



Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 01:08 PM UTC

PDB ID : 6VXK / pdb_00006vxk
EMDB ID : EMD-21442
Title : Cryo-EM Structure of the full-length A39R/PlexinC1 complex
Authors : Kuo, Y.-C.; Chen, H.; Shang, G.; Uchikawa, E.; Tian, H.; Bai, X.; Zhang, X.
Deposited on : 2020-02-22
Resolution : 3.10 Å (reported)
Based on initial model : 3NVN

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

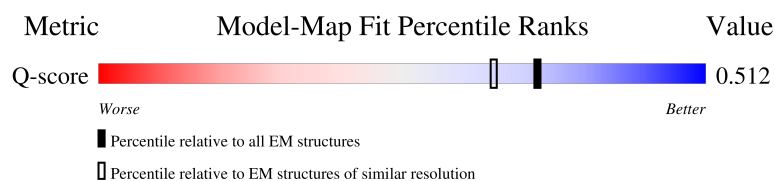
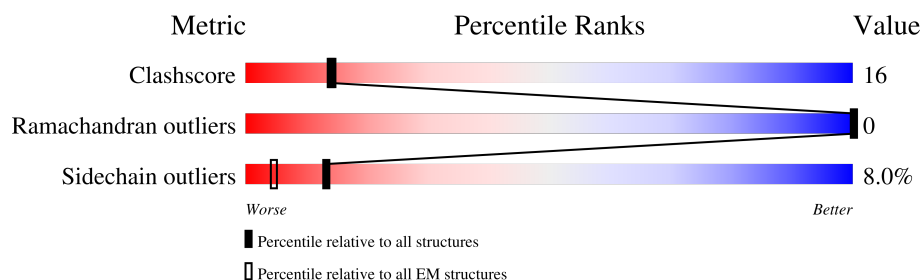
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.10 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14724 (2.60 - 3.60)

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	398	
1	C	398	
2	B	1545	
2	D	1545	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17418 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 Semaphorin-like protein 139.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	380	Total	C	N	O	S	0	0
			3022	1926	500	585	11		
1	C	380	Total	C	N	O	S	0	0
			3022	1926	500	585	11		

There are 26 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	GLU	-	expression tag	UNP Q8JL80
A	13	LEU	-	expression tag	UNP Q8JL80
A	14	GLU	-	expression tag	UNP Q8JL80
A	400	GLY	-	expression tag	UNP Q8JL80
A	401	THR	-	expression tag	UNP Q8JL80
A	402	HIS	-	expression tag	UNP Q8JL80
A	403	HIS	-	expression tag	UNP Q8JL80
A	404	HIS	-	expression tag	UNP Q8JL80
A	405	HIS	-	expression tag	UNP Q8JL80
A	406	HIS	-	expression tag	UNP Q8JL80
A	407	HIS	-	expression tag	UNP Q8JL80
A	408	HIS	-	expression tag	UNP Q8JL80
A	409	HIS	-	expression tag	UNP Q8JL80
C	12	GLU	-	expression tag	UNP Q8JL80
C	13	LEU	-	expression tag	UNP Q8JL80
C	14	GLU	-	expression tag	UNP Q8JL80
C	400	GLY	-	expression tag	UNP Q8JL80
C	401	THR	-	expression tag	UNP Q8JL80
C	402	HIS	-	expression tag	UNP Q8JL80
C	403	HIS	-	expression tag	UNP Q8JL80
C	404	HIS	-	expression tag	UNP Q8JL80
C	405	HIS	-	expression tag	UNP Q8JL80
C	406	HIS	-	expression tag	UNP Q8JL80
C	407	HIS	-	expression tag	UNP Q8JL80
C	408	HIS	-	expression tag	UNP Q8JL80
C	409	HIS	-	expression tag	UNP Q8JL80

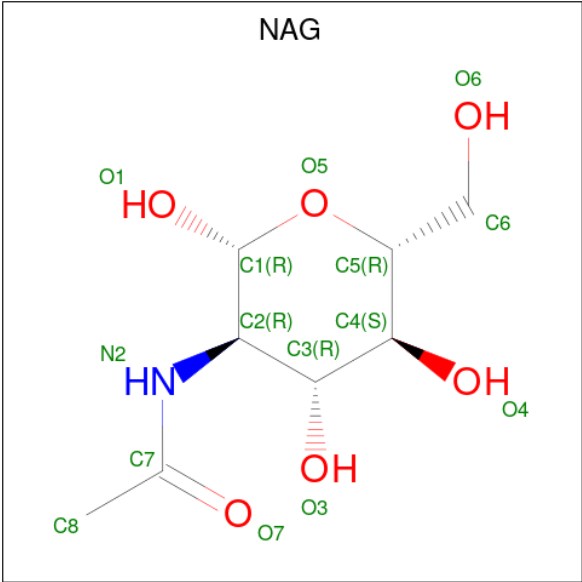
- Molecule 2 is a protein called Plexin-C1.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	747	Total	C	N	O	S	0	0
			5561	3496	971	1056	38		
2	D	747	Total	C	N	O	S	0	0
			5561	3496	971	1056	38		

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	1569	GLY	-	expression tag	UNP O60486
B	1570	THR	-	expression tag	UNP O60486
B	1571	SER	-	expression tag	UNP O60486
B	1572	SER	-	expression tag	UNP O60486
B	1573	GLY	-	expression tag	UNP O60486
B	1574	LEU	-	expression tag	UNP O60486
B	1575	GLU	-	expression tag	UNP O60486
B	1576	VAL	-	expression tag	UNP O60486
B	1577	LEU	-	expression tag	UNP O60486
B	1578	PHE	-	expression tag	UNP O60486
B	1579	GLN	-	expression tag	UNP O60486
D	1569	GLY	-	expression tag	UNP O60486
D	1570	THR	-	expression tag	UNP O60486
D	1571	SER	-	expression tag	UNP O60486
D	1572	SER	-	expression tag	UNP O60486
D	1573	GLY	-	expression tag	UNP O60486
D	1574	LEU	-	expression tag	UNP O60486
D	1575	GLU	-	expression tag	UNP O60486
D	1576	VAL	-	expression tag	UNP O60486
D	1577	LEU	-	expression tag	UNP O60486
D	1578	PHE	-	expression tag	UNP O60486
D	1579	GLN	-	expression tag	UNP O60486

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

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



ILE	VAL	LYS	TYR	PHE	ASP	GLU	ILE	LEU	LEU	LYS	LEU	GLU	ARG	GLU	ARG	GLY	LEU	GLU	GLU	ALA	GLN	LYS	GLN	LEU	LEU	HIS	VAL	LYS	VAL	LEU	LEU	PHE	ASP	GLU	LYS	LYS	CYS	CYS	LYS	TRP	MET	GLY	THR	SER	SER	GLY	LEU	LEU	GLU	VAL	LEU	PHE	ILE
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Chain D: 31% 16% 52%



[illegible]

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	143750	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.059	Depositor
Minimum map value	-0.020	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.009	Depositor
Map size (Å)	298.08002, 298.08002, 298.08002	wwPDB
Map dimensions	360, 360, 360	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.82800007, 0.82800007, 0.82800007	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	0.58	0/3093	0.51	0/4195
1	C	0.58	0/3093	0.51	0/4195
2	B	0.46	0/5663	0.49	3/7689 (0.0%)
2	D	0.46	0/5663	0.48	4/7689 (0.1%)
All	All	0.50	0/17512	0.49	7/23768 (0.0%)

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	411	ASN	CA-C-N	-5.85	112.83	120.67
2	B	411	ASN	C-N-CA	-5.85	112.83	120.67
2	D	411	ASN	CA-C-N	-5.85	112.83	120.67
2	D	411	ASN	C-N-CA	-5.85	112.83	120.67
2	D	806	CYS	CA-CB-SG	5.12	126.17	114.40
2	B	806	CYS	CA-CB-SG	5.10	126.13	114.40
2	D	801	CYS	N-CA-C	5.03	117.32	109.52

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	3022	0	2956	91	0
1	C	3022	0	2956	89	0
2	B	5561	0	5301	173	0
2	D	5561	0	5301	181	0
3	A	14	0	13	0	0
3	B	112	0	104	4	0
3	C	14	0	13	0	0
3	D	112	0	104	4	0
All	All	17418	0	16748	530	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 16.

All (530) 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:D:507:PRO:HA	2:D:524:VAL:O	1.45	1.14
2:B:507:PRO:HA	2:B:524:VAL:O	1.45	1.12
2:D:536:VAL:O	2:D:544:GLU:HA	1.62	0.99
2:B:536:VAL:O	2:B:544:GLU:HA	1.62	0.99
2:B:783:ASP:H	2:B:828:VAL:HG12	1.43	0.82
2:D:783:ASP:H	2:D:828:VAL:HG12	1.43	0.82
2:B:402:VAL:HG12	2:B:413:PRO:HB3	1.71	0.73
2:D:402:VAL:HG12	2:D:413:PRO:HB3	1.71	0.72
2:B:446:GLU:OE1	2:B:448:ARG:NH2	2.23	0.71
2:D:510:GLN:O	2:D:521:VAL:HA	1.91	0.71
2:B:510:GLN:O	2:B:521:VAL:HA	1.90	0.71
1:C:36:LEU:HB3	1:C:47:PHE:HB3	1.73	0.71
1:A:345:ILE:HD11	1:A:369:LEU:HD22	1.73	0.70
2:B:430:VAL:HG23	2:B:440:TYR:HB2	1.73	0.70
2:D:247:PRO:HG3	2:D:264:MET:HE2	1.73	0.70
1:C:345:ILE:HD11	1:C:369:LEU:HD22	1.73	0.70
2:D:430:VAL:HG23	2:D:440:TYR:HB2	1.73	0.70
1:C:44:VAL:HG21	1:C:75:VAL:HG11	1.74	0.69
1:C:331:LYS:HB2	1:C:374:VAL:HG11	1.73	0.69
2:D:446:GLU:OE1	2:D:448:ARG:NH2	2.23	0.69
1:A:36:LEU:HB3	1:A:47:PHE:HB3	1.73	0.69
1:A:331:LYS:HB2	1:A:374:VAL:HG11	1.73	0.69
2:B:247:PRO:HG3	2:B:264:MET:HE2	1.73	0.69
1:A:44:VAL:HG21	1:A:75:VAL:HG11	1.74	0.67
2:B:98:ARG:NH1	2:B:395:GLY:O	2.28	0.67
1:A:216:GLU:HB2	1:A:310:ILE:HD11	1.77	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:GLN:HE21	2:B:88:THR:HA	1.59	0.66
2:D:827:ARG:HH21	2:D:830:ASP:H	1.43	0.66
1:C:216:GLU:HB2	1:C:310:ILE:HD11	1.77	0.66
2:B:311:SER:HB2	2:B:326:THR:HG22	1.78	0.66
2:D:98:ARG:NH1	2:D:395:GLY:O	2.28	0.66
1:A:73:THR:O	1:A:73:THR:OG1	2.14	0.66
2:D:44:GLN:HE21	2:D:88:THR:HA	1.59	0.65
1:A:214:GLU:OE2	1:C:181:ARG:NH2	2.27	0.65
1:C:60:ASN:HD22	1:C:80:ASN:HB2	1.61	0.65
2:D:311:SER:HB2	2:D:326:THR:HG22	1.78	0.65
2:B:827:ARG:HH21	2:B:830:ASP:H	1.43	0.65
2:B:175:TRP:O	2:B:210:THR:OG1	2.12	0.65
2:D:784:ASN:HD21	2:D:827:ARG:HH11	1.45	0.65
1:A:60:ASN:HD22	1:A:80:ASN:HB2	1.60	0.65
2:D:700:THR:HG22	2:D:702:THR:H	1.62	0.65
2:B:784:ASN:HD21	2:B:827:ARG:HH11	1.45	0.64
1:A:283:PRO:HB3	1:A:301:ILE:HD13	1.79	0.64
2:D:175:TRP:O	2:D:210:THR:OG1	2.12	0.64
1:A:369:LEU:HD23	1:A:382:ALA:HB2	1.79	0.64
1:C:369:LEU:HD23	1:C:382:ALA:HB2	1.79	0.64
2:B:700:THR:HG22	2:B:702:THR:H	1.63	0.64
1:C:283:PRO:HB3	1:C:301:ILE:HD13	1.79	0.64
1:C:127:GLU:HB3	2:D:350:ALA:HB1	1.80	0.64
1:A:116:GLU:HB2	1:A:138:PRO:HG2	1.79	0.63
2:D:766:ILE:N	2:D:841:ARG:O	2.25	0.63
1:C:116:GLU:HB2	1:C:138:PRO:HG2	1.79	0.63
2:B:205:ILE:HD12	2:B:223:LEU:HD23	1.80	0.63
1:C:48:SER:O	1:C:51:GLU:HB2	1.98	0.63
1:A:24:GLU:OE2	1:A:45:TYR:OH	2.16	0.63
1:A:48:SER:O	1:A:51:GLU:HB2	1.98	0.62
1:A:181:ARG:HD2	1:C:225:ARG:NH2	2.14	0.62
2:B:766:ILE:N	2:B:841:ARG:O	2.25	0.62
1:A:333:LYS:HE3	1:A:341:ARG:HH21	1.64	0.62
2:D:780:ASP:N	2:D:780:ASP:OD1	2.30	0.62
2:B:726:SER:OG	2:B:727:ARG:N	2.32	0.62
2:B:780:ASP:OD1	2:B:780:ASP:N	2.30	0.62
1:C:333:LYS:HE3	1:C:341:ARG:HH21	1.64	0.62
1:C:24:GLU:OE2	1:C:45:TYR:OH	2.16	0.62
1:C:236:ASP:OD2	1:C:338:ARG:NH2	2.32	0.62
2:D:104:SER:OG	2:D:105:PHE:N	2.32	0.61
2:D:205:ILE:HD12	2:D:223:LEU:HD23	1.80	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:442:THR:HG23	2:D:447:VAL:HG22	1.82	0.61
2:B:442:THR:HG23	2:B:447:VAL:HG22	1.82	0.61
1:C:247:SER:OG	1:C:251:LYS:O	2.18	0.61
1:A:236:ASP:OD2	1:A:338:ARG:NH2	2.32	0.61
2:D:227:GLU:OE1	2:D:227:GLU:N	2.33	0.61
2:D:726:SER:OG	2:D:727:ARG:N	2.32	0.61
2:B:475:CYS:O	2:B:479:GLN:N	2.34	0.61
2:D:287:HIS:ND1	2:D:324:THR:O	2.34	0.61
1:A:247:SER:OG	1:A:251:LYS:O	2.18	0.61
2:D:660:GLN:NE2	2:D:689:ARG:O	2.34	0.60
2:D:889:LEU:HA	2:D:909:ILE:HG12	1.83	0.60
2:B:660:GLN:NE2	2:B:689:ARG:O	2.34	0.60
2:D:324:THR:O	2:D:324:THR:OG1	2.19	0.60
2:B:104:SER:OG	2:B:105:PHE:N	2.32	0.60
1:C:70:VAL:HG23	1:C:71:GLU:H	1.67	0.60
2:D:475:CYS:O	2:D:479:GLN:N	2.34	0.60
1:A:246:ASP:OD1	1:A:247:SER:N	2.34	0.60
1:C:246:ASP:OD1	1:C:247:SER:N	2.34	0.60
2:B:287:HIS:ND1	2:B:324:THR:O	2.34	0.60
1:C:73:THR:O	1:C:73:THR:OG1	2.14	0.59
1:C:333:LYS:NZ	1:C:354:ASP:OD2	2.26	0.59
2:D:789:HIS:O	2:D:793:GLY:N	2.36	0.59
2:B:889:LEU:HA	2:B:909:ILE:HG12	1.83	0.59
2:D:42:SER:OG	2:D:43:GLU:N	2.35	0.59
1:A:70:VAL:HG23	1:A:71:GLU:H	1.67	0.59
2:B:42:SER:OG	2:B:43:GLU:N	2.35	0.58
1:A:225:ARG:NH2	1:C:181:ARG:HD2	2.19	0.58
2:B:789:HIS:O	2:B:793:GLY:N	2.36	0.58
2:D:700:THR:OG1	2:D:729:GLU:OE2	2.16	0.58
1:A:309:ASP:OD1	1:A:310:ILE:N	2.35	0.58
2:B:227:GLU:OE1	2:B:227:GLU:N	2.33	0.58
1:A:60:ASN:OD1	1:A:60:ASN:N	2.38	0.57
2:B:324:THR:O	2:B:324:THR:OG1	2.19	0.57
1:C:309:ASP:OD1	1:C:310:ILE:N	2.35	0.57
2:B:172:ASN:OD1	2:B:172:ASN:N	2.36	0.57
2:D:172:ASN:OD1	2:D:172:ASN:N	2.36	0.57
1:A:266:PHE:HA	1:A:307:LEU:HD11	1.87	0.57
1:C:220:ASP:OD1	1:C:222:ARG:NH2	2.38	0.57
2:D:44:GLN:N	2:D:44:GLN:OE1	2.38	0.57
2:B:784:ASN:ND2	2:B:827:ARG:HH11	2.02	0.57
1:A:127:GLU:HB3	2:B:350:ALA:HB1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:ASP:OD1	1:A:222:ARG:NH2	2.38	0.56
2:B:44:GLN:N	2:B:44:GLN:OE1	2.38	0.56
2:D:696:ILE:HB	2:D:734:CYS:SG	2.46	0.56
2:B:730:MET:HA	2:B:749:SER:HA	1.87	0.56
2:B:696:ILE:HB	2:B:734:CYS:SG	2.46	0.56
2:B:580:SER:HG	2:B:581:TRP:HD1	1.53	0.56
1:C:132:TRP:NE1	1:C:191:MET:SD	2.78	0.56
2:D:784:ASN:ND2	2:D:827:ARG:HH11	2.02	0.56
1:A:252:SER:OG	1:A:322:PRO:O	2.20	0.56
1:A:132:TRP:NE1	1:A:191:MET:SD	2.78	0.56
1:A:224:TYR:OH	1:A:320:GLU:OE2	2.20	0.56
1:C:252:SER:OG	1:C:322:PRO:O	2.20	0.55
1:C:266:PHE:HA	1:C:307:LEU:HD11	1.87	0.55
2:B:326:THR:HG21	2:B:376:LEU:H	1.71	0.55
2:D:326:THR:HG21	2:D:376:LEU:H	1.71	0.55
2:B:766:ILE:HA	2:B:840:TYR:HB3	1.88	0.55
2:D:421:GLU:N	2:D:421:GLU:OE1	2.40	0.55
2:B:784:ASN:HD21	2:B:827:ARG:HD3	1.72	0.55
2:D:300:VAL:HG22	2:D:381:GLY:HA3	1.89	0.55
2:D:783:ASP:HB2	2:D:828:VAL:HA	1.89	0.55
2:D:785:LEU:HD11	2:D:824:VAL:HB	1.89	0.55
1:C:46:THR:OG1	1:C:53:ASN:O	2.24	0.55
2:D:730:MET:HA	2:D:749:SER:HA	1.88	0.55
2:B:783:ASP:HB2	2:B:828:VAL:HA	1.89	0.55
1:C:60:ASN:OD1	1:C:60:ASN:N	2.37	0.55
2:B:421:GLU:OE1	2:B:421:GLU:N	2.40	0.55
2:B:786:ILE:HG13	2:B:832:TYR:HE1	1.72	0.55
1:C:44:VAL:HG22	1:C:64:ILE:HG21	1.89	0.54
1:C:375:THR:OG1	1:C:376:SER:N	2.41	0.54
2:D:784:ASN:HD21	2:D:827:ARG:HD3	1.72	0.54
1:A:222:ARG:NH1	1:A:320:GLU:OE1	2.41	0.54
2:B:110:LEU:HD11	2:B:166:VAL:HG13	1.90	0.54
2:D:766:ILE:HA	2:D:840:TYR:HB3	1.88	0.54
2:D:786:ILE:HG13	2:D:832:TYR:HE1	1.72	0.54
2:B:660:GLN:OE1	2:B:660:GLN:N	2.39	0.54
2:D:52:SER:OG	2:D:56:GLY:O	2.25	0.54
2:D:110:LEU:HD11	2:D:166:VAL:HG13	1.90	0.54
2:D:820:THR:N	2:D:840:TYR:O	2.41	0.54
2:D:827:ARG:HA	2:D:831:THR:O	2.08	0.54
1:C:45:TYR:CE2	1:C:54:LYS:HB2	2.43	0.53
2:D:660:GLN:OE1	2:D:660:GLN:N	2.40	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:785:LEU:HD11	2:B:824:VAL:HB	1.89	0.53
2:D:403:ILE:HD13	2:D:470:PRO:HD3	1.90	0.53
2:B:300:VAL:HG22	2:B:381:GLY:HA3	1.89	0.53
2:B:573:ASN:HA	2:B:586:ARG:HA	1.90	0.53
2:D:573:ASN:HA	2:D:586:ARG:HA	1.90	0.53
1:C:222:ARG:NH1	1:C:320:GLU:OE1	2.41	0.53
1:A:44:VAL:HG22	1:A:64:ILE:HG21	1.89	0.53
2:B:403:ILE:HD13	2:B:470:PRO:HD3	1.90	0.53
1:A:375:THR:OG1	1:A:376:SER:N	2.41	0.53
2:B:820:THR:N	2:B:840:TYR:O	2.41	0.53
1:A:287:LEU:HD23	1:A:291:LYS:HB3	1.91	0.53
1:C:228:ILE:HD11	1:C:246:ASP:HB2	1.90	0.53
2:B:785:LEU:HD12	2:B:786:ILE:H	1.74	0.53
2:D:785:LEU:HD12	2:D:786:ILE:H	1.74	0.53
1:A:45:TYR:CE2	1:A:54:LYS:HB2	2.43	0.53
2:B:52:SER:OG	2:B:56:GLY:O	2.25	0.53
2:B:782:ILE:HD11	2:B:826:LEU:HD13	1.91	0.53
3:B:1608:NAG:H83	3:B:1608:NAG:H3	1.91	0.53
2:D:98:ARG:HH11	2:D:424:PRO:HB3	1.74	0.53
2:D:782:ILE:HD11	2:D:826:LEU:HD13	1.91	0.53
1:C:220:ASP:HB2	1:C:222:ARG:HE	1.73	0.52
2:B:492:ASN:OD1	2:B:492:ASN:N	2.42	0.52
2:B:536:VAL:O	2:B:544:GLU:CA	2.48	0.52
2:B:575:MET:HE3	2:B:577:SER:HB2	1.92	0.52
2:D:390:LEU:HB2	2:D:402:VAL:HG22	1.91	0.52
2:D:575:MET:HE3	2:D:577:SER:HB2	1.91	0.52
1:C:287:LEU:HD23	1:C:291:LYS:HB3	1.91	0.52
2:B:827:ARG:HA	2:B:831:THR:O	2.08	0.52
1:A:46:THR:OG1	1:A:53:ASN:O	2.24	0.52
1:A:220:ASP:HB2	1:A:222:ARG:HE	1.73	0.52
2:D:678:SER:OG	2:D:679:ASN:OD1	2.25	0.52
3:D:1604:NAG:O7	3:D:1604:NAG:O3	2.25	0.52
3:D:1608:NAG:H83	3:D:1608:NAG:H3	1.91	0.52
2:B:44:GLN:NE2	2:B:87:CYS:O	2.43	0.52
2:B:765:TRP:HZ3	2:B:930:GLY:HA3	1.75	0.52
2:D:44:GLN:NE2	2:D:87:CYS:O	2.43	0.52
2:D:675:LEU:HD12	2:D:753:LEU:HD21	1.92	0.52
2:D:824:VAL:HG23	2:D:835:CYS:HB2	1.92	0.52
1:A:228:ILE:HD11	1:A:246:ASP:HB2	1.90	0.52
2:B:870:PHE:HB2	2:B:872:ILE:HD11	1.92	0.52
2:D:492:ASN:OD1	2:D:492:ASN:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:870:PHE:HB2	2:D:872:ILE:HD11	1.92	0.52
2:B:98:ARG:HH11	2:B:424:PRO:HB3	1.74	0.52
2:B:268:ALA:HB3	2:B:274:LEU:HB3	1.91	0.51
2:D:761:PRO:HG2	2:D:772:ILE:HD13	1.92	0.51
1:A:27:ILE:HD13	1:A:63:TYR:HB3	1.92	0.51
2:B:824:VAL:HG23	2:B:835:CYS:HB2	1.92	0.51
1:C:19:LYS:HA	1:C:385:GLY:HA3	1.93	0.51
1:C:27:ILE:HD13	1:C:63:TYR:HB3	1.92	0.51
2:B:344:SER:HB2	2:B:349:THR:OG1	2.11	0.51
2:B:761:PRO:HG2	2:B:772:ILE:HD13	1.92	0.51
2:D:268:ALA:HB3	2:D:274:LEU:HB3	1.91	0.51
1:A:298:PHE:HA	1:A:301:ILE:HG22	1.93	0.51
2:B:700:THR:OG1	2:B:729:GLU:OE2	2.16	0.51
2:B:675:LEU:HD12	2:B:753:LEU:HD21	1.92	0.51
1:C:16:GLU:OE1	1:C:18:HIS:NE2	2.43	0.51
2:B:390:LEU:HB2	2:B:402:VAL:HG22	1.91	0.51
2:B:580:SER:HG	2:B:581:TRP:CD1	2.29	0.51
2:D:765:TRP:HZ3	2:D:930:GLY:HA3	1.75	0.51
2:D:872:ILE:HD12	2:D:872:ILE:H	1.75	0.51
2:B:694:THR:HG22	2:B:709:GLN:HE22	1.76	0.50
2:B:872:ILE:HD12	2:B:872:ILE:H	1.75	0.50
1:C:349:THR:OG1	1:C:364:GLN:OE1	2.29	0.50
1:A:16:GLU:OE1	1:A:18:HIS:NE2	2.43	0.50
2:D:344:SER:HB2	2:D:349:THR:OG1	2.11	0.50
1:C:79:ASN:OD1	1:C:84:LYS:HB3	2.11	0.50
1:C:298:PHE:HA	1:C:301:ILE:HG22	1.93	0.50
1:A:72:ASP:HB2	1:A:87:LYS:HD2	1.93	0.50
1:A:79:ASN:OD1	1:A:84:LYS:HB3	2.11	0.50
1:A:349:THR:OG1	1:A:364:GLN:OE1	2.29	0.50
1:C:72:ASP:HB2	1:C:87:LYS:HD2	1.93	0.50
1:A:19:LYS:HA	1:A:385:GLY:HA3	1.93	0.50
2:B:820:THR:O	2:B:840:TYR:N	2.41	0.50
2:D:91:VAL:HG22	2:D:105:PHE:HZ	1.77	0.50
2:D:871:ASN:HB3	3:D:1608:NAG:O5	2.11	0.50
2:B:802:VAL:HG22	2:B:803:ALA:H	1.77	0.49
1:C:236:ASP:OD1	1:C:236:ASP:N	2.43	0.49
2:D:755:HIS:CE1	2:D:777:ARG:HB2	2.47	0.49
2:D:802:VAL:HG22	2:D:803:ALA:H	1.77	0.49
2:B:678:SER:OG	2:B:679:ASN:OD1	2.25	0.49
2:D:694:THR:HG22	2:D:709:GLN:HE22	1.76	0.49
2:D:407:ASN:OD1	2:D:407:ASN:N	2.36	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:580:SER:HG	2:D:581:TRP:HD1	1.59	0.49
2:B:532:SER:OG	2:B:533:LYS:N	2.46	0.49
2:D:879:ILE:HA	2:D:926:ARG:O	2.12	0.49
1:A:218:ASP:OD1	1:A:218:ASP:N	2.45	0.49
2:B:871:ASN:HB3	3:B:1608:NAG:O5	2.11	0.49
2:B:764:THR:O	2:B:840:TYR:HA	2.13	0.49
1:C:224:TYR:OH	1:C:320:GLU:OE2	2.20	0.49
2:B:879:ILE:HA	2:B:926:ARG:O	2.12	0.49
1:A:60:ASN:ND2	1:A:80:ASN:HB2	2.28	0.49
2:B:755:HIS:CE1	2:B:777:ARG:HB2	2.47	0.48
2:D:764:THR:O	2:D:840:TYR:HA	2.13	0.48
1:A:236:ASP:N	1:A:236:ASP:OD1	2.44	0.48
1:C:218:ASP:N	1:C:218:ASP:OD1	2.45	0.48
1:C:372:VAL:HG22	1:C:380:PHE:HD1	1.78	0.48
2:D:679:ASN:HB3	2:D:720:LYS:HE2	1.94	0.48
2:D:697:LEU:HA	2:D:732:ASP:O	2.13	0.48
2:B:697:LEU:HA	2:B:732:ASP:O	2.13	0.48
2:D:457:LYS:HE3	2:D:458:HIS:CE1	2.49	0.48
1:A:372:VAL:HG22	1:A:380:PHE:HD1	1.78	0.48
2:B:227:GLU:H	2:B:227:GLU:CD	2.22	0.48
2:B:407:ASN:OD1	2:B:407:ASN:N	2.36	0.48
2:B:679:ASN:HB3	2:B:720:LYS:HE2	1.94	0.48
1:A:264:HIS:CE1	1:A:268:THR:HG21	2.49	0.48
2:B:874:LYS:HG2	2:B:889:LEU:HD22	1.96	0.48
1:C:264:HIS:CE1	1:C:268:THR:HG21	2.49	0.48
2:D:660:GLN:HE21	2:D:689:ARG:HB3	1.78	0.48
2:D:761:PRO:HD2	2:D:772:ILE:HG23	1.94	0.48
1:A:201:SER:OG	2:B:215:LEU:O	2.17	0.48
2:B:91:VAL:HG22	2:B:105:PHE:HZ	1.77	0.48
1:C:201:SER:OG	2:D:215:LEU:O	2.22	0.48
1:A:181:ARG:NH2	1:C:214:GLU:OE2	2.38	0.48
2:B:457:LYS:HE3	2:B:458:HIS:CE1	2.49	0.47
1:C:26:ILE:HD13	1:C:40:VAL:HG23	1.96	0.47
1:C:60:ASN:ND2	1:C:80:ASN:HB2	2.28	0.47
1:C:280:SER:OG	1:C:281:PRO:HD3	2.14	0.47
1:A:168:LYS:HE2	1:A:286:CYS:SG	2.55	0.47
1:A:280:SER:OG	1:A:281:PRO:HD3	2.14	0.47
2:B:761:PRO:HD2	2:B:772:ILE:HG23	1.94	0.47
3:B:1604:NAG:O7	3:B:1604:NAG:O3	2.25	0.47
2:D:536:VAL:O	2:D:544:GLU:CA	2.48	0.47
2:D:874:LYS:HG2	2:D:889:LEU:HD22	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:GLU:HG3	1:A:218:ASP:OD1	2.15	0.47
1:A:235:THR:OG1	1:A:238:ASP:O	2.20	0.47
2:B:765:TRP:O	2:B:768:GLY:N	2.45	0.47
1:C:68:ILE:HG21	1:C:111:ILE:HG12	1.96	0.47
1:A:26:ILE:HD13	1:A:40:VAL:HG23	1.96	0.47
1:A:37:TYR:CE1	1:A:46:THR:HG22	2.50	0.47
2:B:324:THR:HB	2:B:372:ILE:HG21	1.97	0.47
2:B:676:GLY:O	2:B:829:GLN:HG3	2.15	0.47
1:C:33:ASP:N	1:C:33:ASP:OD2	2.47	0.47
2:B:660:GLN:HE21	2:B:689:ARG:HB3	1.78	0.47
2:B:536:VAL:HG12	2:B:574:VAL:HG13	1.96	0.47
1:C:37:TYR:CE1	1:C:46:THR:HG22	2.50	0.47
1:C:168:LYS:HE2	1:C:286:CYS:SG	2.55	0.47
2:D:344:SER:O	2:D:344:SER:OG	2.29	0.47
2:D:671:LYS:NZ	2:D:780:ASP:OD2	2.48	0.47
2:D:676:GLY:O	2:D:829:GLN:HG3	2.15	0.47
2:D:765:TRP:O	2:D:768:GLY:N	2.45	0.47
2:B:99:PRO:HG2	2:B:314:ALA:HB3	1.97	0.47
2:B:580:SER:OG	2:B:581:TRP:HD1	1.98	0.47
2:B:671:LYS:NZ	2:B:780:ASP:OD2	2.48	0.47
2:D:532:SER:OG	2:D:533:LYS:N	2.46	0.47
2:B:98:ARG:NH2	2:B:318:GLN:OE1	2.46	0.47
2:B:475:CYS:O	2:B:479:GLN:CA	2.63	0.46
2:D:99:PRO:HG2	2:D:314:ALA:HB3	1.97	0.46
2:D:227:GLU:H	2:D:227:GLU:CD	2.22	0.46
2:D:426:PHE:HB3	2:D:442:THR:HB	1.97	0.46
2:D:580:SER:OG	2:D:581:TRP:HD1	1.98	0.46
1:C:216:GLU:HG3	1:C:218:ASP:OD1	2.15	0.46
2:B:326:THR:OG1	2:B:373:HIS:O	2.28	0.46
2:B:841:ARG:HB2	2:B:870:PHE:CZ	2.51	0.46
2:D:475:CYS:O	2:D:479:GLN:CA	2.63	0.46
2:D:841:ARG:HB2	2:D:870:PHE:CZ	2.51	0.46
1:A:33:ASP:OD2	1:A:33:ASP:N	2.47	0.46
2:B:108:LEU:HD23	2:B:108:LEU:HA	1.66	0.46
1:A:68:ILE:HG21	1:A:111:ILE:HG12	1.96	0.46
2:D:324:THR:HB	2:D:372:ILE:HG21	1.97	0.46
2:D:153:VAL:HG21	2:D:215:LEU:HD12	1.98	0.46
2:D:536:VAL:HG12	2:D:574:VAL:HG13	1.96	0.46
2:B:426:PHE:HB3	2:B:442:THR:HB	1.97	0.46
1:C:40:VAL:HG12	1:C:43:ALA:O	2.16	0.46
1:A:40:VAL:HG12	1:A:43:ALA:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:787:ILE:HG22	2:B:822:VAL:HG21	1.98	0.46
1:C:15:ILE:HA	1:C:388:VAL:O	2.16	0.45
2:D:751:ILE:HD13	2:D:751:ILE:HA	1.85	0.45
2:B:236:ASP:OD1	2:B:237:ALA:N	2.47	0.45
2:B:248:TYR:OH	2:B:278:GLN:NE2	2.49	0.45
2:D:446:GLU:HB2	2:D:448:ARG:HH21	1.82	0.45
2:D:580:SER:HG	2:D:581:TRP:CD1	2.34	0.45
1:C:349:THR:HG23	1:C:363:ALA:O	2.17	0.45
2:D:827:ARG:NH2	2:D:830:ASP:H	2.13	0.45
1:A:15:ILE:HA	1:A:388:VAL:O	2.16	0.45
2:B:287:HIS:CG	2:B:288:PRO:HD2	2.52	0.45
1:C:372:VAL:HG22	1:C:380:PHE:CD1	2.52	0.45
2:D:797:VAL:HB	2:D:811:PRO:HG3	1.98	0.45
2:B:665:LYS:N	2:B:683:THR:O	2.50	0.45
2:B:850:ARG:HA	2:B:859:LEU:HA	1.99	0.45
1:C:216:GLU:O	1:C:313:PRO:HD3	2.17	0.45
2:B:153:VAL:HG21	2:B:215:LEU:HD12	1.98	0.45
2:B:297:SER:HB2	2:B:306:TRP:HZ2	1.82	0.45
2:D:406:GLU:HG2	2:D:407:ASN:N	2.32	0.45
2:D:820:THR:O	2:D:840:TYR:N	2.41	0.45
2:B:754:PRO:HB3	2:B:778:ASN:O	2.17	0.45
2:B:769:GLY:N	2:B:810:ALA:O	2.43	0.45
2:D:98:ARG:NH2	2:D:318:GLN:OE1	2.46	0.45
2:D:248:TYR:OH	2:D:278:GLN:NE2	2.49	0.45
2:D:297:SER:HB2	2:D:306:TRP:HZ2	1.82	0.45
1:A:188:ILE:HG22	1:A:213:VAL:HG23	1.99	0.45
1:A:216:GLU:O	1:A:313:PRO:HD3	2.17	0.45
2:B:446:GLU:HB2	2:B:448:ARG:HH21	1.82	0.45
2:D:850:ARG:HA	2:D:859:LEU:HA	1.99	0.45
2:B:797:VAL:HB	2:B:811:PRO:HG3	1.98	0.44
1:A:239:THR:O	1:A:259:MET:HB2	2.17	0.44
2:B:406:GLU:HG2	2:B:407:ASN:N	2.32	0.44
1:C:179:THR:OG1	1:C:180:LYS:N	2.50	0.44
2:D:287:HIS:CG	2:D:288:PRO:HD2	2.52	0.44
2:D:754:PRO:HB3	2:D:778:ASN:O	2.17	0.44
2:B:735:ILE:O	2:B:743:SER:OG	2.31	0.44
1:A:349:THR:HG23	1:A:363:ALA:O	2.17	0.44
2:D:665:LYS:N	2:D:683:THR:O	2.50	0.44
1:A:87:LYS:HD3	1:A:87:LYS:HA	1.66	0.44
1:A:372:VAL:HG22	1:A:380:PHE:CD1	2.52	0.44
2:B:225:LEU:HD11	2:B:232:LEU:HD22	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:80:TYR:CD2	2:D:87:CYS:HB3	2.53	0.44
2:D:787:ILE:HG22	2:D:822:VAL:HG21	1.98	0.44
1:C:76:CYS:HA	1:C:85:CYS:HA	1.99	0.44
2:D:326:THR:OG1	2:D:373:HIS:O	2.28	0.44
2:D:405:GLY:N	2:D:409:THR:O	2.41	0.44
2:D:735:ILE:O	2:D:743:SER:OG	2.31	0.44
2:D:351:GLU:OE2	2:D:352:SER:OG	2.29	0.44
2:B:168:ARG:HD3	2:B:175:TRP:CZ2	2.53	0.44
2:B:482:THR:OG1	2:B:483:PHE:N	2.51	0.44
2:B:874:LYS:HE2	2:B:874:LYS:HB3	1.74	0.44
1:C:239:THR:O	1:C:259:MET:HB2	2.17	0.44
2:D:225:LEU:HD11	2:D:232:LEU:HD22	1.99	0.44
1:C:188:ILE:HG22	1:C:213:VAL:HG23	1.99	0.43
2:D:827:ARG:O	2:D:827:ARG:HG3	2.18	0.43
2:D:187:GLU:N	2:D:188:PRO:HD3	2.33	0.43
2:B:187:GLU:N	2:B:188:PRO:HD3	2.33	0.43
2:D:482:THR:OG1	2:D:483:PHE:N	2.51	0.43
2:B:691:SER:OG	2:B:692:ASN:N	2.51	0.43
2:B:723:LEU:HA	2:B:724:PRO:HD3	1.89	0.43
1:C:162:LYS:NZ	1:C:165:THR:O	2.52	0.43
2:D:176:TYR:CZ	2:D:271:THR:HG23	2.53	0.43
2:D:734:CYS:HB2	2:D:742:CYS:HB3	1.47	0.43
2:B:185:LEU:HA	2:B:185:LEU:HD23	1.67	0.43
1:A:19:LYS:HB3	1:A:19:LYS:HE2	1.80	0.43
2:B:80:TYR:CD2	2:B:87:CYS:HB3	2.53	0.43
2:B:176:TYR:CZ	2:B:271:THR:HG23	2.53	0.43
2:B:752:ALA:HB3	2:B:778:ASN:ND2	2.33	0.43
2:D:168:ARG:HD3	2:D:175:TRP:CZ2	2.53	0.43
2:D:248:TYR:CZ	2:D:263:SER:HB2	2.54	0.43
1:A:179:THR:OG1	1:A:180:LYS:N	2.50	0.43
2:D:687:PHE:CD2	2:D:719:MET:HG2	2.54	0.43
2:D:694:THR:HG22	2:D:709:GLN:NE2	2.34	0.43
2:B:254:THR:OG1	2:B:255:SER:N	2.52	0.43
2:B:248:TYR:CZ	2:B:263:SER:HB2	2.54	0.43
2:B:757:SER:OG	2:B:776:GLY:HA2	2.19	0.43
2:D:304:ASP:OD1	2:D:304:ASP:N	2.51	0.43
2:D:691:SER:OG	2:D:692:ASN:N	2.51	0.43
2:D:752:ALA:HB3	2:D:778:ASN:ND2	2.33	0.43
1:A:76:CYS:HA	1:A:85:CYS:HA	1.99	0.42
1:A:171:ILE:HG13	1:A:189:ALA:HB3	2.01	0.42
1:A:298:PHE:CE2	1:A:302:GLU:HG3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:61:SER:OG	2:D:62:GLY:N	2.52	0.42
2:D:874:LYS:HE2	2:D:874:LYS:HB3	1.74	0.42
1:A:127:GLU:HG3	1:A:128:GLY:H	1.84	0.42
2:D:306:TRP:HB2	2:D:333:MET:SD	2.60	0.42
2:B:304:ASP:OD1	2:B:304:ASP:N	2.51	0.42
2:B:400:LEU:HB3	2:B:415:VAL:HA	2.01	0.42
2:D:254:THR:OG1	2:D:255:SER:N	2.52	0.42
2:D:328:LEU:HD22	2:D:392:LEU:HD21	2.02	0.42
2:D:786:ILE:HG13	2:D:832:TYR:CE1	2.53	0.42
1:A:67:SER:HB3	1:A:75:VAL:HG22	2.01	0.42
2:B:728:LYS:HE3	2:B:752:ALA:HB2	2.01	0.42
2:B:827:ARG:HG3	2:B:827:ARG:O	2.18	0.42
2:D:396:ASP:OD1	2:D:396:ASP:N	2.53	0.42
2:D:659:LEU:HD23	2:D:659:LEU:HA	1.88	0.42
2:B:126:GLY:HA2	2:B:134:CYS:HA	2.01	0.42
2:B:461:CYS:O	2:B:464:CYS:N	2.51	0.42
2:B:694:THR:HG22	2:B:709:GLN:NE2	2.34	0.42
1:C:31:LEU:HD11	1:C:375:THR:HG22	2.02	0.42
1:C:171:ILE:HG13	1:C:189:ALA:HB3	2.01	0.42
2:D:126:GLY:HA2	2:D:134:CYS:HA	2.01	0.42
2:D:665:LYS:H	2:D:684:GLY:HA2	1.85	0.42
2:D:690:ALA:HB3	2:D:693:ILE:HD11	2.02	0.42
2:B:753:LEU:HD23	2:B:753:LEU:HA	1.80	0.42
1:C:127:GLU:HG3	1:C:128:GLY:H	1.84	0.42
1:C:336:GLU:OE1	1:C:356:LYS:HD2	2.19	0.42
2:D:478:LEU:HG	2:D:480:ARG:HB2	2.01	0.42
2:D:757:SER:OG	2:D:776:GLY:HA2	2.19	0.42
1:A:68:ILE:HD13	1:A:111:ILE:HD11	2.02	0.42
1:A:152:LYS:HA	1:A:152:LYS:HD3	1.88	0.42
1:A:336:GLU:OE1	1:A:356:LYS:HD2	2.19	0.42
2:B:306:TRP:HB2	2:B:333:MET:SD	2.60	0.42
2:B:396:ASP:OD1	2:B:396:ASP:N	2.53	0.42
2:D:185:LEU:HA	2:D:185:LEU:HD23	1.67	0.42
1:A:52:LEU:HD23	1:A:52:LEU:HA	1.79	0.42
1:A:100:GLY:HA3	1:A:135:PHE:CZ	2.55	0.42
2:B:61:SER:OG	2:B:62:GLY:N	2.52	0.42
2:D:236:ASP:OD1	2:D:237:ALA:N	2.47	0.42
2:D:384:VAL:HG13	2:D:470:PRO:HB2	2.00	0.42
2:B:328:LEU:HD22	2:B:392:LEU:HD21	2.02	0.42
2:B:687:PHE:CD2	2:B:719:MET:HG2	2.54	0.42
1:C:189:ALA:HA	1:C:211:LEU:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:PHE:CE2	1:C:302:GLU:HG3	2.54	0.42
2:D:728:LYS:HE3	2:D:752:ALA:HB2	2.01	0.42
1:A:189:ALA:HA	1:A:211:LEU:O	2.19	0.42
2:B:384:VAL:HG13	2:B:470:PRO:HB2	2.00	0.42
2:D:231:SER:HG	2:D:253:TYR:HD2	1.66	0.42
1:A:37:TYR:CD1	1:A:46:THR:HG22	2.54	0.41
2:B:326:THR:HB	2:B:376:LEU:HB2	2.03	0.41
2:B:432:ASP:HA	2:B:433:PRO:HD3	1.90	0.41
2:B:478:LEU:HG	2:B:480:ARG:HB2	2.02	0.41
2:B:825:LYS:HE3	2:B:825:LYS:HB2	1.82	0.41
1:C:37:TYR:CD1	1:C:46:THR:HG22	2.54	0.41
2:D:825:LYS:HB2	2:D:825:LYS:HE3	1.82	0.41
2:B:97:ALA:HB3	2:B:100:ARG:HD2	2.01	0.41
2:B:339:ARG:NH1	2:B:362:ARG:O	2.53	0.41
1:C:67:SER:HB3	1:C:75:VAL:HG22	2.01	0.41
2:D:248:TYR:CE1	2:D:263:SER:HB2	2.55	0.41
2:D:264:MET:HE3	2:D:264:MET:HB2	1.87	0.41
2:D:339:ARG:NH1	2:D:362:ARG:O	2.53	0.41
2:D:400:LEU:HB3	2:D:415:VAL:HA	2.01	0.41
2:D:475:CYS:O	2:D:479:GLN:HA	2.20	0.41
2:D:662:PHE:HZ	2:D:689:ARG:O	2.04	0.41
1:A:191:MET:HE2	1:A:191:MET:HB3	1.94	0.41
2:B:475:CYS:O	2:B:479:GLN:HA	2.20	0.41
1:C:68:ILE:HD13	1:C:111:ILE:HD11	2.02	0.41
2:D:474:TRP:NE1	2:D:479:GLN:OE1	2.52	0.41
1:A:162:LYS:HE3	1:A:162:LYS:HB3	1.86	0.41
2:D:142:LEU:HD23	2:D:142:LEU:HA	1.78	0.41
2:D:461:CYS:O	2:D:464:CYS:N	2.51	0.41
2:D:769:GLY:N	2:D:810:ALA:O	2.43	0.41
2:B:166:VAL:HA	2:B:176:TYR:O	2.21	0.41
2:B:710:VAL:HG22	2:B:721:PHE:CZ	2.55	0.41
1:A:31:LEU:HD11	1:A:375:THR:HG22	2.02	0.41
1:A:236:ASP:CG	1:A:338:ARG:HH21	2.24	0.41
2:B:672:VAL:HG23	2:B:677:LYS:HB2	2.03	0.41
1:C:100:GLY:HA3	1:C:135:PHE:CZ	2.55	0.41
2:D:97:ALA:HB3	2:D:100:ARG:HD2	2.01	0.41
1:A:211:LEU:HG	1:A:301:ILE:HD11	2.03	0.41
1:A:250:SER:C	1:A:323:SER:HB3	2.46	0.41
1:A:287:LEU:HB3	1:A:291:LYS:HB2	2.03	0.41
2:B:159:GLN:OE1	2:B:159:GLN:N	2.48	0.41
2:B:662:PHE:HZ	2:B:689:ARG:O	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:690:ALA:HB3	2:B:693:ILE:HD11	2.02	0.41
2:B:764:THR:HG22	2:B:765:TRP:N	2.36	0.41
2:D:149:ASN:O	2:D:214:SER:HA	2.21	0.41
1:A:301:ILE:HD12	1:A:301:ILE:HA	1.80	0.41
2:B:406:GLU:HG2	2:B:407:ASN:H	1.85	0.41
2:D:166:VAL:HA	2:D:176:TYR:O	2.21	0.41
2:D:329:CYS:HB3	2:D:331:PHE:CE1	2.56	0.41
2:D:406:GLU:HG2	2:D:407:ASN:H	1.85	0.41
2:D:710:VAL:HG22	2:D:721:PHE:CZ	2.55	0.41
1:A:222:ARG:H	1:A:222:ARG:HG2	1.66	0.41
2:B:248:TYR:CE1	2:B:263:SER:HB2	2.55	0.41
2:B:255:SER:OG	3:B:1604:NAG:N2	2.54	0.41
2:B:329:CYS:HB3	2:B:331:PHE:CE1	2.56	0.41
2:B:734:CYS:HB2	2:B:742:CYS:HB3	1.47	0.41
2:B:751:ILE:HD13	2:B:751:ILE:HA	1.85	0.41
2:B:878:GLU:O	2:B:927:VAL:HA	2.21	0.41
1:C:87:LYS:HA	1:C:87:LYS:HD3	1.66	0.41
1:C:200:SER:O	1:C:204:SER:HB2	2.21	0.41
2:D:159:GLN:OE1	2:D:159:GLN:N	2.48	0.41
2:D:406:GLU:H	2:D:406:GLU:CD	2.28	0.41
2:D:432:ASP:HA	2:D:433:PRO:HD3	1.90	0.41
2:D:715:ASN:C	2:D:717:THR:N	2.78	0.41
2:D:878:GLU:O	2:D:927:VAL:HA	2.21	0.41
1:A:200:SER:O	1:A:204:SER:HB2	2.21	0.41
2:B:185:LEU:O	2:B:187:GLU:N	2.50	0.41
2:B:728:LYS:H	2:B:728:LYS:HG3	1.74	0.41
1:C:222:ARG:H	1:C:222:ARG:HG2	1.66	0.41
2:B:172:ASN:HD21	2:B:174:ARG:HE	1.69	0.40
1:C:211:LEU:HG	1:C:301:ILE:HD11	2.03	0.40
1:C:236:ASP:CG	1:C:338:ARG:HH21	2.24	0.40
2:D:726:SER:HB3	2:D:750:TYR:CE2	2.56	0.40
2:D:779:PHE:HD1	2:D:779:PHE:HA	1.74	0.40
2:D:875:LYS:HE2	2:D:875:LYS:HB2	1.86	0.40
2:B:149:ASN:OD1	2:B:150:GLY:N	2.49	0.40
1:C:251:LYS:N	1:C:323:SER:HB3	2.37	0.40
2:D:326:THR:HB	2:D:376:LEU:HB2	2.02	0.40
2:B:264:MET:HE3	2:B:264:MET:HB2	1.87	0.40
2:B:665:LYS:H	2:B:684:GLY:HA2	1.85	0.40
2:B:715:ASN:C	2:B:717:THR:N	2.78	0.40
1:C:52:LEU:HD23	1:C:52:LEU:HA	1.79	0.40
1:C:61:ASN:ND2	1:C:80:ASN:HD22	2.18	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:SER:C	1:C:323:SER:HB3	2.46	0.40
2:D:110:LEU:HA	2:D:111:PRO:HD3	1.86	0.40
2:B:413:PRO:HD2	2:B:703:CYS:SG	2.62	0.40
1:C:192:CYS:N	1:C:209:THR:OG1	2.45	0.40
1:C:287:LEU:HB3	1:C:291:LYS:HB2	2.03	0.40
2:D:391:PHE:CZ	2:D:452:VAL:HB	2.57	0.40
2:D:672:VAL:HG23	2:D:677:LYS:HB2	2.03	0.40
1:A:272:GLY:HA2	1:A:308:ASP:HB2	2.03	0.40
2:B:498:ASP:OD1	2:B:500:SER:N	2.53	0.40
2:D:255:SER:OG	3:D:1604:NAG:N2	2.54	0.40
2:D:413:PRO:HD2	2:D:703:CYS:SG	2.62	0.40
2:D:696:ILE:HG12	2:D:707:VAL:HG22	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	378/398 (95%)	341 (90%)	37 (10%)	0	100	100
1	C	378/398 (95%)	342 (90%)	36 (10%)	0	100	100
2	B	721/1545 (47%)	642 (89%)	79 (11%)	0	100	100
2	D	721/1545 (47%)	642 (89%)	79 (11%)	0	100	100
All	All	2198/3886 (57%)	1967 (90%)	231 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	339/358 (95%)	313 (92%)	26 (8%)	12	38
1	C	339/358 (95%)	314 (93%)	25 (7%)	13	40
2	B	587/1370 (43%)	538 (92%)	49 (8%)	10	35
2	D	587/1370 (43%)	538 (92%)	49 (8%)	10	35
All	All	1852/3456 (54%)	1703 (92%)	149 (8%)	13	37

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	33	ASP
1	A	49	ASN
1	A	52	LEU
1	A	55	THR
1	A	60	ASN
1	A	67	SER
1	A	71	GLU
1	A	73	THR
1	A	74	LEU
1	A	75	VAL
1	A	78	THR
1	A	114	HIS
1	A	124	ILE
1	A	165	THR
1	A	213	VAL
1	A	219	ILE
1	A	230	SER
1	A	237	ASN
1	A	256	THR
1	A	295	HIS
1	A	325	VAL
1	A	365	VAL
1	A	375	THR
1	A	379	LEU
1	A	388	VAL
2	B	42	SER
2	B	49	ILE

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Mol	Chain	Res	Type
2	B	66	ASP
2	B	67	GLN
2	B	68	LEU
2	B	79	LEU
2	B	113	ARG
2	B	125	THR
2	B	128	THR
2	B	151	THR
2	B	155	SER
2	B	172	ASN
2	B	177	LEU
2	B	194	CYS
2	B	231	SER
2	B	255	SER
2	B	259	THR
2	B	263	SER
2	B	267	ILE
2	B	311	SER
2	B	322	SER
2	B	324	THR
2	B	370	THR
2	B	400	LEU
2	B	402	VAL
2	B	409	THR
2	B	423	THR
2	B	430	VAL
2	B	434	VAL
2	B	446	GLU
2	B	487	CYS
2	B	506	CYS
2	B	522	THR
2	B	672	VAL
2	B	674	THR
2	B	683	THR
2	B	708	ILE
2	B	741	ASN
2	B	756	CYS
2	B	765	TRP
2	B	780	ASP
2	B	801	CYS
2	B	806	CYS
2	B	822	VAL

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Mol	Chain	Res	Type
2	B	834	ASP
2	B	879	ILE
2	B	881	LEU
2	B	929	LEU
2	B	934	LEU
1	C	31	LEU
1	C	33	ASP
1	C	49	ASN
1	C	52	LEU
1	C	55	THR
1	C	60	ASN
1	C	67	SER
1	C	71	GLU
1	C	73	THR
1	C	74	LEU
1	C	75	VAL
1	C	78	THR
1	C	114	HIS
1	C	124	ILE
1	C	165	THR
1	C	213	VAL
1	C	219	ILE
1	C	230	SER
1	C	256	THR
1	C	295	HIS
1	C	325	VAL
1	C	365	VAL
1	C	375	THR
1	C	379	LEU
1	C	388	VAL
2	D	42	SER
2	D	49	ILE
2	D	66	ASP
2	D	67	GLN
2	D	68	LEU
2	D	79	LEU
2	D	113	ARG
2	D	125	THR
2	D	128	THR
2	D	151	THR
2	D	155	SER
2	D	172	ASN

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Mol	Chain	Res	Type
2	D	177	LEU
2	D	194	CYS
2	D	231	SER
2	D	255	SER
2	D	259	THR
2	D	263	SER
2	D	267	ILE
2	D	311	SER
2	D	322	SER
2	D	324	THR
2	D	370	THR
2	D	400	LEU
2	D	402	VAL
2	D	409	THR
2	D	423	THR
2	D	430	VAL
2	D	434	VAL
2	D	446	GLU
2	D	487	CYS
2	D	506	CYS
2	D	522	THR
2	D	672	VAL
2	D	674	THR
2	D	683	THR
2	D	708	ILE
2	D	741	ASN
2	D	756	CYS
2	D	765	TRP
2	D	780	ASP
2	D	801	CYS
2	D	806	CYS
2	D	822	VAL
2	D	834	ASP
2	D	879	ILE
2	D	881	LEU
2	D	929	LEU
2	D	934	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN

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Mol	Chain	Res	Type
1	A	80	ASN
1	A	205	HIS
1	A	264	HIS
1	A	295	HIS
2	B	67	GLN
2	B	74	HIS
2	B	145	ASN
2	B	218	GLN
2	B	278	GLN
2	B	353	HIS
2	B	670	GLN
2	B	718	HIS
2	B	784	ASN
2	B	794	ASN
2	B	829	GLN
1	C	59	ASN
1	C	80	ASN
1	C	205	HIS
1	C	264	HIS
1	C	295	HIS
2	D	67	GLN
2	D	74	HIS
2	D	145	ASN
2	D	218	GLN
2	D	278	GLN
2	D	353	HIS
2	D	458	HIS
2	D	670	GLN
2	D	718	HIS
2	D	784	ASN
2	D	794	ASN
2	D	829	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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](#)

18 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	$\# Z > 2$
3	NAG	C	501	1	14,14,15	0.14	0	17,19,21	0.56	0
3	NAG	D	1608	2	14,14,15	0.34	0	17,19,21	1.31	2 (11%)
3	NAG	D	1602	2	14,14,15	0.31	0	17,19,21	0.53	0
3	NAG	D	1605	2	14,14,15	0.16	0	17,19,21	0.51	0
3	NAG	B	1603	2	14,14,15	0.21	0	17,19,21	0.53	0
3	NAG	B	1601	2	14,14,15	0.20	0	17,19,21	0.46	0
3	NAG	B	1606	2	14,14,15	0.36	0	17,19,21	0.58	0
3	NAG	D	1601	2	14,14,15	0.20	0	17,19,21	0.46	0
3	NAG	A	501	1	14,14,15	0.15	0	17,19,21	0.57	0
3	NAG	D	1606	2	14,14,15	0.35	0	17,19,21	0.59	0
3	NAG	B	1604	2	14,14,15	0.35	0	17,19,21	0.57	0
3	NAG	D	1603	2	14,14,15	0.20	0	17,19,21	0.53	0
3	NAG	D	1607	2	14,14,15	0.31	0	17,19,21	0.78	1 (5%)
3	NAG	B	1605	2	14,14,15	0.16	0	17,19,21	0.51	0
3	NAG	D	1604	2	14,14,15	0.35	0	17,19,21	0.57	0
3	NAG	B	1608	2	14,14,15	0.33	0	17,19,21	1.31	2 (11%)
3	NAG	B	1607	2	14,14,15	0.31	0	17,19,21	0.77	1 (5%)
3	NAG	B	1602	2	14,14,15	0.31	0	17,19,21	0.53	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
3	NAG	C	501	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	D	1608	2	-	6/6/23/26	0/1/1/1
3	NAG	D	1602	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1605	2	-	1/6/23/26	0/1/1/1
3	NAG	B	1603	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1601	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1606	2	-	0/6/23/26	0/1/1/1
3	NAG	D	1601	2	-	2/6/23/26	0/1/1/1
3	NAG	A	501	1	-	3/6/23/26	0/1/1/1
3	NAG	D	1606	2	-	0/6/23/26	0/1/1/1
3	NAG	B	1604	2	-	3/6/23/26	0/1/1/1
3	NAG	D	1603	2	-	2/6/23/26	0/1/1/1
3	NAG	D	1607	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1605	2	-	1/6/23/26	0/1/1/1
3	NAG	D	1604	2	-	3/6/23/26	0/1/1/1
3	NAG	B	1608	2	-	6/6/23/26	0/1/1/1
3	NAG	B	1607	2	-	2/6/23/26	0/1/1/1
3	NAG	B	1602	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	1608	NAG	C2-N2-C7	4.52	128.96	122.90
3	D	1608	NAG	C2-N2-C7	4.52	128.96	122.90
3	D	1607	NAG	C1-O5-C5	2.46	115.48	112.19
3	B	1607	NAG	C1-O5-C5	2.44	115.45	112.19
3	B	1608	NAG	C1-C2-N2	2.13	113.80	110.43
3	D	1608	NAG	C1-C2-N2	2.13	113.80	110.43

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	501	NAG	C4-C5-C6-O6
3	C	501	NAG	C4-C5-C6-O6
3	B	1601	NAG	C4-C5-C6-O6
3	D	1601	NAG	C4-C5-C6-O6
3	A	501	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
3	C	501	NAG	O5-C5-C6-O6
3	B	1602	NAG	C4-C5-C6-O6
3	D	1602	NAG	C4-C5-C6-O6
3	B	1601	NAG	O5-C5-C6-O6
3	D	1601	NAG	O5-C5-C6-O6
3	B	1607	NAG	O5-C5-C6-O6
3	D	1607	NAG	O5-C5-C6-O6
3	B	1608	NAG	C4-C5-C6-O6
3	D	1608	NAG	C4-C5-C6-O6
3	B	1608	NAG	O5-C5-C6-O6
3	D	1608	NAG	O5-C5-C6-O6
3	B	1602	NAG	O5-C5-C6-O6
3	D	1602	NAG	O5-C5-C6-O6
3	B	1603	NAG	C4-C5-C6-O6
3	D	1603	NAG	C4-C5-C6-O6
3	B	1607	NAG	C4-C5-C6-O6
3	D	1607	NAG	C4-C5-C6-O6
3	B	1608	NAG	C8-C7-N2-C2
3	B	1608	NAG	O7-C7-N2-C2
3	D	1608	NAG	C8-C7-N2-C2
3	D	1608	NAG	O7-C7-N2-C2
3	B	1603	NAG	O5-C5-C6-O6
3	D	1603	NAG	O5-C5-C6-O6
3	B	1605	NAG	O5-C5-C6-O6
3	D	1605	NAG	O5-C5-C6-O6
3	B	1608	NAG	C1-C2-N2-C7
3	D	1608	NAG	C1-C2-N2-C7
3	B	1604	NAG	C3-C2-N2-C7
3	B	1608	NAG	C3-C2-N2-C7
3	D	1604	NAG	C3-C2-N2-C7
3	D	1608	NAG	C3-C2-N2-C7
3	A	501	NAG	C1-C2-N2-C7
3	C	501	NAG	C1-C2-N2-C7
3	B	1604	NAG	O5-C5-C6-O6
3	D	1604	NAG	O5-C5-C6-O6
3	B	1604	NAG	C4-C5-C6-O6
3	D	1604	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	1608	NAG	2	0
3	B	1604	NAG	2	0
3	D	1604	NAG	2	0
3	B	1608	NAG	2	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.

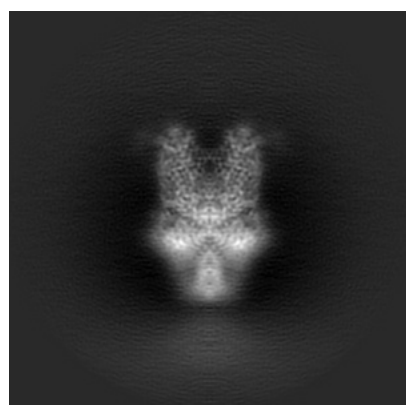
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-21442. These allow visual inspection of the internal detail of the map and identification of artifacts.

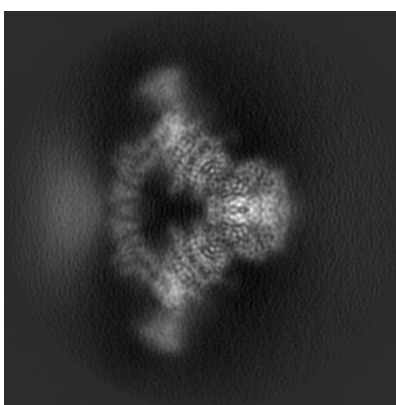
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

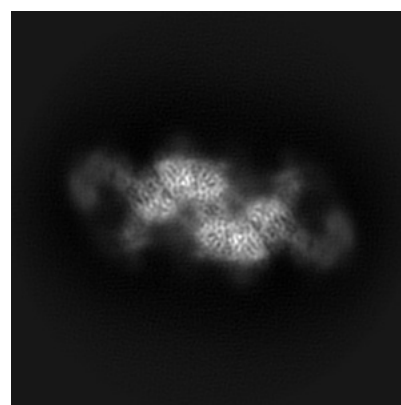
6.1.1 Primary map



X



Y

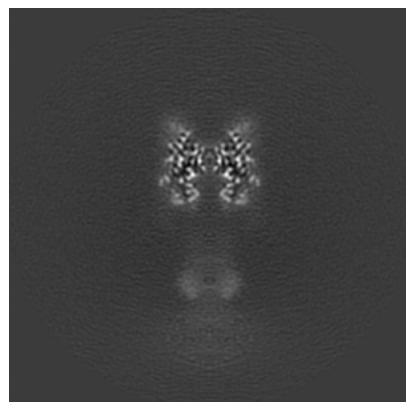


Z

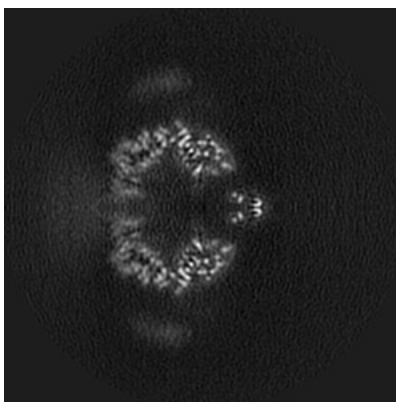
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

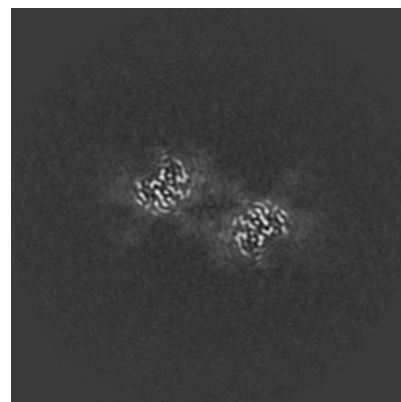
6.2.1 Primary map



X Index: 180



Y Index: 180

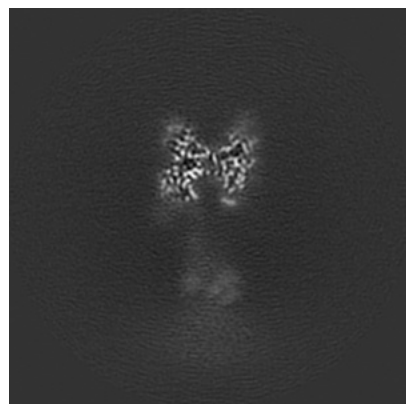


Z Index: 180

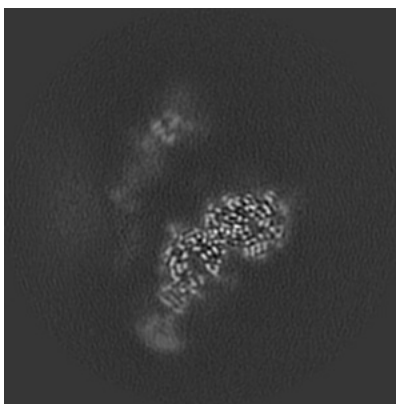
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

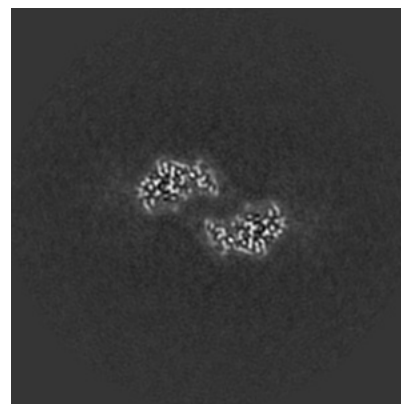
6.3.1 Primary map



X Index: 185



Y Index: 206

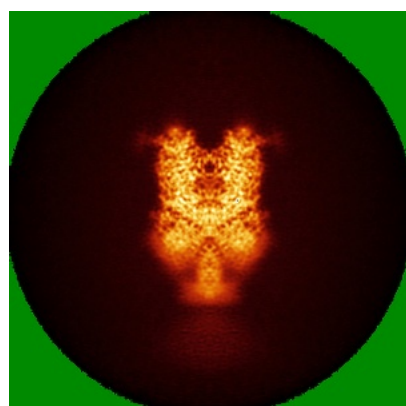


Z Index: 187

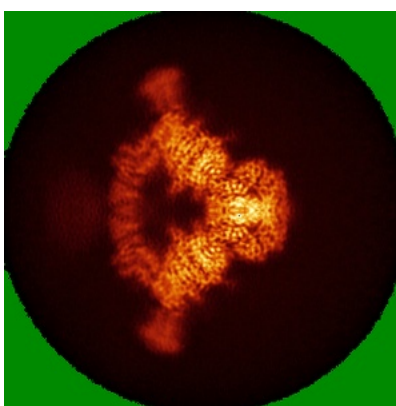
The images above show the largest variance slices of the map in three orthogonal directions.

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

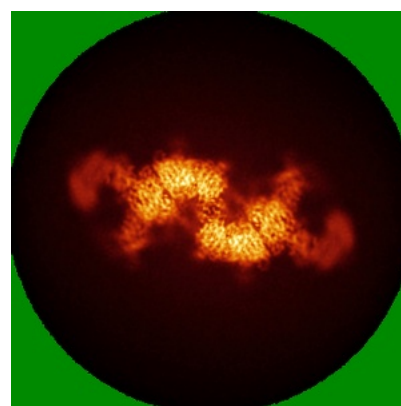
6.4.1 Primary map



X



Y



Z

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

6.5 Orthogonal surface views

This section was not generated.

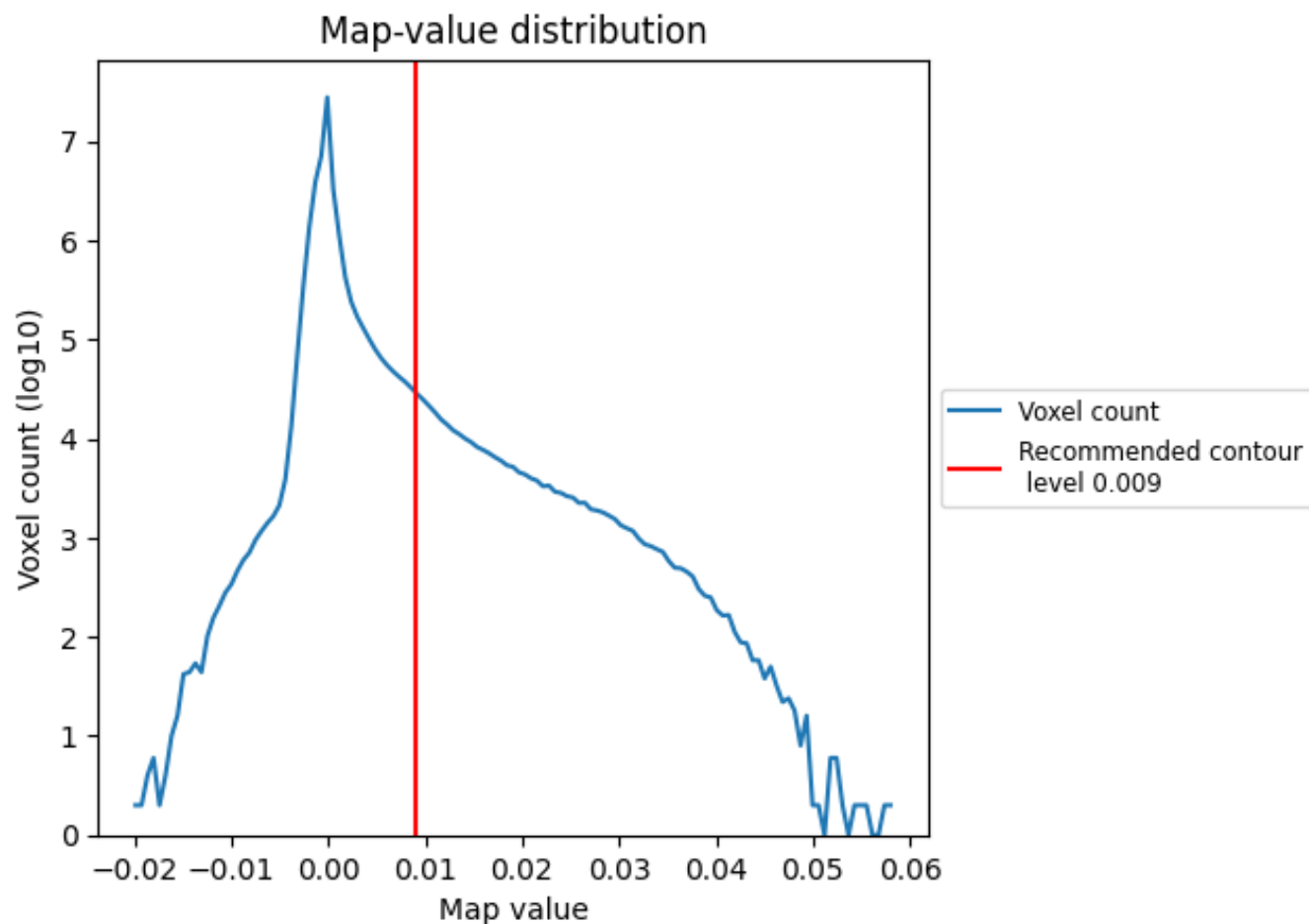
6.6 Mask visualisation

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

7 Map analysis [i](#)

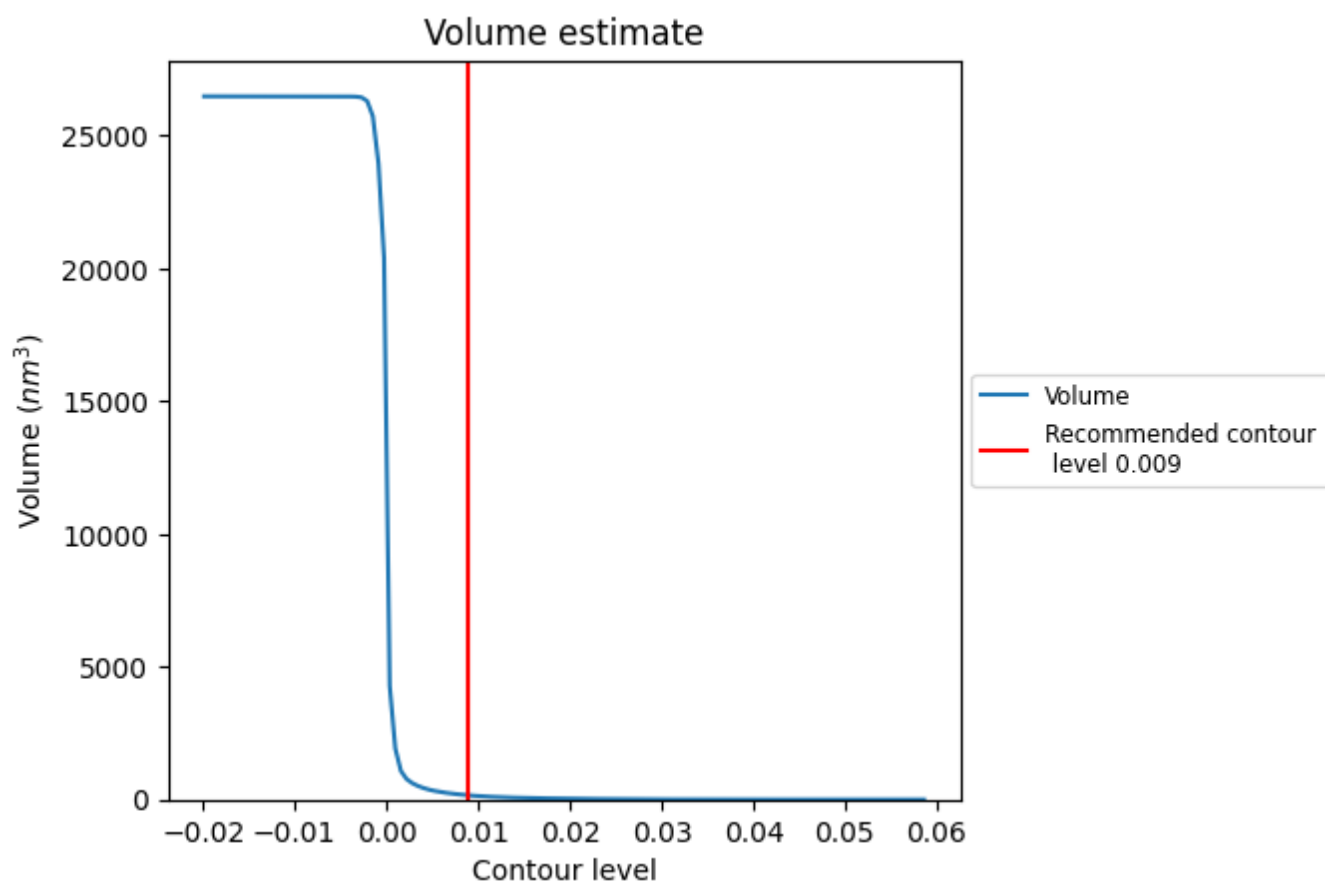
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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

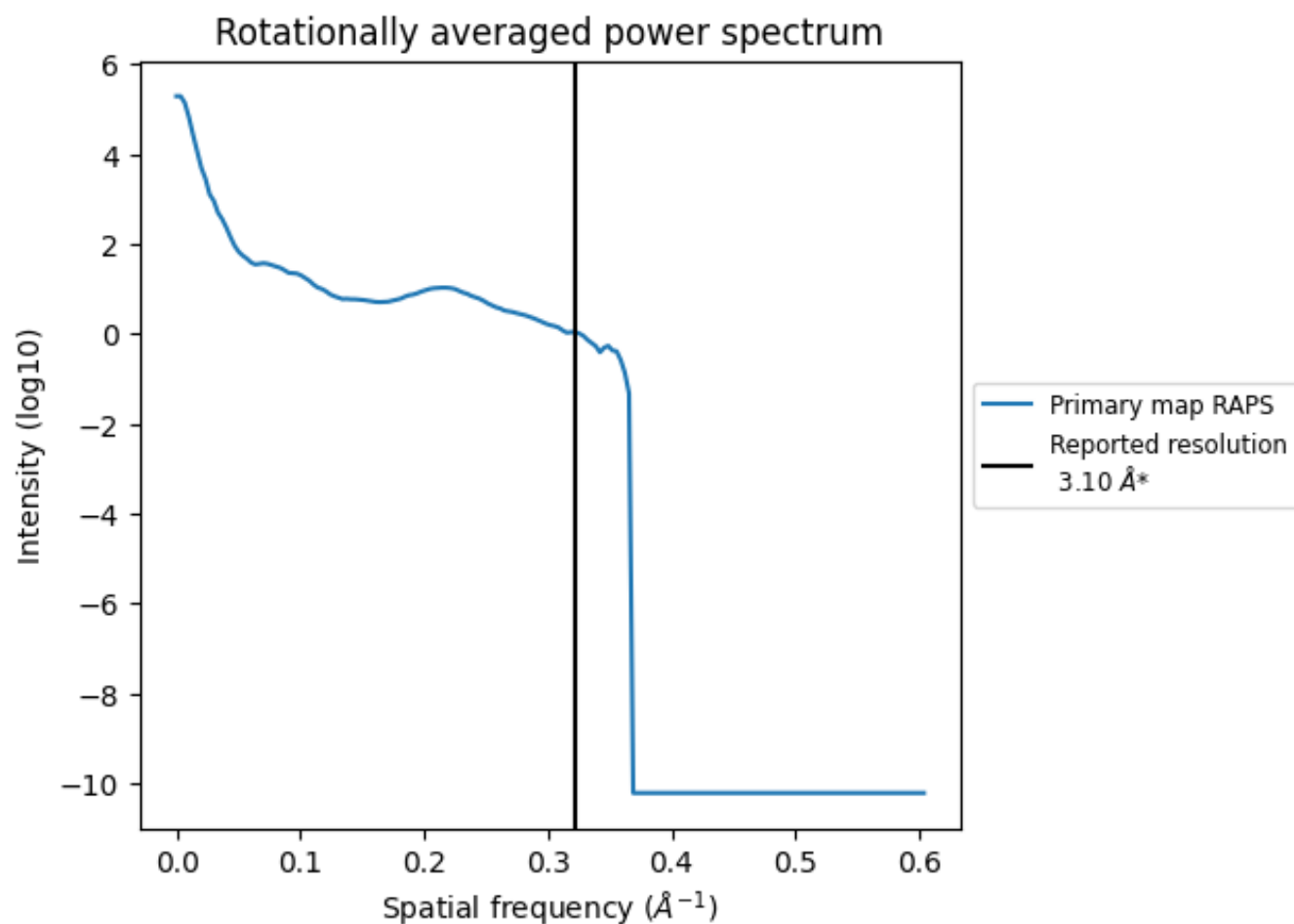
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 159 nm^3 ; this corresponds to an approximate mass of 143 kDa.

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

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.323 Å⁻¹

8 Fourier-Shell correlation ⓘ

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

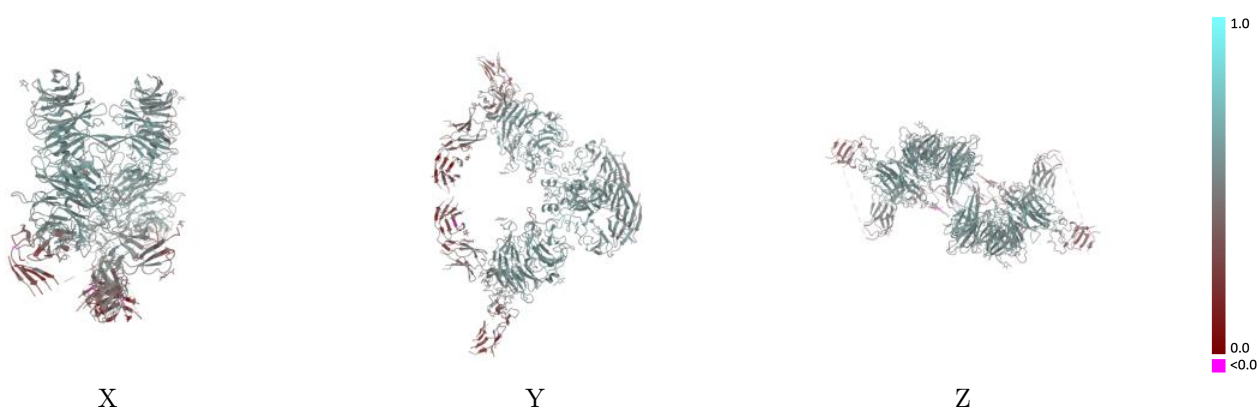
9 Map-model fit [i](#)

This section contains information regarding the fit between EMD map EMD-21442 and PDB model 6VXK. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)

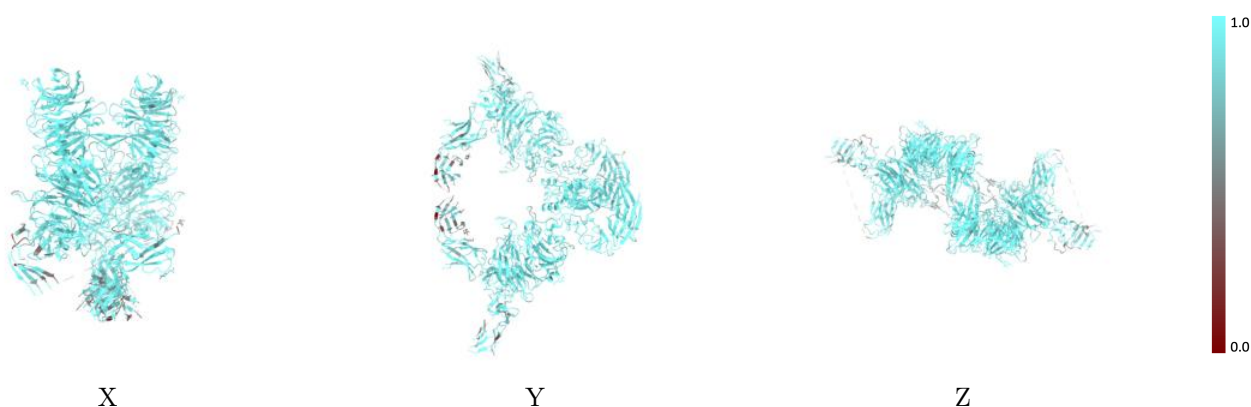
This section was not generated.

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



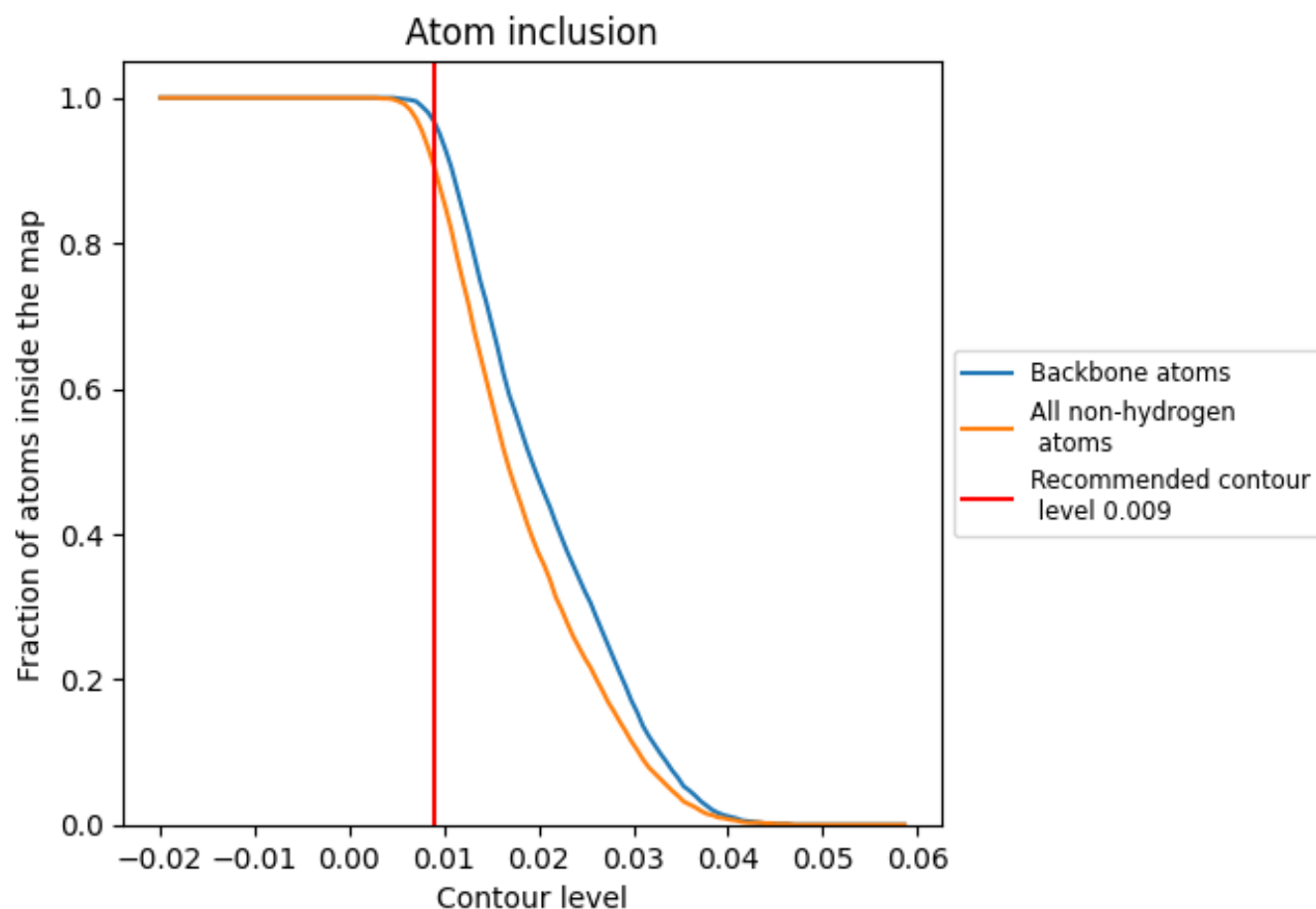
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.009).

9.4 Atom inclusion [i](#)



At the recommended contour level, 97% of all backbone atoms, 90% 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 (0.009) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9050	0.5120
A	0.9390	0.5510
B	0.8860	0.4920
C	0.9390	0.5500
D	0.8860	0.4910

