Full wwPDB EM Validation Report (i)

Nov 6, 2022 – 12:10 PM EST

PDB ID	:	6BSP
EMDB ID	:	EMD-7136
Title	:	High-Resolution Structure Analysis of Antibody V5 and U4 Conformational Epitope on Human Papillomavirus 16
Authors	:	Guan, J.; Bywaters, S.M.; Brendle, S.A.; Ashley, R.E.; Makhov, A.M.; Conway, J.F.; Christenson, N.D.; Hafenstein, S.
Deposited on	:	2017-12-04
Resolution	:	4.70 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 (i)) were used in the production of this report:

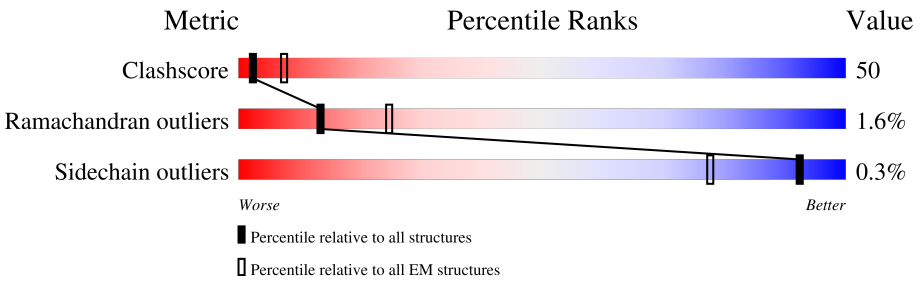
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

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 4.70 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	109	81%; 26%, 73%, •
2	B	110	85%; 26%, 74%
3	C	469	17%; 47%, 48%, • •
3	D	469	•; 15%, 77%, 6%, •
3	E	469	•; 47%, 50%, • •
3	F	469	6%; 46%, 50%, • •
3	G	469	•; 47%, 47%, 5%, •
3	H	469	7%; 46%, 50%, • •

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 23690 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 U4 Heavy chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	109	851	534	145	167	5	0	0

- Molecule 2 is a protein called U4 Light chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	110	850	541	135	170	4	0	0

- Molecule 3 is a protein called Major capsid protein L1.

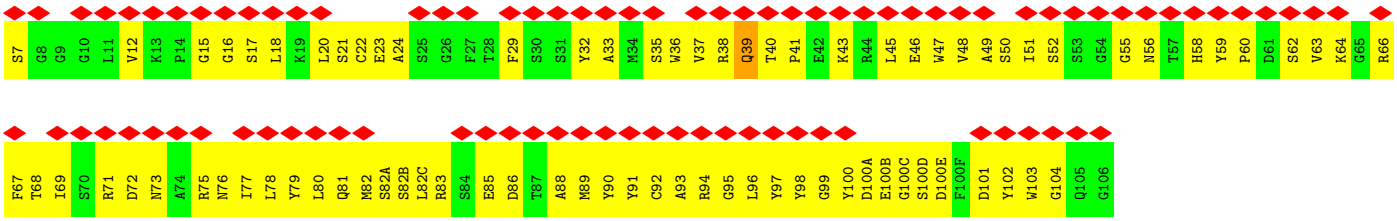
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	468	3675	2347	617	690	21	0	0
3	D	460	3614	2304	609	680	21	0	0
3	E	469	3686	2356	618	691	21	0	0
3	F	468	3675	2347	617	690	21	0	0
3	G	467	3666	2341	615	689	21	0	0
3	H	468	3673	2345	617	690	21	0	0

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.

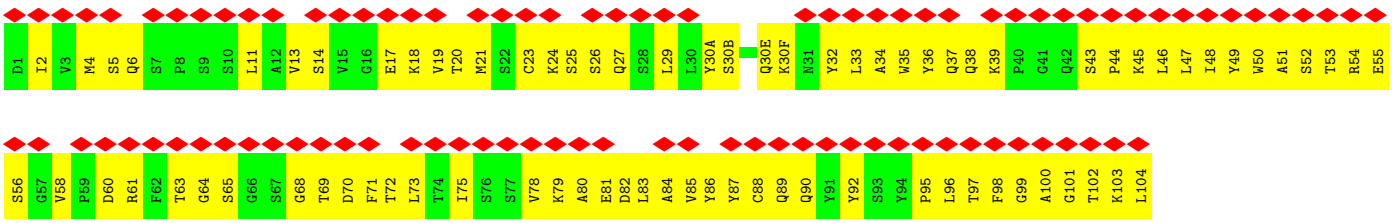
- Molecule 1: U4 Heavy chain

Chain A: 81% 26% 73%



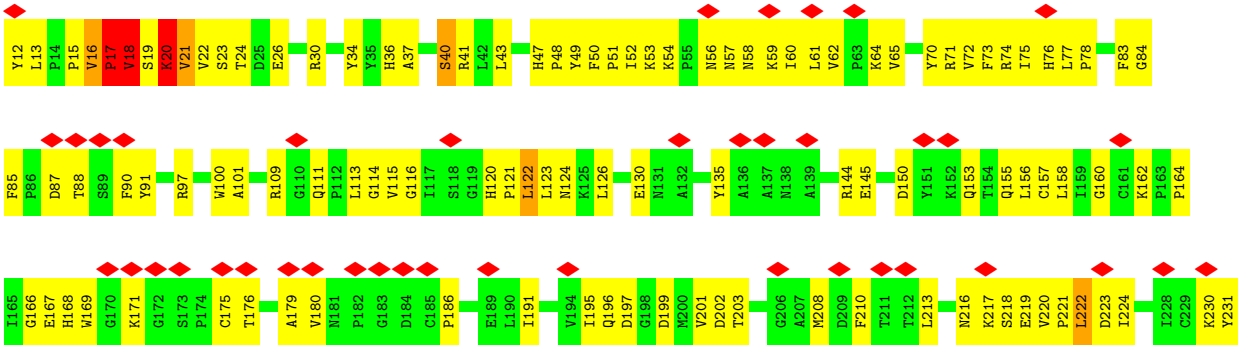
- Molecule 2: U4 Light chain

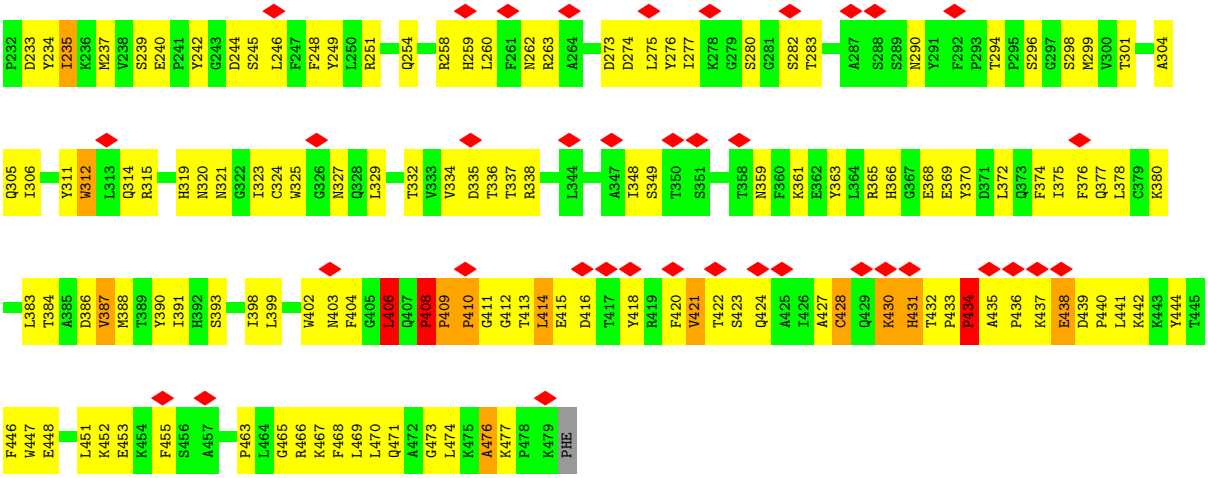
Chain B: 85% 26% 74%



- Molecule 3: Major capsid protein L1

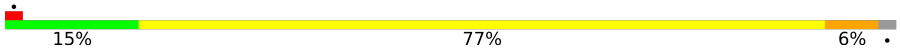
Chain C: 17% 47% 48%

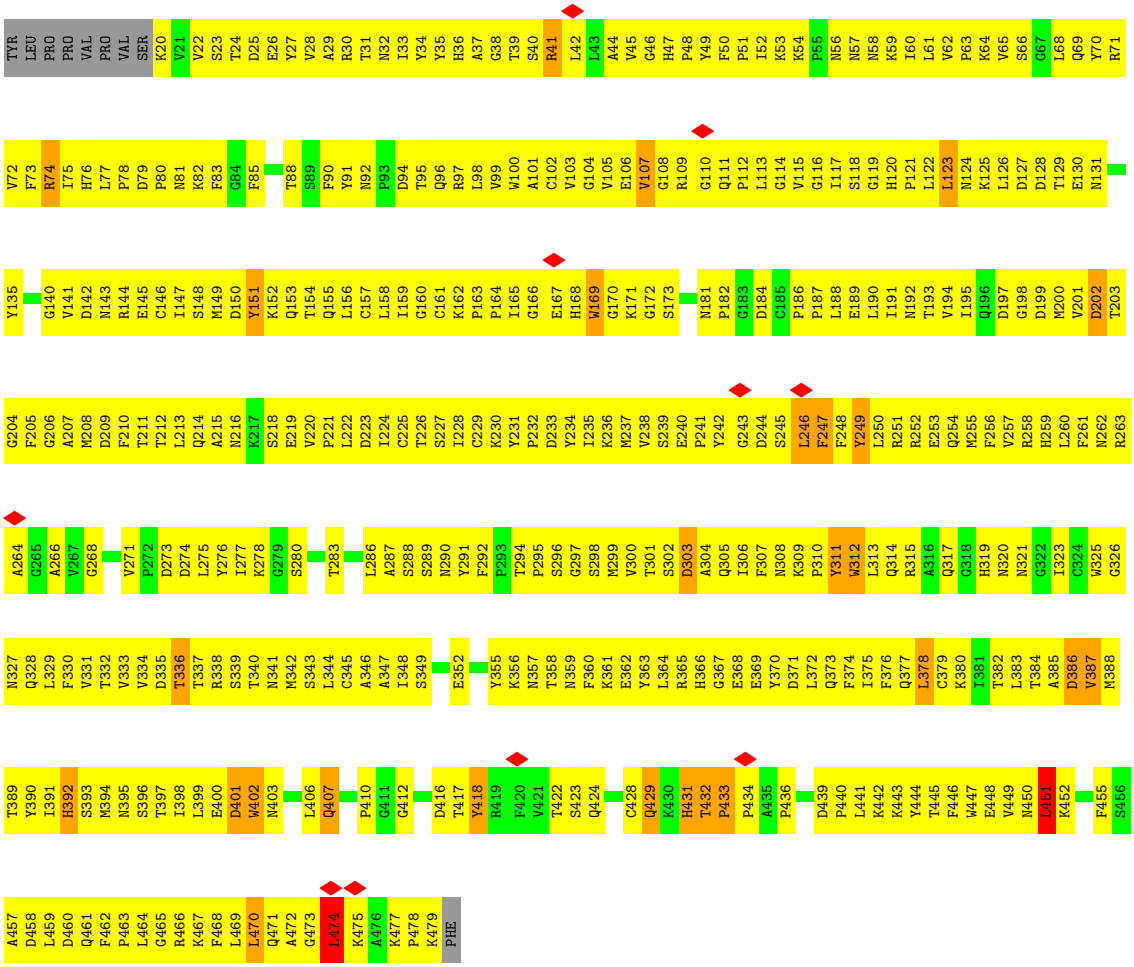




- Molecule 3: Major capsid protein L1

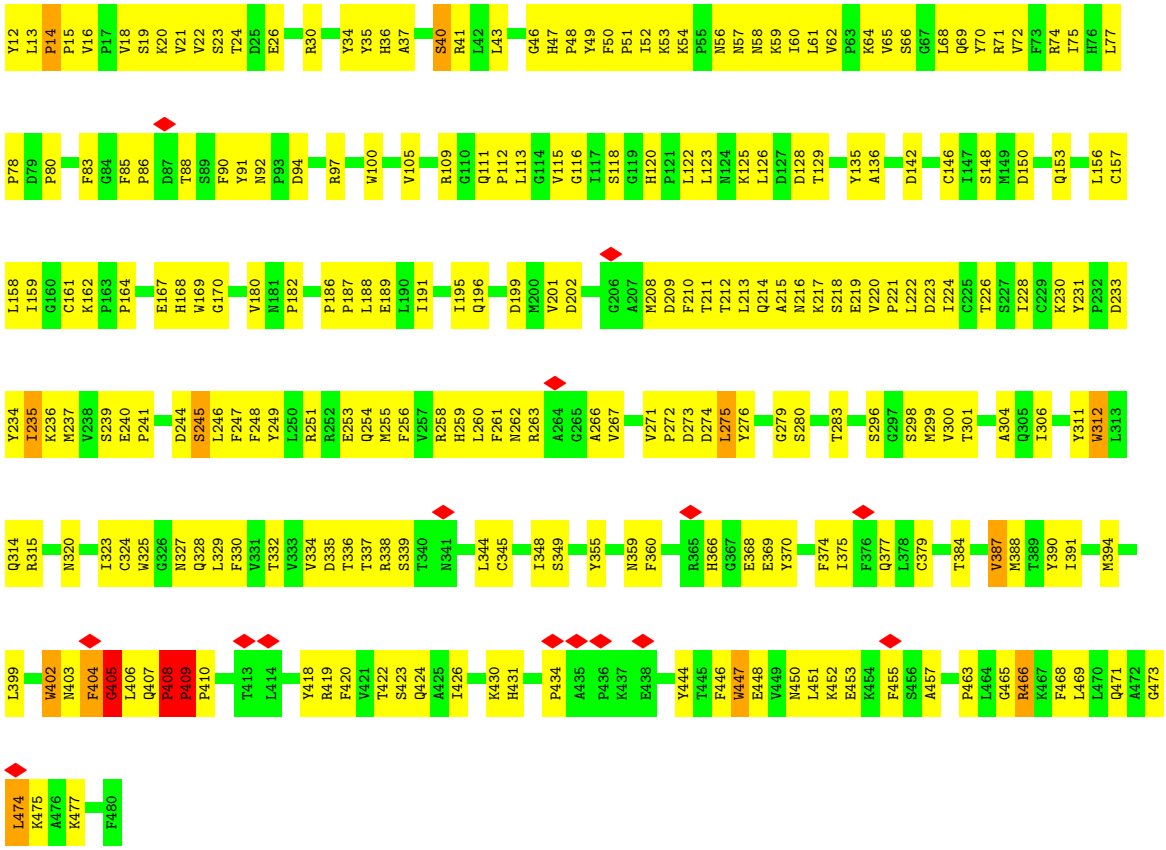
Chain D:





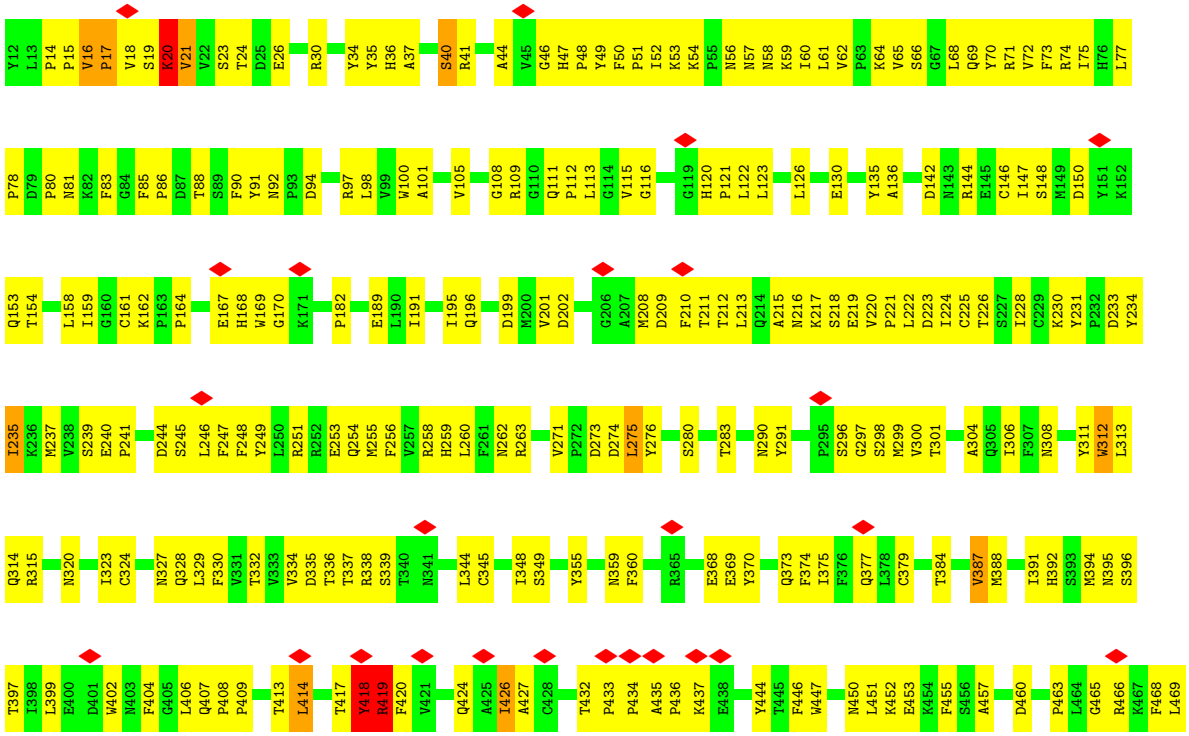
- Molecule 3: Major capsid protein L1

Chain E:



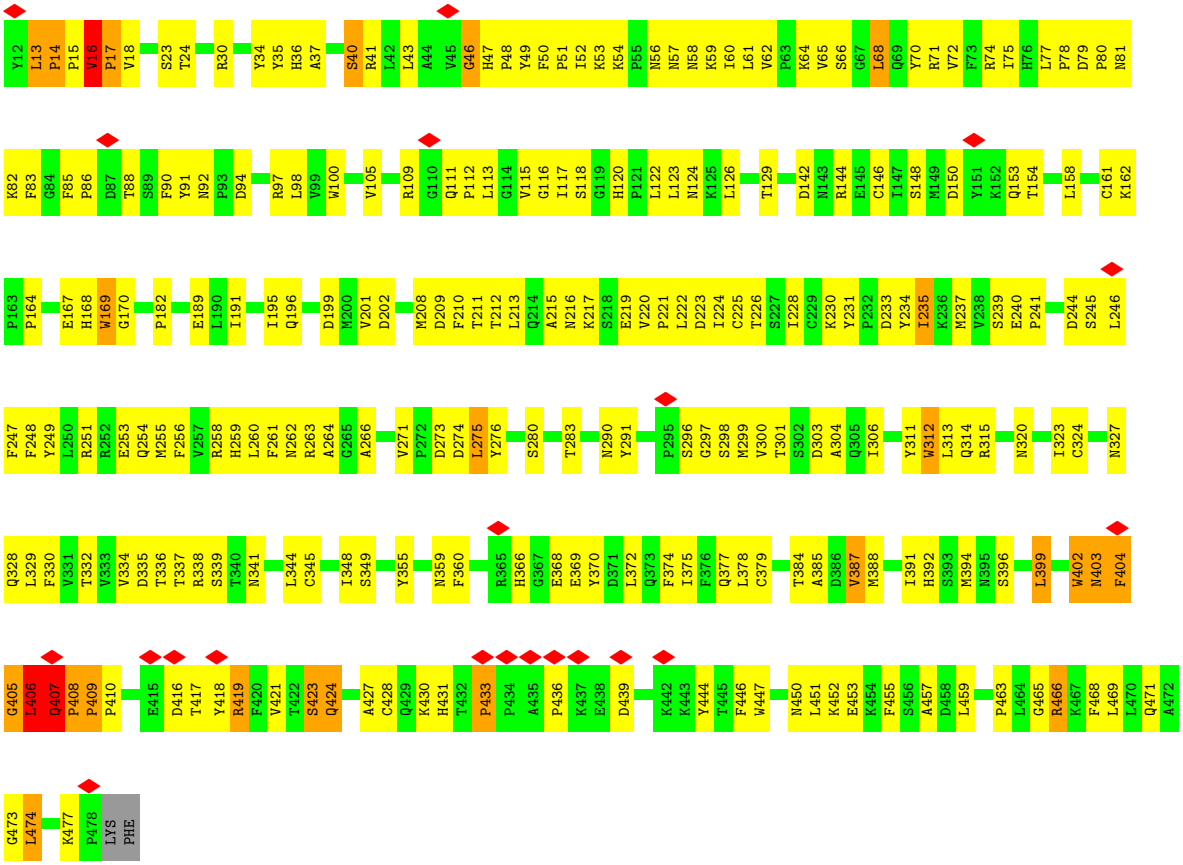
- Molecule 3: Major capsid protein L1

Chain F:



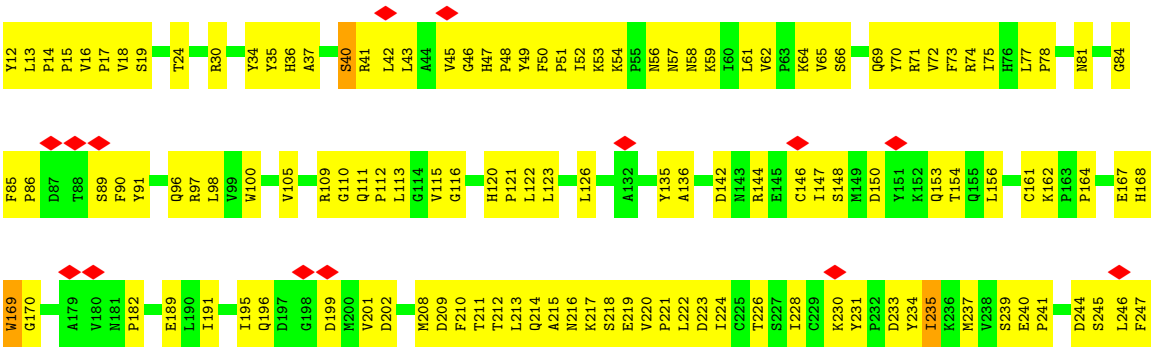
• Molecule 3: Major capsid protein L1

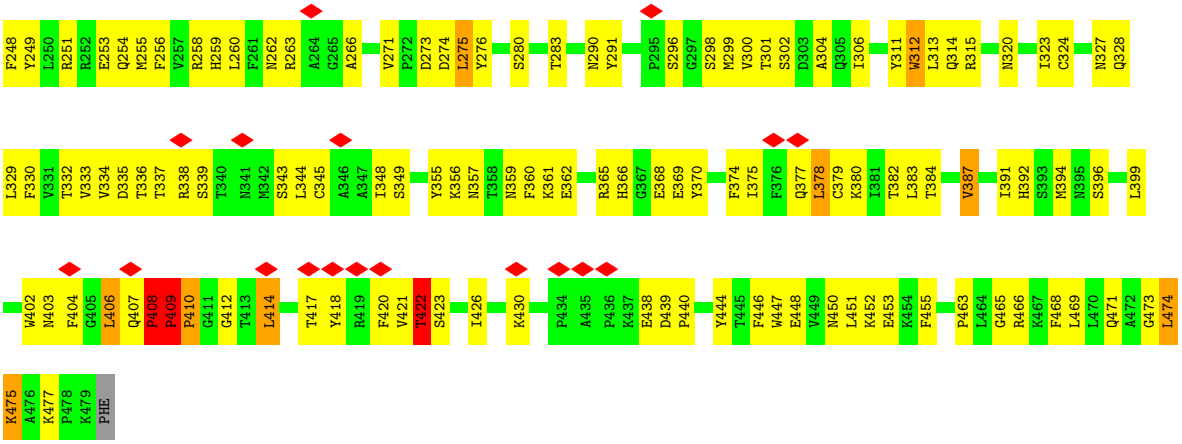
Chain G:



• Molecule 3: Major capsid protein L1

Chain H:




F248 Y249 L250 R251 R252 E253 Q254 M255 F256 V257 R258 H259 L260 F261 N262 R263 A264 G265 A266 V271 P272 D273 D274 L275 Y276 S280 T283 N290 Y291 P295 S296 G297 S298 M299 V300 T301 S302 D303 A304 Q305 I306 Y311 W312 L313 Q314 R315 N320 I323 C324 N327 Q328
L329 F330 V331 T332 V333 V334 D335 T336 T337 R338 S339 T340 N341 M342 S343 L344 C345 A346 A347 I348 S349 Y355 K356 N357 T358 N359 F360 K361 E362 R365 H366 G367 E368 E369 Y370 F374 I375 F376 Q377 L378 C379 K380 I381 T382 L383 T384 V387 I391 H392 S393 M394 N395 S396 L399
W402 N403 F404 G405 L406 Q407 P408 P409 P410 G411 G412 T413 L414 T417 Y418 R419 F420 V421 T422 S423 I426 K430 P434 A435 P436 K437 E438 D439 P440 Y444 T445 F446 W447 E448 V449 N450 L451 K452 E453 K454 F455 P463 L464 G465 R466 K467 F468 L469 L470 Q471 A472 G473 L474
K475 A476 K477 P478 K479 PHE

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	17612	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI POLARA 300	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	7, 7	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k), FEI FALCON II (4k x 4k)	Depositor
Maximum map value	14.058	Depositor
Minimum map value	-8.247	Depositor
Average map value	0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	2.1	Depositor
Map size (Å)	779.95996, 779.95996, 779.95996	wwPDB
Map dimensions	680, 680, 680	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.147, 1.147, 1.147	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	0.50	1/873 (0.1%)	0.71	1/1177 (0.1%)
2	B	0.44	0/870	0.76	0/1181
3	C	0.96	10/3776 (0.3%)	0.93	22/5142 (0.4%)
3	D	0.82	4/3711 (0.1%)	0.95	6/5049 (0.1%)
3	E	0.76	4/3788 (0.1%)	0.79	7/5158 (0.1%)
3	F	0.73	1/3776 (0.0%)	0.79	11/5142 (0.2%)
3	G	0.75	6/3767 (0.2%)	0.82	11/5131 (0.2%)
3	H	0.75	5/3774 (0.1%)	0.85	13/5139 (0.3%)
All	All	0.78	31/24335 (0.1%)	0.85	71/33119 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
3	C	0	12
3	D	0	21
3	E	0	2
3	F	0	7
3	G	0	9
3	H	0	5
All	All	0	57

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	18	VAL	CA-CB	28.75	2.15	1.54
3	C	18	VAL	CB-CG1	21.24	1.97	1.52
3	C	17	PRO	CA-C	14.74	1.82	1.52
3	E	402	TRP	CB-CG	-10.49	1.31	1.50
3	H	409	PRO	N-CA	9.26	1.62	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	17	PRO	N-CA	7.90	1.60	1.47
3	D	312	TRP	CB-CG	-7.79	1.36	1.50
3	C	16	VAL	C-N	7.79	1.49	1.34
3	D	169	TRP	CB-CG	-7.52	1.36	1.50
3	G	402	TRP	CB-CG	-7.48	1.36	1.50
3	C	406	LEU	CG-CD2	-7.08	1.25	1.51
3	C	18	VAL	CA-C	7.04	1.71	1.52
3	C	175	CYS	CB-SG	-6.90	1.70	1.82
3	C	18	VAL	N-CA	6.79	1.59	1.46
3	C	409	PRO	C-N	6.19	1.46	1.34
3	H	410	PRO	CA-C	6.07	1.65	1.52
3	E	447	TRP	CB-CG	-5.84	1.39	1.50
3	G	13	LEU	N-CA	5.69	1.57	1.46
3	H	402	TRP	CB-CG	-5.69	1.40	1.50
3	D	402	TRP	CB-CG	-5.64	1.40	1.50
1	A	39	GLN	C-N	5.63	1.47	1.34
3	E	180	VAL	C-N	-5.55	1.21	1.34
3	G	408	PRO	CB-CG	-5.53	1.22	1.50
3	E	312	TRP	CB-CG	-5.49	1.40	1.50
3	G	169	TRP	CB-CG	-5.37	1.40	1.50
3	G	46	GLY	C-N	-5.36	1.21	1.34
3	H	312	TRP	CB-CG	-5.26	1.40	1.50
3	H	169	TRP	CB-CG	-5.13	1.41	1.50
3	F	312	TRP	CB-CG	-5.11	1.41	1.50
3	G	312	TRP	CB-CG	-5.10	1.41	1.50
3	D	151	TYR	CD1-CE1	-5.01	1.31	1.39

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	409	PRO	C-N-CD	-20.45	75.60	120.60
3	C	17	PRO	C-N-CA	12.92	154.00	121.70
3	G	405	GLY	N-CA-C	-11.90	83.35	113.10
3	G	16	VAL	C-N-CD	-11.61	95.06	120.60
3	C	20	LYS	CD-CE-NZ	-11.38	85.52	111.70
3	C	406	LEU	CA-CB-CG	-10.77	90.53	115.30
3	C	18	VAL	CA-CB-CG1	10.77	127.05	110.90
3	H	409	PRO	CA-N-CD	-10.08	97.39	111.50
3	G	406	LEU	CA-CB-CG	9.86	137.98	115.30
3	C	18	VAL	CB-CA-C	9.66	129.75	111.40
3	C	406	LEU	CB-CG-CD2	-9.29	95.21	111.00
3	C	18	VAL	CA-CB-CG2	8.93	124.30	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	451	LEU	CA-CB-CG	-8.91	94.80	115.30
3	C	122	LEU	CB-CG-CD1	-8.72	96.17	111.00
3	F	474	LEU	CA-CB-CG	8.21	134.18	115.30
3	C	406	LEU	CB-CG-CD1	-8.09	97.25	111.00
3	H	409	PRO	CA-C-N	-7.93	94.91	117.10
3	H	410	PRO	C-N-CA	7.71	138.49	122.30
3	C	175	CYS	CA-CB-SG	-7.66	100.21	114.00
3	C	17	PRO	N-CA-C	7.57	131.78	112.10
3	C	16	VAL	C-N-CD	-7.38	104.36	120.60
3	H	409	PRO	O-C-N	7.22	134.83	121.10
3	H	414	LEU	CA-CB-CG	-7.20	98.75	115.30
3	D	123	LEU	CA-CB-CG	-7.19	98.75	115.30
3	H	412	GLY	N-CA-C	7.14	130.95	113.10
3	D	474	LEU	CA-CB-CG	7.04	131.49	115.30
3	F	414	LEU	CB-CG-CD2	-6.79	99.46	111.00
3	C	19	SER	C-N-CA	-6.66	105.05	121.70
3	C	16	VAL	C-N-CA	6.53	149.41	122.00
3	E	474	LEU	CA-CB-CG	6.48	130.21	115.30
3	C	414	LEU	CA-CB-CG	-6.48	100.39	115.30
3	F	406	LEU	CA-CB-CG	6.42	130.06	115.30
3	H	406	LEU	CA-CB-CG	-6.33	100.73	115.30
3	C	21	VAL	N-CA-C	-6.31	93.97	111.00
3	C	20	LYS	CA-CB-CG	6.26	127.17	113.40
3	H	378	LEU	CB-CG-CD2	-6.22	100.42	111.00
3	D	378	LEU	CA-CB-CG	-6.12	101.22	115.30
3	H	474	LEU	CA-CB-CG	6.11	129.34	115.30
3	C	18	VAL	CA-C-N	6.06	130.54	117.20
3	G	466	ARG	NE-CZ-NH1	-5.96	117.32	120.30
3	F	419	ARG	CG-CD-NE	-5.92	99.37	111.80
3	G	13	LEU	CB-CG-CD1	5.87	120.97	111.00
3	E	405	GLY	C-N-CA	-5.78	107.26	121.70
1	A	99	GLY	N-CA-C	5.75	127.49	113.10
3	E	466	ARG	NE-CZ-NH1	-5.66	117.47	120.30
3	F	275	LEU	CA-CB-CG	-5.59	102.45	115.30
3	H	422	THR	N-CA-CB	5.59	120.91	110.30
3	G	407	GLN	CB-CA-C	5.57	121.55	110.40
3	E	405	GLY	O-C-N	-5.51	113.88	122.70
3	F	68	LEU	CA-CB-CG	-5.51	102.62	115.30
3	H	275	LEU	CA-CB-CG	-5.50	102.65	115.30
3	C	19	SER	O-C-N	-5.47	113.95	122.70
3	H	409	PRO	N-CA-C	5.43	126.21	112.10
3	C	312	TRP	CA-CB-CG	-5.41	103.42	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	F	418	TYR	N-CA-C	-5.41	96.39	111.00
3	G	68	LEU	CA-CB-CG	-5.30	103.10	115.30
3	D	429	GLN	N-CA-C	5.30	125.31	111.00
3	F	414	LEU	CB-CG-CD1	-5.28	102.02	111.00
3	E	434	PRO	C-N-CA	5.28	134.90	121.70
3	E	275	LEU	CA-CB-CG	-5.22	103.28	115.30
3	D	470	LEU	CA-CB-CG	-5.21	103.31	115.30
3	G	474	LEU	CA-CB-CG	5.21	127.28	115.30
3	G	275	LEU	CA-CB-CG	-5.18	103.38	115.30
3	E	312	TRP	CA-CB-CG	-5.13	103.95	113.70
3	G	399	LEU	CA-CB-CG	-5.12	103.54	115.30
3	G	14	PRO	C-N-CD	5.11	139.14	128.40
3	C	20	LYS	C-N-CA	5.08	134.40	121.70
3	F	435	ALA	C-N-CD	5.07	139.06	128.40
3	F	16	VAL	C-N-CD	5.03	138.96	128.40
3	C	222	LEU	CB-CG-CD2	-5.02	102.47	111.00
3	F	475	LYS	CB-CA-C	-5.01	100.39	110.40

There are no chirality outliers.

All (57) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	TYR	Peptide
3	C	17	PRO	Peptide
3	C	18	VAL	Peptide
3	C	20	LYS	Peptide
3	C	408	PRO	Mainchain,Peptide
3	C	416	ASP	Peptide
3	C	421	VAL	Peptide
3	C	428	CYS	Peptide
3	C	430	LYS	Peptide
3	C	431	HIS	Peptide
3	C	434	PRO	Peptide
3	C	438	GLU	Peptide
3	D	107	VAL	Peptide
3	D	202	ASP	Peptide
3	D	232	PRO	Peptide
3	D	246	LEU	Peptide
3	D	249	TYR	Peptide
3	D	311	TYR	Peptide
3	D	313	LEU	Peptide
3	D	336	THR	Peptide

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Mol	Chain	Res	Type	Group
3	D	407	GLN	Peptide
3	D	412	GLY	Peptide
3	D	418	TYR	Peptide
3	D	428	CYS	Peptide
3	D	429	GLN	Peptide
3	D	431	HIS	Peptide
3	D	432	THR	Peptide
3	D	433	PRO	Peptide
3	D	451	LEU	Peptide
3	D	474	LEU	Peptide
3	D	478	PRO	Peptide
3	D	63	PRO	Peptide
3	D	74	ARG	Peptide
3	E	408	PRO	Peptide
3	E	409	PRO	Peptide
3	F	20	LYS	Peptide
3	F	21	VAL	Peptide
3	F	418	TYR	Peptide
3	F	419	ARG	Peptide
3	F	420	PHE	Peptide
3	F	424	GLN	Peptide
3	F	474	LEU	Peptide
3	G	403	ASN	Peptide
3	G	404	PHE	Peptide
3	G	406	LEU	Peptide
3	G	407	GLN	Peptide
3	G	418	TYR	Peptide
3	G	419	ARG	Peptide
3	G	423	SER	Peptide
3	G	433	PRO	Peptide
3	G	439	ASP	Peptide
3	H	408	PRO	Peptide
3	H	409	PRO	Mainchain
3	H	422	THR	Peptide
3	H	438	GLU	Peptide
3	H	475	LYS	Peptide

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	851	0	792	120	0
2	B	850	0	831	126	0
3	C	3675	0	3592	289	0
3	D	3614	0	3528	811	0
3	E	3686	0	3601	295	0
3	F	3675	0	3592	280	0
3	G	3666	0	3579	281	0
3	H	3673	0	3585	292	0
All	All	23690	0	23100	2321	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 50.

All (2321) 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:C:17:PRO:C	3:C:17:PRO:CA	1.82	1.43
3:C:18:VAL:CB	3:C:18:VAL:CG1	1.97	1.39
3:F:19:SER:O	3:F:20:LYS:HG2	1.15	1.33
3:C:18:VAL:CB	3:C:18:VAL:CA	2.15	1.25
3:G:16:VAL:HB	3:G:17:PRO:CD	1.67	1.25
3:G:16:VAL:CB	3:G:17:PRO:HD2	1.67	1.22
3:F:19:SER:O	3:F:20:LYS:CG	1.87	1.20
3:D:76:HIS:HB2	3:D:450:ASN:HA	1.34	1.09
3:D:160:GLY:HA3	3:D:246:LEU:HA	1.31	1.08
3:C:52:ILE:HB	3:C:62:VAL:HB	1.35	1.06
2:B:86:TYR:HB2	2:B:102:THR:HB	1.41	1.02
3:D:109:ARG:HH22	3:D:111:GLN:HG2	1.21	1.02
3:H:162:LYS:HB2	3:H:245:SER:HA	1.41	1.02
3:D:468:PHE:HA	3:D:471:GLN:HB3	1.40	1.01
3:D:47:HIS:HE1	3:D:49:TYR:HB2	1.26	1.00
3:D:234:TYR:O	3:D:238:VAL:N	1.93	1.00
3:D:459:LEU:HD23	3:D:462:PHE:HB2	1.39	1.00
3:F:426:ILE:HG22	3:F:427:ALA:H	1.26	0.99
3:D:103:VAL:H	3:D:376:PHE:HA	1.24	0.98
3:C:111:GLN:HB2	3:C:338:ARG:HD3	1.46	0.98
3:D:25:ASP:HA	3:D:28:VAL:HB	1.45	0.98
3:F:162:LYS:HB2	3:F:245:SER:HA	1.46	0.97
3:D:168:HIS:O	3:D:191:ILE:N	1.97	0.97
3:G:463:PRO:HA	3:G:466:ARG:HH12	1.29	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:162:LYS:HB2	3:G:245:SER:HA	1.47	0.96
3:G:16:VAL:HB	3:G:17:PRO:HD2	0.97	0.96
3:D:24:THR:HG21	3:D:323:ILE:HG13	1.47	0.95
3:E:463:PRO:HA	3:E:466:ARG:HH12	1.30	0.95
1:A:81:GLN:NE2	1:A:82:MET:O	1.99	0.94
3:C:406:LEU:HD11	3:C:411:GLY:N	1.81	0.94
3:D:207:ALA:HA	3:D:229:CYS:HB2	1.49	0.94
3:G:417:THR:HB	3:G:419:ARG:HE	1.31	0.94
2:B:6:GLN:H	2:B:100:ALA:HB3	1.30	0.93
3:D:114:GLY:H	3:D:338:ARG:HA	1.31	0.93
3:C:18:VAL:CA	3:C:18:VAL:HB	1.96	0.93
3:D:399:LEU:HD23	3:D:402:TRP:HB2	1.51	0.93
3:D:389:THR:O	3:D:393:SER:N	2.00	0.92
3:D:287:ALA:HB3	3:H:121:PRO:HB3	1.49	0.92
3:G:109:ARG:NH1	3:G:369:GLU:O	2.01	0.92
3:C:62:VAL:HG13	3:H:426:ILE:HD11	1.48	0.92
3:D:36:HIS:CE1	3:D:37:ALA:O	2.23	0.91
3:F:74:ARG:HB2	3:F:446:PHE:HE1	1.35	0.91
3:D:38:GLY:HA3	3:D:373:GLN:HG2	1.50	0.91
3:F:109:ARG:NH1	3:F:369:GLU:O	2.04	0.91
3:H:422:THR:OG1	3:H:430:LYS:NZ	2.04	0.91
2:B:80:ALA:O	2:B:83:LEU:N	2.04	0.91
3:G:74:ARG:HB2	3:G:446:PHE:HE1	1.33	0.91
3:C:109:ARG:NH1	3:C:369:GLU:O	2.03	0.91
3:H:109:ARG:NH1	3:H:369:GLU:O	2.03	0.90
3:D:349:SER:O	3:D:359:ASN:ND2	2.03	0.90
3:H:219:GLU:OE1	3:H:263:ARG:NH1	2.04	0.90
3:E:162:LYS:HB2	3:E:245:SER:HA	1.52	0.90
3:G:424:GLN:NE2	3:G:428:CYS:O	2.04	0.89
3:E:109:ARG:NH1	3:E:369:GLU:O	2.06	0.89
3:D:113:LEU:HA	3:D:338:ARG:HG2	1.53	0.89
3:D:210:PHE:O	3:D:214:GLN:N	2.05	0.89
3:D:115:VAL:N	3:D:340:THR:OG1	2.04	0.89
3:D:240:GLU:HG2	3:D:242:TYR:H	1.37	0.88
1:A:66:ARG:HA	3:C:176:THR:HB	1.56	0.88
3:H:74:ARG:HB2	3:H:446:PHE:HE1	1.36	0.88
3:D:216:ASN:N	3:H:345:CYS:SG	2.46	0.88
3:D:301:THR:HG23	3:D:304:ALA:H	1.37	0.88
3:F:463:PRO:HA	3:F:466:ARG:HH12	1.37	0.88
3:D:114:GLY:N	3:D:338:ARG:HA	1.88	0.87
3:F:418:TYR:HB2	3:F:419:ARG:HH11	1.38	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:15:PRO:HB2	3:C:17:PRO:HD2	1.56	0.87
3:D:111:GLN:HB2	3:D:338:ARG:HD3	1.55	0.87
3:D:355:TYR:OH	3:D:357:ASN:ND2	2.08	0.87
3:G:16:VAL:HG23	3:G:17:PRO:N	1.88	0.87
3:C:74:ARG:NH1	3:C:439:ASP:OD2	2.07	0.87
3:G:16:VAL:CB	3:G:17:PRO:CD	2.27	0.87
3:F:219:GLU:OE1	3:F:263:ARG:NH1	2.07	0.87
3:H:407:GLN:HB2	3:H:408:PRO:HD3	1.57	0.87
3:G:219:GLU:OE1	3:G:263:ARG:NH1	2.07	0.86
3:C:406:LEU:HD11	3:C:411:GLY:H	1.38	0.86
1:A:100(C):GLY:HA3	2:B:50:TRP:HB2	1.57	0.86
3:F:216:ASN:ND2	3:F:219:GLU:OE2	2.09	0.86
3:D:314:GLN:HG3	3:D:315:ARG:H	1.38	0.86
3:D:77:LEU:HB2	3:D:327:ASN:HB3	1.58	0.86
3:H:404:PHE:CE1	3:H:409:PRO:HD3	2.10	0.86
3:H:463:PRO:HA	3:H:466:ARG:HH12	1.37	0.86
2:B:36:TYR:HB2	2:B:87:TYR:HB2	1.55	0.86
3:D:70:TYR:OH	3:D:230:LYS:O	1.92	0.86
3:D:468:PHE:O	3:D:472:ALA:N	2.08	0.86
3:D:310:PRO:HB2	3:D:312:TRP:HE1	1.41	0.86
3:C:420:PHE:HA	3:H:41:ARG:HD3	1.58	0.85
3:D:257:VAL:HA	3:D:295:PRO:HA	1.58	0.85
3:D:119:GLY:HA3	3:D:148:SER:HA	1.57	0.85
3:D:39:THR:OG1	3:D:371:ASP:OD1	1.92	0.85
3:D:46:GLY:O	3:D:366:HIS:N	2.09	0.84
3:D:118:SER:N	3:D:151:TYR:OH	2.10	0.84
3:D:259:HIS:O	3:D:294:THR:N	2.11	0.84
3:E:74:ARG:HB2	3:E:446:PHE:HE1	1.42	0.84
3:C:415:GLU:HA	3:D:241:PRO:HG3	1.58	0.84
3:F:19:SER:O	3:F:20:LYS:CD	2.25	0.84
3:D:47:HIS:CE1	3:D:49:TYR:HB2	2.12	0.84
3:D:360:PHE:HE1	3:E:215:ALA:HB3	1.42	0.84
3:D:240:GLU:OE1	3:D:244:ASP:N	2.08	0.84
3:D:385:ALA:O	3:D:389:THR:N	2.09	0.84
3:E:463:PRO:HA	3:E:466:ARG:NH1	1.91	0.84
3:C:97:ARG:NH2	3:C:402:TRP:HB3	1.93	0.84
3:D:126:LEU:N	3:D:262:ASN:O	2.10	0.84
3:D:262:ASN:ND2	3:D:290:ASN:O	2.09	0.84
3:G:116:GLY:N	3:G:339:SER:OG	2.11	0.84
2:B:86:TYR:N	2:B:102:THR:O	2.09	0.84
3:D:273:ASP:HA	3:D:276:TYR:CZ	2.12	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:411:GLY:O	3:D:20:LYS:N	2.10	0.83
3:D:202:ASP:HB2	3:D:204:GLY:H	1.43	0.83
3:G:453:GLU:O	3:H:12:TYR:N	2.10	0.83
3:C:162:LYS:HB2	3:C:245:SER:HA	1.59	0.83
3:D:44:ALA:HB3	3:D:368:GLU:HB2	1.61	0.83
3:D:382:THR:HG22	3:D:383:LEU:H	1.43	0.83
3:D:386:ASP:O	3:D:390:TYR:N	2.11	0.83
3:D:263:ARG:HB2	3:D:290:ASN:HB3	1.61	0.83
3:G:463:PRO:HA	3:G:466:ARG:NH1	1.91	0.83
3:D:209:ASP:O	3:D:212:THR:OG1	1.94	0.83
3:D:459:LEU:O	3:D:466:ARG:NE	2.10	0.83
3:H:216:ASN:ND2	3:H:219:GLU:OE2	2.11	0.83
3:H:52:ILE:HG22	3:H:61:LEU:HB3	1.61	0.82
3:D:210:PHE:HB3	3:D:214:GLN:HB2	1.59	0.82
3:E:219:GLU:OE1	3:E:263:ARG:NH1	2.12	0.82
3:D:287:ALA:HB1	3:H:146:CYS:HB2	1.60	0.82
3:G:16:VAL:CG2	3:G:17:PRO:HD2	2.08	0.82
3:D:150:ASP:OD2	3:D:258:ARG:NH2	2.12	0.82
3:D:135:TYR:OH	3:D:286:LEU:O	1.97	0.82
3:F:111:GLN:HB2	3:F:338:ARG:HD3	1.62	0.82
3:H:54:LYS:HB3	3:H:57:ASN:HB3	1.60	0.82
3:D:96:GLN:NE2	3:D:382:THR:OG1	2.12	0.82
3:D:188:LEU:HD22	3:H:45:VAL:HG11	1.61	0.82
3:E:422:THR:HA	3:E:426:ILE:HD12	1.60	0.82
3:G:216:ASN:ND2	3:G:219:GLU:OE2	2.13	0.81
2:B:2:ILE:O	2:B:97:THR:OG1	1.98	0.81
3:G:52:ILE:HG22	3:G:61:LEU:HB3	1.62	0.81
1:A:59:TYR:HB2	1:A:64:LYS:HD2	1.62	0.81
3:C:74:ARG:HB2	3:C:446:PHE:HE1	1.45	0.81
3:F:116:GLY:N	3:F:339:SER:OG	2.11	0.81
3:D:169:TRP:N	3:D:207:ALA:O	2.13	0.81
3:F:54:LYS:HB3	3:F:57:ASN:HB3	1.63	0.81
1:A:94:ARG:NH2	1:A:101:ASP:OD2	2.14	0.80
3:F:19:SER:C	3:F:20:LYS:HG2	2.01	0.80
3:D:69:GLN:HB3	3:D:198:GLY:HA2	1.62	0.80
3:D:108:GLY:N	3:D:371:ASP:O	2.14	0.80
3:D:397:THR:HA	3:D:400:GLU:CD	2.01	0.80
3:D:117:ILE:HG13	3:D:149:MET:O	1.82	0.80
3:F:463:PRO:HA	3:F:466:ARG:NH1	1.95	0.80
3:F:70:TYR:OH	3:F:230:LYS:O	2.00	0.80
3:H:463:PRO:HA	3:H:466:ARG:NH1	1.96	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:116:GLY:N	3:H:339:SER:OG	2.12	0.80
3:D:109:ARG:O	3:D:308:ASN:ND2	2.14	0.80
3:C:126:LEU:HB3	3:C:262:ASN:HB2	1.63	0.80
3:E:54:LYS:HB3	3:E:57:ASN:HB3	1.62	0.79
3:F:83:PHE:HD1	3:G:13:LEU:HD12	1.48	0.79
1:A:59:TYR:CG	1:A:64:LYS:HA	2.17	0.79
3:H:312:TRP:CH2	3:H:468:PHE:HD1	2.01	0.79
3:C:164:PRO:HB2	3:C:195:ILE:HD12	1.65	0.79
3:G:120:HIS:ND1	3:G:122:LEU:O	2.16	0.79
3:H:469:LEU:O	3:H:473:GLY:N	2.16	0.78
3:H:120:HIS:ND1	3:H:122:LEU:O	2.15	0.78
3:D:54:LYS:HB3	3:D:57:ASN:HB3	1.65	0.78
3:D:155:GLN:OE1	3:D:305:GLN:NE2	2.17	0.78
1:A:24:ALA:HB3	1:A:76:ASN:HB3	1.66	0.78
3:D:69:GLN:HB2	3:D:71:ARG:NH2	1.99	0.78
3:D:165:ILE:HG12	3:D:194:VAL:HA	1.66	0.78
2:B:29:LEU:HB2	2:B:68:GLY:HA2	1.66	0.78
3:C:428:CYS:HA	3:C:430:LYS:O	1.82	0.78
3:D:159:ILE:HD12	3:D:248:PHE:CD2	2.18	0.78
3:D:166:GLY:N	3:D:195:ILE:HG13	1.99	0.78
3:C:463:PRO:HA	3:C:466:ARG:HH12	1.48	0.77
3:C:54:LYS:HB3	3:C:57:ASN:HB3	1.65	0.77
3:D:101:ALA:N	3:D:377:GLN:O	2.17	0.77
3:D:102:CYS:HA	3:D:376:PHE:HD1	1.49	0.77
3:E:37:ALA:HB2	3:E:455:PHE:HA	1.65	0.77
3:E:18:VAL:H	3:E:19:SER:HA	1.49	0.77
3:D:109:ARG:HH11	3:D:110:GLY:H	1.29	0.77
3:D:162:LYS:HB2	3:D:245:SER:HA	1.65	0.77
3:D:366:HIS:ND1	3:D:368:GLU:OE2	2.17	0.77
3:F:37:ALA:HB2	3:F:455:PHE:HA	1.65	0.77
3:H:37:ALA:HB2	3:H:455:PHE:HA	1.65	0.77
1:A:39:GLN:H	1:A:88:ALA:HB1	1.50	0.77
3:D:72:VAL:N	3:D:197:ASP:OD1	2.18	0.77
3:G:37:ALA:HB2	3:G:455:PHE:HA	1.66	0.77
3:D:44:ALA:O	3:D:368:GLU:N	2.18	0.77
3:D:335:ASP:OD2	3:D:337:THR:OG1	2.03	0.77
2:B:32:TYR:HD2	2:B:92:TYR:HB2	1.47	0.76
3:D:416:ASP:O	3:D:417:THR:OG1	2.03	0.76
3:F:120:HIS:ND1	3:F:122:LEU:O	2.19	0.76
1:A:29:PHE:CD2	1:A:73:ASN:HA	2.20	0.76
1:A:82(A):SER:HB2	3:C:179:ALA:HB2	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ILE:HD13	2:B:25:SER:HB2	1.65	0.76
3:D:22:VAL:HB	3:D:26:GLU:HG3	1.66	0.76
3:G:74:ARG:HB2	3:G:446:PHE:CE1	2.18	0.76
1:A:22:CYS:HB3	1:A:78:LEU:HB3	1.66	0.76
2:B:30(A):TYR:O	2:B:30(E):GLN:NE2	2.19	0.76
3:D:76:HIS:ND1	3:D:449:VAL:O	2.15	0.76
3:D:182:PRO:HB2	3:H:348:ILE:HG13	1.66	0.76
3:H:52:ILE:O	3:H:61:LEU:N	2.18	0.76
3:D:120:HIS:ND1	3:D:122:LEU:O	2.17	0.76
3:E:70:TYR:OH	3:E:230:LYS:O	2.02	0.76
3:F:220:VAL:HB	3:F:224:ILE:HD11	1.68	0.76
3:D:302:SER:OG	3:E:253:GLU:N	2.19	0.76
3:G:81:ASN:HD21	3:G:98:LEU:H	1.34	0.76
3:H:220:VAL:HB	3:H:224:ILE:HD11	1.67	0.76
3:C:258:ARG:NH2	3:C:296:SER:OG	2.17	0.76
3:F:210:PHE:HE2	3:F:224:ILE:HD12	1.51	0.76
3:D:96:GLN:HG2	3:D:382:THR:HA	1.65	0.76
3:D:372:LEU:HB3	3:D:374:PHE:CZ	2.21	0.76
3:G:406:LEU:HA	3:G:408:PRO:HD3	1.67	0.75
3:F:418:TYR:HB3	3:F:419:ARG:HA	1.68	0.75
3:F:74:ARG:HB2	3:F:446:PHE:CE1	2.20	0.75
2:B:13:VAL:HG11	2:B:19:VAL:HA	1.67	0.75
3:C:312:TRP:CH2	3:C:468:PHE:HD1	2.05	0.75
3:E:52:ILE:HG22	3:E:61:LEU:HB3	1.67	0.75
3:F:52:ILE:HG22	3:F:61:LEU:HB3	1.69	0.75
3:C:399:LEU:HB3	3:C:404:PHE:CE1	2.21	0.75
3:D:47:HIS:HA	3:D:365:ARG:HA	1.66	0.75
3:D:99:VAL:O	3:D:379:CYS:N	2.17	0.75
3:C:53:LYS:HA	3:C:61:LEU:H	1.52	0.74
3:G:421:VAL:HG12	3:G:423:SER:H	1.52	0.74
3:D:109:ARG:NH2	3:D:111:GLN:HG2	1.99	0.74
3:E:312:TRP:CH2	3:E:468:PHE:HD1	2.06	0.74
1:A:72:ASP:HB3	1:A:79:TYR:HE2	1.51	0.74
3:G:46:GLY:HA3	3:G:65:VAL:HB	1.69	0.74
3:D:162:LYS:N	3:D:244:ASP:O	2.21	0.74
3:D:299:MET:HA	3:E:256:PHE:HB3	1.70	0.74
3:C:158:LEU:HB2	3:C:332:THR:HB	1.70	0.74
3:E:120:HIS:ND1	3:E:122:LEU:O	2.21	0.74
3:F:312:TRP:CH2	3:F:468:PHE:HD1	2.06	0.74
3:C:97:ARG:HH22	3:C:404:PHE:N	1.85	0.74
2:B:37:GLN:N	2:B:45:LYS:O	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:157:CYS:HA	3:D:333:VAL:HG22	1.70	0.74
3:D:461:GLN:OE1	3:D:461:GLN:N	2.20	0.74
3:G:312:TRP:CH2	3:G:468:PHE:HD1	2.06	0.74
3:H:70:TYR:OH	3:H:230:LYS:O	2.06	0.74
3:D:277:ILE:HD11	3:H:216:ASN:O	1.88	0.74
3:F:57:ASN:OD1	3:F:58:ASN:N	2.21	0.74
1:A:93:ALA:HA	1:A:103:TRP:HB2	1.70	0.73
3:D:401:ASP:N	3:D:401:ASP:OD1	2.17	0.73
3:E:220:VAL:HB	3:E:224:ILE:HD11	1.70	0.73
3:G:421:VAL:HB	3:G:430:LYS:HZ1	1.53	0.73
3:D:258:ARG:N	3:D:294:THR:O	2.22	0.73
3:E:216:ASN:ND2	3:E:219:GLU:OE2	2.21	0.73
3:G:421:VAL:HB	3:G:430:LYS:NZ	2.02	0.73
3:H:57:ASN:OD1	3:H:58:ASN:N	2.22	0.73
1:A:68:THR:O	1:A:81:GLN:N	2.18	0.73
3:D:306:ILE:O	3:D:311:TYR:OH	2.05	0.73
3:F:418:TYR:HB2	3:F:419:ARG:HD3	1.68	0.73
3:D:169:TRP:HB2	3:D:208:MET:HB3	1.70	0.73
3:G:54:LYS:HB3	3:G:57:ASN:HB3	1.69	0.73
3:G:70:TYR:OH	3:G:230:LYS:O	2.06	0.73
3:C:463:PRO:HA	3:C:466:ARG:NH1	2.03	0.73
3:D:111:GLN:O	3:D:338:ARG:NE	2.22	0.73
3:D:391:ILE:O	3:D:395:ASN:N	2.22	0.73
3:E:74:ARG:HB2	3:E:446:PHE:CE1	2.24	0.73
3:E:469:LEU:O	3:E:473:GLY:N	2.22	0.73
3:G:220:VAL:HB	3:G:224:ILE:HD11	1.71	0.73
3:G:403:ASN:HB3	3:G:405:GLY:HA2	1.71	0.73
3:G:469:LEU:O	3:G:473:GLY:N	2.21	0.73
3:G:57:ASN:OD1	3:G:58:ASN:N	2.22	0.73
3:C:120:HIS:HB2	3:C:221:PRO:HA	1.71	0.72
3:D:187:PRO:HA	3:D:188:LEU:HD12	1.71	0.72
3:G:97:ARG:NH2	3:G:404:PHE:O	2.22	0.72
3:C:469:LEU:O	3:C:473:GLY:N	2.22	0.72
3:E:57:ASN:OD1	3:E:58:ASN:N	2.22	0.72
3:C:427:ALA:HB1	3:D:173:SER:H	1.54	0.72
3:H:384:THR:O	3:H:387:VAL:HB	1.89	0.72
3:D:57:ASN:OD1	3:D:58:ASN:N	2.23	0.72
3:D:129:THR:OG1	3:D:130:GLU:N	2.22	0.72
3:C:312:TRP:HH2	3:C:468:PHE:HD1	1.36	0.72
3:D:240:GLU:CD	3:D:244:ASP:H	1.92	0.72
3:D:468:PHE:CZ	3:D:472:ALA:HB2	2.25	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:459:LEU:HB3	3:D:466:ARG:HB3	1.70	0.72
3:E:406:LEU:HB2	3:E:408:PRO:HB3	1.72	0.72
1:A:83:ARG:HB3	1:A:85:GLU:HG2	1.70	0.72
1:A:93:ALA:HA	1:A:103:TRP:CB	2.20	0.72
3:D:189:GLU:HG2	3:D:190:LEU:N	2.03	0.72
3:E:46:GLY:HA3	3:E:65:VAL:HB	1.70	0.72
3:G:406:LEU:HA	3:G:408:PRO:CD	2.20	0.72
3:H:210:PHE:HE2	3:H:224:ILE:HD12	1.55	0.71
2:B:38:GLN:OE1	2:B:87:TYR:OH	2.09	0.71
3:D:390:TYR:O	3:D:394:MET:N	2.21	0.71
3:E:52:ILE:O	3:E:61:LEU:N	2.23	0.71
3:D:188:LEU:HD21	3:H:365:ARG:HG3	1.73	0.71
3:D:479:LYS:HD2	3:E:22:VAL:HG11	1.72	0.71
3:H:51:PRO:HD3	3:H:64:LYS:HD2	1.72	0.71
3:C:50:PHE:HA	3:C:64:LYS:HD2	1.72	0.71
3:C:325:TRP:HZ3	3:C:402:TRP:CH2	2.08	0.71
3:D:211:THR:OG1	3:D:225:CYS:O	2.08	0.71
3:D:384:THR:H	3:D:387:VAL:HB	1.56	0.71
3:C:306:ILE:O	3:C:311:TYR:OH	2.09	0.71
3:D:168:HIS:N	3:D:191:ILE:O	2.19	0.71
3:G:405:GLY:O	3:G:408:PRO:HD3	1.91	0.71
1:A:17:SER:HA	1:A:82(A):SER:HA	1.71	0.71
3:D:255:MET:HG2	3:D:256:PHE:N	2.06	0.71
3:H:126:LEU:HB3	3:H:262:ASN:HB2	1.71	0.71
3:G:335:ASP:OD1	3:G:336:THR:N	2.24	0.71
3:D:103:VAL:N	3:D:376:PHE:HA	2.04	0.70
3:D:170:GLY:N	3:D:189:GLU:O	2.18	0.70
3:G:111:GLN:HB2	3:G:338:ARG:HD3	1.71	0.70
3:H:74:ARG:HB2	3:H:446:PHE:CE1	2.23	0.70
3:D:459:LEU:HD13	3:D:465:GLY:C	2.11	0.70
3:D:52:ILE:HG21	3:D:61:LEU:HD23	1.73	0.70
1:A:12:VAL:HG21	1:A:18:LEU:HD13	1.71	0.70
3:C:301:THR:HG23	3:C:304:ALA:H	1.56	0.70
3:D:383:LEU:HA	3:D:387:VAL:HG11	1.73	0.70
3:D:79:ASP:HA	3:D:327:ASN:HD21	1.57	0.70
3:D:127:ASP:O	3:D:262:ASN:N	2.21	0.70
3:D:159:ILE:HD12	3:D:248:PHE:HD2	1.55	0.70
3:F:301:THR:HG23	3:F:304:ALA:H	1.56	0.70
3:H:312:TRP:HH2	3:H:468:PHE:HD1	1.38	0.70
3:D:79:ASP:HB3	3:D:82:LYS:HG2	1.73	0.70
3:D:389:THR:HA	3:D:392:HIS:HB3	1.74	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:148:SER:OG	3:H:260:LEU:HD23	1.92	0.70
3:H:56:ASN:OD1	3:H:57:ASN:N	2.25	0.69
3:C:47:HIS:HE1	3:C:49:TYR:HB2	1.57	0.69
3:D:216:ASN:HA	3:H:360:PHE:CE2	2.27	0.69
3:D:298:SER:OG	3:D:299:MET:N	2.25	0.69
3:D:372:LEU:HD22	3:D:374:PHE:HZ	1.56	0.69
3:D:220:VAL:HB	3:D:224:ILE:HD11	1.72	0.69
3:D:106:GLU:N	3:D:373:GLN:O	2.25	0.69
3:C:404:PHE:O	3:C:406:LEU:N	2.19	0.69
3:D:70:TYR:H	3:D:199:ASP:N	1.91	0.69
3:D:172:GLY:H	3:D:187:PRO:C	1.95	0.69
3:E:111:GLN:HB2	3:E:338:ARG:HD3	1.73	0.69
3:E:164:PRO:HB2	3:E:195:ILE:HD12	1.75	0.69
2:B:65:SER:N	2:B:72:THR:O	2.25	0.69
3:E:116:GLY:N	3:E:339:SER:OG	2.14	0.69
1:A:67:PHE:HB3	1:A:80:LEU:HD11	1.75	0.69
1:A:100(E):ASP:HB3	2:B:49:TYR:CD2	2.28	0.69
3:D:109:ARG:NH1	3:D:110:GLY:H	1.91	0.69
3:D:256:PHE:HB3	3:H:299:MET:HA	1.75	0.69
3:D:464:LEU:O	3:D:467:LYS:N	2.21	0.69
3:E:384:THR:O	3:E:387:VAL:HB	1.93	0.69
3:F:426:ILE:HG22	3:F:427:ALA:N	2.06	0.69
3:G:16:VAL:CG2	3:G:17:PRO:CD	2.70	0.69
3:H:53:LYS:HA	3:H:61:LEU:H	1.58	0.69
1:A:38:ARG:NH1	1:A:86:ASP:HA	2.07	0.69
3:E:43:LEU:HD12	3:E:368:GLU:O	1.93	0.69
3:F:392:HIS:O	3:F:396:SER:OG	2.11	0.69
3:G:126:LEU:HB3	3:G:262:ASN:HB2	1.73	0.69
3:D:148:SER:OG	3:E:260:LEU:HD23	1.92	0.68
3:H:97:ARG:NH2	3:H:403:ASN:HB2	2.06	0.68
3:D:104:GLY:O	3:D:375:ILE:N	2.27	0.68
3:D:106:GLU:OE2	3:D:309:LYS:N	2.25	0.68
3:D:166:GLY:N	3:D:193:THR:O	2.26	0.68
3:D:216:ASN:HB3	3:D:219:GLU:HG2	1.74	0.68
3:E:18:VAL:HB	3:E:20:LYS:HG3	1.74	0.68
2:B:37:GLN:HG3	2:B:84:ALA:HB1	1.75	0.68
3:C:76:HIS:HB3	3:C:452:LYS:HE3	1.73	0.68
3:D:118:SER:O	3:D:149:MET:N	2.19	0.68
3:D:171:LYS:HG3	3:D:186:PRO:HB2	1.76	0.68
3:D:254:GLN:OE1	3:D:299:MET:O	2.11	0.68
3:E:407:GLN:HB2	3:E:408:PRO:O	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:426:ILE:CG2	3:F:427:ALA:H	2.01	0.68
3:C:49:TYR:HB3	3:C:222:LEU:CD2	2.23	0.68
3:D:216:ASN:OD1	3:D:219:GLU:OE2	2.11	0.68
3:D:391:ILE:HA	3:D:394:MET:HB3	1.74	0.68
3:F:18:VAL:HG12	3:F:19:SER:N	2.09	0.68
3:F:335:ASP:OD1	3:F:336:THR:N	2.27	0.68
1:A:37:VAL:N	1:A:91:TYR:O	2.26	0.68
3:D:165:ILE:HG23	3:D:193:THR:C	2.14	0.68
3:H:46:GLY:HA3	3:H:65:VAL:HB	1.74	0.68
3:D:360:PHE:CE1	3:E:215:ALA:HB3	2.29	0.68
3:E:126:LEU:HB3	3:E:262:ASN:HB2	1.76	0.68
3:D:352:GLU:OE1	3:D:352:GLU:N	2.26	0.68
3:F:56:ASN:OD1	3:F:57:ASN:N	2.26	0.68
3:F:306:ILE:O	3:F:311:TYR:OH	2.10	0.68
3:G:306:ILE:O	3:G:311:TYR:OH	2.11	0.68
3:E:210:PHE:HE2	3:E:224:ILE:HD12	1.58	0.68
3:F:384:THR:O	3:F:387:VAL:HB	1.94	0.68
3:D:153:GLN:NE2	3:D:299:MET:O	2.22	0.67
3:D:399:LEU:HA	3:D:402:TRP:HB2	1.74	0.67
3:F:254:GLN:NE2	3:F:298:SER:HB3	2.09	0.67
1:A:35:SER:OG	1:A:49:ALA:O	2.10	0.67
3:C:37:ALA:HB2	3:C:455:PHE:HA	1.76	0.67
3:D:468:PHE:CA	3:D:471:GLN:HB3	2.21	0.67
3:E:404:PHE:HB2	3:E:405:GLY:O	1.95	0.67
3:C:97:ARG:CZ	3:C:402:TRP:HB3	2.24	0.67
3:E:312:TRP:HH2	3:E:468:PHE:HD1	1.42	0.67
1:A:33:ALA:HB3	1:A:95:GLY:HA3	1.77	0.67
1:A:45:LEU:HB2	2:B:98:PHE:CD2	2.30	0.67
3:C:40:SER:OG	3:C:41:ARG:N	2.28	0.67
3:C:404:PHE:C	3:C:406:LEU:H	1.97	0.67
3:G:52:ILE:O	3:G:61:LEU:N	2.26	0.67
1:A:83:ARG:HD3	1:A:85:GLU:OE2	1.95	0.67
1:A:94:ARG:HH21	1:A:101:ASP:HB3	1.60	0.67
2:B:54:ARG:NH1	2:B:63:THR:OG1	2.28	0.67
3:D:263:ARG:HG2	3:D:292:PHE:CD2	2.30	0.67
2:B:61:ARG:NE	2:B:82:ASP:OD1	2.17	0.67
3:C:90:PHE:HD1	3:C:380:LYS:HZ1	1.42	0.67
3:D:160:GLY:HA2	3:D:247:PHE:CZ	2.29	0.67
3:D:356:LYS:HB3	3:D:358:THR:HG23	1.76	0.67
3:C:156:LEU:HG	3:C:334:VAL:HB	1.77	0.67
3:D:109:ARG:HB3	3:D:308:ASN:HD21	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:255:MET:HG2	3:D:256:PHE:H	1.59	0.66
3:F:469:LEU:O	3:F:473:GLY:N	2.27	0.66
3:C:196:GLN:HE21	3:C:444:TYR:HD1	1.44	0.66
3:E:254:GLN:NE2	3:E:298:SER:HB3	2.10	0.66
3:G:97:ARG:HH21	3:G:404:PHE:N	1.92	0.66
3:G:210:PHE:HE2	3:G:224:ILE:HD12	1.59	0.66
3:D:268:GLY:HA3	3:H:362:GLU:O	1.94	0.66
1:A:86:ASP:O	1:A:90:TYR:OH	2.13	0.66
3:C:49:TYR:HB3	3:C:222:LEU:HD22	1.77	0.66
3:D:345:CYS:SG	3:E:216:ASN:N	2.66	0.66
3:D:107:VAL:HA	3:D:372:LEU:HD23	1.76	0.66
3:D:361:LYS:HA	3:E:266:ALA:O	1.95	0.66
3:D:159:ILE:O	3:D:248:PHE:N	2.29	0.66
3:D:273:ASP:O	3:D:276:TYR:N	2.28	0.66
3:E:41:ARG:HH21	3:E:369:GLU:HG3	1.59	0.66
3:G:258:ARG:NH2	3:G:296:SER:OG	2.29	0.66
3:H:109:ARG:NH2	3:H:338:ARG:HD2	2.11	0.66
1:A:69:ILE:HD11	1:A:78:LEU:HD11	1.78	0.66
3:C:17:PRO:HG2	3:C:386:ASP:OD1	1.95	0.66
3:D:235:ILE:O	3:D:239:SER:OG	2.11	0.66
3:D:247:PHE:O	3:D:317:GLN:NE2	2.29	0.66
3:D:348:ILE:HG13	3:E:182:PRO:HB2	1.78	0.66
3:E:51:PRO:HD3	3:E:64:LYS:HD2	1.77	0.66
2:B:38:GLN:HG3	2:B:44:PRO:HG3	1.78	0.66
3:C:57:ASN:OD1	3:C:58:ASN:N	2.29	0.66
3:C:406:LEU:CD1	3:C:411:GLY:H	2.09	0.66
3:C:258:ARG:HG2	3:C:259:HIS:ND1	2.10	0.65
3:D:73:PHE:HD1	3:D:447:TRP:CD1	2.14	0.65
3:E:148:SER:OG	3:F:260:LEU:HD23	1.97	0.65
3:E:407:GLN:HB3	3:E:410:PRO:HD2	1.78	0.65
3:C:70:TYR:OH	3:C:230:LYS:O	2.15	0.65
3:C:72:VAL:HB	3:C:446:PHE:HB2	1.76	0.65
3:D:66:SER:O	3:D:71:ARG:NH2	2.29	0.65
3:D:162:LYS:HB3	3:D:163:PRO:HD2	1.78	0.65
3:F:47:HIS:HE1	3:F:49:TYR:HB2	1.61	0.65
2:B:4:MET:O	2:B:100:ALA:N	2.28	0.65
3:D:345:CYS:SG	3:E:215:ALA:N	2.70	0.65
3:G:421:VAL:HG12	3:G:423:SER:N	2.12	0.65
3:H:258:ARG:HG2	3:H:259:HIS:ND1	2.11	0.65
3:C:169:TRP:HB2	3:C:208:MET:HB3	1.78	0.65
3:E:56:ASN:OD1	3:E:57:ASN:N	2.30	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:404:PHE:HE1	3:H:409:PRO:CD	2.09	0.65
3:C:312:TRP:CE2	3:C:471:GLN:NE2	2.65	0.65
3:G:312:TRP:CE2	3:G:471:GLN:NE2	2.65	0.65
3:D:42:LEU:N	3:D:370:TYR:O	2.30	0.65
3:D:105:VAL:HA	3:D:374:PHE:HD1	1.62	0.65
3:C:219:GLU:OE1	3:C:263:ARG:NH1	2.29	0.65
3:F:15:PRO:C	3:F:17:PRO:HD3	2.17	0.65
3:G:223:ASP:OD1	3:G:224:ILE:N	2.30	0.65
1:A:100(A):ASP:OD2	2:B:53:THR:OG1	2.14	0.65
3:D:102:CYS:HA	3:D:376:PHE:CD1	2.31	0.65
3:D:450:ASN:OD1	3:D:451:LEU:N	2.30	0.65
3:H:335:ASP:OD1	3:H:336:THR:N	2.30	0.65
3:D:128:ASP:OD1	3:D:129:THR:N	2.29	0.64
3:F:15:PRO:HB2	3:F:17:PRO:HD3	1.79	0.64
2:B:35:TRP:CB	2:B:47:LEU:HB2	2.27	0.64
3:C:325:TRP:HZ3	3:C:402:TRP:HH2	1.43	0.64
3:D:124:ASN:O	3:D:263:ARG:NH1	2.31	0.64
3:F:52:ILE:O	3:F:61:LEU:N	2.28	0.64
2:B:5:SER:O	2:B:23:CYS:HA	1.98	0.64
3:D:72:VAL:HB	3:D:197:ASP:HB2	1.79	0.64
3:F:258:ARG:NH2	3:F:296:SER:OG	2.31	0.64
1:A:33:ALA:O	1:A:95:GLY:N	2.20	0.64
3:D:50:PHE:HA	3:D:64:LYS:HD2	1.80	0.64
3:D:156:LEU:N	3:D:334:VAL:O	2.22	0.64
3:D:249:TYR:OH	3:D:251:ARG:NH1	2.30	0.64
3:D:406:LEU:HA	3:D:407:GLN:HB2	1.79	0.64
3:G:120:HIS:HB2	3:G:221:PRO:HA	1.78	0.64
3:G:234:TYR:OH	3:G:251:ARG:HD3	1.98	0.64
3:D:222:LEU:O	3:D:225:CYS:HB3	1.97	0.64
3:G:273:ASP:OD1	3:G:274:ASP:N	2.31	0.64
3:G:301:THR:HG23	3:G:304:ALA:H	1.61	0.64
3:H:47:HIS:HE1	3:H:49:TYR:HB2	1.62	0.64
3:D:61:LEU:HG	3:D:62:VAL:HG23	1.79	0.64
3:D:246:LEU:HD22	3:D:249:TYR:HB3	1.79	0.64
3:E:301:THR:HG23	3:E:304:ALA:H	1.62	0.64
3:E:348:ILE:HG13	3:F:182:PRO:HB2	1.80	0.64
3:G:345:CYS:SG	3:H:215:ALA:N	2.71	0.64
3:H:301:THR:HG23	3:H:304:ALA:H	1.60	0.64
3:D:130:GLU:HA	3:H:147:ILE:HG23	1.79	0.64
3:D:156:LEU:O	3:D:333:VAL:HG13	1.97	0.64
3:D:158:LEU:HD12	3:D:332:THR:CG2	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:391:ILE:O	3:F:394:MET:N	2.31	0.64
3:G:56:ASN:OD1	3:G:57:ASN:N	2.31	0.64
3:D:71:ARG:O	3:D:332:THR:HG23	1.98	0.64
3:D:222:LEU:H	3:D:222:LEU:HD12	1.62	0.64
3:H:273:ASP:OD1	3:H:274:ASP:N	2.31	0.64
2:B:13:VAL:HG21	2:B:19:VAL:HG12	1.79	0.64
2:B:34:ALA:HB3	2:B:89:GLN:HB3	1.78	0.64
3:C:262:ASN:ND2	3:C:290:ASN:O	2.30	0.64
3:D:103:VAL:H	3:D:376:PHE:CA	2.06	0.64
3:D:144:ARG:NH2	3:E:279:GLY:HA2	2.13	0.64
3:G:345:CYS:SG	3:H:216:ASN:N	2.63	0.64
2:B:6:GLN:N	2:B:100:ALA:HB3	2.08	0.63
3:F:46:GLY:HA3	3:F:65:VAL:HB	1.80	0.63
3:G:85:PHE:HB2	3:G:88:THR:HG22	1.80	0.63
3:G:391:ILE:O	3:G:394:MET:N	2.31	0.63
3:D:45:VAL:HA	3:D:367:GLY:HA2	1.81	0.63
3:D:76:HIS:HD1	3:D:449:VAL:C	2.01	0.63
3:D:121:PRO:HA	3:D:146:CYS:SG	2.37	0.63
3:D:124:ASN:HB3	3:D:263:ARG:HH11	1.63	0.63
3:D:470:LEU:O	3:D:473:GLY:N	2.31	0.63
3:E:335:ASP:OD1	3:E:336:THR:N	2.31	0.63
3:D:109:ARG:HH22	3:D:111:GLN:CG	2.06	0.63
3:D:310:PRO:HB2	3:D:312:TRP:NE1	2.13	0.63
3:F:97:ARG:HH22	3:F:404:PHE:HB2	1.64	0.63
3:G:408:PRO:HB2	3:G:409:PRO:HD3	1.79	0.63
2:B:64:GLY:HA2	2:B:73:LEU:HA	1.81	0.63
3:D:129:THR:O	3:H:147:ILE:HG12	1.98	0.63
3:E:72:VAL:O	3:E:447:TRP:HB3	1.99	0.63
3:F:477:LYS:HZ2	3:G:23:SER:HB2	1.63	0.63
3:D:208:MET:O	3:D:228:ILE:HA	1.99	0.63
3:F:273:ASP:OD1	3:F:274:ASP:N	2.32	0.63
3:G:312:TRP:HH2	3:G:468:PHE:HD1	1.47	0.63
1:A:52:SER:OG	1:A:56:ASN:N	2.30	0.63
3:D:53:LYS:HA	3:D:61:LEU:H	1.64	0.63
3:D:70:TYR:OH	3:D:201:VAL:HA	1.99	0.63
3:D:240:GLU:HG2	3:D:242:TYR:N	2.08	0.63
3:D:300:VAL:HG22	3:E:255:MET:H	1.64	0.63
3:D:443:LYS:O	3:D:445:THR:HG23	1.99	0.63
3:F:51:PRO:HD3	3:F:64:LYS:HD2	1.80	0.63
3:F:223:ASP:OD1	3:F:224:ILE:N	2.30	0.63
3:F:234:TYR:OH	3:F:251:ARG:HD3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:372:LEU:HB3	3:D:374:PHE:CE2	2.33	0.63
3:E:234:TYR:OH	3:E:251:ARG:HD3	1.99	0.63
3:G:53:LYS:HA	3:G:61:LEU:H	1.63	0.63
3:G:474:LEU:HD12	3:G:474:LEU:O	1.99	0.63
3:H:404:PHE:CE1	3:H:409:PRO:CD	2.81	0.63
3:D:209:ASP:HB2	3:D:228:ILE:HG13	1.79	0.62
3:D:169:TRP:CD1	3:D:207:ALA:N	2.68	0.62
3:D:235:ILE:O	3:D:238:VAL:HB	1.98	0.62
3:D:85:PHE:H	3:D:88:THR:HG22	1.63	0.62
3:D:150:ASP:OD2	3:D:297:GLY:N	2.30	0.62
3:D:344:LEU:HD21	3:D:363:TYR:HD2	1.64	0.62
3:E:97:ARG:NH2	3:E:404:PHE:N	2.47	0.62
3:E:403:ASN:C	3:E:405:GLY:O	2.36	0.62
3:F:299:MET:HA	3:G:256:PHE:HB3	1.80	0.62
3:D:299:MET:HG2	3:D:300:VAL:N	2.15	0.62
3:F:345:CYS:SG	3:G:215:ALA:N	2.71	0.62
3:G:384:THR:O	3:G:387:VAL:HB	1.99	0.62
3:H:81:ASN:HD21	3:H:98:LEU:H	1.46	0.62
3:D:215:ALA:N	3:H:345:CYS:SG	2.72	0.62
3:E:109:ARG:NH2	3:E:338:ARG:HD2	2.15	0.62
3:C:210:PHE:HE2	3:C:224:ILE:HD12	1.65	0.62
3:D:77:LEU:HD23	3:D:451:LEU:HB2	1.82	0.62
3:D:80:PRO:HD3	3:D:100:TRP:NE1	2.15	0.62
3:E:223:ASP:OD1	3:E:224:ILE:N	2.33	0.62
1:A:66:ARG:HA	3:C:176:THR:CB	2.27	0.62
2:B:4:MET:HB2	2:B:99:GLY:HA2	1.82	0.62
3:C:150:ASP:OD1	3:C:296:SER:HA	1.99	0.62
3:D:46:GLY:CA	3:D:65:VAL:HB	2.30	0.62
3:F:348:ILE:HG13	3:G:182:PRO:HB2	1.80	0.62
1:A:38:ARG:HA	1:A:90:TYR:HA	1.81	0.62
3:D:114:GLY:O	3:D:339:SER:N	2.33	0.62
3:D:123:LEU:HD11	3:D:263:ARG:HH12	1.65	0.62
3:G:71:ARG:O	3:G:332:THR:HG23	2.00	0.62
1:A:22:CYS:O	1:A:78:LEU:N	2.26	0.62
3:E:280:SER:N	3:E:283:THR:OG1	2.29	0.62
3:E:387:VAL:O	3:E:391:ILE:HD12	2.00	0.62
3:D:125:LYS:NZ	3:D:127:ASP:HA	2.15	0.61
3:D:152:LYS:HE3	3:D:203:THR:C	2.21	0.61
3:F:450:ASN:OD1	3:F:452:LYS:HG3	2.00	0.61
3:H:52:ILE:HB	3:H:62:VAL:HB	1.82	0.61
3:C:219:GLU:OE1	3:C:263:ARG:CZ	2.48	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:142:ASP:OD1	3:D:144:ARG:NE	2.27	0.61
3:D:162:LYS:HB2	3:D:245:SER:CA	2.30	0.61
3:D:397:THR:O	3:D:400:GLU:HB2	2.00	0.61
3:E:299:MET:HA	3:F:256:PHE:HB3	1.80	0.61
3:F:312:TRP:HH2	3:F:468:PHE:HD1	1.45	0.61
3:H:254:GLN:OE1	3:H:298:SER:HB3	1.99	0.61
2:B:47:LEU:HD21	2:B:86:TYR:CE1	2.35	0.61
3:D:113:LEU:HA	3:D:338:ARG:CG	2.28	0.61
3:D:335:ASP:OD1	3:D:337:THR:HG23	2.00	0.61
3:D:384:THR:O	3:D:388:MET:N	2.16	0.61
3:E:306:ILE:O	3:E:311:TYR:OH	2.17	0.61
2:B:4:MET:HB3	2:B:23:CYS:SG	2.40	0.61
3:C:101:ALA:O	3:C:377:GLN:N	2.31	0.61
3:F:126:LEU:HB3	3:F:262:ASN:HB2	1.81	0.61
3:C:71:ARG:HG3	3:C:370:TYR:OH	1.99	0.61
3:D:57:ASN:CG	3:D:59:LYS:H	2.03	0.61
3:D:390:TYR:O	3:D:393:SER:HB2	2.00	0.61
3:E:273:ASP:OD1	3:E:274:ASP:N	2.34	0.61
3:F:15:PRO:CB	3:F:17:PRO:HD3	2.30	0.61
3:F:148:SER:OG	3:G:260:LEU:HD23	1.99	0.61
3:H:223:ASP:OD1	3:H:224:ILE:N	2.33	0.61
3:D:44:ALA:CB	3:D:368:GLU:HB2	2.29	0.61
3:D:233:ASP:CG	3:D:236:LYS:H	2.04	0.61
3:G:51:PRO:HD3	3:G:64:LYS:HD2	1.81	0.61
3:C:47:HIS:CE1	3:C:49:TYR:HB2	2.35	0.61
3:C:431:HIS:ND1	3:C:433:PRO:O	2.33	0.61
3:D:100:TRP:HA	3:D:378:LEU:HA	1.81	0.61
3:G:465:GLY:O	3:G:468:PHE:N	2.33	0.61
3:H:40:SER:OG	3:H:41:ARG:N	2.34	0.61
1:A:59:TYR:CB	1:A:64:LYS:HD2	2.30	0.61
2:B:14:SER:N	2:B:17:GLU:OE1	2.25	0.61
3:D:69:GLN:OE1	3:D:71:ARG:NH2	2.34	0.61
3:D:200:MET:HB2	3:D:228:ILE:O	2.01	0.61
3:D:307:PHE:O	3:D:309:LYS:HG3	2.00	0.61
3:D:344:LEU:HD22	3:E:186:PRO:HD2	1.83	0.61
3:H:30:ARG:HD3	3:H:379:CYS:SG	2.40	0.61
3:C:109:ARG:NH2	3:C:338:ARG:HD2	2.15	0.61
3:D:32:ASN:H	3:D:33:ILE:HD12	1.65	0.61
3:D:303:ASP:OD1	3:D:303:ASP:N	2.29	0.61
3:C:37:ALA:HB2	3:C:455:PHE:HD1	1.66	0.61
3:C:90:PHE:HD1	3:C:380:LYS:NZ	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:124:ASN:ND2	3:C:219:GLU:OE2	2.33	0.61
3:D:116:GLY:N	3:D:339:SER:OG	2.25	0.61
3:E:258:ARG:NH2	3:E:296:SER:OG	2.34	0.61
3:E:406:LEU:HB2	3:E:408:PRO:CB	2.30	0.61
3:E:418:TYR:HB3	3:E:420:PHE:CE2	2.36	0.61
3:H:164:PRO:HB2	3:H:195:ILE:HD12	1.83	0.61
3:E:404:PHE:HB2	3:E:405:GLY:CA	2.31	0.60
3:C:56:ASN:OD1	3:C:57:ASN:N	2.34	0.60
3:C:349:SER:N	3:C:359:ASN:OD1	2.30	0.60
3:D:66:SER:OG	3:D:68:LEU:N	2.34	0.60
3:E:345:CYS:SG	3:F:215:ALA:N	2.74	0.60
3:G:258:ARG:HB2	3:G:296:SER:HB2	1.82	0.60
3:G:405:GLY:O	3:G:408:PRO:CD	2.48	0.60
3:D:223:ASP:OD1	3:D:224:ILE:N	2.34	0.60
3:F:16:VAL:O	3:F:16:VAL:HG12	2.01	0.60
3:G:258:ARG:HG2	3:G:259:HIS:ND1	2.16	0.60
3:G:348:ILE:HG13	3:H:182:PRO:HB2	1.82	0.60
3:G:387:VAL:O	3:G:391:ILE:HD12	2.01	0.60
3:H:70:TYR:HD1	3:H:334:VAL:HG21	1.65	0.60
2:B:85:VAL:HG22	2:B:103:LYS:HG3	1.83	0.60
3:D:50:PHE:CE2	3:E:271:VAL:HA	2.37	0.60
3:F:105:VAL:HG13	3:F:374:PHE:CE1	2.35	0.60
3:D:78:PRO:HD3	3:D:452:LYS:HA	1.82	0.60
3:D:216:ASN:HD21	3:D:218:SER:HB2	1.67	0.60
3:F:335:ASP:OD2	3:F:337:THR:OG1	2.19	0.60
3:C:43:LEU:HD23	3:H:421:VAL:HG13	1.84	0.60
3:C:424:GLN:OE1	3:C:430:LYS:HB3	2.02	0.60
3:D:24:THR:HA	3:D:27:TYR:CZ	2.37	0.60
3:D:99:VAL:N	3:D:379:CYS:O	2.28	0.60
3:D:100:TRP:HA	3:D:378:LEU:HD12	1.82	0.60
3:D:459:LEU:HD13	3:D:466:ARG:N	2.16	0.60
3:G:16:VAL:HG23	3:G:17:PRO:CD	2.31	0.60
3:D:170:GLY:O	3:D:189:GLU:N	2.34	0.60
3:D:261:PHE:HD2	3:D:294:THR:HG1	1.46	0.60
3:E:164:PRO:HG2	3:E:195:ILE:HB	1.82	0.60
3:G:235:ILE:O	3:G:239:SER:N	2.33	0.60
3:H:306:ILE:O	3:H:311:TYR:OH	2.20	0.60
3:D:280:SER:N	3:D:283:THR:OG1	2.28	0.60
3:D:466:ARG:HA	3:D:469:LEU:HB2	1.83	0.60
3:E:335:ASP:OD2	3:E:337:THR:OG1	2.20	0.60
3:F:263:ARG:HB2	3:F:290:ASN:HD22	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLY:H	1:A:82(C):LEU:HB2	1.67	0.60
3:D:70:TYR:CE1	3:D:201:VAL:HG22	2.37	0.60
3:D:101:ALA:O	3:D:377:GLN:N	2.32	0.60
3:D:223:ASP:OD1	3:D:223:ASP:N	2.28	0.60
3:D:398:ILE:HA	3:D:401:ASP:OD2	2.02	0.60
3:E:169:TRP:HB2	3:E:208:MET:HB3	1.83	0.60
3:E:258:ARG:HG2	3:E:259:HIS:ND1	2.16	0.60
3:G:170:GLY:O	3:G:189:GLU:N	2.34	0.60
3:G:399:LEU:HD13	3:G:404:PHE:HZ	1.66	0.60
3:G:408:PRO:HB2	3:G:409:PRO:CD	2.32	0.60
3:D:158:LEU:N	3:D:332:THR:O	2.34	0.60
3:D:221:PRO:HD2	3:D:224:ILE:HD11	1.83	0.60
3:D:441:LEU:HG	3:D:444:TYR:HE2	1.65	0.60
3:F:120:HIS:CD2	3:F:222:LEU:HD12	2.36	0.60
3:G:280:SER:N	3:G:283:THR:OG1	2.32	0.60
1:A:16:GLY:O	1:A:82(B):SER:N	2.35	0.59
3:D:104:GLY:C	3:D:375:ILE:H	2.05	0.59
3:D:340:THR:HG22	3:D:341:ASN:O	2.02	0.59
3:F:418:TYR:CB	3:F:419:ARG:HA	2.31	0.59
3:H:120:HIS:HB2	3:H:221:PRO:HA	1.83	0.59
2:B:19:VAL:HB	2:B:104:LEU:HD21	1.85	0.59
2:B:29:LEU:HB2	2:B:68:GLY:CA	2.31	0.59
3:C:406:LEU:HD13	3:C:409:PRO:O	2.02	0.59
3:D:77:LEU:HD22	3:D:455:PHE:CZ	2.37	0.59
3:D:141:VAL:HG13	3:H:357:ASN:H	1.67	0.59
3:D:287:ALA:HB3	3:H:121:PRO:CB	2.28	0.59
3:D:123:LEU:H	3:D:145:GLU:H	1.50	0.59
3:D:395:ASN:OD1	3:D:396:SER:N	2.35	0.59
3:E:240:GLU:HG3	3:E:241:PRO:HD2	1.83	0.59
3:E:258:ARG:HB2	3:E:296:SER:HB2	1.84	0.59
3:C:47:HIS:CE1	3:C:49:TYR:H	2.20	0.59
3:E:120:HIS:CD2	3:E:222:LEU:HD12	2.37	0.59
3:H:234:TYR:OH	3:H:251:ARG:HD3	2.02	0.59
1:A:68:THR:HB	1:A:81:GLN:HB3	1.83	0.59
2:B:35:TRP:HB3	2:B:47:LEU:HB2	1.82	0.59
3:C:90:PHE:CE1	3:C:91:TYR:HD2	2.19	0.59
3:C:404:PHE:C	3:C:406:LEU:N	2.54	0.59
3:D:109:ARG:CZ	3:D:369:GLU:O	2.50	0.59
3:D:449:VAL:HG12	3:D:451:LEU:HD21	1.84	0.59
1:A:22:CYS:N	1:A:78:LEU:O	2.33	0.59
3:C:23:SER:O	3:C:26:GLU:HG2	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:302:SER:O	3:D:305:GLN:HB2	2.01	0.59
3:D:384:THR:O	3:D:387:VAL:HB	2.03	0.59
3:C:72:VAL:O	3:C:447:TRP:HB3	2.01	0.59
3:D:23:SER:HA	3:D:319:HIS:HB3	1.84	0.59
3:G:24:THR:HG21	3:G:320:ASN:HA	1.83	0.59
3:G:211:THR:OG1	3:G:226:THR:O	2.21	0.59
3:H:474:LEU:O	3:H:474:LEU:HD12	2.03	0.59
3:C:84:GLY:HA2	3:H:84:GLY:HA3	1.85	0.59
3:C:124:ASN:HA	3:C:144:ARG:HG2	1.83	0.59
3:D:25:ASP:HA	3:D:28:VAL:CB	2.28	0.59
3:D:53:LYS:HB3	3:D:60:ILE:HA	1.83	0.59
3:D:171:LYS:HB2	3:D:213:LEU:HD21	1.84	0.59
3:D:274:ASP:N	3:D:274:ASP:OD1	2.30	0.59
3:E:71:ARG:HG3	3:E:370:TYR:OH	2.02	0.59
2:B:2:ILE:HD11	2:B:27:GLN:HB2	1.84	0.59
3:D:70:TYR:H	3:D:199:ASP:H	1.49	0.59
3:D:258:ARG:HG2	3:D:259:HIS:NE2	2.18	0.59
3:D:335:ASP:OD1	3:D:337:THR:N	2.26	0.59
3:H:71:ARG:O	3:H:332:THR:HG23	2.03	0.59
3:H:391:ILE:O	3:H:394:MET:N	2.35	0.59
1:A:38:ARG:HH12	1:A:86:ASP:HA	1.67	0.59
3:D:221:PRO:HB2	3:D:224:ILE:HG12	1.85	0.59
3:D:345:CYS:HB2	3:D:360:PHE:CD1	2.38	0.59
3:E:116:GLY:H	3:E:339:SER:HG	1.46	0.59
3:F:85:PHE:HB2	3:F:88:THR:HG22	1.85	0.59
3:G:153:GLN:NE2	3:G:300:VAL:HG12	2.18	0.59
2:B:11:LEU:HD11	2:B:104:LEU:HD22	1.85	0.58
3:D:69:GLN:HB2	3:D:71:ARG:HH22	1.66	0.58
3:E:474:LEU:HD12	3:E:474:LEU:O	2.03	0.58
3:C:115:VAL:HG12	3:C:116:GLY:O	2.03	0.58
3:E:404:PHE:HB2	3:E:405:GLY:C	2.23	0.58
1:A:37:VAL:HB	1:A:91:TYR:HB2	1.84	0.58
3:D:91:TYR:HB3	3:D:380:LYS:NZ	2.18	0.58
3:D:157:CYS:O	3:D:158:LEU:HD23	2.02	0.58
3:D:422:THR:O	3:D:423:SER:OG	2.20	0.58
3:F:71:ARG:HG3	3:F:370:TYR:OH	2.03	0.58
3:G:70:TYR:HD1	3:G:334:VAL:HG21	1.67	0.58
2:B:47:LEU:HB3	2:B:48:ILE:HG12	1.85	0.58
3:C:16:VAL:CG1	3:C:17:PRO:HD3	2.33	0.58
3:C:406:LEU:HD13	3:C:409:PRO:C	2.23	0.58
3:C:406:LEU:CD2	3:C:408:PRO:C	2.72	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:31:THR:O	3:D:377:GLN:OE1	2.22	0.58
3:D:259:HIS:N	3:D:294:THR:O	2.32	0.58
3:E:53:LYS:HA	3:E:61:LEU:H	1.68	0.58
3:F:53:LYS:HA	3:F:61:LEU:H	1.69	0.58
3:F:153:GLN:NE2	3:F:300:VAL:HG12	2.18	0.58
3:D:77:LEU:CD2	3:D:451:LEU:HB2	2.32	0.58
3:F:150:ASP:OD1	3:F:296:SER:HA	2.04	0.58
3:G:416:ASP:O	3:G:417:THR:OG1	2.21	0.58
3:C:383:LEU:HD23	3:C:387:VAL:HG11	1.85	0.58
3:D:45:VAL:HA	3:D:366:HIS:O	2.04	0.58
3:D:57:ASN:OD1	3:D:59:LYS:N	2.35	0.58
3:D:112:PRO:HB3	3:E:231:TYR:CE1	2.39	0.58
3:D:248:PHE:CG	3:D:249:TYR:N	2.72	0.58
3:D:360:PHE:O	3:E:266:ALA:N	2.36	0.58
2:B:35:TRP:CE3	2:B:88:CYS:HB3	2.38	0.58
3:C:431:HIS:HD1	3:C:433:PRO:C	2.07	0.58
3:D:92:ASN:HB3	3:D:95:THR:OG1	2.03	0.58
3:D:236:LYS:C	3:D:239:SER:H	2.07	0.58
3:D:249:TYR:HE1	3:D:251:ARG:HG2	1.68	0.58
3:F:120:HIS:HB2	3:F:221:PRO:HA	1.86	0.58
3:H:153:GLN:NE2	3:H:300:VAL:HG12	2.19	0.58
3:D:274:ASP:OD1	3:D:275:LEU:HG	2.03	0.58
3:D:377:GLN:HG2	3:D:378:LEU:N	2.19	0.58
3:D:459:LEU:HB2	3:D:469:LEU:CD1	2.33	0.58
3:F:109:ARG:NH2	3:F:338:ARG:HD2	2.17	0.58
1:A:75:ARG:O	1:A:77:ILE:HG13	2.04	0.58
3:D:24:THR:O	3:D:28:VAL:HG23	2.03	0.58
3:D:70:TYR:HB2	3:D:199:ASP:H	1.69	0.58
3:E:349:SER:O	3:E:359:ASN:ND2	2.34	0.58
3:F:52:ILE:HB	3:F:62:VAL:HB	1.85	0.58
3:D:40:SER:OG	3:D:41:ARG:N	2.35	0.58
3:D:97:ARG:HG3	3:D:402:TRP:CE3	2.39	0.58
3:D:106:GLU:H	3:D:374:PHE:HD1	1.51	0.58
3:D:109:ARG:NH1	3:D:369:GLU:O	2.36	0.58
3:D:167:GLU:CD	3:D:233:ASP:HB2	2.24	0.58
3:D:231:TYR:CZ	3:H:112:PRO:HA	2.39	0.58
3:E:41:ARG:NH2	3:E:369:GLU:HG3	2.18	0.58
3:F:164:PRO:HB2	3:F:195:ILE:HD12	1.84	0.58
3:G:164:PRO:HB2	3:G:195:ILE:HD12	1.86	0.58
3:H:54:LYS:HD2	3:H:57:ASN:HB2	1.85	0.58
3:D:77:LEU:HD22	3:D:455:PHE:HZ	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:154:THR:HG23	3:D:252:ARG:O	2.04	0.57
3:D:374:PHE:HB2	3:D:376:PHE:CZ	2.38	0.57
3:H:168:HIS:CE1	3:H:191:ILE:HB	2.39	0.57
3:C:57:ASN:OD1	3:C:59:LYS:N	2.31	0.57
3:F:47:HIS:CG	3:F:48:PRO:HD2	2.39	0.57
1:A:92:CYS:O	1:A:103:TRP:HB2	2.02	0.57
2:B:54:ARG:HH22	3:D:431:HIS:CE1	2.22	0.57
3:C:220:VAL:HB	3:C:224:ILE:HD11	1.86	0.57
3:C:223:ASP:OD1	3:C:224:ILE:N	2.37	0.57
3:D:128:ASP:HA	3:D:261:PHE:CD1	2.39	0.57
3:H:387:VAL:O	3:H:391:ILE:HD12	2.05	0.57
3:C:167:GLU:CD	3:C:233:ASP:HB2	2.24	0.57
3:D:52:ILE:O	3:D:61:LEU:N	2.38	0.57
3:D:68:LEU:O	3:D:201:VAL:HG23	2.04	0.57
3:D:91:TYR:HB3	3:D:380:LYS:HZ1	1.69	0.57
3:D:103:VAL:HB	3:D:375:ILE:HG22	1.86	0.57
3:D:46:GLY:HA2	3:D:365:ARG:HD2	1.87	0.57
3:D:236:LYS:HA	3:D:239:SER:HB2	1.87	0.57
3:D:314:GLN:HG3	3:D:315:ARG:N	2.14	0.57
3:E:47:HIS:CG	3:E:48:PRO:HD2	2.39	0.57
3:F:90:PHE:CE1	3:F:91:TYR:HD2	2.22	0.57
3:G:109:ARG:NH2	3:G:338:ARG:HD2	2.20	0.57
3:H:71:ARG:HG3	3:H:370:TYR:OH	2.05	0.57
3:C:18:VAL:CG1	3:C:18:VAL:CG2	2.80	0.57
3:D:47:HIS:CE1	3:D:49:TYR:H	2.22	0.57
3:D:126:LEU:HB3	3:D:262:ASN:CB	2.34	0.57
3:D:371:ASP:OD2	3:D:372:LEU:N	2.38	0.57
3:D:465:GLY:O	3:D:468:PHE:N	2.38	0.57
3:H:335:ASP:OD2	3:H:337:THR:OG1	2.22	0.57
3:D:172:GLY:O	3:D:187:PRO:HG2	2.03	0.57
3:D:441:LEU:HG	3:D:444:TYR:CE2	2.40	0.57
3:D:45:VAL:HG12	3:D:365:ARG:HB3	1.87	0.57
3:D:70:TYR:CE2	3:D:200:MET:O	2.57	0.57
3:D:156:LEU:HG	3:D:334:VAL:HB	1.87	0.57
3:D:249:TYR:HE1	3:D:251:ARG:CG	2.18	0.57
3:E:407:GLN:N	3:E:408:PRO:HA	2.19	0.57
3:F:35:TYR:CD1	3:F:457:ALA:HA	2.40	0.57
3:G:105:VAL:HG13	3:G:374:PHE:CE1	2.40	0.57
3:C:17:PRO:C	3:C:17:PRO:HA	2.10	0.57
3:C:195:ILE:HA	3:C:230:LYS:NZ	2.20	0.57
3:D:96:GLN:OE1	3:D:380:LYS:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:122:LEU:HB3	3:D:144:ARG:HB3	1.86	0.57
3:D:158:LEU:HD12	3:D:332:THR:HG22	1.87	0.57
3:D:357:ASN:OD1	3:E:142:ASP:N	2.36	0.57
3:G:47:HIS:CG	3:G:48:PRO:HD2	2.40	0.57
3:D:106:GLU:O	3:D:373:GLN:N	2.33	0.57
3:D:109:ARG:HH11	3:D:110:GLY:N	2.02	0.57
3:G:40:SER:OG	3:G:41:ARG:N	2.38	0.57
3:G:335:ASP:OD2	3:G:337:THR:OG1	2.21	0.57
3:D:30:ARG:HA	3:D:379:CYS:SG	2.45	0.56
3:D:119:GLY:HA2	3:D:221:PRO:HG3	1.87	0.56
3:F:418:TYR:CB	3:F:419:ARG:HH11	2.15	0.56
3:H:404:PHE:CZ	3:H:409:PRO:HD3	2.39	0.56
1:A:63:VAL:HG11	1:A:67:PHE:CE2	2.40	0.56
2:B:21:MET:SD	2:B:102:THR:HG21	2.45	0.56
2:B:35:TRP:HB2	2:B:48:ILE:H	1.70	0.56
3:C:428:CYS:O	3:C:432:THR:HG23	2.06	0.56
3:D:162:LYS:CB	3:D:245:SER:HA	2.35	0.56
3:E:16:VAL:O	3:E:18:VAL:HG23	2.05	0.56
3:E:153:GLN:NE2	3:E:300:VAL:HG12	2.19	0.56
2:B:24:LYS:CE	2:B:70:ASP:HB2	2.35	0.56
2:B:85:VAL:HA	2:B:103:LYS:HA	1.86	0.56
3:C:164:PRO:HG2	3:C:195:ILE:HB	1.85	0.56
3:C:406:LEU:HD22	3:C:409:PRO:HA	1.86	0.56
3:D:47:HIS:O	3:D:65:VAL:N	2.38	0.56
3:D:70:TYR:HE2	3:D:230:LYS:HB2	1.71	0.56
3:D:266:ALA:HB3	3:H:360:PHE:O	2.06	0.56
3:E:83:PHE:CE1	3:F:14:PRO:HD3	2.40	0.56
3:F:71:ARG:O	3:F:332:THR:HG23	2.04	0.56
3:F:72:VAL:O	3:F:447:TRP:HB3	2.06	0.56
3:F:280:SER:N	3:F:283:THR:OG1	2.33	0.56
2:B:11:LEU:HD11	2:B:20:THR:O	2.05	0.56
3:C:312:TRP:NE1	3:C:471:GLN:NE2	2.50	0.56
3:D:56:ASN:OD1	3:D:57:ASN:N	2.39	0.56
3:D:109:ARG:HH12	3:D:369:GLU:HB3	1.70	0.56
3:D:117:ILE:HA	3:D:151:TYR:CE2	2.40	0.56
3:D:273:ASP:OD1	3:D:274:ASP:N	2.38	0.56
3:D:326:GLY:O	3:D:328:GLN:HB2	2.05	0.56
3:E:35:TYR:HD1	3:E:457:ALA:HA	1.69	0.56
3:C:153:GLN:HG3	3:C:336:THR:OG1	2.06	0.56
3:D:70:TYR:CZ	3:D:201:VAL:HA	2.40	0.56
3:D:155:GLN:HA	3:D:335:ASP:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:221:PRO:O	3:D:224:ILE:HG12	2.05	0.56
3:D:234:TYR:O	3:D:237:MET:N	2.38	0.56
3:G:167:GLU:CD	3:G:233:ASP:HB2	2.25	0.56
1:A:51:ILE:HD13	1:A:71:ARG:HG3	1.88	0.56
2:B:19:VAL:HG13	2:B:78:VAL:HG11	1.88	0.56
2:B:24:LYS:HE3	2:B:70:ASP:HB2	1.87	0.56
3:C:273:ASP:OD1	3:C:274:ASP:N	2.38	0.56
3:C:372:LEU:HB3	3:C:374:PHE:CZ	2.40	0.56
3:C:421:VAL:HA	3:C:424:GLN:NE2	2.21	0.56
3:D:123:LEU:H	3:D:145:GLU:N	2.04	0.56
3:C:43:LEU:CD2	3:H:421:VAL:HG13	2.36	0.56
3:C:324:CYS:SG	3:C:329:LEU:HD12	2.45	0.56
3:D:220:VAL:HB	3:D:224:ILE:CD1	2.36	0.56
3:D:305:GLN:NE2	3:D:305:GLN:HA	2.20	0.56
3:C:421:VAL:O	3:C:424:GLN:HG3	2.05	0.56
3:C:439:ASP:O	3:C:442:LYS:N	2.30	0.56
3:D:167:GLU:HA	3:D:192:ASN:HA	1.88	0.56
3:D:236:LYS:HA	3:D:239:SER:CB	2.35	0.56
3:G:392:HIS:O	3:G:396:SER:OG	2.24	0.56
3:H:349:SER:O	3:H:359:ASN:ND2	2.39	0.56
2:B:33:LEU:HG	2:B:35:TRP:NE1	2.21	0.56
2:B:50:TRP:O	2:B:52:SER:N	2.32	0.56
3:C:51:PRO:N	3:C:64:LYS:HB2	2.20	0.56
3:C:365:ARG:HH12	3:H:426:ILE:HG21	1.70	0.56
3:D:128:ASP:HA	3:D:261:PHE:HD1	1.71	0.56
3:D:259:HIS:HB2	3:D:294:THR:HB	1.88	0.56
3:E:233:ASP:N	3:E:237:MET:HE2	2.21	0.56
3:F:258:ARG:HG2	3:F:259:HIS:ND1	2.20	0.56
3:G:399:LEU:HD22	3:G:404:PHE:CE1	2.41	0.56
3:G:431:HIS:HB3	3:G:433:PRO:HD2	1.88	0.56
3:H:150:ASP:OD1	3:H:296:SER:HA	2.05	0.56
3:C:20:LYS:O	3:C:21:VAL:HG23	2.05	0.56
3:C:410:PRO:O	3:D:20:LYS:HB2	2.06	0.56
3:D:126:LEU:HB3	3:D:262:ASN:HB3	1.88	0.56
3:D:416:ASP:HB3	3:D:418:TYR:CE2	2.41	0.56
3:F:70:TYR:HD2	3:F:199:ASP:HB2	1.70	0.56
1:A:50:SER:HB2	1:A:58:HIS:HB2	1.88	0.55
2:B:37:GLN:HG3	2:B:84:ALA:CB	2.35	0.55
3:D:159:ILE:O	3:D:246:LEU:HB2	2.06	0.55
3:E:325:TRP:HZ3	3:E:402:TRP:CH2	2.24	0.55
3:H:85:PHE:HB3	3:H:86:PRO:HD2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:TRP:HZ2	1:A:50:SER:HG	1.55	0.55
3:C:40:SER:HB3	3:H:418:TYR:HB3	1.88	0.55
3:D:233:ASP:OD1	3:D:236:LYS:N	2.34	0.55
3:D:256:PHE:O	3:D:296:SER:N	2.32	0.55
3:D:263:ARG:HG2	3:D:292:PHE:HD2	1.72	0.55
3:E:47:HIS:HE1	3:E:49:TYR:HB2	1.71	0.55
3:E:465:GLY:O	3:E:468:PHE:N	2.39	0.55
1:A:17:SER:HB2	1:A:81:GLN:HE22	1.71	0.55
1:A:32:TYR:CD1	1:A:96:LEU:HA	2.42	0.55
3:C:167:GLU:HG2	3:C:231:TYR:O	2.06	0.55
3:C:418:TYR:HD2	3:D:239:SER:HB3	1.71	0.55
3:D:209:ASP:OD2	3:D:211:THR:HB	2.06	0.55
3:D:372:LEU:HD22	3:D:374:PHE:CZ	2.38	0.55
3:E:406:LEU:HB2	3:E:408:PRO:CA	2.37	0.55
2:B:2:ILE:HD12	2:B:90:GLN:NE2	2.22	0.55
3:D:42:LEU:HB2	3:D:370:TYR:N	2.21	0.55
3:D:309:LYS:HB2	3:D:311:TYR:CE1	2.41	0.55
3:F:47:HIS:CE1	3:F:49:TYR:HB2	2.40	0.55
3:F:169:TRP:HB2	3:F:208:MET:HB3	1.88	0.55
3:F:233:ASP:N	3:F:237:MET:HE2	2.21	0.55
3:H:47:HIS:CG	3:H:48:PRO:HD2	2.41	0.55
1:A:60:PRO:HD2	1:A:63:VAL:HG22	1.89	0.55
3:D:34:TYR:CE1	3:D:377:GLN:HG3	2.42	0.55
3:D:200:MET:CG	3:D:227:SER:HB2	2.36	0.55
3:D:214:GLN:HG2	3:H:344:LEU:HA	1.89	0.55
3:E:71:ARG:O	3:E:332:THR:HG23	2.06	0.55
3:E:408:PRO:HB2	3:E:409:PRO:CD	2.37	0.55
3:F:168:HIS:CE1	3:F:191:ILE:HB	2.40	0.55
3:G:120:HIS:CD2	3:G:222:LEU:HD12	2.42	0.55
3:G:169:TRP:HB2	3:G:208:MET:HB3	1.88	0.55
1:A:59:TYR:CD2	1:A:64:LYS:HA	2.42	0.55
3:C:120:HIS:ND1	3:C:122:LEU:O	2.40	0.55
3:D:277:ILE:HG22	3:D:278:LYS:H	1.72	0.55
3:F:300:VAL:HG22	3:G:255:MET:O	2.06	0.55
3:G:48:PRO:HA	3:G:66:SER:HB2	1.89	0.55
3:G:201:VAL:HG12	3:G:202:ASP:O	2.06	0.55
3:H:244:ASP:OD1	3:H:320:ASN:HB2	2.07	0.55
3:C:97:ARG:HH22	3:C:404:PHE:H	1.52	0.55
3:C:109:ARG:HB3	3:C:338:ARG:CZ	2.37	0.55
3:D:165:ILE:HA	3:D:194:VAL:HA	1.87	0.55
3:D:464:LEU:O	3:D:466:ARG:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:54:LYS:HD2	3:F:57:ASN:HB2	1.88	0.55
3:F:83:PHE:HD1	3:G:13:LEU:CD1	2.16	0.55
3:H:169:TRP:HB2	3:H:208:MET:HB3	1.88	0.55
3:C:22:VAL:O	3:C:319:HIS:HB3	2.07	0.55
3:D:355:TYR:CD2	3:E:142:ASP:HB2	2.42	0.55
3:E:50:PHE:HA	3:E:64:LYS:HD2	1.89	0.55
3:E:97:ARG:HH21	3:E:404:PHE:N	2.05	0.55
3:E:120:HIS:HB2	3:E:221:PRO:HA	1.87	0.55
1:A:100(E):ASP:HB3	2:B:49:TYR:CE2	2.42	0.55
3:D:235:ILE:O	3:D:239:SER:N	2.39	0.55
3:D:299:MET:HG2	3:D:300:VAL:H	1.71	0.55
3:E:170:GLY:O	3:E:189:GLU:N	2.37	0.55
1:A:17:SER:HB2	1:A:81:GLN:NE2	2.22	0.55
3:D:50:PHE:C	3:D:64:LYS:HB2	2.28	0.55
3:D:140:GLY:O	3:D:143:ASN:ND2	2.40	0.55
3:D:463:PRO:HA	3:D:466:ARG:HH12	1.72	0.55
3:E:14:PRO:HG2	3:E:15:PRO:HD2	1.89	0.55
3:E:450:ASN:HD21	3:E:452:LYS:HD2	1.71	0.55
3:D:159:ILE:N	3:D:248:PHE:O	2.29	0.54
3:E:48:PRO:HA	3:E:66:SER:HB2	1.89	0.54
3:E:450:ASN:OD1	3:E:452:LYS:HG3	2.06	0.54
3:F:387:VAL:O	3:F:391:ILE:HD12	2.07	0.54
3:H:85:PHE:CZ	3:H:378:LEU:HD21	2.42	0.54
3:C:109:ARG:HH21	3:C:338:ARG:HD2	1.71	0.54
3:C:168:HIS:CE1	3:C:191:ILE:HB	2.42	0.54
3:C:171:LYS:HB2	3:C:213:LEU:HD11	1.88	0.54
3:D:48:PRO:HG3	3:D:364:LEU:HD13	1.90	0.54
3:D:233:ASP:OD1	3:D:235:ILE:N	2.40	0.54
3:D:395:ASN:OD1	3:D:397:THR:N	2.35	0.54
3:E:54:LYS:HD2	3:E:57:ASN:HB2	1.89	0.54
3:E:146:CYS:HG	3:F:291:TYR:HH	1.55	0.54
3:C:384:THR:O	3:C:387:VAL:HB	2.07	0.54
3:C:408:PRO:HD2	3:C:412:GLY:H	1.73	0.54
3:D:142:ASP:OD2	3:D:144:ARG:NH2	2.38	0.54
3:D:450:ASN:OD1	3:D:452:LYS:HG3	2.07	0.54
3:E:35:TYR:CD1	3:E:457:ALA:HA	2.43	0.54
3:E:85:PHE:HB2	3:E:88:THR:HG22	1.88	0.54
3:E:407:GLN:CB	3:E:410:PRO:HD2	2.38	0.54
3:F:70:TYR:HD1	3:F:334:VAL:HG21	1.73	0.54
3:G:115:VAL:HG12	3:G:116:GLY:O	2.06	0.54
3:H:51:PRO:CA	3:H:64:LYS:HB2	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:39:LYS:NZ	2:B:81:GLU:HB3	2.22	0.54
2:B:82:ASP:O	2:B:86:TYR:OH	2.23	0.54
3:D:23:SER:HB3	3:D:26:GLU:OE2	2.08	0.54
3:D:36:HIS:CE1	3:D:37:ALA:C	2.80	0.54
3:D:105:VAL:HA	3:D:374:PHE:CD1	2.41	0.54
3:D:120:HIS:CE1	3:D:122:LEU:H	2.25	0.54
3:D:152:LYS:HG2	3:D:203:THR:HA	1.90	0.54
3:D:280:SER:O	3:D:283:THR:OG1	2.17	0.54
3:F:78:PRO:HD2	3:F:455:PHE:CZ	2.43	0.54
3:G:233:ASP:N	3:G:237:MET:HE2	2.22	0.54
3:H:233:ASP:N	3:H:237:MET:HE2	2.22	0.54
3:C:248:PHE:CG	3:C:249:TYR:N	2.76	0.54
3:C:365:ARG:NH1	3:H:426:ILE:HG21	2.23	0.54
3:D:65:VAL:HA	3:D:69:GLN:HE22	1.72	0.54
3:D:161:CYS:SG	3:D:244:ASP:HB3	2.48	0.54
3:D:194:VAL:O	3:D:230:LYS:NZ	2.41	0.54
3:D:223:ASP:O	3:D:226:THR:OG1	2.14	0.54
3:E:240:GLU:CG	3:E:241:PRO:HD2	2.38	0.54
3:E:300:VAL:HG22	3:F:255:MET:O	2.06	0.54
3:G:72:VAL:O	3:G:447:TRP:HB3	2.08	0.54
3:G:384:THR:H	3:G:387:VAL:HB	1.73	0.54
3:C:17:PRO:C	3:C:17:PRO:CB	2.71	0.54
3:D:76:HIS:HB2	3:D:450:ASN:CA	2.24	0.54
3:D:147:ILE:HG12	3:E:129:THR:O	2.07	0.54
3:C:123:LEU:N	3:C:145:GLU:O	2.40	0.54
3:D:36:HIS:CG	3:D:37:ALA:N	2.75	0.54
3:D:378:LEU:HG	3:D:379:CYS:N	2.22	0.54
3:E:211:THR:OG1	3:E:226:THR:O	2.26	0.54
3:E:403:ASN:O	3:E:405:GLY:N	2.41	0.54
3:H:384:THR:H	3:H:387:VAL:HB	1.73	0.54
1:A:24:ALA:N	1:A:76:ASN:O	2.30	0.54
3:C:421:VAL:O	3:C:423:SER:N	2.41	0.54
3:D:111:GLN:HB2	3:D:338:ARG:CD	2.32	0.54
3:F:30:ARG:HD3	3:F:379:CYS:SG	2.47	0.54
3:H:15:PRO:HB3	3:H:17:PRO:HD3	1.90	0.54
3:H:24:THR:HG21	3:H:320:ASN:HA	1.89	0.54
3:H:47:HIS:CE1	3:H:49:TYR:HB2	2.41	0.54
3:H:258:ARG:HB2	3:H:296:SER:HB2	1.89	0.54
2:B:36:TYR:O	2:B:86:TYR:HA	2.08	0.54
3:D:459:LEU:O	3:D:466:ARG:CZ	2.56	0.54
3:E:92:ASN:OD1	3:E:94:ASP:N	2.31	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:150:ASP:OD1	3:E:296:SER:HA	2.08	0.54
3:F:97:ARG:NH2	3:F:404:PHE:H	2.05	0.54
2:B:19:VAL:HG13	2:B:78:VAL:HG21	1.90	0.54
3:D:344:LEU:HD11	3:D:363:TYR:CD2	2.43	0.54
3:D:399:LEU:HD23	3:D:402:TRP:CB	2.32	0.54
3:E:167:GLU:CD	3:E:233:ASP:HB2	2.28	0.54
3:F:244:ASP:OD1	3:F:320:ASN:HB2	2.08	0.54
3:G:360:PHE:CE2	3:H:216:ASN:HA	2.42	0.54
1:A:92:CYS:HB3	1:A:104:GLY:HA3	1.89	0.53
3:D:79:ASP:OD2	3:D:81:ASN:HB2	2.09	0.53
3:G:30:ARG:HD3	3:G:379:CYS:SG	2.49	0.53
3:H:314:GLN:HG3	3:H:315:ARG:N	2.22	0.53
2:B:30(A):TYR:HH	2:B:92:TYR:HH	1.56	0.53
2:B:38:GLN:HB2	2:B:44:PRO:HB3	1.91	0.53
3:C:62:VAL:HG22	3:H:426:ILE:HG12	1.89	0.53
3:D:76:HIS:CE1	3:D:449:VAL:H	2.26	0.53
3:D:273:ASP:HA	3:D:276:TYR:CE2	2.43	0.53
3:D:312:TRP:CH2	3:D:468:PHE:HB2	2.43	0.53
3:D:389:THR:HG22	3:D:393:SER:OG	2.07	0.53
3:H:258:ARG:NH2	3:H:296:SER:OG	2.41	0.53
1:A:21:SER:C	1:A:36:TRP:HH2	2.12	0.53
3:D:72:VAL:HG13	3:D:332:THR:OG1	2.08	0.53
3:D:187:PRO:CA	3:D:188:LEU:HD12	2.37	0.53
3:E:61:LEU:HG	3:E:62:VAL:HG23	1.89	0.53
3:F:51:PRO:CA	3:F:64:LYS:HB2	2.39	0.53
3:G:298:SER:OG	3:G:299:MET:N	2.40	0.53
1:A:59:TYR:HD1	1:A:63:VAL:HG23	1.74	0.53
3:C:406:LEU:HD22	3:C:409:PRO:CA	2.37	0.53
3:D:152:LYS:HD2	3:D:202:ASP:O	2.09	0.53
3:D:159:ILE:HG22	3:D:247:PHE:CE1	2.43	0.53
3:H:120:HIS:CD2	3:H:222:LEU:HD12	2.44	0.53
1:A:29:PHE:HD2	1:A:73:ASN:HA	1.73	0.53
3:C:273:ASP:HA	3:C:276:TYR:CE2	2.43	0.53
3:E:298:SER:OG	3:E:299:MET:N	2.41	0.53
3:G:57:ASN:CG	3:G:59:LYS:H	2.12	0.53
1:A:39:GLN:N	1:A:88:ALA:HB1	2.20	0.53
3:C:90:PHE:CE1	3:C:91:TYR:CD2	2.96	0.53
3:D:46:GLY:HA3	3:D:65:VAL:HB	1.89	0.53
3:D:231:TYR:CD1	3:H:112:PRO:HB3	2.43	0.53
3:E:406:LEU:HB2	3:E:408:PRO:HA	1.91	0.53
3:E:407:GLN:HB2	3:E:408:PRO:C	2.28	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:170:GLY:O	3:F:189:GLU:N	2.39	0.53
3:G:36:HIS:HD2	3:G:375:ILE:HD13	1.73	0.53
3:H:383:LEU:HD23	3:H:387:VAL:HG11	1.91	0.53
2:B:79:LYS:O	2:B:82:ASP:HB2	2.09	0.53
3:C:20:LYS:HB2	3:C:21:VAL:O	2.08	0.53
3:C:273:ASP:O	3:C:276:TYR:N	2.30	0.53
3:C:418:TYR:CD2	3:D:239:SER:HB3	2.44	0.53
3:C:420:PHE:HA	3:H:41:ARG:CD	2.36	0.53
3:D:157:CYS:SG	3:D:158:LEU:N	2.81	0.53
3:D:431:HIS:O	3:D:433:PRO:HD2	2.08	0.53
3:F:47:HIS:CE1	3:F:49:TYR:H	2.26	0.53
3:F:235:ILE:O	3:F:239:SER:N	2.39	0.53
3:G:70:TYR:HD2	3:G:199:ASP:HB2	1.73	0.53
3:C:171:LYS:HG3	3:C:186:PRO:HB2	1.91	0.53
3:D:153:GLN:HE22	3:D:299:MET:C	2.11	0.53
3:D:440:PRO:HG2	3:D:441:LEU:HD13	1.90	0.53
3:F:50:PHE:CE2	3:G:271:VAL:HG22	2.43	0.53
3:G:47:HIS:HE1	3:G:49:TYR:HB2	1.74	0.53
3:G:71:ARG:HG3	3:G:370:TYR:OH	2.08	0.53
3:G:146:CYS:SG	3:H:291:TYR:OH	2.65	0.53
3:H:210:PHE:O	3:H:214:GLN:N	2.32	0.53
3:C:441:LEU:O	3:C:444:TYR:N	2.42	0.53
3:D:66:SER:HB3	3:D:69:GLN:HG3	1.90	0.53
3:D:309:LYS:HB3	3:D:310:PRO:HD2	1.91	0.53
3:E:57:ASN:CG	3:E:59:LYS:H	2.12	0.53
3:F:40:SER:OG	3:F:41:ARG:N	2.42	0.53
3:F:83:PHE:CD1	3:G:13:LEU:HD12	2.36	0.53
3:G:150:ASP:OD1	3:G:296:SER:HA	2.09	0.53
3:C:437:LYS:HG2	3:C:438:GLU:H	1.74	0.53
3:D:36:HIS:CE1	3:D:373:GLN:HB3	2.44	0.53
3:C:431:HIS:HA	3:C:433:PRO:HD2	1.90	0.52
3:D:62:VAL:HG11	3:D:365:ARG:HE	1.74	0.52
3:D:96:GLN:HG2	3:D:382:THR:CA	2.37	0.52
3:D:469:LEU:O	3:D:472:ALA:HB3	2.08	0.52
3:E:70:TYR:HD1	3:E:334:VAL:HG21	1.74	0.52
3:F:35:TYR:HD1	3:F:457:ALA:HA	1.74	0.52
3:F:320:ASN:ND2	3:F:323:ILE:O	2.30	0.52
3:F:436:PRO:O	3:F:437:LYS:HB2	2.10	0.52
3:H:298:SER:OG	3:H:299:MET:N	2.41	0.52
3:C:259:HIS:H	3:C:294:THR:HB	1.73	0.52
3:F:97:ARG:HE	3:F:402:TRP:HB3	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:335:ASP:OD1	3:F:337:THR:HG23	2.10	0.52
3:G:299:MET:HA	3:H:256:PHE:HB3	1.90	0.52
1:A:43:LYS:HZ3	2:B:103:LYS:HE2	1.74	0.52
2:B:35:TRP:CZ3	2:B:88:CYS:HB3	2.44	0.52
3:C:70:TYR:N	3:C:199:ASP:O	2.28	0.52
3:D:108:GLY:H	3:D:371:ASP:C	2.11	0.52
3:D:470:LEU:C	3:D:473:GLY:H	2.13	0.52
3:F:258:ARG:HB2	3:F:296:SER:HB2	1.90	0.52
3:G:52:ILE:HB	3:G:62:VAL:H	1.74	0.52
3:H:258:ARG:HG2	3:H:259:HIS:CE1	2.45	0.52
3:C:406:LEU:CG	3:C:411:GLY:H	2.21	0.52
3:D:79:ASP:HA	3:D:327:ASN:ND2	2.25	0.52
3:D:187:PRO:C	3:D:188:LEU:HD12	2.30	0.52
3:D:234:TYR:OH	3:D:251:ARG:HD3	2.09	0.52
3:D:439:ASP:HB3	3:D:442:LYS:HB2	1.92	0.52
3:E:244:ASP:OD1	3:E:320:ASN:HB2	2.10	0.52
2:B:35:TRP:O	2:B:46:LEU:HD12	2.09	0.52
3:C:97:ARG:NH2	3:C:404:PHE:N	2.56	0.52
3:D:120:HIS:ND1	3:D:122:LEU:N	2.57	0.52
3:D:468:PHE:O	3:D:471:GLN:N	2.43	0.52
3:E:408:PRO:HB2	3:E:409:PRO:HD2	1.92	0.52
3:F:18:VAL:HG12	3:F:19:SER:H	1.74	0.52
3:F:201:VAL:HG12	3:F:202:ASP:O	2.10	0.52
3:F:256:PHE:HE2	3:F:298:SER:HB2	1.75	0.52
1:A:69:ILE:HG13	1:A:79:TYR:O	2.10	0.52
3:C:201:VAL:HG12	3:C:202:ASP:O	2.10	0.52
3:D:129:THR:HG21	3:H:148:SER:OG	2.10	0.52
3:D:387:VAL:O	3:D:389:THR:N	2.42	0.52
3:E:52:ILE:HB	3:E:62:VAL:HB	1.91	0.52
3:F:18:VAL:CG1	3:F:19:SER:N	2.73	0.52
3:G:450:ASN:OD1	3:G:452:LYS:HG3	2.10	0.52
1:A:60:PRO:HB3	2:B:95:PRO:HB3	1.92	0.52
1:A:94:ARG:HH21	1:A:101:ASP:CB	2.21	0.52
1:A:100:TYR:O	1:A:100(B):GLU:HG3	2.09	0.52
2:B:54:ARG:CZ	2:B:60:ASP:HA	2.39	0.52
3:D:123:LEU:O	3:D:144:ARG:HA	2.09	0.52
3:D:202:ASP:CB	3:D:204:GLY:H	2.20	0.52
3:F:324:CYS:SG	3:F:329:LEU:HD12	2.50	0.52
3:G:273:ASP:HA	3:G:276:TYR:CE2	2.45	0.52
3:G:384:THR:OG1	3:G:387:VAL:HG23	2.10	0.52
3:H:18:VAL:HG12	3:H:19:SER:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:235:ILE:O	3:H:239:SER:N	2.39	0.52
3:D:23:SER:O	3:D:26:GLU:HG2	2.10	0.52
3:D:104:GLY:N	3:D:375:ILE:O	2.28	0.52
3:E:30:ARG:HD3	3:E:379:CYS:SG	2.50	0.52
3:E:34:TYR:HE1	3:E:377:GLN:HG3	1.74	0.52
3:E:51:PRO:CA	3:E:64:LYS:HB2	2.40	0.52
3:G:320:ASN:ND2	3:G:323:ILE:O	2.30	0.52
3:C:387:VAL:O	3:C:391:ILE:HD12	2.09	0.52
3:D:38:GLY:HA2	3:D:372:LEU:O	2.10	0.52
3:D:52:ILE:HB	3:D:62:VAL:H	1.75	0.52
3:D:73:PHE:O	3:D:331:VAL:N	2.38	0.52
3:F:48:PRO:HA	3:F:66:SER:HB2	1.92	0.52
3:G:70:TYR:HE1	3:G:201:VAL:HG22	1.75	0.52
3:H:164:PRO:HG2	3:H:195:ILE:HB	1.92	0.52
3:H:201:VAL:HG12	3:H:202:ASP:O	2.09	0.52
3:H:324:CYS:SG	3:H:329:LEU:HD12	2.50	0.52
1:A:100(A):ASP:HB3	2:B:50:TRP:CD2	2.44	0.52
3:D:72:VAL:HG22	3:D:332:THR:CG2	2.40	0.52
3:D:123:LEU:HG	3:D:124:ASN:N	2.24	0.52
3:D:165:ILE:HA	3:D:195:ILE:H	1.75	0.52
3:D:289:SER:HA	3:D:291:TYR:CE2	2.45	0.52
3:F:97:ARG:NH2	3:F:404:PHE:N	2.58	0.52
3:H:465:GLY:O	3:H:468:PHE:N	2.43	0.52
2:B:30(E):GLN:O	2:B:30(F):LYS:HD2	2.10	0.51
3:C:101:ALA:N	3:C:377:GLN:O	2.40	0.51
3:C:312:TRP:HH2	3:C:468:PHE:CD1	2.22	0.51
3:D:113:LEU:N	3:D:113:LEU:HD12	2.24	0.51
3:D:122:LEU:HD22	3:D:144:ARG:HB2	1.91	0.51
3:D:168:HIS:HB2	3:D:207:ALA:O	2.10	0.51
3:D:249:TYR:CE1	3:D:251:ARG:HG2	2.45	0.51
3:D:255:MET:O	3:H:300:VAL:HG22	2.10	0.51
3:D:346:ALA:O	3:D:360:PHE:HA	2.10	0.51
3:D:361:LYS:NZ	3:E:267:VAL:O	2.42	0.51
3:E:120:HIS:CE1	3:E:122:LEU:H	2.28	0.51
3:H:245:SER:OG	3:H:246:LEU:N	2.44	0.51
3:H:466:ARG:O	3:H:469:LEU:HB2	2.10	0.51
3:G:120:HIS:CE1	3:G:122:LEU:H	2.27	0.51
3:G:314:GLN:HG3	3:G:315:ARG:N	2.24	0.51
3:H:15:PRO:CB	3:H:16:VAL:HA	2.40	0.51
3:H:312:TRP:HH2	3:H:468:PHE:CD1	2.24	0.51
2:B:2:ILE:HG12	2:B:26:SER:OG	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:47:HIS:CD2	3:D:48:PRO:HD2	2.45	0.51
3:D:273:ASP:HA	3:D:276:TYR:CE1	2.46	0.51
3:D:382:THR:HG22	3:D:383:LEU:N	2.20	0.51
3:E:201:VAL:HG12	3:E:202:ASP:O	2.10	0.51
3:E:391:ILE:O	3:E:394:MET:N	2.43	0.51
3:H:90:PHE:CE1	3:H:91:TYR:HD2	2.28	0.51
2:B:35:TRP:HB2	2:B:47:LEU:HB2	1.92	0.51
3:D:69:GLN:HB2	3:D:71:ARG:CZ	2.41	0.51
3:E:245:SER:OG	3:E:246:LEU:N	2.43	0.51
3:F:196:GLN:HE21	3:F:444:TYR:HD1	1.56	0.51
3:H:167:GLU:CD	3:H:233:ASP:HB2	2.31	0.51
3:H:475:LYS:O	3:H:477:LYS:HG3	2.10	0.51
1:A:63:VAL:HA	1:A:66:ARG:HB2	1.91	0.51
3:C:312:TRP:CH2	3:C:468:PHE:CD1	2.94	0.51
3:D:460:ASP:HB3	3:D:461:GLN:OE1	2.11	0.51
3:D:466:ARG:HA	3:D:469:LEU:CB	2.40	0.51
3:G:85:PHE:HB3	3:G:86:PRO:HD2	1.93	0.51
3:H:116:GLY:H	3:H:339:SER:HG	1.53	0.51
3:H:450:ASN:OD1	3:H:452:LYS:HG3	2.11	0.51
3:D:106:GLU:OE1	3:D:309:LYS:O	2.29	0.51
3:D:195:ILE:HA	3:D:230:LYS:HZ3	1.75	0.51
3:E:403:ASN:O	3:E:404:PHE:C	2.49	0.51
3:G:34:TYR:HE1	3:G:377:GLN:HG3	1.74	0.51
3:G:399:LEU:HD22	3:G:404:PHE:CZ	2.45	0.51
2:B:55:GLU:HG3	2:B:56:SER:O	2.11	0.51
3:C:87:ASP:OD1	3:H:89:SER:HB3	2.11	0.51
3:C:406:LEU:HD23	3:C:406:LEU:C	2.31	0.51
3:D:54:LYS:HB3	3:D:57:ASN:CB	2.36	0.51
3:D:182:PRO:CB	3:H:348:ILE:HG13	2.37	0.51
3:D:200:MET:HG3	3:D:227:SER:HB2	1.92	0.51
3:D:447:TRP:CD1	3:D:448:GLU:N	2.78	0.51
3:D:461:GLN:HE21	3:E:20:LYS:HG2	1.75	0.51
3:G:16:VAL:HB	3:G:17:PRO:HD3	1.77	0.51
3:G:97:ARG:NH2	3:G:404:PHE:N	2.59	0.51
2:B:6:GLN:HB2	2:B:101:GLY:N	2.26	0.51
3:C:235:ILE:O	3:C:239:SER:N	2.42	0.51
3:C:242:TYR:HE1	3:C:390:TYR:HH	1.59	0.51
3:C:254:GLN:NE2	3:C:298:SER:HB3	2.26	0.51
3:D:32:ASN:N	3:D:33:ILE:HD12	2.26	0.51
3:D:46:GLY:N	3:D:366:HIS:O	2.43	0.51
3:D:222:LEU:H	3:D:222:LEU:CD1	2.23	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:301:THR:CG2	3:G:304:ALA:H	2.23	0.51
3:H:161:CYS:SG	3:H:244:ASP:HB3	2.50	0.51
2:B:47:LEU:HD11	2:B:86:TYR:CD1	2.46	0.51
3:C:197:ASP:HB3	3:C:446:PHE:HA	1.92	0.51
3:C:249:TYR:HE1	3:C:251:ARG:NH1	2.08	0.51
3:D:144:ARG:HH21	3:E:279:GLY:HA2	1.75	0.51
3:D:466:ARG:HA	3:D:469:LEU:CG	2.41	0.51
3:F:413:THR:O	3:F:414:LEU:HB2	2.11	0.51
3:G:83:PHE:HZ	3:H:13:LEU:HB3	1.76	0.51
1:A:89:MET:SD	1:A:91:TYR:OH	2.69	0.51
2:B:54:ARG:NH2	2:B:60:ASP:OD1	2.43	0.51
3:D:168:HIS:CE1	3:D:191:ILE:HD12	2.46	0.51
3:D:258:ARG:HB3	3:D:294:THR:HG22	1.93	0.51
3:F:19:SER:O	3:F:20:LYS:HD3	2.08	0.51
3:F:349:SER:O	3:F:359:ASN:ND2	2.41	0.51
3:D:466:ARG:HA	3:D:469:LEU:HG	1.93	0.50
3:E:40:SER:OG	3:E:41:ARG:N	2.39	0.50
3:F:432:THR:HA	3:F:434:PRO:HD2	1.92	0.50
3:G:90:PHE:CE1	3:G:91:TYR:HD2	2.29	0.50
3:G:240:GLU:HG3	3:G:241:PRO:HD2	1.93	0.50
3:G:320:ASN:OD1	3:G:323:ILE:N	2.22	0.50
3:H:263:ARG:HB2	3:H:290:ASN:HD22	1.77	0.50
3:H:273:ASP:O	3:H:276:TYR:N	2.38	0.50
2:B:50:TRP:CZ3	2:B:52:SER:HB2	2.45	0.50
2:B:61:ARG:O	2:B:75:ILE:HG12	2.12	0.50
3:C:36:HIS:HD2	3:C:375:ILE:HD13	1.75	0.50
3:C:43:LEU:HD12	3:C:368:GLU:O	2.11	0.50
3:D:141:VAL:HA	3:H:357:ASN:OD1	2.11	0.50
3:D:246:LEU:HD13	3:D:248:PHE:N	2.27	0.50
3:F:41:ARG:HH21	3:F:369:GLU:HG3	1.76	0.50
3:F:384:THR:OG1	3:F:387:VAL:HG23	2.11	0.50
3:H:70:TYR:HE1	3:H:201:VAL:HG22	1.76	0.50
1:A:59:TYR:CD2	1:A:64:LYS:HD2	2.47	0.50
1:A:60:PRO:HG2	1:A:62:SER:OG	2.11	0.50
3:D:349:SER:H	3:D:359:ASN:HD21	1.57	0.50
3:D:384:THR:H	3:D:387:VAL:CB	2.22	0.50
3:E:47:HIS:CE1	3:E:49:TYR:HB2	2.46	0.50
3:E:90:PHE:CE1	3:E:91:TYR:HD2	2.29	0.50
3:G:81:ASN:ND2	3:G:98:LEU:O	2.45	0.50
3:G:324:CYS:SG	3:G:329:LEU:HD12	2.51	0.50
3:D:45:VAL:HG12	3:D:46:GLY:N	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:51:PRO:N	3:E:64:LYS:HB2	2.27	0.50
3:E:57:ASN:OD1	3:E:59:LYS:N	2.41	0.50
3:E:320:ASN:ND2	3:E:323:ILE:O	2.30	0.50
3:F:70:TYR:HE1	3:F:201:VAL:HG22	1.76	0.50
3:G:254:GLN:OE1	3:G:298:SER:HB3	2.10	0.50
3:H:53:LYS:HA	3:H:61:LEU:N	2.23	0.50
1:A:36:TRP:CZ2	1:A:78:LEU:HG	2.46	0.50
3:D:97:ARG:HH21	3:D:403:ASN:H	1.59	0.50
3:D:114:GLY:N	3:D:337:THR:O	2.41	0.50
3:E:235:ILE:O	3:E:239:SER:N	2.37	0.50
3:F:465:GLY:O	3:F:468:PHE:HB3	2.12	0.50
3:H:274:ASP:OD1	3:H:275:LEU:HG	2.12	0.50
3:H:421:VAL:O	3:H:422:THR:HG23	2.12	0.50
3:C:85:PHE:CD2	3:C:88:THR:HG22	2.47	0.50
3:D:70:TYR:N	3:D:199:ASP:O	2.44	0.50
3:D:150:ASP:CG	3:D:297:GLY:H	2.14	0.50
3:D:344:LEU:O	3:D:362:GLU:HA	2.12	0.50
3:D:384:THR:H	3:D:387:VAL:CG2	2.25	0.50
3:E:47:HIS:CE1	3:E:49:TYR:H	2.30	0.50
3:E:159:ILE:HG22	3:E:247:PHE:CZ	2.46	0.50
3:G:16:VAL:CG2	3:G:17:PRO:N	2.59	0.50
3:H:48:PRO:HA	3:H:66:SER:HB2	1.93	0.50
3:D:24:THR:HA	3:D:27:TYR:OH	2.12	0.50
3:D:90:PHE:HD1	3:D:380:LYS:HZ1	1.58	0.50
3:D:90:PHE:CE1	3:D:91:TYR:CD2	3.00	0.50
3:D:216:ASN:CB	3:D:219:GLU:HG2	2.40	0.50
3:D:320:ASN:CG	3:D:323:ILE:HB	2.32	0.50
3:D:374:PHE:CB	3:D:376:PHE:CZ	2.94	0.50
3:D:384:THR:O	3:D:388:MET:HG3	2.12	0.50
3:C:169:TRP:HB2	3:C:208:MET:CB	2.41	0.50
3:D:120:HIS:O	3:D:146:CYS:HA	2.12	0.50
3:D:271:VAL:HG13	3:D:275:LEU:HD12	1.94	0.50
3:D:386:ASP:N	3:D:386:ASP:OD1	2.36	0.50
3:E:78:PRO:HD2	3:E:455:PHE:CZ	2.47	0.50
3:F:120:HIS:CE1	3:F:122:LEU:H	2.30	0.50
3:F:146:CYS:SG	3:G:291:TYR:OH	2.70	0.50
3:F:466:ARG:O	3:F:469:LEU:HB2	2.11	0.50
3:G:219:GLU:OE1	3:G:263:ARG:CZ	2.58	0.50
3:H:301:THR:CG2	3:H:304:ALA:H	2.25	0.50
1:A:94:ARG:HG2	1:A:102:TYR:O	2.12	0.50
3:C:57:ASN:CG	3:C:59:LYS:H	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:466:ARG:O	3:C:469:LEU:HB2	2.11	0.50
3:D:127:ASP:H	3:D:262:ASN:HB2	1.77	0.50
3:D:287:ALA:CB	3:H:146:CYS:HB2	2.39	0.50
3:F:57:ASN:CG	3:F:59:LYS:H	2.15	0.50
1:A:39:GLN:HB2	1:A:91:TYR:HE2	1.75	0.49
3:C:16:VAL:N	3:C:17:PRO:CD	2.75	0.49
3:D:157:CYS:HA	3:D:333:VAL:HA	1.92	0.49
3:D:159:ILE:HD12	3:D:248:PHE:CE2	2.48	0.49
3:E:406:LEU:CB	3:E:408:PRO:HA	2.41	0.49
1:A:22:CYS:O	1:A:77:ILE:HA	2.12	0.49
3:D:299:MET:CA	3:E:256:PHE:HB3	2.39	0.49
3:D:466:ARG:O	3:D:470:LEU:N	2.42	0.49
3:F:240:GLU:HG3	3:F:241:PRO:HD2	1.93	0.49
1:A:52:SER:OG	1:A:55:GLY:N	2.45	0.49
3:D:389:THR:O	3:D:392:HIS:N	2.46	0.49
3:E:47:HIS:CD2	3:E:48:PRO:HD2	2.47	0.49
3:F:360:PHE:CE2	3:G:216:ASN:HA	2.48	0.49
3:G:78:PRO:HD2	3:G:455:PHE:CZ	2.47	0.49
3:G:406:LEU:CA	3:G:408:PRO:HD3	2.40	0.49
3:H:36:HIS:HD2	3:H:375:ILE:HD13	1.77	0.49
3:H:61:LEU:HG	3:H:62:VAL:HG23	1.94	0.49
3:H:70:TYR:CE1	3:H:201:VAL:HG22	2.47	0.49
3:H:78:PRO:HD2	3:H:455:PHE:CZ	2.48	0.49
3:H:349:SER:N	3:H:359:ASN:OD1	2.44	0.49
3:D:109:ARG:NH1	3:D:110:GLY:N	2.59	0.49
3:D:167:GLU:HB2	3:D:192:ASN:OD1	2.13	0.49
3:D:234:TYR:CZ	3:D:251:ARG:HD3	2.47	0.49
3:D:357:ASN:CG	3:E:142:ASP:H	2.15	0.49
3:E:97:ARG:HH21	3:E:403:ASN:C	2.15	0.49
3:E:196:GLN:HE21	3:E:444:TYR:HD1	1.61	0.49
3:E:258:ARG:HG2	3:E:259:HIS:CE1	2.47	0.49
3:F:450:ASN:HD21	3:F:452:LYS:HD2	1.76	0.49
3:H:240:GLU:HG3	3:H:241:PRO:HD2	1.92	0.49
3:D:142:ASP:HA	3:H:355:TYR:CE2	2.48	0.49
3:D:147:ILE:HG23	3:E:129:THR:O	2.11	0.49
3:D:236:LYS:HA	3:D:239:SER:OG	2.13	0.49
3:E:18:VAL:CB	3:E:20:LYS:HG3	2.43	0.49
3:F:211:THR:OG1	3:F:226:THR:O	2.28	0.49
3:H:111:GLN:HB2	3:H:338:ARG:HD3	1.93	0.49
3:H:170:GLY:O	3:H:189:GLU:N	2.45	0.49
3:H:314:GLN:HG3	3:H:315:ARG:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:43:LYS:NZ	2:B:103:LYS:HE2	2.27	0.49
3:D:45:VAL:HG22	3:E:169:TRP:HH2	1.77	0.49
3:E:335:ASP:OD1	3:E:337:THR:HG23	2.12	0.49
3:F:147:ILE:HG23	3:G:129:THR:O	2.13	0.49
3:F:167:GLU:CD	3:F:233:ASP:HB2	2.32	0.49
3:G:300:VAL:HG22	3:H:255:MET:O	2.12	0.49
3:G:312:TRP:CZ3	3:G:468:PHE:HD1	2.30	0.49
3:H:51:PRO:N	3:H:64:LYS:HB2	2.28	0.49
1:A:100(A):ASP:O	2:B:50:TRP:NE1	2.46	0.49
2:B:18:LYS:HE2	2:B:75:ILE:O	2.13	0.49
3:C:273:ASP:HA	3:C:276:TYR:CZ	2.47	0.49
3:C:384:THR:H	3:C:387:VAL:HB	1.77	0.49
3:D:62:VAL:HG11	3:D:365:ARG:NE	2.27	0.49
3:D:307:PHE:HZ	3:D:335:ASP:HB2	1.78	0.49
3:F:164:PRO:HG2	3:F:195:ILE:HB	1.94	0.49
3:H:320:ASN:OD1	3:H:323:ILE:N	2.27	0.49
3:H:384:THR:OG1	3:H:387:VAL:HG23	2.12	0.49
1:A:23:GLU:HG2	1:A:24:ALA:O	2.13	0.49
1:A:32:TYR:CG	1:A:96:LEU:HA	2.47	0.49
2:B:18:LYS:HA	2:B:78:VAL:CG2	2.42	0.49
3:C:348:ILE:N	3:C:359:ASN:O	2.30	0.49
3:D:159:ILE:HG22	3:D:247:PHE:HE1	1.77	0.49
3:F:36:HIS:HD2	3:F:375:ILE:HD13	1.78	0.49
3:H:167:GLU:OE2	3:H:233:ASP:HB2	2.13	0.49
3:C:298:SER:OG	3:C:299:MET:N	2.44	0.49
3:D:71:ARG:HH12	3:D:198:GLY:HA2	1.77	0.49
3:D:79:ASP:HB3	3:D:82:LYS:CG	2.40	0.49
3:D:170:GLY:C	3:D:189:GLU:HB3	2.33	0.49
3:D:212:THR:OG1	3:D:213:LEU:N	2.46	0.49
3:D:335:ASP:OD1	3:D:336:THR:N	2.46	0.49
3:D:355:TYR:CE2	3:E:142:ASP:HB2	2.48	0.49
3:D:402:TRP:N	3:D:402:TRP:CD1	2.77	0.49
3:E:125:LYS:HE2	3:E:261:PHE:CG	2.48	0.49
3:F:418:TYR:N	3:F:419:ARG:NH1	2.61	0.49
3:G:57:ASN:OD1	3:G:59:LYS:N	2.44	0.49
3:H:247:PHE:HE1	3:H:313:LEU:HD13	1.77	0.49
3:C:47:HIS:CG	3:C:48:PRO:HD2	2.48	0.49
3:D:80:PRO:HD3	3:D:100:TRP:HE1	1.77	0.49
3:D:209:ASP:O	3:D:213:LEU:N	2.31	0.49
3:D:213:LEU:O	3:H:344:LEU:HB2	2.13	0.49
3:D:377:GLN:HG2	3:D:378:LEU:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:459:LEU:HA	3:D:462:PHE:HB2	1.94	0.49
3:G:258:ARG:HG2	3:G:259:HIS:CE1	2.48	0.49
3:H:328:GLN:HE21	3:H:330:PHE:HE1	1.61	0.49
3:C:160:GLY:HA3	3:C:246:LEU:HA	1.95	0.48
3:D:160:GLY:HA2	3:D:247:PHE:CE1	2.48	0.48
3:D:347:ALA:HB1	3:D:359:ASN:ND2	2.28	0.48
3:E:335:ASP:OD1	3:E:337:THR:N	2.38	0.48
3:F:298:SER:OG	3:F:299:MET:N	2.44	0.48
3:F:460:ASP:OD2	3:F:477:LYS:HE2	2.12	0.48
3:G:50:PHE:CE2	3:H:271:VAL:HG22	2.48	0.48
3:G:81:ASN:ND2	3:G:98:LEU:H	2.05	0.48
3:H:35:TYR:HD2	3:H:100:TRP:CH2	2.30	0.48
2:B:54:ARG:HD3	2:B:58:VAL:HG12	1.95	0.48
3:C:240:GLU:OE1	3:C:245:SER:N	2.37	0.48
3:C:432:THR:O	3:C:434:PRO:HD2	2.13	0.48
3:D:117:ILE:HA	3:D:151:TYR:OH	2.13	0.48
3:D:149:MET:O	3:D:151:TYR:CZ	2.65	0.48
3:D:371:ASP:CG	3:D:372:LEU:N	2.66	0.48
3:D:398:ILE:O	3:D:401:ASP:HB2	2.13	0.48
3:D:459:LEU:O	3:D:466:ARG:NH2	2.46	0.48
3:E:43:LEU:HA	3:E:368:GLU:O	2.12	0.48
3:F:48:PRO:O	3:F:64:LYS:HE3	2.12	0.48
3:F:301:THR:CG2	3:F:304:ALA:H	2.24	0.48
3:G:247:PHE:HE1	3:G:313:LEU:HD13	1.78	0.48
3:H:109:ARG:HB3	3:H:338:ARG:CZ	2.43	0.48
2:B:55:GLU:O	2:B:58:VAL:HB	2.13	0.48
3:C:258:ARG:HG2	3:C:259:HIS:CE1	2.48	0.48
3:C:366:HIS:CE1	3:C:368:GLU:OE2	2.66	0.48
3:D:206:GLY:O	3:D:208:MET:HG2	2.13	0.48
3:E:18:VAL:HG12	3:E:20:LYS:H	1.78	0.48
3:E:256:PHE:HE2	3:E:298:SER:HB2	1.79	0.48
3:G:53:LYS:HA	3:G:61:LEU:N	2.28	0.48
3:H:48:PRO:O	3:H:64:LYS:HE3	2.14	0.48
3:H:335:ASP:OD1	3:H:337:THR:HG23	2.13	0.48
1:A:18:LEU:HB3	1:A:82:MET:HB2	1.95	0.48
2:B:19:VAL:HB	2:B:104:LEU:CD2	2.43	0.48
2:B:36:TYR:HA	2:B:46:LEU:HA	1.95	0.48
2:B:38:GLN:CG	2:B:44:PRO:HG3	2.43	0.48
3:D:39:THR:OG1	3:D:41:ARG:N	2.46	0.48
3:D:106:GLU:O	3:D:372:LEU:HA	2.12	0.48
3:D:159:ILE:HB	3:D:248:PHE:HB3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:377:GLN:HG2	3:D:378:LEU:H	1.78	0.48
3:D:450:ASN:OD1	3:D:452:LYS:N	2.38	0.48
3:D:459:LEU:C	3:D:462:PHE:H	2.16	0.48
3:E:161:CYS:SG	3:E:244:ASP:HB3	2.54	0.48
3:G:167:GLU:OE2	3:G:233:ASP:HB2	2.13	0.48
1:A:23:GLU:HA	1:A:77:ILE:HA	1.94	0.48
1:A:63:VAL:O	1:A:66:ARG:N	2.38	0.48
1:A:82(B):SER:OG	3:C:180:VAL:N	2.47	0.48
3:C:421:VAL:HA	3:C:424:GLN:HE21	1.78	0.48
3:C:432:THR:OG1	3:C:433:PRO:HD3	2.13	0.48
3:D:31:THR:HG21	3:D:378:LEU:HB3	1.95	0.48
3:D:389:THR:O	3:D:390:TYR:C	2.51	0.48
3:E:301:THR:CG2	3:E:304:ALA:H	2.26	0.48
3:G:51:PRO:CA	3:G:64:LYS:HB2	2.43	0.48
3:D:29:ALA:HB3	3:D:380:LYS:O	2.13	0.48
3:D:53:LYS:HD3	3:D:58:ASN:HA	1.95	0.48
3:D:115:VAL:HA	3:D:339:SER:OG	2.14	0.48
3:D:214:GLN:OE1	3:H:343:SER:O	2.32	0.48
3:D:441:LEU:HB3	3:D:444:TYR:HD2	1.77	0.48
3:E:314:GLN:HG3	3:E:315:ARG:N	2.28	0.48
3:F:90:PHE:CE1	3:F:91:TYR:CD2	3.00	0.48
3:F:161:CYS:SG	3:F:244:ASP:HB3	2.54	0.48
3:G:161:CYS:SG	3:G:244:ASP:HB3	2.53	0.48
2:B:32:TYR:CD2	2:B:92:TYR:HB2	2.38	0.48
3:C:348:ILE:HG22	3:C:359:ASN:HA	1.96	0.48
3:D:276:TYR:HE1	3:D:278:LYS:NZ	2.12	0.48
3:D:348:ILE:HG22	3:D:359:ASN:OD1	2.14	0.48
3:E:70:TYR:HD2	3:E:199:ASP:HB2	1.79	0.48
3:E:120:HIS:HD2	3:E:222:LEU:HD12	1.79	0.48
3:E:418:TYR:HB3	3:E:420:PHE:CZ	2.48	0.48
3:G:349:SER:O	3:G:359:ASN:ND2	2.45	0.48
3:H:120:HIS:ND1	3:H:122:LEU:N	2.59	0.48
3:H:120:HIS:CE1	3:H:122:LEU:O	2.67	0.48
3:H:216:ASN:OD1	3:H:218:SER:HB2	2.13	0.48
3:C:135:TYR:CD2	3:C:282:SER:HB2	2.49	0.48
3:D:42:LEU:HD12	3:D:370:TYR:HB2	1.96	0.48
3:D:50:PHE:CE1	3:E:272:PRO:HD3	2.49	0.48
3:D:75:ILE:HG22	3:D:77:LEU:HG	1.95	0.48
3:D:153:GLN:NE2	3:D:300:VAL:HG12	2.29	0.48
3:D:156:LEU:HD13	3:D:158:LEU:HD21	1.96	0.48
3:D:314:GLN:O	3:D:321:ASN:ND2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:416:ASP:HB3	3:D:418:TYR:CD2	2.49	0.48
3:G:122:LEU:HB3	3:G:144:ARG:HD2	1.96	0.48
3:G:244:ASP:OD1	3:G:320:ASN:HB2	2.14	0.48
3:D:166:GLY:O	3:D:193:THR:N	2.33	0.48
3:D:371:ASP:CG	3:D:372:LEU:H	2.17	0.48
3:F:384:THR:H	3:F:387:VAL:HB	1.79	0.48
3:G:450:ASN:HD21	3:G:452:LYS:HD2	1.79	0.48
3:H:35:TYR:HD2	3:H:100:TRP:HH2	1.60	0.48
3:H:383:LEU:HA	3:H:387:VAL:HG11	1.96	0.48
2:B:13:VAL:HG13	2:B:104:LEU:HD11	1.96	0.48
3:C:467:LYS:HA	3:C:470:LEU:HB3	1.96	0.48
3:D:259:HIS:C	3:D:260:LEU:HD12	2.34	0.48
3:E:35:TYR:HD2	3:E:100:TRP:HH2	1.62	0.48
3:E:216:ASN:O	3:E:217:LYS:HB3	2.13	0.48
3:F:245:SER:OG	3:F:246:LEU:N	2.46	0.48
3:F:273:ASP:HA	3:F:276:TYR:CE2	2.48	0.48
3:G:335:ASP:OD1	3:G:337:THR:HG23	2.13	0.48
3:H:105:VAL:HG13	3:H:374:PHE:CE1	2.49	0.48
3:H:216:ASN:O	3:H:217:LYS:HB3	2.14	0.48
1:A:38:ARG:HD3	1:A:46:GLU:HG2	1.95	0.47
3:D:156:LEU:CG	3:D:334:VAL:HB	2.44	0.47
3:D:170:GLY:H	3:D:189:GLU:C	2.14	0.47
3:D:258:ARG:HG2	3:D:259:HIS:CD2	2.49	0.47
3:D:260:LEU:HD23	3:H:148:SER:OG	2.14	0.47
3:D:349:SER:OG	3:D:352:GLU:OE1	2.30	0.47
3:D:459:LEU:HD22	3:D:466:ARG:H	1.79	0.47
3:G:61:LEU:HG	3:G:62:VAL:HG23	1.96	0.47
3:G:80:PRO:HD3	3:G:100:TRP:CD1	2.49	0.47
3:G:120:HIS:ND1	3:G:122:LEU:N	2.58	0.47
3:H:47:HIS:CD2	3:H:48:PRO:HD2	2.49	0.47
1:A:7:SER:HB3	1:A:21:SER:O	2.14	0.47
3:C:70:TYR:HD2	3:C:199:ASP:HB2	1.79	0.47
3:D:142:ASP:HA	3:H:355:TYR:HE2	1.78	0.47
3:D:169:TRP:HD1	3:D:207:ALA:N	2.13	0.47
3:D:321:ASN:N	3:D:323:ILE:HG12	2.29	0.47
3:E:52:ILE:HB	3:E:62:VAL:H	1.80	0.47
3:E:70:TYR:HE1	3:E:201:VAL:HG22	1.78	0.47
3:E:210:PHE:O	3:E:214:GLN:N	2.34	0.47
3:F:314:GLN:HG3	3:F:315:ARG:N	2.29	0.47
3:D:165:ILE:HA	3:D:195:ILE:N	2.28	0.47
3:F:47:HIS:CD2	3:F:48:PRO:HD2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:57:ASN:OD1	3:F:59:LYS:N	2.46	0.47
3:F:474:LEU:HD12	3:F:474:LEU:O	2.14	0.47
3:H:406:LEU:HD23	3:H:406:LEU:HA	1.63	0.47
1:A:48:VAL:HG13	1:A:67:PHE:CE2	2.49	0.47
3:C:167:GLU:OE2	3:C:233:ASP:HB2	2.15	0.47
3:C:280:SER:O	3:C:283:THR:OG1	2.16	0.47
3:D:220:VAL:HB	3:D:224:ILE:CG1	2.44	0.47
3:D:277:ILE:O	3:D:278:LYS:HD2	2.14	0.47
3:D:288:SER:O	3:D:291:TYR:CZ	2.68	0.47
3:G:48:PRO:O	3:G:64:LYS:HE3	2.15	0.47
3:D:72:VAL:HB	3:D:197:ASP:CB	2.45	0.47
3:D:216:ASN:ND2	3:D:218:SER:HB2	2.30	0.47
3:E:36:HIS:HD2	3:E:375:ILE:HD13	1.79	0.47
3:E:85:PHE:HB3	3:E:86:PRO:HD2	1.96	0.47
3:F:120:HIS:HE1	3:F:122:LEU:HB2	1.79	0.47
3:H:115:VAL:HG12	3:H:116:GLY:O	2.14	0.47
3:H:120:HIS:CE1	3:H:122:LEU:H	2.32	0.47
2:B:84:ALA:HB3	2:B:86:TYR:CE1	2.50	0.47
3:D:121:PRO:HA	3:D:146:CYS:CB	2.45	0.47
3:G:306:ILE:HG22	3:G:311:TYR:OH	2.15	0.47
2:B:84:ALA:HB3	2:B:86:TYR:CZ	2.49	0.47
3:C:437:LYS:O	3:C:438:GLU:HG3	2.15	0.47
3:D:115:VAL:H	3:D:340:THR:HG1	1.55	0.47
3:D:117:ILE:HA	3:D:151:TYR:HE2	1.80	0.47
3:D:280:SER:O	3:D:283:THR:N	2.48	0.47
3:E:74:ARG:O	3:E:75:ILE:HD13	2.15	0.47
3:E:120:HIS:ND1	3:E:122:LEU:N	2.58	0.47
3:E:209:ASP:O	3:E:213:LEU:HB2	2.15	0.47
3:E:219:GLU:OE1	3:E:263:ARG:CZ	2.63	0.47
3:E:466:ARG:O	3:E:469:LEU:HB2	2.15	0.47
3:F:115:VAL:HG12	3:F:116:GLY:O	2.14	0.47
3:F:196:GLN:NE2	3:F:444:TYR:HD1	2.13	0.47
3:G:79:ASP:HB3	3:G:82:LYS:HG2	1.97	0.47
3:H:50:PHE:HA	3:H:64:LYS:HD2	1.95	0.47
3:H:57:ASN:CG	3:H:59:LYS:H	2.18	0.47
1:A:38:ARG:HB2	1:A:88:ALA:CB	2.44	0.47
3:C:77:LEU:HD22	3:C:455:PHE:HZ	1.80	0.47
3:C:77:LEU:O	3:C:327:ASN:HB3	2.14	0.47
3:D:116:GLY:H	3:D:339:SER:CB	2.24	0.47
3:E:50:PHE:CE2	3:F:271:VAL:HG22	2.50	0.47
3:E:320:ASN:OD1	3:E:323:ILE:N	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:34:TYR:HE1	3:F:377:GLN:HG3	1.80	0.47
3:F:248:PHE:CG	3:F:249:TYR:N	2.83	0.47
3:H:90:PHE:HD1	3:H:380:LYS:HZ1	1.63	0.47
3:H:256:PHE:HE2	3:H:298:SER:HB2	1.80	0.47
3:C:74:ARG:HB2	3:C:446:PHE:CE1	2.37	0.47
3:C:210:PHE:CE2	3:C:220:VAL:HG11	2.49	0.47
3:C:447:TRP:CG	3:C:448:GLU:N	2.83	0.47
3:C:474:LEU:HD12	3:C:476:ALA:N	2.30	0.47
3:D:70:TYR:CZ	3:D:200:MET:O	2.67	0.47
3:D:109:ARG:HD2	3:D:109:ARG:HA	1.54	0.47
3:D:152:LYS:HE3	3:D:203:THR:O	2.13	0.47
3:D:162:LYS:HD3	3:D:162:LYS:HA	1.42	0.47
3:D:249:TYR:CZ	3:D:251:ARG:NH1	2.83	0.47
3:E:13:LEU:N	3:E:14:PRO:HA	2.30	0.47
3:F:258:ARG:HG2	3:F:259:HIS:CE1	2.50	0.47
3:F:355:TYR:HD2	3:G:142:ASP:HB2	1.79	0.47
3:G:274:ASP:OD1	3:G:275:LEU:HG	2.14	0.47
3:C:474:LEU:C	3:C:476:ALA:H	2.18	0.47
3:D:74:ARG:HD3	3:D:448:GLU:OE2	2.15	0.47
3:D:79:ASP:OD1	3:D:81:ASN:N	2.46	0.47
3:D:168:HIS:C	3:D:190:LEU:HD12	2.35	0.47
3:D:317:GLN:H	3:D:317:GLN:CD	2.16	0.47
3:D:391:ILE:HA	3:D:394:MET:CB	2.43	0.47
3:E:111:GLN:O	3:E:113:LEU:HD12	2.14	0.47
3:F:109:ARG:HB3	3:F:338:ARG:CZ	2.44	0.47
3:F:312:TRP:CZ3	3:F:468:PHE:HD1	2.33	0.47
3:G:52:ILE:HB	3:G:62:VAL:HB	1.96	0.47
3:H:47:HIS:CE1	3:H:49:TYR:H	2.33	0.47
3:H:167:GLU:HA	3:H:191:ILE:O	2.15	0.47
1:A:38:ARG:HG2	1:A:48:VAL:HG23	1.97	0.46
2:B:13:VAL:HG22	2:B:104:LEU:HD11	1.98	0.46
3:C:70:TYR:CE1	3:C:201:VAL:HG22	2.50	0.46
3:C:85:PHE:HB2	3:C:88:THR:CG2	2.45	0.46
3:D:92:ASN:OD1	3:D:94:ASP:N	2.36	0.46
3:D:391:ILE:O	3:D:394:MET:N	2.47	0.46
3:E:360:PHE:CE2	3:F:216:ASN:HA	2.50	0.46
3:F:74:ARG:O	3:F:75:ILE:HD13	2.16	0.46
3:F:146:CYS:HG	3:G:291:TYR:HH	1.61	0.46
3:G:407:GLN:O	3:G:410:PRO:HD3	2.15	0.46
3:H:34:TYR:HE1	3:H:377:GLN:HG3	1.80	0.46
3:H:109:ARG:HH21	3:H:338:ARG:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:TYR:CG	1:A:103:TRP:N	2.84	0.46
2:B:35:TRP:HB3	2:B:47:LEU:HD12	1.98	0.46
2:B:54:ARG:NE	2:B:60:ASP:HA	2.30	0.46
3:C:22:VAL:HB	3:C:26:GLU:HG3	1.96	0.46
3:C:30:ARG:HB3	3:C:377:GLN:OE1	2.15	0.46
3:C:155:GLN:OE1	3:C:306:ILE:HG12	2.16	0.46
3:D:258:ARG:HB2	3:D:296:SER:HB2	1.98	0.46
3:D:343:SER:HA	3:D:363:TYR:O	2.15	0.46
3:F:65:VAL:HA	3:F:69:GLN:OE1	2.16	0.46
3:H:465:GLY:O	3:H:468:PHE:HB3	2.15	0.46
1:A:72:ASP:CB	1:A:79:TYR:HE2	2.24	0.46
1:A:100(D):SER:C	2:B:49:TYR:HB2	2.36	0.46
2:B:32:TYR:HE2	2:B:92:TYR:CD1	2.34	0.46
3:D:202:ASP:HB3	3:D:229:CYS:HB3	1.96	0.46
3:D:385:ALA:O	3:D:388:MET:N	2.48	0.46
3:E:384:THR:OG1	3:E:387:VAL:HG23	2.16	0.46
3:F:15:PRO:HG2	3:F:17:PRO:HD3	1.97	0.46
3:F:120:HIS:ND1	3:F:122:LEU:N	2.59	0.46
3:F:274:ASP:OD1	3:F:275:LEU:HG	2.14	0.46
3:G:344:LEU:HB2	3:H:213:LEU:O	2.15	0.46
3:H:51:PRO:CD	3:H:64:LYS:HD2	2.43	0.46
2:B:50:TRP:C	2:B:52:SER:H	2.18	0.46
3:D:79:ASP:HB3	3:D:82:LYS:HZ2	1.79	0.46
3:D:98:LEU:C	3:D:378:LEU:HD21	2.35	0.46
3:D:115:VAL:O	3:D:340:THR:HA	2.16	0.46
3:D:299:MET:HG3	3:E:256:PHE:HD2	1.80	0.46
3:D:347:ALA:HA	3:D:359:ASN:O	2.16	0.46
3:D:373:GLN:OE1	3:D:463:PRO:HD2	2.15	0.46
3:D:389:THR:CA	3:D:392:HIS:HB3	2.43	0.46
3:F:222:LEU:O	3:F:225:CYS:N	2.32	0.46
3:G:168:HIS:CE1	3:G:191:ILE:HB	2.49	0.46
3:G:280:SER:O	3:G:283:THR:N	2.47	0.46
3:H:216:ASN:C	3:H:218:SER:H	2.18	0.46
3:H:248:PHE:CG	3:H:249:TYR:N	2.83	0.46
1:A:51:ILE:HG12	1:A:55:GLY:HA2	1.97	0.46
1:A:88:ALA:HB3	1:A:90:TYR:CE1	2.50	0.46
3:D:46:GLY:C	3:D:366:HIS:H	2.14	0.46
3:D:459:LEU:HD22	3:D:465:GLY:N	2.30	0.46
3:D:475:LYS:O	3:D:477:LYS:N	2.46	0.46
3:E:105:VAL:HG13	3:E:374:PHE:CE1	2.51	0.46
3:F:51:PRO:CD	3:F:64:LYS:HD2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:120:HIS:CE1	3:G:122:LEU:O	2.68	0.46
3:H:70:TYR:HD2	3:H:199:ASP:HB2	1.80	0.46
3:H:377:GLN:CG	3:H:378:LEU:H	2.29	0.46
1:A:94:ARG:NE	1:A:102:TYR:HB3	2.30	0.46
3:C:17:PRO:HG2	3:C:386:ASP:CG	2.34	0.46
3:C:111:GLN:HB2	3:C:338:ARG:CD	2.31	0.46
3:D:50:PHE:CZ	3:E:272:PRO:HD3	2.51	0.46
3:D:274:ASP:OD1	3:D:275:LEU:N	2.49	0.46
3:E:109:ARG:HB3	3:E:338:ARG:CZ	2.46	0.46
3:E:109:ARG:HH21	3:E:338:ARG:HD2	1.79	0.46
3:G:70:TYR:CE1	3:G:201:VAL:HG22	2.51	0.46
3:G:120:HIS:HE1	3:G:122:LEU:HB2	1.80	0.46
2:B:55:GLU:HB3	2:B:58:VAL:CG2	2.46	0.46
3:C:274:ASP:OD1	3:C:275:LEU:N	2.49	0.46
3:D:236:LYS:O	3:D:239:SER:N	2.49	0.46
3:D:242:TYR:N	3:D:242:TYR:CD2	2.84	0.46
3:E:355:TYR:HD2	3:F:142:ASP:HB2	1.81	0.46
3:H:377:GLN:HG2	3:H:378:LEU:N	2.31	0.46
3:H:417:THR:HG1	3:H:418:TYR:HD2	1.63	0.46
3:C:16:VAL:HG13	3:C:17:PRO:HD3	1.97	0.46
3:D:309:LYS:HB3	3:D:309:LYS:HE2	1.40	0.46
3:G:167:GLU:HA	3:G:191:ILE:O	2.15	0.46
3:H:196:GLN:HE21	3:H:444:TYR:HD1	1.64	0.46
1:A:60:PRO:HD2	1:A:63:VAL:CG2	2.44	0.46
3:C:16:VAL:N	3:C:17:PRO:HD2	2.31	0.46
3:C:85:PHE:HB2	3:C:88:THR:HG23	1.98	0.46
3:C:384:THR:H	3:C:387:VAL:CG2	2.29	0.46
3:D:156:LEU:HD11	3:D:334:VAL:HG23	1.98	0.46
3:D:166:GLY:HA3	3:D:230:LYS:CE	2.46	0.46
3:D:181:ASN:HB2	3:D:184:ASP:OD1	2.16	0.46
3:D:277:ILE:CG2	3:G:355:TYR:HB2	2.46	0.46
3:D:338:ARG:O	3:D:340:THR:N	2.49	0.46
3:D:474:LEU:HA	3:D:475:LYS:HZ3	1.80	0.46
3:E:23:SER:O	3:E:26:GLU:HG2	2.16	0.46
3:F:77:LEU:O	3:F:327:ASN:HB3	2.16	0.46
3:F:451:LEU:O	3:F:453:GLU:N	2.49	0.46
3:G:109:ARG:NH1	3:G:370:TYR:CE1	2.84	0.46
3:G:222:LEU:O	3:G:225:CYS:N	2.39	0.46
3:G:263:ARG:HB2	3:G:290:ASN:HD22	1.80	0.46
3:G:355:TYR:HD2	3:H:142:ASP:HB2	1.80	0.46
3:G:407:GLN:N	3:G:408:PRO:HD3	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:79:ASP:CB	3:D:82:LYS:HG2	2.43	0.46
3:D:97:ARG:HG3	3:D:402:TRP:CZ3	2.51	0.46
3:D:300:VAL:HG22	3:E:255:MET:N	2.29	0.46
3:E:112:PRO:HB3	3:F:231:TYR:CD1	2.51	0.46
3:E:366:HIS:CE1	3:E:368:GLU:OE2	2.69	0.46
3:F:167:GLU:HA	3:F:191:ILE:O	2.16	0.46
3:F:450:ASN:HD21	3:F:452:LYS:CD	2.29	0.46
3:G:50:PHE:HA	3:G:64:LYS:HD2	1.98	0.46
3:G:424:GLN:OE1	3:G:427:ALA:HB3	2.14	0.46
3:H:15:PRO:HB3	3:H:16:VAL:HA	1.97	0.46
3:H:156:LEU:HD12	3:H:333:VAL:HA	1.98	0.46
3:D:70:TYR:N	3:D:199:ASP:H	2.14	0.45
3:D:274:ASP:O	3:H:217:LYS:NZ	2.38	0.45
3:E:324:CYS:SG	3:E:329:LEU:HD12	2.57	0.45
3:F:216:ASN:O	3:F:217:LYS:HB3	2.16	0.45
3:G:312:TRP:CH2	3:G:468:PHE:CD1	2.97	0.45
3:H:211:THR:OG1	3:H:226:THR:O	2.34	0.45
3:H:312:TRP:CE2	3:H:471:GLN:OE1	2.69	0.45
3:D:85:PHE:H	3:D:88:THR:CG2	2.27	0.45
3:D:307:PHE:CZ	3:D:335:ASP:HB2	2.50	0.45
3:D:459:LEU:CB	3:D:466:ARG:HB3	2.43	0.45
3:E:404:PHE:HB2	3:E:405:GLY:HA3	1.96	0.45
3:F:384:THR:O	3:F:388:MET:HG3	2.16	0.45
3:G:216:ASN:O	3:G:217:LYS:HB3	2.17	0.45
3:G:335:ASP:OD1	3:G:337:THR:N	2.46	0.45
3:H:209:ASP:O	3:H:213:LEU:HB2	2.16	0.45
3:H:209:ASP:OD2	3:H:212:THR:HG23	2.16	0.45
3:C:47:HIS:O	3:C:65:VAL:N	2.44	0.45
3:D:38:GLY:CA	3:D:373:GLN:HG2	2.35	0.45
3:D:65:VAL:HA	3:D:69:GLN:NE2	2.30	0.45
3:D:70:TYR:O	3:D:198:GLY:N	2.23	0.45
3:D:189:GLU:OE2	3:D:191:ILE:HG12	2.16	0.45
3:D:463:PRO:HA	3:D:466:ARG:NH1	2.31	0.45
3:F:24:THR:HG21	3:F:320:ASN:HA	1.97	0.45
3:F:208:MET:O	3:F:228:ILE:HG23	2.16	0.45
3:F:426:ILE:CG2	3:F:427:ALA:N	2.73	0.45
3:F:477:LYS:HZ2	3:G:23:SER:CB	2.28	0.45
3:G:209:ASP:O	3:G:213:LEU:HB2	2.15	0.45
1:A:94:ARG:HH21	1:A:101:ASP:CG	2.20	0.45
3:C:97:ARG:HH12	3:C:403:ASN:H	1.63	0.45
3:F:312:TRP:CE2	3:F:471:GLN:OE1	2.69	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:417:THR:O	3:F:418:TYR:CD1	2.70	0.45
3:G:47:HIS:CE1	3:G:49:TYR:HB2	2.52	0.45
3:H:72:VAL:O	3:H:447:TRP:HB3	2.16	0.45
3:H:384:THR:H	3:H:387:VAL:CG2	2.30	0.45
2:B:35:TRP:O	2:B:46:LEU:HA	2.16	0.45
3:C:74:ARG:O	3:C:75:ILE:HD13	2.17	0.45
3:C:90:PHE:CD1	3:C:91:TYR:HD2	2.34	0.45
3:C:374:PHE:HB3	3:C:376:PHE:CE2	2.51	0.45
3:C:421:VAL:HG12	3:C:422:THR:HA	1.99	0.45
3:H:123:LEU:HD12	3:H:218:SER:O	2.16	0.45
3:H:384:THR:H	3:H:387:VAL:CB	2.30	0.45
1:A:100(A):ASP:O	2:B:30(F):LYS:HG2	2.16	0.45
3:C:325:TRP:CE3	3:C:398:ILE:HD13	2.51	0.45
3:D:125:LYS:HA	3:D:263:ARG:HA	1.98	0.45
3:D:168:HIS:O	3:D:190:LEU:HD12	2.16	0.45
3:E:157:CYS:SG	3:E:158:LEU:N	2.89	0.45
3:E:404:PHE:CB	3:E:405:GLY:CA	2.94	0.45
3:F:97:ARG:HH12	3:F:404:PHE:HD2	1.63	0.45
3:F:312:TRP:HH2	3:F:468:PHE:CD1	2.30	0.45
3:C:431:HIS:CE1	3:C:434:PRO:HA	2.52	0.45
3:C:474:LEU:O	3:C:476:ALA:O	2.35	0.45
3:D:71:ARG:HD3	3:D:71:ARG:HA	1.57	0.45
3:F:81:ASN:HD21	3:F:98:LEU:N	2.14	0.45
3:F:408:PRO:N	3:F:409:PRO:HD2	2.32	0.45
3:H:216:ASN:HB3	3:H:219:GLU:HG2	1.99	0.45
3:H:273:ASP:HA	3:H:276:TYR:CE2	2.52	0.45
3:H:403:ASN:O	3:H:404:PHE:HB2	2.17	0.45
3:D:153:GLN:OE1	3:D:254:GLN:OE1	2.35	0.45
3:D:164:PRO:HB2	3:D:195:ILE:HB	1.99	0.45
3:D:188:LEU:HD12	3:D:188:LEU:N	2.32	0.45
3:D:395:ASN:OD1	3:D:397:THR:HG23	2.17	0.45
3:E:109:ARG:HD2	3:E:369:GLU:O	2.17	0.45
3:G:81:ASN:HD21	3:G:98:LEU:N	2.09	0.45
3:G:209:ASP:OD2	3:G:212:THR:HG23	2.17	0.45
3:H:312:TRP:CZ3	3:H:468:PHE:HD1	2.32	0.45
3:C:276:TYR:HD1	3:C:277:ILE:O	2.00	0.45
3:D:30:ARG:HD3	3:D:379:CYS:SG	2.57	0.45
3:D:156:LEU:CD2	3:D:334:VAL:HB	2.47	0.45
3:D:201:VAL:HG12	3:D:202:ASP:O	2.17	0.45
3:D:248:PHE:CD2	3:D:249:TYR:N	2.84	0.45
3:D:325:TRP:O	3:D:328:GLN:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:70:TYR:CE1	3:E:201:VAL:HG22	2.52	0.45
3:E:236:LYS:O	3:E:239:SER:HB2	2.17	0.45
3:E:275:LEU:HD23	3:E:275:LEU:HA	1.72	0.45
3:E:312:TRP:CE2	3:E:471:GLN:OE1	2.70	0.45
3:F:216:ASN:HB3	3:F:219:GLU:HG2	1.98	0.45
3:F:465:GLY:O	3:F:468:PHE:N	2.49	0.45
3:C:49:TYR:HB3	3:C:222:LEU:HD23	1.97	0.45
3:C:465:GLY:O	3:C:468:PHE:HB3	2.17	0.45
3:D:24:THR:CG2	3:D:323:ILE:HG13	2.34	0.45
3:D:51:PRO:HB3	3:D:64:LYS:H	1.82	0.45
3:D:124:ASN:HB3	3:D:263:ARG:NH1	2.32	0.45
3:D:291:TYR:OH	3:H:121:PRO:HG3	2.17	0.45
3:D:369:GLU:O	3:D:370:TYR:CG	2.70	0.45
3:F:223:ASP:OD1	3:F:224:ILE:HG23	2.17	0.45
3:F:306:ILE:HG22	3:F:311:TYR:OH	2.17	0.45
3:G:417:THR:HB	3:G:419:ARG:NE	2.15	0.45
3:H:280:SER:N	3:H:283:THR:OG1	2.34	0.45
3:C:51:PRO:CD	3:C:64:LYS:HB2	2.47	0.44
3:D:128:ASP:OD2	3:D:131:ASN:N	2.32	0.44
3:D:205:PHE:O	3:D:210:PHE:HZ	2.00	0.44
3:D:235:ILE:HA	3:D:238:VAL:HB	1.99	0.44
3:D:240:GLU:HB3	3:D:243:GLY:HA2	1.99	0.44
3:D:257:VAL:HG13	3:D:294:THR:O	2.17	0.44
3:D:310:PRO:HD3	3:D:467:LYS:NZ	2.32	0.44
3:D:371:ASP:O	3:D:372:LEU:HD23	2.16	0.44
3:D:468:PHE:O	3:D:469:LEU:C	2.52	0.44
3:E:34:TYR:HE1	3:E:377:GLN:CG	2.29	0.44
3:E:125:LYS:HE2	3:E:261:PHE:CD1	2.51	0.44
3:F:61:LEU:HG	3:F:62:VAL:HG23	1.98	0.44
3:H:90:PHE:CE1	3:H:91:TYR:CD2	3.05	0.44
3:H:420:PHE:HB3	3:H:430:LYS:CE	2.47	0.44
2:B:19:VAL:HG22	2:B:75:ILE:HD12	1.97	0.44
2:B:89:GLN:OE1	2:B:96:LEU:HB3	2.17	0.44
3:D:42:LEU:HB2	3:D:370:TYR:H	1.81	0.44
3:D:78:PRO:HD2	3:D:455:PHE:CZ	2.53	0.44
3:E:208:MET:O	3:E:228:ILE:HG23	2.17	0.44
3:E:248:PHE:CG	3:E:249:TYR:N	2.85	0.44
3:F:120:HIS:HD2	3:F:222:LEU:HD12	1.79	0.44
3:F:159:ILE:HG22	3:F:247:PHE:CZ	2.52	0.44
3:G:47:HIS:CE1	3:G:49:TYR:H	2.35	0.44
3:G:74:ARG:O	3:G:75:ILE:HD13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:36:TRP:CE2	1:A:78:LEU:HG	2.53	0.44
2:B:2:ILE:HG23	2:B:26:SER:H	1.81	0.44
3:C:233:ASP:N	3:C:237:MET:HE2	2.32	0.44
3:C:411:GLY:O	3:C:413:THR:HG23	2.17	0.44
3:D:261:PHE:HD2	3:D:294:THR:OG1	1.99	0.44
3:D:378:LEU:HG	3:D:379:CYS:H	1.82	0.44
3:G:248:PHE:CG	3:G:249:TYR:N	2.85	0.44
3:G:404:PHE:CD2	3:G:409:PRO:HD2	2.53	0.44
3:H:335:ASP:OD2	3:H:338:ARG:NH1	2.50	0.44
3:C:24:THR:HG21	3:C:320:ASN:HA	1.98	0.44
3:C:361:LYS:HB3	3:C:363:TYR:CZ	2.52	0.44
3:C:430:LYS:NZ	3:D:189:GLU:HG3	2.32	0.44
3:D:74:ARG:HH11	3:D:446:PHE:HE1	1.64	0.44
3:D:125:LYS:HG3	3:D:262:ASN:O	2.17	0.44
3:E:35:TYR:HD2	3:E:100:TRP:CH2	2.36	0.44
3:E:465:GLY:O	3:E:468:PHE:HB3	2.16	0.44
3:F:18:VAL:CG1	3:F:19:SER:H	2.30	0.44
3:F:30:ARG:HD2	3:F:377:GLN:OE1	2.18	0.44
3:G:404:PHE:HD2	3:G:409:PRO:HD2	1.83	0.44
3:H:109:ARG:NH1	3:H:370:TYR:CE1	2.86	0.44
1:A:38:ARG:CZ	1:A:86:ASP:HA	2.47	0.44
1:A:41:PRO:C	1:A:43:LYS:H	2.21	0.44
3:C:12:TYR:CD2	3:C:13:LEU:HG	2.53	0.44
3:C:114:GLY:N	3:C:337:THR:O	2.47	0.44
3:C:203:THR:HG21	3:C:224:ILE:HD13	1.98	0.44
3:D:276:TYR:HE1	3:D:278:LYS:HZ2	1.64	0.44
3:F:70:TYR:CE1	3:F:201:VAL:HG22	2.53	0.44
3:F:97:ARG:HH22	3:F:404:PHE:N	2.16	0.44
3:G:47:HIS:CD2	3:G:48:PRO:HD2	2.53	0.44
3:G:109:ARG:HB3	3:G:338:ARG:CZ	2.47	0.44
3:G:123:LEU:N	3:G:144:ARG:HB3	2.33	0.44
3:G:223:ASP:OD1	3:G:224:ILE:HG23	2.18	0.44
3:H:111:GLN:O	3:H:113:LEU:HD12	2.18	0.44
3:C:40:SER:HG	3:H:420:PHE:HD2	1.64	0.44
3:C:469:LEU:HD21	3:C:477:LYS:NZ	2.32	0.44
3:D:74:ARG:HD3	3:D:448:GLU:CD	2.38	0.44
3:D:162:LYS:HB2	3:D:245:SER:N	2.33	0.44
3:D:287:ALA:HB1	3:H:146:CYS:CB	2.39	0.44
3:E:423:SER:O	3:E:424:GLN:HB2	2.18	0.44
3:F:44:ALA:HB3	3:F:368:GLU:HB2	1.99	0.44
3:G:78:PRO:HD3	3:G:452:LYS:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:312:TRP:HH2	3:G:468:PHE:CD1	2.31	0.44
3:G:372:LEU:HA	3:G:372:LEU:HD23	1.75	0.44
3:C:399:LEU:HB3	3:C:404:PHE:CD1	2.53	0.44
3:D:91:TYR:CD2	3:D:91:TYR:N	2.85	0.44
3:G:43:LEU:HD12	3:G:368:GLU:O	2.17	0.44
3:G:52:ILE:HB	3:G:62:VAL:N	2.32	0.44
3:G:77:LEU:HA	3:G:77:LEU:HD23	1.77	0.44
3:G:245:SER:OG	3:G:246:LEU:N	2.49	0.44
3:H:377:GLN:HG2	3:H:378:LEU:H	1.83	0.44
1:A:100(E):ASP:HA	2:B:46:LEU:HD21	1.99	0.44
3:D:123:LEU:CD1	3:D:263:ARG:HH12	2.29	0.44
3:D:189:GLU:CD	3:D:191:ILE:HG12	2.37	0.44
3:D:342:MET:O	3:D:364:LEU:HD23	2.17	0.44
3:D:391:ILE:O	3:D:392:HIS:C	2.56	0.44
3:E:115:VAL:HG12	3:E:116:GLY:O	2.18	0.44
3:E:120:HIS:CE1	3:E:122:LEU:O	2.70	0.44
3:H:219:GLU:OE1	3:H:263:ARG:CZ	2.65	0.44
3:C:84:GLY:HA2	3:H:84:GLY:CA	2.47	0.44
3:C:439:ASP:OD1	3:C:440:PRO:HD2	2.18	0.44
3:D:92:ASN:ND2	3:D:95:THR:HG23	2.33	0.44
3:D:109:ARG:N	3:D:308:ASN:OD1	2.50	0.44
3:D:168:HIS:CE1	3:D:191:ILE:HB	2.52	0.44
3:D:170:GLY:CA	3:D:189:GLU:HB3	2.47	0.44
3:D:208:MET:N	3:D:228:ILE:HG23	2.33	0.44
3:E:80:PRO:HD3	3:E:100:TRP:CD1	2.52	0.44
3:F:50:PHE:HA	3:F:64:LYS:HD2	1.99	0.44
3:F:344:LEU:HB2	3:G:213:LEU:O	2.18	0.44
3:G:196:GLN:HE21	3:G:444:TYR:HD1	1.66	0.44
1:A:100(C):GLY:O	2:B:49:TYR:HD1	2.01	0.43
3:C:62:VAL:HG13	3:H:426:ILE:CD1	2.34	0.43
3:C:113:LEU:HD21	3:C:305:GLN:NE2	2.33	0.43
3:D:124:ASN:OD1	3:D:264:ALA:N	2.31	0.43
3:E:399:LEU:HA	3:E:399:LEU:HD23	1.71	0.43
3:F:111:GLN:OE1	3:F:369:GLU:OE1	2.36	0.43
3:F:120:HIS:CE1	3:F:122:LEU:O	2.70	0.43
3:G:112:PRO:HB3	3:H:231:TYR:CD1	2.52	0.43
3:G:341:ASN:OD1	3:G:366:HIS:HD2	2.01	0.43
1:A:38:ARG:HD3	1:A:46:GLU:CG	2.49	0.43
3:D:47:HIS:HD2	3:D:364:LEU:O	2.00	0.43
3:D:97:ARG:NH2	3:D:403:ASN:H	2.16	0.43
3:D:252:ARG:HD3	3:D:252:ARG:HA	1.87	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:321:ASN:H	3:D:323:ILE:HG12	1.83	0.43
3:D:321:ASN:C	3:D:323:ILE:HG12	2.38	0.43
3:D:344:LEU:CD2	3:D:363:TYR:HB2	2.49	0.43
3:E:158:LEU:C	3:E:159:ILE:HG13	2.38	0.43
3:F:23:SER:O	3:F:26:GLU:HG2	2.18	0.43
3:G:54:LYS:HD2	3:G:57:ASN:HB2	2.00	0.43
3:G:189:GLU:HG2	3:G:191:ILE:HG13	1.99	0.43
3:G:209:ASP:OD1	3:G:211:THR:N	2.52	0.43
3:G:377:GLN:HG2	3:G:378:LEU:N	2.33	0.43
3:H:366:HIS:CE1	3:H:368:GLU:OE2	2.71	0.43
1:A:40:THR:HA	1:A:41:PRO:HD3	1.79	0.43
1:A:94:ARG:CZ	1:A:102:TYR:HB3	2.48	0.43
3:F:135:TYR:CG	3:F:136:ALA:N	2.86	0.43
3:F:167:GLU:OE2	3:F:233:ASP:HB2	2.18	0.43
3:F:320:ASN:OD1	3:F:323:ILE:N	2.22	0.43
3:F:407:GLN:HB3	3:F:409:PRO:HD2	2.01	0.43
3:G:118:SER:O	3:G:148:SER:HB2	2.18	0.43
3:H:208:MET:O	3:H:228:ILE:HG23	2.19	0.43
3:C:144:ARG:NH1	3:C:218:SER:OG	2.51	0.43
3:D:36:HIS:HE1	3:D:373:GLN:CB	2.31	0.43
3:D:39:THR:HG23	3:D:372:LEU:H	1.83	0.43
3:D:277:ILE:HD12	3:H:144:ARG:NH1	2.33	0.43
3:D:468:PHE:HA	3:D:471:GLN:OE1	2.18	0.43
3:E:123:LEU:HD12	3:E:218:SER:O	2.19	0.43
3:F:109:ARG:NH1	3:F:370:TYR:CE1	2.86	0.43
3:F:219:GLU:OE1	3:F:263:ARG:CZ	2.63	0.43
3:H:439:ASP:OD1	3:H:440:PRO:HD2	2.18	0.43
3:D:73:PHE:CD1	3:D:447:TRP:CD1	3.02	0.43
3:D:462:PHE:O	3:D:464:LEU:N	2.51	0.43
3:E:24:THR:HG21	3:E:320:ASN:HA	1.99	0.43
3:E:148:SER:HB3	3:F:291:TYR:CE1	2.53	0.43
3:E:384:THR:O	3:E:388:MET:HG3	2.19	0.43
3:E:450:ASN:OD1	3:E:452:LYS:N	2.31	0.43
3:F:73:PHE:HZ	3:F:370:TYR:CD2	2.36	0.43
3:F:150:ASP:OD2	3:F:297:GLY:N	2.51	0.43
3:F:154:THR:HG23	3:F:253:GLU:HB3	1.99	0.43
3:F:275:LEU:HD23	3:F:275:LEU:HA	1.67	0.43
3:H:74:ARG:O	3:H:75:ILE:HD13	2.17	0.43
3:H:120:HIS:HE1	3:H:122:LEU:HB2	1.82	0.43
2:B:83:LEU:O	2:B:84:ALA:HB2	2.19	0.43
3:C:83:PHE:HD2	3:C:85:PHE:CE1	2.37	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:113:LEU:N	3:D:113:LEU:CD1	2.82	0.43
3:D:259:HIS:CA	3:D:294:THR:HB	2.49	0.43
3:D:275:LEU:C	3:H:217:LYS:HD3	2.39	0.43
3:D:329:LEU:HG	3:D:330:PHE:H	1.82	0.43
3:E:65:VAL:HA	3:E:69:GLN:OE1	2.18	0.43
3:G:34:TYR:CE1	3:G:377:GLN:HG3	2.53	0.43
3:G:399:LEU:HD23	3:G:399:LEU:HA	1.69	0.43
3:G:459:LEU:HD12	3:G:477:LYS:HZ3	1.83	0.43
1:A:63:VAL:HG12	1:A:66:ARG:HH11	1.82	0.43
2:B:32:TYR:HE2	2:B:92:TYR:HD1	1.67	0.43
3:C:248:PHE:CD2	3:C:249:TYR:N	2.87	0.43
3:D:100:TRP:CA	3:D:378:LEU:HD12	2.49	0.43
3:D:150:ASP:C	3:D:151:TYR:CD1	2.92	0.43
3:D:216:ASN:ND2	3:D:216:ASN:C	2.71	0.43
3:D:216:ASN:CG	3:D:218:SER:H	2.22	0.43
3:E:384:THR:H	3:E:387:VAL:CG2	2.31	0.43
3:G:92:ASN:OD1	3:G:94:ASP:N	2.41	0.43
3:H:70:TYR:CD1	3:H:334:VAL:HG21	2.50	0.43
3:H:306:ILE:HG22	3:H:311:TYR:OH	2.19	0.43
2:B:11:LEU:HD13	2:B:20:THR:OG1	2.19	0.43
3:D:119:GLY:O	3:D:221:PRO:HA	2.19	0.43
3:D:250:LEU:HA	3:D:250:LEU:HD23	1.54	0.43
3:D:397:THR:O	3:D:401:ASP:OD1	2.36	0.43
3:D:474:LEU:HD12	3:D:474:LEU:O	2.18	0.43
3:E:116:GLY:HA3	3:E:339:SER:O	2.18	0.43
3:E:209:ASP:OD2	3:E:212:THR:HG23	2.19	0.43
3:F:80:PRO:HD3	3:F:100:TRP:CD1	2.53	0.43
3:F:150:ASP:CG	3:F:297:GLY:H	2.21	0.43
2:B:21:MET:HB2	2:B:102:THR:OG1	2.19	0.43
3:C:12:TYR:CE2	3:C:13:LEU:HG	2.54	0.43
3:C:77:LEU:HA	3:C:77:LEU:HD23	1.82	0.43
3:E:46:GLY:CA	3:E:65:VAL:HB	2.45	0.43
3:E:52:ILE:HB	3:E:62:VAL:N	2.34	0.43
3:E:128:ASP:OD1	3:E:129:THR:N	2.52	0.43
3:E:135:TYR:CG	3:E:136:ALA:N	2.87	0.43
3:E:475:LYS:C	3:E:477:LYS:H	2.22	0.43
3:F:153:GLN:CD	3:F:300:VAL:HG12	2.39	0.43
3:F:399:LEU:HD23	3:F:399:LEU:HA	1.79	0.43
3:F:433:PRO:HG2	3:F:434:PRO:HD3	2.01	0.43
3:G:314:GLN:HG3	3:G:315:ARG:H	1.83	0.43
3:G:366:HIS:CE1	3:G:368:GLU:OE2	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:12:TYR:C	3:H:14:PRO:HD2	2.39	0.43
3:H:74:ARG:NH2	3:H:439:ASP:OD2	2.52	0.43
1:A:100(B):GLU:HB2	2:B:30(F):LYS:CB	2.48	0.43
2:B:18:LYS:HA	2:B:78:VAL:HG23	2.01	0.43
3:D:70:TYR:CE2	3:D:230:LYS:HB2	2.53	0.43
3:D:242:TYR:CZ	3:D:394:MET:HG3	2.53	0.43
3:F:74:ARG:CB	3:F:446:PHE:HE1	2.20	0.43
3:F:108:GLY:HA2	3:F:308:ASN:OD1	2.19	0.43
3:F:116:GLY:HA3	3:F:339:SER:O	2.19	0.43
3:G:90:PHE:CE1	3:G:91:TYR:CD2	3.07	0.43
3:D:249:TYR:HE1	3:D:251:ARG:CB	2.31	0.42
3:D:254:GLN:O	3:D:255:MET:HB2	2.19	0.42
3:D:309:LYS:HB2	3:D:311:TYR:CZ	2.54	0.42
3:F:60:ILE:O	3:F:60:ILE:HG13	2.19	0.42
3:G:208:MET:O	3:G:228:ILE:HG23	2.19	0.42
3:H:74:ARG:HB3	3:H:448:GLU:OE1	2.18	0.42
1:A:100(B):GLU:OE1	2:B:30(F):LYS:HB2	2.19	0.42
3:C:274:ASP:OD1	3:C:275:LEU:HG	2.18	0.42
3:C:314:GLN:HG3	3:C:315:ARG:N	2.35	0.42
3:C:321:ASN:O	3:C:323:ILE:HG12	2.19	0.42
3:D:126:LEU:HB3	3:D:262:ASN:HB2	2.01	0.42
3:D:312:TRP:HH2	3:D:468:PHE:HB2	1.83	0.42
3:D:387:VAL:C	3:D:389:THR:H	2.21	0.42
3:F:52:ILE:HB	3:F:62:VAL:H	1.84	0.42
3:F:387:VAL:O	3:F:388:MET:C	2.57	0.42
3:F:450:ASN:OD1	3:F:451:LEU:N	2.53	0.42
3:F:450:ASN:OD1	3:F:452:LYS:N	2.35	0.42
3:G:68:LEU:HA	3:G:68:LEU:HD23	1.68	0.42
2:B:33:LEU:HD22	2:B:71:PHE:CE2	2.54	0.42
3:C:34:TYR:HD1	3:C:377:GLN:HA	1.84	0.42
3:C:78:PRO:HD2	3:C:455:PHE:CZ	2.55	0.42
3:C:234:TYR:HA	3:C:237:MET:HE3	2.01	0.42
3:D:42:LEU:HD23	3:D:42:LEU:HA	1.66	0.42
3:D:75:ILE:HG12	3:D:329:LEU:O	2.19	0.42
3:D:450:ASN:OD1	3:D:450:ASN:C	2.56	0.42
3:E:34:TYR:CE1	3:E:377:GLN:HG3	2.54	0.42
3:E:118:SER:O	3:E:148:SER:HB2	2.18	0.42
3:F:328:GLN:HE21	3:F:330:PHE:HE1	1.68	0.42
3:G:153:GLN:HE22	3:G:300:VAL:HG12	1.84	0.42
1:A:38:ARG:NH1	1:A:46:GLU:OE2	2.53	0.42
3:C:120:HIS:CE1	3:C:122:LEU:H	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:130:GLU:HA	3:C:260:LEU:HD22	2.01	0.42
3:C:439:ASP:O	3:C:441:LEU:N	2.53	0.42
3:D:159:ILE:HB	3:D:248:PHE:HD2	1.84	0.42
3:D:385:ALA:O	3:D:386:ASP:C	2.56	0.42
3:D:459:LEU:HB2	3:D:469:LEU:HD11	2.00	0.42
3:E:21:VAL:HG13	3:E:390:TYR:OH	2.19	0.42
3:E:109:ARG:NH1	3:E:370:TYR:CE1	2.88	0.42
3:H:30:ARG:HD2	3:H:377:GLN:OE1	2.19	0.42
3:D:112:PRO:HB3	3:E:231:TYR:CZ	2.55	0.42
3:D:164:PRO:C	3:D:195:ILE:HB	2.40	0.42
3:D:271:VAL:HG12	3:D:276:TYR:HE2	1.84	0.42
3:D:289:SER:O	3:D:291:TYR:CD2	2.73	0.42
3:D:300:VAL:O	3:E:254:GLN:HB2	2.20	0.42
3:D:344:LEU:HD21	3:D:363:TYR:HB2	2.01	0.42
3:E:306:ILE:HG22	3:E:311:TYR:OH	2.19	0.42
3:E:450:ASN:OD1	3:E:451:LEU:N	2.52	0.42
3:F:15:PRO:HG2	3:F:17:PRO:CD	2.49	0.42
3:G:35:TYR:HD1	3:G:457:ALA:HA	1.85	0.42
3:G:169:TRP:O	3:G:208:MET:HA	2.20	0.42
3:G:451:LEU:O	3:G:453:GLU:N	2.52	0.42
2:B:24:LYS:CD	2:B:70:ASP:HB2	2.50	0.42
3:D:107:VAL:HG12	3:D:108:GLY:O	2.19	0.42
3:D:123:LEU:HD12	3:D:218:SER:O	2.20	0.42
3:D:155:GLN:HE22	3:D:306:ILE:H	1.68	0.42
3:D:248:PHE:CZ	3:D:250:LEU:HG	2.55	0.42
3:D:323:ILE:HG22	3:D:325:TRP:CZ2	2.54	0.42
3:D:335:ASP:CG	3:D:337:THR:H	2.15	0.42
3:D:391:ILE:HG22	3:D:395:ASN:O	2.20	0.42
3:E:451:LEU:O	3:E:453:GLU:N	2.53	0.42
3:F:70:TYR:CD2	3:F:199:ASP:HB2	2.54	0.42
3:F:121:PRO:HA	3:F:146:CYS:SG	2.60	0.42
3:F:158:LEU:C	3:F:159:ILE:HG13	2.40	0.42
3:F:216:ASN:OD1	3:F:218:SER:HB2	2.19	0.42
3:C:18:VAL:CG1	3:C:20:LYS:NZ	2.82	0.42
3:C:47:HIS:ND1	3:C:49:TYR:N	2.66	0.42
3:C:399:LEU:HA	3:C:402:TRP:HB2	2.02	0.42
3:C:414:LEU:HD23	3:C:414:LEU:HA	1.67	0.42
3:D:53:LYS:CB	3:D:60:ILE:HA	2.49	0.42
3:D:71:ARG:HB2	3:D:333:VAL:O	2.19	0.42
3:D:83:PHE:CD2	3:D:85:PHE:HD1	2.37	0.42
3:D:169:TRP:HA	3:D:190:LEU:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:169:TRP:HE1	3:D:207:ALA:H	1.68	0.42
3:E:153:GLN:HE22	3:E:300:VAL:HG12	1.85	0.42
3:E:167:GLU:OE2	3:E:233:ASP:HB2	2.19	0.42
3:E:246:LEU:HD12	3:E:246:LEU:O	2.20	0.42
3:E:273:ASP:HA	3:E:276:TYR:CE2	2.55	0.42
3:F:85:PHE:HB3	3:F:86:PRO:HD2	2.02	0.42
3:F:280:SER:O	3:F:283:THR:N	2.45	0.42
3:F:474:LEU:O	3:F:475:LYS:HB2	2.20	0.42
3:G:77:LEU:O	3:G:327:ASN:HB3	2.20	0.42
3:G:403:ASN:O	3:G:404:PHE:HB2	2.20	0.42
3:H:273:ASP:O	3:H:275:LEU:N	2.53	0.42
2:B:6:GLN:HE21	2:B:101:GLY:CA	2.33	0.42
3:C:77:LEU:HD13	3:C:100:TRP:CG	2.55	0.42
3:C:84:GLY:HA2	3:H:84:GLY:N	2.35	0.42
3:D:432:THR:C	3:D:434:PRO:HD3	2.39	0.42
3:D:468:PHE:HA	3:D:471:GLN:CB	2.28	0.42
3:D:475:LYS:HE2	3:D:475:LYS:HB2	1.81	0.42
3:F:92:ASN:OD1	3:F:94:ASP:N	2.34	0.42
3:G:51:PRO:CD	3:G:64:LYS:HD2	2.48	0.42
3:G:60:ILE:O	3:G:60:ILE:HG13	2.19	0.42
1:A:59:TYR:HB2	1:A:64:LYS:CD	2.43	0.42
3:C:18:VAL:HG13	3:C:20:LYS:HZ3	1.85	0.42
3:D:120:HIS:CE1	3:D:122:LEU:HB2	2.55	0.42
3:D:459:LEU:HD12	3:D:469:LEU:HG	2.01	0.42
3:E:49:TYR:C	3:E:64:LYS:HE3	2.40	0.42
3:E:77:LEU:O	3:E:327:ASN:HB3	2.20	0.42
3:E:167:GLU:HA	3:E:191:ILE:O	2.19	0.42
3:F:101:ALA:HB3	3:F:377:GLN:HB3	2.02	0.42
3:H:85:PHE:CE2	3:H:378:LEU:HD21	2.54	0.42
3:H:153:GLN:C	3:H:154:THR:HG1	2.23	0.42
3:H:414:LEU:HD23	3:H:414:LEU:HA	1.62	0.42
3:C:20:LYS:HB2	3:C:21:VAL:H	1.36	0.42
3:C:157:CYS:SG	3:C:158:LEU:N	2.92	0.42
3:C:195:ILE:HA	3:C:230:LYS:HZ2	1.83	0.42
3:C:197:ASP:CB	3:C:446:PHE:HA	2.50	0.42
3:D:36:HIS:CE1	3:D:373:GLN:CB	3.03	0.42
3:D:109:ARG:HB3	3:D:308:ASN:ND2	2.28	0.42
3:D:128:ASP:OD1	3:D:130:GLU:N	2.53	0.42
3:D:158:LEU:HD12	3:D:332:THR:HB	2.02	0.42
3:D:401:ASP:O	3:D:402:TRP:HD1	2.03	0.42
3:D:464:LEU:HD23	3:D:465:GLY:HA2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:473:GLY:O	3:D:474:LEU:HG	2.20	0.42
3:E:68:LEU:HD23	3:E:68:LEU:HA	1.78	0.42
3:E:74:ARG:HB3	3:E:448:GLU:OE1	2.20	0.42
3:E:126:LEU:CB	3:E:262:ASN:HB2	2.48	0.42
3:E:209:ASP:OD1	3:E:211:THR:N	2.53	0.42
3:E:259:HIS:CE1	3:F:130:GLU:OE2	2.73	0.42
3:F:101:ALA:N	3:F:377:GLN:O	2.49	0.42
3:F:246:LEU:HD12	3:F:246:LEU:O	2.20	0.42
3:C:85:PHE:CZ	3:C:378:LEU:HD22	2.55	0.41
3:E:156:LEU:C	3:E:156:LEU:HD12	2.41	0.41
3:E:168:HIS:CE1	3:E:191:ILE:HB	2.54	0.41
3:G:70:TYR:CD1	3:G:334:VAL:HG21	2.51	0.41
3:G:261:PHE:O	3:G:291:TYR:HA	2.20	0.41
3:H:96:GLN:HG2	3:H:382:THR:HA	2.01	0.41
3:H:223:ASP:OD1	3:H:224:ILE:HG23	2.20	0.41
3:H:451:LEU:O	3:H:453:GLU:N	2.52	0.41
1:A:100(B):GLU:OE1	2:B:30(F):LYS:HD3	2.20	0.41
2:B:23:CYS:HB3	2:B:35:TRP:CH2	2.55	0.41
2:B:37:GLN:HA	2:B:85:VAL:O	2.20	0.41
3:D:120:HIS:HA	3:D:121:PRO:HD3	1.94	0.41
3:D:202:ASP:HB2	3:D:204:GLY:N	2.23	0.41
3:D:336:THR:O	3:D:338:ARG:N	2.53	0.41
3:D:399:LEU:O	3:D:402:TRP:O	2.38	0.41
3:E:97:ARG:NH2	3:E:403:ASN:C	2.72	0.41
3:F:94:ASP:HA	3:F:404:PHE:CE2	2.55	0.41
3:G:154:THR:HG23	3:G:253:GLU:HB3	2.02	0.41
3:G:384:THR:O	3:G:388:MET:HG3	2.20	0.41
3:H:320:ASN:ND2	3:H:323:ILE:O	2.32	0.41
1:A:18:LEU:HD21	1:A:90:TYR:HE2	1.84	0.41
1:A:39:GLN:HB3	1:A:89:MET:H	1.86	0.41
1:A:96:LEU:HG	1:A:97:TYR:H	1.84	0.41
2:B:49:TYR:CZ	2:B:53:THR:HG22	2.54	0.41
3:C:15:PRO:CB	3:C:17:PRO:HD2	2.39	0.41
3:D:141:VAL:CG1	3:H:356:LYS:HA	2.50	0.41
3:D:231:TYR:CE1	3:H:112:PRO:HA	2.55	0.41
3:D:469:LEU:O	3:D:473:GLY:N	2.53	0.41
3:D:470:LEU:HD12	3:D:470:LEU:HA	1.62	0.41
3:E:19:SER:O	3:E:20:LYS:HB2	2.21	0.41
3:E:187:PRO:C	3:E:188:LEU:HD12	2.40	0.41
3:E:216:ASN:OD1	3:E:218:SER:HB2	2.20	0.41
3:E:366:HIS:ND1	3:E:368:GLU:OE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:111:GLN:O	3:F:113:LEU:HD12	2.20	0.41
3:F:216:ASN:C	3:F:218:SER:H	2.23	0.41
3:F:360:PHE:O	3:G:266:ALA:HB3	2.20	0.41
3:G:385:ALA:HA	3:G:388:MET:HE3	2.02	0.41
3:H:312:TRP:CH2	3:H:468:PHE:CD1	2.92	0.41
2:B:6:GLN:HE21	2:B:101:GLY:H	1.68	0.41
2:B:43:SER:HB2	2:B:45:LYS:HE3	2.03	0.41
3:C:414:LEU:O	3:C:415:GLU:HB2	2.20	0.41
3:C:420:PHE:CD1	3:H:41:ARG:NH1	2.88	0.41
3:D:51:PRO:N	3:D:64:LYS:HB2	2.35	0.41
3:D:161:CYS:O	3:D:162:LYS:HD3	2.19	0.41
3:E:78:PRO:HD3	3:E:452:LYS:HA	2.01	0.41
3:E:90:PHE:CE1	3:E:91:TYR:CD2	3.08	0.41
3:E:344:LEU:HB2	3:F:213:LEU:O	2.20	0.41
3:E:387:VAL:O	3:E:388:MET:C	2.58	0.41
3:F:97:ARG:HH22	3:F:404:PHE:H	1.69	0.41
3:F:112:PRO:HB3	3:G:231:TYR:CD1	2.56	0.41
3:G:77:LEU:HD22	3:G:455:PHE:HZ	1.86	0.41
3:G:116:GLY:HA3	3:G:339:SER:O	2.20	0.41
3:H:156:LEU:O	3:H:333:VAL:HG13	2.21	0.41
3:H:256:PHE:CE2	3:H:298:SER:HB2	2.56	0.41
2:B:11:LEU:HD12	2:B:104:LEU:HD13	2.02	0.41
3:D:35:TYR:HD1	3:D:457:ALA:HA	1.85	0.41
3:D:53:LYS:HB3	3:D:53:LYS:HE2	1.72	0.41
3:D:76:HIS:ND1	3:D:449:VAL:C	2.70	0.41
3:D:127:ASP:O	3:D:261:PHE:HA	2.20	0.41
3:D:246:LEU:HD13	3:D:248:PHE:CA	2.50	0.41
3:F:16:VAL:N	3:F:17:PRO:HD3	2.36	0.41
3:F:335:ASP:OD1	3:F:337:THR:N	2.48	0.41
3:F:395:ASN:CG	3:F:397:THR:HG1	2.14	0.41
3:H:77:LEU:O	3:H:327:ASN:HB3	2.21	0.41
3:H:154:THR:HG23	3:H:253:GLU:HB3	2.03	0.41
3:H:156:LEU:HD12	3:H:156:LEU:C	2.40	0.41
3:H:420:PHE:HB3	3:H:430:LYS:HE3	2.02	0.41
2:B:6:GLN:NE2	2:B:101:GLY:CA	2.83	0.41
3:C:50:PHE:CE1	3:C:52:ILE:HD13	2.55	0.41
3:C:387:VAL:O	3:C:388:MET:C	2.58	0.41
3:D:106:GLU:N	3:D:374:PHE:HD1	2.17	0.41
3:D:123:LEU:HD12	3:D:123:LEU:HA	1.65	0.41
3:D:172:GLY:C	3:D:187:PRO:HG2	2.41	0.41
3:D:253:GLU:HG2	3:H:302:SER:OG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:258:ARG:HB2	3:D:295:PRO:O	2.20	0.41
3:D:387:VAL:C	3:D:389:THR:N	2.74	0.41
3:D:416:ASP:O	3:D:418:TYR:CZ	2.74	0.41
3:E:60:ILE:O	3:E:60:ILE:HG13	2.21	0.41
3:E:345:CYS:SG	3:F:216:ASN:N	2.73	0.41
3:F:51:PRO:N	3:F:64:LYS:HB2	2.36	0.41
3:F:72:VAL:HG12	3:F:446:PHE:CD1	2.56	0.41
3:H:52:ILE:HB	3:H:62:VAL:N	2.36	0.41
3:H:52:ILE:HB	3:H:62:VAL:H	1.86	0.41
3:H:73:PHE:HZ	3:H:370:TYR:CD2	2.38	0.41
3:H:135:TYR:CG	3:H:136:ALA:N	2.89	0.41
3:H:392:HIS:O	3:H:396:SER:OG	2.34	0.41
3:H:406:LEU:O	3:H:407:GLN:C	2.59	0.41
2:B:24:LYS:HG3	2:B:69:THR:C	2.41	0.41
3:C:60:ILE:O	3:C:60:ILE:HG13	2.21	0.41
3:C:153:GLN:OE1	3:C:337:THR:HG22	2.20	0.41
3:D:40:SER:C	3:D:41:ARG:HG2	2.41	0.41
3:D:72:VAL:HG22	3:D:332:THR:HG21	2.02	0.41
3:D:475:LYS:C	3:D:477:LYS:H	2.22	0.41
3:E:48:PRO:O	3:E:64:LYS:HE3	2.21	0.41
3:E:50:PHE:HD1	3:E:51:PRO:O	2.04	0.41
3:E:51:PRO:CD	3:E:64:LYS:HD2	2.47	0.41
3:E:419:ARG:C	3:E:420:PHE:CD1	2.94	0.41
3:F:77:LEU:HA	3:F:77:LEU:HD23	1.83	0.41
3:G:35:TYR:HD2	3:G:100:TRP:HH2	1.68	0.41
3:G:83:PHE:CZ	3:H:13:LEU:HB3	2.56	0.41
3:G:164:PRO:HG2	3:G:195:ILE:HB	2.01	0.41
3:G:273:ASP:O	3:G:276:TYR:N	2.38	0.41
3:G:301:THR:HG23	3:G:303:ASP:N	2.36	0.41
3:G:404:PHE:HE2	3:G:409:PRO:CG	2.34	0.41
3:H:78:PRO:HD3	3:H:452:LYS:HA	2.02	0.41
2:B:88:CYS:SG	2:B:99:GLY:HA3	2.61	0.41
3:C:18:VAL:HG13	3:C:20:LYS:NZ	2.35	0.41
3:C:34:TYR:HE1	3:C:377:GLN:CG	2.34	0.41
3:C:73:PHE:CD1	3:C:447:TRP:HD1	2.38	0.41
3:C:171:LYS:HB2	3:C:213:LEU:CD1	2.51	0.41
3:C:335:ASP:OD2	3:C:338:ARG:NH1	2.53	0.41
3:D:70:TYR:N	3:D:199:ASP:N	2.65	0.41
3:D:80:PRO:HD3	3:D:100:TRP:CD1	2.55	0.41
3:D:103:VAL:N	3:D:375:ILE:O	2.53	0.41
3:D:106:GLU:N	3:D:374:PHE:CD1	2.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:344:LEU:HD21	3:D:363:TYR:CD2	2.49	0.41
3:D:382:THR:C	3:D:383:LEU:HD23	2.41	0.41
3:E:223:ASP:OD1	3:E:224:ILE:HG23	2.20	0.41
3:E:328:GLN:HE21	3:E:330:PHE:HE1	1.68	0.41
3:F:408:PRO:N	3:F:409:PRO:CD	2.84	0.41
3:G:46:GLY:CA	3:G:65:VAL:HB	2.44	0.41
3:G:222:LEU:O	3:G:223:ASP:C	2.59	0.41
3:G:328:GLN:HE21	3:G:330:PHE:HE1	1.68	0.41
3:H:123:LEU:N	3:H:144:ARG:HB3	2.35	0.41
1:A:18:LEU:HG	1:A:20:LEU:HD13	2.01	0.41
3:C:78:PRO:HD3	3:C:452:LYS:HG2	2.02	0.41
3:C:83:PHE:CG	3:C:84:GLY:N	2.89	0.41
3:C:156:LEU:C	3:C:156:LEU:HD12	2.41	0.41
3:C:162:LYS:HG2	3:C:244:ASP:HB3	2.02	0.41
3:C:390:TYR:O	3:C:393:SER:HB2	2.21	0.41
3:D:76:HIS:H	3:D:451:LEU:HD12	1.86	0.41
3:D:112:PRO:HD3	3:E:231:TYR:CD2	2.56	0.41
3:D:115:VAL:HA	3:D:339:SER:HG	1.85	0.41
3:D:189:GLU:HG2	3:D:190:LEU:C	2.41	0.41
3:D:349:SER:H	3:D:359:ASN:ND2	2.18	0.41
3:D:431:HIS:C	3:D:433:PRO:HD2	2.40	0.41
3:D:451:LEU:HD23	3:D:451:LEU:HA	1.76	0.41
3:D:458:ASP:HB2	3:D:461:GLN:OE1	2.20	0.41
3:D:459:LEU:HB2	3:D:469:LEU:HD12	2.03	0.41
3:E:12:TYR:CD1	3:E:12:TYR:O	2.74	0.41
3:E:142:ASP:CG	3:F:283:THR:HG21	2.41	0.41
3:E:404:PHE:CB	3:E:405:GLY:O	2.67	0.41
3:F:97:ARG:NH1	3:F:404:PHE:HD2	2.19	0.41
3:F:98:LEU:HD23	3:F:98:LEU:HA	1.83	0.41
3:F:222:LEU:O	3:F:223:ASP:C	2.58	0.41
3:F:247:PHE:HE1	3:F:313:LEU:HD13	1.86	0.41
3:G:111:GLN:O	3:G:113:LEU:HD12	2.21	0.41
3:G:209:ASP:HA	3:G:228:ILE:HG13	2.03	0.41
3:G:377:GLN:CG	3:G:378:LEU:H	2.34	0.41
3:H:42:LEU:HD23	3:H:42:LEU:HA	1.92	0.41
3:H:65:VAL:HA	3:H:69:GLN:OE1	2.20	0.41
3:H:450:ASN:HD21	3:H:452:LYS:HD2	1.86	0.41
1:A:15:GLY:O	1:A:82(B):SER:HA	2.21	0.41
3:C:21:VAL:HG12	3:C:22:VAL:N	2.36	0.41
3:C:216:ASN:O	3:C:217:LYS:HB3	2.21	0.41
3:C:424:GLN:HA	3:H:43:LEU:HD23	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:375:ILE:HG22	3:D:376:PHE:N	2.35	0.41
3:D:433:PRO:O	3:D:436:PRO:HD3	2.21	0.41
3:E:196:GLN:NE2	3:E:444:TYR:HD1	2.18	0.41
3:F:209:ASP:OD2	3:F:212:THR:HG23	2.21	0.41
3:G:255:MET:HG2	3:G:256:PHE:N	2.36	0.41
3:G:387:VAL:O	3:G:388:MET:C	2.59	0.41
3:G:402:TRP:N	3:G:402:TRP:CD1	2.88	0.41
3:H:46:GLY:CA	3:H:65:VAL:HB	2.46	0.41
3:H:280:SER:O	3:H:283:THR:OG1	2.23	0.41
3:H:377:GLN:CG	3:H:378:LEU:N	2.84	0.41
1:A:24:ALA:HB2	1:A:29:PHE:HD1	1.85	0.40
2:B:30(A):TYR:CG	2:B:30(B):SER:N	2.89	0.40
3:C:451:LEU:O	3:C:453:GLU:N	2.54	0.40
3:D:53:LYS:HB2	3:D:59:LYS:O	2.21	0.40
3:D:266:ALA:HB2	3:H:357:ASN:O	2.21	0.40
3:D:442:LYS:HE3	3:D:442:LYS:HB3	1.79	0.40
3:D:459:LEU:HA	3:D:462:PHE:CB	2.51	0.40
3:E:36:HIS:CE1	3:E:37:ALA:O	2.74	0.40
3:E:113:LEU:HD12	3:E:113:LEU:N	2.36	0.40
3:E:384:THR:H	3:E:387:VAL:HB	1.85	0.40
3:F:111:GLN:HB2	3:F:338:ARG:CD	2.43	0.40
3:G:36:HIS:CE1	3:G:37:ALA:O	2.74	0.40
3:G:105:VAL:HG13	3:G:374:PHE:CD1	2.57	0.40
3:G:150:ASP:CG	3:G:297:GLY:H	2.24	0.40
3:H:422:THR:HG23	3:H:430:LYS:HG3	2.04	0.40
3:C:34:TYR:CE2	3:C:468:PHE:HZ	2.39	0.40
3:C:120:HIS:HA	3:C:121:PRO:HD3	1.94	0.40
3:D:52:ILE:HB	3:D:62:VAL:N	2.36	0.40
3:D:70:TYR:HD2	3:D:199:ASP:HB2	1.85	0.40
3:D:105:VAL:HG13	3:D:374:PHE:CE1	2.55	0.40
3:D:156:LEU:C	3:D:156:LEU:HD12	2.42	0.40
3:D:161:CYS:HG	3:D:244:ASP:HB3	1.85	0.40
3:D:162:LYS:CA	3:D:245:SER:HA	2.51	0.40
3:D:268:GLY:HA2	3:H:361:LYS:HB3	2.03	0.40
3:D:355:TYR:OH	3:D:357:ASN:HA	2.22	0.40
3:D:382:THR:O	3:D:383:LEU:HD23	2.21	0.40
3:E:72:VAL:HG12	3:E:446:PHE:CD1	2.56	0.40
3:G:35:TYR:HD2	3:G:100:TRP:CH2	2.39	0.40
3:G:275:LEU:HD23	3:G:275:LEU:HA	1.71	0.40
3:G:335:ASP:CG	3:G:337:THR:H	2.23	0.40
3:C:155:GLN:HE22	3:C:305:GLN:HA	1.87	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:435:ALA:HA	3:C:436:PRO:HD2	1.91	0.40
3:D:119:GLY:HA3	3:D:147:ILE:O	2.21	0.40
3:D:276:TYR:HD1	3:D:277:ILE:O	2.03	0.40
3:D:479:LYS:NZ	3:E:19:SER:O	2.47	0.40
3:F:15:PRO:CG	3:F:17:PRO:HD3	2.51	0.40
3:F:373:GLN:O	3:F:374:PHE:HD1	2.04	0.40
3:F:477:LYS:HZ2	3:G:23:SER:N	2.19	0.40
3:G:408:PRO:C	3:G:410:PRO:HD3	2.41	0.40
1:A:47:TRP:HZ2	1:A:50:SER:OG	2.04	0.40
1:A:63:VAL:CA	1:A:66:ARG:HB2	2.51	0.40
3:C:406:LEU:HD11	3:C:410:PRO:HA	2.04	0.40
3:D:123:LEU:N	3:D:145:GLU:O	2.53	0.40
3:D:172:GLY:H	3:D:188:LEU:N	2.19	0.40
3:D:259:HIS:C	3:D:294:THR:HB	2.42	0.40
3:D:386:ASP:O	3:D:390:TYR:HB3	2.21	0.40
3:D:451:LEU:O	3:D:452:LYS:C	2.59	0.40
3:D:465:GLY:C	3:D:467:LYS:N	2.73	0.40
3:E:312:TRP:CZ3	3:E:468:PHE:HD1	2.38	0.40
3:F:109:ARG:HH21	3:F:338:ARG:HD2	1.84	0.40
3:F:255:MET:HG2	3:F:256:PHE:N	2.36	0.40
3:G:117:ILE:HG12	3:G:118:SER:N	2.36	0.40
3:G:158:LEU:HD23	3:G:158:LEU:HA	1.91	0.40
3:G:466:ARG:O	3:G:469:LEU:HB2	2.21	0.40
3:H:57:ASN:OD1	3:H:59:LYS:N	2.49	0.40
1:A:37:VAL:O	1:A:91:TYR:N	2.46	0.40
2:B:13:VAL:O	2:B:13:VAL:HG23	2.21	0.40
2:B:30(B):SER:O	2:B:30(E):GLN:HG2	2.21	0.40
3:C:84:GLY:O	3:C:85:PHE:HD1	2.04	0.40
3:C:166:GLY:N	3:C:195:ILE:HG13	2.36	0.40
3:D:157:CYS:CA	3:D:333:VAL:HG22	2.45	0.40
3:E:18:VAL:N	3:E:19:SER:HA	2.21	0.40
3:E:216:ASN:HB3	3:E:219:GLU:HG2	2.04	0.40
3:E:430:LYS:O	3:E:431:HIS:CG	2.74	0.40
3:F:123:LEU:O	3:F:144:ARG:HA	2.22	0.40
3:F:451:LEU:O	3:F:452:LYS:C	2.59	0.40
3:G:124:ASN:OD1	3:G:264:ALA:N	2.52	0.40
3:G:158:LEU:HB2	3:G:332:THR:O	2.21	0.40
3:G:360:PHE:O	3:H:266:ALA:HB3	2.22	0.40
3:H:84:GLY:C	3:H:85:PHE:CD1	2.95	0.40
3:H:110:GLY:HA3	3:H:369:GLU:OE2	2.20	0.40
3:H:246:LEU:HD12	3:H:246:LEU:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:399:LEU:HA	3:H:399:LEU:HD23	1.89	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	107/109 (98%)	95 (89%)	12 (11%)	0	100	100
2	B	108/110 (98%)	101 (94%)	6 (6%)	1 (1%)	17	56
3	C	466/469 (99%)	425 (91%)	33 (7%)	8 (2%)	9	43
3	D	458/469 (98%)	401 (88%)	54 (12%)	3 (1%)	22	62
3	E	467/469 (100%)	425 (91%)	33 (7%)	9 (2%)	8	40
3	F	466/469 (99%)	421 (90%)	36 (8%)	9 (2%)	8	40
3	G	465/469 (99%)	425 (91%)	29 (6%)	11 (2%)	6	35
3	H	466/469 (99%)	431 (92%)	28 (6%)	7 (2%)	10	46
All	All	3003/3033 (99%)	2724 (91%)	231 (8%)	48 (2%)	13	45

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	409	PRO
3	F	20	LYS
3	G	16	VAL
3	G	17	PRO
3	H	410	PRO
3	C	410	PRO
3	C	476	ALA
3	E	404	PHE
3	E	408	PRO

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Mol	Chain	Res	Type
3	F	426	ILE
3	H	422	THR
3	H	423	SER
3	C	18	VAL
3	C	408	PRO
3	E	405	GLY
3	F	475	LYS
3	G	409	PRO
3	G	424	GLN
2	B	51	ALA
3	E	14	PRO
3	E	387	VAL
3	F	40	SER
3	G	18	VAL
3	G	387	VAL
3	H	40	SER
3	H	387	VAL
3	C	40	SER
3	C	387	VAL
3	C	434	PRO
3	D	41	ARG
3	E	40	SER
3	E	235	ILE
3	F	387	VAL
3	F	474	LEU
3	G	40	SER
3	D	410	PRO
3	E	245	SER
3	F	17	PRO
3	F	235	ILE
3	G	235	ILE
3	G	436	PRO
3	H	235	ILE
3	C	235	ILE
3	D	387	VAL
3	G	15	PRO
3	F	21	VAL
3	H	408	PRO
3	G	14	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	89/89 (100%)	89 (100%)	0	100	100
2	B	96/96 (100%)	96 (100%)	0	100	100
3	C	407/408 (100%)	405 (100%)	2 (0%)	88	93
3	D	399/408 (98%)	393 (98%)	6 (2%)	65	80
3	E	408/408 (100%)	408 (100%)	0	100	100
3	F	407/408 (100%)	407 (100%)	0	100	100
3	G	406/408 (100%)	406 (100%)	0	100	100
3	H	406/408 (100%)	406 (100%)	0	100	100
All	All	2618/2633 (99%)	2610 (100%)	8 (0%)	92	95

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	C	17	PRO
3	C	406	LEU
3	D	247	PHE
3	D	303	ASP
3	D	386	ASP
3	D	392	HIS
3	D	401	ASP
3	D	424	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

There are no ligands in this entry.

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.

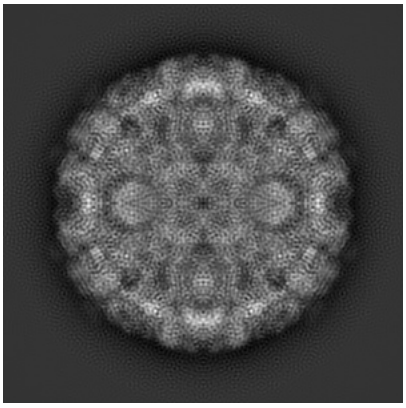
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-7136. These allow visual inspection of the internal detail of the map and identification of artifacts.

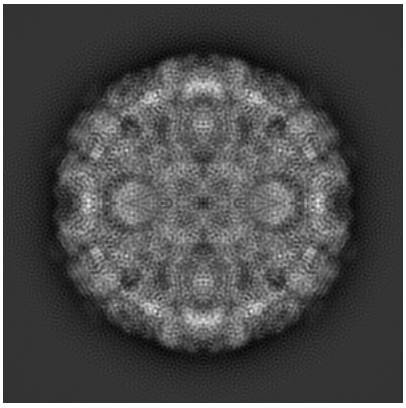
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

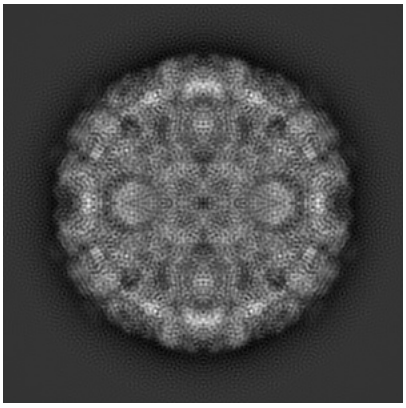
6.1.1 Primary map



X



Y

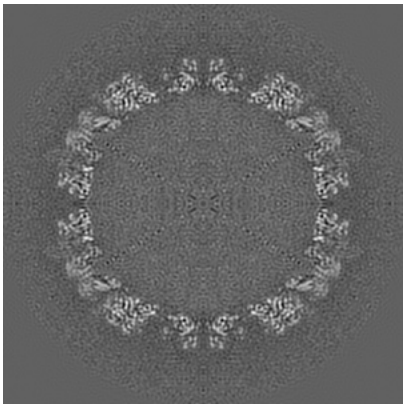


Z

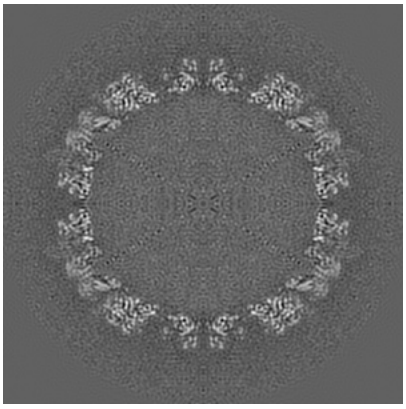
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

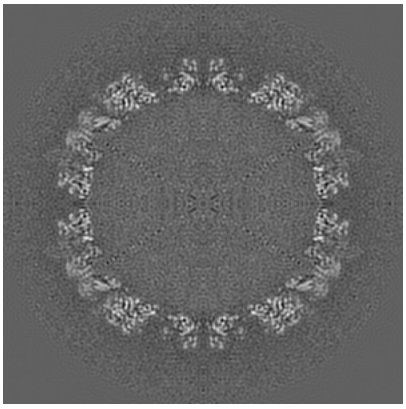
6.2.1 Primary map



X Index: 340



Y Index: 340

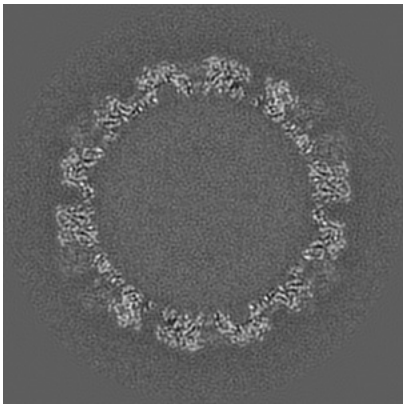


Z Index: 340

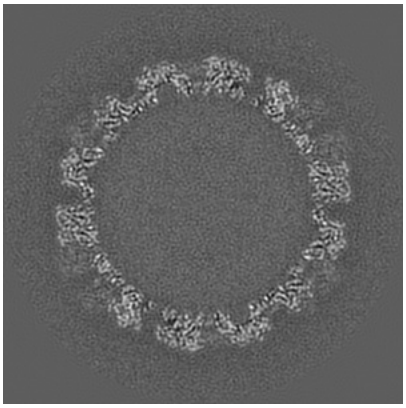
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

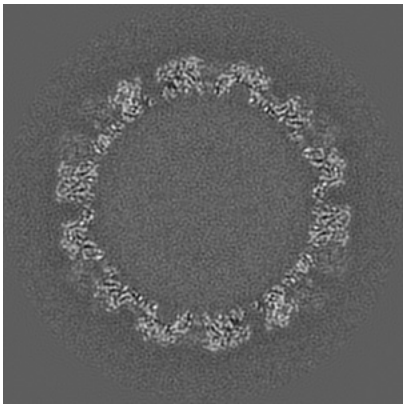
6.3.1 Primary map



X Index: 288



Y Index: 288

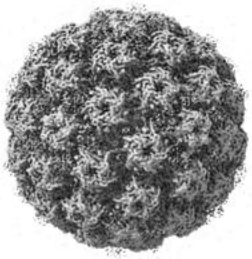


Z Index: 392

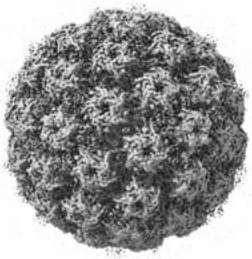
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

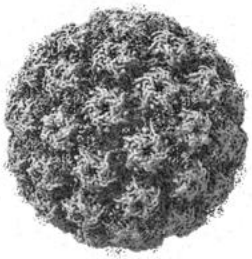
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 2.1. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

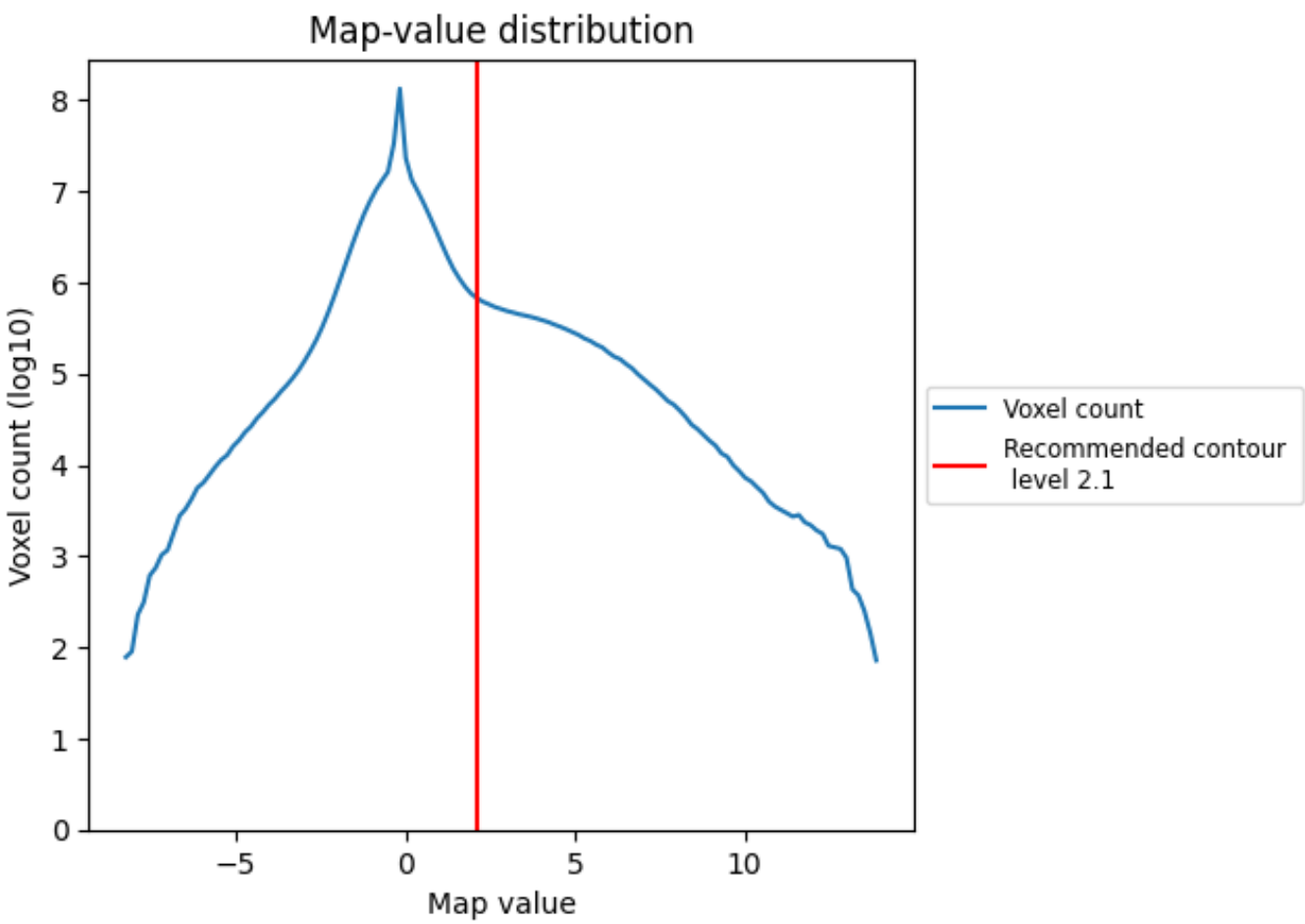
6.5 Mask visualisation (i)

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

7 Map analysis (i)

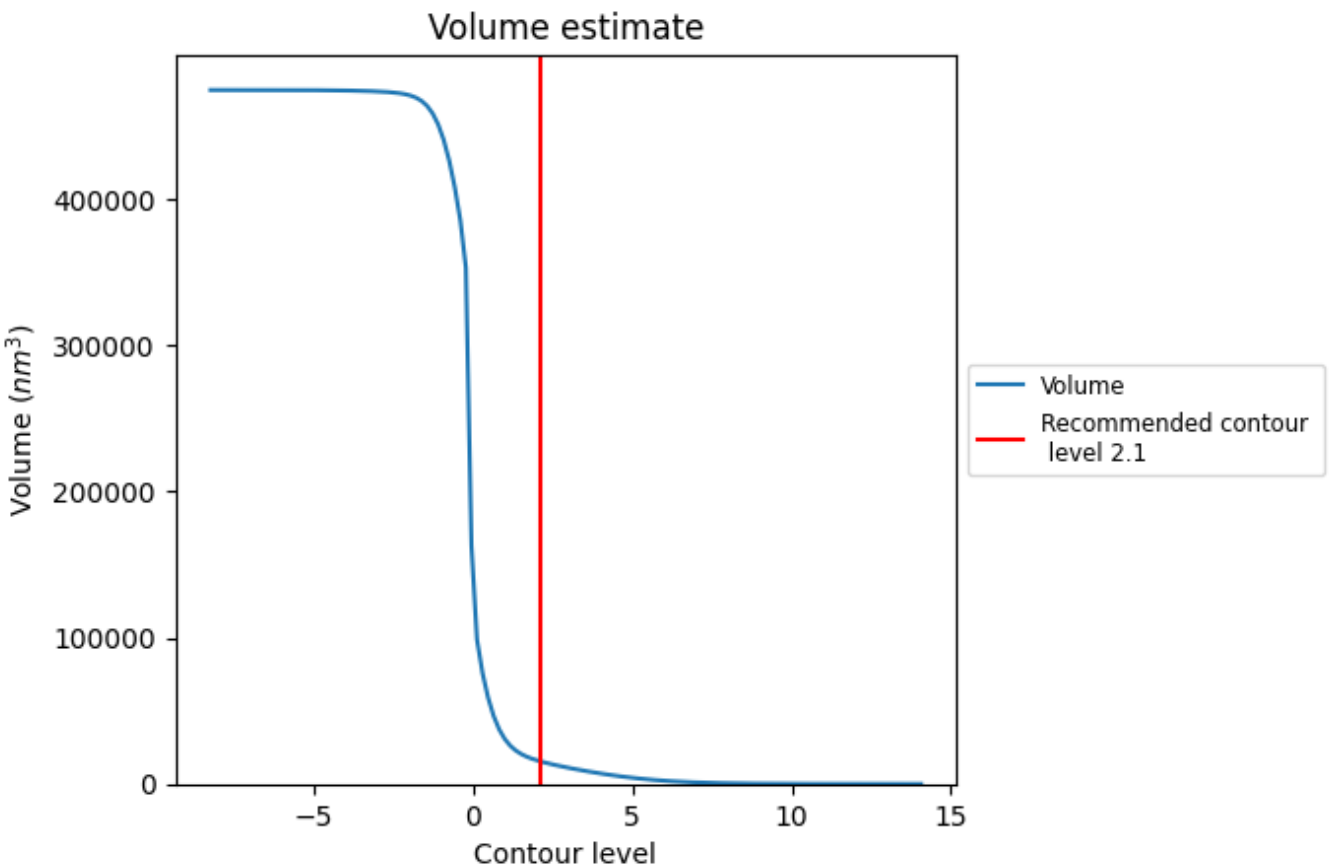
This section contains the results of statistical analysis of the map.

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.

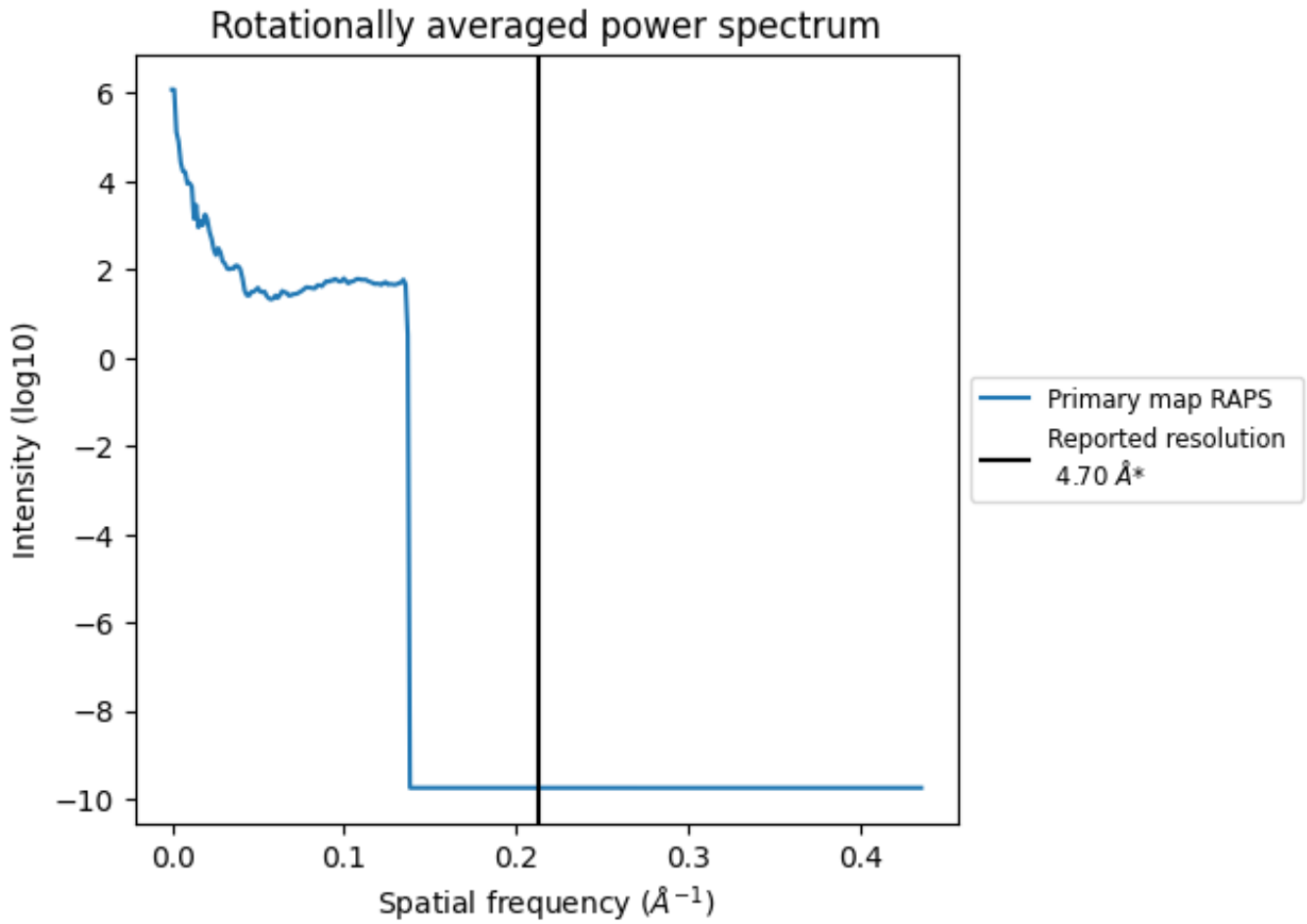
7.2 Volume estimate (i)



The volume at the recommended contour level is 15512 nm^3; this corresponds to an approximate mass of 14013 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.213 Å^{-1}

8 Fourier-Shell correlation (i)

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

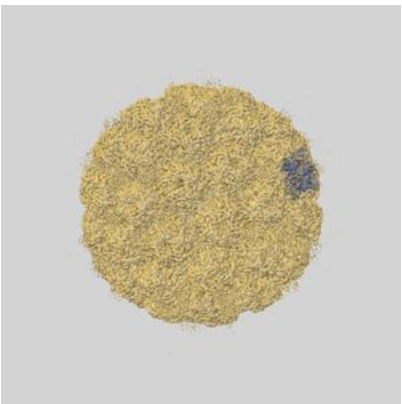
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-7136 and PDB model 6BSP. Per-residue inclusion information can be found in section 3 on page 4.

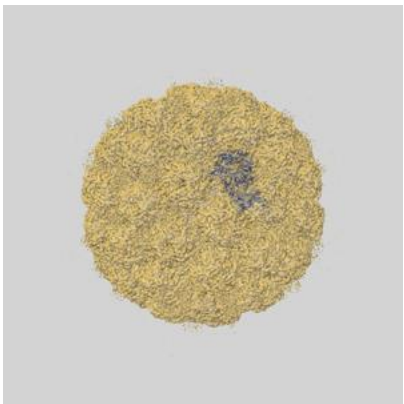
9.1 Map-model overlays

9.1.1 Map-model overlay (i)

X

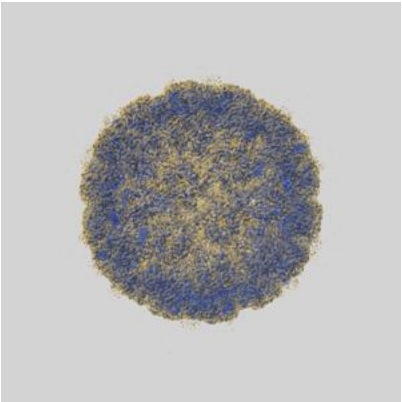


Y

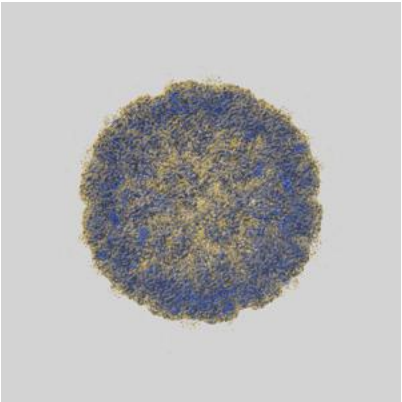


Z

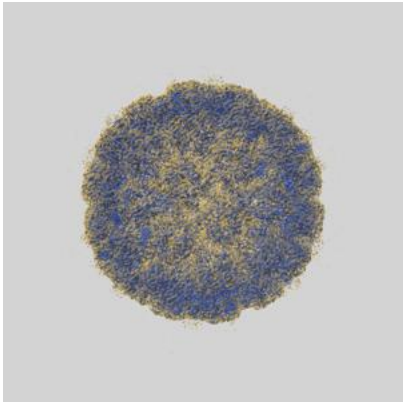
9.1.2 Map-model assembly overlay (i)



X



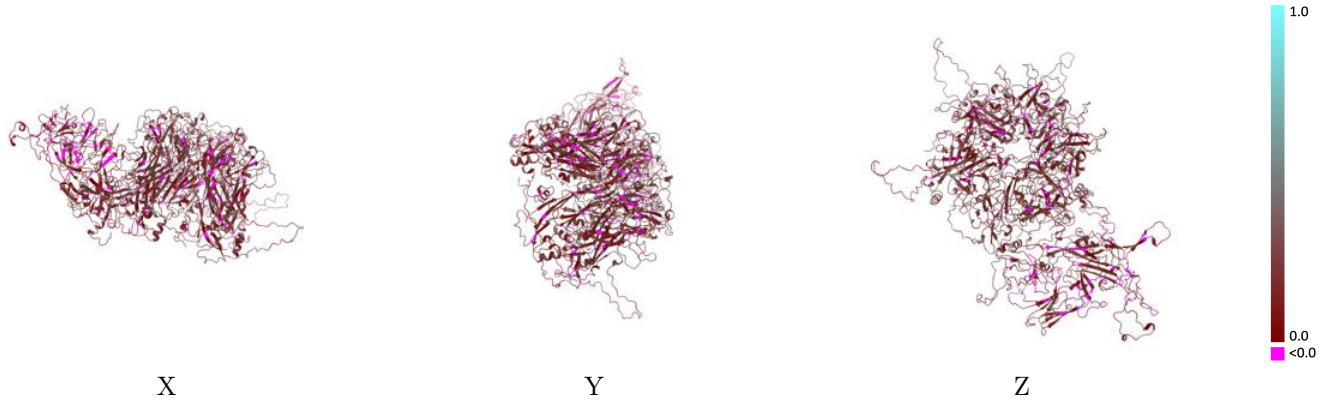
Y



Z

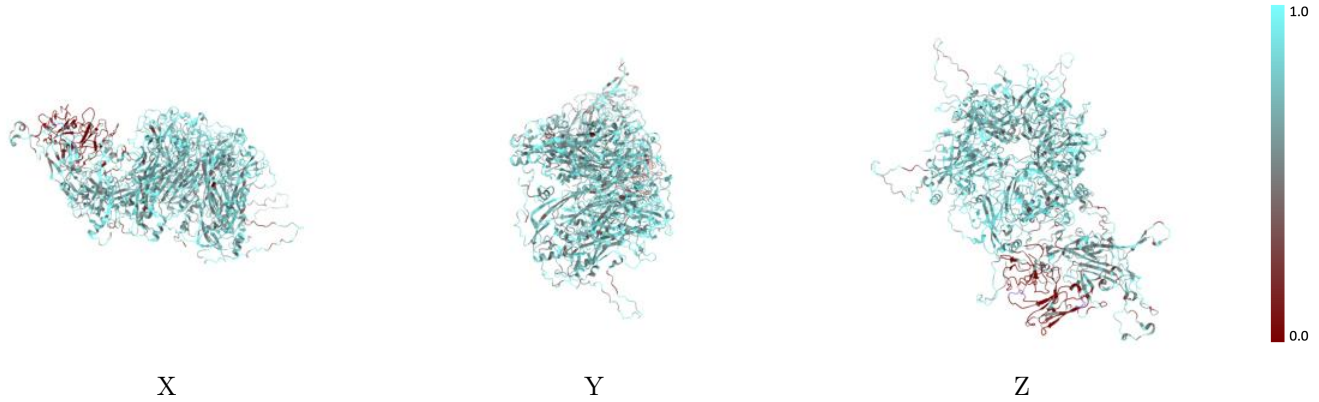
The images above show the 3D surface view of the map at the recommended contour level 2.1 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



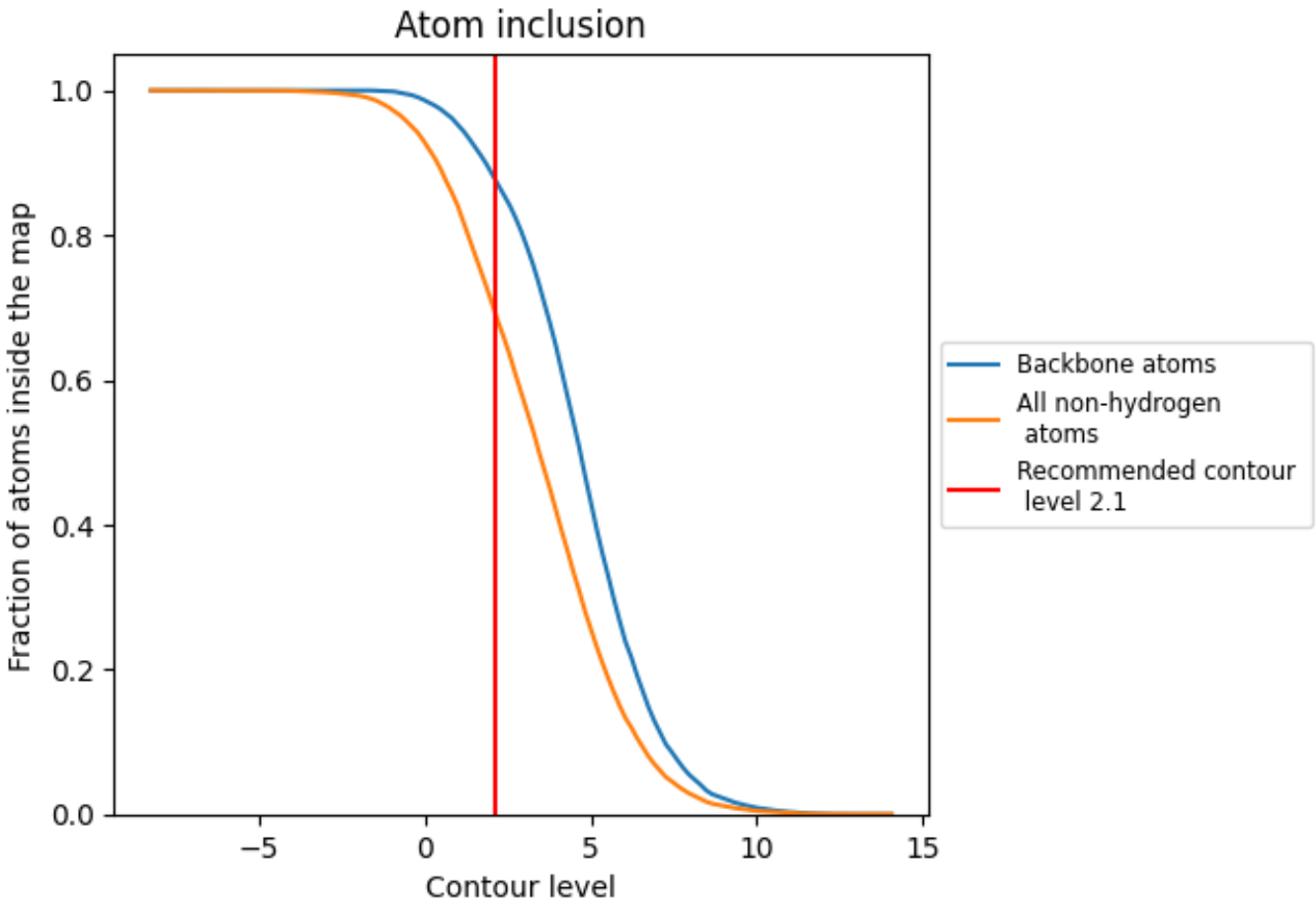
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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)



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 (2.1).

9.4 Atom inclusion (i)



At the recommended contour level, 88% of all backbone atoms, 70% 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 (2.1) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6951	0.1930
A	0.1212	0.1620
B	0.1210	0.1410
C	0.6492	0.1550
D	0.8416	0.2590
E	0.7405	0.1890
F	0.7419	0.1960
G	0.7352	0.1910
H	0.7279	0.1870