53
2:B:4:ILE:CG2	2:B:136:GLN:HG2	2.38	0.53
2:B:68:VAL:HG12	2:B:149:MET:CE	2.38	0.53
2:B:204:ILE:HD13	2:B:231:VAL:HG13	1.89	0.53
2:B:325:MET:O	2:B:329:ASP:HB2	2.07	0.53
2:B:431:GLU:O	2:B:434:GLN:CG	2.56	0.53
3:D:176:LEU:CG	3:D:181:GLN:HG3	2.22	0.53
4:F:407:TRP:CD2	2:G:257:VAL:HG23	2.43	0.53
2:G:307:PRO:O	2:G:308:ARG:HD2	2.09	0.53
2:B:273:ALA:CB	2:B:274:PRO:HD3	2.31	0.53
4:F:21:TRP:CZ3	4:F:63:PRO:HB3	2.43	0.53
2:B:198:THR:HG22	2:B:265:LEU:CD2	2.39	0.53
2:B:311:ARG:HG2	2:B:311:ARG:HH11	1.71	0.53
2:B:322:ARG:HG3	2:B:322:ARG:HH11	1.73	0.53
2:G:216:THR:HG21	2:G:299:LYS:HD3	1.90	0.53
1:A:5:ILE:O	1:A:136:SER:N	2.40	0.53
1:A:150:THR:O	1:A:151:SER:C	2.47	0.53
1:A:121:ARG:O	1:A:125:LEU:HB2	2.08	0.53
2:B:141:LEU:HA	2:B:147:SER:HB3	1.91	0.53
2:B:345:GLU:C	2:B:347:ILE:H	2.13	0.53
1:A:215:ARG:C	1:A:216:ASN:HD22	2.12	0.53
1:A:275:VAL:HG21	1:A:300:ASN:OD1	2.09	0.53
2:B:107:HIS:HD2	2:B:151:THR:HG22	1.72	0.53
2:B:179:ASP:HB2	8:B:600:GDP:H3'	1.90	0.53
3:D:113:ASP:CB	4:F:262:TYR:CZ	2.91	0.53
2:G:2:ARG:O	2:G:3:GLU:HB2	2.09	0.53
2:G:383:ALA:O	2:G:386:GLU:HB2	2.08	0.53
1:A:11:GLN:CG	1:A:74:VAL:HG11	2.28	0.52
1:A:283:HIS:O	1:A:284:GLU:C	2.47	0.52
2:B:210:TYR:CD2	2:B:227:LEU:HD21	2.44	0.52
2:B:212:ILE:O	2:B:216:THR:HB	2.10	0.52
2:B:229:HIS:ND1	2:B:229:HIS:C	2.62	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:400:LYS:HE2	12:D:629:HOH:O	2.09	0.52
2:G:140:SER:O	2:G:147:SER:HB2	2.10	0.52
1:A:173:PRO:HB2	1:A:391:LEU:HD11	1.91	0.52
2:B:425:MET:O	2:B:428:LEU:HB3	2.10	0.52
1:A:101:ASN:ND2	7:B:500:GTP:O3G	2.42	0.52
1:A:345:ASP:OD2	1:A:439:SER:HB3	2.10	0.52
1:A:362:VAL:HG13	1:A:368:LEU:CD1	2.38	0.52
2:B:331:GLN:O	2:B:335:VAL:HG23	2.08	0.52
2:B:360:PRO:HB2	9:B:601:TA1:H281	1.91	0.52
3:D:345:GLY:C	3:D:402:LEU:HD11	2.29	0.52
4:F:249:ASN:CB	4:F:255:PHE:HD2	2.21	0.52
2:G:16:ILE:HG22	2:G:17:GLY:N	2.25	0.52
1:A:196:GLU:C	1:A:197:HIS:CD2	2.82	0.52
1:A:231:ILE:HD13	1:A:231:ILE:N	2.24	0.52
1:A:239:THR:O	1:A:240:ALA:C	2.48	0.52
2:B:5:VAL:HG23	2:B:5:VAL:O	2.09	0.52
2:B:8:GLN:OE1	2:B:14:ASN:ND2	2.42	0.52
2:B:226:ASP:O	2:B:227:LEU:C	2.46	0.52
2:G:287:THR:O	2:G:288:VAL:HB	2.09	0.52
2:B:70:LEU:HD12	2:B:145:THR:HG23	1.91	0.52
2:G:36:TYR:HD1	2:G:37:HIS:H	1.58	0.52
1:A:182:VAL:O	1:A:184:PRO:N	2.41	0.52
2:B:297:ASP:OD1	2:B:298:ALA:N	2.39	0.52
3:D:85:GLN:CD	3:D:85:GLN:N	2.62	0.52
1:A:206:ASN:OD1	1:A:227:LEU:CD1	2.57	0.52
2:B:128:SER:OG	2:B:129:CYS:N	2.34	0.52
2:B:200:GLU:N	2:B:265:LEU:HD13	2.25	0.52
2:B:251:ASP:O	2:B:252:LEU:C	2.49	0.52
2:B:273:ALA:HB3	2:B:274:PRO:CD	2.29	0.52
2:B:277:SER:OG	2:B:281:GLN:HB2	2.10	0.52
4:F:198:SER:CB	4:F:265:ILE:CD1	2.66	0.52
1:A:191:THR:HG23	1:A:192:HIS:N	2.25	0.52
2:B:49:ILE:O	2:B:50:ASN:C	2.48	0.52
2:B:188:THR:HA	2:B:425:MET:CE	2.40	0.52
2:G:241:CYS:HB3	2:G:248:LEU:HD12	1.92	0.52
1:A:4:CYS:HA	1:A:134:GLY:O	2.10	0.52
3:D:402:LEU:O	3:D:402:LEU:CD1	2.48	0.52
4:F:10:GLY:O	4:F:13:GLY:N	2.43	0.52
4:F:270:ALA:HB3	4:F:302:MET:HG3	1.92	0.52
1:A:8:HIS:HB3	1:A:13:GLY:O	2.09	0.52
1:A:234:ILE:HB	1:A:302:MET:HE1	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:149:MET:O	2:B:153:LEU:HD22	2.10	0.52
2:B:226:ASP:O	2:B:229:HIS:N	2.42	0.52
2:B:295:MET:SD	2:B:375:ALA:O	2.68	0.52
4:F:271:THR:HG23	4:F:301:GLN:HA	1.91	0.52
2:G:11:GLN:HG3	2:G:74:THR:CG2	2.40	0.52
1:A:244:PHE:CD2	1:A:245:ASP:N	2.76	0.51
3:D:214:THR:OG1	3:D:289:GLN:HB2	2.10	0.51
1:A:243:ARG:NH2	1:A:251:ASP:OD1	2.43	0.51
2:B:260:VAL:HG23	2:B:260:VAL:O	2.10	0.51
2:B:314:THR:CG2	2:B:315:VAL:N	2.73	0.51
2:G:205:ASP:OD1	2:G:207:GLU:N	2.43	0.51
1:A:119:LEU:HD11	1:A:156:ARG:CD	2.39	0.51
1:A:344:VAL:HG12	1:A:345:ASP:H	1.74	0.51
3:D:192:SER:OG	3:D:259:VAL:HG11	2.10	0.51
4:F:105:ARG:HD2	4:F:411:GLU:OE1	2.10	0.51
4:F:407:TRP:CG	2:G:257:VAL:HG23	2.45	0.51
2:G:295:MET:O	2:G:295:MET:HG2	2.11	0.51
1:A:24:TYR:CE2	1:A:240:ALA:HB2	2.45	0.51
1:A:67:PHE:HE1	1:A:87:PHE:CE2	2.29	0.51
1:A:151:SER:HB3	1:A:193:THR:CG2	2.34	0.51
1:A:251:ASP:OD1	1:A:252:LEU:N	2.43	0.51
2:B:149:MET:O	2:B:149:MET:HG2	2.10	0.51
2:B:264:ARG:HE	2:B:264:ARG:HA	1.74	0.51
2:G:241:CYS:HB3	2:G:248:LEU:CD1	2.41	0.51
1:A:201:ALA:O	1:A:267:PHE:HA	2.10	0.51
1:A:231:ILE:CA	1:A:234:ILE:HG22	2.38	0.51
2:B:107:HIS:CD2	2:B:151:THR:HG22	2.45	0.51
2:B:296:PHE:CZ	2:B:315:VAL:HG11	2.46	0.51
3:D:238:ASP:CA	2:G:419:THR:C	2.77	0.51
1:A:417:GLU:HA	1:A:417:GLU:OE1	2.10	0.51
2:B:168:THR:CB	2:B:201:THR:HG23	2.38	0.51
4:F:239:THR:O	4:F:241:SER:N	2.44	0.51
4:F:270:ALA:O	4:F:302:MET:CG	2.58	0.51
2:G:3:GLU:HG2	2:G:64:ARG:NH2	2.25	0.51
1:A:264:ARG:C	1:A:266:HIS:N	2.60	0.51
2:B:5:VAL:CG2	2:B:135:PHE:CD2	2.94	0.51
2:B:103:TRP:CE2	2:B:189:LEU:HB3	2.45	0.51
2:G:336:GLN:CD	2:G:351:VAL:HG11	2.30	0.51
2:B:253:ARG:O	2:B:257:VAL:N	2.33	0.51
2:B:259:MET:HG2	2:B:314:THR:CG2	2.38	0.51
4:F:252:LEU:O	4:F:254:GLU:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:320:ARG:NH1	2:G:360:PRO:HG3	2.26	0.51
1:A:16:ILE:HG23	1:A:17:GLY:N	2.26	0.51
1:A:196:GLU:O	1:A:197:HIS:CD2	2.64	0.51
1:A:234:ILE:CG1	1:A:270:ALA:HB1	2.38	0.51
2:B:320:ARG:HA	2:B:356:CYS:HB3	1.92	0.51
2:B:413:MET:HG3	2:B:414:ASP:N	2.22	0.51
2:B:431:GLU:OE1	2:B:432:TYR:CA	2.57	0.51
3:D:85:GLN:NE2	12:D:646:HOH:O	2.44	0.51
2:G:44:LEU:O	2:G:49:ILE:HG22	2.11	0.51
2:G:298:ALA:C	2:G:300:ASN:H	2.14	0.51
1:A:119:LEU:HA	1:A:122:ILE:HG12	1.93	0.51
1:A:140:SER:O	1:A:142:GLY:N	2.44	0.51
1:A:147:SER:CB	1:A:190:THR:OG1	2.52	0.51
1:A:171:ILE:O	1:A:171:ILE:HG22	2.10	0.51
2:B:49:ILE:HG13	2:B:50:ASN:H	1.76	0.51
4:F:8:HIS:HE1	4:F:21:TRP:HE1	1.59	0.51
4:F:340:THR:O	4:F:340:THR:HG22	2.11	0.51
2:G:180:THR:CG2	2:G:182:VAL:HG22	2.41	0.51
3:D:328:ALA:CA	4:F:409:VAL:CG1	2.88	0.50
2:G:404:PHE:HD1	2:G:404:PHE:H	1.58	0.50
1:A:261:PRO:HB2	1:A:262:TYR:CD1	2.46	0.50
2:B:323:MET:HG3	2:B:328:VAL:CG2	2.41	0.50
4:F:315:CYS:SG	4:F:377:MET:CE	2.99	0.50
2:B:113:GLU:HG3	2:B:114:LEU:N	2.26	0.50
2:G:2:ARG:NH1	2:G:133:GLN:HA	2.27	0.50
2:G:29:GLY:O	2:G:36:TYR:HA	2.11	0.50
2:B:240:THR:HG23	2:B:241:CYS:H	1.76	0.50
2:B:333:LEU:O	2:B:336:GLN:N	2.44	0.50
4:F:270:ALA:O	4:F:302:MET:HG2	2.12	0.50
2:G:163:ASP:OD1	2:G:164:ARG:HD2	2.11	0.50
1:A:310:GLY:HA3	1:A:383:ALA:N	2.26	0.50
1:A:402:ARG:O	1:A:403:ALA:O	2.29	0.50
2:B:265:LEU:O	2:B:266:HIS:O	2.29	0.50
2:B:369:ARG:C	2:B:369:ARG:HD2	2.32	0.50
1:A:9:VAL:HG21	1:A:149:PHE:CD1	2.46	0.50
1:A:115:ILE:CG2	1:A:116:ASP:N	2.75	0.50
1:A:305:CYS:O	1:A:306:ASP:C	2.49	0.50
2:B:173:PRO:HB3	2:B:183:GLU:HG2	1.93	0.50
2:G:7:ILE:O	2:G:137:LEU:HA	2.12	0.50
1:A:133:GLN:HB3	1:A:243:ARG:HH12	1.76	0.50
1:A:231:ILE:O	1:A:235:VAL:HG23	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:3:GLU:HA	2:B:51:VAL:HA	1.93	0.50
2:B:21:TRP:HZ2	2:B:65:ALA:HB2	1.76	0.50
2:B:176:LYS:CE	2:B:207:GLU:HG3	2.39	0.50
1:A:132:LEU:CD2	1:A:164:LYS:HE3	2.41	0.50
2:B:156:LYS:HA	2:B:156:LYS:CE	2.38	0.50
2:B:209:LEU:O	2:B:210:TYR:C	2.48	0.50
4:F:176:GLN:H	4:F:176:GLN:HE21	1.58	0.50
2:G:236:SER:O	2:G:240:THR:HG23	2.11	0.50
1:A:11:GLN:O	1:A:14:VAL:HB	2.12	0.49
1:A:115:ILE:HD11	1:A:119:LEU:HG	1.92	0.49
2:B:168:THR:O	2:B:201:THR:HA	2.12	0.49
1:A:105:ARG:HH11	1:A:105:ARG:HG3	1.77	0.49
2:B:102:ASN:HB3	2:B:105:LYS:HB2	1.94	0.49
2:B:336:GLN:HE22	2:B:349:ASN:ND2	2.10	0.49
2:B:345:GLU:O	2:B:347:ILE:N	2.45	0.49
2:G:153:LEU:O	2:G:157:ILE:HG12	2.11	0.49
2:G:165:ILE:HD11	2:G:252:LEU:HG	1.93	0.49
2:G:251:ASP:HB2	2:G:254:LYS:HD2	1.94	0.49
1:A:133:GLN:CB	1:A:243:ARG:HH12	2.24	0.49
1:A:414:GLU:OE1	1:A:414:GLU:N	2.46	0.49
2:B:69:ASP:HA	2:B:145:THR:HG21	1.95	0.49
3:D:101:CYS:O	3:D:124:CYS:HA	2.12	0.49
3:D:114:LEU:CG	4:F:263:PRO:HG3	2.41	0.49
3:D:217:GLU:HG2	3:D:226:LEU:HD21	1.95	0.49
3:D:345:GLY:HA3	3:D:402:LEU:CD1	2.42	0.49
4:F:48:SER:O	4:F:243:ARG:O	2.29	0.49
2:G:135:PHE:N	2:G:135:PHE:CD1	2.80	0.49
1:A:238:ILE:O	1:A:242:LEU:HB2	2.11	0.49
1:A:244:PHE:CD2	1:A:244:PHE:C	2.83	0.49
3:D:112:VAL:N	4:F:431:ASP:OD1	2.45	0.49
1:A:227:LEU:O	1:A:231:ILE:HG12	2.12	0.49
2:B:262:PHE:O	2:B:264:ARG:N	2.45	0.49
2:B:269:MET:HB3	2:B:303:ALA:HB2	1.94	0.49
1:A:149:PHE:HE1	1:A:153:LEU:HD22	1.77	0.49
1:A:283:HIS:O	1:A:285:GLN:N	2.45	0.49
3:D:140:ARG:HG3	3:D:140:ARG:HH11	1.76	0.49
1:A:158:SER:OG	1:A:197:HIS:HB3	2.13	0.49
2:B:24:ILE:HG22	2:B:25:SER:N	2.27	0.49
2:B:431:GLU:OE1	2:B:432:TYR:N	2.46	0.49
3:D:325:MET:HG3	4:F:412:GLY:N	2.28	0.49
2:G:225:GLY:O	2:G:227:LEU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LEU:HD23	1:A:236:SER:CB	2.37	0.49
1:A:328:VAL:C	1:A:330:ALA:H	2.16	0.49
2:B:173:PRO:HB3	2:B:183:GLU:CG	2.42	0.49
2:B:176:LYS:HG3	2:B:177:VAL:H	1.78	0.49
2:B:199:ASP:O	2:B:200:GLU:HG3	2.13	0.49
2:B:280:SER:O	2:B:282:GLN:N	2.45	0.49
2:B:298:ALA:O	2:B:299:LYS:C	2.50	0.49
2:B:431:GLU:HA	2:B:434:GLN:CG	2.43	0.49
3:D:241:GLN:HA	2:G:423:SER:HG	1.72	0.49
2:B:4:ILE:HG22	2:B:5:VAL:N	2.27	0.49
2:B:383:ALA:C	2:B:385:GLN:H	2.15	0.49
3:D:238:ASP:C	2:G:419:THR:C	2.70	0.49
4:F:267:PHE:CD1	4:F:267:PHE:N	2.79	0.49
4:F:313:MET:O	4:F:314:ALA:CB	2.61	0.49
2:G:11:GLN:HG3	2:G:74:THR:HG22	1.95	0.49
1:A:163:LYS:C	1:A:164:LYS:HG2	2.33	0.49
1:A:192:HIS:CD2	1:A:424:ASP:OD2	2.66	0.49
2:B:8:GLN:HB3	2:B:14:ASN:HA	1.94	0.49
3:D:282:SER:HB2	3:D:308:ALA:HA	1.94	0.49
1:A:392:ASP:O	1:A:395:PHE:HB3	2.13	0.48
2:B:211:ASP:OD1	2:B:212:ILE:HG13	2.13	0.48
2:B:387:LEU:HD23	2:B:388:PHE:CD2	2.47	0.48
2:B:399:PHE:O	2:B:400:ARG:C	2.52	0.48
3:D:99:SER:OG	3:D:102:LEU:HB2	2.13	0.48
3:D:201:GLN:O	3:D:205:ARG:HG3	2.12	0.48
3:D:328:ALA:HA	4:F:409:VAL:CG1	2.39	0.48
2:G:393:GLU:O	2:G:397:ALA:HB2	2.12	0.48
1:A:99:ALA:O	1:A:100:ALA:HB3	2.13	0.48
1:A:191:THR:CG2	1:A:192:HIS:N	2.76	0.48
1:A:203:MET:SD	1:A:267:PHE:HB3	2.53	0.48
2:B:4:ILE:HD12	2:B:239:THR:CG2	2.42	0.48
3:D:243:VAL:HG21	3:D:360:GLN:CG	2.44	0.48
2:G:240:THR:HG21	2:G:320:ARG:NE	2.28	0.48
2:G:267:PHE:CD1	2:G:267:PHE:N	2.81	0.48
1:A:118:VAL:HG21	1:A:149:PHE:CE2	2.48	0.48
2:B:49:ILE:HG13	2:B:50:ASN:N	2.28	0.48
2:B:209:LEU:O	2:B:213:CYS:N	2.47	0.48
3:D:270:ARG:CZ	3:D:286:ALA:HB2	2.43	0.48
4:F:90:GLU:HB3	4:F:121:ARG:HD3	1.94	0.48
2:G:177:VAL:O	2:G:177:VAL:CG1	2.61	0.48
2:G:241:CYS:CB	2:G:248:LEU:CD1	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:SER:OG	1:A:193:THR:HG21	2.13	0.48
2:B:133:GLN:NE2	2:B:252:LEU:HB2	2.28	0.48
4:F:239:THR:O	4:F:240:ALA:C	2.52	0.48
1:A:384:ILE:HG22	1:A:388:TRP:CD1	2.49	0.48
2:B:2:ARG:NH1	2:B:251:ASP:OD2	2.46	0.48
2:B:307:PRO:HB3	2:B:312:TYR:CZ	2.49	0.48
3:D:341:ILE:O	3:D:344:LEU:HB3	2.12	0.48
4:F:163:LYS:H	4:F:163:LYS:HG3	1.48	0.48
1:A:96:LYS:O	1:A:97:GLU:O	2.31	0.48
1:A:104:ALA:CB	1:A:408:TYR:HD2	2.26	0.48
1:A:188:ILE:O	1:A:191:THR:HG22	2.13	0.48
4:F:70:LEU:O	4:F:97:GLU:O	2.31	0.48
1:A:9:VAL:HG11	1:A:150:THR:OG1	2.13	0.48
1:A:115:ILE:O	1:A:116:ASP:C	2.51	0.48
1:A:155:GLU:HG2	1:A:197:HIS:CE1	2.49	0.48
1:A:316:CYS:HB3	1:A:378:LEU:HD12	1.95	0.48
2:B:142:GLY:HA3	2:B:183:GLU:OE2	2.13	0.48
2:B:265:LEU:HD12	2:B:266:HIS:O	2.12	0.48
2:G:237:GLY:CA	2:G:376:THR:HG21	2.44	0.48
2:G:291:LEU:HD21	2:G:375:ALA:HB3	1.87	0.48
2:B:24:ILE:CD1	2:B:52:TYR:CE1	2.97	0.48
2:B:175:PRO:CD	2:B:207:GLU:OE1	2.61	0.48
2:B:264:ARG:HA	2:B:264:ARG:NE	2.29	0.48
3:D:294:THR:CG2	3:D:297:ARG:HE	2.26	0.48
4:F:102:ASN:O	4:F:103:TYR:C	2.51	0.48
4:F:204:VAL:HG13	4:F:302:MET:HE3	1.96	0.48
4:F:315:CYS:SG	4:F:377:MET:HE2	2.54	0.48
4:F:431:ASP:HA	12:F:606:HOH:O	2.12	0.48
2:G:205:ASP:HB3	2:G:303:ALA:HA	1.96	0.48
2:G:295:MET:SD	2:G:377:PHE:HB2	2.54	0.48
1:A:132:LEU:HD21	1:A:164:LYS:HE3	1.96	0.48
2:B:296:PHE:HZ	2:B:315:VAL:HG11	1.78	0.48
2:B:20:PHE:CG	2:B:235:MET:SD	3.07	0.48
2:G:385:GLN:HE21	2:G:389:LYS:HD2	1.79	0.48
11:G:701:CN2:H15	11:G:701:CN2:C12	2.43	0.48
1:A:286:LEU:CD1	1:A:290:GLU:HG2	2.44	0.47
2:B:137:LEU:HD22	2:B:154:ILE:HG21	1.94	0.47
2:B:175:PRO:O	2:B:176:LYS:C	2.52	0.47
2:B:191:VAL:HG13	2:B:192:HIS:N	2.28	0.47
2:B:209:LEU:CD2	2:B:227:LEU:HD13	2.44	0.47
2:B:297:ASP:OD2	2:B:299:LYS:HE2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:174:SER:HB2	2:G:207:GLU:HB2	1.96	0.47
2:G:180:THR:HG22	2:G:182:VAL:H	1.79	0.47
1:A:97:GLU:HB2	1:A:110:ILE:HD11	1.96	0.47
1:A:242:LEU:C	1:A:244:PHE:N	2.66	0.47
1:A:274:PRO:CB	1:A:371:VAL:HG21	2.43	0.47
1:A:369:ALA:O	1:A:370:LYS:CB	2.62	0.47
4:F:115:ILE:HD13	4:F:119:LEU:HD13	1.95	0.47
4:F:167:LEU:HD11	4:F:256:GLN:NE2	2.27	0.47
4:F:229:ARG:CG	4:F:229:ARG:NH1	2.75	0.47
1:A:339:ARG:C	1:A:341:ILE:N	2.68	0.47
3:D:255:CYS:O	3:D:258:ASP:HB2	2.15	0.47
4:F:98:ASP:CB	2:G:251:ASP:OD2	2.58	0.47
2:G:33:THR:O	2:G:34:GLY:O	2.32	0.47
1:A:6:SER:OG	1:A:65:ALA:HB2	2.14	0.47
1:A:107:HIS:CE1	1:A:152:LEU:HB3	2.49	0.47
1:A:210:TYR:CE2	1:A:227:LEU:HD21	2.49	0.47
1:A:253:THR:O	1:A:254:GLU:C	2.52	0.47
2:B:272:PHE:CE1	9:B:601:TA1:H391	2.50	0.47
3:D:243:VAL:HG21	3:D:360:GLN:HG3	1.96	0.47
3:D:342:ARG:NH1	3:D:402:LEU:HD23	2.28	0.47
2:G:5:VAL:CG2	2:G:135:PHE:CD2	2.97	0.47
2:G:36:TYR:HH	2:G:40:SER:C	2.08	0.47
2:G:209:LEU:HD21	2:G:231:VAL:HG22	1.96	0.47
1:A:148:GLY:O	1:A:151:SER:CB	2.61	0.47
1:A:175:PRO:HD2	1:A:207:GLU:HB3	1.97	0.47
1:A:185:TYR:OH	1:A:399:TYR:HA	2.15	0.47
1:A:217:LEU:CD1	1:A:277:SER:HA	2.44	0.47
1:A:226:ASN:O	1:A:229:ARG:N	2.48	0.47
1:A:384:ILE:HG22	1:A:384:ILE:O	2.15	0.47
1:A:396:ASP:O	1:A:397:LEU:C	2.53	0.47
2:B:20:PHE:O	2:B:24:ILE:HB	2.14	0.47
2:B:387:LEU:O	2:B:387:LEU:HG	2.15	0.47
2:G:200:GLU:OE2	2:G:255:LEU:HD12	2.14	0.47
2:G:248:LEU:HB2	2:G:249:ASN:H	1.46	0.47
1:A:11:GLN:O	1:A:15:GLN:HG3	2.15	0.47
1:A:99:ALA:H	2:B:2:ARG:HH22	1.63	0.47
1:A:120:ASP:O	1:A:124:LYS:HB2	2.15	0.47
1:A:147:SER:O	1:A:190:THR:HG23	2.14	0.47
1:A:155:GLU:OE1	1:A:197:HIS:HE1	1.96	0.47
1:A:407:TRP:O	1:A:411:GLU:CG	2.63	0.47
2:B:226:ASP:O	2:B:229:HIS:HB3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:71:GLU:HG3	4:F:73:THR:OG1	2.15	0.47
1:A:154:MET:HA	1:A:157:LEU:HD12	1.97	0.47
1:A:191:THR:O	1:A:195:LEU:HB2	2.15	0.47
1:A:256:GLN:HA	1:A:260:VAL:HG13	1.97	0.47
2:B:70:LEU:O	2:B:99:ALA:HB2	2.15	0.47
2:B:154:ILE:HG22	2:B:166:MET:CE	2.44	0.47
2:B:198:THR:HG23	2:B:200:GLU:H	1.79	0.47
2:B:237:GLY:O	2:B:241:CYS:CB	2.61	0.47
2:B:242:LEU:CD1	2:B:250:ALA:HB3	2.45	0.47
2:B:308:ARG:HG3	2:B:342:TYR:OH	2.13	0.47
3:D:397:ASP:OD2	3:D:400:LYS:NZ	2.46	0.47
4:F:344:VAL:O	4:F:344:VAL:HG13	2.14	0.47
2:G:259:MET:SD	11:G:701:CN2:H182	2.55	0.47
1:A:224:TYR:CG	2:B:325:MET:HG2	2.50	0.47
1:A:317:LEU:CD1	1:A:351:PHE:CD2	2.97	0.47
2:B:115:VAL:CG2	2:B:152:LEU:HD23	2.44	0.47
2:B:185:TYR:HD2	2:B:395:PHE:CE1	2.33	0.47
2:B:307:PRO:C	2:B:309:HIS:H	2.18	0.47
4:F:395:PHE:C	4:F:395:PHE:CD2	2.87	0.47
2:G:107:HIS:ND1	2:G:152:LEU:HB2	2.29	0.47
1:A:241:SER:HB3	1:A:320:ARG:NH2	2.30	0.47
1:A:255:PHE:O	1:A:256:GLN:C	2.53	0.47
4:F:70:LEU:HD23	4:F:110:ILE:CG2	2.40	0.47
4:F:191:THR:HA	4:F:194:THR:HG22	1.96	0.47
1:A:145:THR:O	1:A:149:PHE:HB3	2.15	0.47
1:A:154:MET:HE3	1:A:166:LYS:HB3	1.97	0.47
1:A:243:ARG:NH2	1:A:252:LEU:HB2	2.30	0.47
1:A:386:GLU:O	1:A:388:TRP:N	2.47	0.47
2:B:101:ASN:ND2	2:B:101:ASN:O	2.48	0.47
2:B:287:THR:N	2:B:290:GLU:OE1	2.48	0.47
2:B:360:PRO:O	2:B:369:ARG:C	2.54	0.47
2:G:154:ILE:HD12	2:G:198:THR:HG22	1.97	0.47
1:A:22:GLU:O	1:A:23:LEU:C	2.54	0.46
1:A:204:VAL:HG21	1:A:231:ILE:HG23	1.97	0.46
1:A:278:ALA:HB2	1:A:369:ALA:CA	2.45	0.46
1:A:436:GLY:O	1:A:438:ASP:N	2.48	0.46
2:B:103:TRP:CE3	2:B:189:LEU:HD13	2.50	0.46
2:B:134:GLY:HA3	2:B:165:ILE:HG12	1.97	0.46
2:B:175:PRO:HD2	2:B:207:GLU:CD	2.35	0.46
4:F:346:TRP:CZ3	4:F:347:CYS:HB2	2.50	0.46
2:B:154:ILE:HG22	2:B:166:MET:HE1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:237:GLY:HA3	2:B:376:THR:OG1	2.15	0.46
3:D:238:ASP:HB3	2:G:419:THR:CB	2.38	0.46
4:F:82:THR:O	4:F:83:TYR:CB	2.63	0.46
4:F:423:GLU:CD	12:F:698:HOH:O	2.51	0.46
1:A:10:GLY:O	1:A:11:GLN:C	2.54	0.46
1:A:19:ALA:HB2	1:A:228:ASN:HB3	1.96	0.46
1:A:34:GLY:C	1:A:61:HIS:N	2.68	0.46
1:A:166:LYS:CE	1:A:199:ASP:OD1	2.62	0.46
1:A:260:VAL:O	1:A:260:VAL:CG2	2.63	0.46
1:A:335:ILE:O	1:A:337:THR:N	2.48	0.46
2:B:137:LEU:HD22	2:B:154:ILE:HG23	1.97	0.46
1:A:114:ILE:O	1:A:118:VAL:HG23	2.16	0.46
1:A:324:VAL:HG12	1:A:326:LYS:H	1.81	0.46
1:A:392:ASP:OD2	1:A:422:ARG:NE	2.48	0.46
2:B:384:ILE:O	2:B:384:ILE:HG23	2.14	0.46
3:D:332:LYS:HG3	3:D:333:SER:N	2.31	0.46
2:G:62:VAL:HG22	2:G:62:VAL:O	2.15	0.46
1:A:95:GLY:C	1:A:97:GLU:N	2.69	0.46
1:A:117:LEU:HD11	1:A:121:ARG:NH2	2.30	0.46
1:A:117:LEU:HD12	1:A:121:ARG:HH12	1.80	0.46
1:A:155:GLU:HA	1:A:197:HIS:CE1	2.49	0.46
1:A:224:TYR:HD1	2:B:247:GLN:HB3	1.80	0.46
1:A:388:TRP:HA	1:A:388:TRP:HE3	1.79	0.46
2:B:408:TYR:O	2:B:411:GLU:HB2	2.15	0.46
4:F:26:LEU:HD21	4:F:364:PRO:HD3	1.96	0.46
2:G:102:ASN:OD1	2:G:105:LYS:HB2	2.15	0.46
2:G:336:GLN:OE1	2:G:351:VAL:CG1	2.58	0.46
1:A:23:LEU:CD2	1:A:232:GLY:O	2.64	0.46
1:A:25:CYS:SG	1:A:83:TYR:HE2	2.38	0.46
1:A:196:GLU:C	1:A:197:HIS:HD2	2.19	0.46
1:A:210:TYR:CZ	1:A:227:LEU:HD11	2.51	0.46
2:B:133:GLN:O	2:B:165:ILE:CD1	2.64	0.46
2:B:224:TYR:O	2:B:225:GLY:C	2.53	0.46
9:B:601:TA1:H463	9:B:601:TA1:C26	2.46	0.46
4:F:87:PHE:CD2	4:F:87:PHE:N	2.82	0.46
2:G:308:ARG:C	2:G:310:GLY:H	2.19	0.46
2:G:320:ARG:HA	2:G:356:CYS:O	2.15	0.46
1:A:241:SER:C	1:A:244:PHE:HB3	2.36	0.46
1:A:243:ARG:NH2	1:A:252:LEU:CB	2.78	0.46
1:A:265:GLY:O	1:A:266:HIS:O	2.33	0.46
1:A:288:VAL:HA	1:A:291:ILE:HG12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:196:GLU:O	2:B:197:ASN:OD1	2.34	0.46
4:F:313:MET:HG3	4:F:380:ASN:O	2.15	0.46
2:G:112:ALA:HA	2:G:115:VAL:CG2	2.45	0.46
1:A:132:LEU:H	1:A:132:LEU:CD2	2.23	0.46
1:A:345:ASP:C	1:A:347:CYS:N	2.68	0.46
2:G:251:ASP:C	2:G:253:ARG:N	2.64	0.46
1:A:278:ALA:O	1:A:279:GLU:HG2	2.15	0.46
1:A:317:LEU:CD1	1:A:351:PHE:CE2	2.99	0.46
2:B:102:ASN:ND2	2:B:104:ALA:HB3	2.31	0.46
2:B:242:LEU:HD11	2:B:250:ALA:HB3	1.97	0.46
2:B:243:ARG:HA	2:B:243:ARG:HD3	1.62	0.46
4:F:263:PRO:O	4:F:265:ILE:N	2.38	0.46
2:G:116:ASP:O	2:G:120:ASP:HB2	2.16	0.46
1:A:5:ILE:CG2	1:A:6:SER:H	2.29	0.46
1:A:256:GLN:O	1:A:260:VAL:HG13	2.15	0.46
1:A:286:LEU:O	1:A:287:SER:O	2.34	0.46
1:A:344:VAL:CG1	1:A:345:ASP:N	2.79	0.46
2:B:274:PRO:HG2	2:B:371:LEU:CD2	2.43	0.46
3:D:375:MET:HE3	3:D:399:VAL:HG21	1.96	0.46
4:F:183:GLU:HB3	4:F:184:PRO:HD3	1.98	0.46
4:F:346:TRP:HZ2	4:F:435:VAL:HG13	1.80	0.46
2:G:5:VAL:CG2	2:G:135:PHE:HD2	2.28	0.46
1:A:115:ILE:CG1	1:A:152:LEU:HD13	2.46	0.45
1:A:180:ALA:HA	2:B:352:LYS:NZ	2.30	0.45
1:A:308:ARG:O	1:A:309:HIS:HB3	2.17	0.45
1:A:381:THR:O	1:A:383:ALA:N	2.49	0.45
1:A:408:TYR:CG	1:A:418:PHE:HZ	2.34	0.45
1:A:423:GLU:O	1:A:426:ALA:HB3	2.16	0.45
2:B:154:ILE:HD12	2:B:155:SER:N	2.31	0.45
2:B:194:LEU:O	2:B:265:LEU:HD23	2.16	0.45
2:B:208:ALA:O	2:B:212:ILE:HG13	2.16	0.45
2:B:210:TYR:CE2	2:B:227:LEU:HD11	2.51	0.45
2:B:263:PRO:O	2:B:264:ARG:C	2.52	0.45
4:F:87:PHE:N	4:F:87:PHE:HD2	2.13	0.45
1:A:7:ILE:HG13	1:A:137:VAL:HG22	1.98	0.45
1:A:148:GLY:O	1:A:149:PHE:C	2.54	0.45
1:A:203:MET:SD	1:A:267:PHE:CB	3.04	0.45
1:A:286:LEU:HG	1:A:290:GLU:HB2	1.97	0.45
1:A:404:PHE:CD1	1:A:404:PHE:N	2.83	0.45
1:A:413:MET:C	1:A:414:GLU:HG3	2.37	0.45
2:B:6:HIS:HB3	2:B:21:TRP:HZ2	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:243:ARG:HD3	2:B:243:ARG:N	2.26	0.45
4:F:122:ILE:HD11	4:F:157:LEU:HD21	1.99	0.45
1:A:12:ALA:CB	1:A:140:SER:OG	2.60	0.45
1:A:122:ILE:CD1	1:A:157:LEU:HD21	2.35	0.45
1:A:229:ARG:NH1	1:A:229:ARG:HG2	2.31	0.45
1:A:276:ILE:HG12	1:A:277:SER:N	2.31	0.45
1:A:392:ASP:OD2	1:A:422:ARG:CZ	2.65	0.45
2:B:115:VAL:HG21	2:B:152:LEU:HD21	1.98	0.45
2:B:313:LEU:O	2:B:347:ILE:HD12	2.16	0.45
3:D:111:LYS:C	4:F:431:ASP:OD1	2.54	0.45
3:D:342:ARG:NH1	3:D:402:LEU:CB	2.76	0.45
1:A:212:ILE:HD11	1:A:302:MET:H	1.82	0.45
1:A:334:THR:CG2	1:A:335:ILE:N	2.79	0.45
3:D:204:TYR:CA	3:D:207:LEU:HD23	2.40	0.45
2:G:287:THR:HG22	2:G:290:GLU:H	1.81	0.45
2:G:431:GLU:O	2:G:434:GLN:HB2	2.17	0.45
2:B:324:SER:O	2:B:326:LYS:N	2.50	0.45
2:B:324:SER:OG	2:B:326:LYS:HB3	2.15	0.45
4:F:190:THR:CG2	4:F:191:THR:N	2.79	0.45
2:G:273:ALA:HB2	2:G:375:ALA:HB3	1.99	0.45
2:G:342:TYR:N	2:G:342:TYR:HD2	2.15	0.45
1:A:9:VAL:HG21	1:A:149:PHE:HD1	1.80	0.45
1:A:434:GLU:C	1:A:436:GLY:H	2.18	0.45
2:B:113:GLU:CG	2:B:114:LEU:N	2.79	0.45
2:B:209:LEU:HD23	2:B:227:LEU:HD13	1.98	0.45
2:B:409:THR:HA	2:B:413:MET:HB3	1.99	0.45
2:G:265:LEU:O	2:G:266:HIS:C	2.55	0.45
1:A:115:ILE:HG23	1:A:116:ASP:H	1.79	0.45
1:A:182:VAL:O	1:A:184:PRO:CD	2.65	0.45
1:A:204:VAL:HG12	1:A:204:VAL:O	2.17	0.45
1:A:291:ILE:HD12	1:A:375:VAL:HG23	1.99	0.45
2:B:67:LEU:HD12	2:B:92:PHE:CD2	2.51	0.45
2:B:167:ASN:HA	2:B:200:GLU:O	2.17	0.45
4:F:82:THR:O	4:F:83:TYR:HB2	2.17	0.45
4:F:132:LEU:HG	4:F:133:GLN:N	2.31	0.45
4:F:174:ALA:HA	4:F:175:PRO:HD2	1.66	0.45
2:G:150:GLY:O	2:G:154:ILE:HG23	2.17	0.45
1:A:104:ALA:HB1	1:A:413:MET:HG3	1.95	0.45
1:A:231:ILE:HD13	1:A:231:ILE:H	1.82	0.45
1:A:271:THR:O	1:A:376:CYS:HA	2.17	0.45
2:B:11:GLN:O	2:B:14:ASN:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:23:VAL:O	2:B:25:SER:N	2.50	0.45
2:B:102:ASN:OD1	2:B:408:TYR:CZ	2.70	0.45
2:B:194:LEU:C	2:B:196:GLU:N	2.70	0.45
2:B:230:LEU:HD21	2:B:302:MET:HE2	1.98	0.45
2:B:242:LEU:HD22	2:B:250:ALA:O	2.17	0.45
3:D:397:ASP:HA	3:D:400:LYS:NZ	2.32	0.45
4:F:298:PRO:HA	4:F:301:GLN:HE21	1.82	0.45
1:A:110:ILE:CG2	1:A:111:GLY:N	2.71	0.45
1:A:152:LEU:HD12	1:A:152:LEU:C	2.38	0.45
1:A:278:ALA:CA	1:A:282:TYR:OH	2.65	0.45
1:A:346:TRP:HZ2	1:A:435:VAL:HG12	1.82	0.45
3:D:204:TYR:O	3:D:207:LEU:HB2	2.16	0.45
3:D:328:ALA:N	4:F:409:VAL:CG1	2.80	0.45
4:F:244:PHE:N	4:F:245:ASP:HA	2.32	0.45
2:G:178:SER:HB2	2:G:183:GLU:OE1	2.16	0.45
1:A:209:ILE:CD1	1:A:231:ILE:HD11	2.47	0.45
1:A:274:PRO:HB2	1:A:371:VAL:HG21	1.99	0.45
1:A:295:CYS:HB3	1:A:377:MET:HG2	1.99	0.45
1:A:303:VAL:O	1:A:303:VAL:CG1	2.65	0.45
2:B:4:ILE:HD12	2:B:239:THR:HG21	1.99	0.45
2:B:250:ALA:HB1	2:B:254:LYS:CB	2.44	0.45
2:B:288:VAL:N	2:B:289:PRO:HD2	2.32	0.45
2:B:307:PRO:C	2:B:309:HIS:N	2.71	0.45
2:B:323:MET:CE	2:B:328:VAL:HG22	2.46	0.45
4:F:51:THR:HG21	4:F:242:LEU:O	2.17	0.45
4:F:174:ALA:CB	4:F:207:GLU:HB2	2.47	0.45
2:G:250:ALA:CB	11:G:701:CN2:H7	2.46	0.45
1:A:119:LEU:HD11	1:A:156:ARG:HD2	1.97	0.44
1:A:288:VAL:C	1:A:290:GLU:N	2.71	0.44
2:B:135:PHE:CD1	2:B:135:PHE:N	2.84	0.44
2:B:167:ASN:HD21	2:B:252:LEU:HD22	1.82	0.44
2:B:431:GLU:HA	2:B:434:GLN:HG3	1.98	0.44
4:F:292:THR:O	4:F:295:CYS:HB2	2.17	0.44
4:F:318:LEU:HB2	4:F:376:CYS:HB3	1.99	0.44
2:G:269:MET:HA	2:G:270:PRO:HD3	1.75	0.44
2:G:401:ARG:O	2:G:402:LYS:C	2.55	0.44
1:A:4:CYS:SG	1:A:252:LEU:CD1	3.02	0.44
1:A:11:GLN:HE21	1:A:74:VAL:CG2	2.29	0.44
1:A:23:LEU:O	1:A:26:LEU:HB3	2.17	0.44
1:A:103:TYR:CD1	1:A:148:GLY:HA2	2.52	0.44
1:A:210:TYR:CD2	1:A:227:LEU:HD21	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:LEU:HD12	2:B:92:PHE:CE2	2.52	0.44
2:B:242:LEU:HD22	2:B:250:ALA:N	2.19	0.44
2:B:242:LEU:C	2:B:244:PHE:H	2.19	0.44
3:D:330:ILE:O	3:D:334:LEU:HG	2.17	0.44
4:F:315:CYS:SG	4:F:377:MET:HE1	2.57	0.44
1:A:153:LEU:O	1:A:157:LEU:HG	2.18	0.44
1:A:283:HIS:O	1:A:283:HIS:ND1	2.49	0.44
1:A:362:VAL:HG13	1:A:368:LEU:CG	2.48	0.44
2:B:72:PRO:O	2:B:74:THR:N	2.50	0.44
2:B:175:PRO:HG2	2:B:207:GLU:OE1	2.16	0.44
2:B:189:LEU:HD23	2:B:421:ALA:CB	2.47	0.44
2:B:239:THR:O	2:B:240:THR:C	2.56	0.44
2:B:288:VAL:N	2:B:289:PRO:CD	2.80	0.44
3:D:295:LYS:C	3:D:297:ARG:H	2.19	0.44
4:F:97:GLU:OE2	2:G:164:ARG:NH1	2.50	0.44
1:A:286:LEU:O	1:A:287:SER:C	2.55	0.44
2:B:295:MET:SD	2:B:375:ALA:HB3	2.57	0.44
4:F:151:SER:O	4:F:155:GLU:HG2	2.17	0.44
4:F:251:ASP:OD1	4:F:251:ASP:O	2.36	0.44
2:G:308:ARG:NH1	2:G:342:TYR:HE1	2.15	0.44
1:A:12:ALA:HB2	7:B:500:GTP:C8	2.52	0.44
1:A:268:PRO:CA	1:A:379:SER:O	2.65	0.44
2:B:8:GLN:CG	2:B:67:LEU:HD22	2.47	0.44
2:B:106:GLY:O	2:B:149:MET:HB2	2.16	0.44
2:B:182:VAL:O	2:B:183:GLU:C	2.56	0.44
4:F:256:GLN:O	4:F:258:ASN:N	2.51	0.44
1:A:5:ILE:HG22	1:A:6:SER:H	1.78	0.44
2:B:14:ASN:O	2:B:17:GLY:N	2.50	0.44
2:B:108:TYR:CE1	2:B:413:MET:HE1	2.52	0.44
2:B:161:TYR:O	2:B:163:ASP:N	2.51	0.44
4:F:266:HIS:CD2	4:F:266:HIS:H	2.35	0.44
2:G:343:PHE:O	2:G:344:VAL:C	2.55	0.44
1:A:121:ARG:HG2	1:A:121:ARG:HH11	1.83	0.44
1:A:121:ARG:HG2	1:A:121:ARG:NH1	2.33	0.44
1:A:144:GLY:H	7:B:500:GTP:PG	2.41	0.44
3:D:218:ILE:HB	3:D:285:HIS:HB2	1.99	0.44
4:F:164:LYS:H	4:F:164:LYS:HG2	1.68	0.44
2:G:6:HIS:HD2	2:G:136:GLN:HG3	1.83	0.44
1:A:377:MET:O	1:A:377:MET:HG3	2.18	0.44
2:B:26:ASP:C	2:B:28:HIS:H	2.21	0.44
2:B:52:TYR:HE1	2:B:240:THR:HB	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:80:THR:HG22	4:F:81:GLY:N	2.33	0.44
1:A:287:SER:N	1:A:290:GLU:OE1	2.51	0.44
2:B:82:PRO:C	2:B:84:GLY:H	2.20	0.44
2:B:243:ARG:HH21	2:B:252:LEU:N	2.12	0.44
2:B:312:TYR:HA	2:B:381:SER:HA	1.99	0.44
2:B:360:PRO:HG2	2:B:371:LEU:CB	2.38	0.44
4:F:260:VAL:HG23	4:F:260:VAL:O	2.18	0.44
1:A:63:PRO:HG2	1:A:91:GLN:OE1	2.17	0.43
1:A:72:PRO:HG2	1:A:73:THR:H	1.83	0.43
1:A:218:ASP:C	1:A:219:ILE:HG12	2.37	0.43
1:A:252:LEU:O	1:A:253:THR:C	2.56	0.43
1:A:262:TYR:HB3	1:A:263:PRO:HD2	2.00	0.43
2:B:12:CYS:C	2:B:14:ASN:N	2.71	0.43
2:B:103:TRP:HZ3	2:B:108:TYR:CE1	2.27	0.43
2:B:141:LEU:N	2:B:141:LEU:HD12	2.33	0.43
2:B:161:TYR:N	2:B:161:TYR:CD1	2.86	0.43
2:B:229:HIS:HE2	9:B:601:TA1:H361	1.83	0.43
2:B:310:GLY:HA3	2:B:436:GLN:NE2	2.29	0.43
3:D:83:ASN:HB2	12:D:630:HOH:O	2.18	0.43
3:D:170:HIS:CD2	3:D:175:ASP:HA	2.52	0.43
4:F:31:GLN:O	4:F:32:PRO:C	2.56	0.43
1:A:7:ILE:HD11	1:A:137:VAL:CG2	2.44	0.43
1:A:149:PHE:O	1:A:150:THR:C	2.56	0.43
1:A:272:TYR:CE2	1:A:274:PRO:HD2	2.53	0.43
1:A:363:VAL:CG1	1:A:364:PRO:HD2	2.48	0.43
2:B:168:THR:CG2	2:B:201:THR:HG23	2.48	0.43
2:B:301:MET:O	2:B:303:ALA:N	2.51	0.43
3:D:239:SER:N	2:G:419:THR:CG2	2.71	0.43
4:F:273:ALA:HB1	4:F:274:PRO:CD	2.35	0.43
2:G:240:THR:CG2	2:G:320:ARG:CZ	2.95	0.43
2:G:251:ASP:O	2:G:253:ARG:N	2.50	0.43
1:A:230:LEU:O	1:A:231:ILE:C	2.57	0.43
1:A:310:GLY:HA3	1:A:383:ALA:CA	2.49	0.43
2:B:72:PRO:HG2	2:B:73:GLY:H	1.83	0.43
2:B:212:ILE:O	2:B:212:ILE:HG22	2.18	0.43
2:G:378:ILE:HD12	11:G:701:CN2:C4	2.48	0.43
1:A:11:GLN:NE2	1:A:74:VAL:HG22	2.30	0.43
2:B:7:ILE:N	2:B:136:GLN:O	2.51	0.43
2:B:68:VAL:HG11	2:B:153:LEU:HD21	2.00	0.43
2:B:288:VAL:C	2:B:290:GLU:N	2.70	0.43
3:D:283:ARG:HH11	3:D:283:ARG:HD2	1.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:328:ALA:N	4:F:409:VAL:HG12	2.33	0.43
1:A:13:GLY:C	1:A:16:ILE:HG22	2.38	0.43
1:A:132:LEU:HD23	1:A:132:LEU:N	2.25	0.43
1:A:172:TYR:CD1	1:A:173:PRO:N	2.80	0.43
1:A:343:PHE:CE1	1:A:351:PHE:HE1	2.36	0.43
2:B:24:ILE:CG2	2:B:25:SER:N	2.80	0.43
4:F:6:SER:O	4:F:65:ALA:HA	2.19	0.43
2:G:111:GLY:HA2	2:G:149:MET:CE	2.49	0.43
1:A:238:ILE:O	1:A:242:LEU:CB	2.67	0.43
1:A:238:ILE:HD11	1:A:378:LEU:HD23	2.01	0.43
1:A:304:LYS:O	1:A:304:LYS:HG3	2.18	0.43
2:B:187:ALA:O	2:B:188:THR:C	2.57	0.43
2:B:422:GLU:O	2:B:426:ASN:CB	2.67	0.43
4:F:359:PRO:HA	4:F:360:PRO:HD3	1.84	0.43
1:A:101:ASN:ND2	2:B:254:LYS:CD	2.76	0.43
1:A:263:PRO:O	1:A:264:ARG:C	2.56	0.43
1:A:425:MET:O	1:A:428:LEU:N	2.45	0.43
2:B:114:LEU:HD23	2:B:149:MET:HE1	2.01	0.43
2:B:161:TYR:C	2:B:163:ASP:N	2.71	0.43
2:B:383:ALA:C	2:B:385:GLN:N	2.72	0.43
3:D:176:LEU:HB2	3:D:181:GLN:HB2	2.00	0.43
4:F:143:GLY:O	4:F:147:SER:OG	2.33	0.43
4:F:358:GLU:HA	4:F:359:PRO:HD3	1.84	0.43
1:A:21:TRP:HE1	1:A:63:PRO:HB3	1.83	0.43
1:A:63:PRO:C	1:A:64:ARG:CG	2.83	0.43
1:A:76:ASP:O	1:A:79:ARG:N	2.52	0.43
1:A:154:MET:CE	1:A:166:LYS:HB3	2.48	0.43
1:A:209:ILE:CD1	1:A:231:ILE:CD1	2.97	0.43
2:B:210:TYR:O	2:B:214:PHE:N	2.52	0.43
4:F:152:LEU:HA	4:F:155:GLU:HG3	2.01	0.43
4:F:205:ASP:HB2	4:F:303:VAL:HA	2.00	0.43
2:G:118:VAL:O	2:G:122:VAL:HG13	2.19	0.43
2:G:298:ALA:O	2:G:300:ASN:N	2.52	0.43
2:G:400:ARG:HE	2:G:400:ARG:HB2	1.56	0.43
1:A:378:LEU:HD12	1:A:378:LEU:O	2.19	0.43
2:B:105:LYS:HG2	2:B:110:GLU:CG	2.48	0.43
2:B:192:HIS:NE2	2:B:420:GLU:HG2	2.34	0.43
2:B:311:ARG:HG2	2:B:311:ARG:NH1	2.34	0.43
3:D:167:GLY:HA2	10:D:500:ANP:H8	2.00	0.43
3:D:239:SER:N	2:G:419:THR:CB	2.82	0.43
2:G:209:LEU:HD21	2:G:231:VAL:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:94:PHE:N	2:B:94:PHE:CD2	2.83	0.43
2:B:118:VAL:O	2:B:122:VAL:HG13	2.19	0.43
2:B:333:LEU:O	2:B:334:ASN:C	2.58	0.43
4:F:68:VAL:HG11	4:F:118:VAL:HG21	2.01	0.43
1:A:15:GLN:NE2	7:B:500:GTP:N7	2.67	0.42
1:A:25:CYS:SG	1:A:26:LEU:N	2.92	0.42
1:A:230:LEU:O	1:A:233:GLN:N	2.35	0.42
1:A:409:VAL:C	1:A:411:GLU:N	2.71	0.42
2:B:82:PRO:HB2	2:B:83:PHE:H	1.56	0.42
2:B:359:PRO:CB	2:B:360:PRO:HD2	2.45	0.42
4:F:71:GLU:O	4:F:71:GLU:HG2	2.17	0.42
4:F:210:TYR:CE1	4:F:214:ARG:HD2	2.54	0.42
2:G:141:LEU:HD12	2:G:141:LEU:HA	1.81	0.42
1:A:363:VAL:HG13	1:A:364:PRO:HD2	2.01	0.42
2:B:35:SER:CB	2:B:59:ASN:HA	2.42	0.42
2:B:48:ARG:HG2	2:B:243:ARG:HB3	2.01	0.42
2:B:72:PRO:O	2:B:73:GLY:C	2.58	0.42
2:B:421:ALA:O	2:B:422:GLU:C	2.58	0.42
3:D:85:GLN:NE2	3:D:85:GLN:H	2.16	0.42
4:F:54:SER:O	4:F:56:THR:N	2.52	0.42
1:A:8:HIS:CD2	1:A:138:PHE:CD1	3.07	0.42
1:A:103:TYR:O	1:A:104:ALA:C	2.57	0.42
1:A:231:ILE:C	1:A:233:GLN:N	2.73	0.42
1:A:402:ARG:O	1:A:405:VAL:N	2.49	0.42
2:B:11:GLN:O	2:B:15:GLN:N	2.41	0.42
2:B:280:SER:OG	2:B:281:GLN:N	2.49	0.42
2:G:106:GLY:O	2:G:111:GLY:HA3	2.19	0.42
1:A:8:HIS:HA	1:A:138:PHE:HB2	2.00	0.42
1:A:105:ARG:O	1:A:110:ILE:CG2	2.64	0.42
1:A:436:GLY:C	1:A:438:ASP:N	2.72	0.42
2:B:409:THR:C	2:B:411:GLU:H	2.22	0.42
3:D:237:GLU:OE2	2:G:423:SER:HB3	2.18	0.42
1:A:67:PHE:HB2	1:A:92:LEU:HD23	2.02	0.42
1:A:119:LEU:HD11	1:A:156:ARG:HD3	2.01	0.42
1:A:147:SER:HB2	1:A:186:ASN:O	2.19	0.42
2:B:70:LEU:HB2	2:B:99:ALA:CB	2.49	0.42
2:B:427:ASP:OD1	2:B:427:ASP:C	2.58	0.42
4:F:277:SER:HA	4:F:367:ASP:O	2.19	0.42
4:F:306:ASP:HA	4:F:307:PRO:HD3	1.57	0.42
1:A:328:VAL:C	1:A:330:ALA:N	2.73	0.42
1:A:390:ARG:HG3	1:A:390:ARG:HH11	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:103:TRP:HB2	2:B:186:ASN:HA	2.01	0.42
2:B:106:GLY:O	2:B:149:MET:CA	2.68	0.42
2:B:210:TYR:O	2:B:211:ASP:C	2.57	0.42
2:B:250:ALA:CB	2:B:254:LYS:HE2	2.50	0.42
3:D:112:VAL:HB	4:F:431:ASP:C	2.39	0.42
4:F:84:ARG:HE	4:F:84:ARG:HB3	1.65	0.42
2:G:264:ARG:O	2:G:266:HIS:N	2.51	0.42
2:G:319:PHE:CD1	2:G:319:PHE:N	2.87	0.42
1:A:213:CYS:O	1:A:219:ILE:HG13	2.20	0.42
2:B:6:HIS:HB3	2:B:65:ALA:CB	2.48	0.42
2:B:150:GLY:HA2	2:B:153:LEU:CD2	2.41	0.42
2:B:204:ILE:HD13	2:B:231:VAL:CG2	2.45	0.42
2:B:333:LEU:HD11	2:B:337:ASN:HD21	1.85	0.42
2:B:343:PHE:CD2	2:B:350:ASN:ND2	2.88	0.42
2:B:435:TYR:C	2:B:437:ASP:N	2.72	0.42
3:D:112:VAL:HB	4:F:431:ASP:CA	2.47	0.42
4:F:21:TRP:CH2	4:F:63:PRO:HB3	2.55	0.42
4:F:62:VAL:HA	4:F:63:PRO:HD3	1.85	0.42
4:F:179:THR:HB	4:F:180:ALA:H	1.73	0.42
1:A:95:GLY:C	1:A:97:GLU:H	2.24	0.42
1:A:175:PRO:HG3	1:A:304:LYS:CB	2.50	0.42
1:A:199:ASP:CB	1:A:256:GLN:NE2	2.77	0.42
1:A:207:GLU:O	1:A:210:TYR:N	2.51	0.42
2:B:2:ARG:NH1	2:B:251:ASP:CG	2.73	0.42
2:B:273:ALA:HB1	2:B:291:LEU:HG	2.01	0.42
3:D:113:ASP:O	3:D:114:LEU:HB2	2.19	0.42
4:F:153:LEU:HD22	4:F:157:LEU:HG	2.01	0.42
4:F:407:TRP:CE2	2:G:257:VAL:HA	2.54	0.42
1:A:16:ILE:CG2	1:A:17:GLY:N	2.82	0.42
1:A:384:ILE:C	1:A:386:GLU:N	2.72	0.42
2:B:138:THR:O	2:B:139:HIS:HB3	2.19	0.42
2:B:153:LEU:HD13	2:B:153:LEU:N	2.34	0.42
2:B:171:VAL:HG12	2:B:171:VAL:O	2.20	0.42
2:B:242:LEU:HB3	2:B:250:ALA:O	2.20	0.42
2:B:273:ALA:CB	2:B:274:PRO:CD	2.93	0.42
2:B:399:PHE:O	2:B:401:ARG:N	2.53	0.42
3:D:304:LEU:N	3:D:304:LEU:CD2	2.82	0.42
1:A:210:TYR:OH	2:B:325:MET:HB3	2.20	0.42
1:A:242:LEU:HD11	1:A:250:VAL:HG23	2.02	0.42
1:A:255:PHE:O	1:A:257:THR:N	2.53	0.42
1:A:388:TRP:CE3	1:A:425:MET:HE3	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:188:THR:HA	2:B:425:MET:HE3	2.00	0.42
2:B:240:THR:HG23	2:B:241:CYS:N	2.33	0.42
3:D:335:LEU:CD1	4:F:402:ARG:HG3	2.47	0.42
2:G:231:VAL:HG12	2:G:235:MET:HE2	2.02	0.42
2:G:255:LEU:HD23	11:G:701:CN2:C22	2.50	0.42
1:A:204:VAL:CG1	1:A:209:ILE:HD11	2.42	0.41
1:A:343:PHE:HZ	1:A:351:PHE:CZ	2.36	0.41
4:F:47:ASP:O	4:F:49:PHE:N	2.53	0.41
4:F:274:PRO:HG3	4:F:291:ILE:HG21	2.02	0.41
1:A:175:PRO:CG	1:A:304:LYS:HG2	2.47	0.41
1:A:243:ARG:NH2	1:A:252:LEU:HG	2.35	0.41
2:B:192:HIS:HD1	2:B:424:ASN:CG	2.20	0.41
2:B:242:LEU:HD23	2:B:242:LEU:HA	1.76	0.41
2:B:274:PRO:HD3	2:B:374:SER:HA	2.03	0.41
2:B:413:MET:CG	2:B:414:ASP:H	2.26	0.41
2:B:417:GLU:O	2:B:420:GLU:HB3	2.21	0.41
4:F:230:LEU:HD12	4:F:230:LEU:O	2.20	0.41
2:G:403:ALA:C	2:G:405:LEU:N	2.71	0.41
1:A:152:LEU:C	1:A:152:LEU:CD1	2.89	0.41
1:A:332:ILE:CD1	1:A:353:VAL:HG22	2.51	0.41
1:A:428:LEU:HD12	1:A:428:LEU:HA	1.79	0.41
2:B:175:PRO:O	2:B:177:VAL:N	2.53	0.41
2:B:261:PRO:HB2	2:B:262:PHE:CD1	2.54	0.41
2:B:307:PRO:O	2:B:309:HIS:N	2.53	0.41
2:G:133:GLN:HE21	2:G:252:LEU:CB	2.31	0.41
1:A:104:ALA:HB3	1:A:408:TYR:HD2	1.84	0.41
1:A:110:ILE:O	1:A:111:GLY:C	2.57	0.41
1:A:130:THR:O	1:A:131:GLY:C	2.59	0.41
1:A:305:CYS:SG	1:A:383:ALA:HB1	2.60	0.41
4:F:139:HIS:CD2	4:F:150:THR:HG21	2.55	0.41
4:F:291:ILE:HD12	4:F:375:VAL:HG23	2.03	0.41
2:G:332:MET:CG	2:G:353:THR:HG21	2.38	0.41
1:A:23:LEU:HD11	1:A:361:THR:O	2.21	0.41
1:A:101:ASN:HD21	2:B:254:LYS:NZ	2.19	0.41
1:A:115:ILE:CD1	1:A:115:ILE:C	2.87	0.41
1:A:115:ILE:CG2	1:A:116:ASP:H	2.32	0.41
1:A:166:LYS:HB2	1:A:199:ASP:OD1	2.20	0.41
2:B:119:LEU:O	2:B:122:VAL:HG22	2.21	0.41
2:B:259:MET:HE3	2:B:268:PHE:CE1	2.56	0.41
3:D:73:ILE:HG23	3:D:403:SER:HB3	2.03	0.41
3:D:183:ALA:HB3	3:D:260:ILE:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:171:ILE:HG23	4:F:206:ASN:ND2	2.35	0.41
2:G:416:MET:H	2:G:416:MET:HG3	1.63	0.41
2:G:427:ASP:O	2:G:431:GLU:HG3	2.20	0.41
1:A:172:TYR:HA	1:A:173:PRO:HD3	1.93	0.41
1:A:288:VAL:O	1:A:289:ALA:C	2.59	0.41
2:B:12:CYS:O	2:B:13:GLY:C	2.59	0.41
2:B:202:TYR:CE2	2:B:268:PHE:HD1	2.38	0.41
2:B:409:THR:C	2:B:411:GLU:N	2.73	0.41
3:D:107:GLU:HA	3:D:108:PRO:HD3	1.79	0.41
2:G:198:THR:OG1	2:G:265:LEU:HD22	2.20	0.41
1:A:13:GLY:HA2	1:A:16:ILE:CG2	2.50	0.41
1:A:67:PHE:CE1	1:A:87:PHE:CE2	3.08	0.41
1:A:221:ARG:N	1:A:222:PRO:CD	2.83	0.41
1:A:335:ILE:C	1:A:337:THR:N	2.73	0.41
1:A:414:GLU:C	1:A:416:GLY:N	2.74	0.41
2:B:132:LEU:O	2:B:164:ARG:HD2	2.21	0.41
2:B:135:PHE:CD1	2:B:166:MET:SD	3.14	0.41
2:B:147:SER:CB	2:B:190:SER:HB3	2.42	0.41
2:B:168:THR:HB	2:B:198:THR:HG21	2.03	0.41
2:B:182:VAL:O	2:B:184:PRO:N	2.54	0.41
2:B:380:ASN:C	2:B:380:ASN:HD22	2.24	0.41
2:G:208:ALA:HB2	2:G:304:ALA:N	2.35	0.41
2:G:239:THR:O	2:G:240:THR:C	2.59	0.41
2:G:404:PHE:N	2:G:404:PHE:CD1	2.89	0.41
2:B:98:GLY:C	2:B:100:GLY:H	2.24	0.41
2:B:199:ASP:C	2:B:265:LEU:HD13	2.41	0.41
2:G:54:ASN:O	2:G:62:VAL:O	2.39	0.41
2:G:93:VAL:HG12	2:G:114:LEU:HD11	2.01	0.41
1:A:76:ASP:O	1:A:80:THR:N	2.53	0.41
1:A:149:PHE:CD1	1:A:150:THR:N	2.89	0.41
1:A:273:ALA:O	1:A:275:VAL:N	2.54	0.41
1:A:289:ALA:HB3	1:A:290:GLU:OE2	2.20	0.41
1:A:434:GLU:C	1:A:436:GLY:N	2.74	0.41
2:B:133:GLN:CG	2:B:165:ILE:HD11	2.49	0.41
2:B:239:THR:CG2	2:B:240:THR:N	2.80	0.41
2:B:276:THR:O	9:B:601:TA1:H192	2.21	0.41
2:B:282:GLN:O	2:B:282:GLN:CG	2.65	0.41
2:B:291:LEU:HD21	2:B:373:MET:HG2	2.03	0.41
3:D:217:GLU:HA	3:D:285:HIS:O	2.21	0.41
3:D:237:GLU:O	2:G:423:SER:HB2	2.21	0.41
4:F:115:ILE:HG13	4:F:152:LEU:CD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:190:THR:O	4:F:194:THR:HB	2.20	0.41
4:F:392:ASP:OD1	4:F:429:GLU:OE1	2.38	0.41
2:G:164:ARG:NH2	2:G:253:ARG:HH22	2.18	0.41
2:G:270:PRO:HA	2:G:377:PHE:O	2.21	0.41
1:A:204:VAL:CG1	1:A:231:ILE:HD12	2.42	0.41
1:A:318:LEU:HB2	1:A:376:CYS:SG	2.61	0.41
2:B:11:GLN:HA	2:B:74:THR:HG21	2.03	0.41
2:B:176:LYS:HD2	2:B:207:GLU:HB2	2.03	0.41
2:B:409:THR:O	2:B:412:GLY:N	2.48	0.41
3:D:269:CYS:O	3:D:269:CYS:SG	2.79	0.41
3:D:372:ARG:NH2	12:D:659:HOH:O	2.47	0.41
4:F:227:LEU:O	4:F:231:ILE:HG13	2.20	0.41
2:G:264:ARG:O	2:G:266:HIS:CD2	2.74	0.41
2:G:347:ILE:O	2:G:348:PRO:O	2.39	0.41
1:A:209:ILE:HD13	1:A:231:ILE:HD11	2.03	0.40
2:B:23:VAL:O	2:B:24:ILE:C	2.59	0.40
2:B:70:LEU:HB2	2:B:99:ALA:HB2	2.03	0.40
2:B:118:VAL:O	2:B:121:VAL:N	2.54	0.40
3:D:285:HIS:CD2	3:D:308:ALA:H	2.39	0.40
4:F:205:ASP:CB	4:F:303:VAL:HA	2.51	0.40
4:F:347:CYS:HA	4:F:348:PRO:HD2	1.88	0.40
2:G:62:VAL:HA	2:G:63:PRO:HD2	1.88	0.40
2:G:224:TYR:O	2:G:228:ASN:ND2	2.54	0.40
1:A:273:ALA:HB2	1:A:375:VAL:HB	2.03	0.40
1:A:320:ARG:O	1:A:373:ARG:HA	2.21	0.40
1:A:362:VAL:HG13	1:A:368:LEU:CB	2.50	0.40
2:B:25:SER:O	2:B:28:HIS:N	2.53	0.40
4:F:72:PRO:O	4:F:74:VAL:N	2.55	0.40
2:G:358:ILE:O	2:G:358:ILE:CG2	2.68	0.40
1:A:100:ALA:HB2	1:A:105:ARG:HD3	2.02	0.40
1:A:425:MET:O	1:A:426:ALA:C	2.60	0.40
2:B:20:PHE:CD2	2:B:235:MET:CG	3.04	0.40
4:F:238:ILE:HG23	4:F:255:PHE:HZ	1.86	0.40
2:G:89:PRO:O	2:G:92:PHE:HD1	2.03	0.40
1:A:14:VAL:HG11	1:A:75:ILE:HD13	2.04	0.40
1:A:98:ASP:OD1	1:A:98:ASP:N	2.55	0.40
1:A:217:LEU:HD12	1:A:277:SER:CB	2.49	0.40
1:A:286:LEU:HG	1:A:290:GLU:CB	2.52	0.40
1:A:401:LYS:O	1:A:402:ARG:HB2	2.21	0.40
1:A:413:MET:C	1:A:414:GLU:CG	2.90	0.40
2:B:99:ALA:O	2:B:100:GLY:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:241:GLN:CA	2:G:423:SER:OG	2.54	0.40
3:D:284:SER:O	3:D:308:ALA:HB2	2.22	0.40
1:A:282:TYR:HD2	1:A:284:GLU:HG3	1.86	0.40
1:A:397:LEU:HA	1:A:397:LEU:HD23	1.81	0.40
2:B:274:PRO:CB	2:B:371:LEU:HD21	2.52	0.40
2:B:405:LEU:HD23	2:B:405:LEU:O	2.21	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	408/451 (90%)	266 (65%)	83 (20%)	59 (14%)	0 4
2	B	424/445 (95%)	273 (64%)	95 (22%)	56 (13%)	0 5
2	G	415/445 (93%)	310 (75%)	57 (14%)	48 (12%)	0 6
3	D	291/331 (88%)	275 (94%)	13 (4%)	3 (1%)	15 55
4	F	415/451 (92%)	316 (76%)	59 (14%)	40 (10%)	0 10
All	All	1953/2123 (92%)	1440 (74%)	307 (16%)	206 (10%)	1 8

All (206) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	96	LYS
1	A	97	GLU
1	A	108	TYR
1	A	109	THR
1	A	141	PHE
1	A	183	GLU
1	A	217	LEU
1	A	240	ALA

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Mol	Chain	Res	Type
1	A	249	ASN
1	A	255	PHE
1	A	266	HIS
1	A	280	LYS
1	A	284	GLU
1	A	285	GLN
1	A	289	ALA
1	A	309	HIS
1	A	346	TRP
1	A	370	LYS
1	A	387	ALA
1	A	403	ALA
1	A	437	VAL
2	B	23	VAL
2	B	24	ILE
2	B	32	PRO
2	B	50	ASN
2	B	82	PRO
2	B	97	SER
2	B	128	SER
2	B	176	LYS
2	B	183	GLU
2	B	218	LYS
2	B	238	VAL
2	B	239	THR
2	B	240	THR
2	B	252	LEU
2	B	263	PRO
2	B	266	HIS
2	B	273	ALA
2	B	278	ARG
2	B	280	SER
2	B	281	GLN
2	B	282	GLN
2	B	288	VAL
2	B	294	GLN
2	B	295	MET
2	B	343	PHE
2	B	344	VAL
2	B	346	TRP
2	B	369	ARG
2	B	403	ALA

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Mol	Chain	Res	Type
3	D	238	ASP
3	D	282	SER
4	F	11	GLN
4	F	55	GLU
4	F	62	VAL
4	F	73	THR
4	F	178	SER
4	F	240	ALA
4	F	253	THR
4	F	265	ILE
4	F	266	HIS
4	F	273	ALA
4	F	314	ALA
4	F	345	ASP
4	F	348	PRO
4	F	377	MET
2	G	3	GLU
2	G	11	GLN
2	G	42	LEU
2	G	43	GLN
2	G	60	LYS
2	G	62	VAL
2	G	115	VAL
2	G	159	GLU
2	G	217	LEU
2	G	218	LYS
2	G	220	THR
2	G	264	ARG
2	G	265	LEU
2	G	266	HIS
2	G	273	ALA
2	G	276	THR
2	G	288	VAL
2	G	348	PRO
2	G	371	LEU
2	G	404	PHE
1	A	24	TYR
1	A	63	PRO
1	A	103	TYR
1	A	111	GLY
1	A	131	GLY
1	A	218	ASP

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Mol	Chain	Res	Type
1	A	219	ILE
1	A	238	ILE
1	A	265	GLY
1	A	287	SER
1	A	314	ALA
1	A	339	ARG
1	A	342	GLN
1	A	373	ARG
1	A	386	GLU
2	B	38	GLY
2	B	73	GLY
2	B	175	PRO
2	B	265	LEU
2	B	279	GLY
2	B	298	ALA
2	B	300	ASN
2	B	311	ARG
4	F	72	PRO
4	F	83	TYR
4	F	144	GLY
4	F	164	LYS
4	F	246	GLY
4	F	305	CYS
4	F	350	GLY
4	F	357	TYR
4	F	403	ALA
2	G	34	GLY
2	G	73	GLY
2	G	82	PRO
2	G	109	THR
2	G	163	ASP
2	G	225	GLY
2	G	227	LEU
2	G	245	PRO
2	G	249	ASN
2	G	299	LYS
2	G	308	ARG
2	G	349	ASN
2	G	370	GLY
2	G	400	ARG
2	G	402	LYS
2	G	403	ALA

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Mol	Chain	Res	Type
1	A	104	ALA
1	A	148	GLY
1	A	149	PHE
1	A	173	PRO
1	A	239	THR
1	A	245	ASP
1	A	263	PRO
1	A	279	GLU
1	A	288	VAL
1	A	330	ALA
1	A	336	LYS
1	A	369	ALA
2	B	34	GLY
2	B	83	PHE
2	B	99	ALA
2	B	100	GLY
2	B	302	MET
2	B	386	GLU
4	F	59	GLY
4	F	112	LYS
4	F	175	PRO
4	F	257	THR
4	F	264	ARG
4	F	349	THR
2	G	226	ASP
2	G	244	PHE
2	G	340	SER
1	A	89	PRO
1	A	129	CYS
1	A	256	GLN
1	A	300	ASN
1	A	348	PRO
2	B	96	GLN
2	B	395	PHE
4	F	32	PRO
4	F	48	SER
4	F	101	ASN
4	F	109	THR
4	F	248	LEU
2	G	47	GLU
2	G	99	ALA
2	G	246	GLY

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Mol	Chain	Res	Type
2	G	252	LEU
2	G	344	VAL
1	A	303	VAL
1	A	382	THR
2	B	57	ALA
2	B	74	THR
2	B	285	ALA
2	B	424	ASN
4	F	34	GLY
4	F	241	SER
2	G	37	HIS
2	G	39	ASP
2	G	146	GLY
1	A	31	GLN
1	A	273	ALA
1	A	307	PRO
2	B	51	VAL
2	B	58	GLY
2	B	145	THR
2	B	162	PRO
2	B	400	ARG
3	D	354	ARG
4	F	4	CYS
2	G	240	THR
2	B	195	VAL
4	F	162	GLY
1	A	115	ILE
4	F	274	PRO
2	B	72	PRO
4	F	10	GLY

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	347/377 (92%)	298 (86%)	49 (14%)	3 16

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	367/381 (96%)	307 (84%)	60 (16%)	2	13
2	G	348/381 (91%)	241 (69%)	107 (31%)	0	2
3	D	261/286 (91%)	237 (91%)	24 (9%)	9	29
4	F	336/378 (89%)	229 (68%)	107 (32%)	0	2
All	All	1659/1803 (92%)	1312 (79%)	347 (21%)	3	6

All (347) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	SER
1	A	20	CYS
1	A	21	TRP
1	A	32	PRO
1	A	76	ASP
1	A	82	THR
1	A	98	ASP
1	A	115	ILE
1	A	120	ASP
1	A	125	LEU
1	A	127	ASP
1	A	130	THR
1	A	135	PHE
1	A	141	PHE
1	A	150	THR
1	A	152	LEU
1	A	155	GLU
1	A	169	PHE
1	A	172	TYR
1	A	173	PRO
1	A	183	GLU
1	A	192	HIS
1	A	204	VAL
1	A	219	ILE
1	A	224	TYR
1	A	231	ILE
1	A	234	ILE
1	A	243	ARG
1	A	244	PHE
1	A	253	THR
1	A	260	VAL
1	A	267	PHE

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Mol	Chain	Res	Type
1	A	269	LEU
1	A	276	ILE
1	A	284	GLU
1	A	303	VAL
1	A	325	PRO
1	A	334	THR
1	A	345	ASP
1	A	352	LYS
1	A	368	LEU
1	A	376	CYS
1	A	378	LEU
1	A	380	ASN
1	A	404	PHE
1	A	415	GLU
1	A	417	GLU
1	A	431	ASP
1	A	432	TYR
2	B	14	ASN
2	B	24	ILE
2	B	26	ASP
2	B	32	PRO
2	B	41	ASP
2	B	68	VAL
2	B	76	ASP
2	B	90	ASP
2	B	94	PHE
2	B	101	ASN
2	B	122	VAL
2	B	129	CYS
2	B	135	PHE
2	B	141	LEU
2	B	145	THR
2	B	149	MET
2	B	153	LEU
2	B	161	TYR
2	B	163	ASP
2	B	165	ILE
2	B	174	SER
2	B	198	THR
2	B	201	THR
2	B	203	CYS
2	B	207	GLU

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Mol	Chain	Res	Type
2	B	211	ASP
2	B	214	PHE
2	B	215	ARG
2	B	224	TYR
2	B	227	LEU
2	B	230	LEU
2	B	236	SER
2	B	240	THR
2	B	244	PHE
2	B	265	LEU
2	B	267	PHE
2	B	275	LEU
2	B	282	GLN
2	B	283	TYR
2	B	284	ARG
2	B	289	PRO
2	B	299	LYS
2	B	306	ASP
2	B	309	HIS
2	B	322	ARG
2	B	324	SER
2	B	325	MET
2	B	343	PHE
2	B	344	VAL
2	B	349	ASN
2	B	369	ARG
2	B	380	ASN
2	B	387	LEU
2	B	413	MET
2	B	414	ASP
2	B	424	ASN
2	B	427	ASP
2	B	431	GLU
2	B	432	TYR
2	B	437	ASP
3	D	73	ILE
3	D	97	VAL
3	D	119	GLU
3	D	175	ASP
3	D	182	ASN
3	D	213	VAL
3	D	215	PHE

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Mol	Chain	Res	Type
3	D	239	SER
3	D	240	ARG
3	D	241	GLN
3	D	242	GLN
3	D	244	GLN
3	D	249	GLN
3	D	280	ASN
3	D	281	SER
3	D	283	ARG
3	D	297	ARG
3	D	302	PHE
3	D	311	GLU
3	D	342	ARG
3	D	370	ASN
3	D	387	GLU
3	D	390	LEU
3	D	398	ARG
4	F	2	ARG
4	F	4	CYS
4	F	9	VAL
4	F	16	ILE
4	F	20	CYS
4	F	22	GLU
4	F	27	GLU
4	F	36	MET
4	F	50	ASN
4	F	51	THR
4	F	62	VAL
4	F	68	VAL
4	F	73	THR
4	F	74	VAL
4	F	79	ARG
4	F	80	THR
4	F	82	THR
4	F	85	GLN
4	F	87	PHE
4	F	88	HIS
4	F	90	GLU
4	F	91	GLN
4	F	94	THR
4	F	97	GLU
4	F	101	ASN

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Mol	Chain	Res	Type
4	F	105	ARG
4	F	110	ILE
4	F	112	LYS
4	F	114	ILE
4	F	115	ILE
4	F	116	ASP
4	F	120	ASP
4	F	122	ILE
4	F	123	ARG
4	F	124	LYS
4	F	128	GLN
4	F	140	SER
4	F	141	PHE
4	F	145	THR
4	F	147	SER
4	F	153	LEU
4	F	155	GLU
4	F	163	LYS
4	F	165	SER
4	F	176	GLN
4	F	178	SER
4	F	182	VAL
4	F	183	GLU
4	F	187	SER
4	F	193	THR
4	F	194	THR
4	F	195	LEU
4	F	198	SER
4	F	199	ASP
4	F	200	CYS
4	F	206	ASN
4	F	211	ASP
4	F	212	ILE
4	F	220	GLU
4	F	223	THR
4	F	225	THR
4	F	226	ASN
4	F	227	LEU
4	F	230	LEU
4	F	234	ILE
4	F	241	SER
4	F	242	LEU

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Mol	Chain	Res	Type
4	F	250	VAL
4	F	251	ASP
4	F	256	GLN
4	F	257	THR
4	F	258	ASN
4	F	265	ILE
4	F	271	THR
4	F	287	SER
4	F	288	VAL
4	F	306	ASP
4	F	313	MET
4	F	315	CYS
4	F	316	CYS
4	F	329	ASN
4	F	340	THR
4	F	341	ILE
4	F	343	PHE
4	F	344	VAL
4	F	349	THR
4	F	355	ILE
4	F	356	ASN
4	F	358	GLU
4	F	362	VAL
4	F	363	VAL
4	F	367	ASP
4	F	368	LEU
4	F	370	LYS
4	F	371	VAL
4	F	377	MET
4	F	379	SER
4	F	381	THR
4	F	384	ILE
4	F	394	LYS
4	F	397	LEU
4	F	401	LYS
4	F	405	VAL
4	F	413	MET
4	F	414	GLU
4	F	415	GLU
4	F	430	LYS
2	G	2	ARG
2	G	4	ILE

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Mol	Chain	Res	Type
2	G	5	VAL
2	G	11	GLN
2	G	12	CYS
2	G	16	ILE
2	G	23	VAL
2	G	26	ASP
2	G	31	ASP
2	G	33	THR
2	G	36	TYR
2	G	39	ASP
2	G	40	SER
2	G	42	LEU
2	G	43	GLN
2	G	49	ILE
2	G	55	GLU
2	G	61	TYR
2	G	62	VAL
2	G	71	GLU
2	G	76	ASP
2	G	77	SER
2	G	80	SER
2	G	83	PHE
2	G	91	ASN
2	G	101	ASN
2	G	102	ASN
2	G	109	THR
2	G	120	ASP
2	G	122	VAL
2	G	130	ASP
2	G	137	LEU
2	G	138	THR
2	G	141	LEU
2	G	147	SER
2	G	151	THR
2	G	154	ILE
2	G	155	SER
2	G	156	LYS
2	G	158	ARG
2	G	164	ARG
2	G	166	MET
2	G	170	SER
2	G	171	VAL

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Mol	Chain	Res	Type
2	G	174	SER
2	G	176	LYS
2	G	177	VAL
2	G	179	ASP
2	G	181	VAL
2	G	190	SER
2	G	193	GLN
2	G	195	VAL
2	G	197	ASN
2	G	198	THR
2	G	200	GLU
2	G	209	LEU
2	G	216	THR
2	G	223	THR
2	G	224	TYR
2	G	226	ASP
2	G	230	LEU
2	G	241	CYS
2	G	242	LEU
2	G	243	ARG
2	G	244	PHE
2	G	251	ASP
2	G	253	ARG
2	G	257	VAL
2	G	258	ASN
2	G	265	LEU
2	G	269	MET
2	G	275	LEU
2	G	276	THR
2	G	286	LEU
2	G	287	THR
2	G	292	THR
2	G	294	GLN
2	G	295	MET
2	G	300	ASN
2	G	302	MET
2	G	308	ARG
2	G	313	LEU
2	G	318	VAL
2	G	320	ARG
2	G	323	MET
2	G	325	MET

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Mol	Chain	Res	Type
2	G	336	GLN
2	G	341	SER
2	G	345	GLU
2	G	350	ASN
2	G	357	ASP
2	G	358	ILE
2	G	371	LEU
2	G	374	SER
2	G	376	THR
2	G	380	ASN
2	G	384	ILE
2	G	400	ARG
2	G	401	ARG
2	G	402	LYS
2	G	405	LEU
2	G	415	GLU
2	G	416	MET
2	G	419	THR
2	G	423	SER
2	G	425	MET
2	G	430	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	15	GLN
1	A	28	HIS
1	A	128	GLN
1	A	133	GLN
1	A	139	HIS
1	A	197	HIS
1	A	216	ASN
1	A	226	ASN
1	A	256	GLN
1	A	309	HIS
1	A	380	ASN
2	B	14	ASN
2	B	91	ASN
2	B	101	ASN
2	B	102	ASN
2	B	107	HIS

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Mol	Chain	Res	Type
2	B	136	GLN
2	B	139	HIS
2	B	282	GLN
2	B	331	GLN
2	B	334	ASN
2	B	337	ASN
2	B	349	ASN
2	B	380	ASN
2	B	406	HIS
2	B	436	GLN
3	D	85	GLN
3	D	182	ASN
3	D	208	ASN
3	D	244	GLN
3	D	285	HIS
3	D	370	ASN
3	D	391	ASN
4	F	8	HIS
4	F	88	HIS
4	F	91	GLN
4	F	101	ASN
4	F	107	HIS
4	F	133	GLN
4	F	139	HIS
4	F	176	GLN
4	F	206	ASN
4	F	256	GLN
4	F	258	ASN
4	F	266	HIS
4	F	301	GLN
4	F	329	ASN
4	F	372	GLN
2	G	6	HIS
2	G	43	GLN
2	G	54	ASN
2	G	136	GLN
2	G	139	HIS
2	G	294	GLN
2	G	300	ASN
2	G	339	ASN
2	G	350	ASN
2	G	380	ASN

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Mol	Chain	Res	Type
2	G	385	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 11 ligands modelled in this entry, 4 are monoatomic - leaving 7 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	$\#\|Z\| > 2$
8	GDP	F	603	-	24,30,30	1.24	2 (8%)	30,47,47	1.57	7 (23%)
7	GTP	B	500	6	26,34,34	1.31	4 (15%)	32,54,54	1.11	3 (9%)
7	GTP	F	601	6	26,34,34	1.22	2 (7%)	32,54,54	1.70	9 (28%)
9	TA1	B	601	-	68,68,68	2.01	19 (27%)	105,105,105	1.39	11 (10%)
10	ANP	D	500	6	29,33,33	1.69	4 (13%)	31,52,52	3.40	12 (38%)
11	CN2	G	701	-	27,32,32	3.27	7 (25%)	26,45,45	5.00	11 (42%)
8	GDP	B	600	-	24,30,30	2.59	9 (37%)	30,47,47	2.92	8 (26%)

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
8	GDP	F	603	-	-	3/12/32/32	0/3/3/3
7	GTP	B	500	6	-	3/18/38/38	0/3/3/3
7	GTP	F	601	6	-	4/18/38/38	0/3/3/3
9	TA1	B	601	-	-	9/41/127/127	0/7/7/7
10	ANP	D	500	6	-	9/14/38/38	0/3/3/3
11	CN2	G	701	-	-	2/10/27/27	0/3/3/3
8	GDP	B	600	-	-	4/12/32/32	0/3/3/3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	G	701	CN2	C20-C19	-8.49	1.24	1.38
11	G	701	CN2	C19-C17	-7.83	1.25	1.39
11	G	701	CN2	C15-C16	7.34	1.54	1.39
11	G	701	CN2	C20-C21	-6.77	1.24	1.39
8	B	600	GDP	O4'-C1'	6.20	1.49	1.41
8	B	600	GDP	O6-C6	5.71	1.34	1.23
11	G	701	CN2	O6-C17	5.44	1.45	1.37
9	B	601	TA1	C06-C05	5.25	1.50	1.38
9	B	601	TA1	C18-C10	5.05	1.68	1.57
8	B	600	GDP	C2-N1	4.66	1.49	1.37
9	B	601	TA1	C08-C07	-4.64	1.25	1.38
9	B	601	TA1	C05-C04	4.29	1.46	1.39
10	D	500	ANP	PB-O3A	4.28	1.64	1.59
7	F	601	GTP	C5-C6	-4.12	1.39	1.47
9	B	601	TA1	C45-C24	3.94	1.61	1.54
10	D	500	ANP	PB-O2B	-3.89	1.46	1.56
7	B	500	GTP	C5-C6	-3.84	1.39	1.47
8	B	600	GDP	PB-O2B	-3.78	1.40	1.54
8	F	603	GDP	C5-C6	-3.71	1.39	1.47
9	B	601	TA1	O02-C03	3.59	1.42	1.34
8	B	600	GDP	C8-N7	3.55	1.41	1.35
10	D	500	ANP	C2-N1	3.43	1.40	1.33
9	B	601	TA1	C25-C24	3.33	1.39	1.34
9	B	601	TA1	C36-C31	3.30	1.45	1.39
9	B	601	TA1	C46-C45	3.11	1.59	1.53
11	G	701	CN2	C1-C22	-3.10	1.37	1.43
9	B	601	TA1	C43-C01	3.08	1.60	1.54
9	B	601	TA1	C11-C10	3.06	1.61	1.54
8	B	600	GDP	C5-C6	-2.92	1.41	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	500	ANP	PG-O1G	2.83	1.50	1.46
9	B	601	TA1	C43-C26	2.78	1.58	1.52
7	B	500	GTP	C6-N1	2.63	1.41	1.37
9	B	601	TA1	C26-C25	2.48	1.56	1.51
11	G	701	CN2	C11-N1	-2.46	1.43	1.46
7	B	500	GTP	C8-N7	-2.43	1.30	1.35
9	B	601	TA1	C18-C20	2.43	1.62	1.55
9	B	601	TA1	C04-C03	-2.37	1.44	1.50
9	B	601	TA1	C01-C45	2.36	1.66	1.56
8	B	600	GDP	PB-O3B	2.36	1.63	1.54
8	B	600	GDP	C2-N3	-2.33	1.27	1.33
7	F	601	GTP	O4'-C4'	-2.33	1.39	1.45
8	F	603	GDP	C2-N3	2.24	1.38	1.33
9	B	601	TA1	C16-C15	2.18	1.56	1.52
7	B	500	GTP	O4'-C1'	2.11	1.44	1.41
9	B	601	TA1	C37-C29	2.11	1.54	1.52
9	B	601	TA1	C10-C02	2.11	1.62	1.57
8	B	600	GDP	O3'-C3'	2.05	1.47	1.43

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	G	701	CN2	C19-C20-C21	20.64	146.64	129.68
8	B	600	GDP	C8-N7-C5	9.27	120.65	102.99
11	G	701	CN2	C10-C11-N1	-8.94	93.97	110.04
10	D	500	ANP	O2B-PB-O1B	8.58	127.91	109.92
10	D	500	ANP	O5'-PA-O1A	-7.67	79.12	109.07
10	D	500	ANP	O2B-PB-O3A	-7.64	79.15	104.64
10	D	500	ANP	O3A-PB-N3B	-6.46	88.66	106.59
8	B	600	GDP	N2-C2-N3	6.24	131.89	119.74
8	B	600	GDP	C5-C6-N1	6.10	124.72	113.95
10	D	500	ANP	O2A-PA-O5'	-5.79	80.84	107.75
11	G	701	CN2	C20-C19-C17	5.31	142.56	129.69
9	B	601	TA1	C06-C05-C04	-4.83	114.63	120.34
10	D	500	ANP	C5-C6-N6	4.75	127.57	120.35
11	G	701	CN2	C10-C9-C8	-4.72	103.36	113.68
9	B	601	TA1	C07-C08-C09	4.70	127.35	120.19
11	G	701	CN2	O3-C5-C7	-4.47	116.42	124.12
8	B	600	GDP	O6-C6-C5	-4.24	116.10	124.37
8	B	600	GDP	N2-C2-N1	-4.16	107.86	116.71
9	B	601	TA1	C05-C04-C03	-3.95	111.48	120.40
8	B	600	GDP	C2-N1-C6	-3.74	118.21	125.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	F	601	GTP	PB-O3B-PG	-3.67	120.22	132.83
8	F	603	GDP	C8-N7-C5	3.57	109.78	102.99
9	B	601	TA1	C09-C04-C03	3.52	128.34	120.40
10	D	500	ANP	C5-C6-N1	-3.51	112.40	120.35
10	D	500	ANP	N3-C2-N1	-3.50	123.20	128.68
11	G	701	CN2	O3-C5-C3	3.49	121.29	115.16
11	G	701	CN2	O4-C12-C13	3.44	127.50	121.59
7	F	601	GTP	O3'-C3'-C4'	-3.43	101.12	111.05
7	F	601	GTP	C5-C6-N1	3.42	120.00	113.95
8	B	600	GDP	C2'-C3'-C4'	3.35	109.15	102.64
11	G	701	CN2	C11-N1-C12	3.33	128.63	123.33
11	G	701	CN2	C4-O2-C3	3.27	123.74	114.78
9	B	601	TA1	C17-C18-C20	3.13	109.82	102.59
10	D	500	ANP	C2-N1-C6	3.12	124.08	118.75
8	F	603	GDP	C5-C6-N1	3.12	119.45	113.95
9	B	601	TA1	C45-C01-C02	3.01	115.20	111.91
7	F	601	GTP	O6-C6-C5	-2.97	118.58	124.37
9	B	601	TA1	O04-C11-C14	-2.90	101.75	108.09
7	F	601	GTP	C8-N7-C5	2.83	108.38	102.99
10	D	500	ANP	O1G-PG-N3B	-2.76	107.70	111.77
11	G	701	CN2	O4-C12-N1	2.75	127.59	122.95
8	F	603	GDP	C2-N1-C6	-2.71	120.10	125.10
7	F	601	GTP	C2-N1-C6	-2.66	120.19	125.10
7	B	500	GTP	O2G-PG-O3B	2.65	113.51	104.64
9	B	601	TA1	O01-C01-C43	2.55	113.40	107.03
10	D	500	ANP	O4'-C4'-C3'	-2.44	100.28	105.11
7	F	601	GTP	PA-O3A-PB	-2.43	124.50	132.83
11	G	701	CN2	C5-C3-C1	-2.43	118.42	120.18
7	F	601	GTP	N2-C2-N1	2.27	121.54	116.71
8	F	603	GDP	O3B-PB-O3A	2.26	112.21	104.64
8	B	600	GDP	O2'-C2'-C3'	2.25	119.11	111.82
8	F	603	GDP	O2B-PB-O3A	2.24	112.14	104.64
9	B	601	TA1	C14-C11-C15	-2.16	83.10	85.40
9	B	601	TA1	C10-C18-C17	-2.16	102.33	106.54
8	F	603	GDP	N1-C2-N3	-2.12	119.36	123.32
8	F	603	GDP	O6-C6-C5	-2.12	120.23	124.37
7	B	500	GTP	O5'-C5'-C4'	2.08	116.15	108.99
10	D	500	ANP	O2A-PA-O1A	2.08	122.53	112.24
9	B	601	TA1	O06-C15-C11	2.07	92.91	90.58
7	F	601	GTP	N1-C2-N3	-2.06	119.47	123.32
7	B	500	GTP	O3G-PG-O3B	2.02	111.41	104.64

There are no chirality outliers.

All (34) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	F	601	GTP	C5'-O5'-PA-O1A
8	B	600	GDP	PA-O3A-PB-O2B
8	B	600	GDP	C5'-O5'-PA-O3A
8	B	600	GDP	C5'-O5'-PA-O1A
10	D	500	ANP	PG-N3B-PB-O1B
10	D	500	ANP	PA-O3A-PB-O1B
10	D	500	ANP	PA-O3A-PB-O2B
10	D	500	ANP	C5'-O5'-PA-O1A
10	D	500	ANP	C5'-O5'-PA-O2A
10	D	500	ANP	C5'-O5'-PA-O3A
9	B	601	TA1	O02-C03-C04-C05
9	B	601	TA1	O02-C03-C04-C09
9	B	601	TA1	O03-C03-C04-C09
8	F	603	GDP	O4'-C4'-C5'-O5'
9	B	601	TA1	O03-C03-C04-C05
9	B	601	TA1	N01-C30-C31-C36
9	B	601	TA1	O14-C30-C31-C36
8	F	603	GDP	C3'-C4'-C5'-O5'
10	D	500	ANP	O4'-C4'-C5'-O5'
10	D	500	ANP	C3'-C4'-C5'-O5'
11	G	701	CN2	C7-C5-O3-C6
9	B	601	TA1	N01-C30-C31-C32
9	B	601	TA1	O14-C30-C31-C32
11	G	701	CN2	C3-C5-O3-C6
7	B	500	GTP	C3'-C4'-C5'-O5'
8	F	603	GDP	PA-O3A-PB-O1B
7	F	601	GTP	C5'-O5'-PA-O3A
7	B	500	GTP	O4'-C4'-C5'-O5'
7	F	601	GTP	C5'-O5'-PA-O2A
7	F	601	GTP	PG-O3B-PB-O1B
8	B	600	GDP	PA-O3A-PB-O3B
10	D	500	ANP	PB-O3A-PA-O1A
9	B	601	TA1	C15-C11-O04-C12
7	B	500	GTP	C5'-O5'-PA-O1A

There are no ring outliers.

7 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	F	603	GDP	1	0
7	B	500	GTP	4	0

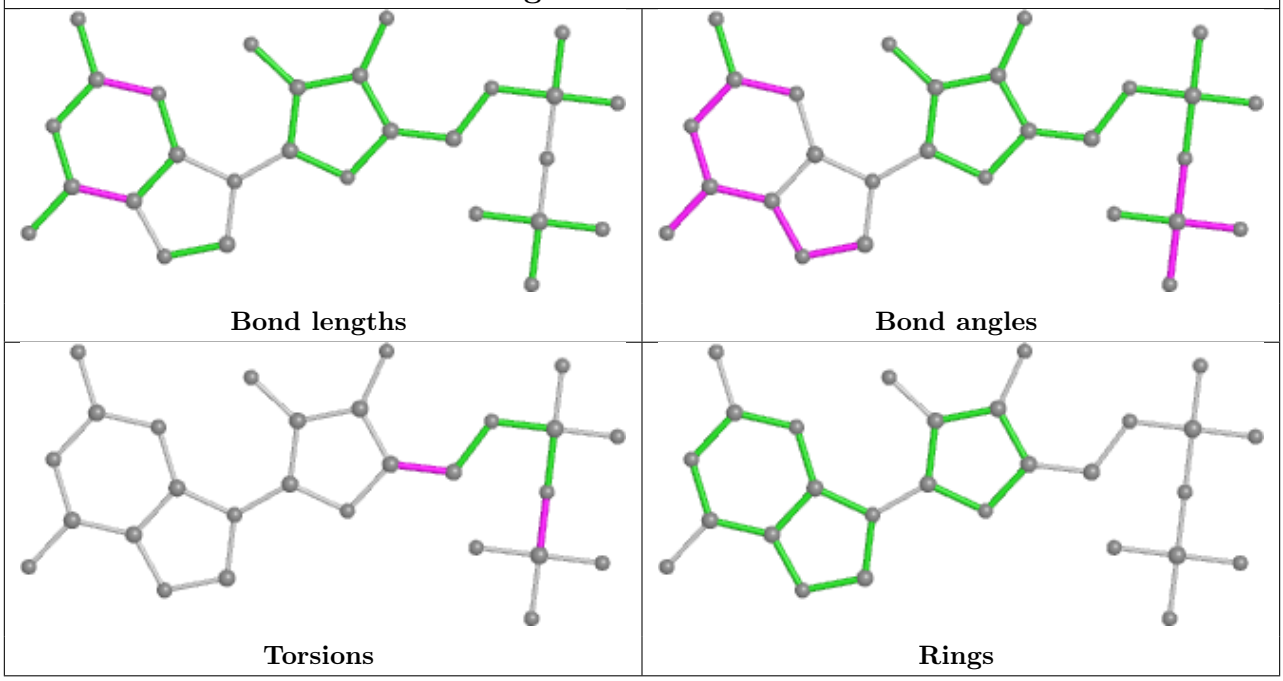
Continued on next page...

Continued from previous page...

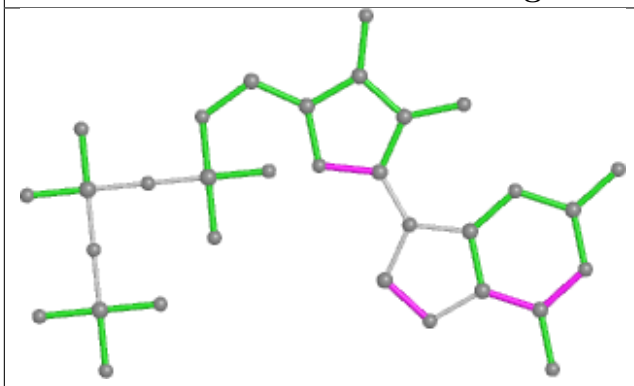
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	F	601	GTP	2	0
9	B	601	TA1	6	0
10	D	500	ANP	3	0
11	G	701	CN2	8	0
8	B	600	GDP	1	0

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.

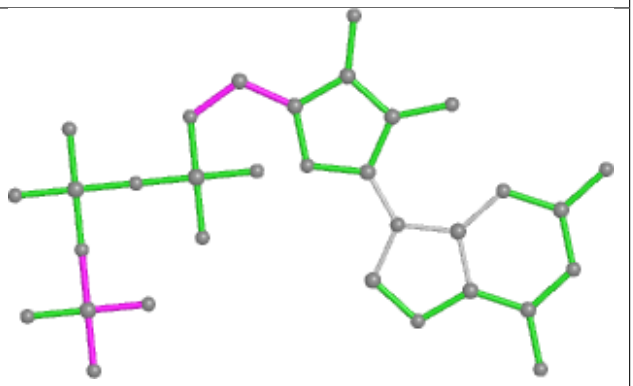
Ligand GDP F 603



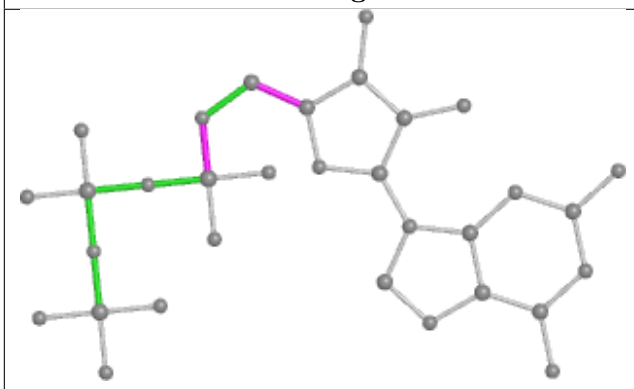
Ligand GTP B 500



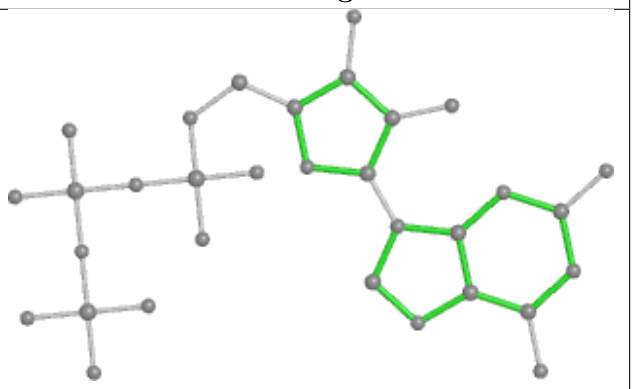
Bond lengths



Bond angles

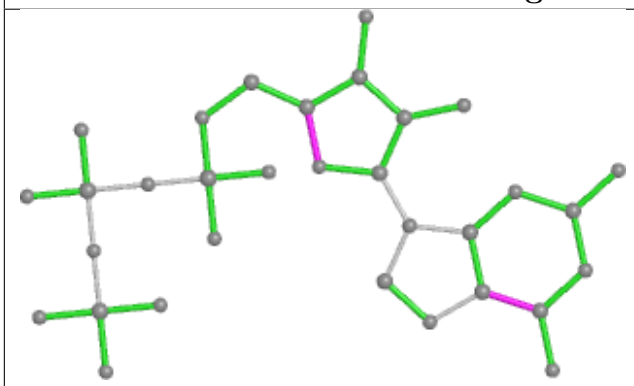


Torsions

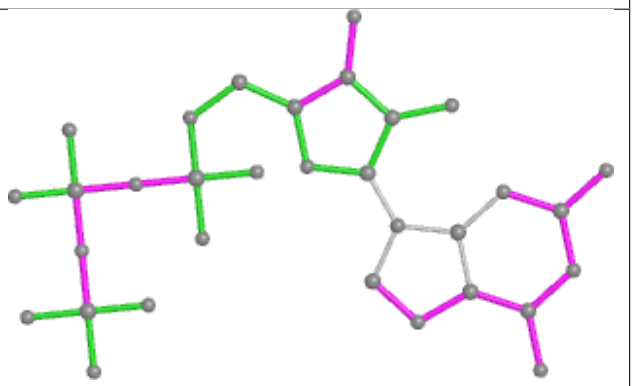


Rings

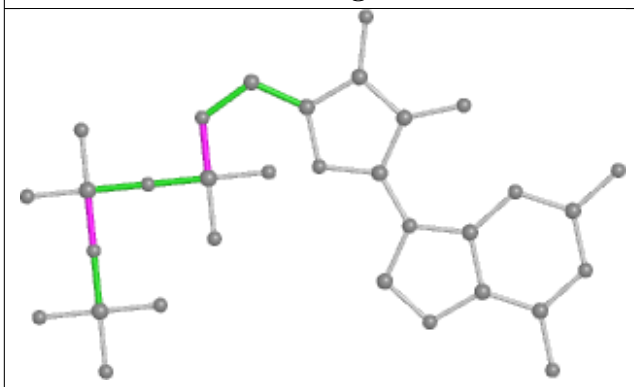
Ligand GTP F 601



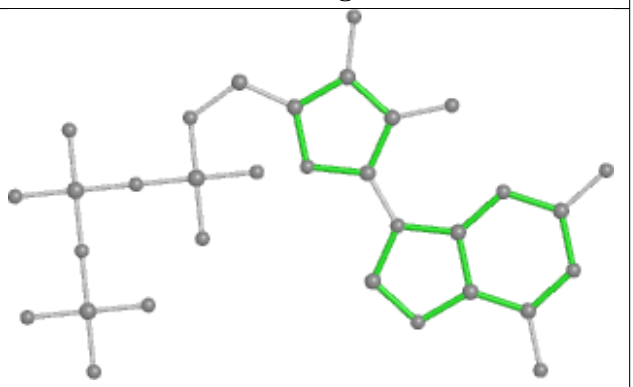
Bond lengths



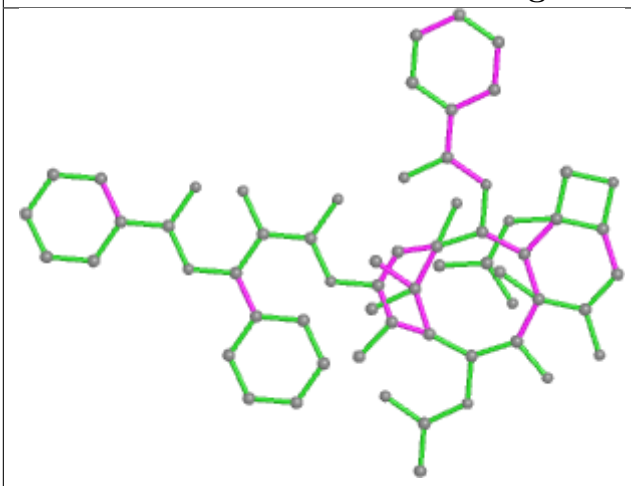
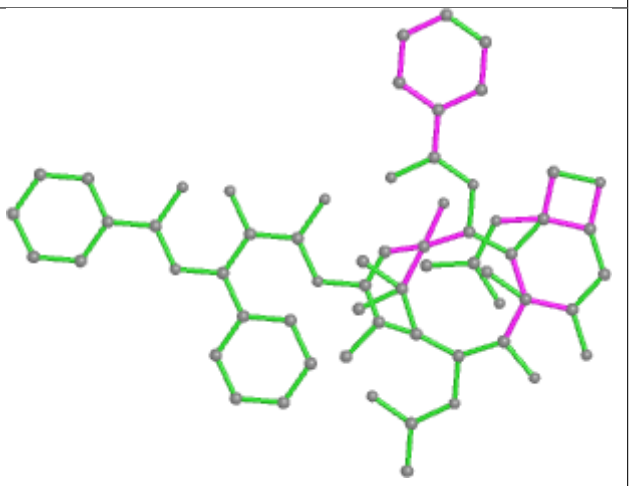
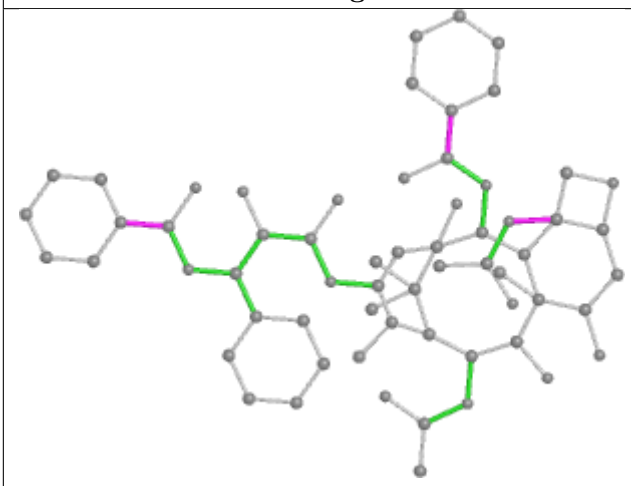
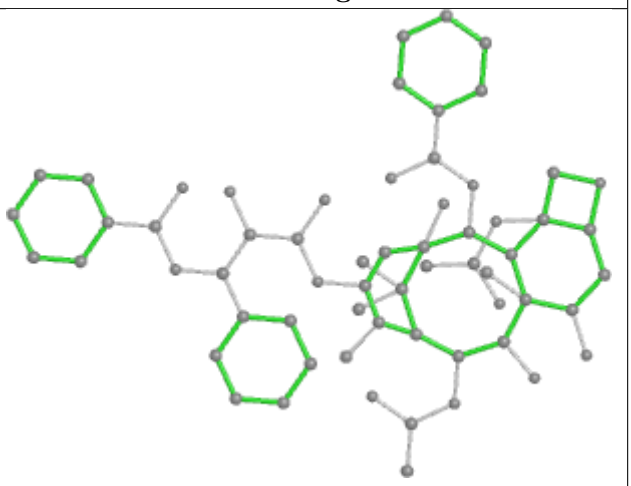
Bond angles



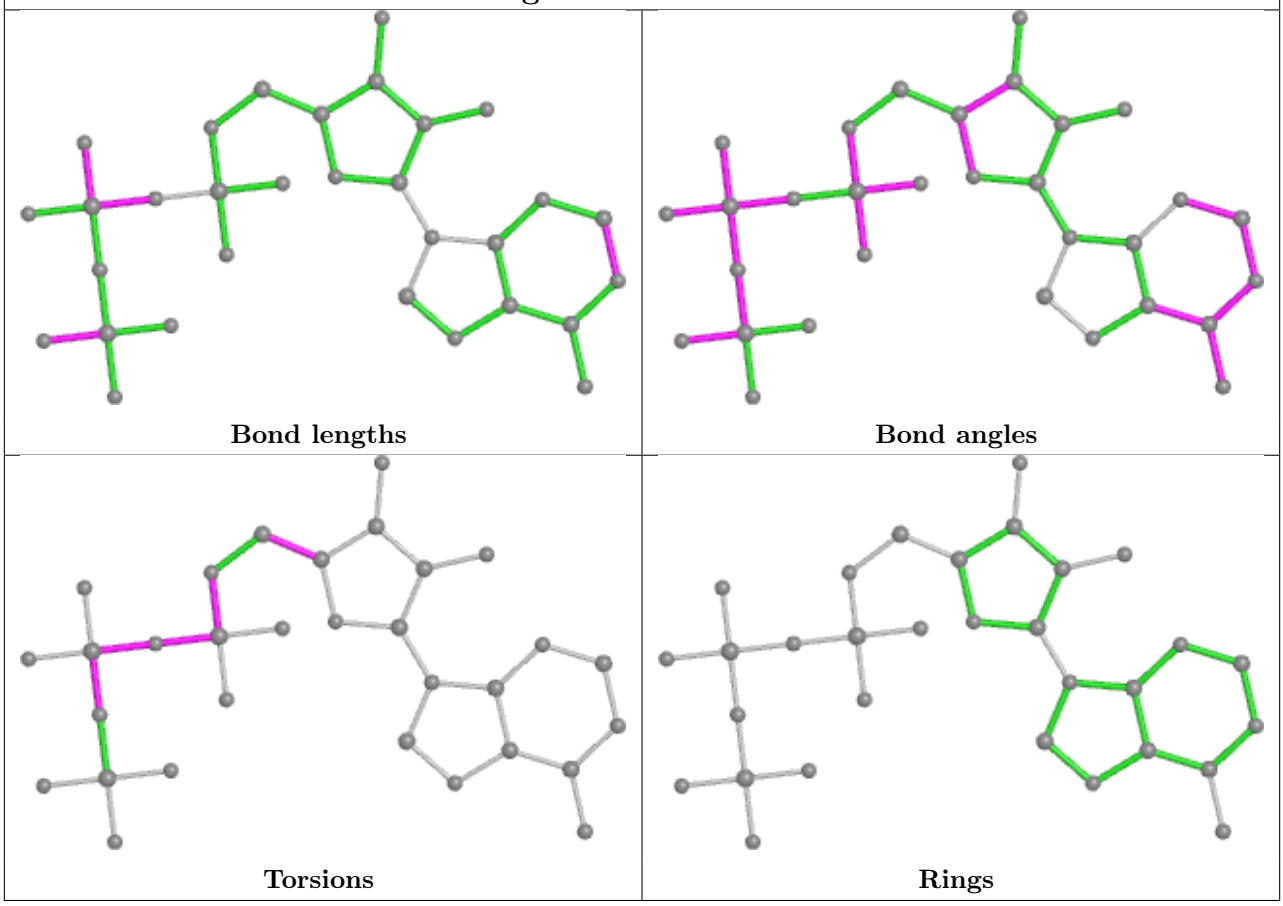
Torsions



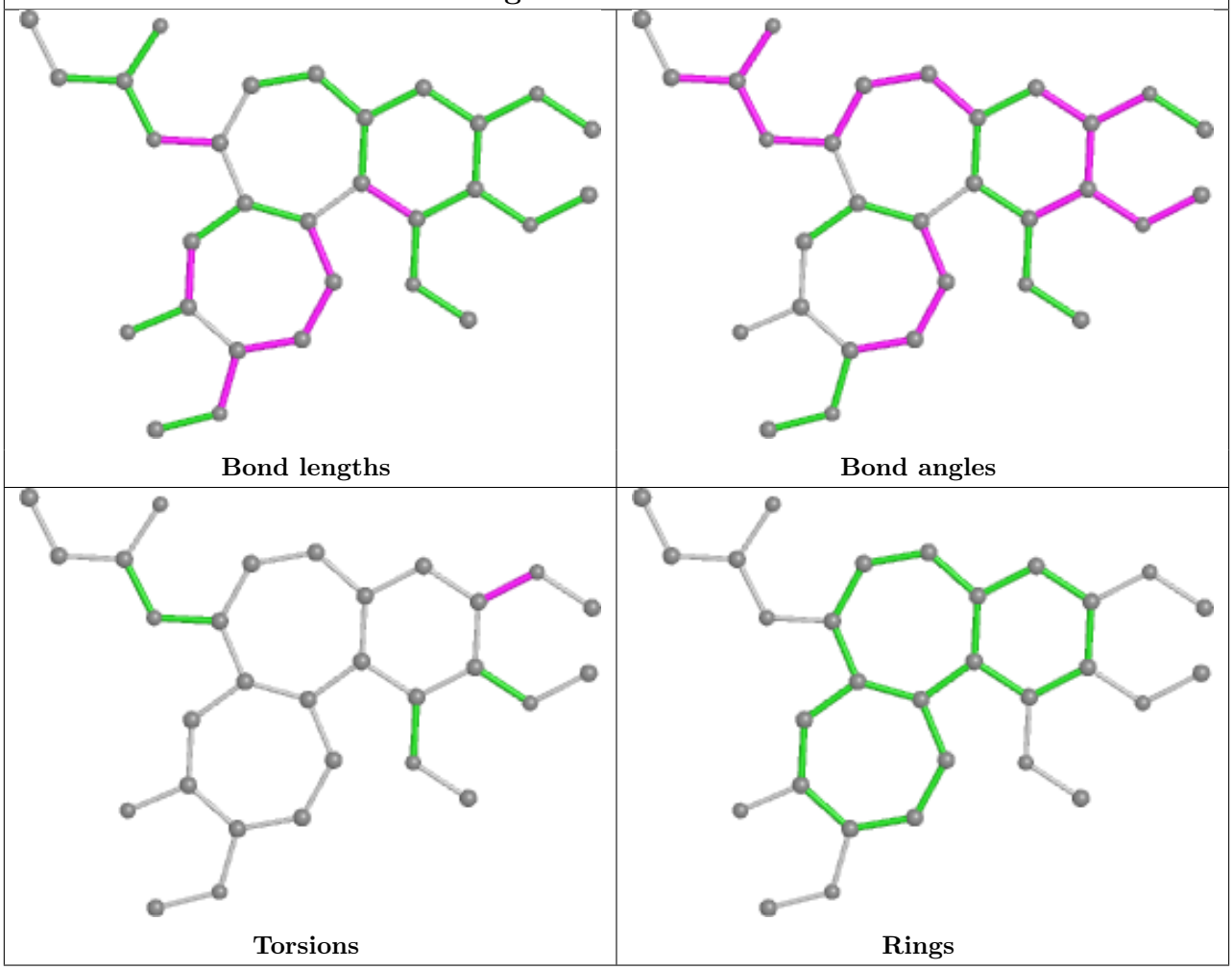
Rings

Ligand TA1 B 601	
 Bond lengths	 Bond angles
 Torsions	 Rings

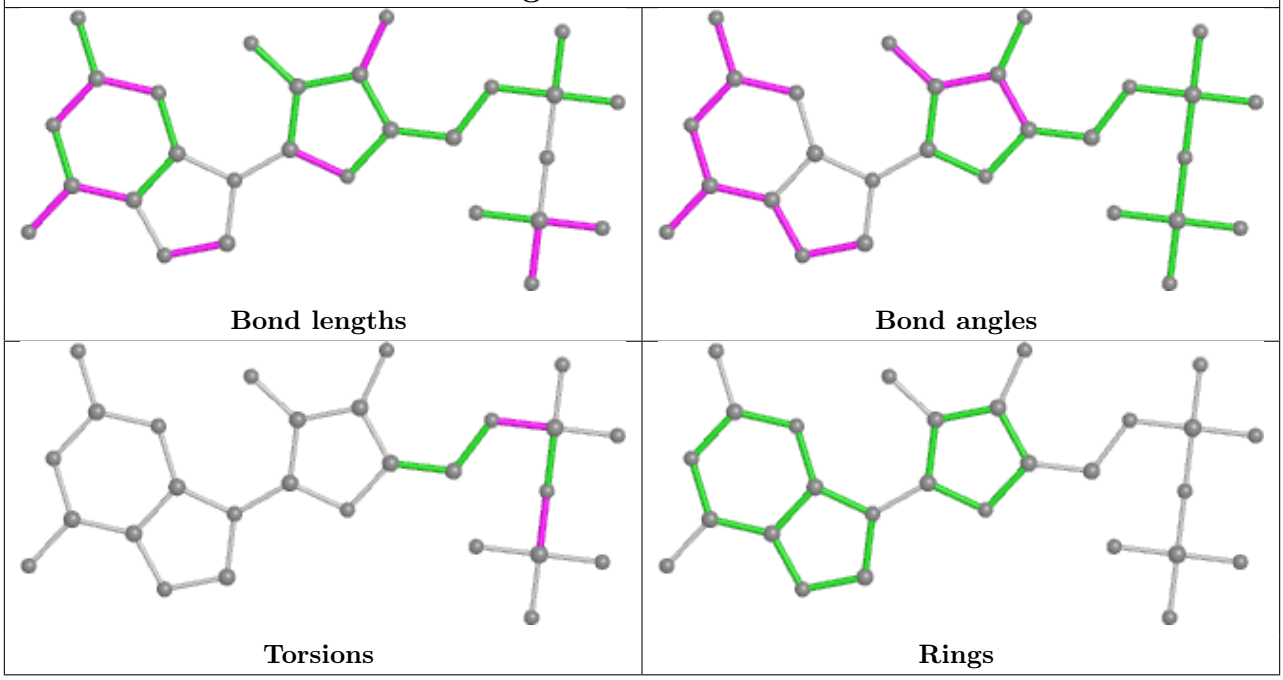
Ligand ANP D 500



Ligand CN2 G 701



Ligand GDP B 600



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.

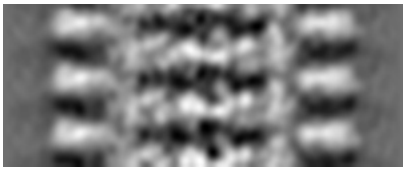
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-5027. These allow visual inspection of the internal detail of the map and identification of artifacts.

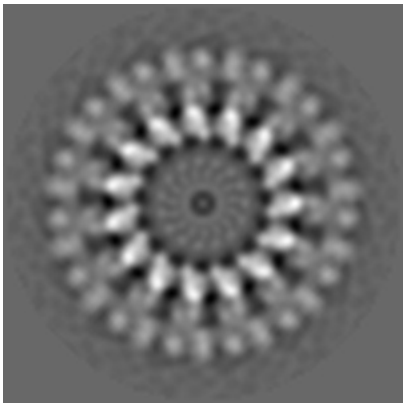
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

6.1.1 Primary map


X

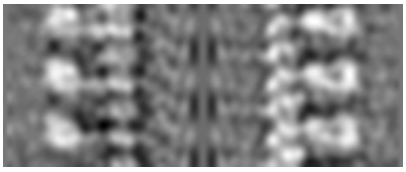
Y


Z

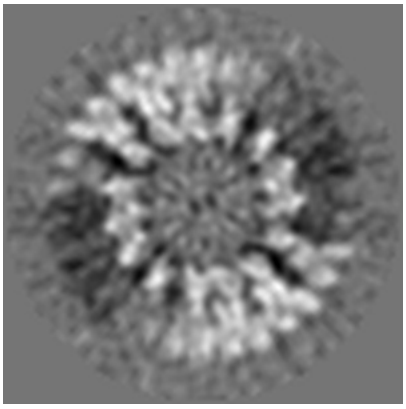
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map


X Index: 50

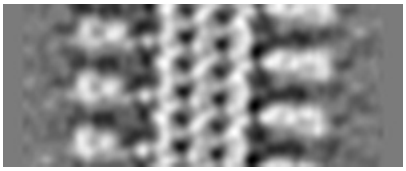
Y Index: 50


Z Index: 20

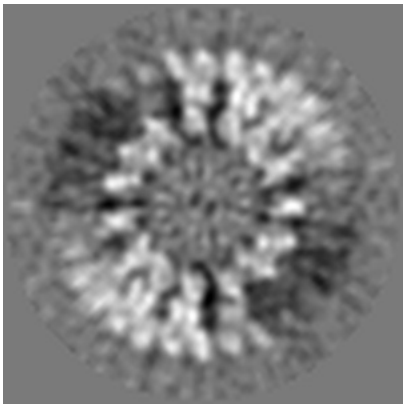
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map


X Index: 71

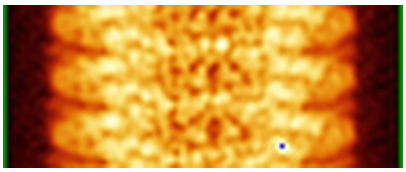
Y Index: 69

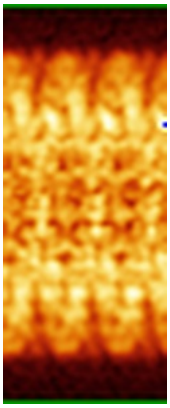

Z Index: 24

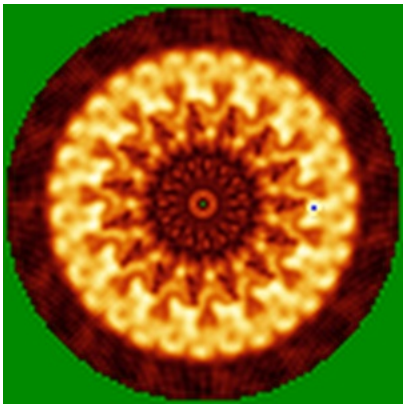
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map


X

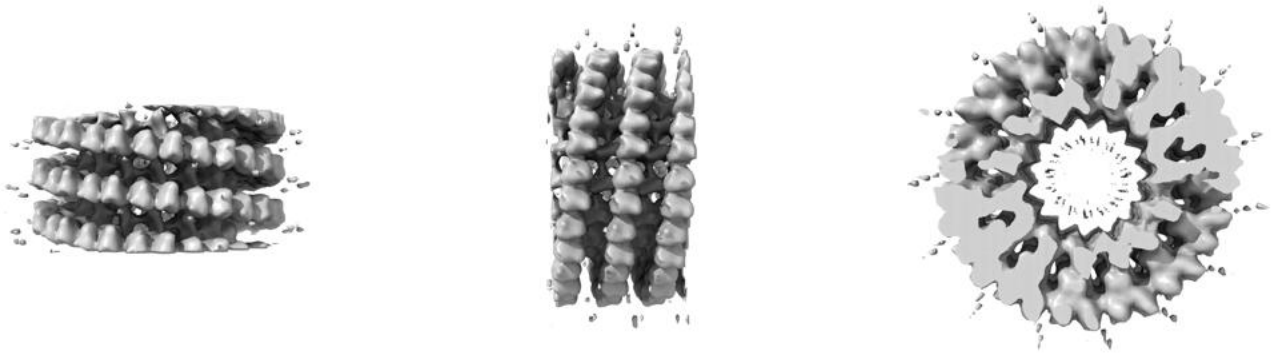

Y


Z

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 11.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

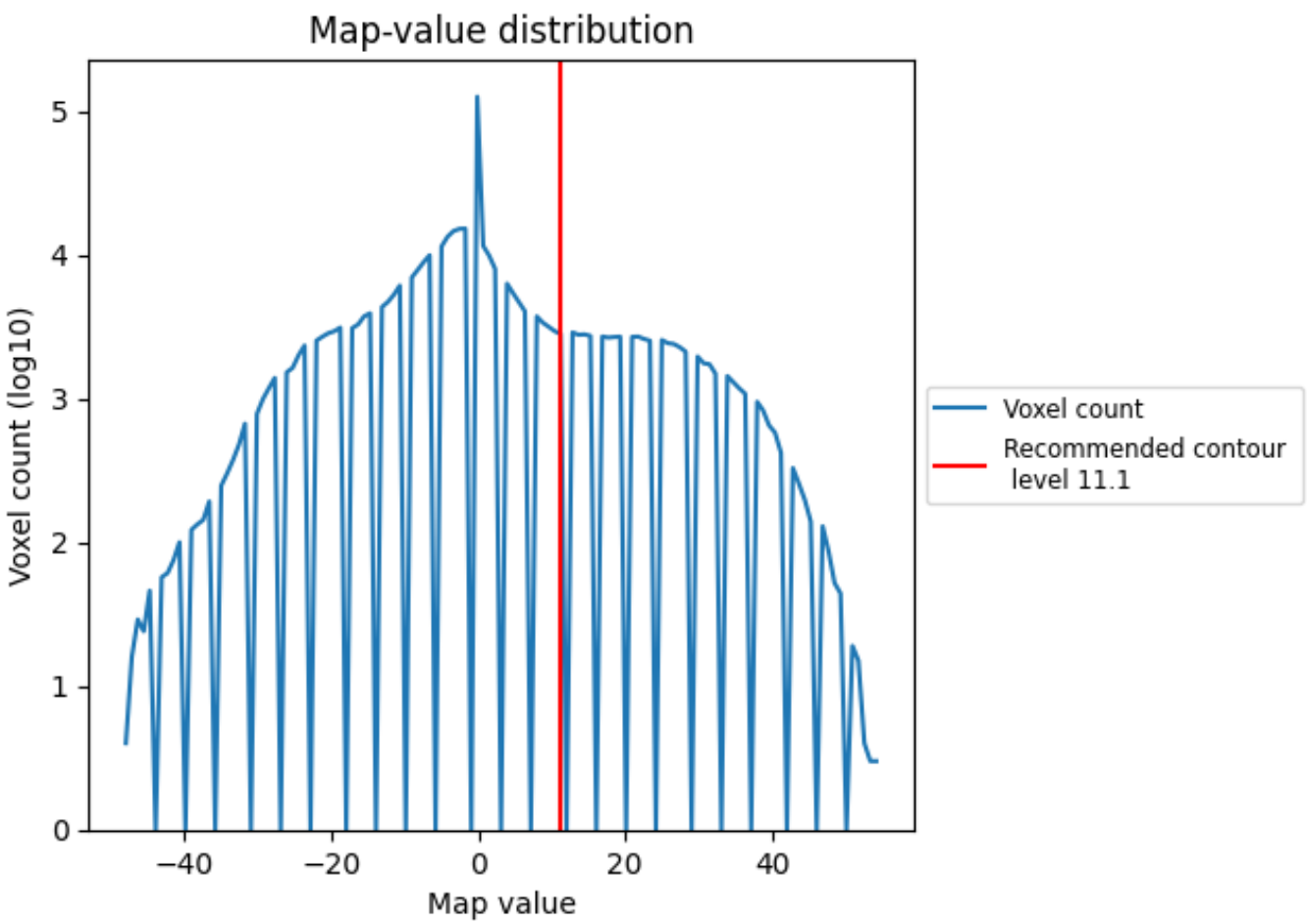
6.6 Mask visualisation (i)

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

7 Map analysis (i)

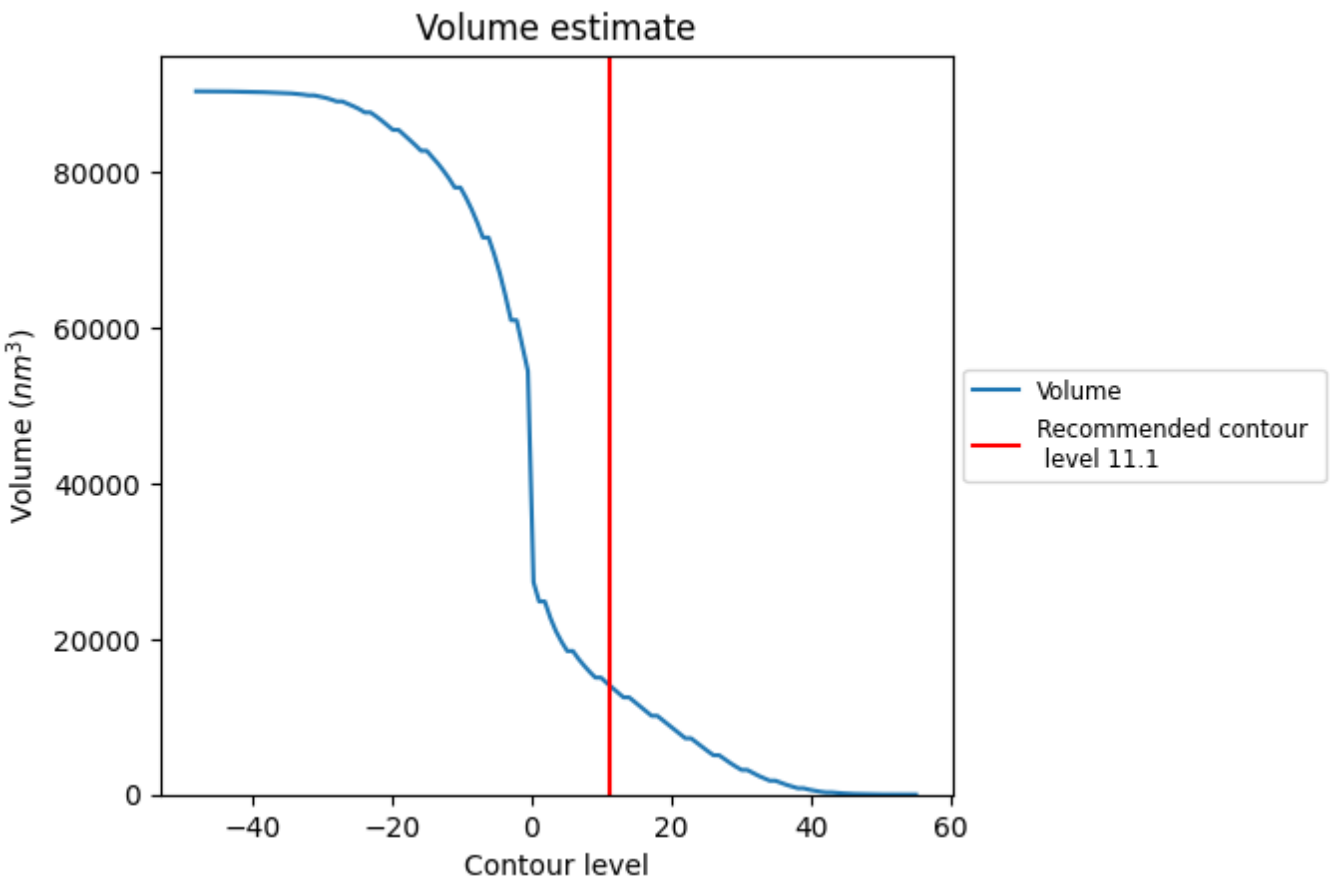
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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 (i)



The volume at the recommended contour level is 14065 nm^3; this corresponds to an approximate mass of 12705 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)

This section was not generated. The rotationally averaged power spectrum is only generated for cubic maps.

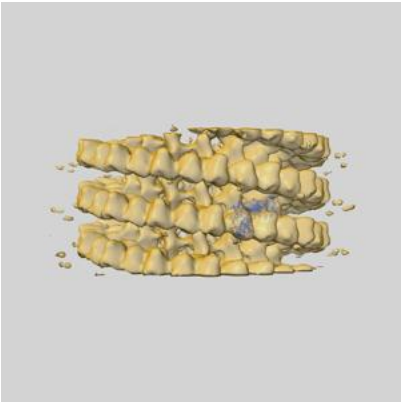
8 Fourier-Shell correlation (i)

This section was not generated. No FSC curve or half-maps provided.

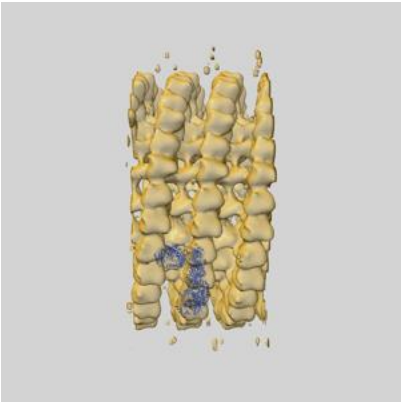
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-5027 and PDB model 3EDL. Per-residue inclusion information can be found in section 3 on page 8.

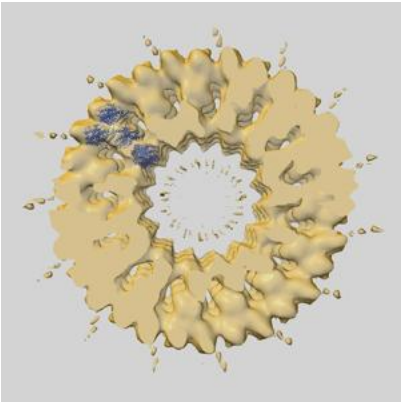
9.1 Map-model overlay (i)



X



Y



Z

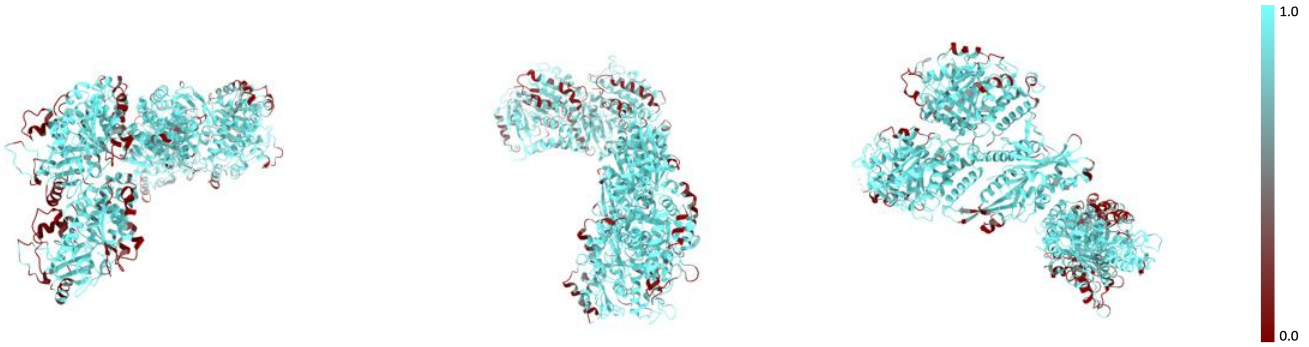
The images above show the 3D surface view of the map at the recommended contour level 11.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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.

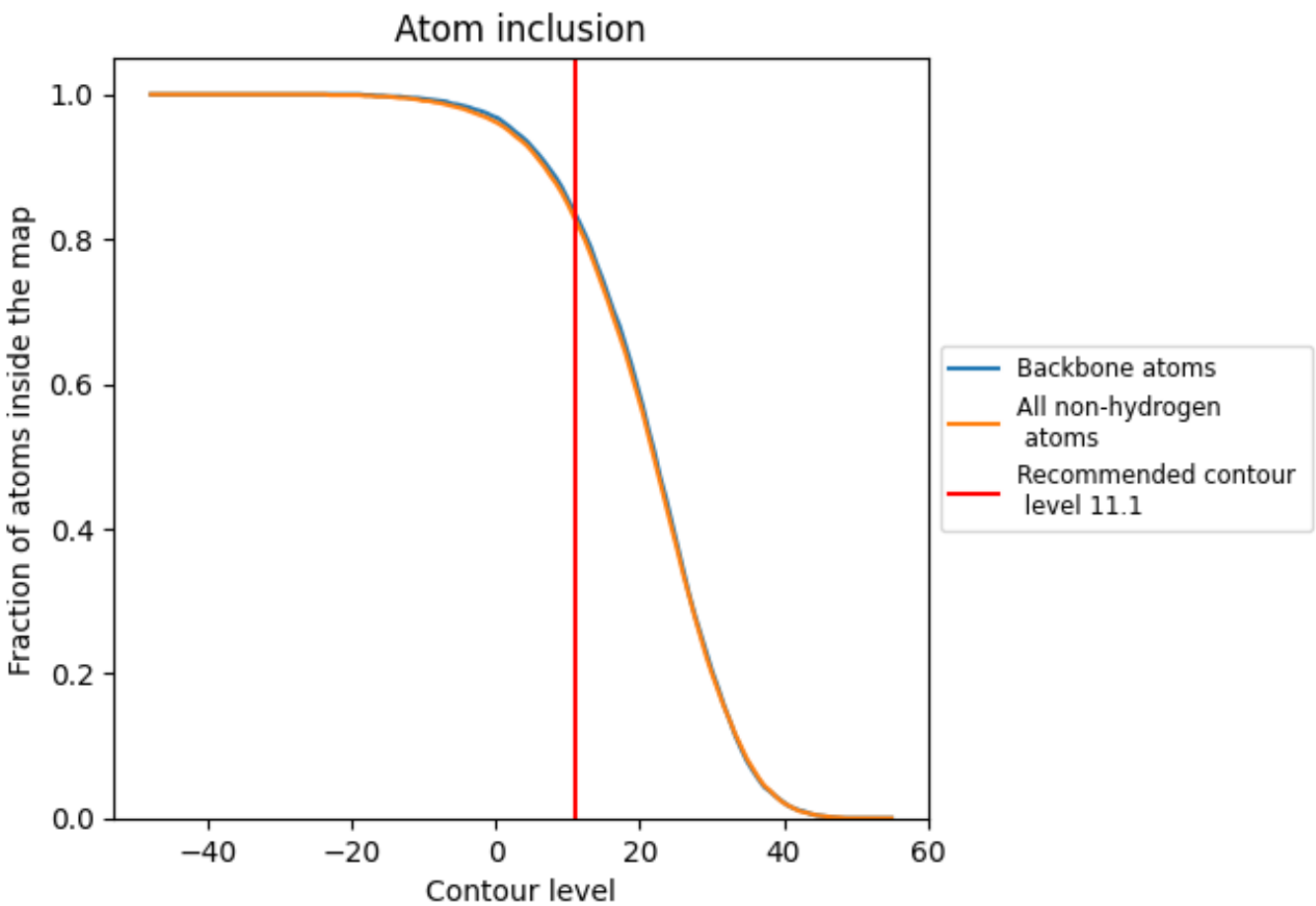
9.3 Atom inclusion mapped to coordinate model (i)



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 (11.1).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 82% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (11.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8250	0.0440
A	0.7400	0.0440
B	0.7690	0.0400
D	0.8900	0.0490
F	0.9020	0.0460
G	0.8470	0.0430