



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 03:41 PM UTC

PDB ID : 7ETJ / pdb_00007etj
EMDB ID : EMD-31298
Title : C5 portal vertex in the partially-enveloped virion capsid
Authors : Li, Z.; Yu, X.
Deposited on : 2021-05-13
Resolution : 4.00 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

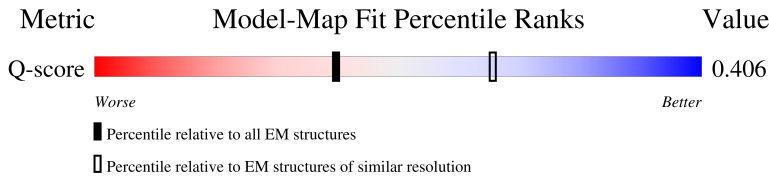
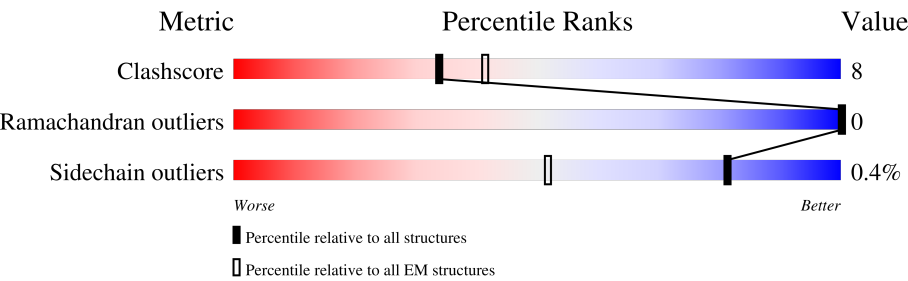
EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 4.00 Å.

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



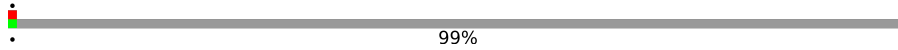
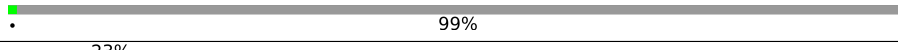
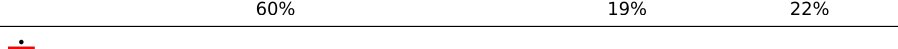
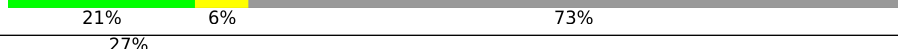
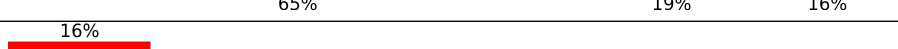
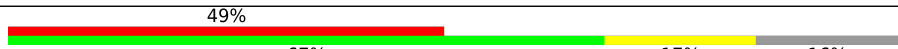
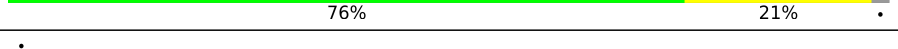
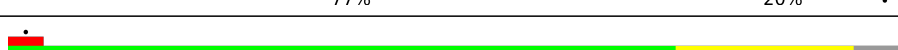
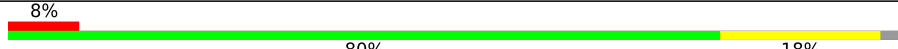
Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	7587 (3.50 - 4.50)

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 $\leq 5\%$. 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	I	306	11% 67% 31% .
1	h	306	11% 74% 24% .
1	n	306	. 78% 18% .
1	o	306	6% 77% 17% 6%

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Mol	Chain	Length	Quality of chain
2	H	2241	
2	P	2241	
3	g	290	
3	m	290	
4	M	594	
5	N	642	
5	O	642	
6	1	1048	
7	R	75	
7	S	75	
7	T	75	
7	i	75	
7	j	75	
8	B	1370	
8	C	1370	
8	D	1370	
8	Y	1370	
8	Z	1370	
8	a	1370	

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 86613 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 Triplex capsid protein 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	h	300	Total	C	N	O	S	0	0
			2384	1528	415	424	17		
1	I	301	Total	C	N	O	S	0	0
			2389	1531	417	424	17		
1	n	294	Total	C	N	O	S	0	0
			2329	1499	401	410	19		
1	o	289	Total	C	N	O	S	0	0
			2291	1473	393	407	18		

- Molecule 2 is a protein called Large tegument protein deneddylase.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	H	20	Total	C	N	O	S	0	0
			172	110	32	29	1		
2	P	20	Total	C	N	O	S	0	0
			172	110	32	29	1		

- Molecule 3 is a protein called Triplex capsid protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	g	227	Total	C	N	O	S	0	0
			1822	1171	319	321	11		
3	m	290	Total	C	N	O	S	0	0
			2325	1485	411	417	12		

- Molecule 4 is a protein called Capsid vertex component 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	M	468	Total	C	N	O	S	0	0
			3848	2408	740	686	14		

- Molecule 5 is a protein called Capsid vertex component 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	N	76	Total	C	N	O	S	0	0
			648	408	127	109	4		
5	O	69	Total	C	N	O	S	0	0
			589	371	113	102	3		

- Molecule 6 is a protein called ORFL92C_UL32.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	1	284	Total	C	N	O	S	0	0
			2320	1463	425	420	12		

- Molecule 7 is a protein called Small capsomere-interacting protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	R	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
7	S	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
7	T	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
7	i	63	Total	C	N	O	S	0	0
			513	321	97	91	4		
7	j	63	Total	C	N	O	S	0	0
			513	321	97	91	4		

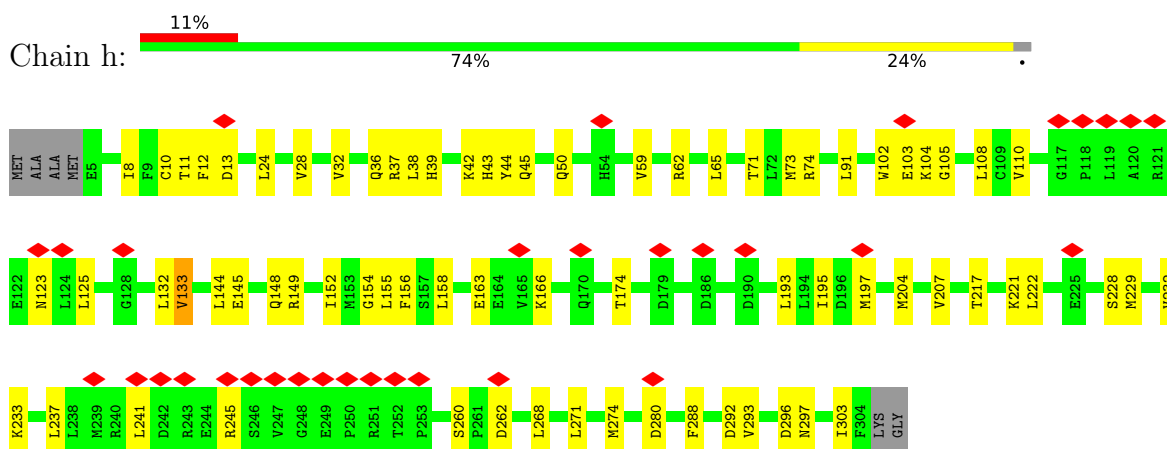
- Molecule 8 is a protein called Major capsid protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	1275	Total	C	N	O	S	0	0
			10079	6410	1756	1855	58		
8	B	1339	Total	C	N	O	S	0	0
			10617	6762	1838	1956	61		
8	C	1331	Total	C	N	O	S	0	0
			10536	6711	1827	1938	60		
8	D	1297	Total	C	N	O	S	0	0
			10269	6538	1785	1887	59		
8	Y	1347	Total	C	N	O	S	0	0
			10676	6799	1850	1966	61		
8	Z	1337	Total	C	N	O	S	0	0
			10582	6740	1831	1952	59		

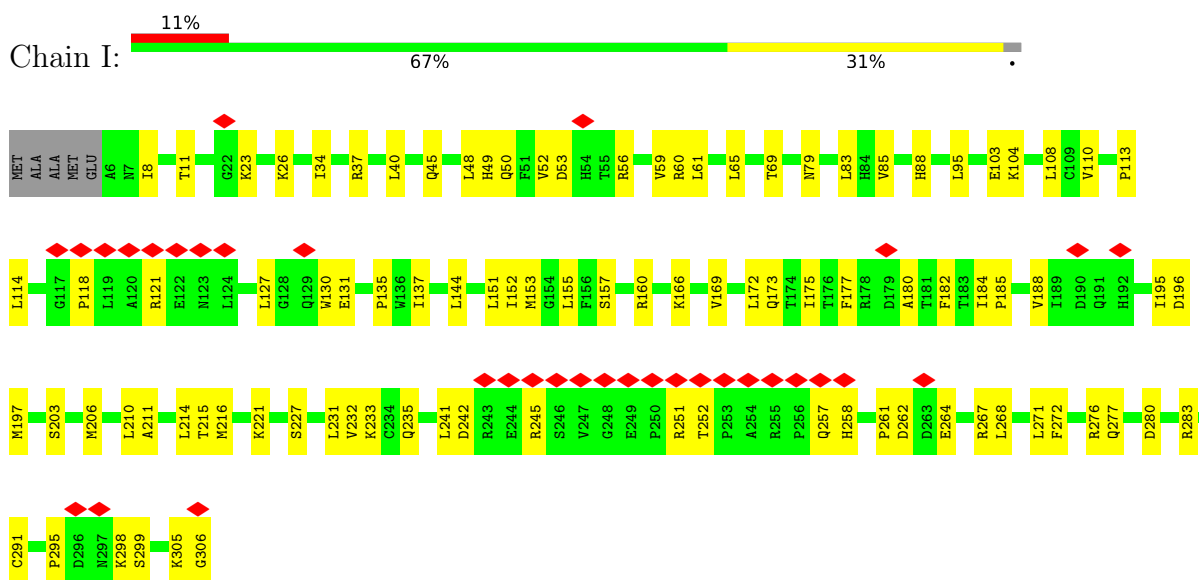
3 Residue-property plots

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.

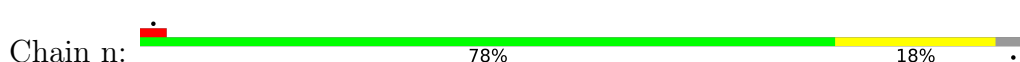
- Molecule 1: Triplex capsid protein 2

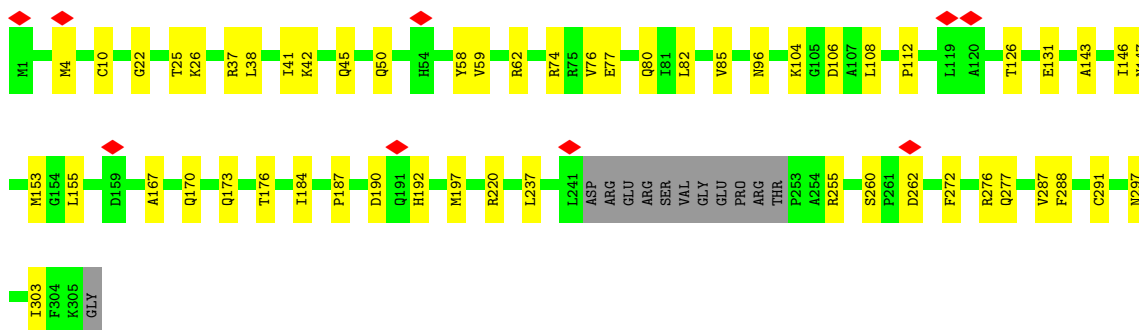


- Molecule 1: Triplex capsid protein 2

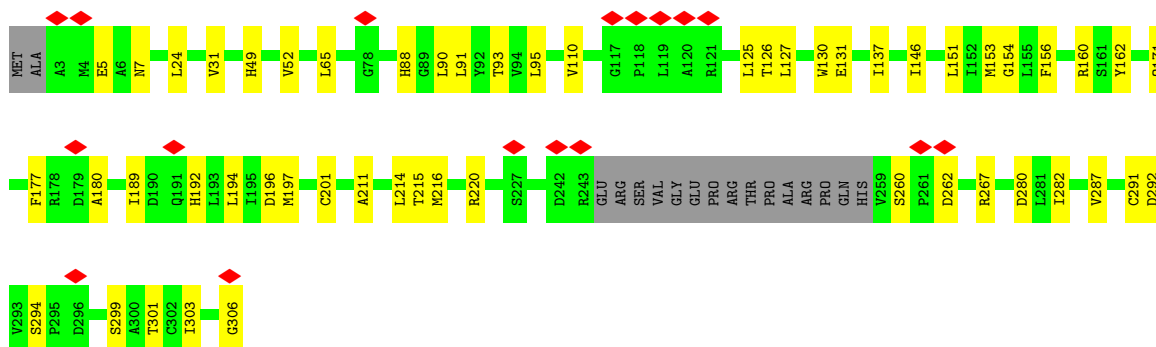
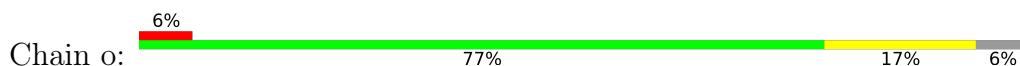


- Molecule 1: Triplex capsid protein 2

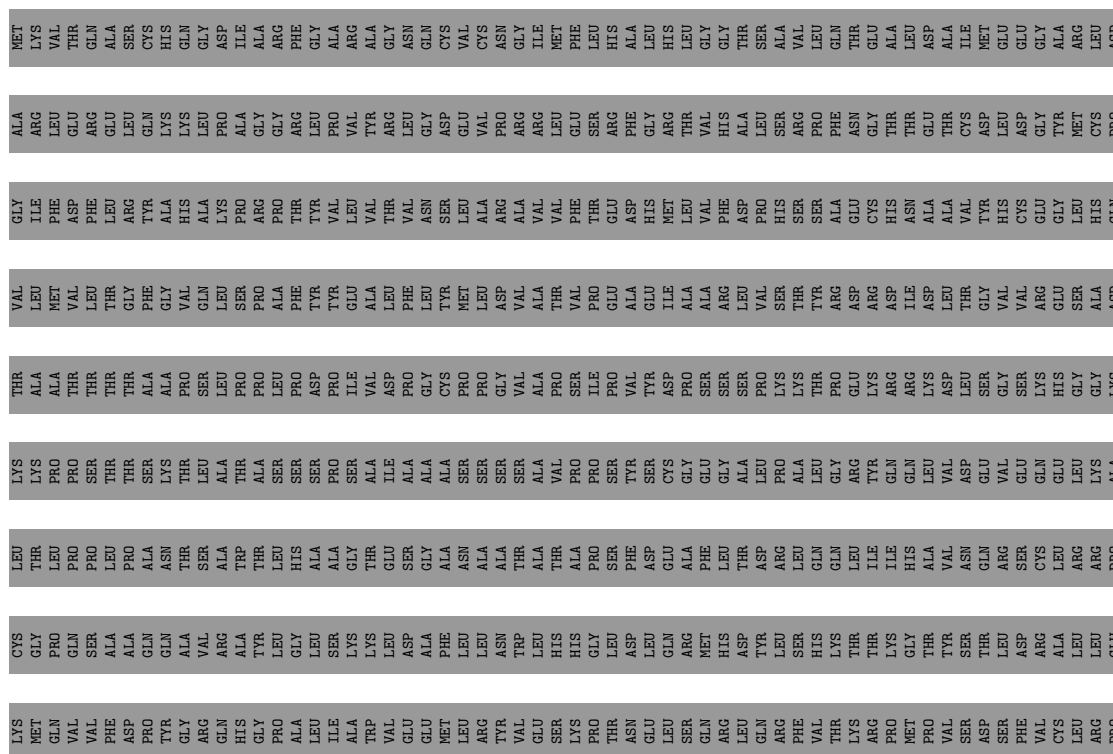




- Molecule 1: Triplex capsid protein 2



- Molecule 2: Large tegument protein deneddylase



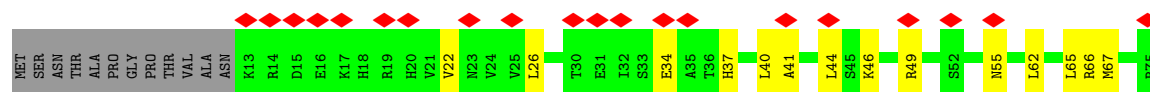




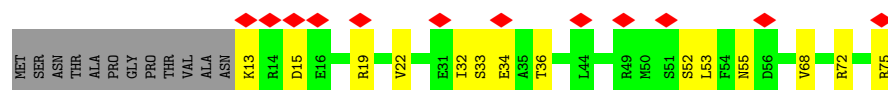




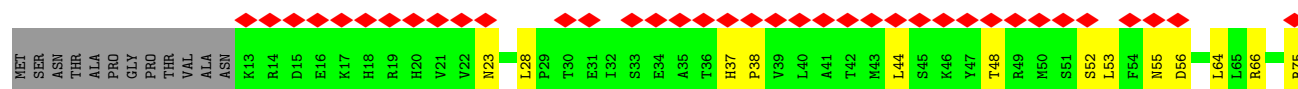




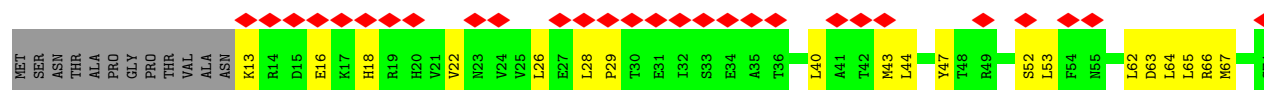
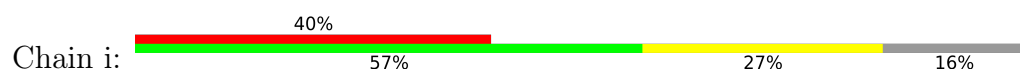
• Molecule 7: Small capsomere-interacting protein



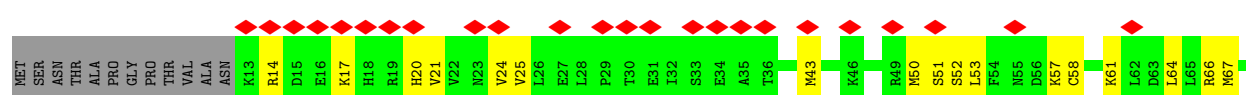
• Molecule 7: Small capsomere-interacting protein



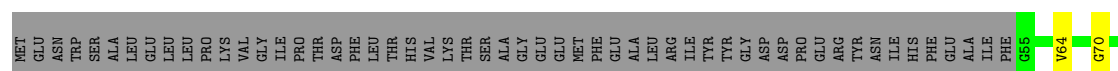
• Molecule 7: Small capsomere-interacting protein

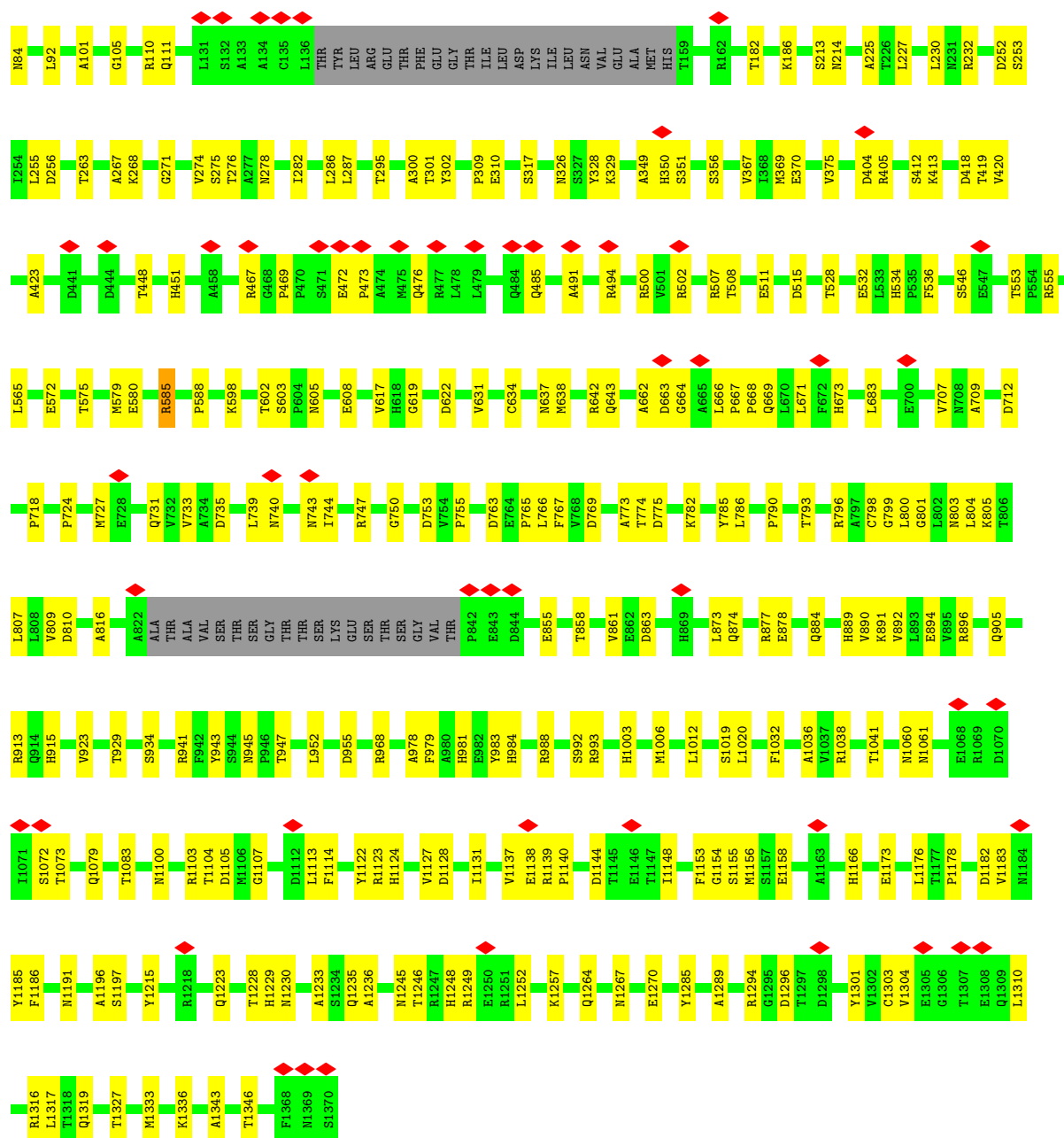


• Molecule 7: Small capsomere-interacting protein



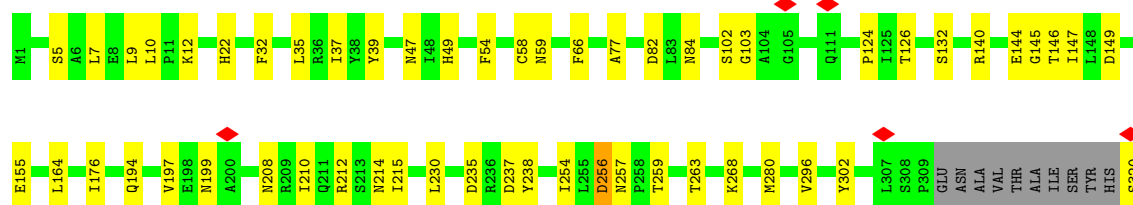
• Molecule 8: Major capsid protein

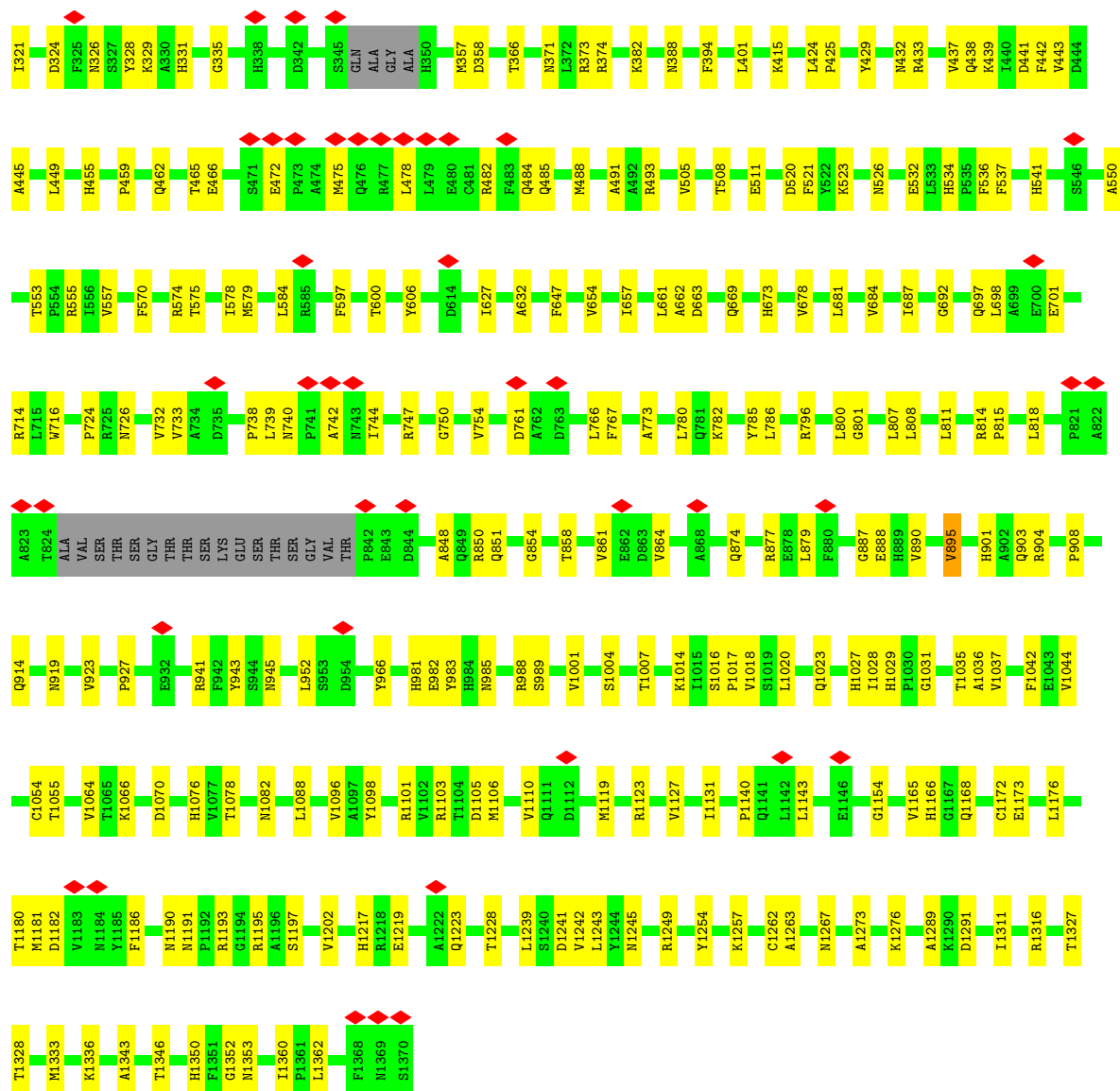




• Molecule 8: Major capsid protein

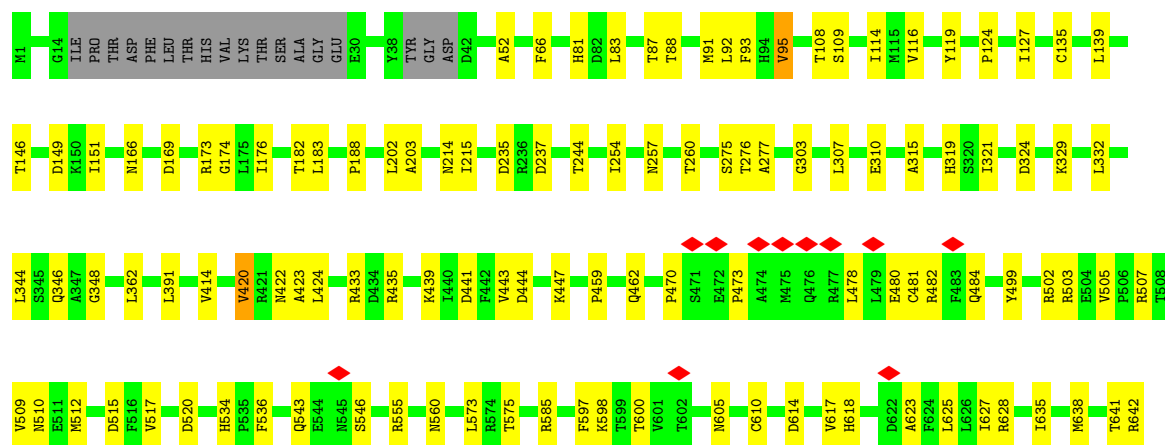
Chain B: 76% 21%

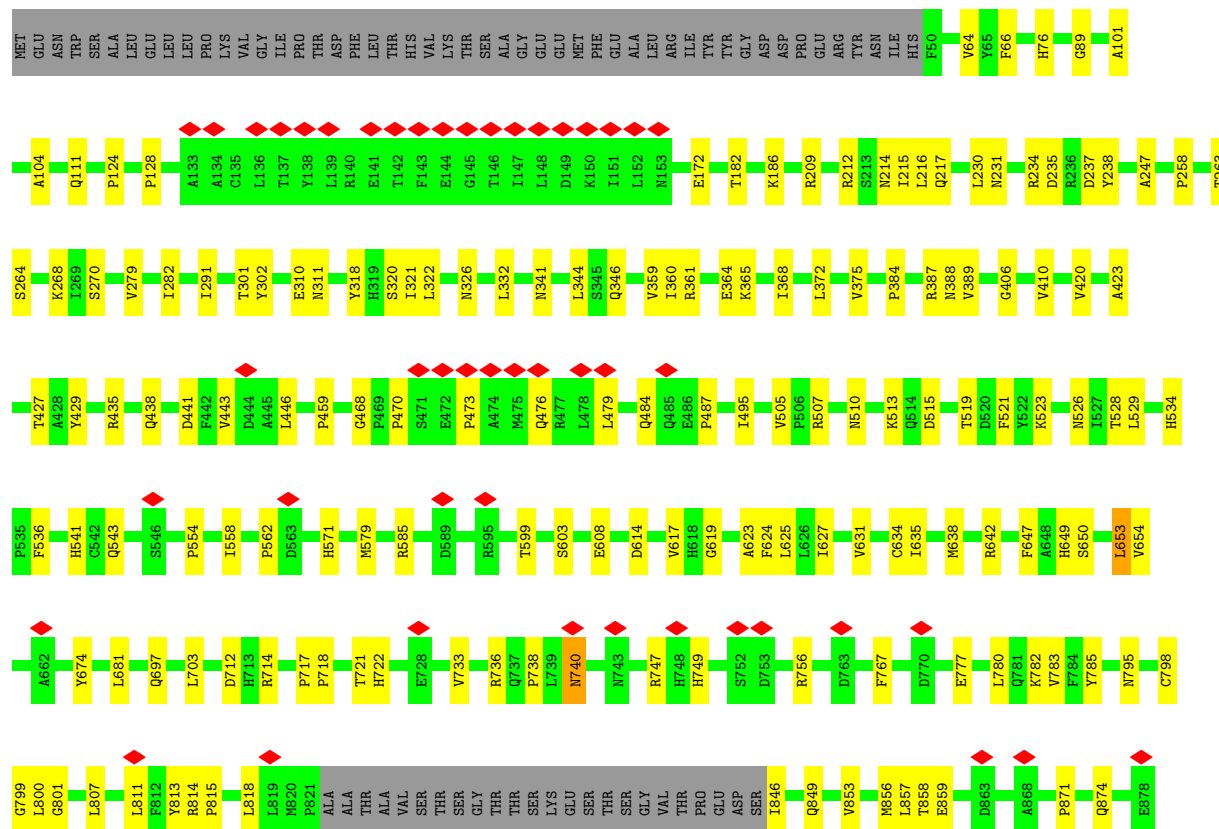


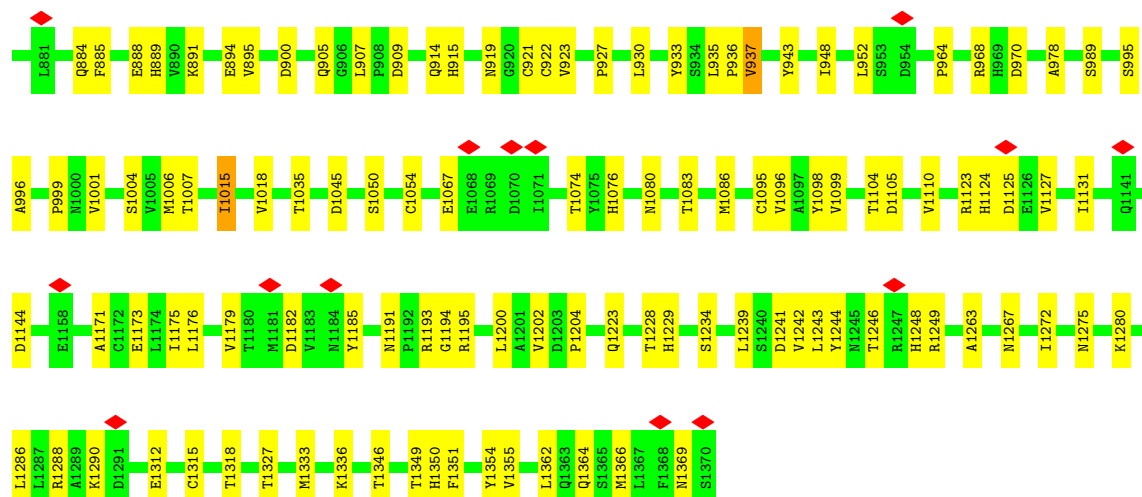


• Molecule 8: Major capsid protein

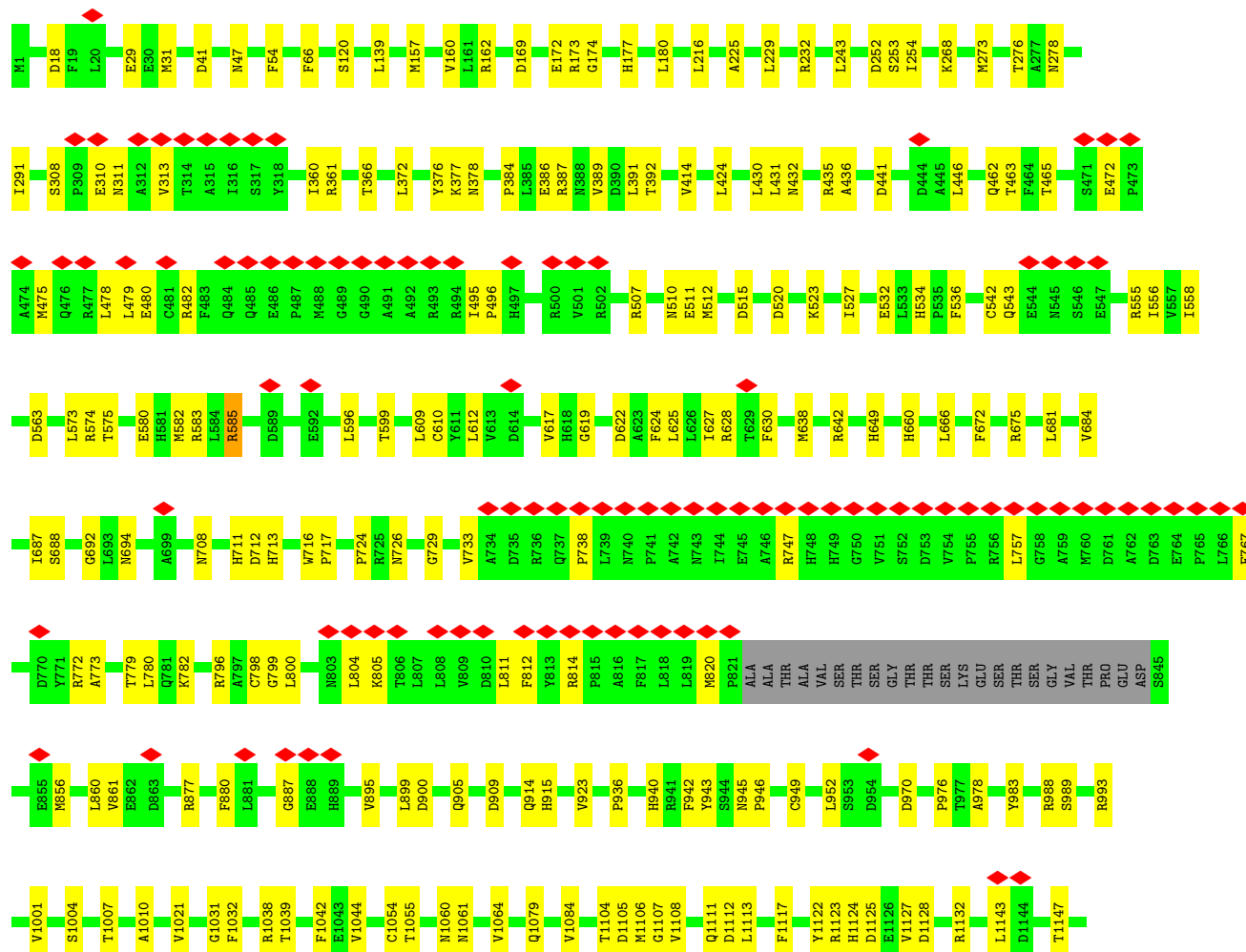
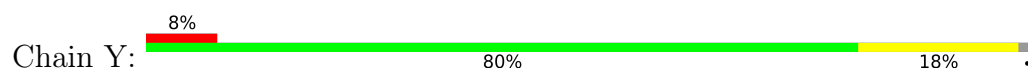
Chain C: 77% 20%

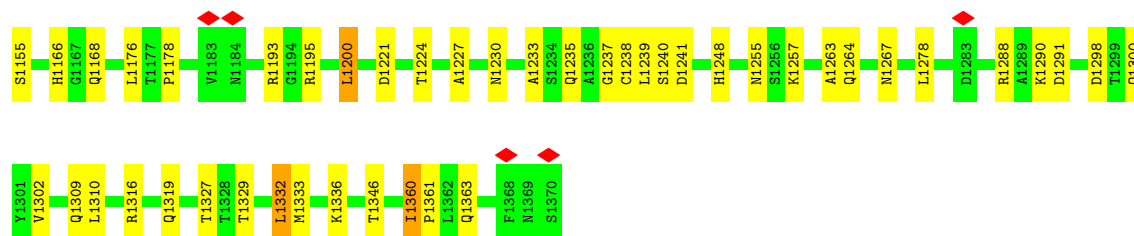






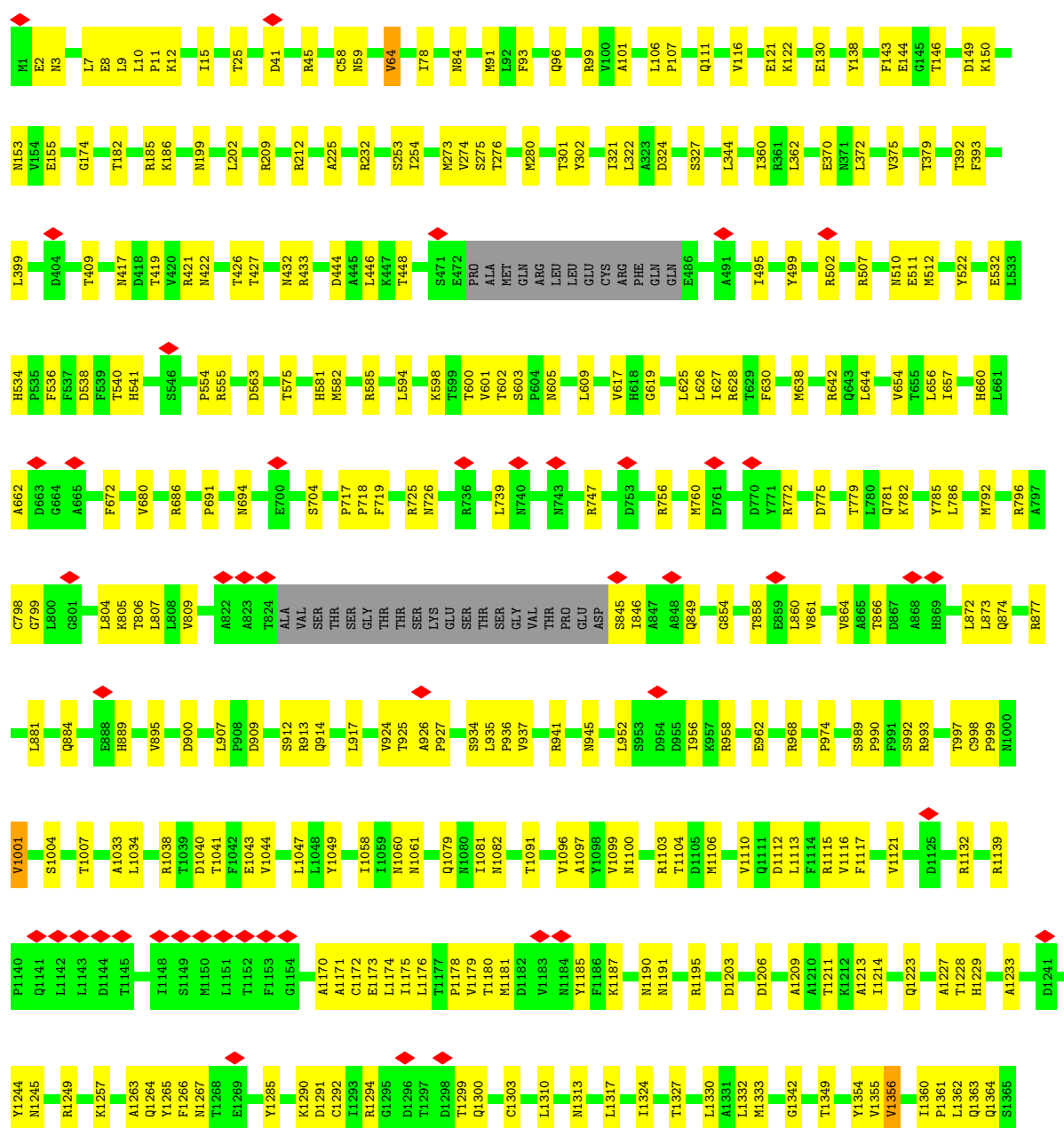
• Molecule 8: Major capsid protein





• Molecule 8: Major capsid protein

Chain Z: 76% 22%



M1366	
L1367	
F1368	
M1369	
S1370	

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	42849	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.093	Depositor
Minimum map value	-0.068	Depositor
Average map value	0.005	Depositor
Map value standard deviation	0.009	Depositor
Recommended contour level	0.015	Depositor
Map size ($\text{\AA}$)	416.0, 416.0, 416.0	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.625, 1.625, 1.625	Depositor

5 Model quality

5.1 Standard geometry

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	I	0.25	0/2436	0.61	0/3310
1	h	0.24	0/2431	0.56	0/3306
1	n	0.24	0/2374	0.51	1/3225 (0.0%)
1	o	0.23	0/2333	0.45	0/3167
2	H	0.19	0/174	0.56	0/233
2	P	0.19	0/174	0.41	0/233
3	g	0.23	0/1860	0.53	0/2521
3	m	0.26	0/2374	0.56	0/3221
4	M	0.26	0/3935	0.56	0/5331
5	N	0.24	0/662	0.63	0/892
5	O	0.21	0/600	0.56	0/808
6	l	0.20	0/2358	0.53	2/3182 (0.1%)
7	R	0.22	0/520	0.58	0/697
7	S	0.22	0/520	0.54	0/697
7	T	0.22	0/520	0.54	0/697
7	i	0.25	0/520	0.63	0/697
7	j	0.24	0/520	0.56	0/697
8	B	0.27	1/10870 (0.0%)	0.55	0/14804
8	C	0.27	0/10786	0.53	1/14692 (0.0%)
8	D	0.24	0/10513	0.50	1/14322 (0.0%)
8	Y	0.24	0/10932	0.50	0/14892
8	Z	0.26	0/10835	0.49	0/14762
8	a	0.27	0/10318	0.55	4/14057 (0.0%)
All	All	0.25	1/88565 (0.0%)	0.53	9/120443 (0.0%)

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
8	C	0	1
8	D	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	Y	0	1
8	Z	0	1
8	a	0	1
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	754	VAL	C-N	5.34	1.40	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	a	735	ASP	CA-C-N	5.51	127.92	120.38
8	a	735	ASP	C-N-CA	5.51	127.92	120.38
8	D	1179	VAL	N-CA-CB	-5.43	106.04	112.39
8	C	1142	LEU	CA-CB-CG	5.39	135.16	116.30
6	1	27	PRO	CA-C-N	5.25	131.56	121.54
6	1	27	PRO	C-N-CA	5.25	131.56	121.54
1	n	287	VAL	N-CA-C	-5.13	108.83	113.71
8	a	753	ASP	CA-C-N	5.03	123.41	120.24
8	a	753	ASP	C-N-CA	5.03	123.41	120.24

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	C	585	ARG	Peptide
8	D	585	ARG	Peptide
8	Y	585	ARG	Peptide
8	Z	585	ARG	Peptide
8	a	585	ARG	Peptide

5.2 Too-close contacts

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	I	2389	0	2480	71	0
1	h	2384	0	2470	52	0
1	n	2329	0	2428	36	0
1	o	2291	0	2383	35	0
2	H	172	0	176	5	0
2	P	172	0	176	7	0
3	g	1822	0	1855	36	0
3	m	2325	0	2363	28	0
4	M	3848	0	3773	72	0
5	N	648	0	648	23	0
5	O	589	0	587	17	0
6	l	2320	0	2351	39	0
7	R	513	0	539	9	0
7	S	513	0	539	11	0
7	T	513	0	539	9	0
7	i	513	0	539	14	0
7	j	513	0	539	16	0
8	B	10617	0	10560	188	0
8	C	10536	0	10477	192	0
8	D	10269	0	10229	172	0
8	Y	10676	0	10618	161	0
8	Z	10582	0	10521	199	0
8	a	10079	0	10035	180	0
All	All	86613	0	86825	1422	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 8.

All (1422) 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)
8:C:782:LYS:O	8:C:786:LEU:HB2	1.78	0.83
8:Z:782:LYS:O	8:Z:786:LEU:HB2	1.81	0.81
8:B:1239:LEU:O	8:B:1243:LEU:HB2	1.81	0.80
8:a:782:LYS:O	8:a:786:LEU:HB2	1.90	0.70
7:R:37:HIS:HD2	7:R:40:LEU:HB2	1.57	0.69
8:D:1050:SER:HG	8:D:1054:CYS:HG	1.40	0.69
1:I:241:LEU:O	1:I:245:ARG:HB2	1.93	0.68
8:Y:507:ARG:HH21	8:Y:511:GLU:HG3	1.59	0.68
8:a:515:ASP:HA	8:a:993:ARG:HH21	1.59	0.68
1:h:245:ARG:HH21	1:I:245:ARG:HH12	1.43	0.67
1:h:36:GLN:HE22	8:a:1153:PHE:HB3	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:1:211:MET:HG3	6:1:215:ARG:HH21	1.60	0.66
3:g:50:PHE:O	3:g:145:LEU:HA	1.96	0.66
4:M:442:ARG:O	4:M:446:GLN:HB2	1.97	0.65
8:D:634:CYS:O	8:D:638:MET:HB2	1.97	0.65
8:Y:446:LEU:HD11	8:Y:1021:VAL:HG12	1.77	0.65
8:B:475:MET:HA	8:B:478:LEU:HG	1.79	0.64
1:I:177:PHE:HB3	1:I:180:ALA:HB3	1.78	0.64
8:Y:1327:THR:HG21	8:Y:1333:MET:HB2	1.80	0.64
8:Z:1324:ILE:HD11	8:Z:1363:GLN:HE21	1.62	0.64
8:B:692:GLY:HA2	8:C:993:ARG:HH12	1.63	0.64
8:B:1054:CYS:SG	8:B:1055:THR:N	2.71	0.64
4:M:510:ARG:HH12	8:a:473:PRO:HB3	1.63	0.64
1:o:127:LEU:HB2	1:o:130:TRP:HB3	1.81	0.63
8:C:798:CYS:SG	8:C:799:GLY:N	2.71	0.63
3:g:66:LEU:HB3	3:g:84:LEU:HD22	1.80	0.62
8:B:534:HIS:HD2	8:B:536:PHE:H	1.47	0.62
8:C:575:THR:HG21	8:C:1007:THR:HA	1.82	0.62
7:T:75:ARG:HH12	8:D:625:LEU:HB3	1.64	0.62
8:C:641:THR:HG23	8:C:642:ARG:HG3	1.82	0.62
8:C:1064:VAL:HG22	8:C:1077:VAL:HG12	1.82	0.62
8:Z:502:ARG:HH12	8:Z:958:ARG:HB3	1.65	0.62
7:i:28:LEU:HD12	7:i:29:PRO:HD2	1.82	0.61
4:M:431:ARG:HH11	4:M:529:LEU:HD23	1.65	0.61
8:B:895:VAL:HG13	8:B:914:GLN:HB3	1.82	0.61
8:C:1181:MET:HG3	8:C:1184:ASN:H	1.65	0.61
8:Y:180:LEU:HD23	8:Y:384:PRO:HG2	1.83	0.61
8:C:941:ARG:HH11	8:C:989:SER:HA	1.65	0.61
8:D:212:ARG:HH22	8:D:1204:PRO:HD3	1.65	0.61
8:Z:1181:MET:SD	8:Z:1181:MET:N	2.72	0.61
1:n:4:MET:SD	1:n:37:ARG:NH2	2.74	0.61
8:B:815:PRO:HA	8:B:818:LEU:HB2	1.82	0.61
3:g:176:GLU:HG3	3:g:178:THR:H	1.65	0.60
8:Y:1235:GLN:HB2	8:Y:1238:CYS:HB3	1.83	0.60
1:n:37:ARG:HH11	1:n:85:VAL:HG11	1.66	0.60
8:a:1032:PHE:HA	8:a:1178:PRO:HD3	1.84	0.60
6:1:166:ARG:HH21	6:1:167:ILE:HD13	1.67	0.60
1:h:103:GLU:HG3	1:h:105:GLY:H	1.67	0.60
8:D:800:LEU:HD22	8:D:923:VAL:HB	1.83	0.60
4:M:556:ARG:HD2	4:M:560:GLN:HE21	1.66	0.60
8:Y:820:MET:HE3	8:Y:877:ARG:HD2	1.83	0.60
1:I:173:GLN:NE2	1:I:184:ILE:O	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:871:PRO:HD2	8:D:874:GLN:HE22	1.66	0.60
8:D:1362:LEU:HD13	8:D:1366:MET:HG3	1.84	0.60
8:Z:538:ASP:HB2	8:Z:555:ARG:HE	1.67	0.60
1:n:10:CYS:O	1:n:80:GLN:HA	2.00	0.60
8:a:213:SER:OG	8:Z:433:ARG:NH1	2.35	0.60
2:H:2229:GLN:HG3	5:N:73:GLN:HB2	1.84	0.60
3:g:234:ARG:HH12	3:g:238:PRO:HA	1.66	0.60
8:D:638:MET:SD	8:D:642:ARG:NH1	2.75	0.60
8:D:798:CYS:SG	8:D:799:GLY:N	2.74	0.60
6:1:248:ASN:HD22	6:1:251:ARG:HH12	1.50	0.60
8:a:230:LEU:HD21	8:a:282:ILE:HG21	1.84	0.60
8:Y:625:LEU:HD13	8:Y:628:ARG:HD2	1.83	0.60
8:B:1217:HIS:HD1	8:B:1228:THR:HG1	1.50	0.60
8:Z:798:CYS:SG	8:Z:799:GLY:N	2.75	0.60
8:C:1139:ARG:HE	8:C:1140:PRO:HD2	1.66	0.59
8:Z:1195:ARG:NH1	8:Z:1227:ALA:O	2.35	0.59
8:Y:856:MET:SD	8:Y:856:MET:N	2.74	0.59
7:S:75:ARG:NH1	8:C:625:LEU:O	2.33	0.59
8:C:174:GLY:HA3	8:D:101:ALA:HB3	1.83	0.59
8:C:1290:LYS:HG2	8:C:1312:GLU:HA	1.83	0.59
6:1:124:ILE:HG22	6:1:127:ARG:HH21	1.66	0.59
8:B:850:ARG:HG3	8:B:858:THR:HG21	1.84	0.59
8:C:480:GLU:HG3	8:C:482:ARG:HH11	1.67	0.59
8:Z:1190:ASN:OD1	8:Z:1223:GLN:NE2	2.35	0.59
8:a:101:ALA:HB3	8:Z:174:GLY:HA3	1.84	0.59
8:D:888:GLU:H	8:D:919:ASN:HD21	1.50	0.59
8:Y:1054:CYS:SG	8:Y:1055:THR:N	2.75	0.59
1:n:108:LEU:HB2	1:n:288:PHE:HB2	1.85	0.59
4:M:533:TRP:HB3	4:M:541:VAL:HB	1.85	0.59
6:1:240:ARG:HA	6:1:251:ARG:HH21	1.67	0.59
8:B:901:HIS:HA	8:B:904:ARG:HB2	1.84	0.59
8:Y:798:CYS:SG	8:Y:799:GLY:N	2.76	0.59
4:M:44:TYR:HB2	4:M:150:ARG:HB2	1.85	0.59
5:N:50:ASP:OD1	5:N:50:ASP:N	2.36	0.59
8:Y:1195:ARG:NH1	8:Y:1227:ALA:O	2.36	0.59
8:Z:895:VAL:HB	8:Z:914:GLN:HB2	1.84	0.59
8:B:662:ALA:HB1	8:C:605:ASN:HD22	1.67	0.58
8:B:747:ARG:HB2	8:B:767:PHE:HB2	1.85	0.58
8:B:807:LEU:O	8:B:811:LEU:HB2	2.02	0.58
8:C:534:HIS:HD2	8:C:536:PHE:H	1.51	0.58
8:Y:139:LEU:HD22	8:Y:160:VAL:HG21	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:1176:LEU:HD22	8:Y:1230:ASN:HB3	1.84	0.58
4:M:103:LEU:O	4:M:107:LEU:HB2	2.03	0.58
8:B:1044:VAL:HG11	8:B:1096:VAL:HG23	1.86	0.58
8:C:1265:TYR:HA	8:C:1319:GLN:HE22	1.68	0.58
8:Y:983:TYR:O	8:Y:988:ARG:NH2	2.36	0.58
8:Y:1155:SER:H	8:Y:1255:ASN:HD21	1.49	0.58
8:Z:448:THR:HG22	8:Z:1113:LEU:HG	1.85	0.58
8:B:541:HIS:HA	8:B:550:ALA:HA	1.85	0.58
8:B:1165:VAL:HG13	8:B:1166:HIS:HD2	1.69	0.58
8:B:437:VAL:HG21	8:C:1183:VAL:HG12	1.86	0.58
8:Z:78:ILE:HB	8:Z:1058:ILE:HG22	1.85	0.58
8:Z:927:PRO:HD2	8:Z:952:LEU:HD21	1.84	0.58
8:C:628:ARG:HB2	8:C:661:LEU:HD21	1.86	0.58
8:Y:174:GLY:HA3	8:Z:101:ALA:HB3	1.86	0.58
7:j:66:ARG:HB2	8:a:884:GLN:HA	1.85	0.58
8:a:534:HIS:HD2	8:a:536:PHE:H	1.52	0.58
8:B:22:HIS:NE2	8:Z:379:THR:O	2.36	0.58
8:B:472:GLU:HB3	8:B:475:MET:HE3	1.84	0.58
8:C:787:CYS:HA	8:C:1008:LEU:HD23	1.86	0.58
2:H:2226:GLN:HG2	5:N:73:GLN:HE22	1.68	0.58
8:a:467:ARG:NH1	8:a:469:PRO:O	2.37	0.58
1:h:228:SER:OG	8:B:1119:MET:SD	2.62	0.57
3:m:67:LEU:HD11	3:m:81:TYR:HB3	1.86	0.57
8:a:1327:THR:HG21	8:a:1333:MET:HB2	1.85	0.57
4:M:41:ARG:HH11	4:M:570:MET:HE3	1.69	0.57
7:R:46:LYS:HA	7:R:49:ARG:HG2	1.86	0.57
8:a:507:ARG:HH11	8:a:511:GLU:HG3	1.69	0.57
8:C:663:ASP:O	8:D:642:ARG:NH2	2.37	0.57
8:C:909:ASP:OD1	8:C:909:ASP:N	2.37	0.57
8:B:401:LEU:HD11	8:B:1352:GLY:H	1.68	0.57
8:Z:138:TYR:O	8:Z:153:ASN:ND2	2.36	0.57
1:I:295:PRO:O	1:I:298:LYS:NZ	2.37	0.57
8:Y:1263:ALA:HB1	8:Y:1267:ASN:HD21	1.70	0.57
1:h:233:LYS:HB3	8:B:1143:LEU:HD11	1.87	0.57
1:h:36:GLN:HG3	1:h:38:LEU:HD23	1.85	0.57
3:g:136:LYS:HB3	3:g:147:THR:HG23	1.87	0.57
5:O:14:VAL:HG22	5:O:16:PHE:H	1.70	0.57
7:R:62:LEU:HA	7:R:65:LEU:HD12	1.87	0.57
8:B:575:THR:HG21	8:B:1007:THR:HA	1.87	0.57
8:D:389:VAL:HG22	8:D:1312:GLU:HB3	1.86	0.57
8:a:555:ARG:HA	8:a:988:ARG:HH12	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:a:804:LEU:HA	8:a:807:LEU:HB3	1.87	0.57
8:Y:694:ASN:O	8:Z:968:ARG:NH1	2.38	0.57
4:M:163:PHE:HB3	4:M:319:ASP:HA	1.87	0.57
8:C:756:ARG:NH2	8:C:888:GLU:OE2	2.38	0.57
2:P:2236:ARG:NH2	5:N:61:LEU:O	2.37	0.57
8:C:324:ASP:OD1	8:C:346:GLN:NE2	2.38	0.57
8:C:507:ARG:NH2	8:C:512:MET:SD	2.78	0.57
1:h:152:ILE:HD12	1:I:268:LEU:HB3	1.86	0.56
8:D:1336:LYS:NZ	8:D:1346:THR:OG1	2.38	0.56
7:i:22:VAL:HA	7:i:26:LEU:HB3	1.87	0.56
1:o:65:LEU:HD21	1:o:110:VAL:HG22	1.86	0.56
1:o:95:LEU:HD12	1:o:299:SER:HB3	1.87	0.56
8:B:210:ILE:O	8:B:214:ASN:ND2	2.38	0.56
8:C:182:THR:HG21	8:C:1083:THR:HG21	1.86	0.56
8:C:1360:ILE:HD12	8:C:1361:PRO:HD2	1.87	0.56
8:Z:600:THR:HG22	8:Z:644:LEU:HB2	1.88	0.56
8:B:733:VAL:HG22	8:B:738:PRO:HB3	1.87	0.56
8:C:709:ALA:HB3	8:C:1012:LEU:HB3	1.88	0.56
8:Z:575:THR:HG21	8:Z:1007:THR:HA	1.88	0.56
8:Y:713:HIS:HE1	8:Y:729:GLY:H	1.52	0.56
1:I:169:VAL:HA	1:I:172:LEU:HB2	1.88	0.56
8:B:146:THR:OG1	8:B:147:ILE:N	2.39	0.56
8:a:64:VAL:HG11	8:a:375:VAL:HG23	1.87	0.56
8:Y:532:GLU:OE1	8:Y:555:ARG:NH1	2.38	0.56
1:h:155:LEU:HA	1:h:197:MET:HE3	1.87	0.56
4:M:47:ASN:HD22	4:M:135:ARG:HB3	1.69	0.56
8:C:716:TRP:H	8:C:914:GLN:HE22	1.53	0.56
8:C:941:ARG:HH12	8:C:971:GLY:HA3	1.71	0.56
8:Y:463:THR:HG21	8:Y:1237:GLY:HA3	1.87	0.56
8:Z:444:ASP:OD1	8:Z:444:ASP:N	2.36	0.56
8:Z:581:HIS:ND1	8:Z:582:MET:SD	2.77	0.56
8:B:532:GLU:OE1	8:B:555:ARG:NH2	2.39	0.56
8:Y:414:VAL:HG12	8:Z:409:THR:HG22	1.87	0.56
8:Z:625:LEU:HD13	8:Z:628:ARG:HD2	1.88	0.56
3:m:74:CYS:HB2	8:C:1150:MET:HE3	1.88	0.56
8:D:922:CYS:SG	8:D:923:VAL:N	2.78	0.56
8:Y:905:GLN:HA	8:Y:1123:ARG:HE	1.71	0.56
3:g:131:THR:HG21	3:g:249:GLN:HE22	1.71	0.55
8:a:472:GLU:O	8:a:476:GLN:NE2	2.35	0.55
8:B:1037:VAL:HG21	8:B:1262:CYS:HB3	1.86	0.55
8:B:1172:CYS:SG	8:B:1173:GLU:N	2.78	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:694:ASN:ND2	8:C:704:SER:OG	2.38	0.55
8:a:803:ASN:OD1	8:a:889:HIS:NE2	2.37	0.55
8:B:1273:ALA:O	8:B:1276:LYS:NZ	2.38	0.55
8:D:697:GLN:HA	8:D:703:LEU:HB2	1.88	0.55
1:h:144:LEU:HD13	1:I:276:ARG:HD2	1.87	0.55
3:g:70:MET:HB3	3:g:129:LEU:HD13	1.88	0.55
8:D:1067:GLU:HB3	8:D:1074:THR:HB	1.88	0.55
8:D:1194:GLY:H	8:D:1234:SER:HB3	1.71	0.55
8:Y:169:ASP:OD2	8:Y:173:ARG:NH2	2.39	0.55
8:a:515:ASP:OD2	8:a:515:ASP:N	2.38	0.55
8:C:424:LEU:HD12	8:C:573:LEU:HG	1.88	0.55
8:D:811:LEU:HD12	8:D:857:LEU:HD13	1.87	0.55
8:Z:199:ASN:HA	8:Z:202:LEU:HD23	1.88	0.55
8:Z:554:PRO:HD3	8:Z:907:LEU:HD12	1.88	0.55
7:j:50:MET:HE1	7:j:53:LEU:HB2	1.88	0.55
8:a:800:LEU:HD22	8:a:952:LEU:HD11	1.88	0.55
8:C:499:TYR:O	8:C:502:ARG:NH2	2.40	0.55
8:C:1043:GLU:OE2	8:C:1101:ARG:NH1	2.40	0.55
8:Y:580:GLU:HG2	8:Y:585:ARG:HB2	1.87	0.55
8:Y:940:HIS:HD2	8:Y:942:PHE:H	1.54	0.55
1:I:103:GLU:OE1	3:g:69:ARG:NH1	2.40	0.55
8:a:300:ALA:HB3	8:a:351:SER:HB2	1.87	0.55
8:D:814:ARG:NH1	8:D:853:VAL:O	2.40	0.55
8:Y:1038:ARG:NH1	8:Y:1107:GLY:O	2.38	0.55
8:B:553:THR:HG21	8:B:983:TYR:HB3	1.89	0.55
8:D:258:PRO:O	8:D:268:LYS:NZ	2.40	0.55
8:Z:507:ARG:HH21	8:Z:512:MET:HA	1.72	0.55
7:T:66:ARG:NH2	8:D:884:GLN:O	2.38	0.55
8:a:709:ALA:HB3	8:a:1012:LEU:HD12	1.89	0.55
8:B:230:LEU:HD12	8:B:1098:TYR:HB2	1.88	0.55
8:D:468:GLY:O	8:D:541:HIS:NE2	2.40	0.55
8:Z:626:LEU:HD11	8:Z:881:LEU:HD13	1.89	0.55
1:n:25:THR:HA	1:n:76:VAL:HG11	1.88	0.55
1:n:143:ALA:O	1:n:147:ASN:ND2	2.40	0.55
3:g:47:THR:OG1	3:g:49:ARG:NH1	2.40	0.55
8:C:1336:LYS:NZ	8:C:1343:ALA:O	2.39	0.55
8:Y:361:ARG:HG2	8:Y:366:THR:HG22	1.89	0.55
8:B:212:ARG:NH2	8:B:1202:VAL:O	2.40	0.55
8:B:1263:ALA:O	8:B:1267:ASN:ND2	2.40	0.55
8:D:905:GLN:O	8:D:1123:ARG:NH2	2.39	0.55
1:I:114:LEU:HD23	1:I:185:PRO:HD2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:255:ARG:HH11	1:o:162:TYR:HB3	1.71	0.54
8:a:274:VAL:HG23	8:a:370:GLU:HB3	1.88	0.54
8:B:485:GLN:OE1	8:B:981:HIS:NE2	2.40	0.54
8:C:668:PRO:HB3	8:D:642:ARG:HA	1.89	0.54
8:Y:495:ILE:HG23	8:Y:496:PRO:HD3	1.89	0.54
6:1:271:LEU:O	6:1:278:TYR:OH	2.26	0.54
8:B:32:PHE:HB2	8:B:35:LEU:HD21	1.88	0.54
8:B:82:ASP:OD1	8:B:82:ASP:N	2.39	0.54
8:B:126:THR:HG23	8:B:1078:THR:HG22	1.88	0.54
8:C:237:ASP:N	8:C:237:ASP:OD1	2.41	0.54
8:Z:1245:ASN:ND2	8:Z:1266:PHE:O	2.40	0.54
7:R:34:GLU:HG2	7:R:44:LEU:HD11	1.90	0.54
7:T:23:ASN:ND2	7:T:28:LEU:O	2.41	0.54
8:a:1038:ARG:NH1	8:a:1107:GLY:O	2.41	0.54
8:Y:216:LEU:HD21	8:Y:1200:LEU:HB3	1.90	0.54
8:Z:8:GLU:OE2	8:Z:45:ARG:NH1	2.37	0.54
1:n:62:ARG:NH1	1:n:147:ASN:OD1	2.41	0.54
8:a:1191:ASN:ND2	8:a:1197:SER:OG	2.40	0.54
1:n:276:ARG:NH2	1:o:282:ILE:O	2.40	0.54
3:g:122:PRO:O	3:g:123:HIS:ND1	2.41	0.54
6:1:175:ARG:NH2	6:1:219:GLU:OE2	2.38	0.54
8:C:435:ARG:NH1	8:C:1363:GLN:O	2.40	0.54
8:D:927:PRO:HD2	8:D:952:LEU:HD21	1.88	0.54
1:h:42:LYS:HD2	1:h:44:TYR:H	1.72	0.54
8:a:420:VAL:HA	8:a:423:ALA:HB3	1.90	0.54
8:C:509:VAL:HA	8:C:512:MET:HB2	1.88	0.54
8:D:470:PRO:HD2	8:D:479:LEU:HD21	1.90	0.54
1:I:37:ARG:HH12	1:I:85:VAL:HG21	1.73	0.54
8:a:1336:LYS:NZ	8:a:1346:THR:OG1	2.41	0.54
8:D:889:HIS:O	8:D:891:LYS:NZ	2.41	0.54
8:Y:638:MET:SD	8:Y:642:ARG:NH2	2.80	0.54
8:Z:209:ARG:HG3	8:Z:212:ARG:HH11	1.71	0.54
8:Z:225:ALA:O	8:Z:232:ARG:NH1	2.40	0.54
8:Z:275:SER:OG	8:Z:276:THR:N	2.40	0.54
8:a:747:ARG:HB2	8:a:767:PHE:HB3	1.90	0.54
8:a:1303:CYS:SG	8:a:1304:VAL:N	2.80	0.54
8:B:747:ARG:NH2	8:B:767:PHE:O	2.40	0.54
8:D:712:ASP:O	8:D:782:LYS:NZ	2.41	0.54
7:j:66:ARG:HH22	8:a:750:GLY:H	1.56	0.54
8:C:543:GLN:HE21	8:C:546:SER:H	1.56	0.54
8:Z:804:LEU:HA	8:Z:807:LEU:HB3	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:n:277:GLN:HE21	3:m:220:ARG:HH22	1.56	0.54
5:O:63:GLN:HE22	7:j:52:SER:HB2	1.73	0.54
7:S:15:ASP:OD1	7:S:19:ARG:NH1	2.40	0.54
8:a:981:HIS:HB3	8:a:984:HIS:HB2	1.90	0.54
8:C:81:HIS:ND1	8:Z:144:GLU:OE2	2.41	0.54
8:C:244:THR:HA	8:C:362:LEU:HD13	1.90	0.54
8:C:1336:LYS:NZ	8:C:1346:THR:OG1	2.41	0.54
1:I:227:SER:HA	1:I:231:LEU:HD21	1.90	0.53
1:o:211:ALA:O	1:o:215:THR:OG1	2.26	0.53
3:g:234:ARG:O	3:g:234:ARG:NH1	2.41	0.53
5:O:56:VAL:HG13	5:O:57:ARG:HE	1.72	0.53
8:a:227:LEU:O	8:a:232:ARG:NH2	2.41	0.53
8:a:418:ASP:N	8:a:418:ASP:OD1	2.40	0.53
8:B:326:ASN:HB3	8:B:1066:LYS:HE3	1.90	0.53
8:Y:252:ASP:OD1	8:Y:252:ASP:N	2.41	0.53
8:Y:712:ASP:O	8:Y:782:LYS:NZ	2.38	0.53
8:a:1060:ASN:O	8:a:1079:GLN:NE2	2.41	0.53
8:Y:1032:PHE:HA	8:Y:1178:PRO:HD3	1.89	0.53
1:I:104:LYS:NZ	1:I:291:CYS:O	2.40	0.53
8:B:373:ARG:O	8:B:373:ARG:NH1	2.41	0.53
8:Y:624:PHE:HE2	8:Y:660:HIS:HB2	1.74	0.53
1:n:173:GLN:HG2	1:n:184:ILE:HB	1.90	0.53
8:a:603:SER:OG	8:a:605:ASN:OD1	2.26	0.53
8:B:1195:ARG:NH2	8:B:1219:GLU:OE1	2.41	0.53
1:I:11:THR:OG1	1:I:79:ASN:ND2	2.41	0.53
1:I:113:PRO:HD3	1:I:135:PRO:HA	1.89	0.53
3:m:123:HIS:HB2	3:m:128:ARG:HH21	1.73	0.53
8:a:310:GLU:OE2	8:a:326:ASN:ND2	2.42	0.53
8:a:1183:VAL:HG11	8:Z:1330:LEU:HD11	1.88	0.53
8:B:237:ASP:OD1	8:B:237:ASP:N	2.41	0.53
8:B:329:LYS:NZ	8:B:329:LYS:O	2.40	0.53
8:B:432:ASN:HD21	8:B:438:GLN:HE21	1.56	0.53
8:B:520:ASP:HA	8:B:523:LYS:HG3	1.90	0.53
8:C:52:ALA:HB3	8:D:89:GLY:HA2	1.91	0.53
8:C:515:ASP:OD1	8:C:515:ASP:N	2.38	0.53
8:D:473:PRO:HA	8:D:476:GLN:HG2	1.89	0.53
8:D:1243:LEU:O	8:D:1249:ARG:NH1	2.40	0.53
1:h:11:THR:OG1	1:h:12:PHE:N	2.41	0.53
1:h:102:TRP:H	1:h:297:ASN:HD21	1.57	0.53
1:o:189:ILE:O	1:o:192:HIS:ND1	2.42	0.53
4:M:372:ARG:HA	4:M:375:ILE:HD12	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:95:VAL:HG13	8:C:114:ILE:HG23	1.90	0.53
8:B:49:HIS:O	8:C:319:HIS:ND1	2.41	0.53
8:B:927:PRO:HD2	8:B:952:LEU:HD21	1.90	0.53
8:Y:1336:LYS:NZ	8:Y:1346:THR:OG1	2.42	0.53
8:Z:747:ARG:HD3	8:Z:756:ARG:HH22	1.73	0.53
4:M:27:LEU:HB3	4:M:31:VAL:HG11	1.89	0.53
4:M:506:ASP:OD2	4:M:512:ARG:NH2	2.41	0.53
8:B:102:SER:OG	8:B:103:GLY:N	2.41	0.53
8:B:263:THR:HA	8:B:296:VAL:HA	1.90	0.53
8:B:382:LYS:NZ	8:C:202:LEU:O	2.40	0.53
8:B:782:LYS:O	8:B:786:LEU:HB2	2.08	0.53
8:B:1154:GLY:O	8:B:1257:LYS:NZ	2.41	0.53
8:C:900:ASP:OD2	8:C:1014:LYS:NZ	2.42	0.53
8:Z:58:CYS:SG	8:Z:59:ASN:N	2.82	0.53
1:h:104:LYS:NZ	1:h:292:ASP:OD1	2.41	0.53
1:n:167:ALA:O	1:n:170:GLN:NE2	2.41	0.53
7:R:22:VAL:HA	7:R:26:LEU:HB2	1.91	0.53
8:B:669:GLN:O	8:B:673:HIS:ND1	2.42	0.53
8:C:481:CYS:SG	8:C:484:GLN:NE2	2.81	0.53
8:D:234:ARG:HH22	8:D:282:ILE:HD13	1.74	0.53
8:D:579:MET:HE3	8:D:1006:MET:HG3	1.91	0.53
8:Y:392:THR:OG1	8:Y:1264:GLN:NE2	2.42	0.53
3:g:170:ASP:N	3:g:170:ASP:OD1	2.42	0.53
8:a:638:MET:HE1	8:a:642:ARG:HH11	1.71	0.53
8:B:254:ILE:HD11	8:B:1088:LEU:HD23	1.91	0.53
8:C:244:THR:HG22	8:C:362:LEU:HB2	1.90	0.53
8:C:954:ASP:OD2	8:C:958:ARG:NH1	2.41	0.53
8:D:1349:THR:HA	8:D:1354:TYR:HA	1.92	0.53
1:o:177:PHE:HB3	1:o:180:ALA:HB3	1.91	0.52
4:M:57:ARG:NH1	4:M:85:GLU:OE2	2.42	0.52
8:B:445:ALA:HA	8:B:1110:VAL:HG11	1.90	0.52
8:B:1191:ASN:ND2	8:B:1197:SER:OG	2.42	0.52
8:D:311:ASN:ND2	8:D:322:LEU:O	2.43	0.52
8:Y:29:GLU:HB3	8:Y:31:MET:HE2	1.90	0.52
8:Y:1298:ASP:OD1	8:Y:1298:ASP:N	2.41	0.52
6:1:60:LEU:HG	6:1:268:LEU:HD22	1.91	0.52
8:C:757:LEU:O	8:C:805:LYS:NZ	2.42	0.52
8:D:846:ILE:O	8:D:849:GLN:NE2	2.42	0.52
8:Z:1332:LEU:HD23	8:Z:1355:VAL:HG23	1.90	0.52
5:N:32:ARG:O	5:N:32:ARG:NH2	2.41	0.52
5:O:68:LEU:HA	5:O:71:ARG:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:54:PHE:HB3	8:C:344:LEU:HD21	1.91	0.52
8:C:433:ARG:NH1	8:C:1166:HIS:O	2.42	0.52
8:C:1038:ARG:NH1	8:C:1107:GLY:O	2.41	0.52
2:P:2236:ARG:HH22	5:N:65:LEU:HB3	1.75	0.52
1:n:76:VAL:O	8:Y:47:ASN:ND2	2.42	0.52
8:B:521:PHE:HA	8:B:526:ASN:HD22	1.74	0.52
8:Y:479:LEU:O	8:Y:482:ARG:NH1	2.42	0.52
8:Z:563:ASP:OD1	8:Z:563:ASP:N	2.40	0.52
1:h:65:LEU:HD21	1:h:110:VAL:HG22	1.91	0.52
1:o:91:LEU:HA	1:o:303:ILE:HA	1.92	0.52
4:M:414:TRP:NE1	4:M:476:ASP:OD2	2.40	0.52
5:N:30:VAL:HA	5:N:33:ARG:HE	1.75	0.52
8:a:532:GLU:O	8:a:1235:GLN:NE2	2.43	0.52
8:C:275:SER:OG	8:C:276:THR:N	2.42	0.52
8:D:915:HIS:NE2	8:D:978:ALA:O	2.41	0.52
8:D:970:ASP:HB3	8:D:996:ALA:HB3	1.92	0.52
8:Y:1291:ASP:OD1	8:Y:1291:ASP:N	2.42	0.52
1:I:272:PHE:O	1:I:276:ARG:HB2	2.09	0.52
1:I:291:CYS:HB2	3:g:150:MET:HE1	1.91	0.52
6:1:129:LEU:HD11	6:1:207:GLY:HA3	1.92	0.52
8:B:462:GLN:NE2	8:B:466:GLU:OE1	2.42	0.52
8:C:235:ASP:OD1	8:C:235:ASP:N	2.42	0.52
8:C:945:ASN:ND2	8:C:947:THR:OG1	2.40	0.52
1:h:10:CYS:SG	1:h:11:THR:N	2.82	0.52
4:M:372:ARG:HH22	5:N:43:ARG:HH12	1.58	0.52
4:M:422:SER:OG	4:M:423:CYS:N	2.42	0.52
8:B:321:ILE:O	8:B:328:TYR:OH	2.27	0.52
8:B:493:ARG:NH1	8:B:761:ASP:O	2.43	0.52
8:D:427:THR:HG22	8:D:441:ASP:HB3	1.91	0.52
8:C:763:ASP:OD1	8:C:763:ASP:N	2.39	0.52
8:Z:1181:MET:SD	8:Z:1229:HIS:ND1	2.83	0.52
1:h:123:ASN:HD22	1:h:133:VAL:HA	1.74	0.51
4:M:479:ARG:NH1	4:M:484:GLN:OE1	2.42	0.51
7:i:52:SER:OG	7:i:53:LEU:N	2.44	0.51
8:C:1324:ILE:HD11	8:C:1363:GLN:HE21	1.75	0.51
8:D:487:PRO:HB3	8:D:736:ARG:HH11	1.74	0.51
1:h:280:ASP:OD1	1:I:283:ARG:NH2	2.38	0.51
1:I:210:LEU:HB2	1:I:271:LEU:HD12	1.92	0.51
4:M:460:GLY:O	4:M:462:ARG:NH1	2.43	0.51
7:j:20:HIS:HA	7:j:24:VAL:HB	1.93	0.51
8:a:605:ASN:HD22	8:Z:662:ALA:HB1	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:65:LEU:HD21	1:I:110:VAL:HG22	1.91	0.51
5:O:63:GLN:NE2	7:j:51:SER:OG	2.43	0.51
6:1:212:ASN:OD1	6:1:215:ARG:NH2	2.42	0.51
6:1:83:ARG:NH1	6:1:206:THR:OG1	2.44	0.51
3:g:192:ASP:HB3	3:g:199:ARG:HB2	1.92	0.51
8:B:1070:ASP:OD1	8:B:1070:ASP:N	2.44	0.51
8:B:1176:LEU:HD11	8:B:1180:THR:HG21	1.93	0.51
1:h:158:LEU:O	1:I:221:LYS:NZ	2.42	0.51
1:n:22:GLY:O	1:n:26:LYS:NZ	2.44	0.51
7:S:13:LYS:HZ2	7:S:15:ASP:HB2	1.76	0.51
8:a:405:ARG:NH2	8:Z:421:ARG:O	2.44	0.51
8:C:257:ASN:HB2	8:C:260:THR:HG22	1.91	0.51
8:C:433:ARG:HH21	8:D:217:GLN:HG2	1.74	0.51
8:Y:432:ASN:ND2	8:Y:436:ALA:O	2.43	0.51
1:o:214:LEU:HD11	1:o:267:ARG:HB3	1.93	0.51
4:M:344:ASP:OD1	4:M:344:ASP:N	2.43	0.51
7:S:52:SER:OG	7:S:53:LEU:N	2.44	0.51
7:j:58:CYS:HB2	8:a:805:LYS:HZ3	1.75	0.51
8:B:326:ASN:O	8:B:329:LYS:HB3	2.11	0.51
8:Y:478:LEU:HD21	8:Y:512:MET:HE2	1.92	0.51
8:a:637:ASN:ND2	8:a:863:ASP:O	2.44	0.51
8:a:1104:THR:OG1	8:a:1105:ASP:N	2.42	0.51
8:D:1095:CYS:SG	8:D:1096:VAL:N	2.84	0.51
8:Y:276:THR:HG21	8:Y:386:GLU:HG3	1.91	0.51
8:Z:779:THR:HA	8:Z:782:LYS:HD3	1.93	0.51
3:g:73:GLY:H	3:g:117:TRP:HB3	1.75	0.51
3:m:56:LEU:HD11	3:m:80:LEU:HD12	1.92	0.51
4:M:146:THR:HA	4:M:164:LEU:HA	1.93	0.51
6:1:99:ARG:O	6:1:103:ARG:HB2	2.11	0.51
8:a:214:ASN:OD1	8:Z:433:ARG:NH2	2.44	0.51
8:D:647:PHE:HB3	8:D:653:LEU:HD23	1.93	0.51
1:I:232:VAL:HG22	4:M:6:TYR:HB2	1.93	0.51
8:C:146:THR:HG23	8:C:149:ASP:H	1.76	0.51
8:C:422:ASN:ND2	8:D:406:GLY:O	2.44	0.51
8:C:618:HIS:O	8:C:721:THR:OG1	2.29	0.51
8:D:1182:ASP:OD1	8:D:1182:ASP:N	2.44	0.51
8:Z:419:THR:HB	8:Z:422:ASN:HB2	1.91	0.51
1:I:95:LEU:HA	1:I:299:SER:HA	1.93	0.50
8:a:915:HIS:NE2	8:a:978:ALA:O	2.44	0.50
8:B:1193:ARG:HH21	8:B:1195:ARG:HB2	1.75	0.50
8:C:66:PHE:HD1	8:C:176:ILE:HG12	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:534:HIS:HD2	8:Z:536:PHE:H	1.59	0.50
8:Z:806:THR:HA	8:Z:809:VAL:HG12	1.92	0.50
1:I:45:GLN:O	1:I:50:GLN:NE2	2.44	0.50
1:n:173:GLN:NE2	1:n:184:ILE:O	2.45	0.50
4:M:428:LEU:HB3	4:M:529:LEU:HD11	1.93	0.50
5:O:33:ARG:HA	8:a:502:ARG:HH21	1.76	0.50
8:a:1183:VAL:HG21	8:Z:1330:LEU:HD21	1.94	0.50
8:B:724:PRO:HA	8:B:773:ALA:HB3	1.93	0.50
8:C:1277:THR:OG1	8:C:1278:LEU:N	2.44	0.50
8:C:1291:ASP:OD1	8:C:1291:ASP:N	2.43	0.50
8:D:1018:VAL:HG12	8:D:1131:ILE:HD11	1.92	0.50
8:Z:726:ASN:OD1	8:Z:726:ASN:N	2.45	0.50
1:n:276:ARG:NH1	3:m:288:GLU:OE2	2.36	0.50
8:a:769:ASP:OD1	8:a:769:ASP:N	2.43	0.50
8:Y:177:HIS:ND1	8:Y:376:TYR:OH	2.38	0.50
8:Z:598:LYS:O	8:Z:602:THR:OG1	2.29	0.50
8:Z:609:LEU:HD21	8:Z:864:VAL:HG11	1.92	0.50
1:o:216:MET:HE3	1:o:220:ARG:HG3	1.93	0.50
4:M:107:LEU:HD12	4:M:112:LEU:HD22	1.92	0.50
8:a:1144:ASP:HB2	8:a:1148:ILE:HB	1.93	0.50
8:B:663:ASP:OD1	8:B:663:ASP:N	2.44	0.50
8:D:1104:THR:OG1	8:D:1105:ASP:N	2.44	0.50
8:D:1110:VAL:HA	8:D:1171:ALA:HB3	1.92	0.50
8:Y:617:VAL:HG13	8:Y:619:GLY:H	1.76	0.50
8:Z:694:ASN:HD22	8:Z:704:SER:HB2	1.75	0.50
8:Z:845:SER:O	8:Z:849:GLN:NE2	2.44	0.50
8:Z:900:ASP:OD1	8:Z:900:ASP:N	2.42	0.50
1:n:126:THR:HG22	1:n:131:GLU:HG2	1.93	0.50
4:M:63:GLU:OE2	4:M:84:ARG:NH1	2.40	0.50
8:a:1105:ASP:HB2	8:a:1166:HIS:HB3	1.93	0.50
8:B:465:THR:HG22	8:B:550:ALA:HB3	1.93	0.50
8:B:698:LEU:HD11	8:B:1127:VAL:HA	1.94	0.50
8:B:785:TYR:O	8:B:943:TYR:OH	2.28	0.50
8:D:900:ASP:OD1	8:D:900:ASP:N	2.43	0.50
8:Y:1104:THR:OG1	8:Y:1105:ASP:N	2.44	0.50
2:P:2228:VAL:HG23	5:N:71:ARG:HH22	1.77	0.50
8:a:798:CYS:SG	8:a:799:GLY:N	2.85	0.50
8:C:169:ASP:OD2	8:C:173:ARG:NE	2.44	0.50
8:C:1193:ARG:HG2	8:C:1234:SER:HA	1.93	0.50
8:D:429:TYR:HA	8:D:438:GLN:O	2.11	0.50
8:D:756:ARG:NH1	8:D:888:GLU:OE2	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:804:LEU:HD22	8:Y:887:GLY:HA3	1.93	0.50
8:Z:1116:VAL:HG13	8:Z:1117:PHE:HD1	1.75	0.50
1:n:106:ASP:OD1	1:n:106:ASP:N	2.42	0.50
7:R:66:ARG:HH21	8:B:750:GLY:H	1.60	0.50
8:B:149:ASP:OD1	8:B:149:ASP:N	2.41	0.50
8:Y:510:ASN:ND2	8:Y:989:SER:OG	2.44	0.50
3:g:169:LYS:HG2	3:g:274:VAL:HG23	1.92	0.50
8:C:420:VAL:HA	8:C:423:ALA:HB3	1.93	0.50
8:Z:1034:LEU:HA	8:Z:1175:ILE:HA	1.94	0.50
8:Z:1211:THR:HA	8:Z:1214:ILE:HG22	1.94	0.50
1:I:264:GLU:HA	1:I:267:ARG:HD2	1.93	0.50
8:B:268:LYS:O	8:B:366:THR:OG1	2.30	0.50
8:C:510:ASN:ND2	8:C:989:SER:OG	2.44	0.50
8:C:1211:THR:HA	8:C:1214:ILE:HG22	1.94	0.50
8:Z:594:LEU:HD12	8:Z:792:MET:HE3	1.92	0.50
4:M:380:ARG:NH2	5:N:36:GLU:OE1	2.44	0.49
7:i:13:LYS:N	7:i:16:GLU:OE2	2.45	0.49
8:C:439:LYS:NZ	8:D:519:THR:OG1	2.43	0.49
8:D:1001:VAL:O	8:D:1004:SER:OG	2.30	0.49
8:Y:253:SER:OG	8:Y:254:ILE:N	2.44	0.49
8:Y:622:ASP:HA	8:Y:625:LEU:HB2	1.93	0.49
8:Z:253:SER:OG	8:Z:254:ILE:N	2.45	0.49
1:I:160:ARG:O	1:I:166:LYS:NZ	2.40	0.49
1:n:190:ASP:OD1	1:n:192:HIS:ND1	2.41	0.49
5:O:40:VAL:HG22	8:a:500:ARG:HD3	1.94	0.49
8:a:412:SER:OG	8:a:413:LYS:NZ	2.45	0.49
8:C:303:GLY:HA3	8:C:348:GLY:HA2	1.93	0.49
8:Y:424:LEU:HD12	8:Y:573:LEU:HB3	1.93	0.49
6:1:73:LEU:HD11	6:1:214:ARG:HH21	1.77	0.49
8:a:712:ASP:O	8:a:782:LYS:NZ	2.39	0.49
8:a:1072:SER:OG	8:a:1073:THR:N	2.44	0.49
8:a:1246:THR:HA	8:a:1249:ARG:HD3	1.94	0.49
8:B:874:GLN:HA	8:B:877:ARG:HG2	1.93	0.49
8:C:988:ARG:HB3	8:C:990:PRO:HD2	1.94	0.49
8:C:1054:CYS:SG	8:C:1055:THR:N	2.85	0.49
8:Y:915:HIS:NE2	8:Y:978:ALA:O	2.44	0.49
1:I:34:ILE:HG13	1:I:69:THR:HG23	1.93	0.49
4:M:388:GLN:O	4:M:389:ARG:NH1	2.43	0.49
8:C:83:LEU:HD11	8:C:1082:ASN:HD21	1.77	0.49
8:D:558:ILE:HG22	8:D:571:HIS:HE1	1.77	0.49
6:1:71:PRO:HB3	6:1:179:PHE:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:52:ALA:HA	8:D:321:ILE:HG22	1.95	0.49
8:D:359:VAL:HG12	8:D:368:ILE:HD13	1.93	0.49
8:D:1144:ASP:OD1	8:D:1144:ASP:N	2.37	0.49
8:Y:563:ASP:N	8:Y:563:ASP:OD1	2.44	0.49
2:P:2221:LEU:HD12	2:P:2222:ARG:HG2	1.94	0.49
1:o:88:HIS:ND1	1:o:306:GLY:OXT	2.44	0.49
3:m:68:ILE:HG21	3:m:129:LEU:HD23	1.94	0.49
7:j:66:ARG:NH2	8:a:884:GLN:O	2.43	0.49
8:B:1018:VAL:HG12	8:B:1131:ILE:HD11	1.94	0.49
8:B:1082:ASN:N	8:B:1082:ASN:OD1	2.44	0.49
8:Y:54:PHE:HB2	8:Z:91:MET:HG2	1.94	0.49
1:n:45:GLN:O	1:n:50:GLN:NE2	2.44	0.49
8:B:505:VAL:O	8:B:966:TYR:OH	2.31	0.49
8:D:361:ARG:NH1	8:D:364:GLU:O	2.45	0.49
8:D:1263:ALA:O	8:D:1267:ASN:ND2	2.45	0.49
8:Z:507:ARG:NH1	8:Z:511:GLU:OE2	2.46	0.49
8:Z:1292:CYS:SG	8:Z:1303:CYS:N	2.80	0.49
8:a:744:ILE:HG22	8:a:765:PRO:HA	1.95	0.49
8:B:66:PHE:HD1	8:B:176:ILE:HG12	1.78	0.49
8:B:1289:ALA:HB1	8:B:1316:ARG:HG2	1.95	0.49
8:C:654:VAL:HA	8:C:657:ILE:HG22	1.95	0.49
8:C:1156:MET:SD	8:C:1294:ARG:NH1	2.86	0.49
8:C:1176:LEU:HD21	8:C:1180:THR:HG21	1.94	0.49
8:Z:1060:ASN:O	8:Z:1079:GLN:NE2	2.45	0.49
8:Z:1264:GLN:OE1	8:Z:1313:ASN:ND2	2.45	0.49
3:m:138:VAL:HA	3:m:146:LEU:HD13	1.95	0.49
4:M:100:PRO:HB3	4:M:125:PHE:HA	1.94	0.49
4:M:169:LEU:HD12	4:M:173:MET:HB2	1.94	0.49
8:a:1003:HIS:HA	8:a:1006:MET:HG2	1.95	0.49
8:Z:10:LEU:O	8:Z:12:LYS:NZ	2.45	0.49
1:I:23:LYS:O	1:I:26:LYS:NZ	2.39	0.49
3:m:258:ASP:OD1	3:m:258:ASP:N	2.42	0.49
8:a:1138:GLU:HG2	8:a:1139:ARG:HG2	1.94	0.49
8:B:449:LEU:HD12	8:B:1020:LEU:HD21	1.95	0.49
8:D:237:ASP:OD1	8:D:237:ASP:N	2.45	0.49
8:Z:1047:LEU:HD22	8:Z:1097:ALA:HB2	1.94	0.49
1:h:274:MET:HE1	3:g:290:VAL:HG21	1.95	0.48
3:m:61:ALA:HA	3:m:138:VAL:HG11	1.95	0.48
8:B:508:THR:HG23	8:B:511:GLU:H	1.78	0.48
8:D:216:LEU:HD22	8:D:1200:LEU:HB2	1.95	0.48
8:D:443:VAL:HA	8:D:446:LEU:HD23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:1185:TYR:OH	8:D:1193:ARG:O	2.31	0.48
8:Y:475:MET:HE1	8:Y:527:ILE:HD12	1.95	0.48
8:Z:1043:GLU:HG3	8:Z:1100:ASN:HB2	1.94	0.48
8:Z:1060:ASN:ND2	8:Z:1061:ASN:O	2.46	0.48
7:S:33:SER:OG	7:S:34:GLU:N	2.46	0.48
8:a:617:VAL:HG23	8:a:619:GLY:H	1.78	0.48
8:a:731:GLN:HG3	8:a:740:ASN:HD21	1.77	0.48
8:C:517:VAL:HG12	8:C:520:ASP:HB2	1.94	0.48
8:C:635:ILE:HG22	8:C:646:VAL:HB	1.95	0.48
8:C:675:ARG:HE	8:D:603:SER:HA	1.78	0.48
8:D:484:GLN:NE2	8:D:543:GLN:O	2.46	0.48
8:D:801:GLY:N	8:D:935:LEU:O	2.46	0.48
1:h:217:THR:HG23	1:h:221:LYS:HE3	1.95	0.48
7:R:66:ARG:HG3	7:R:67:MET:HE2	1.95	0.48
8:a:1124:HIS:HB3	8:a:1127:VAL:HG12	1.95	0.48
8:B:1035:THR:HG23	8:B:1176:LEU:HD22	1.95	0.48
8:B:1336:LYS:NZ	8:B:1346:THR:OG1	2.42	0.48
8:C:694:ASN:HA	8:C:703:LEU:HD12	1.95	0.48
8:C:1001:VAL:O	8:C:1004:SER:OG	2.30	0.48
8:Z:186:LYS:NZ	8:Z:1091:THR:OG1	2.47	0.48
1:n:104:LYS:NZ	1:n:291:CYS:O	2.42	0.48
1:o:189:ILE:HD11	1:o:194:LEU:HD21	1.95	0.48
4:M:364:GLU:HG3	4:M:420:VAL:HA	1.95	0.48
8:B:1101:ARG:HH21	8:C:214:ASN:HD22	1.62	0.48
8:Y:811:LEU:O	8:Y:814:ARG:NH1	2.46	0.48
8:B:657:ILE:HG23	8:B:661:LEU:HD23	1.95	0.48
8:C:712:ASP:O	8:C:782:LYS:NZ	2.36	0.48
8:D:740:ASN:OD1	8:D:740:ASN:N	2.44	0.48
8:Y:278:ASN:OD1	8:Y:278:ASN:N	2.47	0.48
8:Y:724:PRO:HA	8:Y:773:ALA:HB3	1.95	0.48
8:Z:990:PRO:HA	8:Z:993:ARG:HB2	1.96	0.48
1:h:59:VAL:HB	1:h:62:ARG:HH21	1.77	0.48
1:I:151:LEU:HA	1:I:197:MET:HE1	1.94	0.48
1:I:251:ARG:HD3	1:I:252:THR:H	1.77	0.48
7:i:47:TYR:OH	7:i:63:ASP:OD2	2.29	0.48
8:a:309:PRO:HB2	8:C:329:LYS:HG3	1.95	0.48
8:B:740:ASN:HD21	8:B:742:ALA:HB3	1.77	0.48
8:D:263:THR:OG1	8:D:264:SER:N	2.45	0.48
8:D:513:LYS:HG2	8:D:562:PRO:HB3	1.94	0.48
8:D:681:LEU:HG	8:D:783:VAL:HG23	1.95	0.48
8:Y:716:TRP:H	8:Y:914:GLN:HE22	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:153:MET:O	1:I:157:SER:OG	2.31	0.48
4:M:409:HIS:ND1	4:M:480:CYS:SG	2.83	0.48
8:a:707:VAL:HG12	8:a:1019:SER:HA	1.95	0.48
8:a:800:LEU:HD13	8:a:934:SER:HB2	1.95	0.48
8:D:936:PRO:HB3	8:D:952:LEU:HD12	1.95	0.48
4:M:51:ALA:O	4:M:53:ARG:NH2	2.47	0.48
8:a:579:MET:HG3	8:a:1003:HIS:HE1	1.78	0.48
8:B:441:ASP:HB3	8:B:443:VAL:HG22	1.95	0.48
8:D:526:ASN:HB2	8:D:528:THR:HG22	1.95	0.48
8:D:1191:ASN:ND2	8:D:1195:ARG:O	2.45	0.48
8:Y:120:SER:HB3	8:Y:1084:VAL:HG12	1.94	0.48
8:Y:800:LEU:HD23	8:Y:923:VAL:HG11	1.96	0.48
6:1:157:VAL:HB	6:1:158:HIS:HD2	1.78	0.48
8:a:317:SER:O	8:Z:3:ASN:ND2	2.47	0.48
8:B:537:PHE:O	8:B:555:ARG:NE	2.47	0.48
8:B:578:ILE:HG22	8:B:1028:ILE:HD12	1.95	0.48
8:D:231:ASN:OD1	8:D:1099:VAL:N	2.44	0.48
8:D:231:ASN:HD22	8:D:1369:ASN:HD21	1.61	0.48
8:D:1124:HIS:HB3	8:D:1127:VAL:HG12	1.94	0.48
8:D:1327:THR:HG21	8:D:1333:MET:HB2	1.96	0.48
8:Y:41:ASP:OD1	8:Y:41:ASP:N	2.45	0.48
8:Y:1060:ASN:O	8:Y:1079:GLN:NE2	2.44	0.48
8:Z:3:ASN:OD1	8:Z:3:ASN:N	2.45	0.48
8:Z:925:THR:OG1	8:Z:926:ALA:N	2.46	0.48
1:h:163:GLU:HA	1:h:166:LYS:HE3	1.96	0.48
2:H:2238:LEU:HD23	8:a:755:PRO:HB3	1.96	0.48
4:M:305:GLU:HG2	4:M:333:ASN:HD21	1.79	0.48
8:B:388:ASN:HB2	8:B:1311:ILE:HD12	1.94	0.48
8:B:701:GLU:OE1	8:B:714:ARG:NH1	2.46	0.48
8:D:795:ASN:ND2	8:D:995:SER:OG	2.41	0.48
8:D:1045:ASP:HB2	8:D:1098:TYR:HB3	1.96	0.48
8:Z:605:ASN:O	8:Z:642:ARG:NH1	2.46	0.48
8:Z:866:THR:HG21	8:Z:872:LEU:HD12	1.95	0.48
1:h:13:ASP:OD1	1:h:43:HIS:NE2	2.46	0.47
1:I:88:HIS:ND1	1:I:306:GLY:OXT	2.46	0.47
4:M:151:LEU:O	4:M:158:TYR:HA	2.14	0.47
7:S:72:ARG:NE	8:C:820:MET:O	2.43	0.47
8:C:1060:ASN:O	8:C:1079:GLN:NE2	2.46	0.47
8:D:858:THR:OG1	8:D:859:GLU:N	2.47	0.47
8:D:1241:ASP:O	8:D:1248:HIS:ND1	2.39	0.47
8:Y:610:CYS:HB3	8:Y:649:HIS:HE1	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:757:LEU:O	8:Y:805:LYS:NZ	2.47	0.47
1:I:118:PRO:HD2	1:I:121:ARG:HA	1.97	0.47
4:M:505:ARG:HG2	4:M:511:LEU:HA	1.96	0.47
8:a:1155:SER:OG	8:a:1156:MET:N	2.47	0.47
8:C:447:LYS:NZ	8:C:1135:ALA:O	2.46	0.47
8:C:646:VAL:O	8:C:674:TYR:OH	2.29	0.47
8:Y:1200:LEU:HD21	8:Y:1278:LEU:HD13	1.96	0.47
1:I:153:MET:HG3	1:I:172:LEU:HD12	1.96	0.47
1:o:292:ASP:OD1	1:o:301:THR:OG1	2.31	0.47
8:a:1294:ARG:NH2	8:a:1296:ASP:OD2	2.47	0.47
8:B:358:ASP:OD1	8:B:358:ASP:N	2.44	0.47
8:C:470:PRO:HG2	8:C:473:PRO:HB3	1.96	0.47
8:D:599:THR:O	8:D:603:SER:OG	2.32	0.47
8:D:617:VAL:HG13	8:D:619:GLY:H	1.79	0.47
8:D:1246:THR:HA	8:D:1249:ARG:HD3	1.95	0.47
1:I:210:LEU:O	1:I:214:LEU:HB2	2.13	0.47
1:n:237:LEU:O	1:o:267:ARG:NE	2.47	0.47
7:T:52:SER:OG	7:T:53:LEU:N	2.47	0.47
8:a:182:THR:HG21	8:a:1083:THR:HG21	1.96	0.47
8:a:275:SER:OG	8:a:276:THR:N	2.46	0.47
8:D:291:ILE:HG12	8:D:360:ILE:HB	1.96	0.47
8:Y:462:GLN:HA	8:Y:465:THR:HG22	1.95	0.47
8:Y:1329:THR:HG23	8:Y:1332:LEU:H	1.79	0.47
8:Z:417:ASN:OD1	8:Z:422:ASN:ND2	2.47	0.47
4:M:81:ALA:HB1	4:M:556:ARG:HG2	1.95	0.47
8:a:451:HIS:HE2	8:a:1114:PHE:HA	1.79	0.47
8:B:684:VAL:HA	8:B:687:ILE:HG22	1.95	0.47
8:C:124:PRO:HG2	8:D:104:ALA:HB2	1.95	0.47
8:C:968:ARG:HH11	8:C:972:GLY:HA3	1.80	0.47
8:C:1243:LEU:O	8:C:1249:ARG:NH1	2.47	0.47
8:D:654:VAL:HG13	8:D:674:TYR:HD1	1.79	0.47
8:D:1086:MET:HE3	8:D:1086:MET:HB2	1.71	0.47
8:Y:909:ASP:OD1	8:Y:909:ASP:N	2.43	0.47
8:Y:1221:ASP:OD2	8:Y:1224:THR:OG1	2.32	0.47
8:Z:84:ASN:OD1	8:Z:84:ASN:N	2.48	0.47
8:Z:656:LEU:HA	8:Z:660:HIS:HD2	1.79	0.47
8:Z:1245:ASN:O	8:Z:1249:ARG:N	2.47	0.47
7:i:26:LEU:HD21	7:i:64:LEU:HD11	1.96	0.47
8:a:485:GLN:HE21	8:a:913:ARG:HH12	1.62	0.47
8:a:1264:GLN:O	8:a:1319:GLN:NE2	2.41	0.47
8:C:776:ASP:OD1	8:C:776:ASP:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:D:128:PRO:HB3	8:D:1076:HIS:HA	1.97	0.47
8:Z:1360:ILE:HD12	8:Z:1361:PRO:HD2	1.96	0.47
1:I:144:LEU:HD21	3:g:127:ARG:HH22	1.80	0.47
1:I:175:ILE:HG22	1:I:182:PHE:H	1.79	0.47
1:o:280:ASP:N	1:o:280:ASP:OD1	2.41	0.47
3:m:245:THR:HG23	3:m:290:VAL:HG22	1.97	0.47
5:N:22:ASN:HB3	5:O:7:PHE:H	1.79	0.47
6:1:118:VAL:HB	6:1:214:ARG:HH12	1.78	0.47
8:B:256:ASP:OD2	8:B:256:ASP:N	2.48	0.47
8:C:203:ALA:O	8:Z:25:THR:OG1	2.30	0.47
8:C:1104:THR:OG1	8:C:1105:ASP:N	2.46	0.47
8:C:1195:ARG:NH2	8:C:1219:GLU:O	2.41	0.47
8:C:1332:LEU:HD13	8:C:1355:VAL:HG23	1.97	0.47
8:D:624:PHE:HA	8:D:627:ILE:HG22	1.96	0.47
8:Z:146:THR:HG23	8:Z:149:ASP:H	1.79	0.47
8:Z:1001:VAL:O	8:Z:1004:SER:OG	2.32	0.47
8:Z:1038:ARG:HB3	8:Z:1171:ALA:HA	1.97	0.47
8:Z:1342:GLY:H	8:Z:1364:GLN:HE21	1.61	0.47
1:I:196:ASP:N	1:I:196:ASP:OD1	2.48	0.47
1:n:155:LEU:HD22	1:n:197:MET:HG2	1.96	0.47
8:a:727:MET:HE2	8:a:727:MET:HB2	1.87	0.47
8:a:1245:ASN:HD22	8:a:1248:HIS:HB2	1.79	0.47
8:C:617:VAL:HG13	8:C:623:ALA:HB3	1.96	0.47
8:C:702:PRO:HG3	8:D:964:PRO:HB2	1.97	0.47
8:C:981:HIS:O	8:C:985:ASN:ND2	2.48	0.47
8:D:777:GLU:HA	8:D:780:LEU:HB2	1.96	0.47
8:Y:480:GLU:HA	8:Y:482:ARG:HH11	1.80	0.47
8:Y:1176:LEU:HD21	8:Y:1233:ALA:HB2	1.96	0.47
8:Z:510:ASN:OD1	8:Z:989:SER:OG	2.33	0.47
8:Z:1112:ASP:OD1	8:Z:1115:ARG:N	2.42	0.47
8:Z:1173:GLU:O	8:Z:1244:TYR:OH	2.27	0.47
4:M:529:LEU:HD12	4:M:545:VAL:HG11	1.97	0.47
6:1:101:LYS:NZ	6:1:138:MET:SD	2.86	0.47
7:j:52:SER:OG	7:j:53:LEU:N	2.48	0.47
8:a:253:SER:OG	8:a:255:LEU:O	2.33	0.47
8:B:1291:ASP:OD1	8:B:1316:ARG:NH2	2.48	0.47
8:Z:638:MET:HE3	8:Z:864:VAL:HA	1.97	0.47
8:Z:846:ILE:HA	8:Z:849:GLN:HE21	1.80	0.47
1:o:110:VAL:HG12	1:o:287:VAL:HG21	1.97	0.47
8:B:12:LYS:HE2	8:Z:58:CYS:HB2	1.97	0.47
8:C:695:ASN:HD21	8:D:968:ARG:HD2	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:970:ASP:OD1	8:C:992:SER:OG	2.32	0.47
8:D:510:ASN:ND2	8:D:989:SER:OG	2.47	0.47
8:D:534:HIS:HD2	8:D:536:PHE:H	1.63	0.47
8:D:554:PRO:HD3	8:D:907:LEU:HD12	1.96	0.47
8:Y:431:LEU:HD23	8:Y:435:ARG:HA	1.96	0.47
1:I:59:VAL:HB	1:I:196:ASP:HB2	1.95	0.46
1:n:42:LYS:HG3	8:a:105:GLY:HA3	1.96	0.46
1:n:74:ARG:O	1:n:82:LEU:HB3	2.16	0.46
8:C:414:VAL:HG21	8:C:1331:ALA:HB1	1.96	0.46
8:C:684:VAL:HA	8:C:687:ILE:HG22	1.96	0.46
8:Y:596:LEU:HA	8:Y:599:THR:HG22	1.97	0.46
8:Y:672:PHE:HA	8:Y:675:ARG:HG2	1.95	0.46
8:Y:692:GLY:HA2	8:Z:993:ARG:HH12	1.81	0.46
8:Y:1360:ILE:HD12	8:Y:1361:PRO:HD2	1.97	0.46
8:Z:301:THR:OG1	8:Z:302:TYR:N	2.48	0.46
8:Z:393:PHE:HZ	8:Z:1362:LEU:HD11	1.79	0.46
8:Z:1121:VAL:HG12	8:Z:1132:ARG:HH11	1.80	0.46
8:a:894:GLU:OE1	8:a:896:ARG:NE	2.47	0.46
8:a:1191:ASN:ND2	8:a:1319:GLN:O	2.48	0.46
8:B:5:SER:O	8:B:9:LEU:HB2	2.16	0.46
8:B:394:PHE:HA	8:B:1036:ALA:O	2.15	0.46
8:B:1327:THR:OG1	8:B:1328:THR:N	2.49	0.46
8:C:391:LEU:HD12	8:C:1042:PHE:HE2	1.79	0.46
8:C:793:THR:HG23	8:C:796:ARG:H	1.80	0.46
8:D:301:THR:OG1	8:D:302:TYR:N	2.49	0.46
1:h:204:MET:HA	1:h:207:VAL:HG22	1.97	0.46
3:m:101:LEU:O	3:m:104:SER:OG	2.31	0.46
6:1:87:VAL:HG21	6:1:203:LEU:HD22	1.97	0.46
8:a:816:ALA:O	8:a:877:ARG:NH1	2.49	0.46
8:a:1310:LEU:HD12	8:a:1310:LEU:HA	1.83	0.46
8:C:135:CYS:O	8:C:139:LEU:HB2	2.16	0.46
8:C:444:ASP:OD1	8:D:523:LYS:NZ	2.42	0.46
8:D:515:ASP:OD1	8:D:515:ASP:N	2.38	0.46
8:D:785:TYR:O	8:D:943:TYR:OH	2.26	0.46
8:Y:18:ASP:OD1	8:Y:18:ASP:N	2.44	0.46
8:Z:275:SER:HB3	8:Z:280:MET:HG2	1.97	0.46
3:g:169:LYS:HE3	3:g:261:THR:HB	1.97	0.46
4:M:74:ASP:OD2	4:M:74:ASP:N	2.38	0.46
4:M:106:TYR:HA	4:M:109:GLN:HG2	1.96	0.46
4:M:475:ALA:HA	4:M:523:LEU:O	2.16	0.46
5:N:14:VAL:HA	5:O:13:ALA:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:a:941:ARG:HD3	8:a:992:SER:HB3	1.98	0.46
8:D:733:VAL:HG12	8:D:738:PRO:HA	1.97	0.46
8:Y:583:ARG:HH21	8:Z:998:CYS:HA	1.81	0.46
8:Z:1195:ARG:NE	8:Z:1213:ALA:O	2.42	0.46
1:h:28:VAL:HG13	1:h:74:ARG:HA	1.98	0.46
8:a:225:ALA:O	8:a:232:ARG:NH1	2.48	0.46
8:B:155:GLU:HG3	8:Z:9:LEU:HD13	1.97	0.46
8:C:857:LEU:HD21	8:C:876:CYS:HB3	1.97	0.46
8:D:714:ARG:HH21	8:D:900:ASP:HA	1.80	0.46
8:Y:430:LEU:HD12	8:Y:1108:VAL:HG12	1.98	0.46
8:Y:681:LEU:HB3	8:Y:780:LEU:HD22	1.97	0.46
1:I:211:ALA:O	1:I:215:THR:OG1	2.27	0.46
4:M:478:VAL:HG23	4:M:485:VAL:HG12	1.97	0.46
5:O:55:ARG:HH22	5:O:59:ARG:HB2	1.80	0.46
6:1:282:PHE:O	6:1:284:GLN:NE2	2.48	0.46
8:a:1182:ASP:OD1	8:a:1182:ASP:N	2.39	0.46
8:C:166:ASN:ND2	8:D:111:GLN:OE1	2.49	0.46
8:D:521:PHE:O	8:D:526:ASN:ND2	2.48	0.46
8:D:895:VAL:HB	8:D:914:GLN:HB3	1.97	0.46
8:D:895:VAL:N	8:D:914:GLN:O	2.42	0.46
8:Y:556:ILE:HD12	8:Y:899:LEU:HD21	1.97	0.46
8:Z:1044:VAL:HG11	8:Z:1096:VAL:HG13	1.97	0.46
8:Z:1349:THR:HA	8:Z:1354:TYR:HA	1.97	0.46
8:B:1001:VAL:O	8:B:1004:SER:OG	2.33	0.46
8:C:715:LEU:HB3	8:C:782:LYS:HE3	1.98	0.46
8:Y:812:PHE:HB3	8:Y:880:PHE:HE1	1.81	0.46
1:o:154:GLY:HA3	1:o:197:MET:HE2	1.98	0.46
4:M:306:TRP:HA	4:M:333:ASN:HD22	1.80	0.46
6:1:30:ASP:O	6:1:34:HIS:N	2.48	0.46
7:i:62:LEU:HA	7:i:65:LEU:HD12	1.98	0.46
8:a:801:GLY:HA3	8:a:890:VAL:HG11	1.98	0.46
8:a:892:VAL:HG11	8:a:979:PHE:HE1	1.81	0.46
8:C:905:GLN:HG3	8:C:1123:ARG:H	1.81	0.46
8:C:1285:TYR:OH	8:C:1312:GLU:OE1	2.34	0.46
8:Y:1105:ASP:N	8:Y:1105:ASP:OD1	2.48	0.46
8:Z:540:THR:OG1	8:Z:541:HIS:N	2.48	0.46
8:Z:609:LEU:HD23	8:Z:860:LEU:HB3	1.97	0.46
8:Z:845:SER:OG	8:Z:846:ILE:N	2.47	0.46
8:Z:1291:ASP:OD1	8:Z:1291:ASP:N	2.48	0.46
1:h:268:LEU:HD11	1:I:151:LEU:HD22	1.98	0.46
1:n:38:LEU:HB2	1:n:41:ILE:HG22	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:N:28:GLU:HG2	5:O:2:SER:HB3	1.97	0.46
8:a:491:ALA:HA	8:a:494:ARG:HB2	1.98	0.46
8:a:1158:GLU:O	8:a:1301:TYR:OH	2.31	0.46
8:B:35:LEU:HB3	8:B:37:ILE:HD11	1.98	0.46
8:B:208:ASN:OD1	8:B:208:ASN:N	2.49	0.46
8:C:724:PRO:HA	8:C:773:ALA:HB3	1.98	0.46
8:Y:515:ASP:OD2	8:Y:515:ASP:N	2.41	0.46
8:Y:1111:GLN:NE2	8:Y:1112:ASP:O	2.42	0.46
1:h:108:LEU:HB2	1:h:288:PHE:HB2	1.98	0.46
1:h:149:ARG:NH1	1:h:174:THR:O	2.49	0.46
3:m:183:GLN:HG2	3:m:256:ALA:HB2	1.96	0.46
5:N:18:PRO:HA	5:N:22:ASN:HD21	1.81	0.46
7:S:55:ASN:OD1	7:S:55:ASN:N	2.46	0.46
8:a:256:ASP:OD1	8:a:256:ASP:N	2.49	0.46
8:Y:268:LYS:HA	8:Y:268:LYS:HD3	1.82	0.46
8:Y:1128:ASP:OD1	8:Y:1132:ARG:NH2	2.49	0.46
8:Z:941:ARG:NH1	8:Z:992:SER:OG	2.45	0.46
3:m:59:PHE:H	3:m:266:HIS:CD2	2.34	0.45
3:m:250:LYS:HB2	3:m:250:LYS:HE3	1.74	0.45
4:M:366:VAL:HG23	4:M:550:LEU:HD21	1.98	0.45
8:a:598:LYS:O	8:a:602:THR:OG1	2.33	0.45
8:C:775:ASP:OD1	8:C:775:ASP:N	2.48	0.45
8:D:1280:LYS:HE3	8:D:1280:LYS:HB3	1.76	0.45
8:Z:273:MET:HG3	8:Z:1049:TYR:HB2	1.97	0.45
8:Z:1041:THR:OG1	8:Z:1103:ARG:NH1	2.49	0.45
8:a:1185:TYR:OH	8:a:1191:ASN:O	2.23	0.45
8:B:632:ALA:HB2	8:B:661:LEU:HD11	1.98	0.45
8:C:92:LEU:HD23	8:Z:7:LEU:HB2	1.97	0.45
8:C:1298:ASP:OD2	8:D:209:ARG:NH1	2.49	0.45
8:D:1272:ILE:O	8:D:1275:ASN:ND2	2.49	0.45
8:Z:1294:ARG:HG2	8:Z:1303:CYS:HB3	1.98	0.45
1:h:280:ASP:OD2	3:g:287:ARG:NH2	2.50	0.45
4:M:312:SER:OG	4:M:313:ARG:N	2.47	0.45
4:M:321:GLN:NE2	4:M:357:TYR:OH	2.48	0.45
8:B:488:MET:HB2	8:B:491:ALA:HB2	1.97	0.45
8:C:188:PRO:HA	8:C:1286:LEU:HD21	1.97	0.45
8:C:1166:HIS:NE2	8:D:1223:GLN:O	2.48	0.45
8:Z:600:THR:O	8:Z:603:SER:OG	2.34	0.45
3:g:172:TYR:HA	3:g:204:VAL:HG23	1.97	0.45
6:1:103:ARG:HD3	6:1:106:LEU:HD11	1.98	0.45
8:a:662:ALA:HA	8:a:671:LEU:HD23	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:a:1114:PHE:HB2	8:a:1137:VAL:HG11	1.99	0.45
8:a:1154:GLY:HA2	8:a:1257:LYS:HE2	1.99	0.45
8:B:280:MET:HG2	8:B:371:ASN:HB2	1.99	0.45
8:B:320:SER:OG	8:B:321:ILE:N	2.50	0.45
8:C:1216:ASP:OD1	8:C:1219:GLU:N	2.49	0.45
8:D:921:CYS:SG	8:D:922:CYS:N	2.89	0.45
8:D:1173:GLU:O	8:D:1244:TYR:OH	2.30	0.45
8:Y:225:ALA:O	8:Y:232:ARG:NH1	2.50	0.45
1:I:152:ILE:HA	1:I:155:LEU:HG	1.99	0.45
1:I:262:ASP:N	1:I:262:ASP:OD2	2.49	0.45
3:g:267:LYS:HE2	3:g:267:LYS:HB3	1.78	0.45
8:a:1343:ALA:O	8:a:1346:THR:OG1	2.30	0.45
8:B:9:LEU:HD13	8:Z:155:GLU:HG3	1.97	0.45
8:C:657:ILE:HG13	8:C:661:LEU:HD12	1.98	0.45
8:C:811:LEU:HD12	8:C:856:MET:HE1	1.97	0.45
8:C:1111:GLN:HB2	8:C:1172:CYS:HA	1.97	0.45
8:D:495:ILE:HD12	8:D:937:VAL:HG12	1.99	0.45
8:Y:558:ILE:HD11	8:Y:1031:GLY:HA3	1.97	0.45
1:n:260:SER:OG	1:n:262:ASP:OD2	2.34	0.45
3:m:258:ASP:O	3:m:260:HIS:ND1	2.50	0.45
4:M:425:ILE:O	4:M:429:THR:OG1	2.28	0.45
5:N:22:ASN:N	5:N:22:ASN:OD1	2.49	0.45
8:D:638:MET:HE3	8:D:638:MET:HB3	1.84	0.45
8:Y:1193:ARG:NH2	8:Y:1195:ARG:O	2.50	0.45
8:Z:273:MET:HB3	8:Z:273:MET:HE2	1.87	0.45
8:Z:796:ARG:HA	8:Z:945:ASN:HD22	1.81	0.45
8:Z:1362:LEU:HA	8:Z:1366:MET:HG2	1.99	0.45
1:h:195:ILE:HD12	1:h:195:ILE:HA	1.88	0.45
4:M:589:LEU:HD21	8:a:1140:PRO:HB2	1.99	0.45
7:i:40:LEU:O	7:i:44:LEU:HB2	2.17	0.45
8:a:1176:LEU:HD22	8:a:1230:ASN:HB3	1.98	0.45
8:B:144:GLU:HG2	8:B:145:GLY:H	1.82	0.45
8:B:164:LEU:HD23	8:B:164:LEU:HA	1.86	0.45
8:B:424:LEU:HD12	8:B:425:PRO:HD2	1.98	0.45
8:C:87:THR:OG1	8:C:88:THR:N	2.49	0.45
8:C:1323:PRO:HG2	8:C:1359:ILE:HG12	1.99	0.45
8:D:230:LEU:HD12	8:D:279:VAL:HG23	1.98	0.45
8:D:435:ARG:HH21	8:D:1364:GLN:HA	1.82	0.45
8:Y:609:LEU:HD21	8:Y:860:LEU:HB3	1.99	0.45
8:Y:688:SER:OG	8:Y:708:ASN:ND2	2.49	0.45
8:Y:1105:ASP:HB3	8:Y:1166:HIS:HB3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:h:156:PHE:CZ	1:I:261:PRO:HB3	2.52	0.45
1:h:241:LEU:HD21	1:I:267:ARG:HG2	1.99	0.45
1:o:31:VAL:HG21	1:o:137:ILE:HD11	1.98	0.45
4:M:309:ALA:HB1	4:M:332:VAL:HG23	1.98	0.45
4:M:388:GLN:HA	4:M:539:PHE:HA	1.98	0.45
8:a:110:ARG:HH11	8:B:39:TYR:HB2	1.82	0.45
8:a:955:ASP:OD1	8:a:955:ASP:N	2.48	0.45
8:B:1241:ASP:OD1	8:B:1245:ASN:ND2	2.50	0.45
8:C:1100:ASN:OD1	8:C:1100:ASN:N	2.47	0.45
8:C:1220:ALA:HA	8:C:1227:ALA:HB2	1.98	0.45
8:D:182:THR:HG21	8:D:1083:THR:HG21	1.97	0.45
8:Y:936:PRO:HB3	8:Y:952:LEU:HD12	1.99	0.45
1:h:32:VAL:HG23	1:h:71:THR:HG23	1.98	0.45
1:h:204:MET:HG3	1:I:215:THR:HG23	1.99	0.45
2:P:2223:GLN:O	2:P:2227:SER:OG	2.31	0.45
1:o:171:GLN:OE1	6:1:99:ARG:NH2	2.49	0.45
7:T:55:ASN:N	7:T:55:ASN:OD1	2.50	0.45
7:j:14:ARG:HH12	7:j:17:LYS:HB2	1.81	0.45
8:a:84:ASN:OD1	8:a:84:ASN:N	2.47	0.45
8:a:111:GLN:HE21	8:Z:130:GLU:HG2	1.82	0.45
8:a:572:GLU:OE1	8:a:575:THR:OG1	2.35	0.45
8:B:433:ARG:HB3	8:B:1105:ASP:HA	1.98	0.45
8:C:503:ARG:HH12	8:C:505:VAL:HB	1.82	0.45
8:C:1286:LEU:HD23	8:C:1286:LEU:HA	1.84	0.45
8:D:270:SER:HB2	8:D:365:LYS:HE2	1.98	0.45
8:Z:93:PHE:HB2	8:Z:116:VAL:HG12	1.98	0.45
1:I:53:ASP:OD1	1:I:53:ASP:N	2.48	0.45
1:o:5:GLU:O	1:o:7:ASN:ND2	2.50	0.45
7:i:44:LEU:HD23	7:i:47:TYR:HB2	1.98	0.45
8:a:532:GLU:OE2	8:a:555:ARG:NH1	2.50	0.45
8:C:983:TYR:O	8:C:988:ARG:NH2	2.41	0.45
8:D:66:PHE:N	8:D:172:GLU:OE2	2.49	0.45
8:Y:229:LEU:HD12	8:Y:229:LEU:HA	1.81	0.45
8:Y:377:LYS:NZ	8:Y:378:ASN:OD1	2.48	0.45
8:Z:627:ILE:HG22	8:Z:630:PHE:HB3	1.98	0.45
8:Z:725:ARG:HA	8:Z:772:ARG:HB3	1.99	0.45
4:M:102:GLU:HG2	4:M:121:ARG:HH21	1.82	0.44
8:a:349:ALA:O	8:a:350:HIS:ND1	2.50	0.44
8:a:800:LEU:HD23	8:a:923:VAL:HG21	1.98	0.44
8:a:1020:LEU:HD11	8:a:1032:PHE:HZ	1.82	0.44
8:B:627:ILE:HD11	8:B:879:LEU:HD23	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:718:PRO:HD2	8:C:785:TYR:HB3	1.99	0.44
8:D:747:ARG:NH2	8:D:767:PHE:O	2.41	0.44
8:a:1176:LEU:HD21	8:a:1233:ALA:HB2	2.00	0.44
8:B:1190:ASN:OD1	8:B:1223:GLN:NE2	2.50	0.44
8:D:64:VAL:HG21	8:D:375:VAL:HG23	1.99	0.44
8:Y:733:VAL:HG12	8:Y:738:PRO:HA	1.99	0.44
1:h:24:LEU:HD21	1:h:125:LEU:HD13	1.99	0.44
1:h:148:GLN:O	1:h:152:ILE:HG12	2.18	0.44
1:I:203:SER:HA	1:I:206:MET:HG2	1.98	0.44
7:i:66:ARG:NH2	8:Z:884:GLN:O	2.50	0.44
8:a:328:TYR:HD2	8:B:10:LEU:HD12	1.82	0.44
8:a:718:PRO:HD2	8:a:785:TYR:HB3	2.00	0.44
8:a:790:PRO:HA	8:a:793:THR:HG22	1.98	0.44
8:a:873:LEU:HD12	8:a:877:ARG:HH21	1.82	0.44
8:a:1228:THR:OG1	8:a:1229:HIS:N	2.51	0.44
8:C:93:PHE:HB2	8:C:116:VAL:HG13	1.98	0.44
8:C:1149:SER:HA	8:C:1152:THR:HG22	1.99	0.44
8:D:372:LEU:HD23	8:D:372:LEU:HA	1.89	0.44
8:Y:1124:HIS:HB3	8:Y:1127:VAL:HG12	1.99	0.44
8:Z:274:VAL:HG23	8:Z:370:GLU:HB3	1.98	0.44
8:Z:1174:LEU:HD21	8:Z:1233:ALA:HB2	1.99	0.44
1:h:229:MET:HE2	8:B:1140:PRO:HD2	1.99	0.44
1:I:257:GLN:HE21	1:I:258:HIS:HD2	1.66	0.44
2:P:2240:LEU:HG	5:O:61:LEU:HD12	1.98	0.44
3:m:135:VAL:HG21	3:m:146:LEU:HD12	1.99	0.44
8:a:810:ASP:OD2	8:a:810:ASP:N	2.48	0.44
8:B:654:VAL:HA	8:B:657:ILE:HD12	1.99	0.44
8:B:982:GLU:OE2	8:B:989:SER:N	2.50	0.44
8:D:235:ASP:HB3	8:D:238:TYR:HB3	2.00	0.44
8:Y:717:PRO:HB3	8:Y:782:LYS:HA	1.99	0.44
8:Y:1290:LYS:HB3	8:Y:1310:LEU:HB3	1.99	0.44
1:I:108:LEU:HD22	1:I:137:ILE:HG22	1.99	0.44
3:g:64:GLY:HA3	3:g:166:MET:HG2	2.00	0.44
6:l:148:ILE:HD13	8:D:479:LEU:HD13	1.99	0.44
7:R:41:ALA:HA	7:R:44:LEU:HG	2.00	0.44
8:a:70:GLY:N	8:a:370:GLU:OE2	2.50	0.44
8:a:252:ASP:OD1	8:a:252:ASP:N	2.41	0.44
8:B:848:ALA:HA	8:B:851:GLN:HE21	1.83	0.44
8:D:815:PRO:HA	8:D:818:LEU:HB2	1.99	0.44
8:Y:372:LEU:HD23	8:Y:372:LEU:HA	1.86	0.44
8:Y:582:MET:HE3	8:Y:582:MET:HB3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:900:ASP:N	8:Y:900:ASP:OD1	2.49	0.44
8:a:404:ASP:OD1	8:Z:421:ARG:NH1	2.51	0.44
8:a:580:GLU:OE2	8:a:585:ARG:NE	2.44	0.44
8:a:622:ASP:OD1	8:a:622:ASP:N	2.48	0.44
8:C:108:THR:OG1	8:C:109:SER:N	2.50	0.44
8:C:861:VAL:HA	8:C:864:VAL:HG22	1.98	0.44
8:C:1282:ILE:HD13	8:C:1282:ILE:HA	1.87	0.44
8:Y:441:ASP:OD1	8:Y:441:ASP:N	2.49	0.44
8:Z:775:ASP:OD1	8:Z:775:ASP:N	2.50	0.44
8:Z:1081:ILE:O	8:Z:1082:ASN:ND2	2.51	0.44
1:h:156:PHE:HZ	1:I:261:PRO:HB3	1.83	0.44
8:a:546:SER:O	8:a:546:SER:OG	2.32	0.44
8:a:1285:TYR:CG	8:a:1317:LEU:HD22	2.53	0.44
8:B:77:ALA:HB1	8:B:302:TYR:HD1	1.82	0.44
8:Y:684:VAL:HA	8:Y:687:ILE:HG22	1.99	0.44
8:Z:1172:CYS:SG	8:Z:1173:GLU:N	2.84	0.44
1:I:61:LEU:O	1:I:65:LEU:HB2	2.18	0.44
6:1:175:ARG:HD2	6:1:216:SER:HB3	2.00	0.44
7:S:68:VAL:HG11	8:C:818:LEU:HD13	2.00	0.44
8:a:774:THR:OG1	8:a:775:ASP:N	2.50	0.44
8:B:908:PRO:HG3	8:B:1123:ARG:HH22	1.82	0.44
8:B:983:TYR:O	8:B:988:ARG:NH2	2.51	0.44
8:C:598:LYS:HD3	8:C:792:MET:HE3	1.99	0.44
8:C:949:CYS:HB3	8:C:956:ILE:HG21	2.00	0.44
8:D:388:ASN:OD1	8:D:388:ASN:N	2.50	0.44
8:D:608:GLU:HG2	8:D:930:LEU:HD23	2.00	0.44
8:D:721:THR:OG1	8:D:722:HIS:N	2.51	0.44
8:D:948:ILE:HD13	8:D:948:ILE:HA	1.86	0.44
8:D:999:PRO:HB2	8:D:1001:VAL:HG23	2.00	0.44
8:Y:1125:ASP:OD1	8:Y:1125:ASP:N	2.50	0.44
8:Z:1299:THR:OG1	8:Z:1300:GLN:N	2.51	0.44
8:a:667:PRO:HA	8:a:668:PRO:HD3	1.81	0.44
8:a:669:GLN:O	8:a:673:HIS:ND1	2.51	0.44
8:B:557:VAL:HA	8:B:1014:LYS:HA	1.99	0.44
8:Y:1143:LEU:O	8:Y:1147:THR:OG1	2.35	0.44
8:Z:212:ARG:NH1	8:Z:1203:ASP:OD1	2.42	0.44
8:Z:582:MET:HE2	8:Z:691:PRO:HD2	2.00	0.44
8:Z:1033:ALA:HB2	8:Z:1178:PRO:HA	2.00	0.44
3:g:121:GLY:H	3:g:128:ARG:HH12	1.66	0.43
8:B:132:SER:N	8:Z:41:ASP:OD2	2.47	0.43
8:B:1101:ARG:HH22	8:C:202:LEU:HD22	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:1182:ASP:HA	8:B:1186:PHE:HD2	1.83	0.43
8:Y:389:VAL:HG13	8:Y:1044:VAL:HG21	1.99	0.43
8:Z:1110:VAL:HA	8:Z:1171:ALA:HB3	2.00	0.43
1:I:56:ARG:HD3	1:I:60:ARG:HD2	2.00	0.43
3:m:167:ILE:HD12	3:m:168:PRO:HD2	2.00	0.43
8:a:785:TYR:O	8:a:943:TYR:OH	2.27	0.43
8:B:47:ASN:OD1	8:B:47:ASN:N	2.51	0.43
8:B:429:TYR:HE1	8:B:439:LYS:HZ3	1.65	0.43
8:C:119:TYR:OH	8:Z:2:GLU:OE2	2.35	0.43
8:Y:610:CYS:HB3	8:Y:649:HIS:CE1	2.53	0.43
8:Y:627:ILE:HG22	8:Y:630:PHE:HB3	2.00	0.43
8:Z:392:THR:HG21	8:Z:1265:TYR:HE2	1.82	0.43
8:Z:522:TYR:OH	8:Z:1179:VAL:O	2.23	0.43
8:Z:718:PRO:HD2	8:Z:785:TYR:HB3	2.00	0.43
1:o:126:THR:HG22	1:o:131:GLU:HG3	1.99	0.43
3:m:42:ASP:OD1	3:m:42:ASP:N	2.40	0.43
7:T:37:HIS:HD2	7:T:38:PRO:HD2	1.83	0.43
7:j:21:VAL:HA	7:j:25:VAL:HB	1.99	0.43
8:a:286:LEU:HG	8:a:287:LEU:HD12	1.99	0.43
8:B:140:ARG:NE	8:B:324:ASP:OD1	2.51	0.43
8:B:808:LEU:HD13	8:B:808:LEU:HA	1.89	0.43
8:D:459:PRO:HB2	8:D:1242:VAL:HG11	2.00	0.43
8:Y:310:GLU:HA	8:Y:313:VAL:HG22	2.00	0.43
8:Z:182:THR:HG22	8:Z:185:ARG:HH22	1.83	0.43
3:g:258:ASP:HB2	3:g:277:ASP:H	1.84	0.43
6:1:171:LEU:HD12	6:1:212:ASN:HD21	1.84	0.43
6:1:201:ASN:HA	6:1:204:VAL:HG12	1.99	0.43
7:j:17:LYS:HD2	7:j:20:HIS:HD2	1.83	0.43
8:C:183:LEU:HD23	8:C:183:LEU:HA	1.88	0.43
8:C:1124:HIS:HB3	8:C:1127:VAL:HG12	1.99	0.43
8:C:1191:ASN:ND2	8:C:1197:SER:OG	2.51	0.43
8:Z:617:VAL:HG13	8:Z:619:GLY:H	1.83	0.43
3:g:58:GLU:O	3:g:106:TYR:OH	2.30	0.43
7:i:18:HIS:CE1	7:i:44:LEU:HB3	2.53	0.43
8:a:588:PRO:HG2	8:a:683:LEU:HD21	2.00	0.43
8:B:1027:HIS:CD2	8:C:517:VAL:HG11	2.53	0.43
8:B:1106:MET:SD	8:B:1106:MET:N	2.92	0.43
8:C:1060:ASN:OD1	8:C:1060:ASN:N	2.52	0.43
8:D:1175:ILE:HB	8:D:1239:LEU:HD21	2.01	0.43
8:Y:946:PRO:HA	8:Y:949:CYS:HB2	2.01	0.43
8:Y:1241:ASP:O	8:Y:1248:HIS:ND1	2.35	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Z:122:LYS:HG3	8:Z:1082:ASN:HD21	1.83	0.43
8:Z:804:LEU:HD23	8:Z:889:HIS:HD2	1.83	0.43
1:n:59:VAL:HG23	1:n:62:ARG:HH21	1.83	0.43
5:N:28:GLU:OE1	5:O:2:SER:N	2.51	0.43
8:a:419:THR:OG1	8:a:580:GLU:OE1	2.28	0.43
8:a:553:THR:HG21	8:a:983:TYR:HB3	2.01	0.43
8:B:482:ARG:NE	8:B:484:GLN:O	2.51	0.43
8:B:716:TRP:H	8:B:914:GLN:HE22	1.66	0.43
8:C:276:THR:OG1	8:C:277:ALA:N	2.52	0.43
8:C:1277:THR:O	8:C:1281:THR:OG1	2.32	0.43
8:Y:534:HIS:CE1	8:Y:1239:LEU:HB3	2.53	0.43
8:Z:1285:TYR:HB2	8:Z:1317:LEU:HD21	2.01	0.43
1:n:58:TYR:OH	1:n:112:PRO:O	2.32	0.43
8:a:1100:ASN:OD1	8:a:1100:ASN:N	2.52	0.43
8:D:507:ARG:H	8:D:507:ARG:HG2	1.57	0.43
8:Y:1143:LEU:HD23	8:Y:1143:LEU:HA	1.92	0.43
1:h:237:LEU:HD23	1:I:206:MET:HE1	2.01	0.43
4:M:474:TYR:HA	4:M:489:VAL:O	2.19	0.43
8:B:194:GLN:HA	8:B:197:VAL:HG12	2.00	0.43
8:C:605:ASN:O	8:C:642:ARG:NH2	2.51	0.43
8:D:1004:SER:O	8:D:1007:THR:OG1	2.34	0.43
8:Z:499:TYR:OH	8:Z:974:PRO:O	2.31	0.43
8:Z:874:GLN:HA	8:Z:877:ARG:HB2	2.00	0.43
8:Z:1187:LYS:HA	8:Z:1356:VAL:HG23	2.01	0.43
1:I:23:LYS:HB3	1:I:23:LYS:HE3	1.85	0.43
1:I:127:LEU:N	1:I:130:TRP:O	2.51	0.43
3:g:209:ILE:HG21	3:g:215:LEU:HD13	2.01	0.43
4:M:31:VAL:HB	4:M:324:VAL:HG13	2.00	0.43
7:T:53:LEU:HD12	7:T:56:ASP:HB3	2.01	0.43
8:C:329:LYS:HE2	8:C:329:LYS:HB3	1.75	0.43
8:C:610:CYS:O	8:C:614:ASP:N	2.51	0.43
8:Y:574:ARG:NH2	8:Y:1010:ALA:O	2.52	0.43
8:Y:905:GLN:O	8:Y:1123:ARG:NH2	2.50	0.43
8:Z:1263:ALA:HB1	8:Z:1267:ASN:HD21	1.82	0.43
1:I:8:ILE:HB	1:I:83:LEU:HB2	2.00	0.43
1:n:272:PHE:HZ	1:o:151:LEU:HD13	1.84	0.43
4:M:393:HIS:NE2	5:O:20:GLU:OE2	2.50	0.43
4:M:492:ARG:HH11	4:M:507:ARG:HB2	1.84	0.43
6:1:59:TRP:CH2	6:1:227:ARG:HD2	2.54	0.43
8:a:1036:ALA:HA	8:a:1173:GLU:HA	2.00	0.43
8:B:257:ASN:OD1	8:B:259:THR:OG1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:472:GLU:HB2	8:Y:475:MET:HG2	2.01	0.43
8:Y:1001:VAL:O	8:Y:1004:SER:OG	2.36	0.43
8:Z:324:ASP:HB3	8:Z:327:SER:HB3	2.00	0.43
1:o:156:PHE:O	1:o:160:ARG:NE	2.38	0.42
3:m:38:LEU:HD23	8:C:1066:LYS:HD2	2.00	0.42
3:m:148:CYS:SG	3:m:149:VAL:N	2.91	0.42
8:a:92:LEU:HG	8:B:7:LEU:HD13	2.01	0.42
8:B:424:LEU:HD21	8:B:1029:HIS:HB2	2.01	0.42
8:B:570:PHE:HZ	8:B:1031:GLY:HA2	1.84	0.42
8:B:739:LEU:HD23	8:B:744:ILE:HG21	2.01	0.42
8:B:814:ARG:HE	8:B:854:GLY:HA3	1.84	0.42
8:D:215:ILE:HD13	8:D:215:ILE:HA	1.92	0.42
8:D:649:HIS:NE2	8:D:921:CYS:SG	2.91	0.42
8:Y:798:CYS:HA	8:Y:943:TYR:HB3	2.02	0.42
8:Y:1122:TYR:HB2	8:Y:1128:ASP:HB2	2.01	0.42
8:Z:99:ARG:HH11	8:Z:111:GLN:HG3	1.82	0.42
8:Z:495:ILE:HD13	8:Z:937:VAL:HG12	2.01	0.42
8:Z:502:ARG:NH1	8:Z:962:GLU:OE2	2.52	0.42
8:Z:934:SER:OG	8:Z:935:LEU:N	2.51	0.42
3:g:171:MET:HE2	3:g:171:MET:HB3	1.88	0.42
5:N:14:VAL:HG22	5:O:11:PRO:HB2	2.00	0.42
5:N:32:ARG:HA	5:N:32:ARG:HD2	1.87	0.42
8:B:800:LEU:HD23	8:B:923:VAL:HG21	2.01	0.42
8:C:1343:ALA:O	8:C:1346:THR:OG1	2.37	0.42
8:D:631:VAL:O	8:D:635:ILE:HG12	2.19	0.42
8:D:733:VAL:HG22	8:D:894:GLU:HB2	2.01	0.42
8:Y:54:PHE:HB3	8:Z:344:LEU:HD21	1.99	0.42
8:Y:1238:CYS:SG	8:Y:1240:SER:OG	2.69	0.42
8:Z:1038:ARG:HH12	8:Z:1106:MET:HG3	1.84	0.42
8:Z:1040:ASP:OD1	8:Z:1104:THR:OG1	2.33	0.42
1:I:206:MET:HB2	1:I:206:MET:HE3	1.75	0.42
3:g:62:GLN:HG2	3:g:266:HIS:HD2	1.84	0.42
3:g:228:CYS:HA	3:g:231:VAL:HG12	2.02	0.42
3:m:183:GLN:HE21	3:m:256:ALA:HA	1.85	0.42
8:a:874:GLN:NE2	8:a:878:GLU:OE2	2.52	0.42
8:B:58:CYS:SG	8:B:59:ASN:N	2.92	0.42
1:h:228:SER:O	1:h:232:VAL:N	2.49	0.42
1:I:40:LEU:HD21	8:B:124:PRO:HG2	2.01	0.42
4:M:417:TRP:HE3	4:M:485:VAL:HG22	1.84	0.42
4:M:454:PRO:HA	4:M:457:LEU:HB2	2.02	0.42
6:1:92:TYR:HE1	6:1:106:LEU:HD13	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:l:164:VAL:O	6:l:168:GLU:HG2	2.20	0.42
7:i:66:ARG:HB2	8:Z:884:GLN:HA	2.01	0.42
8:a:295:THR:HA	8:a:356:SER:HA	2.02	0.42
8:B:574:ARG:HH11	8:B:1023:GLN:HE22	1.68	0.42
8:B:681:LEU:HB3	8:B:780:LEU:HD22	2.02	0.42
8:C:798:CYS:HB3	8:C:948:ILE:HD11	2.01	0.42
8:D:420:VAL:HA	8:D:423:ALA:HB3	2.01	0.42
8:D:623:ALA:HB2	8:D:885:PHE:CG	2.55	0.42
8:Z:717:PRO:HG3	8:Z:781:GLN:HB3	2.00	0.42
8:Z:1185:TYR:OH	8:Z:1191:ASN:O	2.35	0.42
1:o:24:LEU:HB2	1:o:125:LEU:HD11	2.00	0.42
1:o:196:ASP:OD1	1:o:196:ASP:N	2.53	0.42
4:M:136:CYS:HB3	4:M:141:LEU:HD12	2.02	0.42
7:S:72:ARG:HG3	8:C:820:MET:HB3	2.00	0.42
8:a:724:PRO:HA	8:a:773:ALA:HB3	2.00	0.42
8:B:331:HIS:O	8:B:335:GLY:N	2.53	0.42
8:B:579:MET:HG3	8:B:584:LEU:HB2	2.02	0.42
8:B:796:ARG:O	8:B:945:ASN:ND2	2.52	0.42
8:B:1249:ARG:HB3	8:B:1254:TYR:CG	2.55	0.42
8:D:247:ALA:HB1	8:D:365:LYS:HD3	2.01	0.42
8:D:1315:CYS:HA	8:D:1318:THR:HG22	2.01	0.42
8:Y:387:ARG:HA	8:Y:1309:GLN:HE21	1.85	0.42
8:Y:392:THR:HA	8:Y:1039:THR:HA	2.02	0.42
8:Y:520:ASP:HA	8:Y:523:LYS:HG2	2.01	0.42
8:Z:760:MET:HG2	8:Z:805:LYS:HB2	2.02	0.42
1:I:242:ASP:OD1	1:I:245:ARG:NH1	2.53	0.42
3:g:238:PRO:HG2	4:M:297:ARG:HH22	1.84	0.42
4:M:526:THR:OG1	4:M:528:ASP:OD1	2.36	0.42
7:i:43:MET:HG3	7:i:67:MET:HG3	2.02	0.42
7:j:58:CYS:HB3	8:a:809:VAL:HG11	2.02	0.42
8:a:572:GLU:O	8:a:575:THR:OG1	2.31	0.42
8:B:1064:VAL:HA	8:B:1076:HIS:O	2.20	0.42
8:D:909:ASP:OD1	8:D:909:ASP:N	2.40	0.42
8:D:1286:LEU:O	8:D:1290:LYS:NZ	2.40	0.42
8:Y:534:HIS:CD2	8:Y:536:PHE:H	2.38	0.42
8:Y:575:THR:HG21	8:Y:1007:THR:HG22	2.02	0.42
8:Y:895:VAL:HB	8:Y:914:GLN:HB3	2.01	0.42
8:Z:909:ASP:OD2	8:Z:909:ASP:N	2.42	0.42
1:h:91:LEU:HD13	1:h:303:ILE:HG12	2.00	0.42
1:I:60:ARG:HH11	1:I:195:ILE:HG23	1.84	0.42
4:M:588:ARG:HH22	8:a:1252:LEU:HB2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:a:905:GLN:O	8:a:1123:ARG:NH1	2.53	0.42
8:a:1215:TYR:CZ	8:a:1236:ALA:HB2	2.55	0.42
8:B:744:ILE:HG22	8:B:766:LEU:H	1.85	0.42
8:B:1327:THR:HG22	8:B:1333:MET:HE2	2.02	0.42
8:C:151:ILE:HD12	8:D:332:LEU:HG	2.00	0.42
8:C:627:ILE:HD12	8:C:627:ILE:HA	1.89	0.42
8:D:717:PRO:HA	8:D:718:PRO:HD3	1.90	0.42
8:Y:747:ARG:HD2	8:Y:767:PHE:HB3	2.01	0.42
1:o:291:CYS:HA	3:m:150:MET:HE3	2.00	0.42
4:M:102:GLU:HG3	4:M:123:ARG:HA	2.01	0.42
4:M:305:GLU:O	4:M:309:ALA:HB2	2.20	0.42
4:M:391:ALA:HB2	4:M:501:LEU:HB2	2.02	0.42
7:j:43:MET:SD	7:j:67:MET:HG3	2.59	0.42
8:a:448:THR:HG23	8:a:1113:LEU:HG	2.02	0.42
8:a:643:GLN:HB2	8:Z:672:PHE:HE2	1.84	0.42
8:a:1131:ILE:HD13	8:a:1131:ILE:HA	1.92	0.42
8:C:1163:ALA:HB2	8:D:1202:VAL:HG12	2.02	0.42
8:C:1336:LYS:HE2	8:C:1355:VAL:HG11	2.01	0.42
8:D:341:ASN:HB2	8:D:346:GLN:HE21	1.85	0.42
8:Y:711:HIS:HA	8:Y:779:THR:HG22	2.02	0.42
8:Y:713:HIS:CE1	8:Y:729:GLY:H	2.35	0.42
8:Y:1061:ASN:OD1	8:Y:1061:ASN:N	2.50	0.42
8:Z:322:LEU:HD12	8:Z:322:LEU:HA	1.88	0.42
8:Z:372:LEU:HD23	8:Z:372:LEU:HA	1.93	0.42
8:Z:654:VAL:HA	8:Z:657:ILE:HD12	2.01	0.42
8:Z:1113:LEU:HA	8:Z:1116:VAL:HG12	2.01	0.42
8:Z:1176:LEU:HD23	8:Z:1176:LEU:HA	1.83	0.42
1:h:104:LYS:HZ3	1:h:293:VAL:H	1.67	0.42
2:H:2237:PHE:HB3	8:a:755:PRO:HB2	2.01	0.42
1:n:77:GLU:HG3	1:n:80:GLN:HB3	2.02	0.42
4:M:475:ALA:O	4:M:489:VAL:HB	2.20	0.42
6:1:14:VAL:HA	6:1:17:VAL:HG22	2.02	0.42
6:1:83:ARG:HE	6:1:202:LYS:HE3	1.85	0.42
7:j:57:LYS:HG3	7:j:61:LYS:HE3	2.01	0.42
8:a:733:VAL:HB	8:a:894:GLU:HB3	2.00	0.42
8:B:482:ARG:O	8:B:485:GLN:NE2	2.47	0.42
8:B:732:VAL:HG13	8:B:739:LEU:HD13	2.01	0.42
8:B:903:GLN:HE21	8:B:1016:SER:HB2	1.85	0.42
8:Y:583:ARG:HE	8:Z:999:PRO:HD3	1.85	0.42
8:Y:609:LEU:O	8:Y:612:LEU:HB2	2.20	0.42
8:Y:1106:MET:SD	8:Y:1363:GLN:NE2	2.92	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:Y:1316:ARG:O	8:Y:1319:GLN:NE2	2.50	0.42
3:g:239:ARG:HA	3:g:239:ARG:HD3	1.90	0.42
4:M:5:LEU:HD13	4:M:306:TRP:CD2	2.55	0.42
6:1:95:PRO:HA	6:1:99:ARG:HH12	1.85	0.42
6:1:129:LEU:HD22	6:1:204:VAL:HG23	2.02	0.42
7:R:55:ASN:OD1	7:R:55:ASN:N	2.52	0.42
8:B:606:TYR:OH	8:B:647:PHE:N	2.53	0.42
8:B:678:VAL:HA	8:B:681:LEU:HD12	2.01	0.42
8:B:888:GLU:O	8:B:919:ASN:ND2	2.53	0.42
8:D:1350:HIS:CD2	8:D:1351:PHE:H	2.38	0.42
8:Z:1360:ILE:HG23	8:Z:1362:LEU:HD22	2.02	0.42
1:h:145:GLU:OE2	1:h:149:ARG:NE	2.51	0.41
4:M:397:ASN:OD1	4:M:397:ASN:N	2.53	0.41
5:N:8:TRP:HE1	8:Z:1139:ARG:HH21	1.68	0.41
5:N:68:LEU:HD12	5:N:68:LEU:HA	1.91	0.41
6:1:117:ASP:OD1	6:1:117:ASP:N	2.46	0.41
6:1:225:LEU:HA	6:1:228:ILE:HG12	2.02	0.41
8:a:631:VAL:HA	8:a:634:CYS:HB3	2.02	0.41
8:a:763:ASP:HA	8:a:891:LYS:HZ1	1.84	0.41
8:a:1289:ALA:HB1	8:a:1316:ARG:HD2	2.01	0.41
8:B:861:VAL:HA	8:B:864:VAL:HG22	2.01	0.41
8:C:945:ASN:HD22	8:C:948:ILE:HG12	1.84	0.41
8:D:1125:ASP:OD2	8:D:1125:ASP:N	2.53	0.41
8:Y:243:LEU:HD22	8:Y:273:MET:HE1	2.01	0.41
8:Z:121:GLU:O	8:Z:1082:ASN:ND2	2.53	0.41
1:h:45:GLN:O	1:h:50:GLN:NE2	2.53	0.41
1:I:280:ASP:OD1	1:I:280:ASP:N	2.53	0.41
2:H:2238:LEU:HD22	7:j:53:LEU:HD13	2.02	0.41
4:M:124:MET:HE2	4:M:124:MET:HB3	1.88	0.41
6:1:270:LEU:HD12	6:1:270:LEU:HA	1.89	0.41
8:a:263:THR:HB	8:a:267:ALA:HB3	2.02	0.41
8:a:329:LYS:HE2	8:a:329:LYS:HB3	1.83	0.41
8:a:528:THR:O	8:a:528:THR:OG1	2.35	0.41
8:a:1122:TYR:HB2	8:a:1128:ASP:HB2	2.01	0.41
8:B:415:LYS:HB2	8:B:415:LYS:HE3	1.84	0.41
8:B:441:ASP:OD2	8:B:442:PHE:N	2.53	0.41
8:B:597:PHE:HA	8:B:600:THR:HG22	2.02	0.41
8:C:127:ILE:HD13	8:C:127:ILE:HA	1.89	0.41
8:Z:106:LEU:HD12	8:Z:107:PRO:HD2	2.02	0.41
1:o:146:ILE:HD13	1:o:146:ILE:HA	1.90	0.41
1:o:260:SER:OG	1:o:262:ASP:OD2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:m:62:GLN:HA	3:m:63:PRO:HD3	1.95	0.41
8:D:124:PRO:HB3	8:D:1080:ASN:HA	2.02	0.41
8:D:186:LYS:HE2	8:D:186:LYS:HB2	1.94	0.41
8:D:614:ASP:OD2	8:D:650:SER:OG	2.28	0.41
8:Y:666:LEU:HD23	8:Y:666:LEU:HA	1.93	0.41
1:n:42:LYS:HE3	1:n:42:LYS:HB3	1.97	0.41
5:N:31:LEU:HA	5:N:34:LEU:HB2	2.01	0.41
6:1:90:ARG:HA	6:1:90:ARG:HD3	1.92	0.41
8:a:278:ASN:N	8:a:278:ASN:OD1	2.49	0.41
8:a:329:LYS:HD3	8:C:310:GLU:HG3	2.01	0.41
8:a:855:GLU:O	8:a:858:THR:OG1	2.31	0.41
8:a:1267:ASN:ND2	8:a:1270:GLU:OE1	2.54	0.41
8:D:384:PRO:O	8:D:387:ARG:NH1	2.53	0.41
8:D:856:MET:HE1	8:D:933:TYR:HE2	1.85	0.41
8:Y:66:PHE:N	8:Y:172:GLU:OE1	2.51	0.41
8:Z:360:ILE:HD12	8:Z:362:LEU:HD11	2.03	0.41
1:h:125:LEU:HD23	1:h:132:LEU:HB2	2.01	0.41
1:I:48:LEU:HD21	1:I:65:LEU:HD13	2.02	0.41
1:I:233:LYS:HD2	3:g:231:VAL:HG13	2.02	0.41
3:m:188:ILE:HB	3:m:203:TYR:HB2	2.03	0.41
7:S:32:ILE:HD12	7:S:36:THR:HG23	2.02	0.41
8:a:608:GLU:OE1	8:a:929:THR:N	2.51	0.41
8:B:199:ASN:HD21	8:B:215:ILE:HD11	1.85	0.41
8:B:235:ASP:HB3	8:B:238:TYR:HB3	2.03	0.41
8:B:388:ASN:HA	8:B:1042:PHE:O	2.21	0.41
8:B:534:HIS:CD2	8:B:536:PHE:H	2.33	0.41
8:B:726:ASN:OD1	8:B:726:ASN:N	2.48	0.41
8:D:749:HIS:NE2	8:D:885:PHE:HA	2.36	0.41
8:D:807:LEU:HD12	8:D:807:LEU:HA	1.83	0.41
8:D:1336:LYS:HE2	8:D:1355:VAL:HG21	2.01	0.41
8:Y:796:ARG:O	8:Y:945:ASN:ND2	2.53	0.41
8:Y:1168:GLN:HG3	8:Y:1300:GLN:HG2	2.02	0.41
8:Y:1288:ARG:HA	8:Y:1288:ARG:HD3	1.92	0.41
8:Z:321:ILE:HD13	8:Z:321:ILE:HA	1.88	0.41
8:Z:532:GLU:OE1	8:Z:555:ARG:NH1	2.43	0.41
8:Z:601:VAL:HG13	8:Z:924:VAL:HG11	2.02	0.41
1:I:157:SER:HB3	1:I:188:VAL:HB	2.03	0.41
1:I:216:MET:HE1	1:I:235:GLN:HE21	1.86	0.41
1:I:305:LYS:HA	1:I:305:LYS:HD3	1.91	0.41
1:n:146:ILE:HD13	1:n:146:ILE:HA	1.91	0.41
1:o:153:MET:O	1:o:160:ARG:NH1	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:m:36:ARG:HH21	8:Z:143:PHE:HA	1.84	0.41
3:m:168:PRO:HG2	3:m:171:MET:HG3	2.02	0.41
4:M:513:ARG:HE	5:O:22:ASN:ND2	2.18	0.41
8:a:743:ASN:OD1	8:a:743:ASN:N	2.50	0.41
8:B:1336:LYS:NZ	8:B:1343:ALA:O	2.52	0.41
8:C:459:PRO:HA	8:C:462:GLN:HG2	2.01	0.41
8:C:732:VAL:HG23	8:C:739:LEU:HB2	2.03	0.41
8:Y:1113:LEU:HD13	8:Y:1117:PHE:HE2	1.86	0.41
8:Z:1290:LYS:HB2	8:Z:1310:LEU:HD23	2.02	0.41
1:h:268:LEU:HA	1:h:271:LEU:HB3	2.01	0.41
1:o:294:SER:OG	1:o:299:SER:O	2.34	0.41
3:g:269:LEU:HD23	3:g:269:LEU:HA	1.91	0.41
5:O:62:ARG:HB2	5:O:66:ARG:HH21	1.85	0.41
6:1:99:ARG:HD2	6:1:103:ARG:HH21	1.84	0.41
8:B:54:PHE:HB2	8:C:91:MET:HG3	2.02	0.41
8:B:459:PRO:HB2	8:B:1242:VAL:HG21	2.02	0.41
8:B:801:GLY:HA3	8:B:890:VAL:HG11	2.01	0.41
8:B:1181:MET:SD	8:B:1181:MET:N	2.90	0.41
8:C:81:HIS:HB3	8:Z:144:GLU:HG3	2.01	0.41
8:C:315:ALA:HB2	8:C:321:ILE:HD11	2.02	0.41
8:C:478:LEU:HG	8:C:480:GLU:HB3	2.02	0.41
8:C:597:PHE:O	8:C:600:THR:OG1	2.35	0.41
8:C:638:MET:HE3	8:C:638:MET:HB3	1.84	0.41
8:D:310:GLU:OE1	8:D:326:ASN:ND2	2.53	0.41
8:Y:970:ASP:HB2	8:Y:993:ARG:HG3	2.02	0.41
8:Z:64:VAL:HG21	8:Z:375:VAL:HG12	2.02	0.41
8:Z:146:THR:O	8:Z:150:LYS:NZ	2.54	0.41
8:Z:399:LEU:HD11	8:Z:1180:THR:HG22	2.02	0.41
1:h:8:ILE:HD12	1:h:39:HIS:HA	2.02	0.41
8:a:1041:THR:HG21	8:a:1103:ARG:HH21	1.86	0.41
8:a:1296:ASP:OD1	8:a:1296:ASP:N	2.44	0.41
8:D:1244:TYR:HA	8:D:1249:ARG:HH11	1.86	0.41
8:Z:884:GLN:H	8:Z:884:GLN:HG2	1.67	0.41
8:Z:1257:LYS:HE3	8:Z:1257:LYS:HB3	1.95	0.41
1:I:121:ARG:NH1	1:I:131:GLU:OE1	2.54	0.41
1:o:197:MET:HE3	1:o:201:CYS:HB3	2.02	0.41
7:T:44:LEU:O	7:T:48:THR:OG1	2.30	0.41
8:a:945:ASN:HD21	8:a:947:THR:HB	1.85	0.41
8:B:84:ASN:OD1	8:B:84:ASN:N	2.53	0.41
8:B:357:MET:HE2	8:B:357:MET:HB3	1.84	0.41
8:B:455:HIS:CE1	8:B:1017:PRO:HG3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:B:697:GLN:HG3	8:C:965:HIS:CD2	2.56	0.41
8:B:982:GLU:HA	8:B:985:ASN:HD22	1.86	0.41
8:B:1350:HIS:HB3	8:B:1353:ASN:HB2	2.02	0.41
8:B:1360:ILE:O	8:B:1362:LEU:N	2.54	0.41
8:C:307:LEU:HD23	8:C:307:LEU:HA	1.86	0.41
8:Y:308:SER:N	8:Y:311:ASN:OD1	2.53	0.41
8:Z:99:ARG:NH1	8:Z:111:GLN:HG3	2.36	0.41
8:Z:997:THR:O	8:Z:997:THR:OG1	2.38	0.41
1:h:73:MET:HE3	1:h:74:ARG:N	2.36	0.41
3:m:136:LYS:HG3	3:m:137:THR:HG23	2.03	0.41
7:S:19:ARG:HA	7:S:22:VAL:HG22	2.02	0.41
7:T:64:LEU:HD11	8:D:813:TYR:HE1	1.84	0.41
8:a:1060:ASN:ND2	8:a:1061:ASN:O	2.53	0.41
8:C:215:ILE:HD13	8:C:215:ILE:HA	1.92	0.41
8:C:534:HIS:CE1	8:C:1239:LEU:HD13	2.56	0.41
8:D:558:ILE:HD13	8:D:1015:ILE:HG12	2.02	0.41
8:Y:772:ARG:HD3	8:Y:772:ARG:HA	1.92	0.41
8:Z:426:THR:HG23	8:Z:427:THR:HG23	2.03	0.41
8:Z:686:ARG:HD2	8:Z:691:PRO:HG2	2.03	0.41
8:Z:719:PHE:HE1	8:Z:917:LEU:HD13	1.85	0.41
8:Z:873:LEU:O	8:Z:877:ARG:NH1	2.44	0.41
8:Z:1170:ALA:HB2	8:Z:1300:GLN:HG3	2.03	0.41
1:I:49:HIS:HA	1:I:52:VAL:HG12	2.02	0.40
1:n:153:MET:HE2	1:n:187:PRO:HB2	2.03	0.40
8:a:508:THR:HG23	8:a:511:GLU:H	1.86	0.40
8:a:663:ASP:OD1	8:a:664:GLY:N	2.54	0.40
8:a:668:PRO:HA	8:a:671:LEU:HD13	2.02	0.40
8:a:739:LEU:HG	8:a:766:LEU:HD12	2.03	0.40
8:a:1317:LEU:HD12	8:a:1317:LEU:HA	1.92	0.40
8:B:1101:ARG:HE	8:C:214:ASN:HD22	1.69	0.40
8:C:332:LEU:HD13	8:Z:11:PRO:HD3	2.03	0.40
8:C:433:ARG:HH22	8:D:214:ASN:HD22	1.69	0.40
8:D:749:HIS:CE1	8:D:885:PHE:HA	2.56	0.40
8:Y:970:ASP:OD1	8:Y:970:ASP:N	2.53	0.40
8:Y:1176:LEU:HD23	8:Y:1176:LEU:HA	1.94	0.40
8:Y:1257:LYS:HA	8:Y:1302:VAL:HG22	2.03	0.40
1:h:154:GLY:HA3	1:h:193:LEU:HD21	2.02	0.40
1:h:296:ASP:OD1	1:h:296:ASP:N	2.54	0.40
1:I:216:MET:HE1	1:I:235:GLN:HG2	2.03	0.40
1:o:93:THR:H	8:C:1070:ASP:HB3	1.86	0.40
7:i:72:ARG:HD3	7:i:72:ARG:HA	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:a:369:MET:HB2	8:a:369:MET:HE2	1.80	0.40
8:a:793:THR:HG23	8:a:796:ARG:H	1.87	0.40
8:B:371:ASN:O	8:B:374:ARG:NH1	2.49	0.40
8:B:747:ARG:HH11	8:B:887:GLY:HA2	1.87	0.40
8:C:441:ASP:HB2	8:C:443:VAL:HG12	2.03	0.40
8:C:694:ASN:OD1	8:C:694:ASN:N	2.51	0.40
8:C:1132:ARG:HH22	8:C:1140:PRO:HD3	1.86	0.40
8:D:1035:THR:HG23	8:D:1176:LEU:HB2	2.02	0.40
8:Y:495:ILE:HG13	8:Y:976:PRO:HG2	2.02	0.40
8:Y:542:CYS:SG	8:Y:543:GLN:N	2.94	0.40
8:Y:1060:ASN:OD1	8:Y:1060:ASN:N	2.51	0.40
8:Z:594:LEU:HD21	8:Z:680:VAL:HG21	2.03	0.40
8:Z:854:GLY:O	8:Z:858:THR:OG1	2.28	0.40
1:I:203:SER:OG	1:I:277:GLN:NE2	2.54	0.40
1:n:96:ASN:ND2	1:n:297:ASN:O	2.51	0.40
3:g:167:ILE:HD12	3:g:167:ILE:HA	1.92	0.40
4:M:43:VAL:HG12	4:M:151:LEU:HG	2.03	0.40
4:M:89:TRP:CE2	4:M:150:ARG:HD2	2.56	0.40
6:l:23:LEU:HB3	6:l:69:HIS:HE1	1.86	0.40
8:a:186:LYS:HA	8:a:186:LYS:HD3	1.89	0.40
8:a:666:LEU:HB2	8:a:671:LEU:HD11	2.03	0.40
8:a:1196:ALA:HB2	8:a:1223:GLN:HB2	2.03	0.40
8:B:1103:ARG:NH1	8:B:1168:GLN:OE1	2.54	0.40
8:C:254:ILE:HG23	8:Z:15:ILE:HG21	2.03	0.40
8:C:391:LEU:HD23	8:C:391:LEU:HA	1.86	0.40
8:D:894:GLU:HG2	8:D:915:HIS:CE1	2.57	0.40
8:Y:157:MET:HE3	8:Y:157:MET:HB2	1.98	0.40
8:Y:162:ARG:HB3	8:Z:96:GLN:HE22	1.87	0.40
8:Z:935:LEU:HD12	8:Z:936:PRO:HD2	2.04	0.40
8:Z:1206:ASP:HB3	8:Z:1209:ALA:HB3	2.03	0.40
8:Z:1228:THR:OG1	8:Z:1229:HIS:N	2.54	0.40
8:Z:1327:THR:HG21	8:Z:1333:MET:HB2	2.03	0.40
1:n:220:ARG:H	1:n:220:ARG:HG2	1.70	0.40
1:o:90:LEU:HD23	1:o:90:LEU:HA	1.94	0.40
4:M:130:THR:OG1	4:M:131:THR:N	2.55	0.40
4:M:499:THR:OG1	5:N:20:GLU:OE2	2.35	0.40
8:a:271:GLY:O	8:a:367:VAL:HA	2.21	0.40
8:a:301:THR:OG1	8:a:302:TYR:N	2.55	0.40
8:a:968:ARG:H	8:a:968:ARG:HG3	1.75	0.40
8:B:941:ARG:HE	8:B:941:ARG:HB3	1.73	0.40
8:C:555:ARG:HB3	8:C:560:ASN:HB2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:C:1119:MET:SD	8:C:1119:MET:N	2.78	0.40
8:D:318:TYR:O	8:D:320:SER:N	2.55	0.40
8:D:1228:THR:OG1	8:D:1229:HIS:N	2.54	0.40
8:D:1288:ARG:HA	8:D:1288:ARG:HD3	1.85	0.40
8:Y:713:HIS:ND1	8:Y:726:ASN:O	2.54	0.40
8:Z:912:SER:OG	8:Z:913:ARG:N	2.54	0.40
1:h:37:ARG:HD2	1:h:37:ARG:HA	1.90	0.40
1:h:260:SER:OG	1:h:262:ASP:OD1	2.37	0.40
2:P:2236:ARG:HE	5:N:61:LEU:HD13	1.86	0.40
1:o:49:HIS:HA	1:o:52:VAL:HG23	2.03	0.40
3:g:93:ASN:ND2	3:g:202:ILE:O	2.54	0.40
8:a:268:LYS:HB3	8:a:268:LYS:HE2	1.84	0.40
8:a:1182:ASP:HA	8:a:1186:PHE:HD2	1.87	0.40
8:D:76:HIS:NE2	8:D:344:LEU:O	2.44	0.40
8:D:529:LEU:HD23	8:D:529:LEU:HA	1.94	0.40
8:Y:291:ILE:HG22	8:Y:360:ILE:HG22	2.02	0.40
8:Y:391:LEU:HB2	8:Y:1042:PHE:HE2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	I	299/306 (98%)	287 (96%)	12 (4%)	0	100	100
1	h	298/306 (97%)	283 (95%)	15 (5%)	0	100	100
1	n	290/306 (95%)	273 (94%)	17 (6%)	0	100	100
1	o	285/306 (93%)	274 (96%)	11 (4%)	0	100	100
2	H	18/2241 (1%)	18 (100%)	0	0	100	100
2	P	18/2241 (1%)	18 (100%)	0	0	100	100
3	g	221/290 (76%)	204 (92%)	17 (8%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	m	288/290 (99%)	274 (95%)	14 (5%)	0	100	100
4	M	462/594 (78%)	442 (96%)	20 (4%)	0	100	100
5	N	74/642 (12%)	70 (95%)	4 (5%)	0	100	100
5	O	65/642 (10%)	64 (98%)	1 (2%)	0	100	100
6	1	282/1048 (27%)	269 (95%)	13 (5%)	0	100	100
7	R	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
7	S	61/75 (81%)	60 (98%)	1 (2%)	0	100	100
7	T	61/75 (81%)	59 (97%)	2 (3%)	0	100	100
7	i	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
7	j	61/75 (81%)	58 (95%)	3 (5%)	0	100	100
8	B	1331/1370 (97%)	1260 (95%)	71 (5%)	0	100	100
8	C	1323/1370 (97%)	1268 (96%)	55 (4%)	0	100	100
8	D	1293/1370 (94%)	1210 (94%)	83 (6%)	0	100	100
8	Y	1343/1370 (98%)	1267 (94%)	76 (6%)	0	100	100
8	Z	1331/1370 (97%)	1264 (95%)	67 (5%)	0	100	100
8	a	1269/1370 (93%)	1216 (96%)	53 (4%)	0	100	100
All	All	10795/17807 (61%)	10256 (95%)	539 (5%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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	I	270/273 (99%)	270 (100%)	0	100	100
1	h	270/273 (99%)	268 (99%)	2 (1%)	76	79
1	n	263/273 (96%)	261 (99%)	2 (1%)	73	77
1	o	259/273 (95%)	259 (100%)	0	100	100
2	H	19/1941 (1%)	19 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	P	19/1941 (1%)	19 (100%)	0	100	100
3	g	199/252 (79%)	199 (100%)	0	100	100
3	m	252/252 (100%)	252 (100%)	0	100	100
4	M	395/500 (79%)	392 (99%)	3 (1%)	73	77
5	N	69/526 (13%)	69 (100%)	0	100	100
5	O	64/526 (12%)	64 (100%)	0	100	100
6	l	255/883 (29%)	255 (100%)	0	100	100
7	R	59/68 (87%)	59 (100%)	0	100	100
7	S	59/68 (87%)	59 (100%)	0	100	100
7	T	59/68 (87%)	59 (100%)	0	100	100
7	i	59/68 (87%)	59 (100%)	0	100	100
7	j	59/68 (87%)	58 (98%)	1 (2%)	53	68
8	B	1169/1192 (98%)	1167 (100%)	2 (0%)	87	87
8	C	1156/1192 (97%)	1149 (99%)	7 (1%)	78	81
8	D	1130/1192 (95%)	1124 (100%)	6 (0%)	81	82
8	Y	1174/1192 (98%)	1169 (100%)	5 (0%)	84	84
8	Z	1163/1192 (98%)	1154 (99%)	9 (1%)	73	77
8	a	1110/1192 (93%)	1108 (100%)	2 (0%)	87	87
All	All	9531/15405 (62%)	9492 (100%)	39 (0%)	81	84

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	h	133	VAL
1	h	222	LEU
1	n	176	THR
1	n	303	ILE
4	M	31	VAL
4	M	103	LEU
4	M	363	VAL
7	j	64	LEU
8	a	565	LEU
8	a	861	VAL
8	B	256	ASP
8	B	895	VAL
8	C	95	VAL

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Mol	Chain	Res	Type
8	C	420	VAL
8	C	753	ASP
8	C	754	VAL
8	C	861	VAL
8	C	1000	ASN
8	C	1096	VAL
8	D	410	VAL
8	D	505	VAL
8	D	653	LEU
8	D	740	ASN
8	D	937	VAL
8	D	1015	ILE
8	Y	861	VAL
8	Y	1064	VAL
8	Y	1200	LEU
8	Y	1332	LEU
8	Y	1360	ILE
8	Z	64	VAL
8	Z	432	ASN
8	Z	446	LEU
8	Z	739	LEU
8	Z	861	VAL
8	Z	956	ILE
8	Z	1001	VAL
8	Z	1099	VAL
8	Z	1356	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (198) such sidechains are listed below:

Mol	Chain	Res	Type
1	h	14	HIS
1	h	36	GLN
1	h	80	GLN
1	h	123	ASN
1	h	191	GLN
1	h	277	GLN
1	h	297	ASN
1	I	54	HIS
1	I	79	ASN
1	I	123	ASN
1	I	129	GLN
1	I	171	GLN

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Mol	Chain	Res	Type
1	I	258	HIS
1	n	39	HIS
1	n	43	HIS
1	n	129	GLN
1	n	277	GLN
1	o	7	ASN
1	o	84	HIS
1	o	209	ASN
3	g	126	HIS
3	g	249	GLN
3	m	18	ASN
3	m	31	ASN
3	m	79	HIS
3	m	116	GLN
3	m	266	HIS
4	M	47	ASN
4	M	90	GLN
4	M	145	GLN
4	M	333	ASN
4	M	517	GLN
4	M	560	GLN
4	M	561	ASN
5	N	73	GLN
5	O	22	ASN
5	O	63	GLN
6	1	18	ASN
6	1	70	ASN
6	1	150	GLN
6	1	158	HIS
6	1	201	ASN
6	1	248	ASN
7	R	18	HIS
7	R	37	HIS
7	T	37	HIS
8	a	81	HIS
8	a	111	GLN
8	a	181	GLN
8	a	338	HIS
8	a	485	GLN
8	a	534	HIS
8	a	649	HIS
8	a	694	ASN

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Mol	Chain	Res	Type
8	a	731	GLN
8	a	737	GLN
8	a	849	GLN
8	a	874	GLN
8	a	945	ASN
8	a	1003	HIS
8	a	1061	ASN
8	a	1080	ASN
8	a	1111	GLN
8	a	1124	HIS
8	a	1190	ASN
8	a	1191	ASN
8	a	1245	ASN
8	a	1350	HIS
8	B	76	HIS
8	B	81	HIS
8	B	214	ASN
8	B	231	ASN
8	B	350	HIS
8	B	417	ASN
8	B	438	GLN
8	B	476	GLN
8	B	510	ASN
8	B	534	HIS
8	B	543	GLN
8	B	571	HIS
8	B	711	HIS
8	B	737	GLN
8	B	740	ASN
8	B	749	HIS
8	B	849	GLN
8	B	851	GLN
8	B	874	GLN
8	B	914	GLN
8	B	945	ASN
8	B	985	ASN
8	B	1111	GLN
8	B	1160	ASN
8	B	1166	HIS
8	B	1223	GLN
8	B	1230	ASN
8	B	1319	GLN

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Mol	Chain	Res	Type
8	Z	514	GLN
8	Z	660	HIS
8	Z	697	GLN
8	Z	884	GLN
8	Z	901	HIS
8	Z	984	HIS
8	Z	1060	ASN
8	Z	1076	HIS
8	Z	1082	ASN
8	Z	1141	GLN
8	Z	1223	GLN
8	Z	1230	ASN
8	Z	1264	GLN
8	Z	1313	ASN
8	Z	1319	GLN
8	Z	1353	ASN
8	Z	1363	GLN
8	Z	1364	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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

There are no chain breaks in this entry.

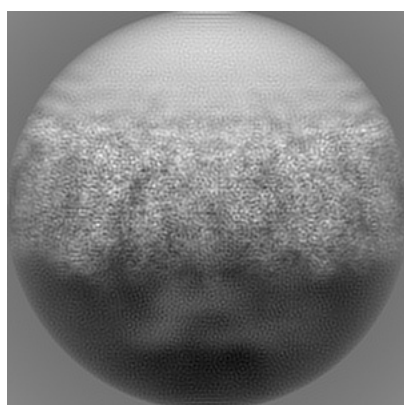
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31298. These allow visual inspection of the internal detail of the map and identification of artifacts.

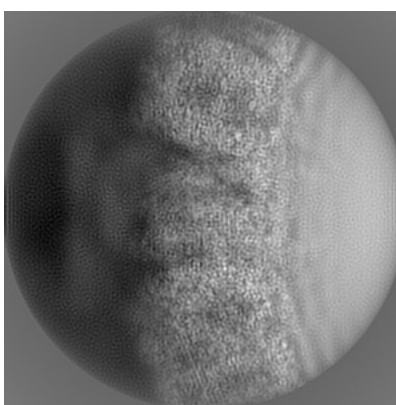
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

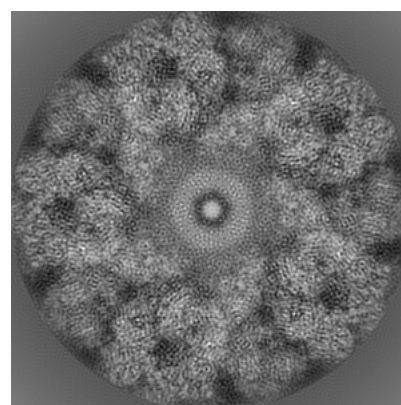
6.1.1 Primary map



X



Y

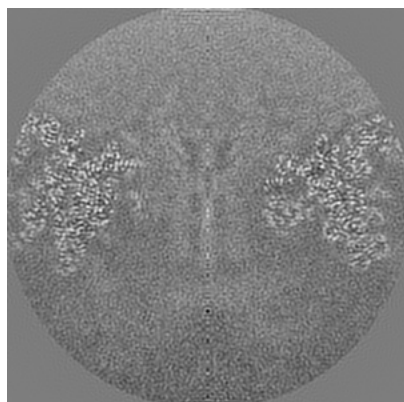


Z

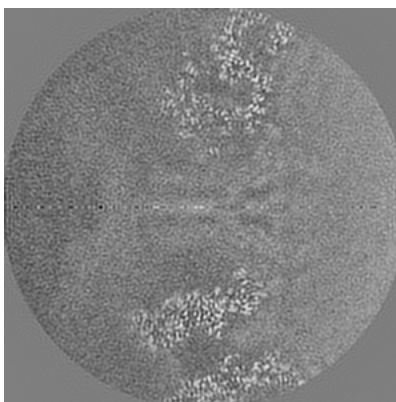
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

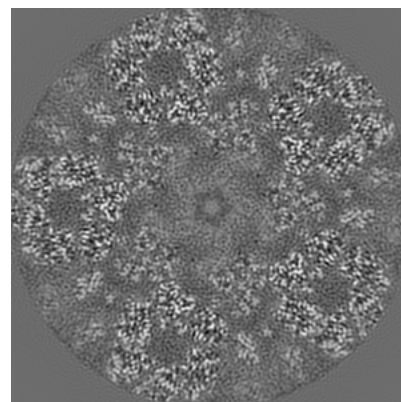
6.2.1 Primary map



X Index: 128



Y Index: 128

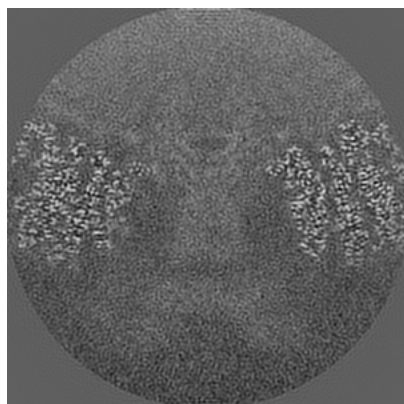


Z Index: 128

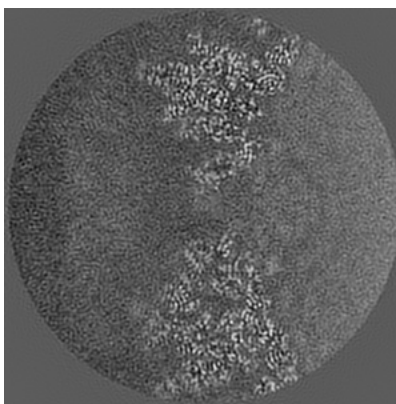
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

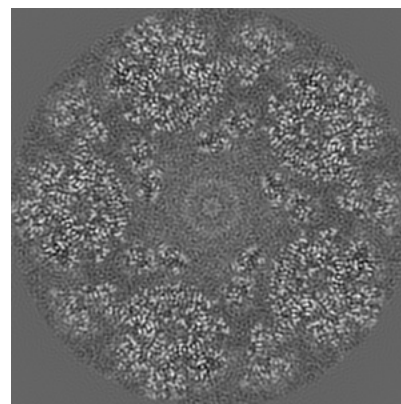
6.3.1 Primary map



X Index: 116



Y Index: 97

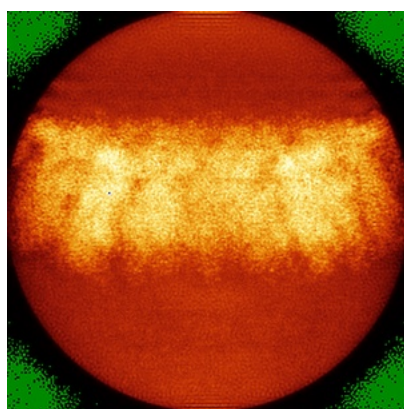


Z Index: 141

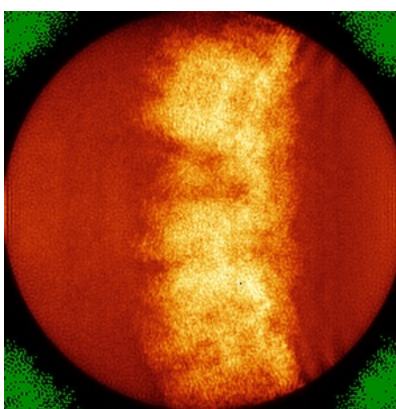
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

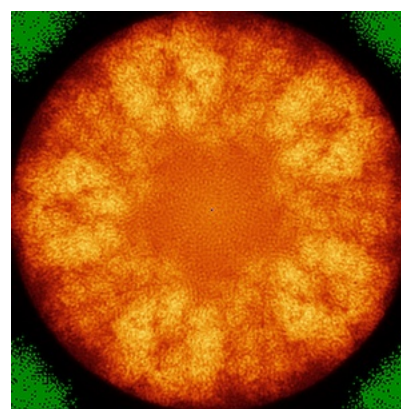
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

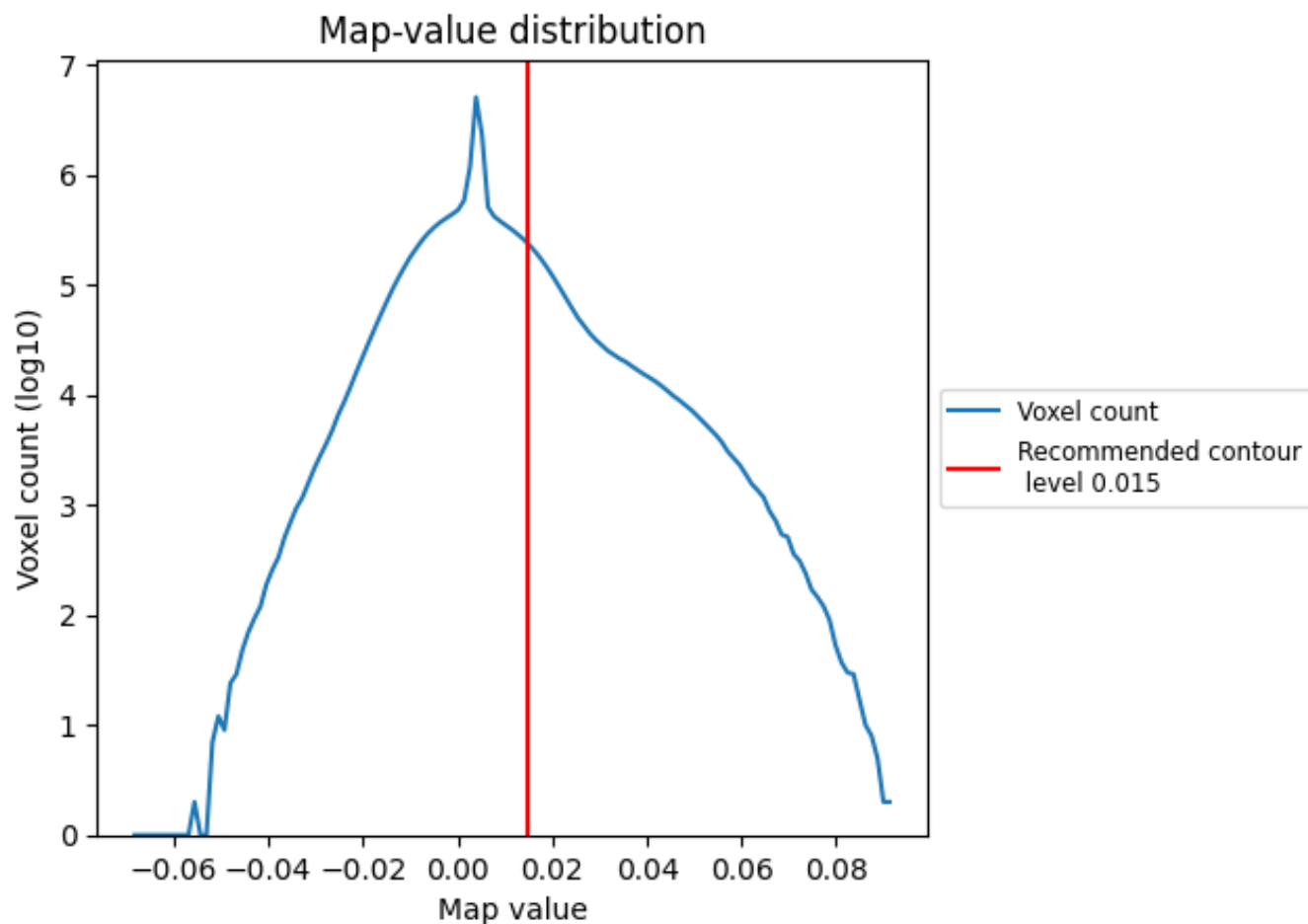
6.6 Mask visualisation

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

7 Map analysis [i](#)

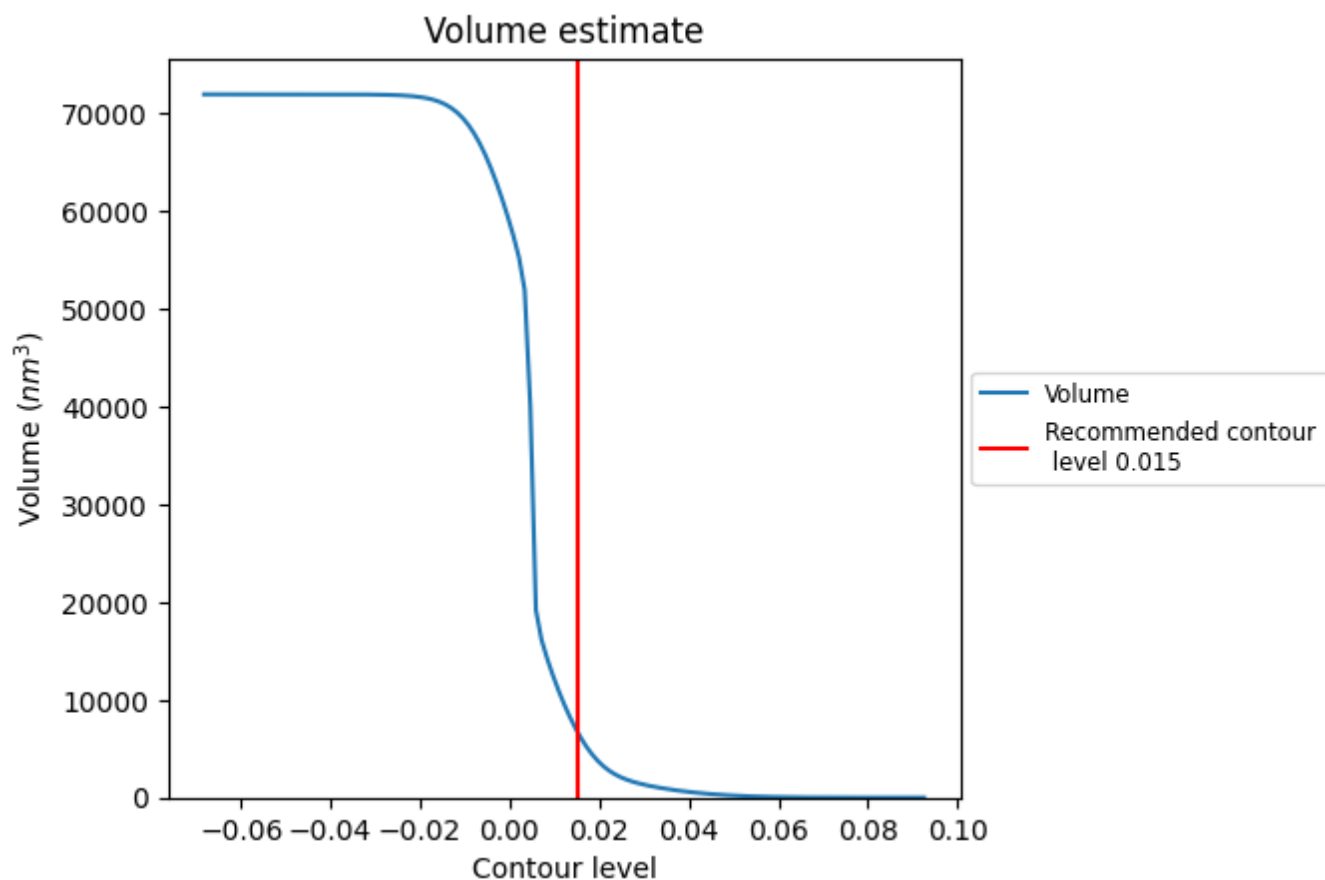
This section contains the results of statistical analysis of the map.

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.

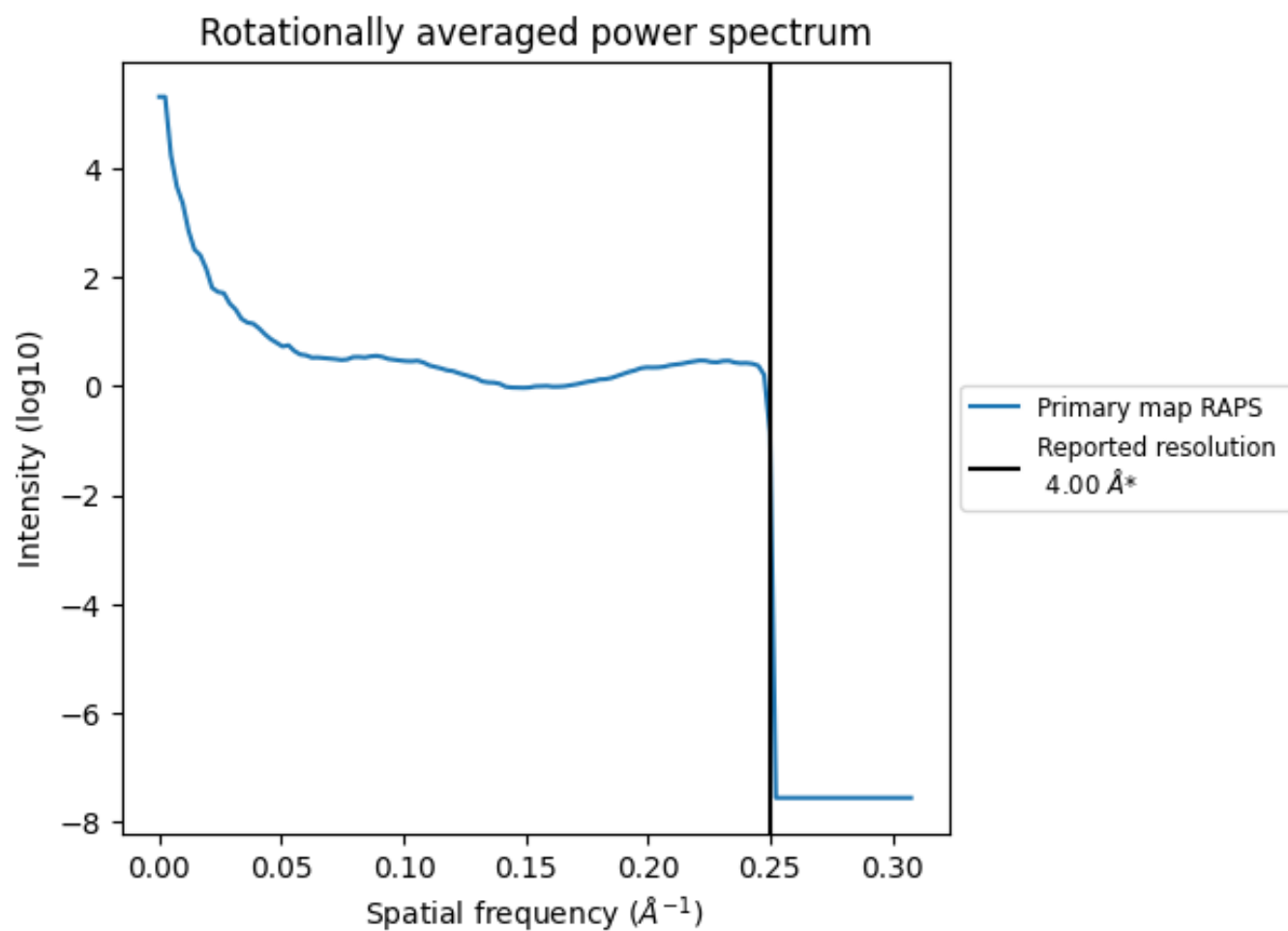
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 6849 nm³; this corresponds to an approximate mass of 6187 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.250 Å⁻¹

8 Fourier-Shell correlation ⓘ

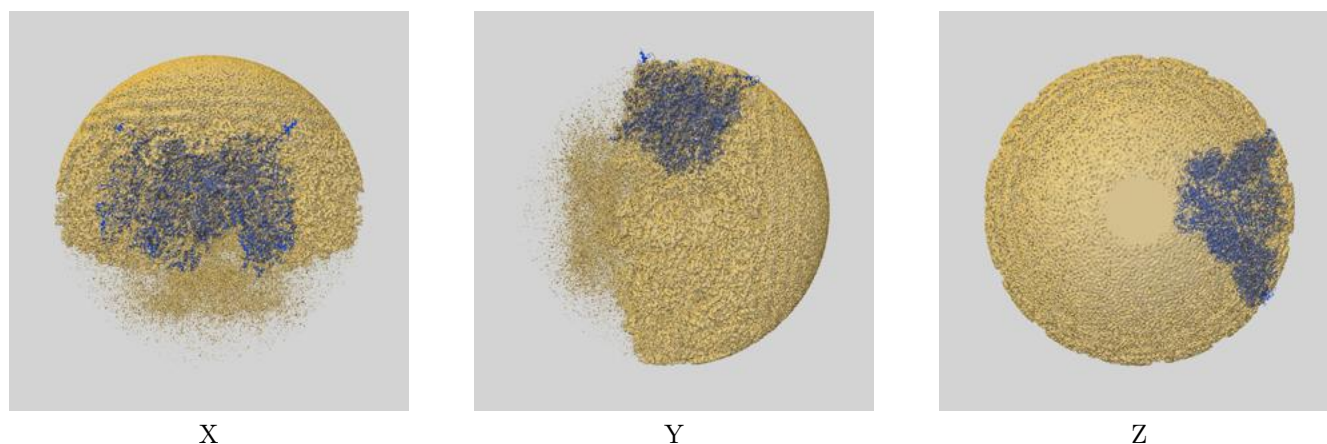
This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

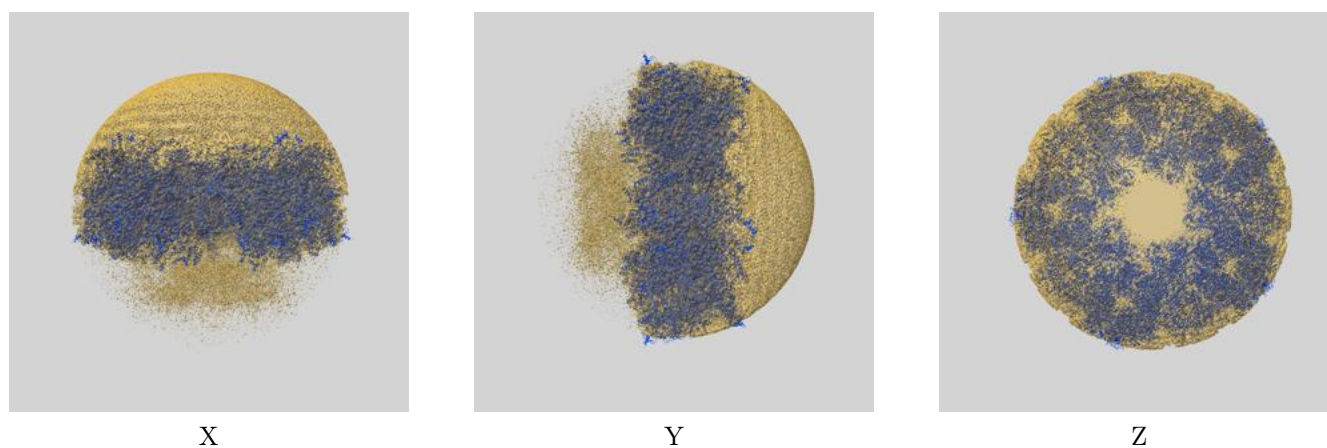
This section contains information regarding the fit between EMDB map EMD-31298 and PDB model 7ETJ. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

9.1.1 Map-model overlay [i](#)

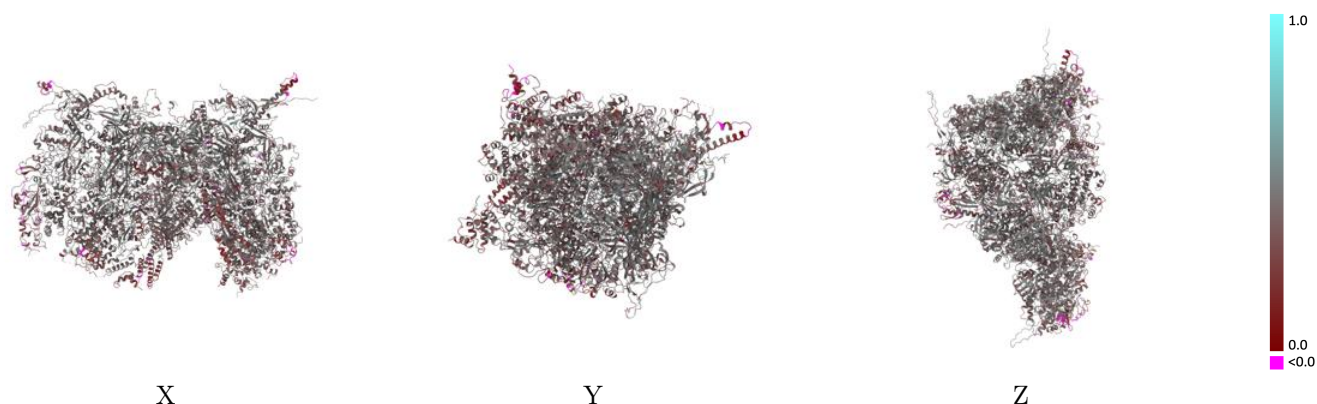


9.1.2 Map-model assembly overlay [i](#)



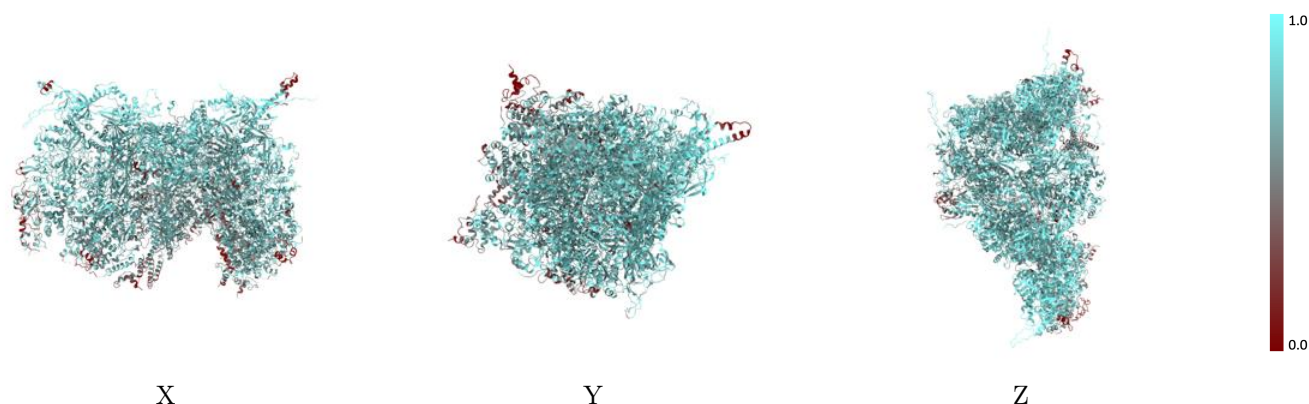
The images above show the 3D surface view of the map at the recommended contour level 0.015 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



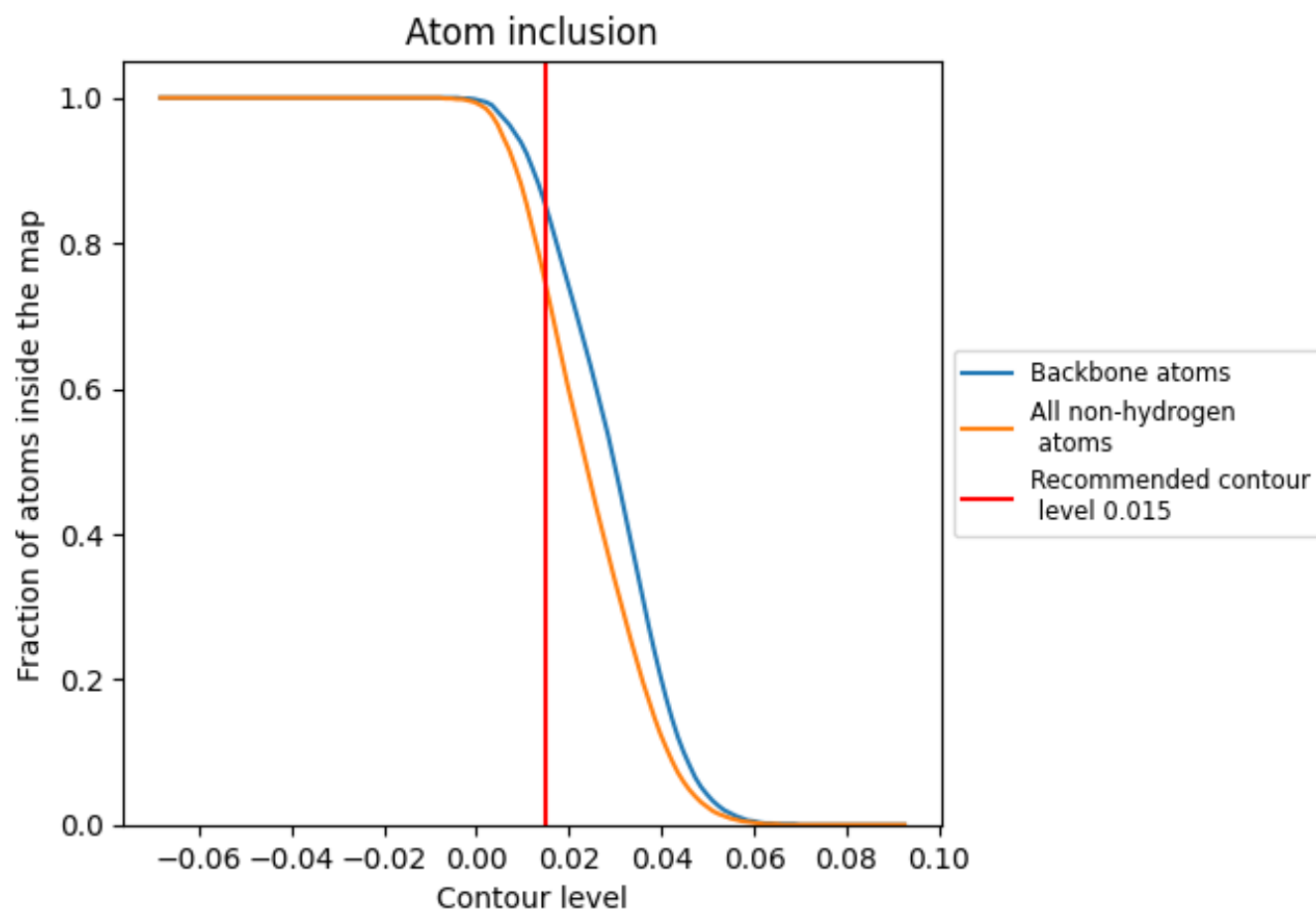
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.015).

9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.015) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7430	 0.4060
1	 0.5070	 0.3130
B	 0.7710	 0.4180
C	 0.7890	 0.4290
D	 0.7800	 0.4160
H	 0.4130	 0.2030
I	 0.6930	 0.3800
M	 0.7210	 0.4020
N	 0.6100	 0.3640
O	 0.5020	 0.2500
P	 0.5330	 0.2810
R	 0.5060	 0.3220
S	 0.5960	 0.3500
T	 0.3030	 0.2460
Y	 0.7570	 0.4060
Z	 0.7860	 0.4280
a	 0.7770	 0.4250
g	 0.5520	 0.3090
h	 0.6850	 0.3930
i	 0.3860	 0.2820
j	 0.4480	 0.3160
m	 0.7790	 0.4300
n	 0.7740	 0.4140
o	 0.7690	 0.4100

