Full wwPDB EM Validation Report ⓘ

Nov 4, 2024 – 04:04 AM JST

PDB ID	:	7E9N
EMDB ID	:	EMD-31033
Title	:	Cryo-EM structure of the SARS-CoV-2 S-6P in complex with 35B5 Fab(1 down RBD, state1)
Authors	:	Wang, X.F.; Zhu, Y.Q.
Deposited on	:	2021-03-04
Resolution	:	3.69 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:

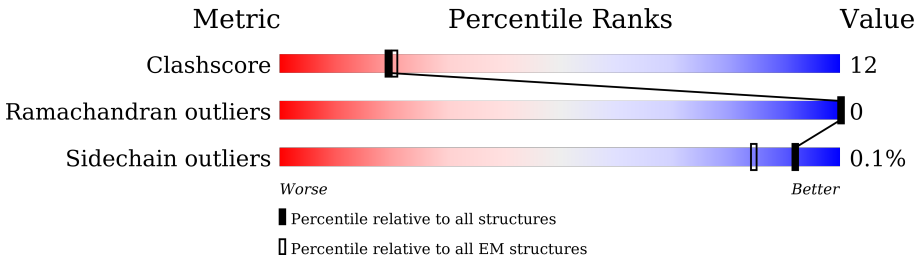
EMDB validation analysis	:	0.0.1.dev113
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.39

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.69 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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

Mol	Chain	Length	Quality of chain
1	A	1121	67% 20% 13%
1	B	1121	68% 21% 11%
1	C	1121	65% 24% 11%
2	L	218	50% 78% 22%
2	O	218	64% 36%
2	X	218	67% 33%
3	H	237	33% 72% 24% 5%
3	P	237	56% 39% 5%

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Mol	Chain	Length	Quality of chain
3	Y	237	

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 33519 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 Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1002	Total	C	N	O	S	0	0
			7805	4985	1294	1491	35		
1	A	977	Total	C	N	O	S	0	0
			7535	4817	1250	1434	34		
1	C	1002	Total	C	N	O	S	0	0
			7823	4997	1300	1491	35		

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	817	PRO	PHE	engineered mutation	UNP P0DTC2
B	892	PRO	ALA	engineered mutation	UNP P0DTC2
B	899	PRO	ALA	engineered mutation	UNP P0DTC2
B	942	PRO	ALA	engineered mutation	UNP P0DTC2
B	986	PRO	LYS	engineered mutation	UNP P0DTC2
B	987	PRO	VAL	engineered mutation	UNP P0DTC2
A	817	PRO	PHE	engineered mutation	UNP P0DTC2
A	892	PRO	ALA	engineered mutation	UNP P0DTC2
A	899	PRO	ALA	engineered mutation	UNP P0DTC2
A	942	PRO	ALA	engineered mutation	UNP P0DTC2
A	986	PRO	LYS	engineered mutation	UNP P0DTC2
A	987	PRO	VAL	engineered mutation	UNP P0DTC2
C	817	PRO	PHE	engineered mutation	UNP P0DTC2
C	892	PRO	ALA	engineered mutation	UNP P0DTC2
C	899	PRO	ALA	engineered mutation	UNP P0DTC2
C	942	PRO	ALA	engineered mutation	UNP P0DTC2
C	986	PRO	LYS	engineered mutation	UNP P0DTC2
C	987	PRO	VAL	engineered mutation	UNP P0DTC2

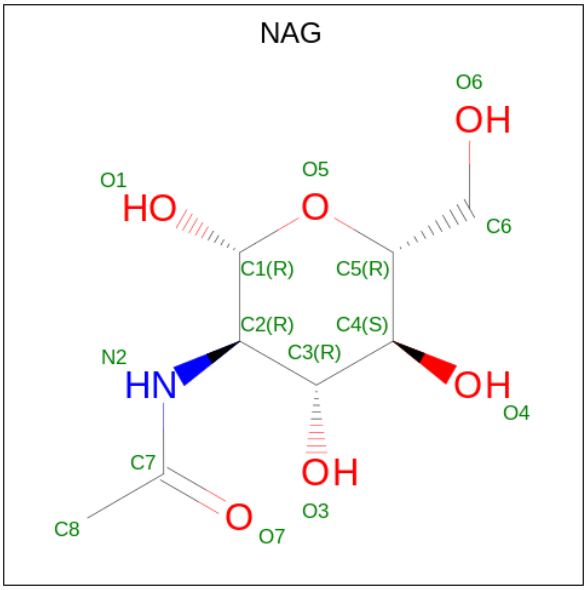
- Molecule 2 is a protein called Light chain of 35B5 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	O	218	Total	C	N	O	S	0	0
			1669	1048	280	335	6		
2	X	218	Total	C	N	O	S	0	0
			1655	1038	274	337	6		
2	L	218	Total	C	N	O	S	0	0
			1669	1047	279	337	6		

- Molecule 3 is a protein called Heavy chain of 35B5 Fab.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	P	226	Total	C	N	O	S	0	0
			1668	1048	285	327	8		
3	Y	226	Total	C	N	O	S	0	0
			1653	1038	281	327	7		
3	H	226	Total	C	N	O	S	0	0
			1664	1046	284	326	8		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	
4	B	1	Total	C	N	O	0
			14	8	1	5	

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Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	B	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	A	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0
4	C	1	Total C N O 14 8 1 5	0

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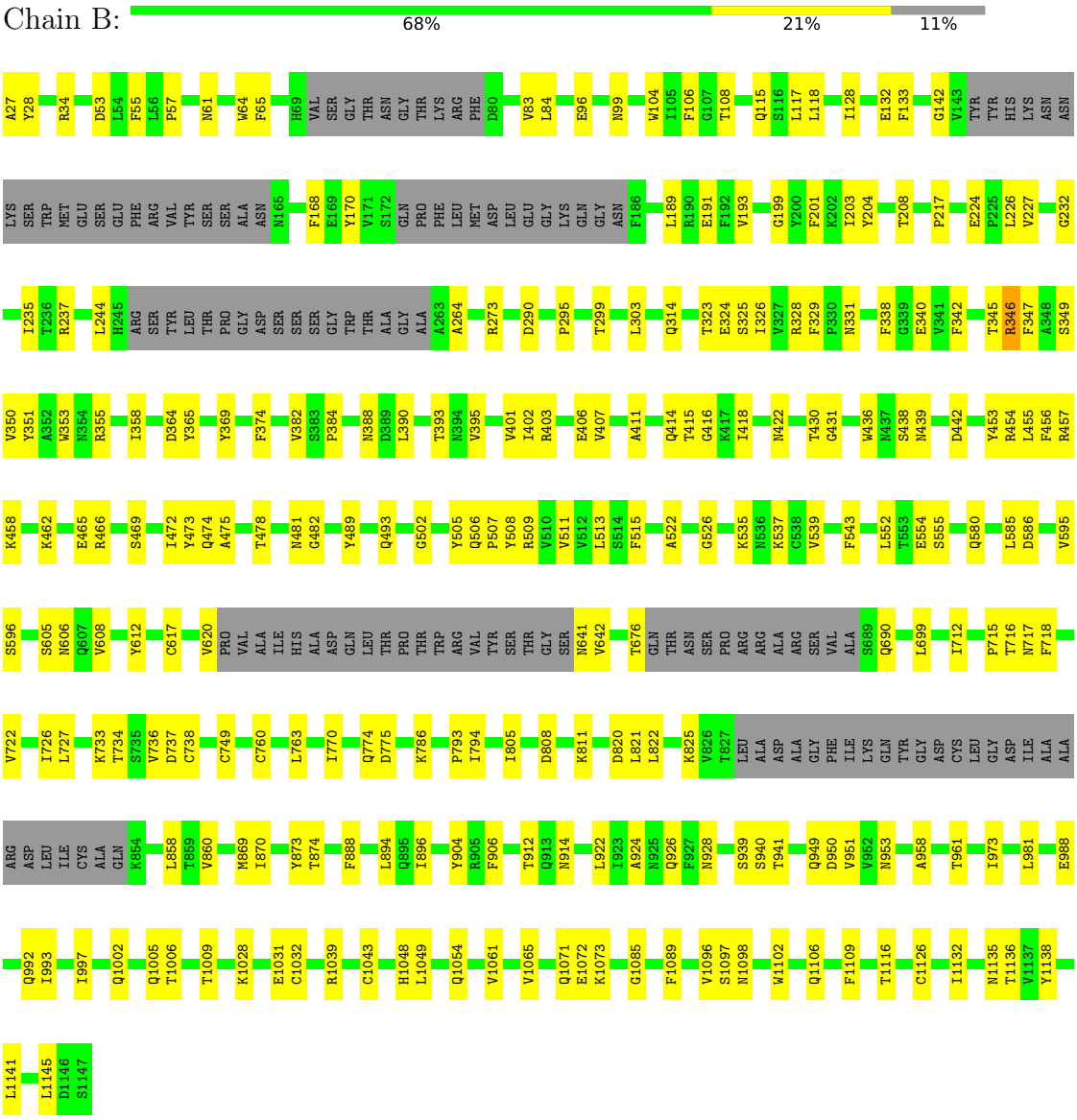
Mol	Chain	Residues	Atoms				AltConf
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	
4	C	1	Total	C	N	O	0
			14	8	1	5	

3 Residue-property plots (i)

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

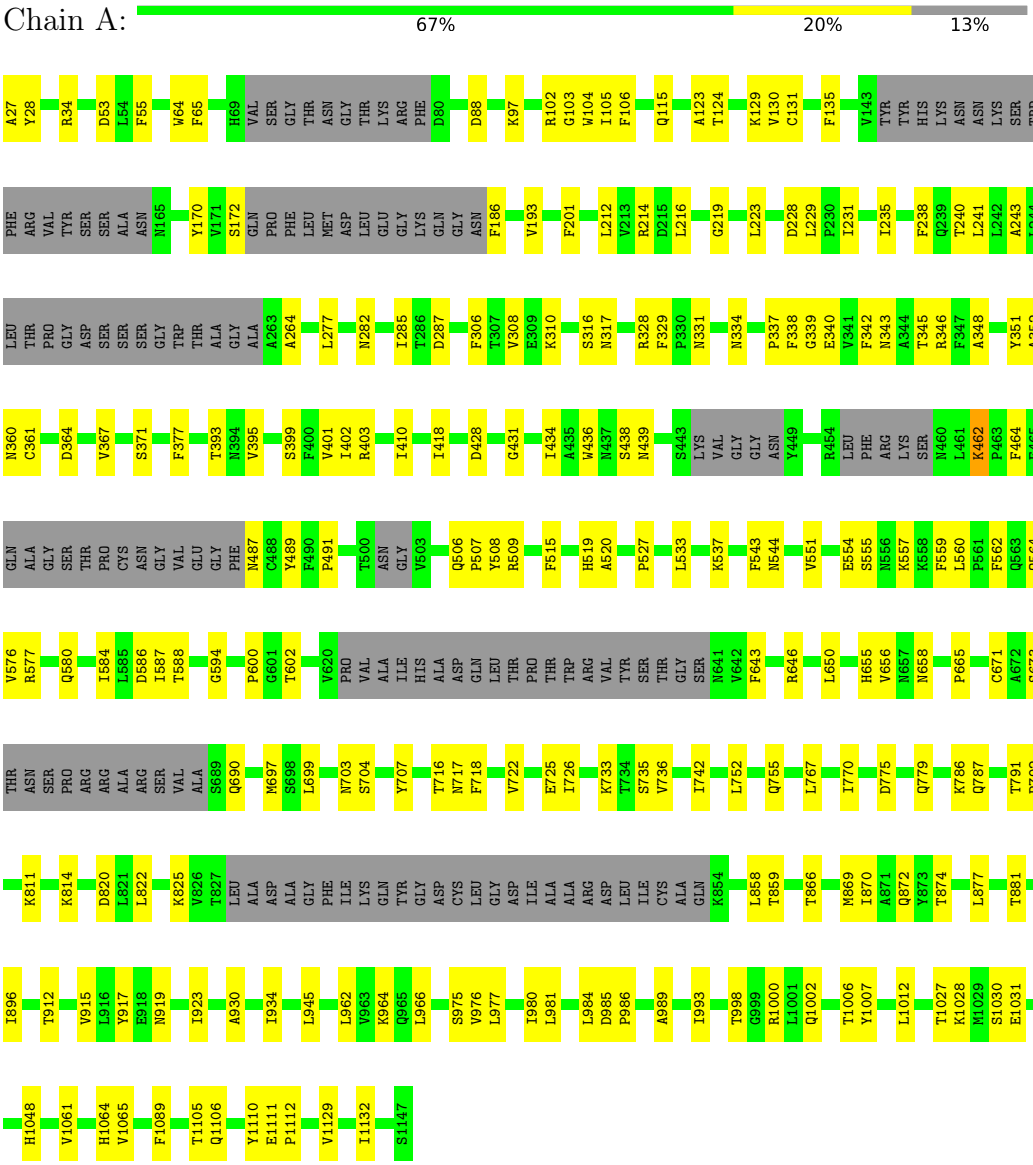
- Molecule 1: Spike glycoprotein

Chain B:



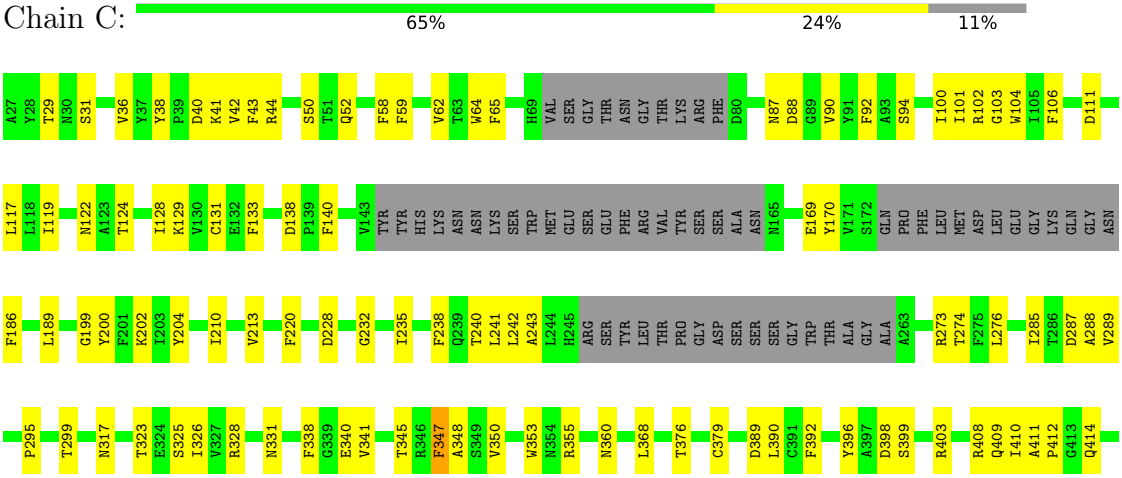
- Molecule 1: Spike glycoprotein

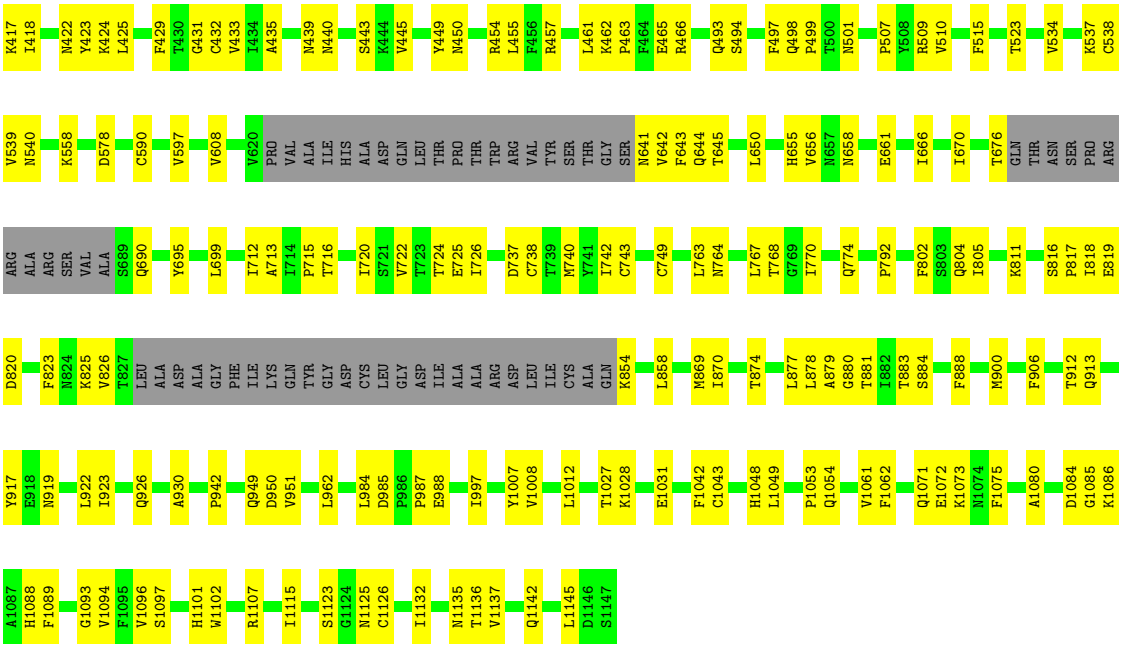
Chain A:



• Molecule 1: Spike glycoprotein

Chain C:



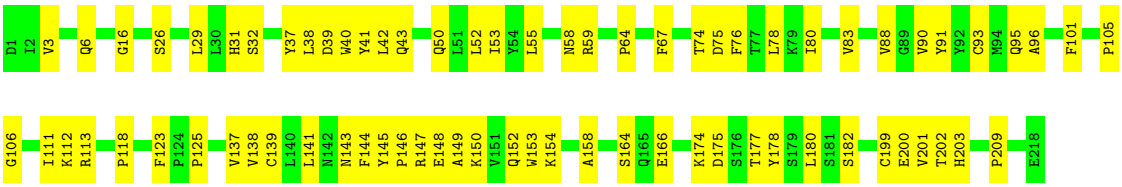


• Molecule 2: Light chain of 35B5 Fab

Chain O:

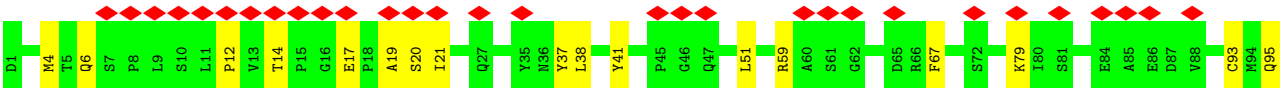
• Molecule 2: Light chain of 35B5 Fab

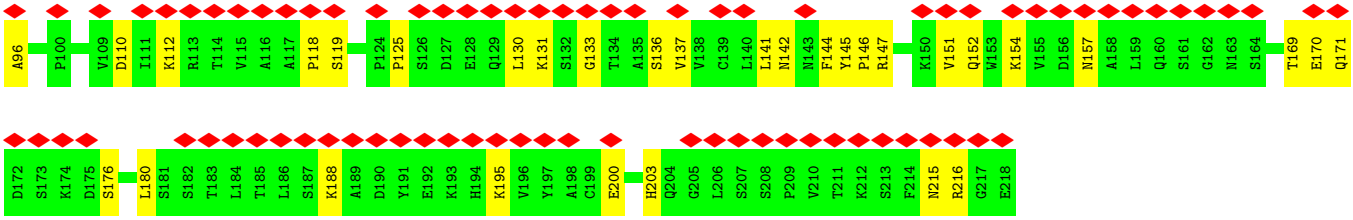
Chain X:



• Molecule 2: Light chain of 35B5 Fab

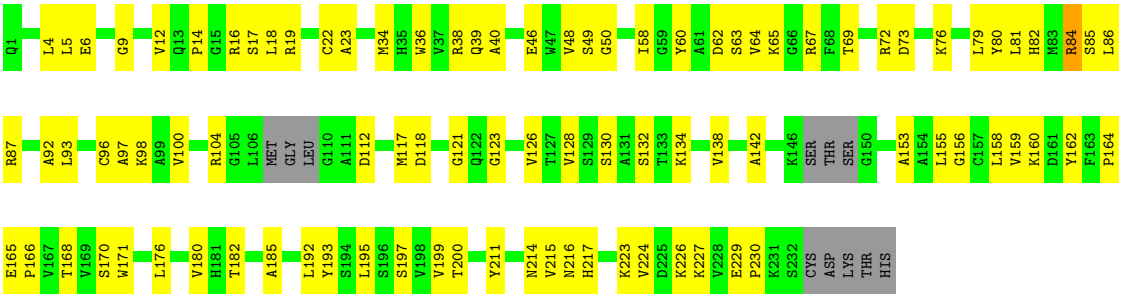
Chain L:





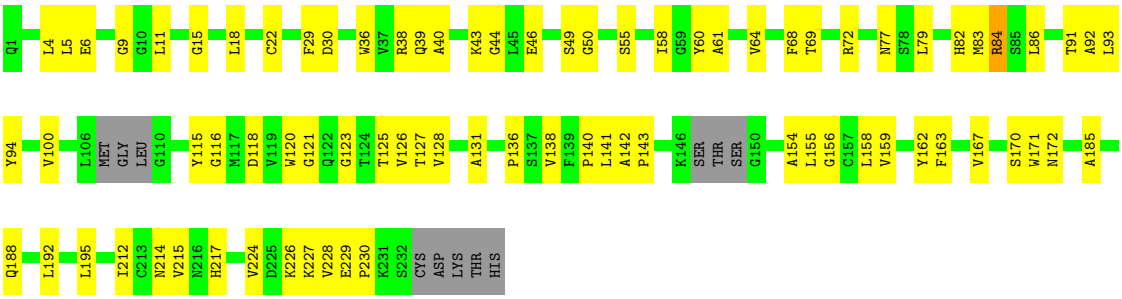
• Molecule 3: Heavy chain of 35B5 Fab

Chain P:



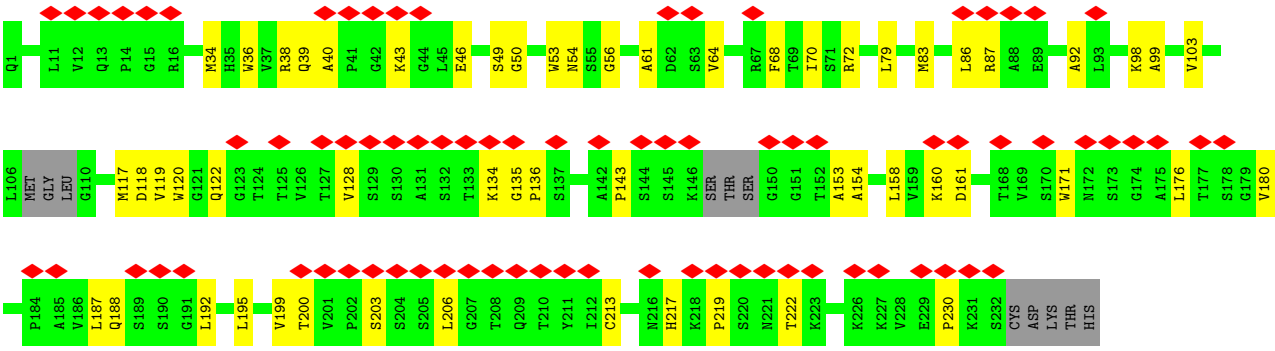
• Molecule 3: Heavy chain of 35B5 Fab

Chain Y:



• Molecule 3: Heavy chain of 35B5 Fab

Chain H:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	62600	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 ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1300	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.434	Depositor
Minimum map value	-0.454	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.048	Depositor
Recommended contour level	0.08	Depositor
Map size (Å)	361.35, 361.35, 361.35	wwPDB
Map dimensions	330, 330, 330	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.095, 1.095, 1.095	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.46	0/7702	0.55	0/10492
1	B	0.45	0/7984	0.55	0/10874
1	C	0.43	0/8002	0.55	0/10893
2	L	0.30	0/1707	0.48	0/2322
2	O	0.30	0/1707	0.52	0/2321
2	X	0.33	0/1693	0.51	0/2307
3	H	0.30	0/1702	0.52	0/2318
3	P	0.31	0/1706	0.52	0/2323
3	Y	0.28	0/1691	0.50	0/2306
All	All	0.41	0/33894	0.54	0/46156

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	A	7535	0	7281	165	0
1	B	7805	0	7588	177	0
1	C	7823	0	7632	193	0
2	L	1669	0	1617	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	1669	0	1624	52	0
2	X	1655	0	1584	64	0
3	H	1664	0	1603	39	0
3	P	1668	0	1609	74	0
3	Y	1653	0	1573	62	0
4	A	126	0	117	3	0
4	B	126	0	117	2	0
4	C	126	0	117	2	0
All	All	33519	0	32462	818	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 12.

All (818) 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)
2:O:38:LEU:HD11	2:O:93:CYS:HB2	1.66	0.78
1:B:115:GLN:HA	1:B:132:GLU:HB3	1.65	0.76
2:O:118:PRO:HB3	2:O:144:PHE:HB3	1.67	0.75
2:O:40:TRP:HB2	2:O:53:ILE:HG22	1.70	0.73
2:X:141:LEU:HB2	2:X:180:LEU:HB3	1.70	0.73
1:A:555:SER:HB2	1:A:586:ASP:HB2	1.70	0.73
1:B:34:ARG:NH1	1:B:191:GLU:OE2	2.23	0.71
1:C:299:THR:HG21	1:C:597:VAL:HG11	1.72	0.71
1:B:1135:ASN:OD1	1:B:1136:THR:N	2.23	0.71
1:B:676:THR:HG22	1:B:690:GLN:HG2	1.72	0.70
2:X:118:PRO:HB3	2:X:144:PHE:HB3	1.73	0.70
2:X:3:VAL:HB	2:X:26:SER:HB3	1.74	0.70
1:B:474:GLN:NE2	1:B:478:THR:O	2.25	0.69
1:B:502:GLY:H	1:B:505:TYR:HB2	1.56	0.69
2:X:123:PHE:HB2	2:X:138:VAL:HB	1.73	0.69
1:C:1053:PRO:O	1:C:1054:GLN:NE2	2.25	0.69
1:B:431:GLY:HA3	1:B:513:LEU:O	1.93	0.69
1:C:355:ARG:HD2	1:C:396:TYR:HD1	1.57	0.69
2:O:38:LEU:HA	2:O:94:MET:O	1.93	0.69
3:Y:156:GLY:HA2	3:Y:171:TRP:HH2	1.58	0.68
1:B:1028:LYS:O	1:B:1032:CYS:HB2	1.93	0.68
1:C:1135:ASN:OD1	1:C:1136:THR:N	2.25	0.68
3:P:34:MET:SD	3:P:79:LEU:HD22	2.34	0.68
2:X:50:GLN:HA	3:Y:120:TRP:CZ3	2.29	0.68
2:X:59:ARG:NH2	2:X:64:PRO:O	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:986:PRO:O	1:A:989:ALA:N	2.27	0.67
3:Y:227:LYS:NZ	3:Y:229:GLU:OE1	2.26	0.67
1:B:422:ASN:O	1:B:454:ARG:NH2	2.22	0.67
1:B:722:VAL:HG22	1:B:1065:VAL:HG22	1.75	0.67
1:B:737:ASP:OD2	1:C:317:ASN:ND2	2.28	0.67
1:A:726:ILE:HG12	1:A:1061:VAL:HG22	1.76	0.67
3:P:63:SER:O	3:P:67:ARG:NH2	2.28	0.67
1:B:418:ILE:HA	1:B:422:ASN:HB2	1.75	0.67
1:A:115:GLN:NE2	1:A:130:VAL:O	2.27	0.67
2:O:195:LYS:NZ	2:O:216:ARG:O	2.28	0.67
1:B:340:GLU:OE1	3:P:104:ARG:NH1	2.27	0.67
1:B:108:THR:O	1:B:237:ARG:NH2	2.28	0.66
1:A:671:CYS:SG	1:A:697:MET:HB3	2.35	0.66
2:O:172:ASP:HB3	2:O:177:THR:HB	1.76	0.66
1:C:811:LYS:NZ	1:C:820:ASP:OD2	2.28	0.66
3:P:138:VAL:HG21	3:P:215:VAL:HG11	1.77	0.66
3:P:12:VAL:HG21	3:P:18:LEU:HD11	1.78	0.66
2:O:166:GLU:HB3	2:O:180:LEU:HD21	1.78	0.66
1:B:793:PRO:HG2	1:B:794:ILE:HD12	1.77	0.66
1:C:412:PRO:HG3	1:C:429:PHE:HD2	1.60	0.65
3:Y:100:VAL:HG23	3:Y:118:ASP:HB3	1.77	0.65
1:A:328:ARG:HE	1:A:533:LEU:HD23	1.60	0.65
1:A:725:GLU:OE1	1:A:1064:HIS:NE2	2.27	0.65
3:Y:15:GLY:H	3:Y:86:LEU:HB2	1.62	0.65
1:C:348:ALA:HB2	3:Y:55:SER:O	1.96	0.65
2:O:3:VAL:HB	2:O:26:SER:HB3	1.79	0.65
3:P:180:VAL:HA	3:P:199:VAL:HG22	1.79	0.65
1:C:1085:GLY:O	1:C:1126:CYS:N	2.22	0.65
2:L:38:LEU:HD11	2:L:93:CYS:HB2	1.78	0.65
2:L:133:GLY:HA2	2:L:188:LYS:HB2	1.79	0.64
2:L:171:GLN:HE21	2:L:176:SER:HB3	1.62	0.64
1:C:443:SER:HB3	1:C:499:PRO:HD3	1.79	0.64
1:B:106:PHE:HB3	1:B:235:ILE:HD11	1.79	0.64
1:B:822:LEU:HD21	1:B:1061:VAL:HG11	1.78	0.64
1:B:388:ASN:HB2	1:B:526:GLY:HA3	1.78	0.64
2:L:147:ARG:O	2:L:147:ARG:NH1	2.31	0.64
2:O:123:PHE:HB2	2:O:138:VAL:HB	1.79	0.64
3:Y:39:GLN:O	3:Y:93:LEU:N	2.23	0.64
3:Y:142:ALA:HB1	3:Y:230:PRO:HA	1.79	0.64
1:B:351:TYR:HB3	1:B:454:ARG:HB2	1.80	0.64
2:O:133:GLY:HA2	2:O:188:LYS:HD2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:676:THR:HA	1:C:690:GLN:HA	1.78	0.64
1:A:104:TRP:HB3	1:A:106:PHE:CE1	2.33	0.64
1:B:369:TYR:HE1	1:B:384:PRO:HB2	1.62	0.63
1:C:103:GLY:HA3	1:C:119:ILE:O	1.98	0.63
3:P:39:GLN:HB3	3:P:93:LEU:HB3	1.80	0.63
1:B:353:TRP:HE1	1:B:466:ARG:HA	1.62	0.63
1:C:328:ARG:NH1	1:C:578:ASP:OD1	2.32	0.63
1:C:1043:CYS:HB3	1:C:1048:HIS:CD2	2.33	0.63
2:X:145:TYR:HA	2:X:147:ARG:H	1.62	0.63
1:B:458:LYS:HD3	1:B:475:ALA:HA	1.78	0.63
3:P:69:THR:HG23	3:P:84:ARG:HH12	1.62	0.63
1:A:317:ASN:HA	1:A:594:GLY:HA2	1.80	0.63
1:A:393:THR:HG21	1:A:519:HIS:H	1.64	0.63
1:B:482:GLY:HA3	3:P:17:SER:H	1.64	0.63
1:C:1126:CYS:HB2	1:C:1132:ILE:HD13	1.81	0.62
1:A:64:TRP:HD1	1:A:65:PHE:N	1.96	0.62
3:P:39:GLN:H	3:P:92:ALA:HB1	1.64	0.62
2:X:40:TRP:HB2	2:X:53:ILE:HG22	1.80	0.62
1:A:557:LYS:NZ	1:A:574:ASP:O	2.32	0.62
1:A:403:ARG:HA	1:A:507:PRO:HA	1.80	0.62
1:A:977:LEU:HA	1:A:980:ILE:HD13	1.81	0.62
3:P:38:ARG:HB2	3:P:48:VAL:HB	1.82	0.62
2:X:145:TYR:CG	2:X:146:PRO:HA	2.35	0.62
1:B:555:SER:OG	1:B:586:ASP:N	2.33	0.61
3:P:168:THR:OG1	3:P:216:ASN:HB2	2.00	0.61
1:B:808:ASP:HB2	1:B:811:LYS:HG2	1.82	0.61
1:B:726:ILE:HG12	1:B:1061:VAL:HG23	1.81	0.61
1:A:170:TYR:HE2	1:A:172:SER:HB3	1.65	0.61
3:P:62:ASP:HA	3:P:65:LYS:HE3	1.82	0.61
2:O:91:TYR:O	2:O:106:GLY:HA2	2.00	0.61
2:O:128:GLU:HA	2:O:131:LYS:HG3	1.82	0.61
1:A:562:PHE:HZ	1:C:38:TYR:HD2	1.48	0.61
1:A:707:TYR:HD2	1:C:792:PRO:HG3	1.65	0.61
3:H:98:LYS:NZ	3:H:99:ALA:O	2.34	0.61
1:A:431:GLY:HA2	1:A:515:PHE:HD1	1.66	0.61
2:L:136:SER:OG	3:H:160:LYS:NZ	2.33	0.60
1:B:118:LEU:HD22	1:B:133:PHE:HZ	1.66	0.60
3:P:12:VAL:HG11	3:P:18:LEU:HD21	1.83	0.60
1:A:402:ILE:HD11	1:A:418:ILE:HG13	1.82	0.60
1:A:277:LEU:HD23	1:A:285:ILE:HD13	1.83	0.60
2:L:6:GLN:NE2	2:L:93:CYS:SG	2.74	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:646:ARG:O	1:A:646:ARG:NH1	2.35	0.60
1:A:703:ASN:OD1	1:A:704:SER:N	2.33	0.60
1:A:228:ASP:OD1	1:A:229:LEU:N	2.35	0.60
1:C:379:CYS:HA	1:C:432:CYS:HA	1.83	0.60
1:B:716:THR:HG21	1:B:1073:LYS:HE3	1.84	0.60
3:P:165:GLU:N	3:P:166:PRO:HD2	2.17	0.60
2:X:153:TRP:NE1	2:X:182:SER:OG	2.35	0.60
1:C:1089:PHE:CE1	1:C:1123:SER:HB3	2.37	0.59
1:C:950:ASP:OD1	1:C:951:VAL:N	2.35	0.59
1:A:825:LYS:HD2	1:A:945:LEU:HD23	1.83	0.59
3:Y:18:LEU:HB2	3:Y:83:MET:HB2	1.84	0.59
1:A:1106:GLN:NE2	1:A:1111:GLU:OE1	2.36	0.59
3:P:134:LYS:HE2	3:P:192:LEU:HD21	1.83	0.59
1:B:128:ILE:HB	1:B:170:TYR:HB3	1.85	0.59
1:B:64:TRP:HD1	1:B:65:PHE:N	2.01	0.59
3:P:5:LEU:O	3:P:22:CYS:HA	2.03	0.59
2:L:118:PRO:HB3	2:L:144:PHE:HB3	1.85	0.59
1:B:346:ARG:HA	1:B:509:ARG:NH2	2.18	0.59
1:C:323:THR:HG21	1:C:537:LYS:HD2	1.85	0.58
3:P:142:ALA:HB1	3:P:230:PRO:HA	1.85	0.58
1:C:722:VAL:HG12	1:C:930:ALA:HB1	1.85	0.58
2:X:29:LEU:HD11	2:X:95:GLN:HB2	1.84	0.58
2:X:37:TYR:HA	2:X:55:LEU:HD22	1.84	0.58
3:Y:138:VAL:HG11	3:Y:215:VAL:HG21	1.85	0.58
3:Y:156:GLY:HA2	3:Y:171:TRP:CH2	2.38	0.58
1:B:353:TRP:O	1:B:466:ARG:NH1	2.36	0.58
1:A:34:ARG:HD2	1:A:216:LEU:HD13	1.84	0.58
1:C:345:THR:O	1:C:509:ARG:NH1	2.29	0.58
1:A:439:ASN:ND2	1:A:506:GLN:OE1	2.36	0.58
1:A:912:THR:O	1:A:915:VAL:HG12	2.01	0.58
1:B:439:ASN:HB2	1:B:506:GLN:HG2	1.85	0.58
3:P:104:ARG:HA	3:P:104:ARG:NE	2.19	0.58
2:X:42:LEU:HB2	2:X:52:LEU:HD11	1.85	0.58
3:Y:30:ASP:HA	3:Y:72:ARG:HH22	1.67	0.58
3:H:83:MET:SD	3:H:86:LEU:HD21	2.44	0.58
3:Y:9:GLY:HA2	3:Y:126:VAL:HG22	1.85	0.58
3:Y:143:PRO:HB3	3:Y:155:LEU:HB3	1.86	0.58
3:H:217:HIS:CD2	3:H:219:PRO:HD2	2.39	0.58
1:C:40:ASP:OD2	1:C:44:ARG:NH1	2.37	0.58
1:B:418:ILE:HD13	1:B:422:ASN:ND2	2.19	0.57
1:C:742:ILE:HD11	1:C:997:ILE:HG23	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1093:GLY:H	1:C:1107:ARG:HH12	1.51	0.57
1:A:722:VAL:HG22	1:A:930:ALA:HB1	1.86	0.57
1:B:715:PRO:HA	1:B:1072:GLU:HA	1.86	0.57
1:B:1098:ASN:HD22	4:B:1308:NAG:H61	1.69	0.57
1:C:138:ASP:HB3	1:C:140:PHE:CE1	2.39	0.57
1:A:770:ILE:HD11	1:A:1012:LEU:HD12	1.85	0.57
2:X:144:PHE:CE2	2:X:180:LEU:HB2	2.39	0.57
1:B:382:VAL:HG21	1:B:390:LEU:HD21	1.85	0.57
1:A:656:VAL:HG12	1:A:658:ASN:H	1.69	0.57
1:C:392:PHE:HD2	1:C:515:PHE:HB3	1.70	0.57
3:P:100:VAL:HG23	3:P:118:ASP:HB3	1.85	0.57
2:X:91:TYR:O	2:X:106:GLY:HA2	2.04	0.57
1:B:1116:THR:HG22	1:B:1138:TYR:HB3	1.87	0.57
1:C:411:ALA:HB3	1:C:414:GLN:HB2	1.86	0.57
3:Y:50:GLY:HA3	3:Y:58:ILE:HD12	1.87	0.57
1:A:736:VAL:HG22	1:A:858:LEU:HD23	1.86	0.57
3:P:227:LYS:NZ	3:P:229:GLU:OE1	2.33	0.57
2:X:143:ASN:HA	2:X:177:THR:HB	1.87	0.56
1:A:316:SER:OG	1:A:317:ASN:N	2.38	0.56
3:H:161:ASP:HA	3:H:192:LEU:HB3	1.87	0.56
3:Y:39:GLN:H	3:Y:92:ALA:HB1	1.71	0.56
3:H:68:PHE:CE1	3:H:83:MET:HG3	2.40	0.56
1:B:924:ALA:O	1:B:928:ASN:ND2	2.39	0.56
1:C:1043:CYS:HB3	1:C:1048:HIS:HD2	1.70	0.56
1:A:733:LYS:NZ	1:A:775:ASP:OD2	2.37	0.56
1:B:894:LEU:HD21	1:C:715:PRO:HD3	1.87	0.56
1:C:295:PRO:HB2	1:C:608:VAL:HG21	1.88	0.56
3:P:17:SER:HB2	3:P:82:HIS:NE2	2.20	0.56
3:H:203:SER:HA	3:H:206:LEU:HG	1.88	0.56
1:B:617:CYS:HA	1:B:620:VAL:HG23	1.86	0.56
2:X:39:ASP:OD1	2:X:55:LEU:HD23	2.05	0.56
1:A:562:PHE:HD2	1:C:41:LYS:HZ2	1.53	0.56
1:B:466:ARG:HH21	3:P:72:ARG:H	1.54	0.56
1:A:115:GLN:HE22	1:A:131:CYS:HA	1.72	0.55
2:O:53:ILE:HD11	2:O:59:ARG:NE	2.20	0.55
2:O:190:ASP:HA	2:O:193:LYS:HG2	1.88	0.55
3:P:138:VAL:HG22	3:P:159:VAL:HG22	1.87	0.55
1:A:811:LYS:NZ	1:A:820:ASP:OD2	2.31	0.55
1:B:347:PHE:HB2	1:B:401:VAL:HG23	1.88	0.55
2:O:141:LEU:HB2	2:O:180:LEU:HB3	1.87	0.55
3:P:6:GLU:HG3	3:P:22:CYS:SG	2.46	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:889:GLY:HA3	1:A:1034:LEU:HD12	1.89	0.55
1:C:742:ILE:HD11	1:C:997:ILE:HA	1.88	0.55
1:B:473:TYR:HD2	1:B:489:TYR:HB2	1.71	0.55
1:A:676:THR:HG22	1:A:690:GLN:HG2	1.88	0.55
1:C:299:THR:CG2	1:C:597:VAL:HG11	2.37	0.55
3:Y:40:ALA:HA	3:Y:92:ALA:HA	1.89	0.55
3:P:9:GLY:HA2	3:P:126:VAL:HG22	1.87	0.55
3:H:176:LEU:HD21	3:H:199:VAL:HG11	1.88	0.55
1:C:716:THR:HG22	1:C:1071:GLN:O	2.07	0.55
1:B:329:PHE:O	1:B:580:GLN:NE2	2.37	0.55
1:A:1043:CYS:HB3	1:A:1048:HIS:CD2	2.41	0.55
1:B:273:ARG:NH1	1:B:290:ASP:OD2	2.40	0.55
1:C:64:TRP:HD1	1:C:65:PHE:N	2.05	0.55
1:B:716:THR:N	1:B:1071:GLN:O	2.29	0.55
1:A:310:LYS:HG3	1:A:600:PRO:HA	1.89	0.55
1:A:802:PHE:HD2	1:A:805:ILE:HD11	1.72	0.55
1:A:980:ILE:HG23	1:A:984:LEU:HD12	1.89	0.55
2:X:67:PHE:HB3	2:X:78:LEU:HD11	1.89	0.55
1:A:229:LEU:HD23	1:A:231:ILE:HD11	1.89	0.54
1:A:328:ARG:NE	1:A:533:LEU:HD23	2.21	0.54
2:O:113:ARG:H	2:O:145:TYR:HE2	1.54	0.54
3:H:153:ALA:HB3	3:H:206:LEU:HD11	1.88	0.54
1:B:811:LYS:NZ	1:B:820:ASP:OD2	2.41	0.54
1:B:993:ILE:O	1:B:997:ILE:HG12	2.07	0.54
1:C:1084:ASP:HB2	1:C:1086:LYS:NZ	2.23	0.54
1:B:401:VAL:HG22	1:B:509:ARG:HG2	1.89	0.54
1:B:712:ILE:HD13	1:A:896:ILE:HD12	1.88	0.54
1:C:422:ASN:HD21	1:C:454:ARG:HD2	1.72	0.54
3:Y:38:ARG:N	3:Y:46:GLU:O	2.41	0.54
1:C:410:ILE:HG12	1:C:433:VAL:HG11	1.89	0.54
1:C:418:ILE:HA	1:C:422:ASN:HD22	1.73	0.54
2:O:38:LEU:HD13	2:O:95:GLN:NE2	2.22	0.54
3:Y:138:VAL:HA	3:Y:158:LEU:O	2.08	0.54
1:B:734:THR:HG22	1:B:860:VAL:HG12	1.89	0.54
1:A:348:ALA:O	1:A:401:VAL:N	2.40	0.54
1:A:487:ASN:N	1:A:489:TYR:HH	2.06	0.54
1:C:92:PHE:HE2	1:C:94:SER:HB2	1.73	0.54
2:O:71:GLY:HA3	2:O:76:PHE:HA	1.90	0.54
1:A:410:ILE:HD11	1:A:418:ILE:HG22	1.90	0.53
1:A:1089:PHE:HE1	1:C:917:TYR:HD1	1.56	0.53
1:A:1105:THR:HG22	1:A:1112:PRO:HA	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:4:MET:HE3	2:L:95:GLN:HB3	1.89	0.53
2:L:141:LEU:HD12	2:L:180:LEU:HD22	1.88	0.53
2:X:74:THR:OG1	2:X:75:ASP:OD2	2.24	0.53
2:X:139:CYS:HB3	2:X:182:SER:HB3	1.89	0.53
1:A:353:TRP:HA	1:A:399:SER:O	2.08	0.53
1:C:879:ALA:O	1:C:883:THR:HG22	2.08	0.53
2:O:6:GLN:HE22	2:O:92:TYR:HA	1.73	0.53
2:O:195:LYS:HE3	2:O:215:ASN:HB3	1.90	0.53
1:A:337:PRO:HB2	1:A:340:GLU:HB2	1.89	0.53
1:C:87:ASN:OD1	1:C:88:ASP:N	2.41	0.53
3:P:6:GLU:HG2	3:P:123:GLY:HA2	1.90	0.53
1:C:104:TRP:HB3	1:C:106:PHE:CE1	2.42	0.53
1:B:462:LYS:N	1:B:465:GLU:OE1	2.38	0.53
1:B:749:CYS:SG	1:B:997:ILE:HD11	2.49	0.53
1:A:722:VAL:HG12	1:A:1065:VAL:HG22	1.90	0.53
1:C:338:PHE:O	1:C:341:VAL:HG12	2.09	0.53
1:C:737:ASP:HB3	1:C:740:MET:HB2	1.90	0.53
2:X:144:PHE:CE1	2:X:147:ARG:HA	2.44	0.53
1:C:106:PHE:CD1	1:C:238:PHE:HB2	2.44	0.53
2:L:19:ALA:O	2:L:79:LYS:HA	2.08	0.53
1:B:106:PHE:HB3	1:B:235:ILE:CD1	2.38	0.53
1:A:346:ARG:HE	3:H:56:GLY:HA3	1.74	0.53
1:B:395:VAL:HG23	1:B:515:PHE:HD1	1.74	0.52
1:A:102:ARG:HE	1:A:243:ALA:HB2	1.74	0.52
1:C:725:GLU:HG2	1:C:1062:PHE:HB2	1.92	0.52
1:C:1027:THR:O	1:C:1031:GLU:HG3	2.09	0.52
2:X:153:TRP:CD1	2:X:164:SER:HB2	2.45	0.52
3:H:118:ASP:OD1	3:H:119:VAL:N	2.42	0.52
1:C:186:PHE:HB3	1:C:213:VAL:HA	1.90	0.52
2:O:42:LEU:O	2:O:50:GLN:N	2.31	0.52
1:A:339:GLY:O	1:A:343:ASN:HB2	2.09	0.52
1:A:334:ASN:ND2	1:A:360:ASN:O	2.40	0.52
3:P:73:ASP:HB2	3:P:80:TYR:HE1	1.73	0.52
3:Y:131:ALA:HB3	3:Y:163:PHE:CE1	2.44	0.52
1:B:106:PHE:CD1	1:B:235:ILE:HD11	2.44	0.52
1:B:595:VAL:HG12	1:B:612:TYR:CD2	2.44	0.52
1:B:736:VAL:HG22	1:B:858:LEU:HD23	1.92	0.52
1:A:338:PHE:HD1	1:A:342:PHE:HE2	1.56	0.52
1:C:38:TYR:CE1	1:C:285:ILE:HG12	2.45	0.52
1:C:410:ILE:HD12	1:C:425:LEU:HD11	1.92	0.52
1:C:802:PHE:HD1	1:C:805:ILE:HD11	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:H:180:VAL:HA	3:H:199:VAL:HG22	1.92	0.52
1:B:555:SER:HG	1:B:586:ASP:N	2.07	0.52
1:B:1089:PHE:HE1	1:A:917:TYR:HD1	1.57	0.52
1:C:725:GLU:OE2	1:C:1028:LYS:HE2	2.10	0.52
3:Y:4:LEU:HB2	3:Y:121:GLY:HA3	1.92	0.52
1:C:537:LYS:O	1:C:539:VAL:HG13	2.10	0.52
1:C:656:VAL:HG12	1:C:658:ASN:H	1.75	0.52
2:X:6:GLN:HG3	2:X:105:PRO:HD2	1.92	0.52
2:X:37:TYR:HB3	2:X:96:ALA:HB3	1.91	0.52
2:X:152:GLN:HB2	2:X:200:GLU:HB3	1.91	0.52
2:L:145:TYR:O	2:L:203:HIS:NE2	2.37	0.52
3:P:156:GLY:HA2	3:P:171:TRP:HH2	1.75	0.51
3:Y:188:GLN:HB2	3:Y:192:LEU:HB2	1.92	0.51
2:L:119:SER:HB2	2:L:142:ASN:OD1	2.09	0.51
1:B:193:VAL:HG22	1:B:204:TYR:HB2	1.92	0.51
1:C:100:ILE:HG22	1:C:242:LEU:HG	1.92	0.51
1:C:985:ASP:OD2	1:C:987:PRO:HD2	2.10	0.51
3:P:164:PRO:HD2	3:P:217:HIS:HE1	1.74	0.51
1:B:346:ARG:HA	1:B:509:ARG:CZ	2.38	0.51
1:A:962:LEU:HD11	1:A:1007:TYR:CD2	2.45	0.51
2:L:154:LYS:HE2	2:L:157:ASN:HA	1.91	0.51
1:A:97:LYS:HB3	1:A:186:PHE:HA	1.91	0.51
1:A:462:LYS:NZ	1:A:464:PHE:O	2.35	0.51
2:O:74:THR:OG1	2:O:75:ASP:OD2	2.25	0.51
1:B:455:LEU:HD22	1:B:493:GLN:HB2	1.91	0.51
1:A:282:ASN:OD1	4:A:1301:NAG:N2	2.44	0.51
1:B:353:TRP:NE1	1:B:465:GLU:O	2.44	0.51
1:B:418:ILE:HA	1:B:422:ASN:HD22	1.75	0.51
1:A:64:TRP:CD1	1:A:65:PHE:N	2.78	0.51
1:A:643:PHE:HB3	1:A:650:LEU:HG	1.92	0.51
1:C:200:TYR:HB3	1:C:228:ASP:OD1	2.10	0.51
1:C:331:ASN:OD1	4:C:1302:NAG:N2	2.43	0.51
3:Y:69:THR:HG23	3:Y:84:ARG:HH12	1.75	0.51
1:B:403:ARG:HB2	1:B:406:GLU:HG2	1.92	0.51
1:A:329:PHE:CE2	1:A:544:ASN:HA	2.46	0.51
1:A:786:LYS:HG3	1:A:787:GLN:HG3	1.92	0.51
1:A:877:LEU:O	1:A:881:THR:HG23	2.11	0.51
3:Y:30:ASP:OD1	3:Y:72:ARG:NH2	2.44	0.51
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.76	0.50
1:A:393:THR:HB	1:A:520:ALA:HB3	1.93	0.50
1:C:661:GLU:O	1:C:695:TYR:OH	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:138:VAL:HG22	3:Y:159:VAL:HG22	1.93	0.50
2:L:37:TYR:HB3	2:L:96:ALA:HB3	1.92	0.50
2:X:40:TRP:CE2	2:X:78:LEU:HB2	2.47	0.50
2:X:153:TRP:HE1	2:X:182:SER:HG	1.53	0.50
2:X:166:GLU:HB2	2:X:180:LEU:HD21	1.93	0.50
1:B:472:ILE:HD11	3:P:84:ARG:HG2	1.94	0.50
1:A:329:PHE:O	1:A:580:GLN:NE2	2.44	0.50
1:B:457:ARG:NH2	1:B:469:SER:OG	2.40	0.50
1:B:458:LYS:HG3	1:B:473:TYR:HE1	1.76	0.50
3:Y:185:ALA:HB2	3:Y:195:LEU:HB3	1.93	0.50
1:A:351:TYR:O	1:A:466:ARG:NH2	2.45	0.50
1:A:775:ASP:O	1:A:779:GLN:HG2	2.12	0.50
1:A:998:THR:O	1:A:1002:GLN:HG2	2.12	0.50
2:X:41:TYR:OH	3:Y:116:GLY:HA2	2.12	0.50
1:A:986:PRO:HA	1:A:989:ALA:HB3	1.93	0.50
1:C:1115:ILE:HG22	1:C:1137:VAL:HG13	1.93	0.50
1:A:53:ASP:HB3	1:A:55:PHE:HE2	1.77	0.49
2:O:37:TYR:HB3	2:O:96:ALA:HB3	1.93	0.49
2:X:40:TRP:CD2	2:X:78:LEU:HB2	2.47	0.49
1:B:770:ILE:O	1:B:774:GLN:HG2	2.13	0.49
3:P:85:SER:O	3:P:87:ARG:NH1	2.44	0.49
1:B:314:GLN:HA	1:B:596:SER:HA	1.94	0.49
1:A:1002:GLN:O	1:A:1006:THR:HG23	2.11	0.49
3:P:185:ALA:HB2	3:P:195:LEU:HB3	1.95	0.49
1:C:643:PHE:HD2	1:C:650:LEU:HD21	1.77	0.49
2:X:146:PRO:HD2	2:X:203:HIS:NE2	2.27	0.49
1:B:328:ARG:HG3	1:B:543:PHE:CE2	2.46	0.49
1:A:912:THR:HG23	1:A:1106:GLN:OE1	2.12	0.49
1:C:129:LYS:HE2	1:C:169:GLU:HB2	1.94	0.49
1:C:742:ILE:HG23	1:C:743:CYS:N	2.27	0.49
1:C:922:LEU:O	1:C:926:GLN:HG3	2.12	0.49
3:Y:83:MET:HB3	3:Y:86:LEU:HD21	1.94	0.49
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.94	0.49
3:P:132:SER:HB2	3:P:134:LYS:NZ	2.28	0.49
2:L:133:GLY:HA2	2:L:188:LYS:HE3	1.92	0.49
3:H:203:SER:O	3:H:206:LEU:HB2	2.13	0.49
1:B:83:VAL:HG11	1:B:237:ARG:HH11	1.76	0.49
1:B:712:ILE:HG21	1:B:1096:VAL:HG12	1.94	0.49
1:C:189:LEU:HB2	1:C:210:ILE:HD13	1.95	0.49
1:C:287:ASP:OD1	1:C:288:ALA:N	2.44	0.49
3:P:138:VAL:HA	3:P:158:LEU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:LEU:HD23	1:B:118:LEU:N	2.27	0.49
1:A:377:PHE:CD1	1:A:434:ILE:HG12	2.48	0.49
1:C:350:VAL:HG21	1:C:418:ILE:HG23	1.95	0.49
2:O:53:ILE:HD11	2:O:59:ARG:HE	1.78	0.49
3:P:50:GLY:HA3	3:P:58:ILE:HD12	1.94	0.49
3:H:61:ALA:HB3	3:H:64:VAL:HG12	1.94	0.49
1:B:1141:LEU:HD22	1:B:1145:LEU:HD23	1.94	0.49
1:A:985:ASP:OD1	1:A:986:PRO:HD2	2.13	0.49
1:C:713:ALA:HA	1:C:1073:LYS:O	2.13	0.49
1:B:27:ALA:HB3	1:B:64:TRP:HB3	1.95	0.49
1:A:551:VAL:HG13	1:A:588:THR:HB	1.94	0.49
2:O:118:PRO:HD2	2:O:206:LEU:HG	1.95	0.48
2:O:122:ILE:HD12	2:O:199:CYS:HB3	1.95	0.48
3:P:97:ALA:HB3	3:P:117:MET:CE	2.43	0.48
3:Y:29:PHE:CD2	3:Y:77:ASN:HA	2.48	0.48
1:B:96:GLU:OE2	1:B:99:ASN:N	2.46	0.48
1:B:481:ASN:O	3:P:16:ARG:HD3	2.14	0.48
1:B:896:ILE:HD12	1:C:712:ILE:HG12	1.95	0.48
1:A:170:TYR:CE2	1:A:172:SER:HB3	2.46	0.48
1:C:338:PHE:HE2	1:C:368:LEU:HD11	1.78	0.48
1:C:725:GLU:CG	1:C:1062:PHE:HB2	2.44	0.48
1:C:854:LYS:HA	1:C:858:LEU:HD11	1.94	0.48
1:C:1102:TRP:HB2	1:C:1135:ASN:ND2	2.28	0.48
1:B:201:PHE:HE2	1:B:203:ILE:HD11	1.78	0.48
1:B:552:LEU:HD13	1:B:585:LEU:HD13	1.94	0.48
1:A:436:TRP:HE1	1:A:509:ARG:HD2	1.78	0.48
1:A:438:SER:HB2	1:A:509:ARG:HG3	1.95	0.48
1:A:870:ILE:O	1:A:874:THR:HG23	2.13	0.48
1:C:106:PHE:CD2	1:C:117:LEU:HD22	2.49	0.48
1:B:350:VAL:HG11	1:B:422:ASN:HB3	1.95	0.48
1:C:455:LEU:HD22	1:C:493:GLN:HB2	1.95	0.48
2:O:113:ARG:NH2	2:O:175:ASP:HA	2.28	0.48
1:B:502:GLY:N	1:B:505:TYR:HB2	2.27	0.48
1:B:949:GLN:HG3	1:B:953:ASN:HD21	1.78	0.48
1:A:129:LYS:HE3	1:A:131:CYS:HB2	1.94	0.48
1:A:364:ASP:HA	1:A:527:PRO:HD3	1.95	0.48
1:C:804:GLN:O	1:C:818:ILE:HG13	2.14	0.48
2:X:6:GLN:NE2	2:X:93:CYS:SG	2.86	0.48
2:X:67:PHE:CE1	2:X:80:ILE:HG12	2.48	0.48
1:B:1005:GLN:O	1:B:1009:THR:HG23	2.14	0.48
1:A:34:ARG:NH1	1:A:219:GLY:O	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:64:TRP:CD1	1:C:65:PHE:N	2.82	0.48
1:C:726:ILE:HG23	1:C:1061:VAL:HG12	1.96	0.48
1:C:988:GLU:OE1	1:C:988:GLU:N	2.47	0.48
2:X:38:LEU:HD13	2:X:76:PHE:HB2	1.95	0.48
3:Y:224:VAL:HG12	3:Y:226:LYS:HG3	1.96	0.48
2:L:59:ARG:NH1	2:L:67:PHE:O	2.45	0.48
3:H:203:SER:HA	3:H:206:LEU:CG	2.44	0.48
1:B:65:PHE:CZ	1:B:84:LEU:HD11	2.49	0.48
1:B:338:PHE:HB3	1:B:342:PHE:HE2	1.77	0.48
1:B:738:CYS:HB3	1:B:760:CYS:HB2	1.73	0.48
2:X:52:LEU:HD22	2:X:67:PHE:CE2	2.48	0.48
3:Y:143:PRO:HD3	3:Y:228:VAL:HG12	1.96	0.48
1:A:989:ALA:O	1:A:993:ILE:HG12	2.14	0.48
1:C:1097:SER:OG	1:C:1101:HIS:O	2.27	0.48
1:C:38:TYR:HE1	1:C:285:ILE:HG12	1.78	0.48
3:H:203:SER:HA	3:H:206:LEU:HD12	1.95	0.48
1:B:727:LEU:HD11	1:B:1028:LYS:HD2	1.96	0.48
1:B:950:ASP:OD1	1:B:951:VAL:N	2.46	0.48
1:C:819:GLU:O	1:C:823:PHE:HD2	1.96	0.48
1:A:358:ILE:HB	1:A:395:VAL:HG13	1.96	0.47
1:A:1089:PHE:CE1	1:C:917:TYR:HD1	2.30	0.47
1:C:31:SER:HB3	1:C:62:VAL:HG13	1.96	0.47
1:C:1075:PHE:HB3	1:C:1096:VAL:HG13	1.95	0.47
2:X:148:GLU:HB3	2:X:203:HIS:CD2	2.49	0.47
3:H:217:HIS:HB3	3:H:222:THR:HG22	1.96	0.47
3:Y:141:LEU:HD12	3:Y:158:LEU:HD11	1.95	0.47
2:L:146:PRO:HD2	2:L:203:HIS:CE1	2.49	0.47
1:B:786:LYS:NZ	1:B:888:PHE:O	2.47	0.47
1:C:439:ASN:OD1	1:C:440:ASN:N	2.47	0.47
1:C:641:ASN:OD1	1:C:642:VAL:N	2.46	0.47
2:X:31:HIS:CG	2:X:32:SER:H	2.32	0.47
3:H:203:SER:HA	3:H:206:LEU:CD1	2.44	0.47
1:C:117:LEU:HD21	1:C:119:ILE:HD11	1.96	0.47
1:B:226:LEU:HB3	1:B:227:VAL:HG23	1.96	0.47
1:A:472:ILE:HA	1:A:491:PRO:HG3	1.96	0.47
1:A:866:THR:O	1:A:869:MET:N	2.44	0.47
1:C:403:ARG:HE	1:C:497:PHE:HE1	1.61	0.47
2:X:144:PHE:HB2	2:X:149:ALA:HB3	1.97	0.47
3:H:49:SER:OG	3:H:50:GLY:N	2.47	0.47
1:B:295:PRO:HB2	1:B:608:VAL:HG21	1.96	0.47
1:C:408:ARG:CZ	1:C:409:GLN:HG2	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:770:ILE:HD11	1:C:1012:LEU:HD23	1.97	0.47
2:O:153:TRP:HE1	2:O:182:SER:HG	1.62	0.47
2:X:153:TRP:CH2	2:X:199:CYS:HB2	2.50	0.47
3:Y:11:LEU:HA	3:Y:127:THR:HB	1.97	0.47
2:L:195:LYS:HD3	2:L:216:ARG:HB2	1.97	0.47
3:H:34:MET:HG2	3:H:72:ARG:CZ	2.45	0.47
1:B:28:TYR:HD2	1:B:61:ASN:HB3	1.80	0.47
1:B:430:THR:OG1	1:B:515:PHE:O	2.33	0.47
1:B:904:TYR:OH	1:C:1094:VAL:HG22	2.15	0.47
1:B:1085:GLY:O	1:B:1126:CYS:N	2.41	0.47
1:A:308:VAL:HG22	1:A:602:THR:HG23	1.96	0.47
1:A:334:ASN:HB2	1:A:361:CYS:HA	1.96	0.47
1:A:537:LYS:HE2	1:A:537:LYS:HB3	1.65	0.47
1:C:870:ILE:O	1:C:874:THR:HG23	2.15	0.47
1:C:877:LEU:O	1:C:881:THR:HG23	2.15	0.47
1:C:922:LEU:HG	1:C:926:GLN:HE21	1.78	0.47
1:C:962:LEU:HD11	1:C:1007:TYR:CD2	2.50	0.47
3:P:38:ARG:HG3	3:P:92:ALA:CB	2.44	0.47
3:P:224:VAL:HG12	3:P:226:LYS:HG3	1.96	0.47
3:Y:155:LEU:HD12	3:Y:171:TRP:HZ3	1.80	0.47
1:B:353:TRP:CZ3	1:B:355:ARG:HB2	2.50	0.47
1:B:364:ASP:OD1	1:B:365:TYR:N	2.48	0.47
1:A:201:PHE:HB3	1:A:229:LEU:HB2	1.97	0.47
1:C:131:CYS:HB2	1:C:133:PHE:CE1	2.49	0.47
2:O:154:LYS:HG2	2:O:158:ALA:O	2.14	0.47
3:Y:82:HIS:CD2	3:Y:84:ARG:HH21	2.33	0.47
1:B:1039:ARG:NH2	1:A:1031:GLU:OE2	2.48	0.47
3:Y:22:CYS:HB2	3:Y:79:LEU:HG	1.97	0.47
2:L:130:LEU:O	2:L:131:LYS:HE2	2.14	0.47
1:B:374:PHE:HA	1:B:436:TRP:HB3	1.96	0.46
1:B:506:GLN:HB2	1:B:508:TYR:HE1	1.80	0.46
1:B:988:GLU:N	1:B:988:GLU:OE1	2.48	0.46
1:A:88:ASP:OD2	1:A:88:ASP:N	2.48	0.46
1:C:129:LYS:HG3	1:C:131:CYS:H	1.80	0.46
2:X:175:ASP:OD1	2:X:177:THR:OG1	2.27	0.46
1:C:199:GLY:HA2	1:C:232:GLY:HA2	1.97	0.46
2:L:41:TYR:OH	3:H:117:MET:N	2.34	0.46
3:P:4:LEU:HB2	3:P:121:GLY:HA3	1.97	0.46
1:B:342:PHE:HE1	1:B:511:VAL:HG11	1.80	0.46
1:A:367:VAL:O	1:A:371:SER:N	2.48	0.46
3:P:19:ARG:NE	3:P:82:HIS:HD1	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:140:PRO:HB3	3:Y:228:VAL:HA	1.98	0.46
2:L:110:ASP:OD1	2:L:110:ASP:N	2.48	0.46
1:B:53:ASP:HB3	1:B:55:PHE:CE1	2.51	0.46
1:A:742:ILE:O	1:A:1000:ARG:NH1	2.41	0.46
1:C:738:CYS:O	1:C:742:ILE:HG22	2.15	0.46
3:P:36:TRP:CD1	3:P:81:LEU:HD12	2.50	0.46
1:C:90:VAL:HG21	1:C:238:PHE:CE1	2.51	0.46
2:O:103:PHE:CD2	3:P:46:GLU:HA	2.51	0.46
3:P:162:TYR:HE2	3:P:165:GLU:O	1.99	0.46
1:B:869:MET:HG2	1:C:699:LEU:HD11	1.97	0.46
1:B:912:THR:HG22	1:B:914:ASN:H	1.81	0.46
1:C:326:ILE:HD11	1:C:534:VAL:HG22	1.97	0.46
1:C:390:LEU:HB3	1:C:392:PHE:CE1	2.51	0.46
1:C:431:GLY:HA2	1:C:515:PHE:CE2	2.51	0.46
1:C:645:THR:OG1	1:C:670:ILE:HD12	2.16	0.46
3:P:171:TRP:HE1	3:P:197:SER:HG	1.64	0.46
1:B:65:PHE:O	1:B:264:ALA:HB1	2.16	0.46
1:B:104:TRP:HB3	1:B:106:PHE:CE2	2.51	0.46
1:A:331:ASN:OD1	4:A:1303:NAG:N2	2.48	0.46
1:C:737:ASP:OD2	1:C:740:MET:HG3	2.16	0.46
3:P:22:CYS:HB2	3:P:79:LEU:CG	2.46	0.46
3:P:73:ASP:OD2	3:P:76:LYS:HG2	2.15	0.46
1:B:64:TRP:CD1	1:B:65:PHE:N	2.82	0.46
1:A:229:LEU:HB3	1:A:231:ILE:HG12	1.98	0.45
1:A:287:ASP:HB3	1:A:306:PHE:HE2	1.81	0.45
1:B:106:PHE:HD1	1:B:235:ILE:HD11	1.81	0.45
1:A:106:PHE:HB3	1:A:235:ILE:HG21	1.98	0.45
1:A:106:PHE:CD1	1:A:238:PHE:HB2	2.51	0.45
1:C:424:LYS:NZ	1:C:463:PRO:HA	2.31	0.45
2:O:67:PHE:CE1	2:O:80:ILE:HG12	2.51	0.45
2:X:40:TRP:HB2	2:X:53:ILE:CG2	2.44	0.45
1:B:388:ASN:O	1:B:526:GLY:N	2.49	0.45
1:B:763:LEU:HD21	1:B:1005:GLN:OE1	2.17	0.45
1:A:586:ASP:OD2	1:A:587:ILE:N	2.49	0.45
2:O:135:ALA:HB3	2:O:186:LEU:HB2	1.97	0.45
1:A:27:ALA:C	1:A:28:TYR:HD2	2.20	0.45
1:C:666:ILE:HB	1:C:670:ILE:O	2.17	0.45
3:P:215:VAL:O	3:P:223:LYS:HA	2.16	0.45
2:X:201:VAL:O	2:X:209:PRO:HA	2.16	0.45
1:B:1089:PHE:CE1	1:A:917:TYR:HD1	2.33	0.45
1:A:212:LEU:HD21	1:A:214:ARG:NH2	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:40:TRP:CE2	2:O:78:LEU:HB2	2.51	0.45
1:B:403:ARG:O	1:B:407:VAL:HG23	2.17	0.45
1:C:52:GLN:HA	1:C:274:THR:HA	1.99	0.45
1:C:111:ASP:N	1:C:111:ASP:OD1	2.47	0.45
1:C:128:ILE:HD12	1:C:170:TYR:HD2	1.81	0.45
3:P:170:SER:OG	3:P:214:ASN:HB2	2.17	0.45
3:Y:15:GLY:H	3:Y:86:LEU:CB	2.27	0.45
1:B:1002:GLN:O	1:B:1006:THR:HG23	2.17	0.45
1:A:103:GLY:HA3	1:A:241:LEU:HB2	1.98	0.45
1:A:557:LYS:NZ	1:A:575:ALA:HB2	2.32	0.45
1:C:878:LEU:HD11	1:C:1054:GLN:HE22	1.81	0.45
1:C:29:THR:HB	1:C:62:VAL:HG23	1.99	0.45
1:C:102:ARG:HB2	1:C:241:LEU:HD12	1.99	0.45
1:C:353:TRP:CE2	1:C:466:ARG:HD3	2.51	0.45
2:O:8:PRO:HG2	2:O:11:LEU:HB3	1.99	0.45
2:X:55:LEU:HD12	2:X:58:ASN:HB2	1.98	0.45
2:X:101:PHE:CE2	3:Y:115:TYR:HB3	2.51	0.45
1:B:821:LEU:HD21	1:B:939:SER:HB3	1.98	0.45
1:A:565:PHE:O	1:C:42:VAL:HA	2.17	0.45
1:A:665:PRO:HA	1:A:671:CYS:HB3	1.99	0.45
1:C:360:ASN:H	1:C:523:THR:HG23	1.80	0.45
1:C:498:GLN:HB3	1:C:501:ASN:OD1	2.17	0.45
3:P:159:VAL:HG12	3:P:162:TYR:CD1	2.52	0.45
2:X:43:GLN:HB3	2:X:90:VAL:CG1	2.47	0.45
2:X:125:PRO:HD3	2:X:137:VAL:HA	1.98	0.45
1:C:742:ILE:HG23	1:C:743:CYS:H	1.81	0.44
2:O:42:LEU:HD22	2:O:52:LEU:HD21	1.99	0.44
3:Y:93:LEU:HD11	3:Y:125:THR:HG22	1.99	0.44
1:B:1043:CYS:HB3	1:B:1048:HIS:ND1	2.32	0.44
1:B:1106:GLN:HE21	1:B:1109:PHE:HB3	1.82	0.44
1:C:58:PHE:HB3	1:C:59:PHE:CD1	2.53	0.44
1:B:1031:GLU:OE2	1:C:1042:PHE:HB2	2.16	0.44
1:A:673:SER:OG	1:A:674:TYR:N	2.51	0.44
3:P:34:MET:HG3	3:P:97:ALA:O	2.16	0.44
3:P:155:LEU:HD21	3:P:211:TYR:CE1	2.52	0.44
3:Y:43:LYS:HE3	3:Y:44:GLY:H	1.81	0.44
1:B:870:ILE:O	1:B:874:THR:HG23	2.16	0.44
1:B:940:SER:OG	1:B:941:THR:N	2.50	0.44
1:C:462:LYS:HB3	1:C:463:PRO:HD2	1.99	0.44
3:Y:30:ASP:HA	3:Y:72:ARG:NH2	2.32	0.44
1:B:349:SER:OG	1:B:350:VAL:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1030:SER:O	1:A:1034:LEU:HB2	2.18	0.44
1:C:826:VAL:HG23	1:C:949:GLN:OE1	2.18	0.44
3:H:136:PRO:HD3	3:H:217:HIS:ND1	2.31	0.44
1:A:105:ILE:HG21	1:A:135:PHE:CZ	2.52	0.44
2:O:66:ARG:HB2	2:O:82:ARG:HB2	1.99	0.44
2:O:125:PRO:HD3	2:O:137:VAL:HA	1.99	0.44
3:P:79:LEU:HD11	3:P:96:CYS:SG	2.58	0.44
2:X:42:LEU:HD23	2:X:43:GLN:N	2.32	0.44
1:B:142:GLY:HA2	1:B:244:LEU:H	1.82	0.44
1:B:323:THR:OG1	1:B:324:GLU:HG2	2.18	0.44
1:C:1093:GLY:N	1:C:1107:ARG:HH12	2.14	0.44
1:A:822:LEU:HD23	1:A:945:LEU:HD21	1.99	0.44
1:C:1080:ALA:HB3	1:C:1132:ILE:HG13	2.00	0.44
2:X:145:TYR:HA	2:X:147:ARG:N	2.29	0.44
3:Y:92:ALA:HB3	3:Y:94:TYR:CZ	2.52	0.44
1:B:402:ILE:O	1:B:508:TYR:HB2	2.18	0.44
1:C:558:LYS:HD2	1:C:558:LYS:HA	1.86	0.44
2:O:16:GLY:H	2:O:83:VAL:HG21	1.82	0.44
2:O:37:TYR:HA	2:O:55:LEU:HD22	2.00	0.44
2:X:141:LEU:HD13	2:X:180:LEU:HD22	1.99	0.44
3:H:188:GLN:HB2	3:H:192:LEU:O	2.17	0.44
1:B:411:ALA:HB3	1:B:414:GLN:HB2	2.00	0.43
1:B:442:ASP:OD2	1:B:509:ARG:NE	2.47	0.43
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.51	0.43
1:C:106:PHE:HB3	1:C:235:ILE:HG21	2.00	0.43
3:P:97:ALA:HB3	3:P:117:MET:HE3	1.99	0.43
1:B:331:ASN:OD1	4:B:1309:NAG:N2	2.51	0.43
1:B:537:LYS:O	1:B:539:VAL:HG13	2.18	0.43
1:B:894:LEU:CD2	1:C:715:PRO:HD3	2.47	0.43
1:A:560:LEU:CD1	1:C:38:TYR:HE2	2.30	0.43
1:A:966:LEU:O	1:A:975:SER:OG	2.36	0.43
1:C:431:GLY:HA2	1:C:515:PHE:HE2	1.83	0.43
1:C:919:ASN:O	1:C:923:ILE:HG13	2.18	0.43
2:O:44:LYS:HB2	2:O:47:GLN:HB2	2.00	0.43
3:Y:6:GLU:HG2	3:Y:123:GLY:HA2	1.99	0.43
2:L:152:GLN:HB2	2:L:200:GLU:HB2	2.00	0.43
1:B:199:GLY:HA2	1:B:232:GLY:HA2	2.00	0.43
1:C:340:GLU:N	1:C:340:GLU:OE1	2.52	0.43
1:C:1072:GLU:N	1:C:1072:GLU:OE1	2.51	0.43
2:O:127:ASP:HA	2:O:130:LEU:HD12	2.00	0.43
3:P:227:LYS:NZ	3:P:229:GLU:HB2	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Y:40:ALA:HB3	3:Y:43:LYS:HB2	1.99	0.43
3:H:38:ARG:HG2	3:H:46:GLU:HB3	2.00	0.43
1:B:717:ASN:OD1	1:B:718:PHE:N	2.51	0.43
1:B:958:ALA:O	1:B:961:THR:OG1	2.30	0.43
1:A:543:PHE:HE2	1:A:576:VAL:HG11	1.84	0.43
1:A:802:PHE:CD2	1:A:805:ILE:HD11	2.54	0.43
2:X:123:PHE:CD2	3:Y:141:LEU:HD21	2.53	0.43
3:H:39:GLN:O	3:H:92:ALA:HB1	2.19	0.43
1:B:699:LEU:HD12	1:A:872:GLN:NE2	2.33	0.43
1:C:273:ARG:HD3	1:C:273:ARG:HA	1.71	0.43
2:L:151:VAL:HA	2:L:200:GLU:O	2.18	0.43
3:H:87:ARG:O	3:H:128:VAL:HG21	2.18	0.43
3:H:171:TRP:CZ3	3:H:213:CYS:HB3	2.54	0.43
1:A:554:GLU:CD	1:A:554:GLU:H	2.20	0.43
1:A:557:LYS:HB2	1:A:584:ILE:HG21	1.99	0.43
1:A:643:PHE:CE1	1:A:655:HIS:HB2	2.54	0.43
1:A:699:LEU:HD11	1:C:869:MET:HG2	2.00	0.43
1:C:417:LYS:HA	1:C:417:LYS:HD3	1.72	0.43
1:C:770:ILE:O	1:C:774:GLN:HG2	2.19	0.43
3:P:14:PRO:O	3:P:16:ARG:NH1	2.52	0.43
3:P:22:CYS:HB2	3:P:79:LEU:HG	2.01	0.43
1:B:456:PHE:HB3	1:B:473:TYR:CD2	2.53	0.43
1:B:873:TYR:CZ	1:C:699:LEU:HD22	2.54	0.43
1:C:435:ALA:HB2	1:C:510:VAL:HG22	2.01	0.43
1:C:816:SER:OG	1:C:819:GLU:HG3	2.19	0.43
1:B:393:THR:HA	1:B:522:ALA:HA	1.99	0.43
1:B:554:GLU:OE1	1:B:555:SER:N	2.49	0.43
1:B:1126:CYS:HB2	1:B:1132:ILE:HD13	2.00	0.43
1:C:825:LYS:HB3	1:C:825:LYS:HE3	1.73	0.43
1:C:1086:LYS:HA	1:C:1125:ASN:HA	2.00	0.43
2:O:55:LEU:HB2	2:O:58:ASN:HB2	2.00	0.43
2:O:144:PHE:HE1	2:O:147:ARG:HA	1.83	0.43
3:H:158:LEU:HD12	3:H:195:LEU:O	2.19	0.43
1:A:348:ALA:HB3	1:A:352:ALA:O	2.19	0.43
1:A:722:VAL:HG23	1:A:722:VAL:O	2.19	0.43
1:A:934:ILE:HD13	1:A:934:ILE:HA	1.87	0.43
1:A:1129:VAL:HG13	1:A:1132:ILE:HB	2.01	0.43
1:C:454:ARG:HH21	1:C:457:ARG:N	2.17	0.43
3:H:53:TRP:CG	3:H:103:VAL:HG21	2.54	0.43
1:B:458:LYS:HG3	1:B:473:TYR:CE1	2.54	0.43
1:B:981:LEU:HD21	1:B:993:ILE:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:345:THR:HG23	1:A:346:ARG:N	2.34	0.43
1:A:555:SER:HB3	1:A:584:ILE:HG22	2.01	0.43
1:C:325:SER:HA	1:C:540:ASN:O	2.19	0.43
1:C:538:CYS:HB2	1:C:590:CYS:HB3	1.74	0.43
1:C:767:LEU:HD23	1:C:767:LEU:HA	1.91	0.43
1:C:1142:GLN:HA	1:C:1145:LEU:HG	1.99	0.43
2:X:113:ARG:H	2:X:145:TYR:HE2	1.65	0.43
2:X:118:PRO:HB3	2:X:144:PHE:CB	2.44	0.43
3:Y:136:PRO:HA	3:Y:162:TYR:HB3	2.01	0.43
1:B:922:LEU:O	1:B:926:GLN:HG3	2.19	0.42
1:C:643:PHE:CZ	1:C:655:HIS:ND1	2.87	0.42
1:B:369:TYR:OH	1:B:384:PRO:O	2.26	0.42
1:A:543:PHE:CE2	1:A:576:VAL:HG11	2.54	0.42
2:O:88:VAL:HG12	2:O:110:ASP:HA	2.01	0.42
2:X:149:ALA:HA	2:X:202:THR:O	2.19	0.42
2:L:41:TYR:CD1	2:L:51:LEU:HA	2.55	0.42
1:B:326:ILE:HD13	1:B:326:ILE:HA	1.86	0.42
1:B:402:ILE:HG13	1:B:407:VAL:HG22	2.01	0.42
1:B:825:LYS:HE2	1:B:825:LYS:HB2	1.65	0.42
4:A:1307:NAG:O6	4:A:1307:NAG:O4	2.30	0.42
1:C:119:ILE:HD12	1:C:128:ILE:HG12	2.01	0.42
1:C:497:PHE:CE2	1:C:507:PRO:HB3	2.55	0.42
1:C:825:LYS:NZ	1:C:942:PRO:HA	2.34	0.42
1:C:1086:LYS:HE2	1:C:1088:HIS:NE2	2.34	0.42
3:H:53:TRP:CE2	3:H:54:ASN:OD1	2.72	0.42
3:P:36:TRP:HB2	3:P:49:SER:OG	2.20	0.42
2:X:112:LYS:HA	2:X:145:TYR:OH	2.19	0.42
2:X:144:PHE:CD1	2:X:147:ARG:HA	2.54	0.42
1:A:240:THR:OG1	1:A:241:LEU:N	2.52	0.42
1:C:742:ILE:CD1	1:C:997:ILE:HG23	2.49	0.42
2:O:43:GLN:HB3	2:O:90:VAL:CG1	2.48	0.42
3:H:154:ALA:HA	3:H:200:THR:HA	2.01	0.42
1:A:506:GLN:NE2	1:A:508:TYR:OH	2.52	0.42
1:C:101:ILE:HD11	1:C:240:THR:OG1	2.19	0.42
1:C:347:PHE:CZ	1:C:399:SER:HB2	2.54	0.42
1:C:715:PRO:HA	1:C:1072:GLU:HA	2.00	0.42
3:Y:83:MET:HE1	3:Y:86:LEU:HD11	2.01	0.42
3:Y:91:THR:HG23	3:Y:128:VAL:HB	2.01	0.42
3:H:70:ILE:HD11	3:H:79:LEU:HD11	2.01	0.42
1:B:57:PRO:HB3	1:B:273:ARG:NH2	2.34	0.42
1:B:733:LYS:NZ	1:B:775:ASP:OD2	2.45	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:436:TRP:NE1	1:A:509:ARG:HD2	2.34	0.42
1:C:202:LYS:HB3	1:C:204:TYR:CE1	2.54	0.42
1:C:743:CYS:SG	1:C:749:CYS:C	2.98	0.42
3:P:86:LEU:HD12	3:P:128:VAL:HG11	2.01	0.42
3:P:182:THR:HA	3:P:197:SER:HA	2.01	0.42
1:C:276:LEU:HB3	1:C:289:VAL:CG2	2.49	0.42
1:C:720:ILE:HG13	1:C:923:ILE:HG23	2.02	0.42
3:P:14:PRO:HD2	3:P:130:SER:HB2	2.01	0.42
3:P:60:TYR:HB3	3:P:64:VAL:HG13	2.00	0.42
2:L:4:MET:CE	2:L:95:GLN:HB3	2.50	0.42
1:B:906:PHE:CD1	1:B:1049:LEU:HD11	2.54	0.42
1:A:317:ASN:N	1:A:317:ASN:OD1	2.52	0.42
1:A:919:ASN:O	1:A:923:ILE:HG13	2.19	0.42
1:C:58:PHE:HB3	1:C:59:PHE:HD1	1.85	0.42
1:C:763:LEU:HD22	1:C:1008:VAL:HG21	2.02	0.42
1:C:984:LEU:HD23	1:C:984:LEU:HA	1.90	0.42
3:P:4:LEU:HA	3:P:23:ALA:O	2.20	0.42
3:P:69:THR:OG1	3:P:82:HIS:HB3	2.20	0.42
3:Y:36:TRP:HB2	3:Y:49:SER:OG	2.20	0.42
2:L:20:SER:C	2:L:21:ILE:HG13	2.40	0.42
3:H:117:MET:O	3:H:120:TRP:NE1	2.41	0.42
1:B:358:ILE:HB	1:B:395:VAL:CG1	2.49	0.42
1:A:791:THR:OG1	1:A:792:PRO:HD2	2.20	0.42
1:C:449:TYR:O	1:C:494:SER:HB2	2.19	0.42
2:X:123:PHE:HZ	3:Y:154:ALA:HB3	1.85	0.42
2:X:154:LYS:HA	2:X:158:ALA:O	2.20	0.42
3:Y:5:LEU:O	3:Y:22:CYS:HA	2.19	0.42
3:H:143:PRO:HG2	3:H:230:PRO:HB3	2.01	0.42
1:B:224:GLU:N	1:B:224:GLU:OE1	2.53	0.41
1:A:551:VAL:CG1	1:A:588:THR:HB	2.50	0.41
1:C:445:VAL:O	1:C:498:GLN:NE2	2.53	0.41
1:C:724:THR:HA	1:C:1062:PHE:O	2.19	0.41
1:C:900:MET:HA	1:C:917:TYR:OH	2.20	0.41
2:O:38:LEU:HD12	2:O:94:MET:O	2.20	0.41
2:L:41:TYR:HD1	2:L:51:LEU:HA	1.85	0.41
1:B:430:THR:OG1	1:B:430:THR:O	2.36	0.41
1:A:64:TRP:HD1	1:A:65:PHE:H	1.64	0.41
2:O:67:PHE:HE1	2:O:80:ILE:HG12	1.84	0.41
2:L:169:THR:OG1	2:L:170:GLU:N	2.53	0.41
1:B:395:VAL:HG23	1:B:515:PHE:CD1	2.55	0.41
1:B:438:SER:OG	1:B:507:PRO:O	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:123:ALA:O	1:A:124:THR:HG22	2.21	0.41
1:A:473:TYR:O	1:A:489:TYR:N	2.52	0.41
1:A:722:VAL:HA	1:A:1064:HIS:O	2.20	0.41
1:C:50:SER:HB2	1:C:276:LEU:HD13	2.01	0.41
1:C:376:THR:HG22	1:C:435:ALA:HB3	2.01	0.41
1:C:912:THR:HG22	1:C:913:GLN:H	1.86	0.41
3:P:176:LEU:HD21	3:P:199:VAL:HG11	2.02	0.41
3:Y:6:GLU:HG3	3:Y:22:CYS:SG	2.60	0.41
3:H:134:LYS:HG2	3:H:135:GLY:N	2.35	0.41
1:B:453:TYR:CE1	1:B:493:GLN:HB3	2.55	0.41
1:B:535:LYS:O	1:B:537:LYS:HG3	2.21	0.41
1:A:431:GLY:HA2	1:A:515:PHE:CD1	2.51	0.41
1:C:122:ASN:O	1:C:124:THR:N	2.53	0.41
1:C:389:ASP:OD1	1:C:390:LEU:N	2.53	0.41
2:X:88:VAL:HG11	2:X:111:ILE:HG12	2.01	0.41
1:B:825:LYS:HZ1	1:B:939:SER:HA	1.86	0.41
1:B:973:ILE:HG13	1:B:992:GLN:OE1	2.21	0.41
1:A:716:THR:HG22	1:A:1110:TYR:HB2	2.01	0.41
1:A:717:ASN:OD1	1:A:718:PHE:N	2.54	0.41
1:A:767:LEU:HD23	1:A:767:LEU:HA	1.87	0.41
1:A:976:VAL:HG23	1:A:976:VAL:O	2.21	0.41
1:C:450:ASN:HD21	3:Y:60:TYR:HD2	1.67	0.41
1:C:644:GLN:HG3	1:C:645:THR:N	2.36	0.41
2:L:14:THR:HG23	2:L:17:GLU:OE1	2.20	0.41
2:L:215:ASN:OD1	2:L:215:ASN:N	2.51	0.41
3:H:40:ALA:HB3	3:H:43:LYS:HB2	2.02	0.41
1:B:189:LEU:HB3	1:B:208:THR:HG23	2.03	0.41
1:A:393:THR:HG21	1:A:520:ALA:H	1.86	0.41
1:A:814:LYS:HA	1:A:814:LYS:HD3	1.81	0.41
2:X:16:GLY:H	2:X:83:VAL:HG21	1.85	0.41
1:B:345:THR:CG2	3:P:112:ASP:HB2	2.51	0.41
1:B:605:SER:OG	1:B:606:ASN:N	2.53	0.41
1:A:193:VAL:HG23	1:A:223:LEU:HD21	2.03	0.41
1:A:964:LYS:HE2	1:A:964:LYS:HB2	1.81	0.41
1:A:1027:THR:O	1:A:1031:GLU:HG3	2.20	0.41
1:C:881:THR:HG22	1:C:888:PHE:HE2	1.85	0.41
2:O:43:GLN:HB3	2:O:90:VAL:HG12	2.03	0.41
3:H:122:GLN:H	3:H:122:GLN:CD	2.24	0.41
1:B:168:PHE:CE2	1:B:170:TYR:HB2	2.56	0.41
1:B:299:THR:O	1:B:303:LEU:HG	2.20	0.41
1:B:415:THR:OG1	1:B:416:GLY:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:PRO:HD3	1:A:894:LEU:HD13	2.03	0.41
1:B:1097:SER:HB3	1:B:1102:TRP:CE3	2.55	0.41
1:A:752:LEU:O	1:A:755:GLN:HG2	2.20	0.41
1:C:36:VAL:HG11	1:C:220:PHE:CZ	2.56	0.41
1:C:242:LEU:HG	1:C:243:ALA:H	1.85	0.41
1:C:398:ASP:OD2	1:C:423:TYR:OH	2.24	0.41
1:C:880:GLY:O	1:C:884:SER:OG	2.29	0.41
3:Y:167:VAL:HG12	3:Y:217:HIS:HA	2.02	0.41
3:Y:170:SER:OG	3:Y:214:ASN:HB2	2.21	0.41
3:H:36:TRP:HE1	3:H:79:LEU:HG	1.85	0.41
1:B:325:SER:O	1:B:326:ILE:HD13	2.21	0.41
1:A:428:ASP:OD1	1:A:428:ASP:N	2.53	0.41
1:C:138:ASP:HB3	1:C:140:PHE:HE1	1.84	0.41
1:C:816:SER:HB2	1:C:817:PRO:HD2	2.01	0.41
1:C:1101:HIS:HD2	4:C:1308:NAG:H5	1.85	0.41
1:B:436:TRP:CE2	1:B:509:ARG:HB2	2.57	0.40
1:A:977:LEU:O	1:A:981:LEU:HG	2.21	0.40
2:O:31:HIS:CG	2:O:32:SER:H	2.40	0.40
2:O:139:CYS:HB3	2:O:182:SER:HB3	2.03	0.40
2:X:145:TYR:CD1	2:X:178:TYR:HE1	2.40	0.40
2:X:150:LYS:O	2:X:201:VAL:HA	2.21	0.40
3:Y:138:VAL:HB	3:Y:226:LYS:HD2	2.03	0.40
3:Y:172:ASN:HA	3:Y:212:ILE:HG13	2.02	0.40
1:B:345:THR:HG23	3:P:112:ASP:H	1.85	0.40
1:B:1102:TRP:HB2	1:B:1135:ASN:ND2	2.37	0.40
1:A:564:GLN:O	1:A:577:ARG:HB3	2.21	0.40
1:C:643:PHE:CD2	1:C:650:LEU:HD21	2.55	0.40
2:O:141:LEU:HB3	2:O:144:PHE:CD2	2.56	0.40
3:P:38:ARG:N	3:P:46:GLU:O	2.54	0.40
3:Y:61:ALA:HB3	3:Y:64:VAL:HG12	2.04	0.40
1:B:189:LEU:HD22	1:B:217:PRO:HG2	2.02	0.40
1:A:559:PHE:HE2	1:A:565:PHE:HA	1.85	0.40
2:X:101:PHE:HE2	3:Y:115:TYR:HB3	1.86	0.40
2:X:144:PHE:HB2	2:X:149:ALA:CB	2.51	0.40
2:X:174:LYS:HG3	2:X:175:ASP:OD1	2.22	0.40
2:L:12:PRO:HB2	2:L:112:LYS:HB2	2.03	0.40
3:H:187:LEU:HD23	3:H:188:GLN:O	2.21	0.40
1:B:805:ILE:HB	1:B:1054:GLN:HE22	1.86	0.40
1:C:43:PHE:C	1:C:44:ARG:HD2	2.41	0.40
1:C:461:LEU:HB3	1:C:465:GLU:HB3	2.03	0.40
1:C:906:PHE:CD1	1:C:1049:LEU:HD11	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:962:LEU:HA	1:C:962:LEU:HD23	1.91	0.40
3:P:18:LEU:O	3:P:82:HIS:HA	2.22	0.40
3:P:38:ARG:NH1	3:P:40:ALA:HB2	2.37	0.40
3:P:98:LYS:HG3	3:P:118:ASP:OD1	2.20	0.40
3:P:160:LYS:HA	3:P:193:TYR:O	2.21	0.40
3:Y:64:VAL:HG21	3:Y:68:PHE:CE2	2.56	0.40
2:L:125:PRO:HD3	2:L:137:VAL:HG22	2.02	0.40
1:B:641:ASN:OD1	1:B:642:VAL:N	2.55	0.40
1:A:345:THR:C	1:A:346:ARG:HG3	2.41	0.40
1:A:735:SER:OG	1:A:859:THR:OG1	2.30	0.40
1:C:764:ASN:O	1:C:768:THR:HG23	2.22	0.40
2:O:113:ARG:HB2	2:O:145:TYR:CE2	2.56	0.40
3:P:153:ALA:O	3:P:200:THR:HA	2.22	0.40
3:Y:39:GLN:HB3	3:Y:93:LEU:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	953/1121 (85%)	871 (91%)	82 (9%)	0	100	100
1	B	986/1121 (88%)	896 (91%)	90 (9%)	0	100	100
1	C	986/1121 (88%)	891 (90%)	95 (10%)	0	100	100
2	L	216/218 (99%)	201 (93%)	15 (7%)	0	100	100
2	O	216/218 (99%)	206 (95%)	10 (5%)	0	100	100
2	X	216/218 (99%)	207 (96%)	9 (4%)	0	100	100
3	H	220/237 (93%)	207 (94%)	13 (6%)	0	100	100
3	P	220/237 (93%)	204 (93%)	16 (7%)	0	100	100
3	Y	220/237 (93%)	209 (95%)	11 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4233/4728 (90%)	3892 (92%)	341 (8%)	0	100 100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	833/975 (85%)	832 (100%)	1 (0%)	92 96
1	B	874/975 (90%)	873 (100%)	1 (0%)	92 96
1	C	878/975 (90%)	877 (100%)	1 (0%)	92 96
2	L	191/192 (100%)	191 (100%)	0	100 100
2	O	191/192 (100%)	191 (100%)	0	100 100
2	X	188/192 (98%)	188 (100%)	0	100 100
3	H	180/195 (92%)	180 (100%)	0	100 100
3	P	181/195 (93%)	180 (99%)	1 (1%)	84 90
3	Y	177/195 (91%)	176 (99%)	1 (1%)	84 90
All	All	3693/4086 (90%)	3688 (100%)	5 (0%)	92 96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	346	ARG
1	A	462	LYS
1	C	347	PHE
3	P	84	ARG
3	Y	84	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	422	ASN
1	B	474	GLN
1	B	928	ASN
1	A	343	ASN
1	A	439	ASN
1	A	506	GLN
1	A	580	GLN
2	L	129	GLN
3	H	82	HIS

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)

27 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	NAG	B	1308	1	14,14,15	1.98	4 (28%)	17,19,21	1.12	1 (5%)
4	NAG	A	1304	1	14,14,15	1.93	4 (28%)	17,19,21	1.36	2 (11%)
4	NAG	A	1307	1	14,14,15	1.92	4 (28%)	17,19,21	1.28	3 (17%)
4	NAG	C	1303	1	14,14,15	1.91	4 (28%)	17,19,21	1.08	2 (11%)
4	NAG	A	1303	1	14,14,15	1.84	3 (21%)	17,19,21	1.29	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	NAG	B	1304	1	14,14,15	1.97	4 (28%)	17,19,21	1.43	3 (17%)
4	NAG	B	1309	1	14,14,15	1.94	3 (21%)	17,19,21	1.31	3 (17%)
4	NAG	A	1309	1	14,14,15	1.90	4 (28%)	17,19,21	1.11	1 (5%)
4	NAG	B	1305	1	14,14,15	1.88	2 (14%)	17,19,21	1.36	4 (23%)
4	NAG	C	1307	1	14,14,15	1.86	2 (14%)	17,19,21	0.87	0
4	NAG	C	1302	1	14,14,15	1.78	3 (21%)	17,19,21	1.38	3 (17%)
4	NAG	C	1306	1	14,14,15	1.83	4 (28%)	17,19,21	1.45	2 (11%)
4	NAG	B	1303	1	14,14,15	1.81	3 (21%)	17,19,21	1.28	2 (11%)
4	NAG	A	1308	1	14,14,15	1.84	4 (28%)	17,19,21	1.25	2 (11%)
4	NAG	A	1302	1	14,14,15	1.89	3 (21%)	17,19,21	1.23	2 (11%)
4	NAG	B	1307	1	14,14,15	1.85	4 (28%)	17,19,21	1.30	4 (23%)
4	NAG	A	1305	1	14,14,15	1.94	4 (28%)	17,19,21	2.05	4 (23%)
4	NAG	C	1308	1	14,14,15	1.86	3 (21%)	17,19,21	1.26	3 (17%)
4	NAG	A	1306	1	14,14,15	1.97	4 (28%)	17,19,21	1.08	2 (11%)
4	NAG	B	1301	1	14,14,15	1.89	3 (21%)	17,19,21	0.83	0
4	NAG	C	1301	1	14,14,15	1.89	4 (28%)	17,19,21	1.11	1 (5%)
4	NAG	A	1301	1	14,14,15	2.03	4 (28%)	17,19,21	1.25	2 (11%)
4	NAG	B	1306	1	14,14,15	1.81	2 (14%)	17,19,21	1.22	1 (5%)
4	NAG	C	1304	1	14,14,15	1.80	4 (28%)	17,19,21	1.15	2 (11%)
4	NAG	C	1305	1	14,14,15	1.91	3 (21%)	17,19,21	1.25	3 (17%)
4	NAG	C	1309	1	14,14,15	1.71	3 (21%)	17,19,21	1.90	3 (17%)
4	NAG	B	1302	1	14,14,15	1.97	4 (28%)	17,19,21	1.34	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1308	1	-	3/6/23/26	0/1/1/1
4	NAG	A	1304	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1303	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	B	1309	1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	A	1309	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1302	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1302	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1305	1	-	3/6/23/26	0/1/1/1
4	NAG	C	1308	1	-	2/6/23/26	0/1/1/1
4	NAG	A	1306	1	-	3/6/23/26	0/1/1/1
4	NAG	B	1301	1	-	4/6/23/26	0/1/1/1
4	NAG	C	1301	1	-	4/6/23/26	0/1/1/1
4	NAG	A	1301	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1306	1	-	1/6/23/26	0/1/1/1
4	NAG	C	1304	1	-	0/6/23/26	0/1/1/1
4	NAG	C	1305	1	-	2/6/23/26	0/1/1/1
4	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
4	NAG	B	1302	1	-	0/6/23/26	0/1/1/1

All (93) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1301	NAG	O5-C1	4.75	1.51	1.43
4	B	1302	NAG	O5-C1	4.71	1.51	1.43
4	B	1309	NAG	O5-C1	4.66	1.51	1.43
4	A	1304	NAG	O5-C1	4.63	1.51	1.43
4	B	1305	NAG	O5-C1	4.63	1.51	1.43
4	B	1308	NAG	O5-C1	4.59	1.51	1.43
4	B	1304	NAG	O5-C1	4.51	1.50	1.43
4	C	1307	NAG	O5-C1	4.49	1.50	1.43
4	C	1301	NAG	O5-C1	4.45	1.50	1.43
4	A	1302	NAG	O5-C1	4.40	1.50	1.43
4	A	1307	NAG	O5-C1	4.39	1.50	1.43
4	C	1305	NAG	O5-C1	4.38	1.50	1.43
4	A	1308	NAG	O5-C1	4.35	1.50	1.43
4	A	1306	NAG	O5-C1	4.33	1.50	1.43
4	A	1305	NAG	O5-C1	4.32	1.50	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1301	NAG	O5-C1	4.31	1.50	1.43
4	C	1306	NAG	O5-C1	4.26	1.50	1.43
4	C	1303	NAG	O5-C1	4.21	1.50	1.43
4	C	1308	NAG	O5-C1	4.20	1.50	1.43
4	A	1303	NAG	O5-C1	4.20	1.50	1.43
4	B	1303	NAG	O5-C1	4.19	1.50	1.43
4	A	1309	NAG	O5-C1	4.19	1.50	1.43
4	B	1307	NAG	O5-C1	4.10	1.50	1.43
4	B	1306	NAG	O5-C1	4.09	1.50	1.43
4	C	1304	NAG	O5-C1	4.07	1.50	1.43
4	C	1302	NAG	O5-C1	3.92	1.50	1.43
4	C	1309	NAG	O5-C1	3.79	1.49	1.43
4	A	1305	NAG	C7-N2	3.58	1.46	1.34
4	A	1306	NAG	C7-N2	3.53	1.46	1.34
4	A	1309	NAG	C7-N2	3.44	1.46	1.34
4	A	1301	NAG	C7-N2	3.43	1.46	1.34
4	C	1303	NAG	C7-N2	3.38	1.46	1.34
4	B	1308	NAG	C7-N2	3.36	1.45	1.34
4	B	1301	NAG	C7-N2	3.33	1.45	1.34
4	A	1302	NAG	C7-N2	3.33	1.45	1.34
4	B	1302	NAG	C7-N2	3.30	1.45	1.34
4	A	1307	NAG	C7-N2	3.29	1.45	1.34
4	C	1309	NAG	C7-N2	3.28	1.45	1.34
4	C	1302	NAG	C7-N2	3.28	1.45	1.34
4	B	1307	NAG	C7-N2	3.26	1.45	1.34
4	B	1306	NAG	C7-N2	3.26	1.45	1.34
4	C	1301	NAG	C7-N2	3.25	1.45	1.34
4	C	1308	NAG	C7-N2	3.22	1.45	1.34
4	A	1303	NAG	C7-N2	3.21	1.45	1.34
4	C	1305	NAG	C7-N2	3.20	1.45	1.34
4	B	1309	NAG	C7-N2	3.20	1.45	1.34
4	A	1304	NAG	C7-N2	3.19	1.45	1.34
4	A	1308	NAG	C7-N2	3.17	1.45	1.34
4	B	1304	NAG	C7-N2	3.17	1.45	1.34
4	C	1307	NAG	C7-N2	3.14	1.45	1.34
4	C	1304	NAG	C7-N2	3.11	1.45	1.34
4	B	1303	NAG	C7-N2	3.04	1.44	1.34
4	C	1306	NAG	C7-N2	3.03	1.44	1.34
4	B	1305	NAG	C7-N2	3.02	1.44	1.34
4	A	1306	NAG	C2-N2	2.63	1.50	1.46
4	A	1305	NAG	C2-N2	2.59	1.50	1.46
4	B	1304	NAG	O5-C5	2.51	1.48	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1301	NAG	C2-N2	2.50	1.50	1.46
4	B	1308	NAG	O5-C5	2.45	1.48	1.43
4	C	1303	NAG	C2-N2	2.41	1.50	1.46
4	B	1304	NAG	C3-C2	-2.38	1.47	1.52
4	A	1309	NAG	C2-N2	2.38	1.50	1.46
4	B	1302	NAG	O5-C5	2.38	1.48	1.43
4	B	1301	NAG	C2-N2	2.34	1.50	1.46
4	A	1304	NAG	O5-C5	2.28	1.48	1.43
4	A	1307	NAG	C3-C2	-2.25	1.47	1.52
4	B	1308	NAG	C2-N2	2.23	1.50	1.46
4	C	1305	NAG	C3-C2	-2.21	1.47	1.52
4	C	1303	NAG	O5-C5	2.17	1.47	1.43
4	C	1306	NAG	O5-C5	2.16	1.47	1.43
4	A	1309	NAG	O5-C5	2.12	1.47	1.43
4	A	1303	NAG	O5-C5	2.12	1.47	1.43
4	B	1309	NAG	O5-C5	2.11	1.47	1.43
4	A	1301	NAG	O5-C5	2.11	1.47	1.43
4	C	1308	NAG	O5-C5	2.10	1.47	1.43
4	C	1309	NAG	C2-N2	2.10	1.49	1.46
4	A	1307	NAG	C2-N2	2.09	1.49	1.46
4	C	1301	NAG	C2-N2	2.09	1.49	1.46
4	A	1308	NAG	C2-N2	2.09	1.49	1.46
4	B	1307	NAG	O5-C5	2.07	1.47	1.43
4	A	1302	NAG	C2-N2	2.06	1.49	1.46
4	A	1305	NAG	O7-C7	-2.06	1.18	1.23
4	A	1304	NAG	C2-N2	2.04	1.49	1.46
4	B	1302	NAG	C2-N2	2.04	1.49	1.46
4	B	1307	NAG	C3-C2	-2.04	1.48	1.52
4	A	1308	NAG	O7-C7	-2.03	1.18	1.23
4	C	1306	NAG	O7-C7	-2.03	1.18	1.23
4	B	1303	NAG	O7-C7	-2.03	1.18	1.23
4	C	1304	NAG	O5-C5	2.02	1.47	1.43
4	C	1302	NAG	C2-N2	2.01	1.49	1.46
4	C	1301	NAG	O7-C7	-2.01	1.18	1.23
4	A	1306	NAG	O5-C5	2.01	1.47	1.43
4	C	1304	NAG	C3-C2	-2.00	1.48	1.52

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1309	NAG	C4-C3-C2	5.63	119.27	111.02
4	A	1305	NAG	C8-C7-N2	5.33	125.12	116.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1306	NAG	C2-N2-C7	-4.05	117.14	122.90
4	A	1305	NAG	C2-N2-C7	3.55	127.96	122.90
4	B	1304	NAG	C2-N2-C7	-3.18	118.38	122.90
4	C	1302	NAG	C1-O5-C5	-3.05	108.06	112.19
4	B	1303	NAG	C2-N2-C7	-2.89	118.79	122.90
4	B	1305	NAG	C2-N2-C7	-2.82	118.89	122.90
4	B	1302	NAG	C2-N2-C7	-2.79	118.93	122.90
4	C	1305	NAG	C2-N2-C7	-2.79	118.93	122.90
4	C	1309	NAG	C3-C4-C5	2.75	115.14	110.24
4	C	1308	NAG	C2-N2-C7	-2.64	119.15	122.90
4	B	1307	NAG	C2-N2-C7	-2.62	119.17	122.90
4	B	1309	NAG	C8-C7-N2	2.61	120.51	116.10
4	C	1301	NAG	C8-C7-N2	2.61	120.51	116.10
4	A	1305	NAG	O7-C7-N2	-2.58	117.22	121.95
4	B	1304	NAG	C8-C7-N2	2.57	120.45	116.10
4	A	1308	NAG	C4-C3-C2	2.57	114.78	111.02
4	C	1308	NAG	C8-C7-N2	2.55	120.42	116.10
4	A	1307	NAG	C8-C7-N2	2.54	120.40	116.10
4	B	1302	NAG	C8-C7-N2	2.53	120.38	116.10
4	B	1309	NAG	C1-O5-C5	2.51	115.60	112.19
4	A	1301	NAG	O5-C1-C2	2.42	115.11	111.29
4	A	1302	NAG	C8-C7-N2	2.40	120.17	116.10
4	C	1306	NAG	C8-C7-N2	2.40	120.17	116.10
4	A	1302	NAG	C2-N2-C7	-2.39	119.51	122.90
4	B	1307	NAG	C6-C5-C4	-2.37	107.45	113.00
4	C	1305	NAG	C8-C7-N2	2.36	120.10	116.10
4	A	1305	NAG	O7-C7-C8	-2.36	117.67	122.06
4	B	1303	NAG	C8-C7-N2	2.36	120.09	116.10
4	A	1301	NAG	C1-O5-C5	2.35	115.37	112.19
4	B	1304	NAG	C4-C3-C2	-2.30	107.64	111.02
4	B	1307	NAG	C8-C7-N2	2.29	119.98	116.10
4	A	1308	NAG	C8-C7-N2	2.28	119.96	116.10
4	C	1308	NAG	C6-C5-C4	-2.27	107.69	113.00
4	C	1304	NAG	C2-N2-C7	-2.26	119.68	122.90
4	C	1302	NAG	C3-C4-C5	2.25	114.26	110.24
4	C	1302	NAG	C8-C7-N2	2.24	119.89	116.10
4	B	1305	NAG	C6-C5-C4	-2.23	107.79	113.00
4	A	1307	NAG	C2-N2-C7	-2.23	119.73	122.90
4	A	1304	NAG	C8-C7-N2	2.20	119.83	116.10
4	B	1308	NAG	O5-C5-C6	2.20	110.66	107.20
4	A	1307	NAG	C6-C5-C4	-2.18	107.90	113.00
4	B	1305	NAG	C1-O5-C5	2.16	115.12	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1306	NAG	C1-C2-N2	-2.16	106.80	110.49
4	B	1309	NAG	C2-N2-C7	-2.16	119.83	122.90
4	A	1303	NAG	C8-C7-N2	2.15	119.74	116.10
4	C	1303	NAG	C3-C4-C5	2.13	114.04	110.24
4	A	1304	NAG	C1-O5-C5	2.11	115.05	112.19
4	C	1305	NAG	C6-C5-C4	-2.10	108.10	113.00
4	A	1303	NAG	C3-C4-C5	2.09	113.97	110.24
4	C	1304	NAG	C1-C2-N2	-2.08	106.94	110.49
4	C	1309	NAG	C8-C7-N2	2.08	119.61	116.10
4	B	1305	NAG	C8-C7-N2	2.07	119.61	116.10
4	A	1309	NAG	C6-C5-C4	-2.06	108.17	113.00
4	B	1307	NAG	C1-O5-C5	2.05	114.97	112.19
4	A	1306	NAG	C2-N2-C7	2.04	125.81	122.90
4	C	1303	NAG	C6-C5-C4	-2.04	108.24	113.00
4	B	1302	NAG	C1-O5-C5	2.03	114.94	112.19
4	A	1306	NAG	O7-C7-C8	-2.03	118.29	122.06

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1308	NAG	O5-C5-C6-O6
4	C	1305	NAG	C4-C5-C6-O6
4	C	1309	NAG	O5-C5-C6-O6
4	C	1301	NAG	O5-C5-C6-O6
4	B	1305	NAG	C4-C5-C6-O6
4	A	1302	NAG	O5-C5-C6-O6
4	A	1306	NAG	O5-C5-C6-O6
4	A	1307	NAG	O5-C5-C6-O6
4	A	1308	NAG	C4-C5-C6-O6
4	C	1309	NAG	C4-C5-C6-O6
4	A	1307	NAG	C4-C5-C6-O6
4	C	1301	NAG	C4-C5-C6-O6
4	C	1303	NAG	C4-C5-C6-O6
4	C	1305	NAG	O5-C5-C6-O6
4	B	1305	NAG	O5-C5-C6-O6
4	C	1303	NAG	O5-C5-C6-O6
4	C	1302	NAG	C1-C2-N2-C7
4	B	1301	NAG	O5-C5-C6-O6
4	B	1307	NAG	O5-C5-C6-O6
4	C	1307	NAG	O5-C5-C6-O6
4	B	1307	NAG	C4-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	A	1305	NAG	C8-C7-N2-C2
4	A	1305	NAG	O7-C7-N2-C2
4	C	1301	NAG	C8-C7-N2-C2
4	C	1301	NAG	O7-C7-N2-C2
4	B	1309	NAG	C4-C5-C6-O6
4	A	1302	NAG	C4-C5-C6-O6
4	C	1302	NAG	O5-C5-C6-O6
4	A	1306	NAG	C1-C2-N2-C7
4	A	1304	NAG	O5-C5-C6-O6
4	B	1301	NAG	C4-C5-C6-O6
4	C	1306	NAG	C4-C5-C6-O6
4	C	1307	NAG	C4-C5-C6-O6
4	A	1303	NAG	O5-C5-C6-O6
4	B	1309	NAG	O5-C5-C6-O6
4	B	1308	NAG	C4-C5-C6-O6
4	A	1306	NAG	C4-C5-C6-O6
4	C	1302	NAG	C4-C5-C6-O6
4	A	1301	NAG	O5-C5-C6-O6
4	C	1306	NAG	O5-C5-C6-O6
4	C	1308	NAG	C4-C5-C6-O6
4	B	1306	NAG	O5-C5-C6-O6
4	A	1304	NAG	C4-C5-C6-O6
4	B	1308	NAG	O5-C5-C6-O6
4	C	1308	NAG	O5-C5-C6-O6
4	B	1308	NAG	C3-C2-N2-C7
4	A	1305	NAG	C3-C2-N2-C7
4	A	1309	NAG	C3-C2-N2-C7
4	B	1303	NAG	C4-C5-C6-O6
4	B	1303	NAG	O5-C5-C6-O6
4	A	1303	NAG	C4-C5-C6-O6
4	B	1301	NAG	C1-C2-N2-C7
4	B	1301	NAG	C3-C2-N2-C7
4	A	1301	NAG	C3-C2-N2-C7
4	C	1302	NAG	C3-C2-N2-C7
4	C	1303	NAG	C3-C2-N2-C7
4	C	1303	NAG	C1-C2-N2-C7

There are no ring outliers.

7 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1308	NAG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1307	NAG	1	0
4	A	1303	NAG	1	0
4	B	1309	NAG	1	0
4	C	1302	NAG	1	0
4	C	1308	NAG	1	0
4	A	1301	NAG	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

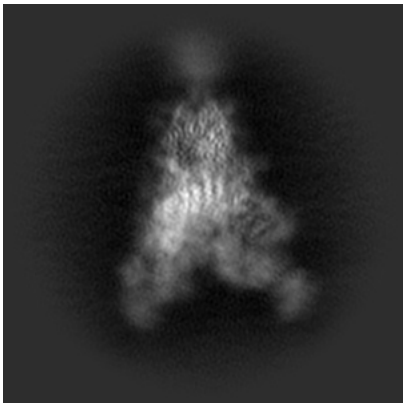
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-31033. These allow visual inspection of the internal detail of the map and identification of artifacts.

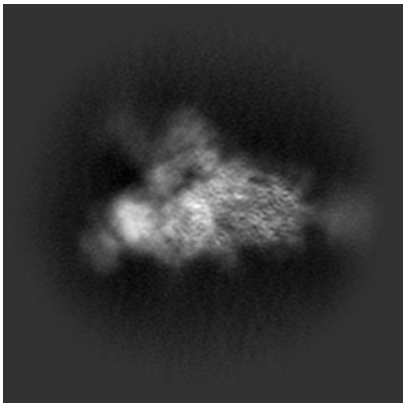
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

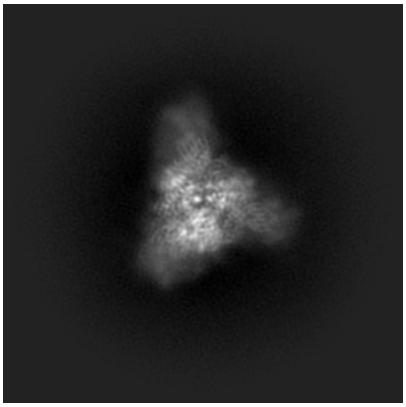
6.1.1 Primary map



X



Y

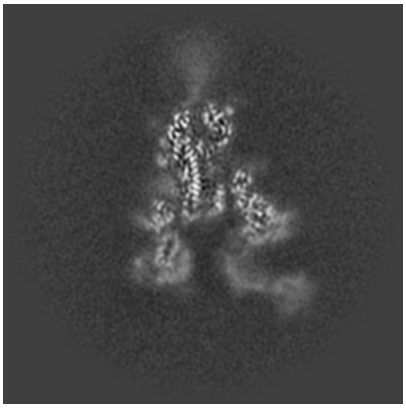


Z

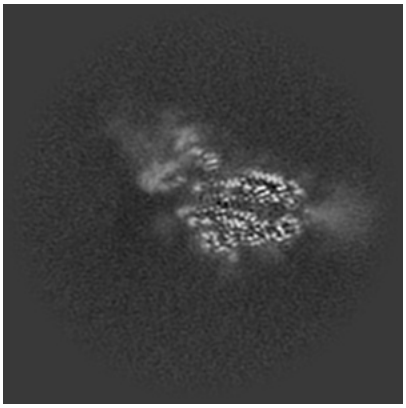
The images above show the map projected in three orthogonal directions.

6.2 Central slices

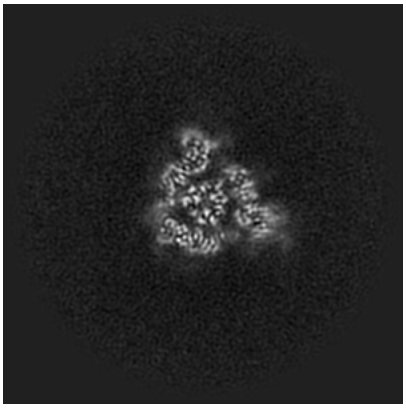
6.2.1 Primary map



X Index: 165



Y Index: 165

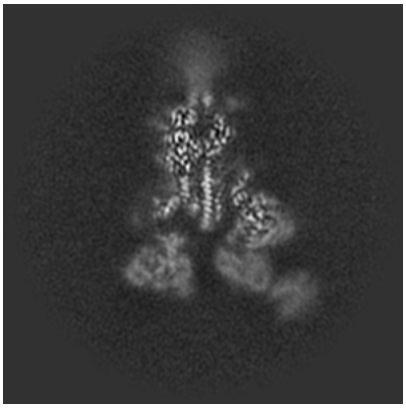


Z Index: 165

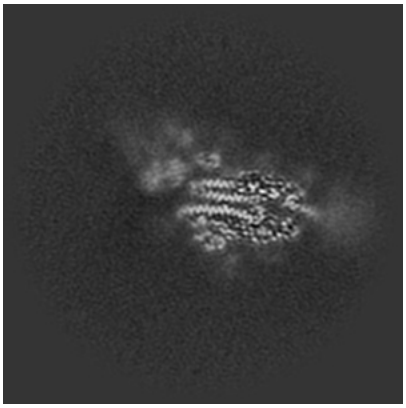
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

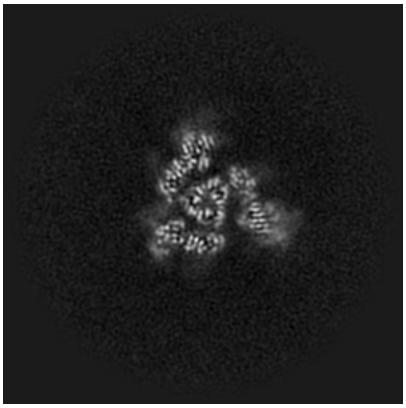
6.3.1 Primary map



X Index: 159



Y Index: 168

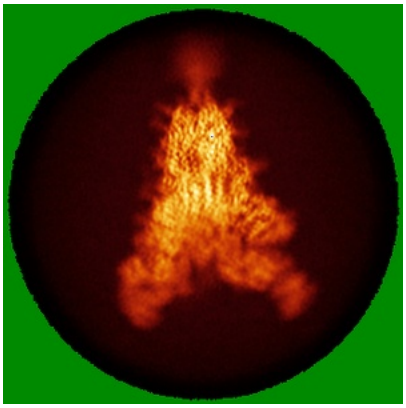


Z Index: 160

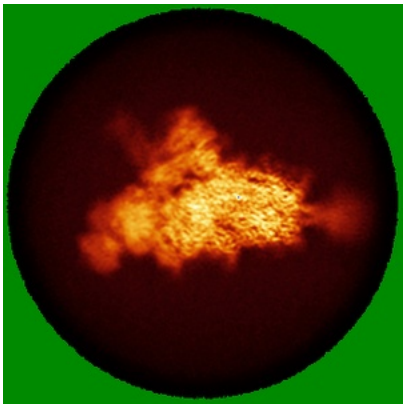
The images above show the largest variance slices of the map in three orthogonal directions.

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

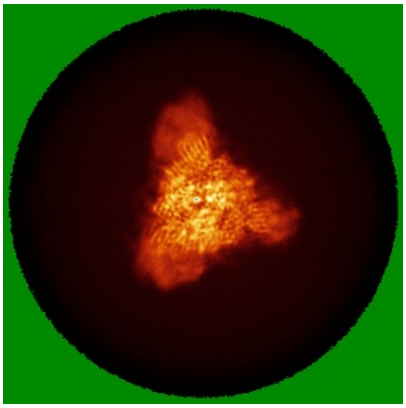
6.4.1 Primary map



X



Y

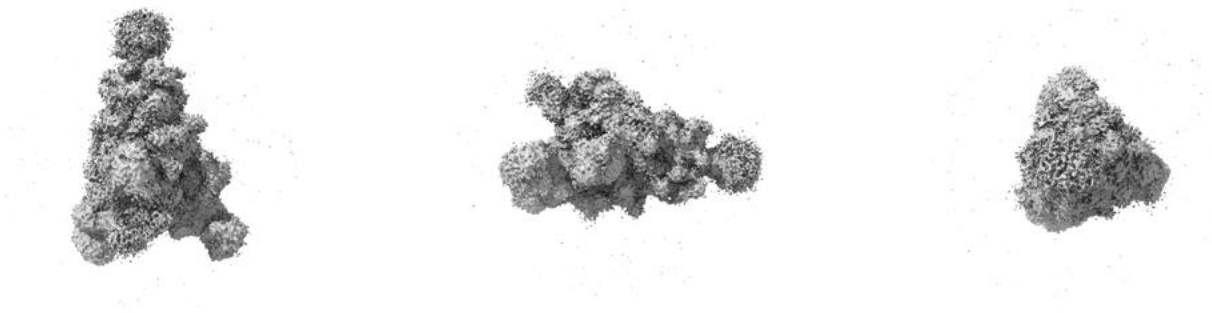


Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.08. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

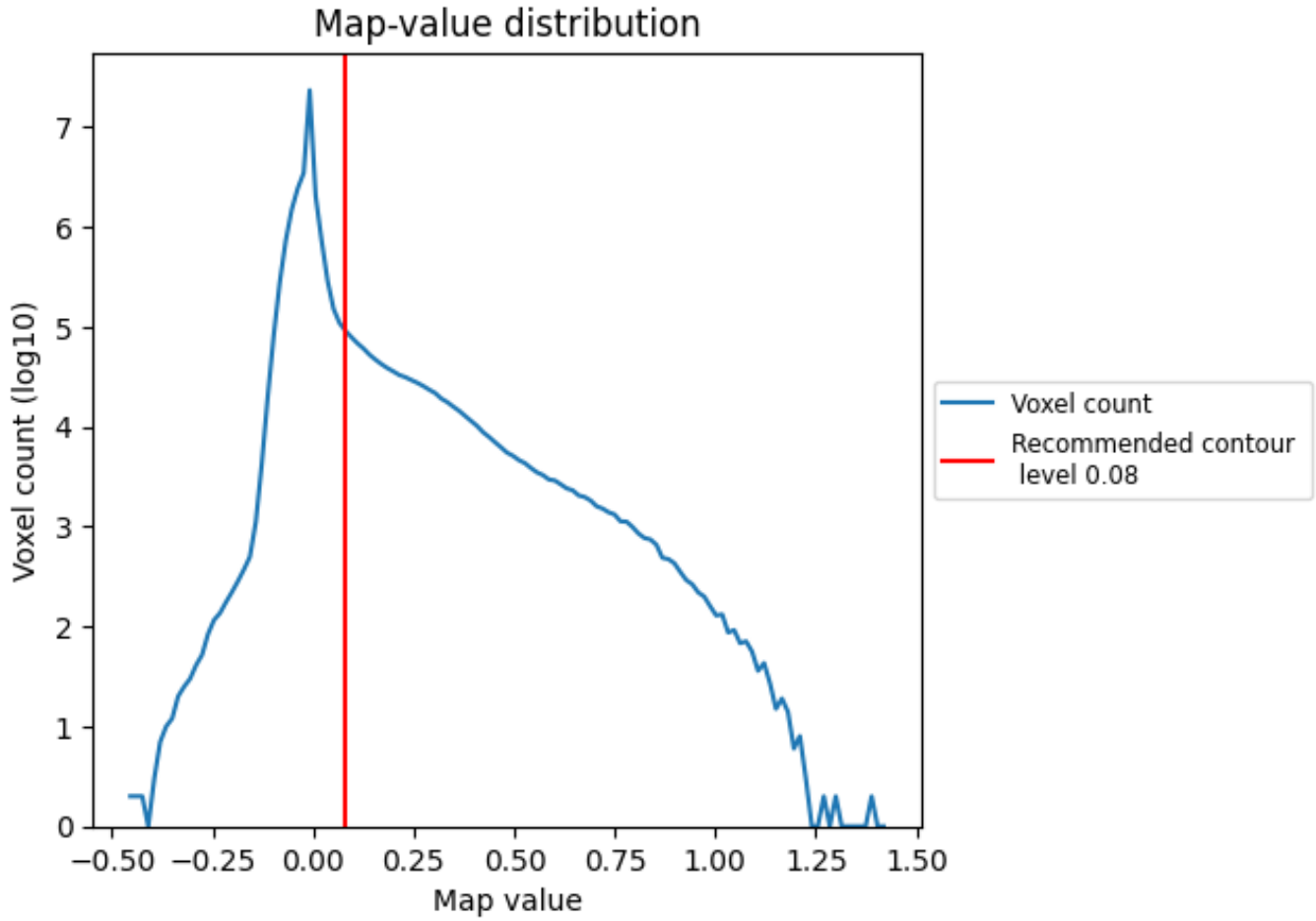
6.6 Mask visualisation (i)

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

7 Map analysis

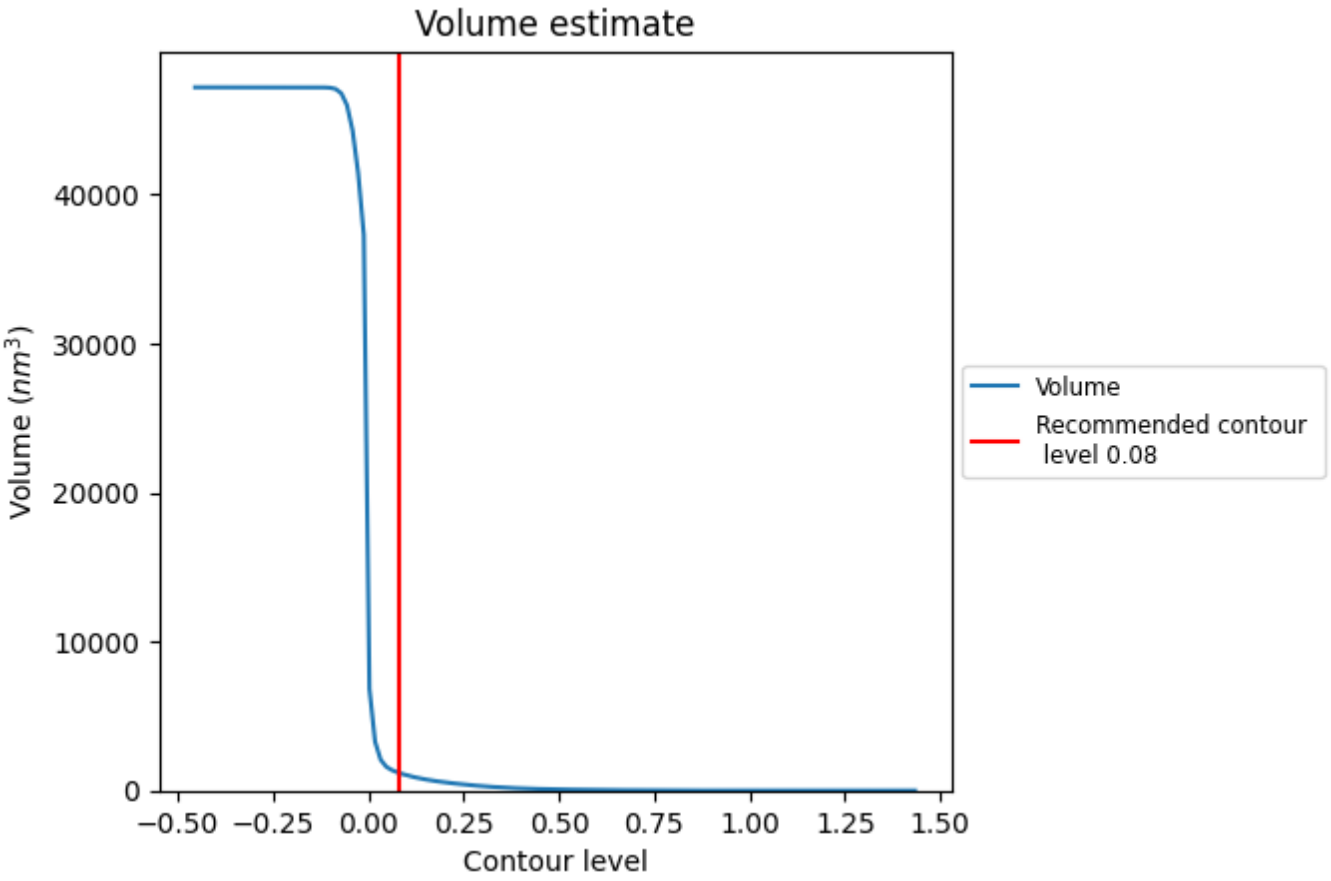
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

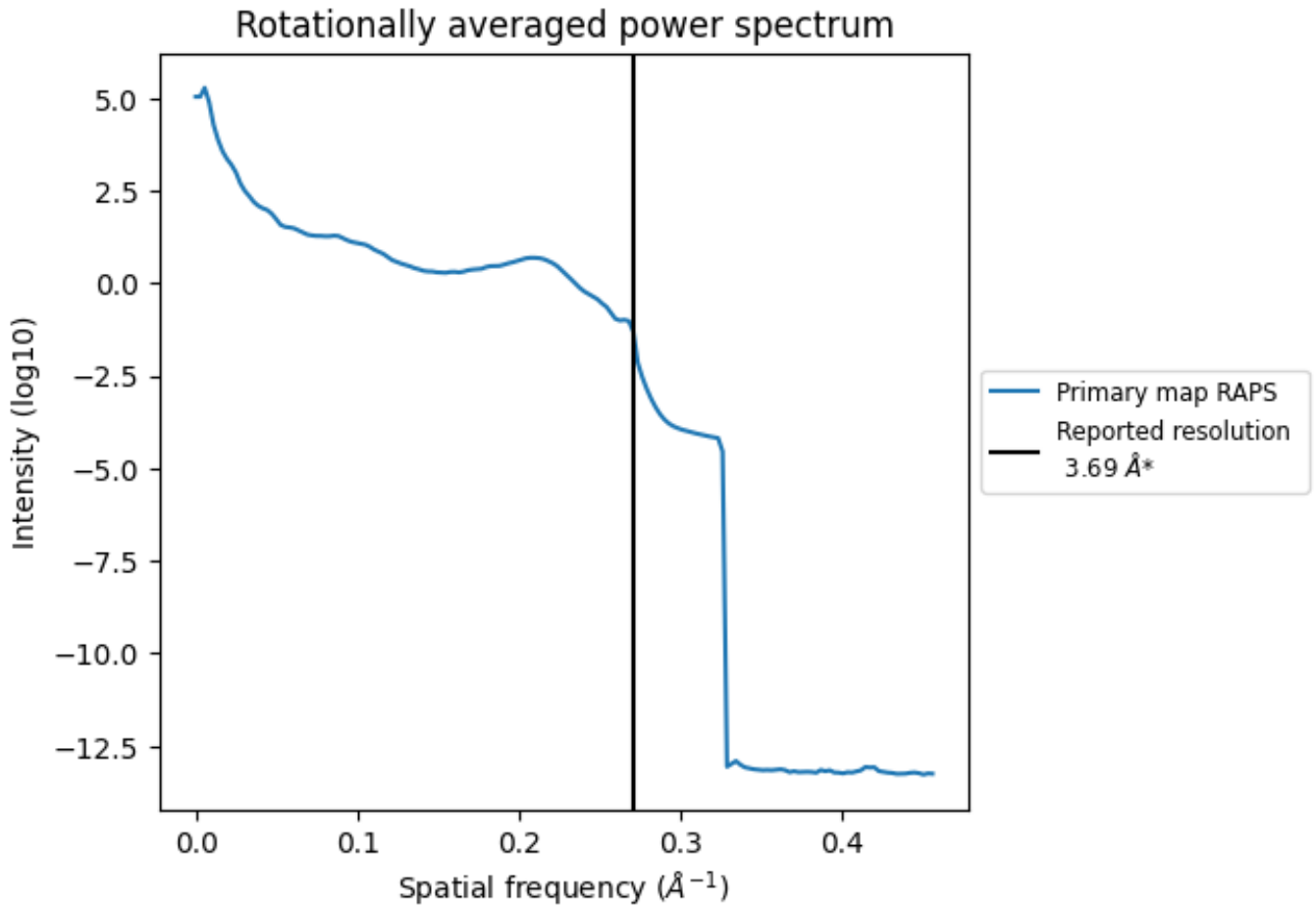
7.2 Volume estimate



The volume at the recommended contour level is 1192 nm^3; this corresponds to an approximate mass of 1077 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.271 $Å^{-1}$

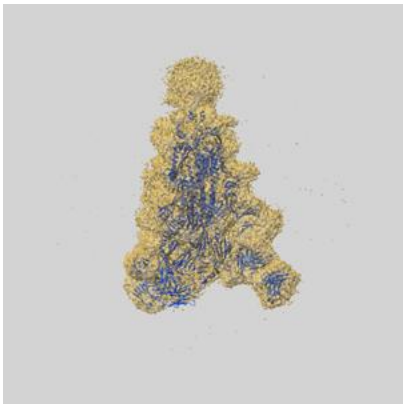
8 Fourier-Shell correlation (i)

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

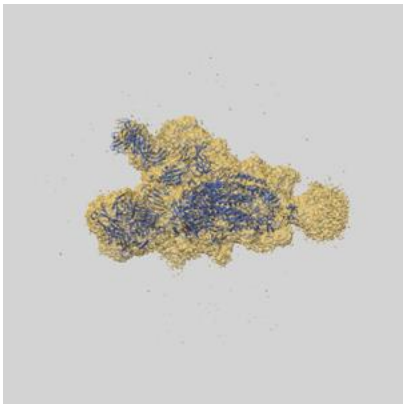
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-31033 and PDB model 7E9N. Per-residue inclusion information can be found in section 3 on page 8.

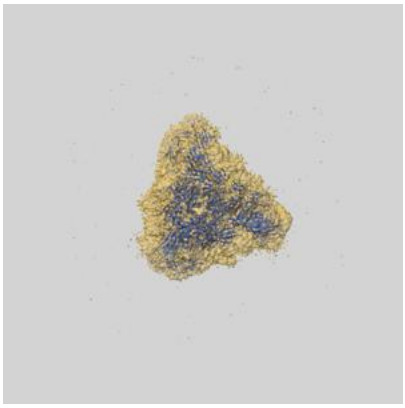
9.1 Map-model overlay



X



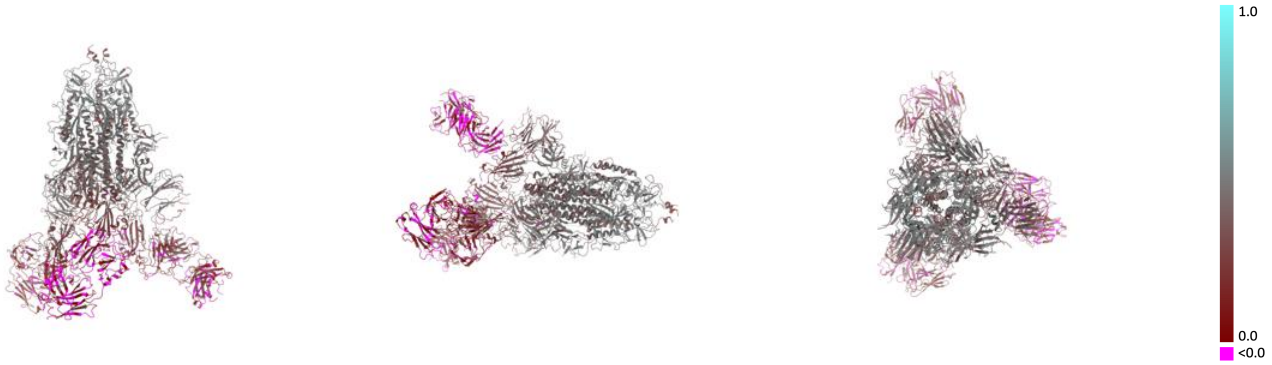
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.08 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.

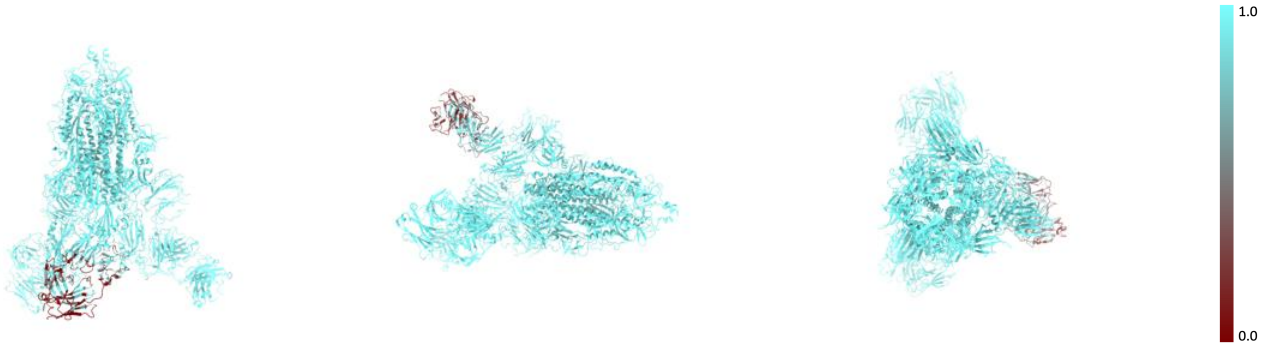
9.2 Q-score mapped to coordinate model



X Y Z

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

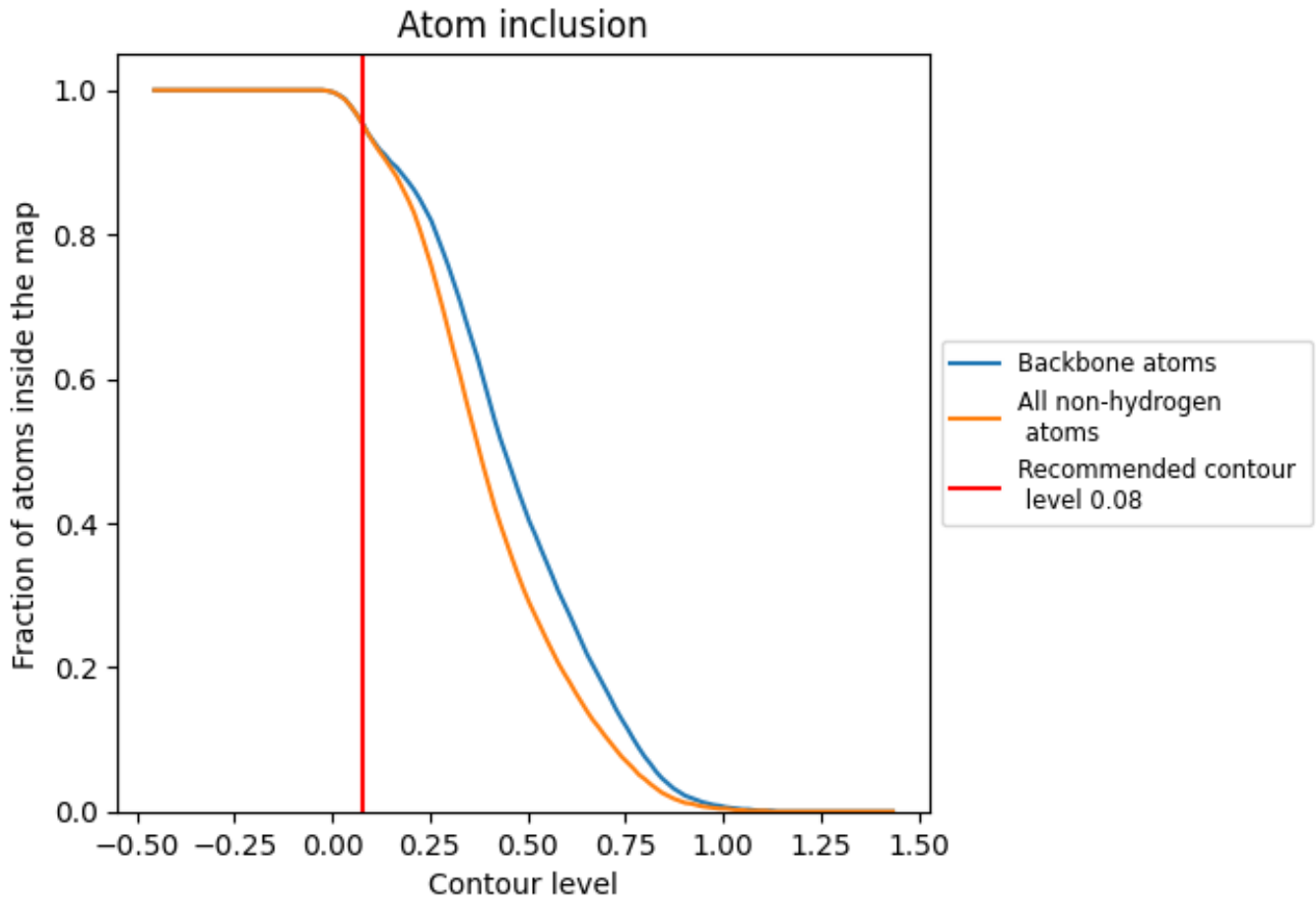
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.08).

9.4 Atom inclusion (i)



At the recommended contour level, 95% of all backbone atoms, 95% 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 (0.08) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9510	0.3100
A	0.9990	0.4020
B	0.9990	0.3900
C	0.9990	0.3830
H	0.6140	0.0190
L	0.4410	0.0440
O	0.9930	0.1240
P	0.9930	0.1540
X	0.9950	0.1650
Y	0.9980	0.2000