



Full wwPDB EM Validation Report ⓘ

Nov 28, 2022 – 04:16 PM JST

PDB ID : 7VHN
EMDB ID : EMD-32000
Title : Spike of SARS-CoV-2 spike protein(1 up)
Authors : Wang, X.
Deposited on : 2021-09-22
Resolution : 3.80 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.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.3

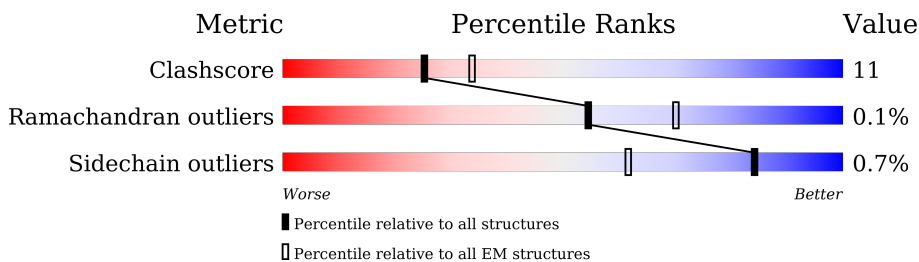
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	A	1135	
1	B	1135	
1	C	1135	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	1206	-	-	X	-
2	NAG	A	1211	X	-	-	-

2 Entry composition i

There are 2 unique types of molecules in this entry. The entry contains 25403 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.

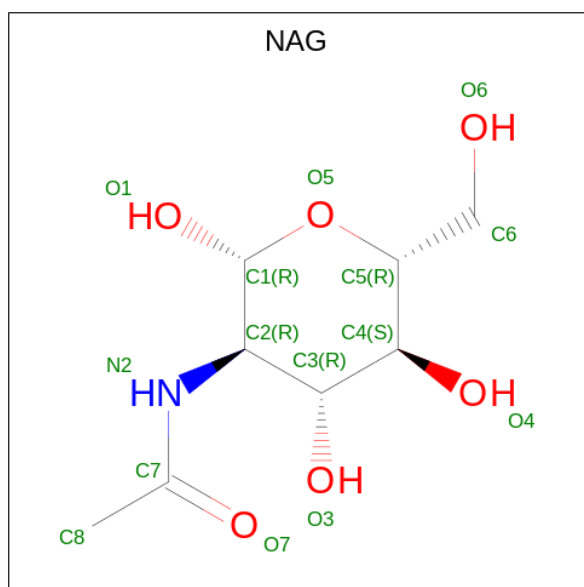
- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1064	8323	5316	1388	1580	39	0	0
1	B	1064	8323	5316	1388	1580	39	0	0
1	C	1064	8323	5316	1388	1580	39	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	501	TYR	ASN	variant	UNP P0DTC2
A	570	ASP	ALA	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	716	ILE	THR	variant	UNP P0DTC2
A	859	ASN	THR	variant	UNP P0DTC2
A	982	ALA	SER	variant	UNP P0DTC2
A	1118	HIS	ASP	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	570	ASP	ALA	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	716	ILE	THR	variant	UNP P0DTC2
B	859	ASN	THR	variant	UNP P0DTC2
B	982	ALA	SER	variant	UNP P0DTC2
B	1118	HIS	ASP	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	570	ASP	ALA	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	716	ILE	THR	variant	UNP P0DTC2
C	859	ASN	THR	variant	UNP P0DTC2
C	982	ALA	SER	variant	UNP P0DTC2
C	1118	HIS	ASP	variant	UNP P0DTC2

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



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
2	A	1	154	88	11	55	0
2	A	1	154	88	11	55	0
2	A	1	154	88	11	55	0
2	A	1	154	88	11	55	0
2	A	1	154	88	11	55	0
2	A	1	154	88	11	55	0
2	A	1	154	88	11	55	0
2	A	1	154	88	11	55	0
2	A	1	154	88	11	55	0
2	A	1	154	88	11	55	0
2	A	1	154	88	11	55	0
2	B	1	140	80	10	50	0
2	B	1	140	80	10	50	0
2	B	1	140	80	10	50	0

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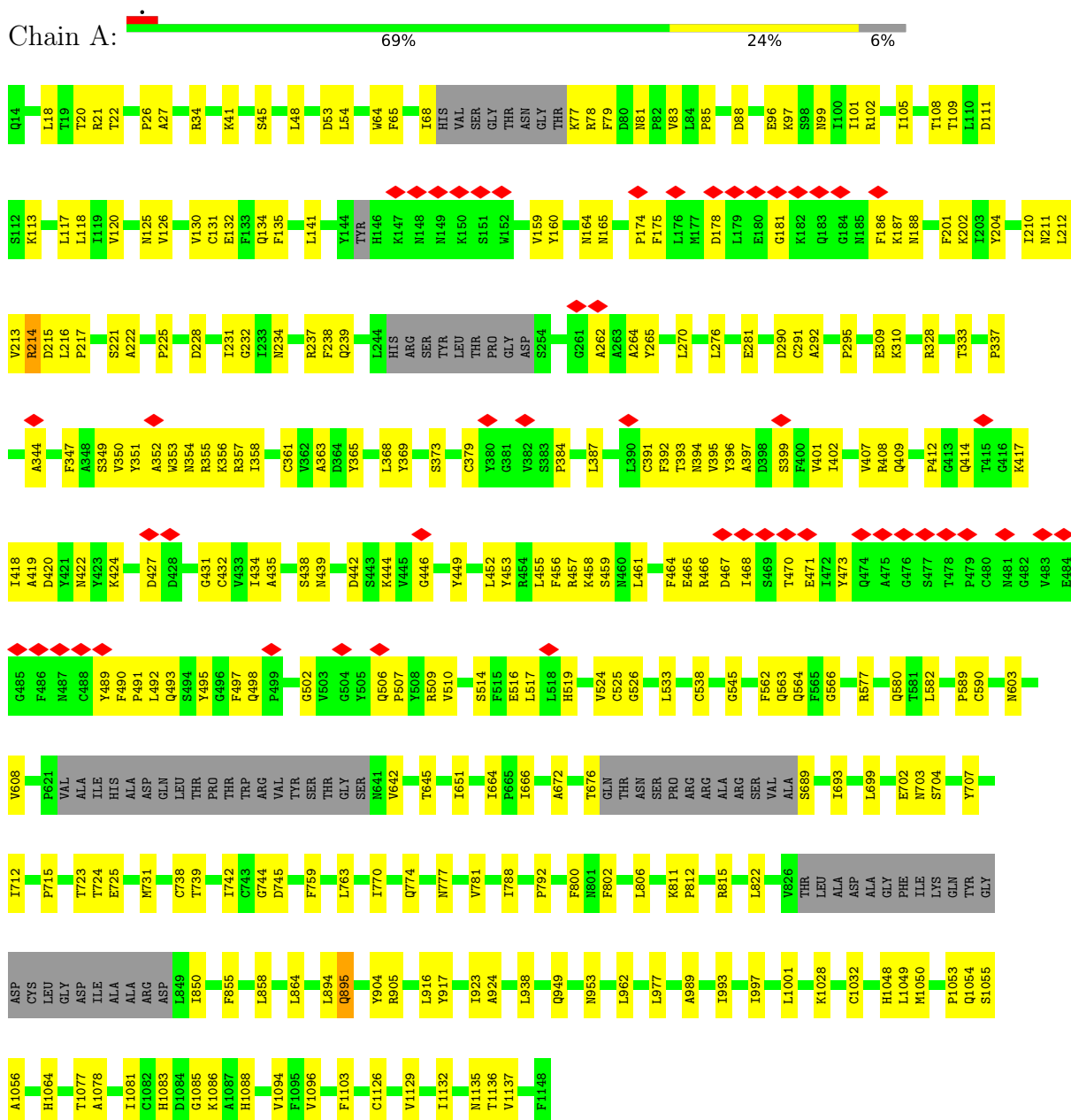
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Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
2	B	1	Total 140	C 80	N 10	O 50	0
2	B	1	Total 140	C 80	N 10	O 50	0
2	B	1	Total 140	C 80	N 10	O 50	0
2	B	1	Total 140	C 80	N 10	O 50	0
2	B	1	Total 140	C 80	N 10	O 50	0
2	B	1	Total 140	C 80	N 10	O 50	0
2	B	1	Total 140	C 80	N 10	O 50	0
2	C	1	Total 140	C 80	N 10	O 50	0
2	C	1	Total 140	C 80	N 10	O 50	0
2	C	1	Total 140	C 80	N 10	O 50	0
2	C	1	Total 140	C 80	N 10	O 50	0
2	C	1	Total 140	C 80	N 10	O 50	0
2	C	1	Total 140	C 80	N 10	O 50	0
2	C	1	Total 140	C 80	N 10	O 50	0
2	C	1	Total 140	C 80	N 10	O 50	0
2	C	1	Total 140	C 80	N 10	O 50	0
2	C	1	Total 140	C 80	N 10	O 50	0

3 Residue-property plots

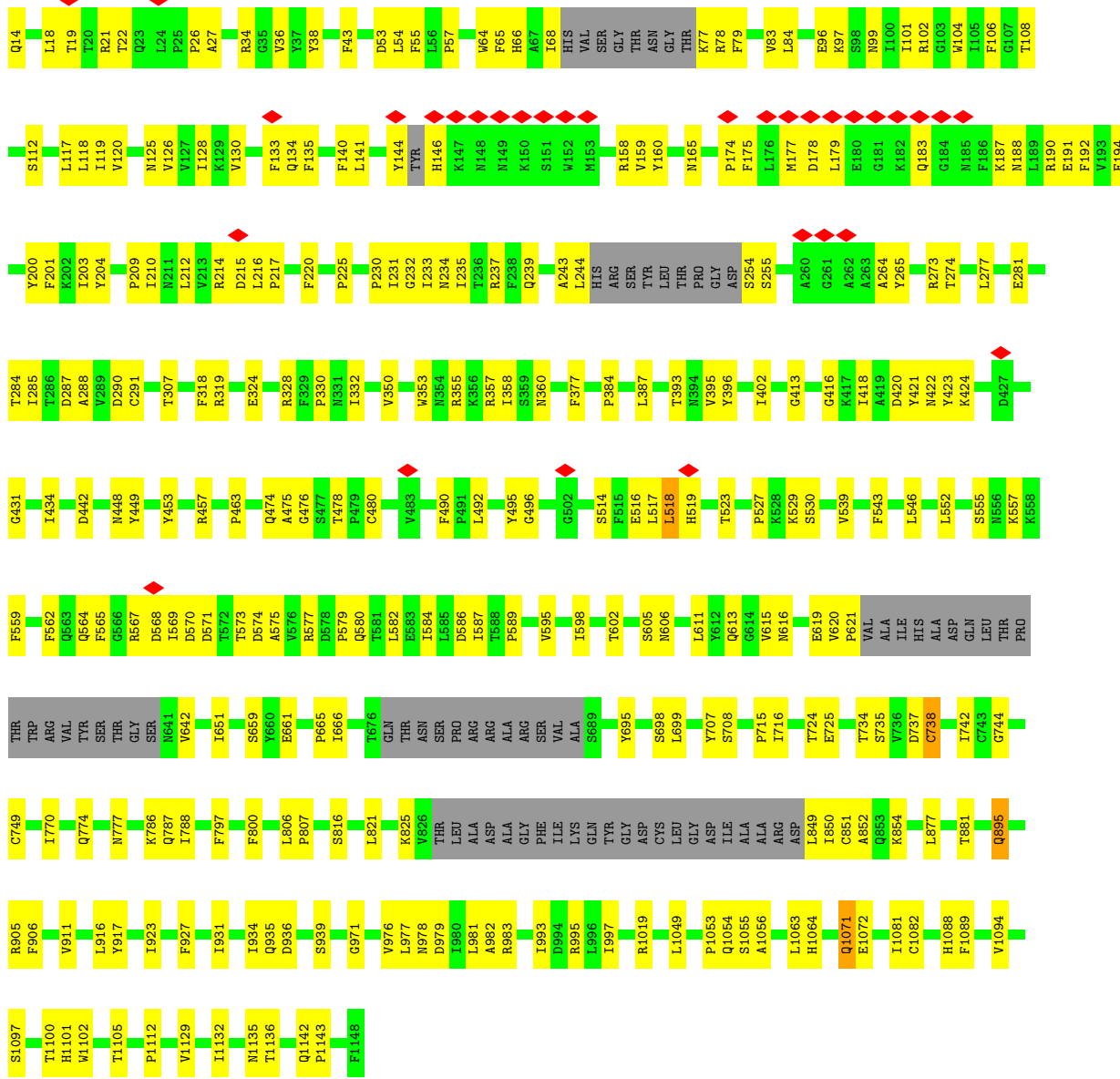
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Spike glycoprotein



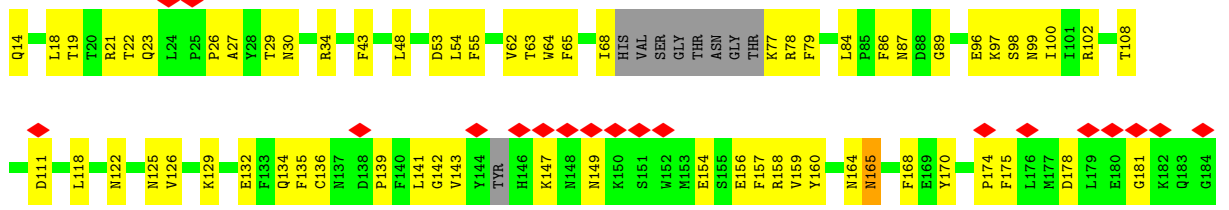
• Molecule 1: Spike glycoprotein

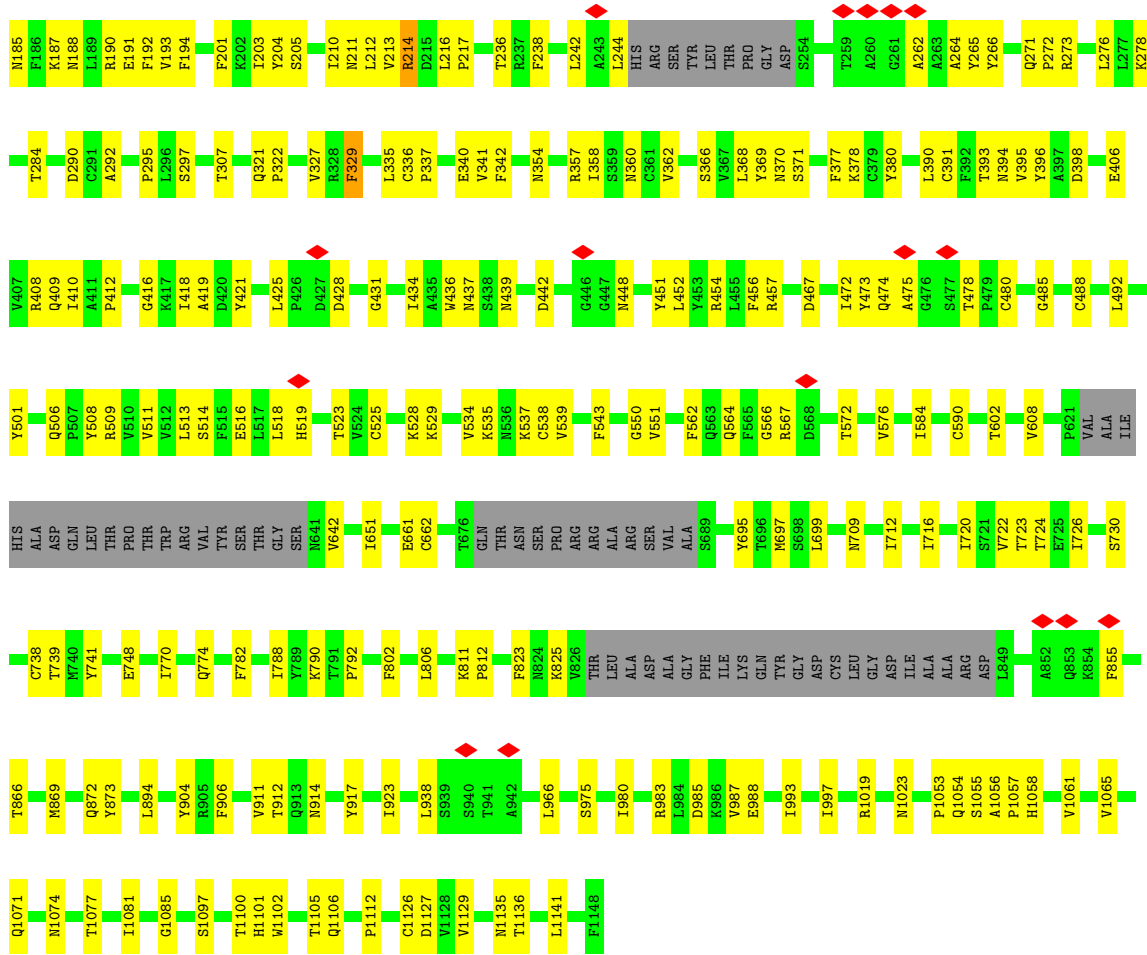
Chain B:  69% 25% 6%



• Molecule 1: Spike glycoprotein

Chain C:  69% 24% 6%





4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	56270	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.875	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	0.084	Depositor
Minimum map value	-0.042	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.01	Depositor
Map size (\AA)	342.40002, 342.40002, 342.40002	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.07, 1.07, 1.07	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.35	0/8513	0.50	0/11578
1	B	0.35	0/8513	0.51	1/11578 (0.0%)
1	C	0.35	0/8513	0.51	0/11578
All	All	0.35	0/25539	0.51	1/34734 (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
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	518	LEU	CA-CB-CG	5.03	126.88	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	738	CYS	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8323	0	8120	208	0
1	B	8323	0	8122	197	0
1	C	8323	0	8122	198	0
2	A	154	0	143	10	0
2	B	140	0	130	3	0
2	C	140	0	130	5	0
All	All	25403	0	24767	576	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 11.

All (576) 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)
1:A:603:ASN:ND2	2:A:1206:NAG:H82	1.72	1.05
2:B:1204:NAG:H3	2:B:1204:NAG:H82	1.48	0.94
1:A:391:CYS:HA	1:A:525:CYS:HB3	1.51	0.93
1:B:318:PHE:HZ	1:B:615:VAL:HG21	1.33	0.92
1:A:603:ASN:ND2	2:A:1206:NAG:C8	2.35	0.89
1:A:603:ASN:HD22	2:A:1206:NAG:H82	1.38	0.87
2:B:1204:NAG:H3	2:B:1204:NAG:C8	2.05	0.85
1:A:125:ASN:HB3	1:A:174:PRO:HA	1.58	0.85
1:C:391:CYS:HA	1:C:525:CYS:HB3	1.59	0.83
1:C:102:ARG:HD2	1:C:141:LEU:HG	1.61	0.83
1:C:1081:ILE:HD11	1:C:1135:ASN:HB3	1.60	0.80
1:B:474:GLN:HB2	1:B:480:CYS:HB2	1.66	0.77
1:C:442:ASP:O	1:C:448:ASN:ND2	2.17	0.76
1:C:661:GLU:O	1:C:695:TYR:OH	2.03	0.75
1:A:109:THR:HG21	1:A:113:LYS:HB2	1.68	0.74
1:A:603:ASN:CG	2:A:1206:NAG:H83	2.07	0.74
1:B:204:TYR:HD1	1:B:225:PRO:HA	1.53	0.74
1:C:125:ASN:HB3	1:C:174:PRO:HA	1.70	0.73
1:C:528:LYS:O	1:C:529:LYS:HG2	1.88	0.73
1:B:201:PHE:CD2	1:B:231:ILE:HG21	2.23	0.73
1:A:905:ARG:NH1	1:A:1049:LEU:O	2.21	0.73
1:A:350:VAL:O	1:A:422:ASN:ND2	2.22	0.73
1:A:354:ASN:HB2	1:A:399:SER:O	1.88	0.72
1:C:393:THR:HG21	1:C:519:HIS:HB2	1.72	0.72
1:C:1135:ASN:OD1	1:C:1136:THR:N	2.22	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:702:GLU:OE2	1:C:790:LYS:NZ	2.23	0.71
1:C:64:TRP:HE1	1:C:264:ALA:HB1	1.55	0.71
1:C:108:THR:HA	1:C:236:THR:HG22	1.73	0.71
1:A:603:ASN:CG	2:A:1206:NAG:C8	2.58	0.71
1:B:231:ILE:HB	1:B:233:ILE:HG12	1.71	0.71
1:B:201:PHE:HD2	1:B:231:ILE:HG21	1.56	0.71
1:C:562:PHE:O	1:C:564:GLN:NE2	2.24	0.71
1:B:442:ASP:O	1:B:448:ASN:ND2	2.23	0.70
1:B:324:GLU:H	1:B:539:VAL:HG12	1.54	0.70
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.74	0.69
1:C:452:LEU:HB3	1:C:492:LEU:HD12	1.75	0.69
1:A:1135:ASN:OD1	1:A:1136:THR:N	2.24	0.69
1:B:125:ASN:HB3	1:B:174:PRO:HA	1.75	0.69
1:B:53:ASP:OD2	1:B:54:LEU:N	2.26	0.69
1:B:330:PRO:HA	1:B:579:PRO:HB2	1.74	0.69
1:C:358:ILE:HB	1:C:395:VAL:HB	1.74	0.69
1:A:379:CYS:HB3	1:A:432:CYS:HA	1.75	0.68
1:A:452:LEU:HB3	1:A:492:LEU:HD22	1.76	0.68
1:C:86:PHE:HB2	1:C:238:PHE:HD1	1.58	0.67
1:A:26:PRO:HB3	1:A:65:PHE:HE2	1.59	0.67
1:A:788:ILE:HD11	1:B:699:LEU:HB2	1.77	0.67
1:A:438:SER:O	1:A:442:ASP:N	2.20	0.67
1:C:216:LEU:HD12	1:C:217:PRO:HD2	1.76	0.67
1:C:1019:ARG:NH1	1:C:1023:ASN:OD1	2.28	0.67
1:A:1053:PRO:O	1:A:1054:GLN:NE2	2.26	0.66
1:A:132:GLU:HG2	2:A:1211:NAG:H81	1.77	0.66
1:A:99:ASN:OD1	1:A:102:ARG:NH2	2.29	0.66
1:A:738:CYS:SG	1:A:739:THR:N	2.69	0.65
1:A:409:GLN:HB3	1:A:419:ALA:HB2	1.79	0.65
1:A:458:LYS:NZ	1:A:471:GLU:OE2	2.30	0.65
1:B:83:VAL:HG13	1:B:239:GLN:HB2	1.79	0.65
1:C:22:THR:O	1:C:78:ARG:NH1	2.29	0.65
1:B:567:ARG:HH21	1:B:573:THR:HA	1.62	0.65
1:A:355:ARG:HH22	1:A:464:PHE:HB3	1.61	0.65
1:B:22:THR:OG1	1:B:77:LYS:O	2.15	0.65
1:C:14:GLN:HG2	1:C:158:ARG:HE	1.61	0.65
1:B:849:LEU:HB3	1:B:852:ALA:HB2	1.79	0.65
1:B:216:LEU:HD12	1:B:217:PRO:HD2	1.77	0.65
1:A:417:LYS:NZ	1:A:495:TYR:OH	2.29	0.64
1:B:188:ASN:HD21	1:B:190:ARG:HE	1.43	0.64
1:C:723:THR:HG22	1:C:724:THR:H	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:THR:OG1	1:A:516:GLU:O	2.13	0.64
1:B:971:GLY:HA3	1:B:995:ARG:HH21	1.61	0.64
1:B:906:PHE:HB3	1:B:911:VAL:HG23	1.78	0.64
1:C:738:CYS:SG	1:C:739:THR:N	2.70	0.64
1:B:34:ARG:NH1	1:B:191:GLU:OE2	2.31	0.64
1:B:101:ILE:O	1:B:102:ARG:NE	2.31	0.64
1:A:164:ASN:HB3	1:A:165:ASN:HD22	1.61	0.64
1:C:1053:PRO:O	1:C:1054:GLN:NE2	2.30	0.64
1:B:744:GLY:H	1:B:977:LEU:HD22	1.62	0.64
1:A:712:ILE:HG13	1:A:1077:THR:HG21	1.78	0.63
1:A:744:GLY:H	1:A:977:LEU:HD23	1.63	0.63
1:A:1129:VAL:HG23	1:C:917:TYR:HB3	1.80	0.63
2:B:1204:NAG:C8	2:B:1204:NAG:C3	2.77	0.63
1:A:562:PHE:O	1:A:564:GLN:NE2	2.30	0.63
1:A:723:THR:HG22	1:A:724:THR:H	1.63	0.63
1:C:34:ARG:NH1	1:C:191:GLU:OE1	2.32	0.63
1:B:725:GLU:OE1	1:B:1064:HIS:NE2	2.28	0.63
1:B:358:ILE:HB	1:B:395:VAL:HB	1.80	0.62
1:C:1019:ARG:O	1:C:1023:ASN:ND2	2.32	0.62
1:A:64:TRP:HE1	1:A:264:ALA:HB1	1.65	0.62
1:A:309:GLU:N	1:A:309:GLU:OE1	2.33	0.62
1:B:27:ALA:HB3	1:B:64:TRP:HB3	1.80	0.62
1:B:214:ARG:O	1:B:214:ARG:NH1	2.33	0.62
1:C:335:LEU:HD13	1:C:362:VAL:HG13	1.82	0.62
1:C:53:ASP:OD1	1:C:54:LEU:N	2.28	0.62
1:B:66:HIS:HE1	1:B:68:ILE:HB	1.65	0.61
1:C:100:ILE:HG23	1:C:242:LEU:HD11	1.82	0.61
1:C:436:TRP:HE3	1:C:509:ARG:HH21	1.48	0.61
1:B:212:LEU:HD21	1:B:215:ASP:HB3	1.81	0.61
1:B:1135:ASN:OD1	1:B:1136:THR:N	2.29	0.61
1:A:703:ASN:OD1	1:A:704:SER:N	2.33	0.61
1:A:1081:ILE:HG23	1:A:1088:HIS:HB2	1.82	0.61
1:B:360:ASN:H	1:B:523:THR:HG22	1.65	0.61
1:B:328:ARG:HG2	1:B:530:SER:HB3	1.83	0.61
1:A:18:LEU:O	1:A:21:ARG:NH1	2.34	0.61
1:A:420:ASP:HA	1:A:424:LYS:HE2	1.82	0.61
1:A:699:LEU:HD11	1:C:869:MET:HG2	1.83	0.61
1:B:34:ARG:NH2	1:B:217:PRO:O	2.34	0.61
1:A:676:THR:OG1	1:A:689:SER:O	2.19	0.60
1:B:65:PHE:HE1	1:B:84:LEU:HD21	1.66	0.60
1:A:210:ILE:HG13	1:A:212:LEU:H	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:474:GLN:OE1	1:B:476:GLY:N	2.27	0.60
1:A:393:THR:HG23	1:A:517:LEU:HD12	1.83	0.60
1:B:570:ASP:OD1	1:B:571:ASP:N	2.34	0.60
1:B:1097:SER:HB3	1:B:1102:TRP:CD2	2.36	0.60
1:B:905:ARG:NH1	1:B:1049:LEU:O	2.30	0.60
1:A:97:LYS:HE3	1:A:181:GLY:HA3	1.83	0.60
1:C:26:PRO:HB3	1:C:65:PHE:HE2	1.67	0.60
1:C:966:LEU:O	1:C:975:SER:OG	2.20	0.60
1:A:715:PRO:HD3	1:C:894:LEU:HD21	1.83	0.60
1:A:802:PHE:HB3	1:A:806:LEU:HD23	1.82	0.60
1:B:917:TYR:HB3	1:C:1129:VAL:HG23	1.84	0.59
1:C:366:SER:O	1:C:370:ASN:ND2	2.36	0.59
1:C:214:ARG:O	1:C:214:ARG:NH1	2.35	0.59
1:B:290:ASP:OD1	1:B:291:CYS:N	2.35	0.59
1:B:431:GLY:HA3	1:B:514:SER:HA	1.85	0.59
1:B:516:GLU:OE2	1:B:519:HIS:ND1	2.25	0.59
1:C:501:TYR:O	1:C:506:GLN:NE2	2.36	0.59
1:B:800:PHE:HD2	1:B:927:PHE:HD2	1.49	0.59
1:B:527:PRO:HB3	1:B:529:LYS:NZ	2.18	0.59
1:C:1085:GLY:O	1:C:1126:CYS:N	2.35	0.59
1:B:144:TYR:O	1:B:146:HIS:N	2.36	0.58
1:B:737:ASP:OD2	1:B:738:CYS:N	2.37	0.58
1:C:21:ARG:HG2	1:C:79:PHE:HB3	1.84	0.58
1:B:976:VAL:HB	1:B:979:ASP:HB2	1.85	0.58
1:C:421:TYR:CD1	1:C:457:ARG:HB2	2.39	0.58
1:C:210:ILE:HG13	1:C:212:LEU:H	1.68	0.58
1:A:187:LYS:NZ	1:A:211:ASN:OD1	2.35	0.58
1:A:949:GLN:NE2	1:A:953:ASN:OD1	2.36	0.57
1:A:1081:ILE:HD11	1:A:1135:ASN:HB3	1.86	0.57
1:A:745:ASP:OD2	1:B:319:ARG:NH1	2.37	0.57
1:A:131:CYS:HB3	1:A:165:ASN:O	2.04	0.57
1:C:185:ASN:ND2	1:C:211:ASN:OD1	2.37	0.57
1:C:329:PHE:CB	1:C:528:LYS:HD3	2.35	0.57
1:A:431:GLY:HA3	1:A:514:SER:HA	1.86	0.57
1:A:603:ASN:CB	2:A:1206:NAG:C8	2.83	0.57
1:C:748:GLU:OE1	1:C:748:GLU:N	2.32	0.57
1:B:1053:PRO:O	1:B:1054:GLN:NE2	2.37	0.57
1:B:1055:SER:OG	1:B:1056:ALA:N	2.38	0.57
1:A:365:TYR:O	1:A:369:TYR:HB2	2.06	0.56
1:C:190:ARG:HG2	1:C:192:PHE:CE2	2.41	0.56
1:A:216:LEU:HD12	1:A:217:PRO:HD2	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:LYS:O	1:A:498:GLN:NE2	2.38	0.56
1:C:132:GLU:OE1	1:C:164:ASN:HB3	2.05	0.56
1:A:290:ASP:OD1	1:A:291:CYS:N	2.39	0.56
1:B:141:LEU:O	1:B:244:LEU:N	2.38	0.56
1:B:318:PHE:CZ	1:B:615:VAL:HG21	2.25	0.56
1:A:894:LEU:HD21	1:B:715:PRO:HD3	1.88	0.56
1:B:99:ASN:ND2	1:B:178:ASP:O	2.39	0.56
1:B:64:TRP:HE1	1:B:264:ALA:HB1	1.71	0.56
1:B:231:ILE:HG13	1:B:232:GLY:N	2.21	0.56
1:A:368:LEU:HD21	1:A:434:ILE:HG12	1.88	0.55
1:C:1105:THR:HG22	1:C:1112:PRO:HA	1.87	0.55
1:B:935:GLN:O	1:B:939:SER:N	2.39	0.55
1:C:141:LEU:O	1:C:244:LEU:N	2.38	0.55
1:A:417:LYS:HD2	1:A:418:ILE:HG23	1.88	0.55
1:C:357:ARG:HH12	1:C:396:TYR:HE2	1.54	0.55
1:B:586:ASP:OD1	1:B:587:ILE:N	2.40	0.55
1:C:421:TYR:HD1	1:C:457:ARG:HB2	1.71	0.55
1:A:117:LEU:HD13	1:A:130:VAL:HG22	1.88	0.55
1:B:14:GLN:HG3	1:B:158:ARG:HD3	1.89	0.55
1:C:68:ILE:HG21	1:C:77:LYS:HB2	1.89	0.55
1:B:806:LEU:HD12	1:B:807:PRO:HD2	1.89	0.54
1:A:725:GLU:OE2	1:A:1064:HIS:NE2	2.40	0.54
1:B:307:THR:HA	1:B:602:THR:HG21	1.90	0.54
1:A:917:TYR:HD2	1:B:1089:PHE:HE2	1.55	0.54
1:C:409:GLN:HB3	1:C:419:ALA:HB2	1.89	0.54
1:B:273:ARG:HG2	1:B:274:THR:H	1.72	0.54
1:A:466:ARG:HH12	1:A:468:ILE:HG22	1.73	0.54
1:C:380:TYR:CE2	1:C:412:PRO:HD3	2.43	0.54
1:A:212:LEU:HD21	1:A:215:ASP:HB3	1.90	0.53
1:A:566:GLY:HA2	1:C:43:PHE:HB3	1.90	0.53
1:C:393:THR:OG1	1:C:518:LEU:N	2.41	0.53
1:C:442:ASP:OD1	1:C:451:TYR:OH	2.26	0.53
1:A:759:PHE:HD2	1:A:1001:LEU:HD21	1.73	0.53
1:C:290:ASP:O	1:C:297:SER:HB3	2.09	0.53
1:A:358:ILE:HB	1:A:395:VAL:HB	1.90	0.53
1:A:438:SER:HB2	1:A:442:ASP:HB2	1.89	0.53
1:C:369:TYR:HA	1:C:377:PHE:HE2	1.74	0.53
1:A:455:LEU:HD22	1:A:456:PHE:CE2	2.44	0.53
1:B:140:PHE:HD2	1:B:244:LEU:HB3	1.72	0.53
1:B:287:ASP:OD1	1:B:288:ALA:N	2.41	0.53
1:C:68:ILE:HB	1:C:78:ARG:HB2	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:VAL:HG23	1:A:160:TYR:HD1	1.74	0.53
1:C:1055:SER:OG	1:C:1056:ALA:N	2.42	0.53
1:A:392:PHE:HA	1:A:517:LEU:HD13	1.89	0.52
1:B:474:GLN:NE2	1:B:478:THR:O	2.42	0.52
1:A:231:ILE:HG13	1:A:232:GLY:H	1.75	0.52
1:B:402:ILE:HG21	1:B:418:ILE:HD13	1.91	0.52
1:B:935:GLN:NE2	1:B:936:ASP:OD1	2.43	0.52
1:C:99:ASN:ND2	1:C:178:ASP:O	2.39	0.52
1:C:157:PHE:HZ	2:C:1209:NAG:HO6	1.56	0.52
1:C:474:GLN:NE2	1:C:478:THR:O	2.43	0.52
1:B:931:ILE:O	1:B:934:ILE:HG22	2.10	0.52
1:C:410:ILE:O	1:C:425:LEU:HD12	2.09	0.52
1:B:53:ASP:HB3	1:B:55:PHE:CE2	2.44	0.52
1:B:418:ILE:HA	1:B:422:ASN:HD21	1.74	0.52
1:B:821:LEU:O	1:B:825:LYS:HG2	2.08	0.52
1:C:68:ILE:HG22	1:C:78:ARG:O	2.10	0.52
1:C:722:VAL:HG22	1:C:1065:VAL:HG22	1.92	0.52
1:A:517:LEU:O	1:A:519:HIS:ND1	2.42	0.52
1:A:770:ILE:O	1:A:774:GLN:HG2	2.10	0.52
1:C:164:ASN:CG	1:C:165:ASN:H	2.14	0.52
1:A:21:ARG:HG2	1:A:79:PHE:HB3	1.91	0.52
1:A:41:LYS:NZ	1:B:564:GLN:OE1	2.42	0.52
1:A:457:ARG:NE	1:A:467:ASP:OD2	2.43	0.51
1:B:96:GLU:O	1:B:188:ASN:HB3	2.10	0.51
1:A:461:LEU:HG	1:A:465:GLU:HB2	1.92	0.51
1:C:136:CYS:O	1:C:139:PRO:HD3	2.09	0.51
1:B:353:TRP:HZ3	1:B:355:ARG:HD3	1.74	0.51
1:B:598:ILE:HG12	1:B:666:ILE:HD11	1.91	0.51
1:C:357:ARG:NH1	1:C:396:TYR:HE2	2.08	0.51
1:B:159:VAL:HG23	1:B:160:TYR:HD1	1.76	0.51
1:B:777:ASN:OD1	1:B:1019:ARG:NH1	2.42	0.51
1:A:603:ASN:CB	2:A:1206:NAG:H83	2.41	0.51
1:B:716:ILE:HG22	1:B:1071:GLN:HB2	1.91	0.51
1:C:642:VAL:HG12	1:C:651:ILE:HG22	1.92	0.51
1:A:800:PHE:CE1	1:A:924:ALA:HA	2.46	0.51
1:B:661:GLU:O	1:B:695:TYR:OH	2.19	0.51
1:B:38:TYR:OH	1:B:284:THR:HA	2.11	0.51
1:B:982:ALA:O	1:C:390:LEU:HD21	2.10	0.51
1:C:360:ASN:HA	1:C:523:THR:HG21	1.92	0.51
1:C:30:ASN:N	2:C:1208:NAG:H81	2.25	0.51
1:C:96:GLU:O	1:C:188:ASN:HB3	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:GLN:HG2	1:C:273:ARG:HH12	1.76	0.50
1:C:18:LEU:O	1:C:21:ARG:NH1	2.44	0.50
1:A:164:ASN:HB3	1:A:165:ASN:ND2	2.24	0.50
1:A:563:GLN:OE1	1:C:43:PHE:HD1	1.94	0.50
1:C:111:ASP:OD1	1:C:134:GLN:NE2	2.41	0.50
1:C:811:LYS:HD2	1:C:812:PRO:HD2	1.94	0.50
1:B:108:THR:OG1	1:B:234:ASN:O	2.29	0.50
1:B:21:ARG:HG2	1:B:79:PHE:HB3	1.94	0.50
1:B:788:ILE:HD11	1:C:699:LEU:HB2	1.93	0.50
1:A:455:LEU:N	1:A:491:PRO:O	2.38	0.50
1:B:43:PHE:O	1:C:566:GLY:HA2	2.11	0.50
1:B:106:PHE:HB3	1:B:235:ILE:HD13	1.93	0.50
1:C:336:CYS:N	1:C:362:VAL:O	2.45	0.50
1:C:1097:SER:HB2	1:C:1102:TRP:CE3	2.47	0.50
1:A:439:ASN:HB2	1:A:506:GLN:HB3	1.94	0.49
1:C:27:ALA:HB3	1:C:64:TRP:HB3	1.94	0.49
1:A:310:LYS:HG3	1:A:664:ILE:HD11	1.94	0.49
1:B:177:MET:SD	1:B:190:ARG:NH2	2.85	0.49
1:B:800:PHE:HD2	1:B:927:PHE:CD2	2.29	0.49
1:A:96:GLU:HB2	1:A:99:ASN:HA	1.94	0.49
1:A:99:ASN:ND2	1:A:178:ASP:O	2.35	0.49
1:A:295:PRO:HB2	1:A:608:VAL:HG21	1.92	0.49
1:A:707:TYR:HB3	1:C:792:PRO:HG2	1.94	0.49
1:B:112:SER:HB3	1:B:134:GLN:HA	1.93	0.49
1:B:577:ARG:HG2	1:B:584:ILE:HA	1.93	0.49
1:A:470:THR:HG22	1:A:492:LEU:HD12	1.94	0.49
1:B:68:ILE:HG21	1:B:77:LYS:HD3	1.94	0.49
1:B:194:PHE:CD1	1:B:203:ILE:HG12	2.46	0.49
1:B:555:SER:OG	1:B:584:ILE:HG12	2.13	0.49
1:C:193:VAL:HG12	1:C:204:TYR:HB2	1.94	0.49
1:A:27:ALA:HB3	1:A:64:TRP:HB3	1.94	0.49
1:B:140:PHE:CD2	1:B:244:LEU:HB3	2.47	0.49
1:A:344:ALA:HB3	1:A:347:PHE:HE2	1.78	0.49
1:B:1105:THR:HG22	1:B:1112:PRO:HA	1.94	0.49
1:B:231:ILE:HG13	1:B:232:GLY:H	1.78	0.49
1:C:126:VAL:HG13	1:C:175:PHE:HZ	1.78	0.49
1:A:53:ASP:OD2	1:A:54:LEU:N	2.34	0.49
1:A:126:VAL:HG13	1:A:175:PHE:CZ	2.47	0.49
1:A:497:PHE:CD2	1:A:507:PRO:HG3	2.48	0.49
1:C:135:PHE:HD2	1:C:136:CYS:O	1.96	0.49
1:A:1083:HIS:CE1	1:A:1137:VAL:H	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:659:SER:HB3	1:B:698:SER:HB3	1.93	0.49
1:C:86:PHE:HB2	1:C:238:PHE:CD1	2.45	0.49
1:C:802:PHE:HB3	1:C:806:LEU:HD23	1.95	0.49
1:A:83:VAL:O	1:A:237:ARG:NH2	2.45	0.48
1:A:97:LYS:HB2	1:A:186:PHE:HD1	1.77	0.48
1:B:190:ARG:HB3	1:B:192:PHE:HE2	1.78	0.48
1:A:48:LEU:HB3	1:A:276:LEU:HD11	1.95	0.48
1:B:66:HIS:CE1	1:B:68:ILE:HB	2.48	0.48
1:B:83:VAL:HG12	1:B:237:ARG:HE	1.78	0.48
1:C:975:SER:OG	1:C:975:SER:O	2.30	0.48
1:B:18:LEU:O	1:B:21:ARG:NH1	2.46	0.48
1:C:290:ASP:OD1	1:C:292:ALA:N	2.40	0.48
1:B:978:ASN:HA	1:B:981:LEU:HB2	1.95	0.48
1:C:122:ASN:ND2	2:C:1209:NAG:C7	2.76	0.48
1:C:168:PHE:CZ	1:C:170:TYR:HB2	2.48	0.48
1:C:406:GLU:HG3	1:C:418:ILE:HD13	1.95	0.48
1:B:1081:ILE:O	1:B:1088:HIS:N	2.46	0.48
1:C:65:PHE:HD1	1:C:265:TYR:CZ	2.32	0.48
1:A:1028:LYS:O	1:A:1032:CYS:HB2	2.13	0.48
1:B:201:PHE:CE2	1:B:231:ILE:HD13	2.49	0.48
1:C:327:VAL:HG12	1:C:528:LYS:HG2	1.95	0.48
1:C:190:ARG:HG2	1:C:192:PHE:HE2	1.77	0.48
1:C:428:ASP:OD1	1:C:428:ASP:N	2.45	0.48
1:B:1082:CYS:N	1:B:1132:ILE:HD11	2.29	0.48
1:C:712:ILE:HG13	1:C:1077:THR:HG21	1.96	0.48
1:A:349:SER:H	1:A:351:TYR:HE1	1.62	0.48
1:B:421:TYR:CD1	1:B:457:ARG:HB2	2.49	0.48
1:B:895:GLN:HE21	1:B:895:GLN:HB3	1.49	0.48
1:C:29:THR:C	2:C:1208:NAG:H81	2.34	0.48
1:B:1097:SER:HB3	1:B:1102:TRP:CE3	2.49	0.47
1:A:18:LEU:HD23	1:A:20:THR:H	1.78	0.47
1:A:516:GLU:OE2	1:A:519:HIS:ND1	2.47	0.47
1:B:424:LYS:HB2	1:B:463:PRO:HA	1.95	0.47
1:C:394:ASN:OD1	1:C:516:GLU:HB3	2.14	0.47
1:A:22:THR:OG1	1:A:77:LYS:O	2.19	0.47
1:B:22:THR:HB	1:B:78:ARG:HG3	1.96	0.47
1:C:89:GLY:HA2	1:C:194:PHE:O	2.14	0.47
1:C:368:LEU:O	1:C:371:SER:OG	2.30	0.47
1:C:782:PHE:HB3	1:C:873:TYR:HD2	1.78	0.47
1:A:34:ARG:NH2	1:A:217:PRO:HG2	2.30	0.47
1:A:165:ASN:HD22	1:A:165:ASN:N	2.11	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:LYS:NZ	1:A:228:ASP:OD1	2.38	0.47
1:A:699:LEU:HD22	1:C:873:TYR:CE1	2.50	0.47
1:A:894:LEU:HD11	1:B:1072:GLU:HG2	1.95	0.47
1:B:125:ASN:HD22	1:B:174:PRO:HG3	1.79	0.47
1:C:307:THR:HA	1:C:602:THR:HG21	1.96	0.47
1:C:738:CYS:O	1:C:741:TYR:N	2.47	0.47
1:C:912:THR:OG1	1:C:1106:GLN:NE2	2.46	0.47
1:A:126:VAL:HG13	1:A:175:PHE:HZ	1.80	0.47
1:A:822:LEU:HD21	1:A:938:LEU:HD13	1.95	0.47
1:B:83:VAL:HG12	1:B:237:ARG:NE	2.30	0.47
1:B:416:GLY:O	1:B:420:ASP:N	2.48	0.47
1:C:19:THR:HA	1:C:21:ARG:NH1	2.29	0.47
1:C:97:LYS:HE3	1:C:181:GLY:HA3	1.95	0.47
1:C:295:PRO:HB2	1:C:608:VAL:HG21	1.96	0.47
1:C:439:ASN:HB3	1:C:506:GLN:HB3	1.97	0.47
1:C:473:TYR:O	1:C:488:CYS:HA	2.14	0.47
1:A:759:PHE:O	1:A:763:LEU:HG	2.15	0.47
1:B:104:TRP:HB3	1:B:106:PHE:HE1	1.79	0.47
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.96	0.47
1:C:143:VAL:HA	1:C:154:GLU:HA	1.97	0.47
1:A:408:ARG:O	1:A:414:GLN:HG3	2.14	0.47
1:B:916:LEU:HD12	1:B:923:ILE:HD12	1.97	0.47
1:B:318:PHE:HD1	1:B:595:VAL:HG13	1.80	0.47
1:C:431:GLY:HA3	1:C:514:SER:HA	1.97	0.47
1:C:912:THR:OG1	1:C:914:ASN:OD1	2.19	0.47
1:A:22:THR:HB	1:A:78:ARG:HG3	1.97	0.46
1:B:543:PHE:HZ	1:B:552:LEU:HD21	1.80	0.46
1:C:474:GLN:HG2	1:C:480:CYS:HB3	1.97	0.46
1:C:584:ILE:O	1:C:584:ILE:HG13	2.15	0.46
1:B:244:LEU:O	1:B:254:SER:N	2.48	0.46
1:B:851:CYS:HA	1:B:854:LYS:HD3	1.96	0.46
1:C:142:GLY:HA3	1:C:156:GLU:HB2	1.97	0.46
1:C:271:GLN:HG3	1:C:272:PRO:HD2	1.97	0.46
1:C:538:CYS:HB3	1:C:551:VAL:HG23	1.96	0.46
1:C:823:PHE:HD1	1:C:1057:PRO:HG3	1.79	0.46
1:C:164:ASN:ND2	1:C:165:ASN:H	2.14	0.46
1:C:377:PHE:CD1	1:C:434:ILE:HG12	2.50	0.46
1:C:434:ILE:HB	1:C:511:VAL:HG13	1.97	0.46
1:C:538:CYS:HA	1:C:550:GLY:O	2.14	0.46
1:A:490:PHE:HB3	1:A:493:GLN:OE1	2.16	0.46
1:A:672:ALA:HA	1:A:693:ILE:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:ILE:HG23	1:B:128:ILE:HG13	1.96	0.46
1:B:422:ASN:OD1	1:B:423:TYR:N	2.49	0.46
1:B:749:CYS:SG	1:B:997:ILE:HD11	2.56	0.46
1:C:454:ARG:NH1	1:C:467:ASP:OD2	2.49	0.46
1:A:164:ASN:C	1:A:165:ASN:HD22	2.19	0.46
1:A:642:VAL:HG12	1:A:651:ILE:HG22	1.98	0.46
1:A:864:LEU:HD11	1:B:665:PRO:HB2	1.97	0.46
1:A:1085:GLY:O	1:A:1126:CYS:N	2.49	0.46
1:B:200:TYR:CD1	1:B:230:PRO:HA	2.51	0.46
1:B:84:LEU:O	1:B:237:ARG:HD2	2.16	0.46
1:B:350:VAL:O	1:B:353:TRP:HD1	1.99	0.46
1:B:786:LYS:HG3	1:B:787:GLN:OE1	2.16	0.46
1:A:603:ASN:HB2	2:A:1206:NAG:C8	2.46	0.46
1:B:118:LEU:HD23	1:B:120:VAL:H	1.81	0.46
1:B:490:PHE:CE2	1:B:492:LEU:HB2	2.51	0.46
1:B:83:VAL:HB	1:B:237:ARG:HH21	1.81	0.45
1:B:807:PRO:HA	1:B:816:SER:HB3	1.97	0.45
1:A:800:PHE:HE1	1:A:924:ALA:HA	1.80	0.45
1:C:273:ARG:HH11	1:C:273:ARG:HB2	1.81	0.45
1:C:662:CYS:HB2	1:C:697:MET:HG3	1.97	0.45
1:A:101:ILE:H	1:A:101:ILE:HD12	1.81	0.45
1:B:200:TYR:HD1	1:B:230:PRO:HA	1.81	0.45
1:C:770:ILE:O	1:C:774:GLN:HG2	2.16	0.45
1:C:825:LYS:NZ	1:C:938:LEU:O	2.33	0.45
1:C:147:LYS:HG3	1:C:149:ASN:H	1.81	0.45
1:A:353:TRP:NE1	1:A:466:ARG:HG3	2.31	0.45
1:B:357:ARG:HD3	1:B:396:TYR:CZ	2.52	0.45
1:B:616:ASN:O	1:B:619:GLU:HG2	2.16	0.45
1:C:408:ARG:HB3	1:C:408:ARG:NH1	2.32	0.45
1:A:365:TYR:HD2	1:A:387:LEU:HD13	1.79	0.45
1:A:895:GLN:HE21	1:A:895:GLN:HB3	1.59	0.45
1:B:413:GLY:HA3	1:C:987:VAL:HG21	1.97	0.45
1:B:559:PHE:CE2	1:B:564:GLN:HA	2.52	0.45
1:B:569:ILE:HG23	1:B:570:ASP:H	1.81	0.45
1:C:431:GLY:HA3	1:C:513:LEU:O	2.17	0.45
1:C:452:LEU:HD22	1:C:492:LEU:HB3	1.99	0.45
1:A:1055:SER:OG	1:A:1056:ALA:N	2.49	0.45
1:A:96:GLU:O	1:A:188:ASN:HB3	2.17	0.45
1:A:351:TYR:CG	1:A:352:ALA:N	2.85	0.45
1:A:412:PRO:HB2	1:A:427:ASP:HA	1.99	0.45
1:B:141:LEU:HB3	1:B:243:ALA:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:384:PRO:HA	1:B:387:LEU:HD13	1.98	0.45
1:C:473:TYR:CZ	1:C:475:ALA:HA	2.51	0.45
1:C:985:ASP:OD1	1:C:988:GLU:HG3	2.17	0.45
1:A:64:TRP:NE1	1:A:264:ALA:HB1	2.32	0.44
1:A:473:TYR:N	1:A:489:TYR:O	2.43	0.44
1:A:989:ALA:O	1:A:993:ILE:HG13	2.16	0.44
1:B:557:LYS:HB2	1:B:584:ILE:HD11	1.99	0.44
1:C:63:THR:O	1:C:266:TYR:HA	2.17	0.44
1:A:337:PRO:HD2	1:A:358:ILE:HD12	1.99	0.44
1:A:792:PRO:HG3	1:B:707:TYR:HB3	1.99	0.44
1:C:141:LEU:HD22	1:C:159:VAL:HG11	1.99	0.44
1:C:213:VAL:HG23	1:C:214:ARG:H	1.82	0.44
1:A:105:ILE:O	1:A:238:PHE:HB2	2.17	0.44
1:A:904:TYR:OH	1:B:1094:VAL:HG12	2.17	0.44
1:B:65:PHE:HB2	1:B:265:TYR:CZ	2.52	0.44
1:B:605:SER:OG	1:B:606:ASN:N	2.51	0.44
1:C:159:VAL:HG23	1:C:160:TYR:CD1	2.51	0.44
1:C:193:VAL:CG1	1:C:204:TYR:HB2	2.48	0.44
1:A:97:LYS:HB2	1:A:186:PHE:CD1	2.53	0.44
1:A:361:CYS:H	1:A:524:VAL:HG12	1.81	0.44
1:B:277:LEU:HD23	1:B:285:ILE:HD13	2.00	0.44
1:B:559:PHE:CG	1:B:584:ILE:HD12	2.53	0.44
1:B:738:CYS:HB3	1:B:742:ILE:HD12	1.99	0.44
1:B:850:ILE:HD12	1:B:850:ILE:H	1.82	0.44
1:B:1129:VAL:HG23	1:B:1132:ILE:HB	1.99	0.44
1:A:290:ASP:OD1	1:A:292:ALA:N	2.26	0.44
1:A:497:PHE:CZ	1:A:507:PRO:HB3	2.53	0.44
1:C:566:GLY:O	1:C:567:ARG:HG3	2.17	0.44
1:A:221:SER:OG	1:A:222:ALA:N	2.48	0.44
1:A:666:ILE:HD11	1:A:672:ALA:HB2	2.00	0.44
1:B:797:PHE:O	1:B:800:PHE:HD1	2.00	0.44
1:C:321:GLN:HA	1:C:322:PRO:HD3	1.86	0.44
1:C:538:CYS:HB3	1:C:590:CYS:HB3	1.94	0.44
1:B:642:VAL:HG12	1:B:651:ILE:HG22	1.99	0.44
1:A:68:ILE:HD12	1:A:262:ALA:HA	1.99	0.44
1:A:118:LEU:HD11	1:A:120:VAL:HG23	2.00	0.44
1:A:453:TYR:CZ	1:A:493:GLN:HB2	2.53	0.44
1:C:68:ILE:HD12	1:C:262:ALA:HA	1.99	0.44
1:A:603:ASN:HB2	2:A:1206:NAG:H83	1.99	0.43
1:B:770:ILE:O	1:B:774:GLN:HG2	2.18	0.43
1:C:396:TYR:HB2	1:C:514:SER:OG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:534:VAL:HG22	1:C:535:LYS:H	1.82	0.43
1:C:730:SER:O	1:C:1058:HIS:HB3	2.18	0.43
1:A:204:TYR:HD1	1:A:225:PRO:HA	1.83	0.43
1:A:811:LYS:HD2	1:A:812:PRO:HD2	2.00	0.43
1:B:393:THR:OG1	1:B:518:LEU:N	2.52	0.43
1:C:1127:ASP:OD1	1:C:1127:ASP:N	2.51	0.43
1:A:135:PHE:HA	1:A:160:TYR:HA	2.00	0.43
1:B:18:LEU:HD12	1:B:255:SER:HA	2.00	0.43
1:B:786:LYS:HG3	1:B:787:GLN:CD	2.38	0.43
1:A:231:ILE:HG13	1:A:232:GLY:N	2.34	0.43
1:A:1126:CYS:HB2	1:A:1132:ILE:HD13	2.00	0.43
1:A:538:CYS:HB2	1:A:590:CYS:HB3	1.64	0.43
1:B:574:ASP:CG	1:B:575:ALA:H	2.22	0.43
1:C:21:ARG:HB2	1:C:23:GLN:OE1	2.18	0.43
1:C:273:ARG:HB2	1:C:273:ARG:NH1	2.33	0.43
1:C:437:ASN:HB3	1:C:508:TYR:CZ	2.54	0.43
1:C:537:LYS:O	1:C:539:VAL:HG13	2.18	0.43
1:C:1100:THR:OG1	1:C:1101:HIS:ND1	2.51	0.43
1:A:214:ARG:HH11	1:A:215:ASP:HA	1.83	0.43
1:B:449:TYR:CE1	1:B:496:GLY:HA2	2.53	0.43
1:A:379:CYS:CB	1:A:432:CYS:HA	2.47	0.43
1:A:394:ASN:OD1	1:A:395:VAL:N	2.52	0.43
1:A:369:TYR:CE1	1:A:384:PRO:HB2	2.53	0.43
1:A:858:LEU:HD21	1:A:962:LEU:HD22	2.00	0.43
1:A:1086:LYS:HB2	1:A:1086:LYS:HE3	1.78	0.43
1:B:36:VAL:HG21	1:B:220:PHE:CZ	2.53	0.43
1:B:377:PHE:CD2	1:B:434:ILE:HG12	2.54	0.43
1:C:53:ASP:HB3	1:C:55:PHE:CE2	2.54	0.43
1:B:133:PHE:HB2	1:B:135:PHE:CE2	2.54	0.43
1:B:906:PHE:HE1	1:B:1049:LEU:HD11	1.84	0.43
1:C:97:LYS:HD2	1:C:98:SER:H	1.83	0.43
1:A:577:ARG:NH1	1:A:582:LEU:HB3	2.34	0.42
1:B:118:LEU:HD21	1:B:120:VAL:HG23	2.01	0.42
1:B:546:LEU:HD22	1:B:565:PHE:CE1	2.54	0.42
1:B:993:ILE:O	1:B:997:ILE:HG12	2.18	0.42
1:C:65:PHE:HE1	1:C:84:LEU:HD11	1.83	0.42
1:C:369:TYR:HA	1:C:377:PHE:CE2	2.53	0.42
1:A:85:PRO:HA	1:A:237:ARG:HD2	2.00	0.42
1:A:213:VAL:HG23	1:A:214:ARG:N	2.33	0.42
1:B:57:PRO:HG3	1:B:273:ARG:HE	1.84	0.42
1:A:365:TYR:CD2	1:A:387:LEU:HD13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:106:PHE:HB3	1:B:235:ILE:HG21	2.00	0.42
1:B:126:VAL:HG13	1:B:175:PHE:CZ	2.54	0.42
1:B:1100:THR:OG1	1:B:1101:HIS:N	2.53	0.42
1:C:185:ASN:OD1	1:C:187:LYS:HE2	2.19	0.42
1:A:201:PHE:HB2	1:A:231:ILE:HD13	2.01	0.42
1:A:1048:HIS:NE2	1:A:1050:MET:O	2.47	0.42
1:A:1077:THR:OG1	1:A:1078:ALA:N	2.53	0.42
1:B:611:LEU:HD22	1:B:613:GLN:HG3	2.01	0.42
1:C:980:ILE:H	1:C:980:ILE:HD12	1.85	0.42
1:A:41:LYS:HE2	1:B:562:PHE:HB2	2.02	0.42
1:A:356:LYS:HB3	1:A:397:ALA:HB3	2.01	0.42
1:A:363:ALA:O	1:A:526:GLY:HA2	2.19	0.42
1:B:83:VAL:HB	1:B:237:ARG:NH2	2.35	0.42
1:C:278:LYS:HB2	1:C:278:LYS:HE3	1.69	0.42
1:A:108:THR:OG1	1:A:234:ASN:O	2.34	0.42
1:B:724:THR:HG22	1:B:1063:LEU:HD23	2.02	0.42
1:B:983:ARG:HG2	1:C:390:LEU:HD11	2.02	0.42
1:A:363:ALA:HB1	1:A:365:TYR:HE1	1.85	0.42
1:A:855:PHE:CE1	1:B:589:PRO:HD2	2.54	0.42
1:B:527:PRO:HB3	1:B:529:LYS:HZ1	1.84	0.42
1:A:111:ASP:OD1	1:A:134:GLN:NE2	2.43	0.42
1:C:191:GLU:O	1:C:205:SER:OG	2.27	0.42
1:A:81:ASN:OD1	1:A:81:ASN:N	2.53	0.42
1:B:579:PRO:O	1:B:580:GLN:HB2	2.20	0.42
1:C:906:PHE:HB3	1:C:911:VAL:HG23	2.01	0.42
1:A:101:ILE:O	1:A:102:ARG:NE	2.53	0.41
1:A:731:MET:HG2	1:A:774:GLN:OE1	2.19	0.41
1:A:916:LEU:HD12	1:A:923:ILE:HD12	2.01	0.41
1:A:1096:VAL:O	1:A:1103:PHE:N	2.47	0.41
1:B:474:GLN:OE1	1:B:475:ALA:N	2.53	0.41
1:C:472:ILE:HG13	1:C:488:CYS:HB3	2.02	0.41
1:A:402:ILE:HD11	1:A:407:VAL:HG12	2.01	0.41
1:A:1094:VAL:HG12	1:C:904:TYR:OH	2.21	0.41
1:C:567:ARG:HA	1:C:572:THR:O	2.20	0.41
1:C:788:ILE:HG21	1:C:872:GLN:HE21	1.85	0.41
1:A:45:SER:OG	1:A:281:GLU:HA	2.21	0.41
1:A:580:GLN:H	1:A:580:GLN:HG2	1.64	0.41
1:C:118:LEU:HD11	1:C:129:LYS:HD2	2.02	0.41
1:C:307:THR:O	1:C:307:THR:HG23	2.20	0.41
1:C:543:PHE:HD2	1:C:576:VAL:HG21	1.85	0.41
1:A:444:LYS:HG2	1:A:446:GLY:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:456:PHE:HD2	1:A:491:PRO:HA	1.85	0.41
1:A:699:LEU:HD22	1:C:873:TYR:CZ	2.56	0.41
1:A:742:ILE:H	1:A:742:ILE:HD12	1.85	0.41
1:A:993:ILE:O	1:A:997:ILE:HG12	2.21	0.41
1:B:453:TYR:HB3	1:B:495:TYR:CE1	2.55	0.41
1:C:329:PHE:HB2	1:C:528:LYS:HD3	2.02	0.41
1:C:354:ASN:O	1:C:398:ASP:HA	2.21	0.41
1:A:564:GLN:OE1	1:A:577:ARG:HD2	2.20	0.41
1:A:777:ASN:O	1:A:781:VAL:HG23	2.21	0.41
1:A:328:ARG:CZ	1:A:533:LEU:HD23	2.51	0.41
1:A:357:ARG:HD3	1:A:396:TYR:CE1	2.56	0.41
1:A:589:PRO:HD3	1:C:855:PHE:CE1	2.55	0.41
1:B:26:PRO:HB3	1:B:65:PHE:CE2	2.56	0.41
1:B:104:TRP:HB3	1:B:106:PHE:CE1	2.56	0.41
1:B:517:LEU:O	1:B:518:LEU:HG	2.20	0.41
1:B:877:LEU:O	1:B:881:THR:OG1	2.25	0.41
1:B:1142:GLN:N	1:B:1143:PRO:HD2	2.36	0.41
1:C:201:PHE:CD1	1:C:203:ILE:HD11	2.55	0.41
1:A:1083:HIS:ND1	1:A:1136:THR:HA	2.36	0.41
1:B:453:TYR:HB3	1:B:495:TYR:HE1	1.86	0.41
1:C:87:ASN:OD1	1:C:87:ASN:N	2.54	0.41
1:C:726:ILE:HG13	1:C:1061:VAL:HG22	2.02	0.41
1:C:1100:THR:HG1	1:C:1101:HIS:CE1	2.39	0.41
1:A:373:SER:O	1:A:373:SER:OG	2.34	0.41
1:A:457:ARG:NH1	1:A:459:SER:OG	2.54	0.41
1:B:620:VAL:N	1:B:621:PRO:HD2	2.35	0.41
1:C:62:VAL:HG22	1:C:266:TYR:HB3	2.03	0.41
1:C:716:ILE:HG22	1:C:1071:GLN:O	2.21	0.41
1:C:866:THR:HG23	1:C:869:MET:H	1.86	0.41
1:A:449:TYR:HA	1:A:495:TYR:O	2.20	0.41
1:A:502:GLY:O	1:A:506:GLN:HG3	2.21	0.41
1:B:99:ASN:OD1	1:B:179:LEU:HD12	2.20	0.41
1:C:378:LYS:HB3	1:C:380:TYR:CE1	2.56	0.41
1:C:485:GLY:H	1:C:488:CYS:HB2	1.85	0.41
1:B:567:ARG:NH2	1:B:573:THR:HA	2.33	0.41
1:A:105:ILE:HG12	1:A:239:GLN:O	2.21	0.40
1:C:337:PRO:O	1:C:340:GLU:HG3	2.21	0.40
1:C:416:GLY:N	1:C:419:ALA:HB3	2.37	0.40
1:C:983:ARG:HB3	1:C:983:ARG:NH1	2.37	0.40
1:A:65:PHE:HD1	1:A:265:TYR:CZ	2.39	0.40
1:A:88:ASP:O	1:A:270:LEU:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:850:ILE:HD12	1:A:850:ILE:H	1.86	0.40
1:C:48:LEU:HB3	1:C:276:LEU:HD11	2.02	0.40
1:A:357:ARG:NH2	2:C:1210:NAG:O3	2.51	0.40
1:A:566:GLY:CA	1:C:43:PHE:HB3	2.50	0.40
1:B:19:THR:HA	1:B:21:ARG:NH1	2.35	0.40
1:B:187:LYS:O	1:B:209:PRO:HA	2.21	0.40
1:B:210:ILE:HG13	1:B:212:LEU:H	1.86	0.40
1:B:734:THR:OG1	1:B:735:SER:N	2.54	0.40
1:C:1141:LEU:HD23	1:C:1141:LEU:O	2.22	0.40
1:A:141:LEU:HD23	1:A:141:LEU:HA	1.88	0.40
1:B:97:LYS:HG3	1:B:183:GLN:HB3	2.04	0.40
1:C:456:PHE:HB3	1:C:473:TYR:CE1	2.56	0.40
1:A:45:SER:HB3	1:B:568:ASP:OD2	2.21	0.40
1:A:435:ALA:HB2	1:A:510:VAL:HG22	2.03	0.40
1:B:546:LEU:HD22	1:B:565:PHE:HE1	1.86	0.40
1:C:720:ILE:HG13	1:C:923:ILE:HG23	2.02	0.40
1:C:723:THR:HG22	1:C:724:THR:N	2.32	0.40
1:C:993:ILE:O	1:C:997:ILE:HG12	2.22	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	1050/1135 (92%)	969 (92%)	80 (8%)	1 (0%)	51	83
1	B	1050/1135 (92%)	970 (92%)	79 (8%)	1 (0%)	51	83
1	C	1050/1135 (92%)	966 (92%)	84 (8%)	0	100	100
All	All	3150/3405 (92%)	2905 (92%)	243 (8%)	2 (0%)	54	83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1071	GLN
1	A	545	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	929/985 (94%)	924 (100%)	5 (0%)	88	94
1	B	929/985 (94%)	922 (99%)	7 (1%)	81	89
1	C	929/985 (94%)	921 (99%)	8 (1%)	78	88
All	All	2787/2955 (94%)	2767 (99%)	20 (1%)	84	91

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	214	ARG
1	A	333	THR
1	A	645	THR
1	A	815	ARG
1	A	895	GLN
1	B	130	VAL
1	B	165	ASN
1	B	281	GLU
1	B	332	ILE
1	B	582	LEU
1	B	708	SER
1	B	895	GLN
1	C	165	ASN
1	C	214	ARG
1	C	284	THR
1	C	329	PHE
1	C	341	VAL
1	C	342	PHE
1	C	709	ASN
1	C	1074	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	334	ASN
1	A	895	GLN
1	B	66	HIS
1	B	125	ASN
1	B	895	GLN
1	C	949	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

31 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	$\# Z > 2$
2	NAG	B	1206	1	14,14,15	0.30	0	17,19,21	0.63	0
2	NAG	B	1210	1	14,14,15	0.38	0	17,19,21	0.51	0
2	NAG	A	1201	1	14,14,15	0.32	0	17,19,21	0.63	0
2	NAG	A	1202	1	14,14,15	0.40	0	17,19,21	0.73	1 (5%)
2	NAG	C	1203	1	14,14,15	0.27	0	17,19,21	0.88	0
2	NAG	A	1205	1	14,14,15	0.32	0	17,19,21	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1207	1	14,14,15	0.32	0	17,19,21	0.99	0
2	NAG	C	1208	1	14,14,15	0.38	0	17,19,21	0.53	0
2	NAG	A	1208	1	14,14,15	0.32	0	17,19,21	0.68	0
2	NAG	C	1210	1	14,14,15	0.38	0	17,19,21	0.53	0
2	NAG	B	1201	1	14,14,15	0.30	0	17,19,21	0.73	1 (5%)
2	NAG	C	1206	1	14,14,15	0.32	0	17,19,21	0.74	0
2	NAG	A	1206	1	14,14,15	0.28	0	17,19,21	0.59	0
2	NAG	C	1201	1	14,14,15	0.31	0	17,19,21	0.66	0
2	NAG	B	1204	1	14,14,15	0.32	0	17,19,21	0.91	1 (5%)
2	NAG	C	1209	1	14,14,15	0.37	0	17,19,21	0.60	0
2	NAG	C	1202	1	14,14,15	0.30	0	17,19,21	0.62	0
2	NAG	C	1205	1	14,14,15	0.31	0	17,19,21	0.68	0
2	NAG	B	1208	1	14,14,15	0.29	0	17,19,21	1.10	2 (11%)
2	NAG	A	1210	1	14,14,15	0.32	0	17,19,21	0.71	0
2	NAG	C	1204	1	14,14,15	0.31	0	17,19,21	0.76	0
2	NAG	A	1211	1	14,14,15	0.39	0	17,19,21	0.77	1 (5%)
2	NAG	A	1207	1	14,14,15	0.33	0	17,19,21	0.72	1 (5%)
2	NAG	B	1202	1	14,14,15	0.32	0	17,19,21	0.60	0
2	NAG	C	1207	1	14,14,15	0.30	0	17,19,21	0.65	0
2	NAG	A	1204	1	14,14,15	0.28	0	17,19,21	0.73	0
2	NAG	A	1203	1	14,14,15	0.32	0	17,19,21	0.58	0
2	NAG	B	1209	1	14,14,15	0.27	0	17,19,21	0.70	0
2	NAG	A	1209	1	14,14,15	0.30	0	17,19,21	0.64	0
2	NAG	B	1205	1	14,14,15	0.36	0	17,19,21	0.75	0
2	NAG	B	1203	1	14,14,15	0.30	0	17,19,21	0.61	0

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
2	NAG	B	1206	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1210	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1201	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1202	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1203	1	-	4/6/23/26	0/1/1/1
2	NAG	A	1205	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1207	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1208	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1208	1	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1210	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1201	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1206	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1206	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1201	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1204	1	-	4/6/23/26	0/1/1/1
2	NAG	C	1209	1	-	5/6/23/26	0/1/1/1
2	NAG	C	1202	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1205	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1208	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1210	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1204	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1211	1	1/1/5/7	1/6/23/26	0/1/1/1
2	NAG	A	1207	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1202	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1207	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1204	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1203	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1209	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1209	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1205	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1203	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1208	NAG	C2-N2-C7	2.94	127.09	122.90
2	B	1201	NAG	C1-O5-C5	2.33	115.36	112.19
2	B	1208	NAG	C1-O5-C5	2.31	115.32	112.19
2	B	1204	NAG	C1-O5-C5	2.30	115.31	112.19
2	A	1207	NAG	C1-O5-C5	2.07	115.00	112.19
2	A	1211	NAG	C1-O5-C5	2.06	114.98	112.19
2	A	1202	NAG	C1-O5-C5	2.01	114.91	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	1211	NAG	C1

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1206	NAG	C8-C7-N2-C2
2	A	1206	NAG	O7-C7-N2-C2
2	B	1203	NAG	C8-C7-N2-C2
2	B	1203	NAG	O7-C7-N2-C2
2	B	1204	NAG	C8-C7-N2-C2
2	B	1204	NAG	O7-C7-N2-C2
2	B	1205	NAG	C8-C7-N2-C2
2	B	1205	NAG	O7-C7-N2-C2
2	B	1208	NAG	C8-C7-N2-C2
2	B	1208	NAG	O7-C7-N2-C2
2	B	1209	NAG	C8-C7-N2-C2
2	B	1209	NAG	O7-C7-N2-C2
2	B	1210	NAG	C8-C7-N2-C2
2	B	1210	NAG	O7-C7-N2-C2
2	C	1202	NAG	O7-C7-N2-C2
2	C	1203	NAG	C1-C2-N2-C7
2	C	1203	NAG	C8-C7-N2-C2
2	C	1203	NAG	O7-C7-N2-C2
2	C	1207	NAG	C8-C7-N2-C2
2	C	1207	NAG	O7-C7-N2-C2
2	C	1208	NAG	C1-C2-N2-C7
2	C	1208	NAG	C8-C7-N2-C2
2	C	1208	NAG	O7-C7-N2-C2
2	C	1209	NAG	C8-C7-N2-C2
2	C	1209	NAG	O7-C7-N2-C2
2	C	1201	NAG	O7-C7-N2-C2
2	C	1202	NAG	C8-C7-N2-C2
2	A	1209	NAG	C8-C7-N2-C2
2	C	1201	NAG	C8-C7-N2-C2
2	B	1208	NAG	C1-C2-N2-C7
2	A	1209	NAG	O7-C7-N2-C2
2	A	1210	NAG	C8-C7-N2-C2
2	C	1210	NAG	C8-C7-N2-C2
2	C	1210	NAG	O7-C7-N2-C2
2	A	1203	NAG	C8-C7-N2-C2
2	A	1210	NAG	O7-C7-N2-C2
2	A	1201	NAG	C8-C7-N2-C2
2	A	1203	NAG	O7-C7-N2-C2

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Mol	Chain	Res	Type	Atoms
2	A	1211	NAG	O5-C5-C6-O6
2	C	1209	NAG	O5-C5-C6-O6
2	A	1201	NAG	O7-C7-N2-C2
2	C	1209	NAG	C3-C2-N2-C7
2	A	1204	NAG	C8-C7-N2-C2
2	A	1207	NAG	C8-C7-N2-C2
2	B	1204	NAG	C1-C2-N2-C7
2	C	1209	NAG	C1-C2-N2-C7
2	B	1210	NAG	C1-C2-N2-C7
2	A	1207	NAG	O7-C7-N2-C2
2	C	1203	NAG	C3-C2-N2-C7
2	A	1204	NAG	O7-C7-N2-C2
2	C	1206	NAG	C8-C7-N2-C2
2	C	1206	NAG	O7-C7-N2-C2
2	C	1205	NAG	C8-C7-N2-C2
2	B	1204	NAG	C3-C2-N2-C7
2	C	1205	NAG	O7-C7-N2-C2

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1208	NAG	2	0
2	C	1210	NAG	1	0
2	A	1206	NAG	9	0
2	B	1204	NAG	3	0
2	C	1209	NAG	2	0
2	A	1211	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

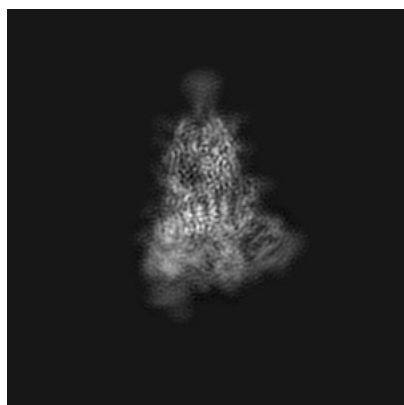
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32000. These allow visual inspection of the internal detail of the map and identification of artifacts.

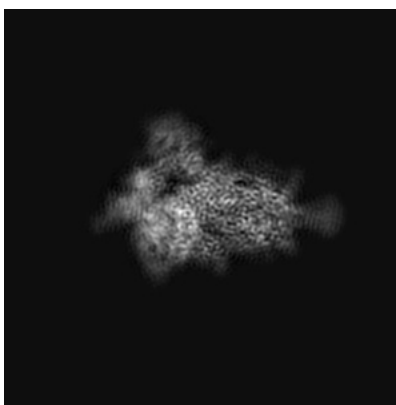
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

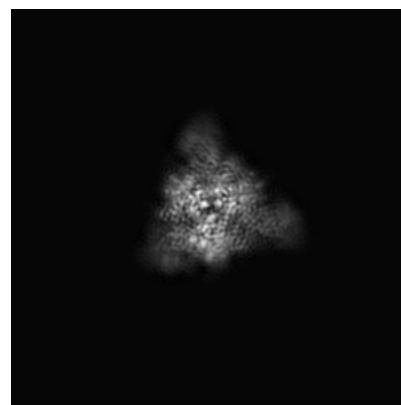
6.1.1 Primary map



X



Y

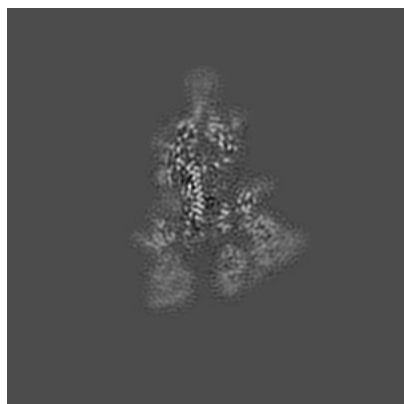


Z

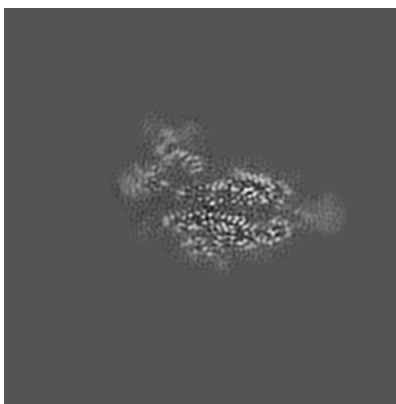
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

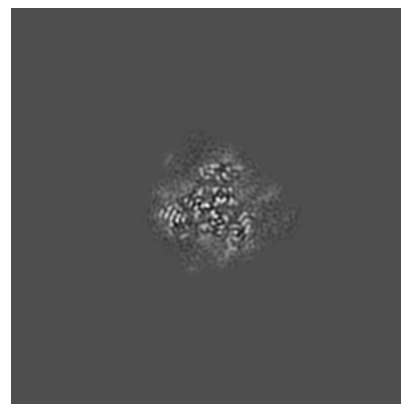
6.2.1 Primary map



X Index: 160



Y Index: 160

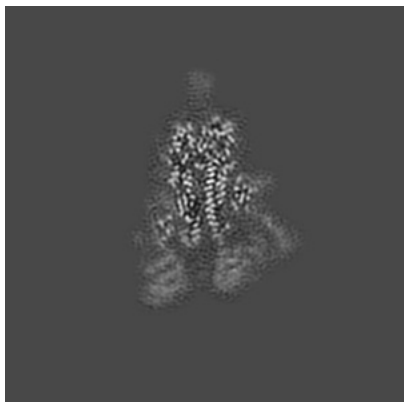


Z Index: 160

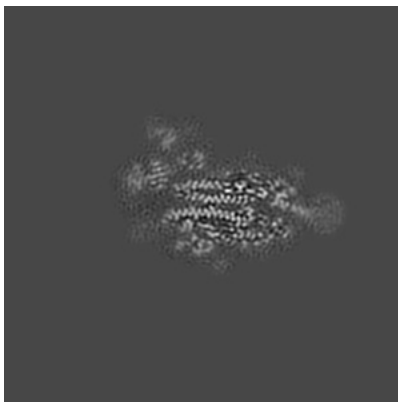
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

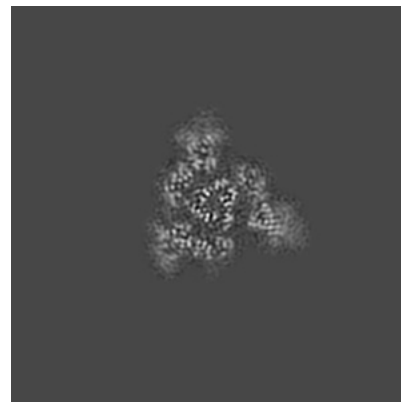
6.3.1 Primary map



X Index: 166



Y Index: 163



Z Index: 142

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

6.4 Orthogonal surface views [i](#)

6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

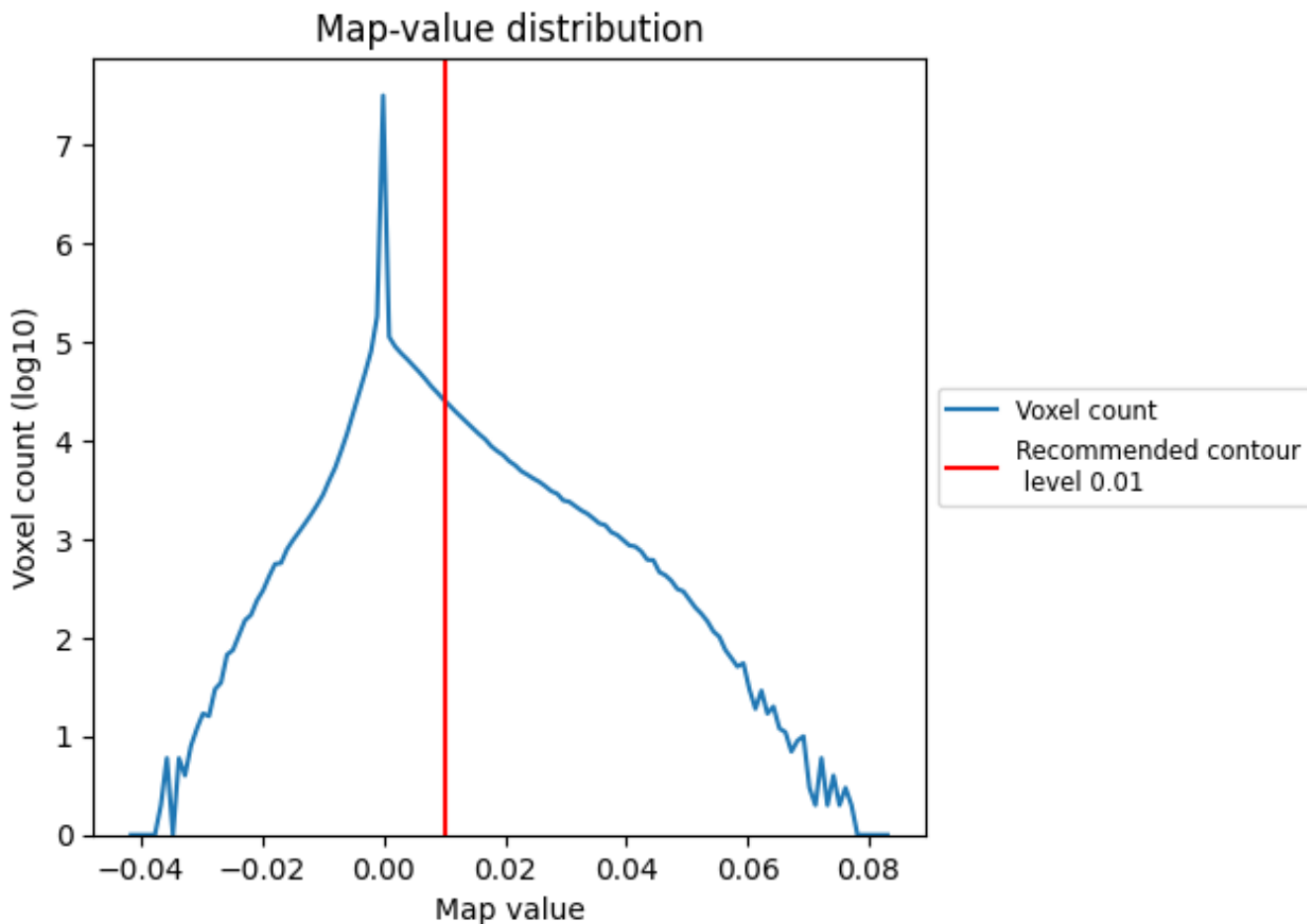
6.5 Mask visualisation

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

7 Map analysis [i](#)

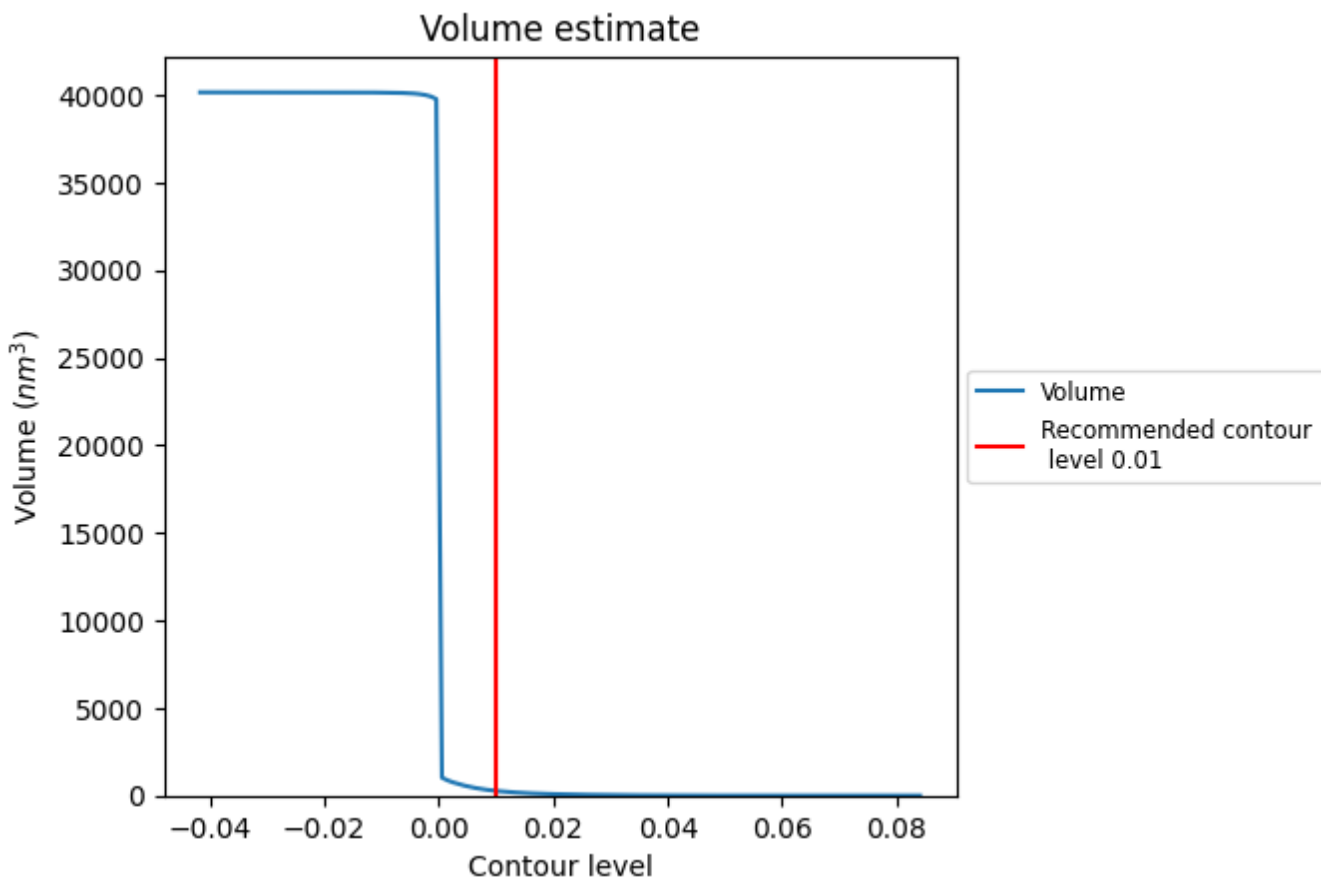
This section contains the results of statistical analysis of the map.

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.

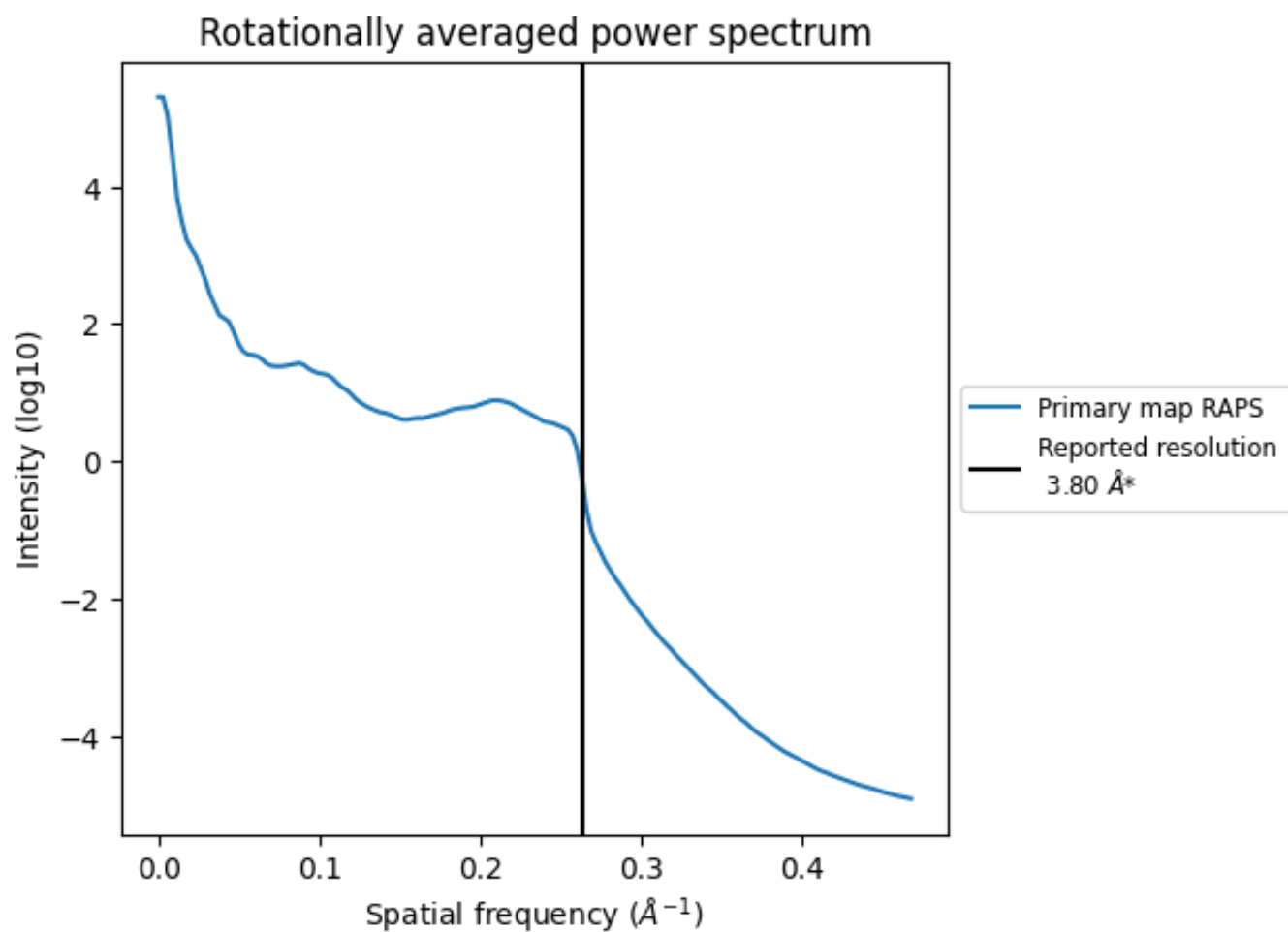
7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 269 nm³; this corresponds to an approximate mass of 243 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 0.263\AA^{-1}

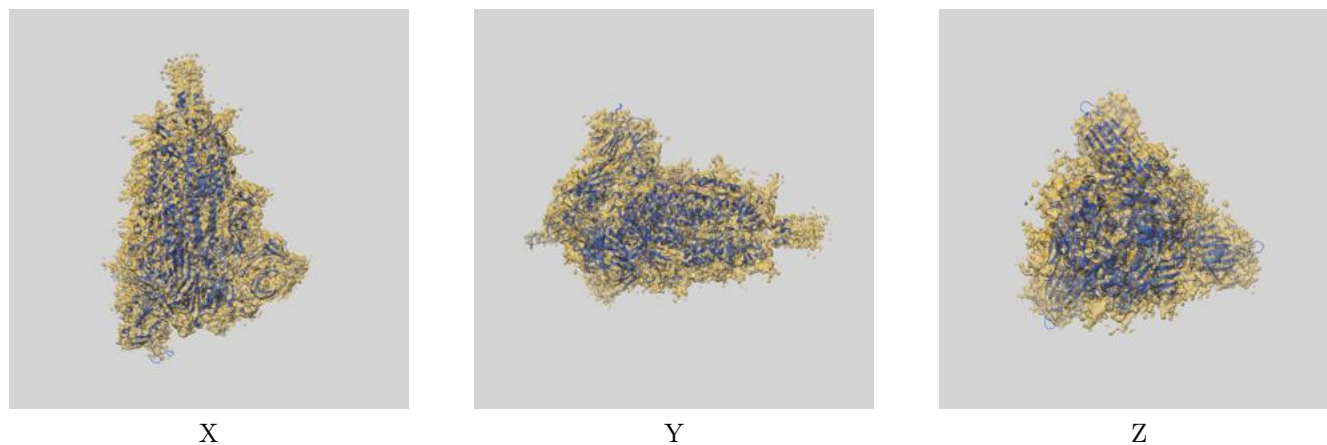
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

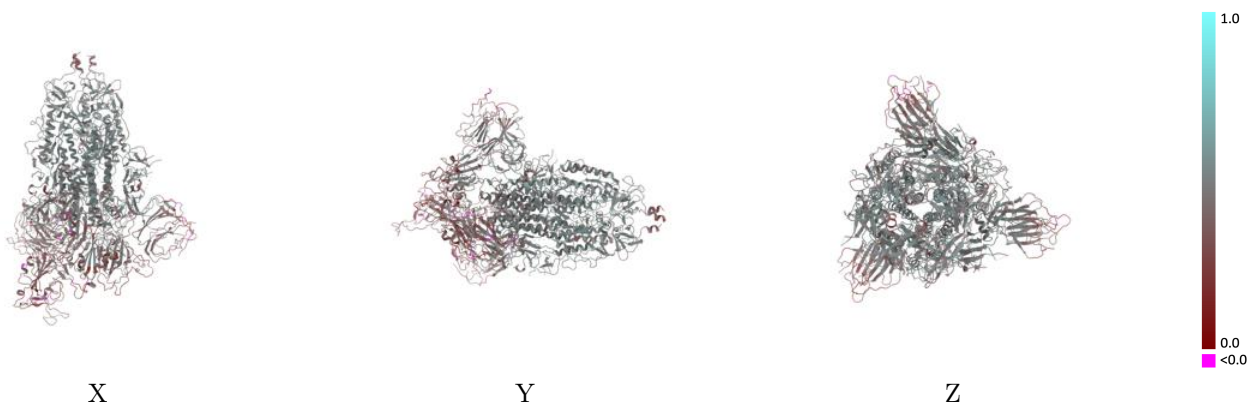
This section contains information regarding the fit between EMDB map EMD-32000 and PDB model 7VHN. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlay [i](#)



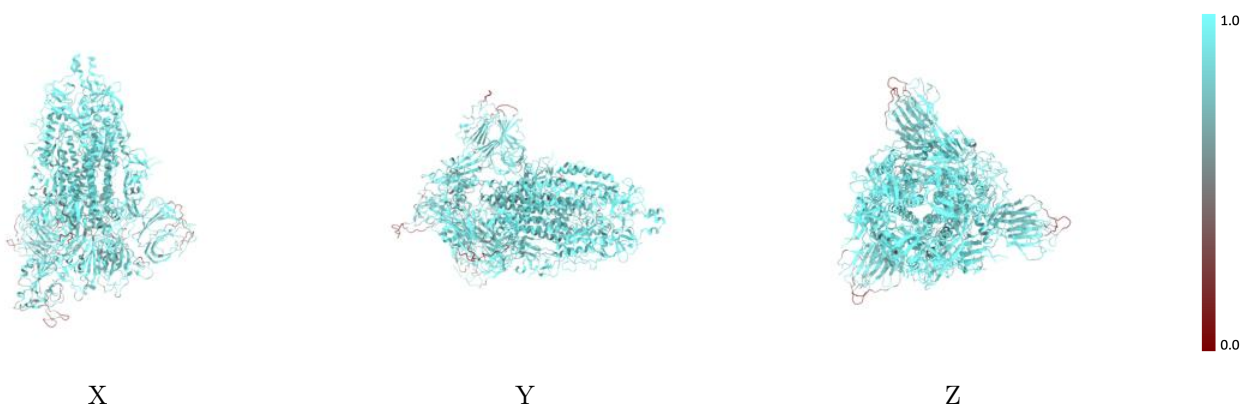
The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



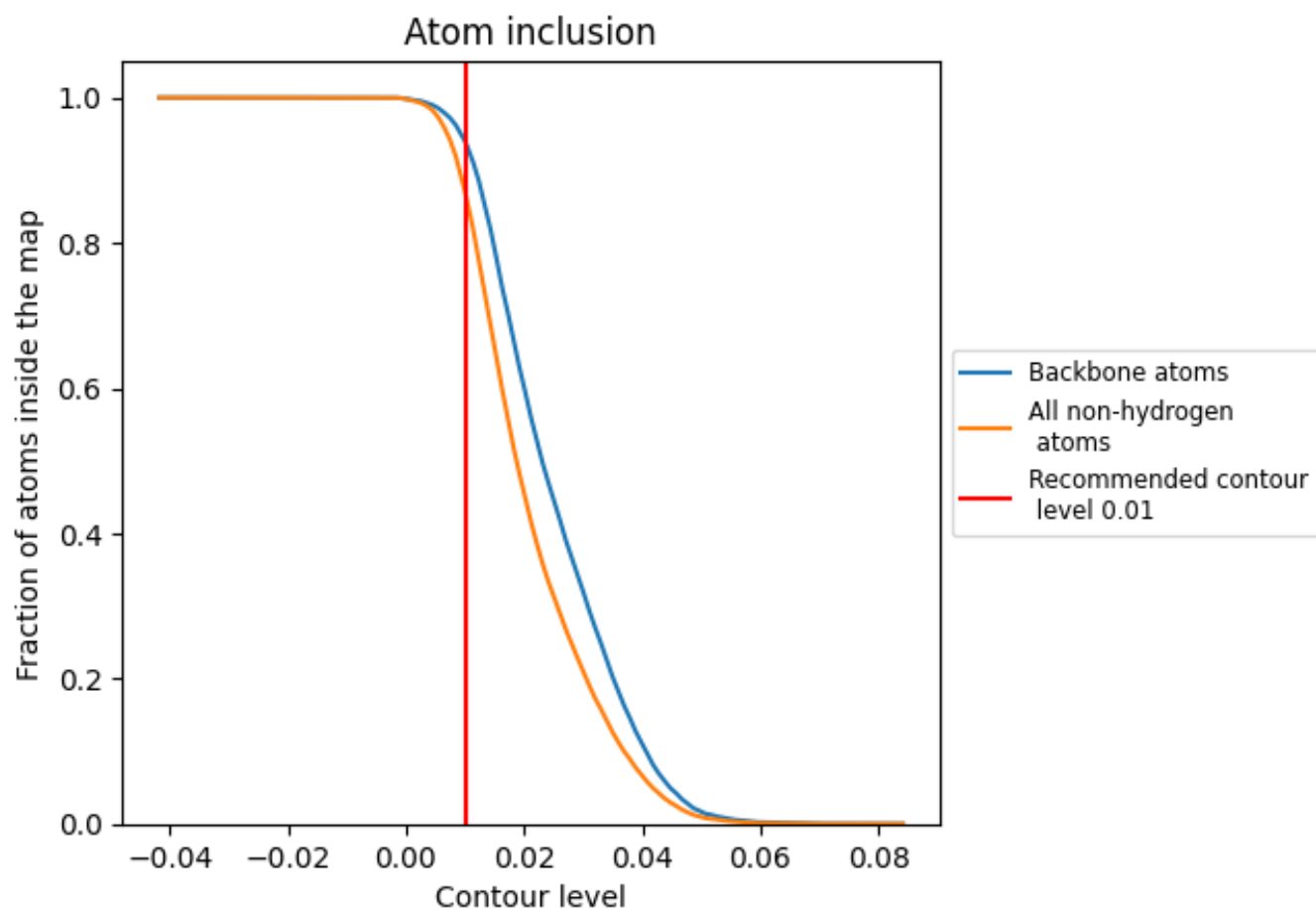
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.01).





9.4 Atom inclusion [i](#)



At the recommended contour level, 94% of all backbone atoms, 87% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.8706	 0.4290
A	 0.8616	 0.4290
B	 0.8790	 0.4330
C	 0.8711	 0.4250

