



Full wwPDB EM Validation Report ⓘ

Mar 8, 2026 – 05:37 PM UTC

PDB ID : 8PBZ / pdb_00008pbz
EMDB ID : EMD-17591
Title : Sub-tomogram average of the Nap adhesion complex from the human pathogen
Mycoplasma genitalium at 11 Angstrom.
Authors : Sprankel, L.; Scheffer, M.P.; Frangakis, A.F.
Deposited on : 2023-06-09
Resolution : 11.00 Å(reported)
Based on initial models : ., 6RUT, 6R43

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:

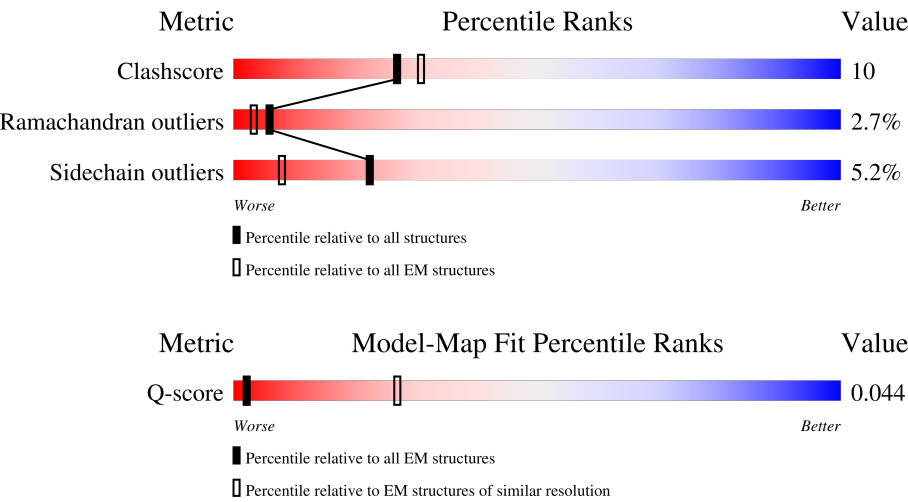
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
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 i

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

The reported resolution of this entry is 11.00 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	97 (10.50 - 11.50)

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

Mol	Chain	Length	Quality of chain
1	A	1053	12% 66% 21% 5% 5%
1	D	1053	13% 65% 22% 5% 5%
2	B	1444	15% 88% 6% .. .
2	E	1444	16% 88% 6% .. .

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Mol	Chain	Length	Quality of chain	
3	C	3		67% 33%
3	F	3		67% 33%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 73330 atoms, of which 36308 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 Mgp-operon protein 3.

Mol	Chain	Residues	Atoms						AltConf	Trace
1	A	1003	Total	C	H	N	O	S	0	0
			15252	4850	7559	1282	1554	7		
1	D	1003	Total	C	H	N	O	S	0	0
			15252	4850	7559	1282	1554	7		

- Molecule 2 is a protein called Adhesin P1.

Mol	Chain	Residues	Atoms						AltConf	Trace
2	B	1380	Total	C	H	N	O	S	0	0
			21334	6843	10558	1823	2095	15		
2	E	1380	Total	C	H	N	O	S	0	0
			21334	6843	10558	1823	2095	15		

- Molecule 3 is an oligosaccharide called N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.

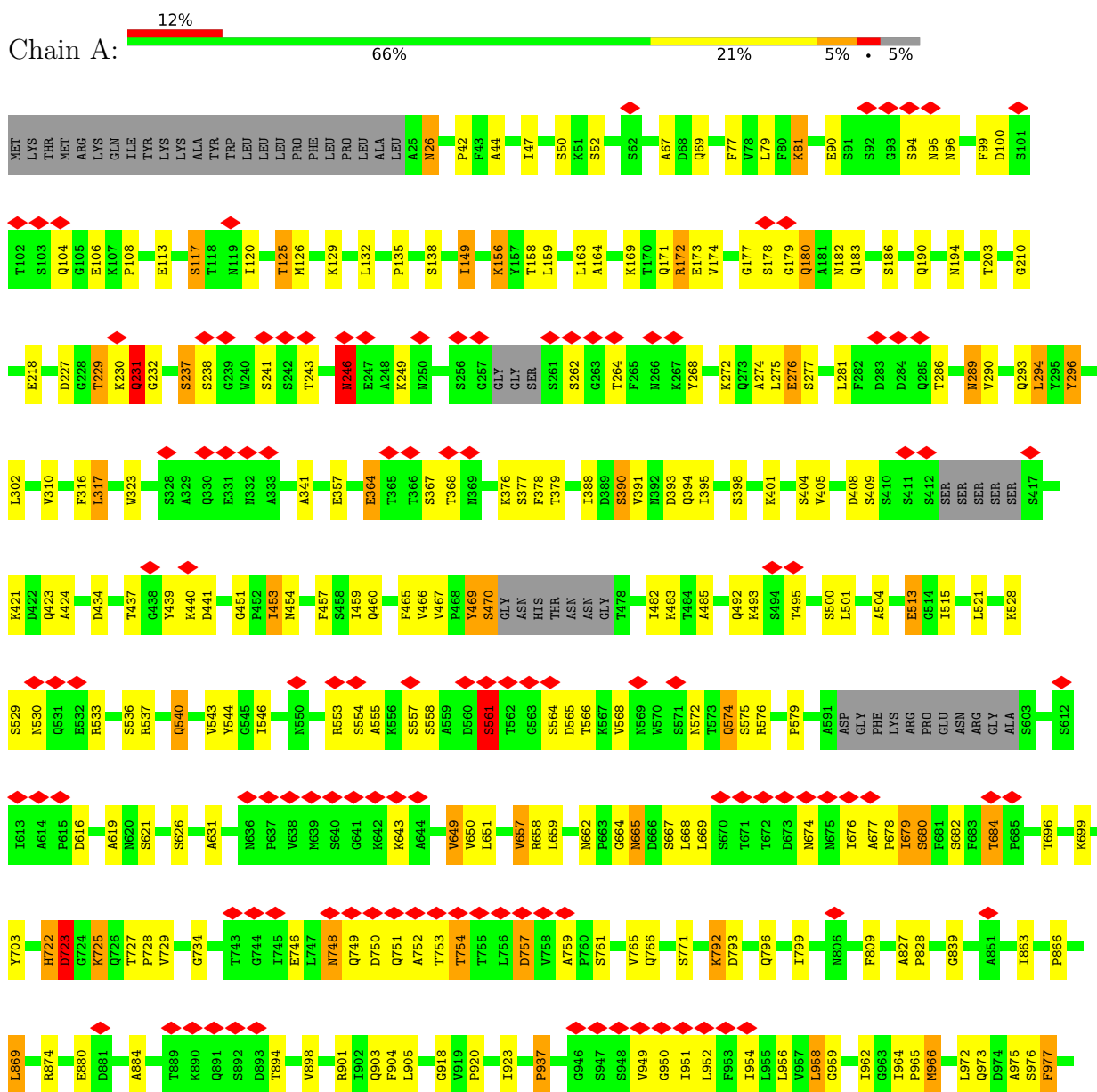


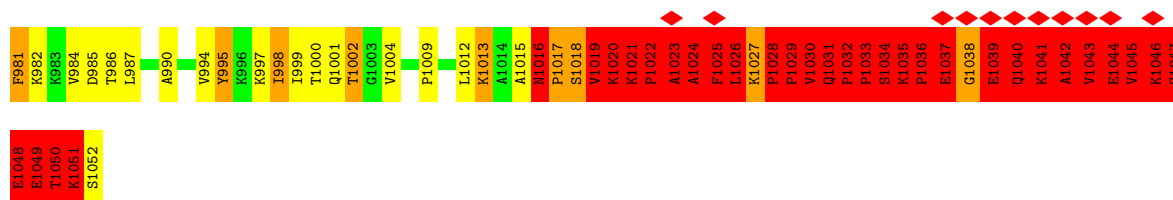
Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	3	Total	C	H	N	O	0	0
			79	23	37	1	18		
3	F	3	Total	C	H	N	O	0	0
			79	23	37	1	18		

3 Residue-property plots

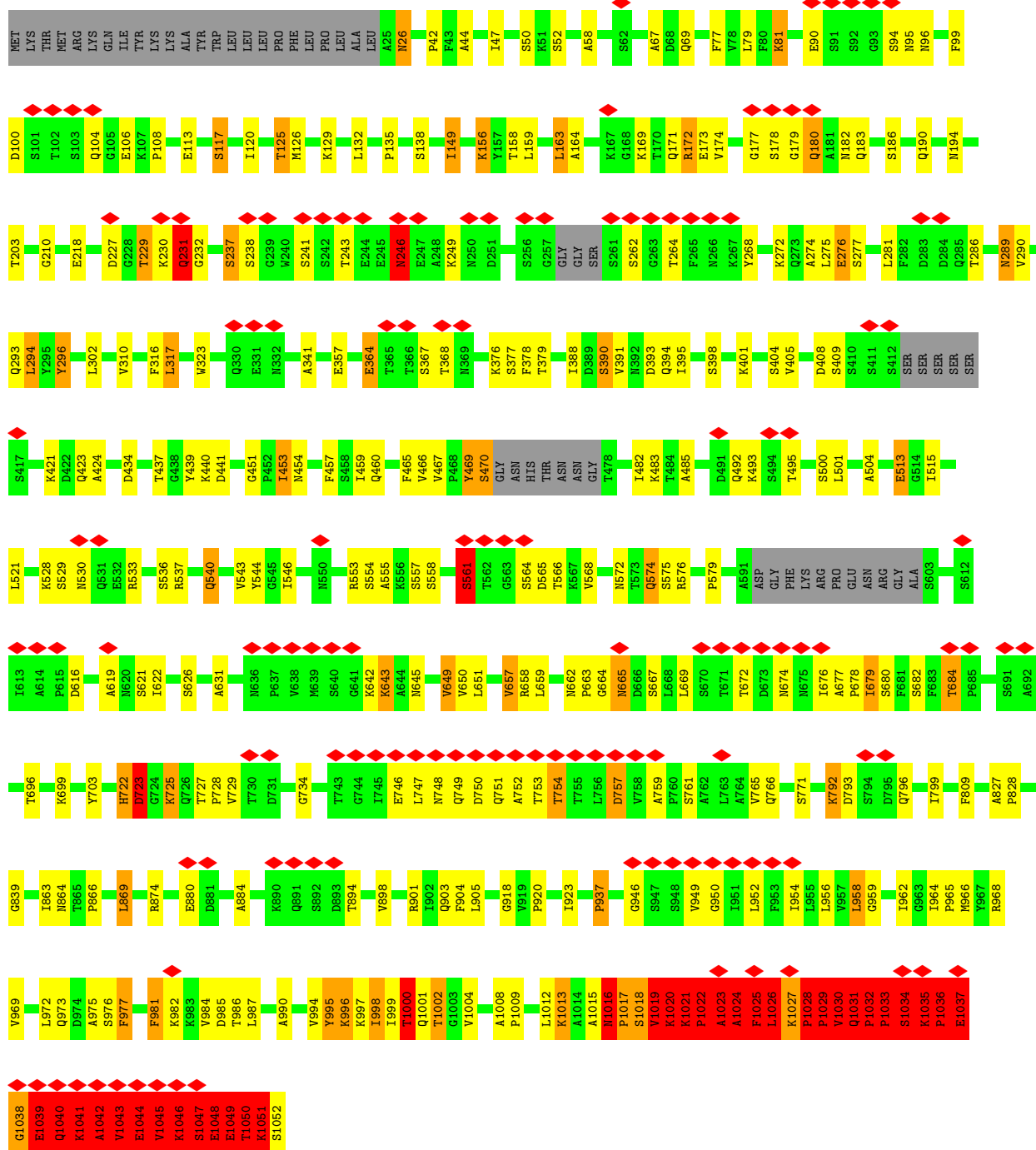
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Mgp-operon protein 3



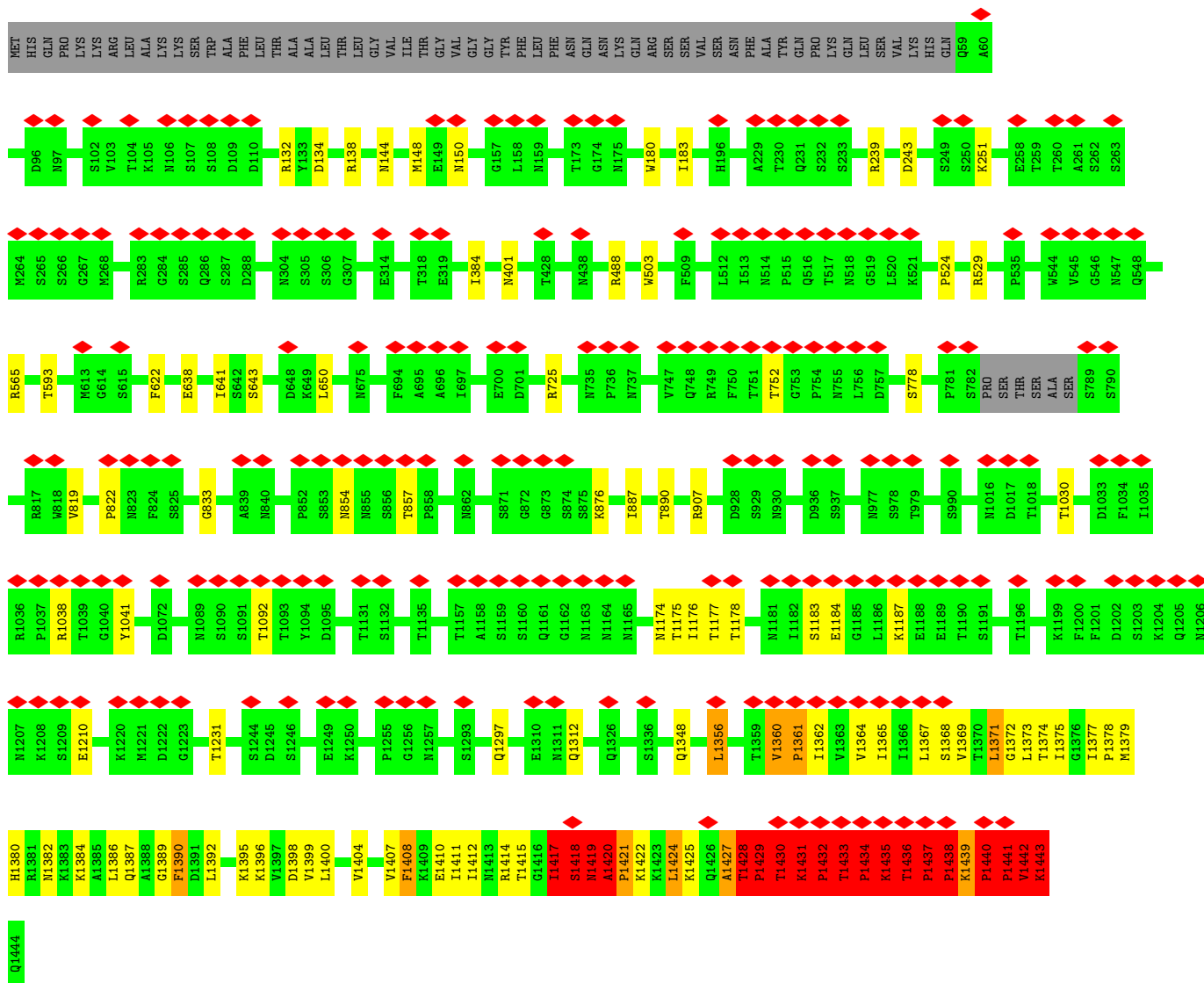


• Molecule 1: Mgp-operon protein 3



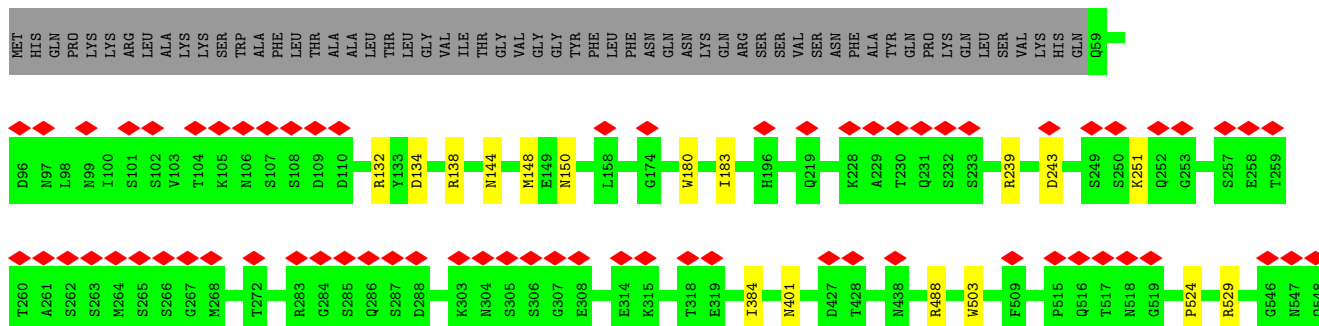
● Molecule 2: Adhesin P1

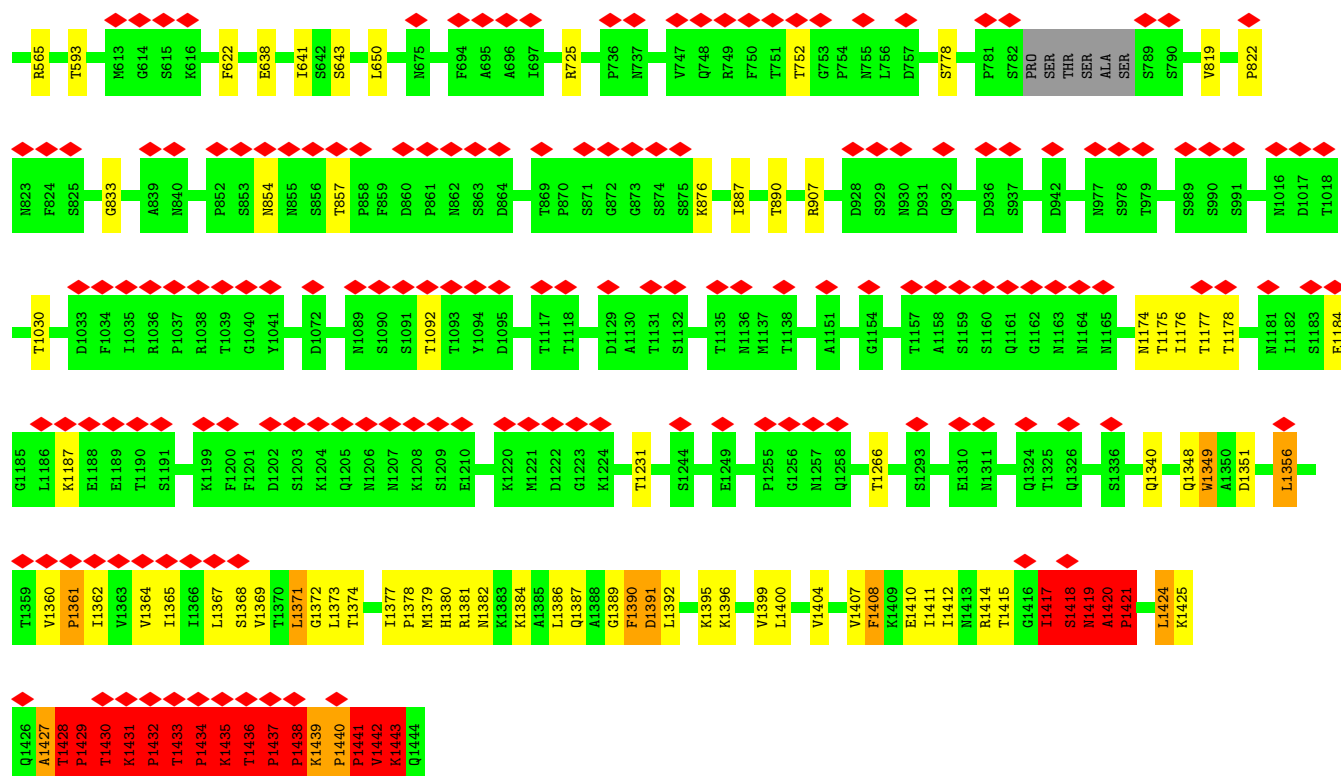
Chain B: 



● Molecule 2: Adhesin P1

Chain E: 





- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain C:



- Molecule 3: N-acetyl-alpha-neuraminic acid-(2-6)-beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain F:



4 Experimental information

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of subtomograms used	36720	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 ($e^-/\text{\AA}^2$)	120	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	105000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	14.746	Depositor
Minimum map value	-6.394	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	1.000	Depositor
Recommended contour level	1.66	Depositor
Map size (Å)	332.8, 332.8, 332.8	wwPDB
Map dimensions	128, 128, 128	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.6, 2.6, 2.6	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GAL, BGC, SIA

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	1.42	52/7851 (0.7%)	1.90	117/10678 (1.1%)
1	D	1.41	56/7851 (0.7%)	1.91	116/10678 (1.1%)
2	B	1.03	30/11047 (0.3%)	1.47	50/15045 (0.3%)
2	E	1.02	31/11047 (0.3%)	1.48	53/15045 (0.4%)
All	All	1.20	169/37796 (0.4%)	1.67	336/51446 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	40
1	D	0	40
2	B	0	21
2	E	0	20
All	All	0	121

All (169) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1024	ALA	C-N	-41.00	0.76	1.33
1	D	1024	ALA	C-N	-40.20	0.77	1.33
2	E	1429	PRO	C-N	-25.21	0.98	1.33
2	B	1429	PRO	C-N	-22.58	1.02	1.33
2	B	1434	PRO	C-N	-19.96	1.05	1.33
1	A	1042	ALA	C-N	-17.35	1.10	1.33
1	A	1022	PRO	C-N	-16.75	1.10	1.33
1	D	1039	GLU	C-N	-16.30	1.10	1.33
1	D	1036	PRO	C-N	-15.58	1.11	1.33
2	E	1434	PRO	C-N	-15.40	1.12	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1039	GLU	C-N	-15.12	1.12	1.33
1	D	1022	PRO	C-N	-15.07	1.12	1.33
1	D	1042	ALA	C-N	-14.74	1.13	1.33
1	A	1036	PRO	C-N	-14.37	1.13	1.33
1	A	1029	PRO	C-N	-14.22	1.14	1.33
1	D	1029	PRO	C-N	-13.64	1.15	1.33
1	D	1002	THR	C-N	-13.62	1.16	1.33
1	D	1048	GLU	C-N	-13.40	1.15	1.33
1	A	1049	GLU	C-N	-12.89	1.15	1.33
1	D	1038	GLY	C-N	-12.57	1.16	1.33
1	A	1038	GLY	C-N	-12.38	1.16	1.33
1	A	1002	THR	C-N	-12.15	1.18	1.33
2	B	1431	LYS	C-N	-12.14	1.05	1.33
1	A	1009	PRO	N-CD	-11.79	1.31	1.47
1	D	1027	LYS	C-N	11.78	1.47	1.33
1	D	1009	PRO	N-CD	-11.76	1.31	1.47
1	D	1013	LYS	C-N	-11.71	1.17	1.34
1	A	1047	SER	C-N	-11.66	1.17	1.33
1	D	1028	PRO	N-CD	-11.48	1.31	1.47
1	A	1028	PRO	N-CD	-11.40	1.31	1.47
1	A	1027	LYS	C-N	11.28	1.46	1.33
1	D	1033	PRO	N-CD	-11.28	1.31	1.47
1	A	1033	PRO	N-CD	-11.28	1.31	1.47
2	B	1421	PRO	N-CD	-11.28	1.31	1.47
2	E	1421	PRO	N-CD	-11.21	1.32	1.47
1	A	1029	PRO	N-CD	-11.08	1.32	1.47
1	D	1029	PRO	N-CD	-11.02	1.32	1.47
1	A	1032	PRO	N-CD	-11.01	1.32	1.47
1	D	1032	PRO	N-CD	-10.99	1.32	1.47
2	B	1429	PRO	N-CD	-10.91	1.32	1.47
2	E	1429	PRO	N-CD	-10.85	1.32	1.47
1	A	1013	LYS	C-N	-10.78	1.19	1.33
1	D	1022	PRO	N-CD	-10.71	1.32	1.47
2	B	1441	PRO	C-N	10.69	1.48	1.33
2	B	1441	PRO	N-CD	-10.69	1.32	1.47
1	D	1041	LYS	C-N	-10.69	1.18	1.33
2	E	1441	PRO	N-CD	-10.68	1.32	1.47
2	E	1437	PRO	N-CD	-10.65	1.32	1.47
2	B	1437	PRO	N-CD	-10.65	1.32	1.47
1	A	1022	PRO	N-CD	-10.62	1.32	1.47
1	A	1041	LYS	C-N	-10.61	1.18	1.33
2	B	1440	PRO	N-CD	-10.45	1.33	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1440	PRO	N-CD	-10.43	1.33	1.47
1	A	1048	GLU	C-N	-10.40	1.19	1.33
2	E	1434	PRO	N-CD	-10.31	1.33	1.47
2	B	1434	PRO	N-CD	-10.29	1.33	1.47
1	D	1047	SER	C-N	-10.22	1.19	1.33
1	D	950	GLY	C-N	10.20	1.46	1.33
1	D	1036	PRO	N-CD	-10.09	1.33	1.47
1	A	1036	PRO	N-CD	-10.08	1.33	1.47
2	B	1438	PRO	N-CD	-9.90	1.33	1.47
2	E	1441	PRO	C-N	9.86	1.47	1.33
2	E	1432	PRO	N-CD	-9.81	1.34	1.47
1	A	1040	GLN	C-N	-9.80	1.20	1.33
1	D	1040	GLN	C-N	-9.69	1.20	1.33
2	B	1432	PRO	N-CD	-9.68	1.34	1.47
2	E	1438	PRO	N-CD	-9.66	1.34	1.47
1	D	1049	GLU	C-N	-9.33	1.20	1.33
1	A	950	GLY	C-N	9.29	1.45	1.33
1	A	1021	LYS	C-N	-9.12	1.12	1.33
2	E	1431	LYS	C-N	-9.10	1.12	1.33
1	A	1033	PRO	C-N	-9.04	1.21	1.33
2	B	1417	ILE	C-N	-9.04	1.21	1.33
1	A	1031	GLN	C-N	8.92	1.44	1.33
2	E	1427	ALA	C-N	-8.88	1.15	1.33
1	A	1017	PRO	N-CD	-8.78	1.35	1.47
1	D	1017	PRO	N-CD	-8.65	1.35	1.47
2	E	1436	THR	C-N	-8.53	1.23	1.33
1	D	1033	PRO	C-N	-8.50	1.21	1.33
1	D	1021	LYS	C-N	-8.44	1.14	1.33
1	A	981	PHE	C-N	-8.32	1.23	1.33
1	D	1043	VAL	C-N	-8.31	1.22	1.33
2	B	1436	THR	C-N	-8.31	1.23	1.33
2	B	1442	VAL	C-N	-8.01	1.22	1.33
2	E	1417	ILE	C-N	-8.01	1.22	1.33
2	B	1361	PRO	C-N	-7.71	1.24	1.33
2	B	1374	THR	C-N	-7.64	1.24	1.33
2	B	1443	LYS	C-N	7.57	1.44	1.33
2	E	1374	THR	C-N	-7.55	1.24	1.33
2	B	1420	ALA	C-N	-7.51	1.16	1.33
2	B	1427	ALA	C-N	-7.44	1.18	1.33
1	A	1016	ASN	C-N	-7.34	1.16	1.33
1	D	981	PHE	C-N	-7.33	1.24	1.33
2	E	1425	LYS	C-N	-7.31	1.23	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	949	VAL	C-N	-7.31	1.24	1.33
2	E	1362	ILE	C-N	-7.26	1.24	1.33
2	E	1361	PRO	C-N	-7.25	1.24	1.33
1	D	1034	SER	C-N	7.22	1.48	1.33
2	B	1425	LYS	C-N	-7.15	1.23	1.33
1	D	1016	ASN	C-N	-7.15	1.17	1.33
1	D	1015	ALA	C-N	-7.14	1.24	1.33
1	A	1034	SER	C-N	7.07	1.48	1.33
2	B	1362	ILE	C-N	-7.07	1.25	1.33
1	A	1043	VAL	C-N	-7.05	1.23	1.33
2	E	1439	LYS	C-N	7.01	1.41	1.33
1	A	401	LYS	C-O	6.97	1.32	1.24
2	E	1443	LYS	C-N	6.95	1.43	1.33
1	A	923	ILE	C-O	6.94	1.32	1.24
1	D	401	LYS	C-O	6.94	1.32	1.24
1	D	923	ILE	C-O	6.90	1.32	1.24
1	A	1035	LYS	C-N	-6.79	1.18	1.33
1	D	949	VAL	C-N	-6.78	1.25	1.33
2	E	1428	THR	C-N	-6.76	1.18	1.33
1	A	1019	VAL	C-N	-6.73	1.24	1.33
2	B	1390	PHE	C-N	-6.61	1.25	1.33
1	D	1035	LYS	C-N	-6.59	1.18	1.33
2	E	1433	THR	C-N	-6.58	1.18	1.33
1	D	1009	PRO	C-N	-6.46	1.25	1.34
2	B	1382	ASN	C-N	-6.38	1.25	1.33
2	E	1382	ASN	C-N	-6.33	1.25	1.33
2	E	1420	ALA	C-N	-6.26	1.19	1.33
1	D	977	PHE	C-N	-6.23	1.26	1.33
2	E	1387	GLN	C-N	-6.23	1.25	1.33
2	B	1432	PRO	C-N	-6.20	1.20	1.33
1	D	649	VAL	C-O	6.15	1.30	1.23
1	A	649	VAL	C-O	6.13	1.30	1.23
2	B	1421	PRO	C-N	-6.10	1.25	1.33
1	D	1046	LYS	C-N	-6.09	1.25	1.33
1	D	920	PRO	C-O	-6.09	1.16	1.23
2	E	1390	PHE	C-N	-6.06	1.26	1.33
1	D	504	ALA	C-O	6.02	1.32	1.23
1	A	504	ALA	C-O	5.99	1.32	1.23
1	A	920	PRO	C-O	-5.98	1.16	1.23
1	A	977	PHE	C-N	-5.95	1.26	1.33
1	A	316	PHE	C-O	-5.91	1.17	1.24
2	B	1387	GLN	C-N	-5.86	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	982	LYS	C-N	-5.84	1.26	1.33
1	A	1015	ALA	C-N	-5.83	1.26	1.33
1	D	1019	VAL	C-N	-5.82	1.25	1.33
1	D	316	PHE	C-O	-5.82	1.17	1.24
1	D	972	LEU	C-N	-5.79	1.26	1.33
1	A	1044	GLU	C-N	-5.79	1.25	1.33
1	A	972	LEU	C-N	-5.76	1.26	1.33
1	D	968	ARG	C-N	-5.63	1.26	1.33
1	D	998	ILE	C-N	-5.62	1.26	1.33
2	B	1439	LYS	C-N	5.57	1.40	1.33
1	A	982	LYS	C-N	-5.54	1.26	1.33
1	D	1017	PRO	C-N	5.42	1.41	1.33
1	A	404	SER	C-O	5.41	1.30	1.24
1	A	998	ILE	C-N	-5.41	1.27	1.33
1	A	880	GLU	C-O	5.40	1.30	1.23
1	D	404	SER	C-O	5.40	1.30	1.24
1	A	1000	THR	C-N	-5.37	1.26	1.33
1	A	246	ASN	C-O	5.36	1.30	1.24
1	D	880	GLU	C-O	5.34	1.30	1.23
1	D	246	ASN	C-O	5.32	1.30	1.24
2	B	1395	LYS	C-N	-5.30	1.27	1.33
1	D	1031	GLN	C-N	5.27	1.39	1.33
2	E	1421	PRO	C-N	-5.26	1.26	1.33
1	D	996	LYS	C-N	-5.25	1.27	1.33
2	E	1369	VAL	C-N	-5.21	1.27	1.33
1	D	975	ALA	C-N	-5.20	1.26	1.33
1	A	828	PRO	C-O	-5.17	1.17	1.23
2	E	1395	LYS	C-N	-5.16	1.27	1.33
1	D	1000	THR	C-N	-5.15	1.26	1.33
2	E	1391	ASP	C-N	-5.14	1.27	1.33
1	D	828	PRO	C-O	-5.12	1.17	1.23
2	B	1369	VAL	C-N	-5.11	1.27	1.33
1	A	975	ALA	C-N	-5.07	1.27	1.33

All (336) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1047	SER	O-C-N	-29.01	84.01	122.59
1	A	1038	GLY	O-C-N	-28.77	85.30	122.70
1	D	1038	GLY	O-C-N	-28.58	85.54	122.70
1	A	1047	SER	O-C-N	-28.13	85.18	122.59
1	D	1036	PRO	O-C-N	-26.64	86.68	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1033	PRO	O-C-N	-25.57	88.12	122.64
1	A	1036	PRO	O-C-N	-25.46	88.27	122.64
1	D	1030	VAL	O-C-N	-24.50	91.95	122.57
1	A	1019	VAL	O-C-N	-24.11	92.43	122.57
1	D	1029	PRO	O-C-N	-23.80	90.52	122.64
1	D	1026	LEU	O-C-N	-23.66	91.12	122.59
1	D	1045	VAL	O-C-N	-23.46	93.25	122.57
1	A	1024	ALA	O-C-N	-23.21	91.73	122.59
1	D	1049	GLU	O-C-N	-23.09	91.88	122.59
1	A	1026	LEU	O-C-N	-23.06	91.92	122.59
2	B	1434	PRO	O-C-N	-22.98	91.61	122.64
1	A	1030	VAL	O-C-N	-22.85	94.01	122.57
1	A	1033	PRO	O-C-N	-22.80	91.86	122.64
1	A	1049	GLU	O-C-N	-22.75	92.33	122.59
1	A	1029	PRO	O-C-N	-22.71	91.99	122.64
2	B	1432	PRO	O-C-N	-22.68	92.02	122.64
1	D	1051	LYS	O-C-N	-22.51	92.65	122.59
1	D	1023	ALA	O-C-N	-22.48	92.69	122.59
2	E	1434	PRO	O-C-N	-22.29	92.55	122.64
1	A	1045	VAL	O-C-N	-22.19	94.84	122.57
1	D	1040	GLN	O-C-N	-21.68	93.75	122.59
1	D	1042	ALA	O-C-N	-21.65	93.79	122.59
2	B	1443	LYS	O-C-N	-21.48	94.03	122.59
1	A	1042	ALA	O-C-N	-21.46	94.04	122.59
1	A	1022	PRO	O-C-N	-21.16	94.08	122.64
1	A	1050	THR	O-C-N	-20.97	94.70	122.59
2	E	1443	LYS	O-C-N	-20.74	95.01	122.59
1	D	1024	ALA	O-C-N	-20.60	95.19	122.59
1	A	1048	GLU	O-C-N	-20.59	95.20	122.59
1	D	1048	GLU	O-C-N	-20.49	95.34	122.59
1	A	1040	GLN	O-C-N	-20.35	95.52	122.59
1	D	1019	VAL	O-C-N	-20.21	97.31	122.57
1	D	1050	THR	O-C-N	-20.16	95.77	122.59
1	A	1051	LYS	O-C-N	-19.98	96.02	122.59
2	E	1432	PRO	O-C-N	-19.90	95.78	122.64
2	B	1417	ILE	O-C-N	-19.65	98.00	122.57
1	D	1022	PRO	O-C-N	-19.63	96.13	122.64
1	A	1034	SER	O-C-N	-19.62	96.50	122.59
1	D	1041	LYS	O-C-N	-19.37	96.83	122.59
1	D	1034	SER	O-C-N	-19.32	96.89	122.59
1	D	1043	VAL	O-C-N	-19.11	98.69	122.57
1	A	1041	LYS	O-C-N	-18.99	97.34	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1417	ILE	O-C-N	-18.91	98.94	122.57
2	B	1435	LYS	O-C-N	-18.57	97.89	122.59
1	A	1023	ALA	O-C-N	-18.45	98.05	122.59
1	D	1039	GLU	O-C-N	-18.42	98.10	122.59
2	E	1431	LYS	O-C-N	-18.16	106.52	121.23
2	E	1435	LYS	O-C-N	-18.07	98.56	122.59
1	A	1043	VAL	O-C-N	-18.00	100.07	122.57
1	A	1020	LYS	O-C-N	-17.79	98.93	122.59
1	D	1027	LYS	O-C-N	-17.77	100.89	121.32
1	D	1020	LYS	O-C-N	-17.52	99.30	122.59
1	A	1027	LYS	O-C-N	-17.51	101.18	121.32
1	D	1046	LYS	O-C-N	-17.11	99.84	122.59
1	A	1027	LYS	CA-C-N	16.80	137.69	120.38
1	A	1027	LYS	C-N-CA	16.80	137.69	120.38
1	A	1039	GLU	O-C-N	-16.73	100.34	122.59
1	D	1032	PRO	O-C-N	-16.36	102.16	121.46
2	B	1433	THR	O-C-N	-16.11	102.79	121.32
1	D	1027	LYS	CA-C-N	15.46	136.30	120.38
1	D	1027	LYS	C-N-CA	15.46	136.30	120.38
2	E	1441	PRO	O-C-N	-15.45	101.78	122.64
2	B	1441	PRO	O-C-N	-15.41	101.84	122.64
1	D	1044	GLU	O-C-N	-15.32	102.21	122.59
2	B	1437	PRO	O-C-N	-15.16	103.58	121.46
2	E	1438	PRO	O-C-N	-14.94	102.48	122.64
1	A	1044	GLU	O-C-N	-14.88	102.80	122.59
1	A	1046	LYS	O-C-N	-14.87	102.81	122.59
2	E	1442	VAL	O-C-N	-14.84	104.02	122.57
2	E	1437	PRO	O-C-N	-14.62	104.22	121.46
2	E	1431	LYS	CA-C-N	14.55	138.03	119.84
2	E	1431	LYS	C-N-CA	14.55	138.03	119.84
2	B	1438	PRO	O-C-N	-14.52	103.03	122.64
2	E	1433	THR	O-C-N	-14.39	104.77	121.32
1	A	1032	PRO	O-C-N	-14.33	104.56	121.46
2	B	1442	VAL	O-C-N	-14.30	104.69	122.57
2	E	1429	PRO	O-C-N	-13.21	104.81	122.64
2	B	1431	LYS	CA-C-N	12.23	135.13	119.84
2	B	1431	LYS	C-N-CA	12.23	135.13	119.84
1	D	1028	PRO	O-C-N	-12.22	107.04	121.46
2	B	1436	THR	O-C-N	-12.22	107.27	121.32
1	A	1037	GLU	O-C-N	-12.16	106.42	122.59
1	A	1021	LYS	O-C-N	-12.15	107.35	121.32
1	D	1037	GLU	O-C-N	-12.09	106.51	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1440	PRO	O-C-N	-12.07	107.21	121.46
1	A	1016	ASN	O-C-N	-11.89	110.60	121.42
2	B	1429	PRO	O-C-N	-11.71	106.83	122.64
1	A	1028	PRO	O-C-N	-11.71	107.65	121.46
2	E	1436	THR	O-C-N	-11.63	107.94	121.32
1	D	1021	LYS	O-C-N	-11.53	108.06	121.32
2	B	1431	LYS	O-C-N	-11.32	108.30	121.32
2	E	1440	PRO	O-C-N	-11.25	108.19	121.46
1	A	1031	GLN	O-C-N	-11.19	108.46	121.32
1	A	1025	PHE	O-C-N	-11.07	107.86	122.59
2	B	1418	SER	O-C-N	-10.90	108.09	122.59
1	A	1028	PRO	CA-C-N	10.72	133.24	119.84
1	A	1028	PRO	C-N-CA	10.72	133.24	119.84
1	D	1016	ASN	O-C-N	-10.33	112.02	121.42
1	D	1031	GLN	O-C-N	-10.23	109.56	121.32
2	B	1348	GLN	N-CA-C	9.97	125.96	110.20
1	D	1004	VAL	O-C-N	-9.92	110.48	122.18
1	D	1035	LYS	O-C-N	-9.87	109.97	121.32
1	D	1033	PRO	CA-C-N	9.70	140.07	121.54
1	D	1033	PRO	C-N-CA	9.70	140.07	121.54
2	E	1439	LYS	O-C-N	-9.66	110.21	121.32
2	E	1418	SER	O-C-N	-9.60	109.82	122.59
2	B	1439	LYS	O-C-N	-9.34	110.58	121.32
1	A	1033	PRO	CA-C-N	9.32	139.35	121.54
1	A	1033	PRO	C-N-CA	9.32	139.35	121.54
2	E	1421	PRO	O-C-N	-8.72	110.87	122.64
2	E	1420	ALA	O-C-N	-8.65	111.37	121.32
1	A	1035	LYS	O-C-N	-8.56	111.47	121.32
2	E	1349	TRP	N-CA-C	8.54	121.54	110.53
2	E	1430	THR	CA-C-N	-8.48	110.55	121.74
2	E	1430	THR	C-N-CA	-8.48	110.55	121.74
1	D	937	PRO	N-CA-C	8.40	129.78	112.47
2	B	1420	ALA	O-C-N	-8.39	111.67	121.32
2	E	1348	GLN	N-CA-C	8.25	122.17	112.93
2	E	1428	THR	O-C-N	-8.23	111.85	121.32
1	D	1028	PRO	CA-C-N	8.22	130.12	119.84
1	D	1028	PRO	C-N-CA	8.22	130.12	119.84
2	E	1421	PRO	CA-C-N	8.02	136.86	121.54
2	E	1421	PRO	C-N-CA	8.02	136.86	121.54
1	D	1016	ASN	CA-C-N	7.89	129.71	119.84
1	D	1016	ASN	C-N-CA	7.89	129.71	119.84
2	B	1421	PRO	O-C-N	-7.85	112.05	122.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1417	ILE	CA-C-N	7.78	136.40	121.54
2	E	1417	ILE	C-N-CA	7.78	136.40	121.54
1	A	1016	ASN	CA-C-N	7.75	129.52	119.84
1	A	1016	ASN	C-N-CA	7.75	129.52	119.84
2	B	1421	PRO	CA-C-N	7.65	136.15	121.54
2	B	1421	PRO	C-N-CA	7.65	136.15	121.54
1	D	1025	PHE	O-C-N	-7.62	112.45	122.59
2	E	1418	SER	CA-C-N	-7.53	111.07	123.04
2	E	1418	SER	C-N-CA	-7.53	111.07	123.04
1	D	1027	LYS	C-N-CD	-7.43	94.54	125.00
1	D	995	TYR	O-C-N	7.40	129.69	122.07
1	A	1030	VAL	CA-C-N	7.32	139.66	121.80
1	A	1030	VAL	C-N-CA	7.32	139.66	121.80
1	A	1027	LYS	C-N-CD	-7.28	95.14	125.00
1	A	995	TYR	O-C-N	7.26	129.55	122.07
2	B	1420	ALA	CA-C-N	7.14	128.77	119.84
2	B	1420	ALA	C-N-CA	7.14	128.77	119.84
2	B	1418	SER	CA-C-N	-7.08	111.78	123.04
2	B	1418	SER	C-N-CA	-7.08	111.78	123.04
2	B	1417	ILE	CA-C-N	7.08	135.07	121.54
2	B	1417	ILE	C-N-CA	7.08	135.07	121.54
1	A	937	PRO	N-CA-C	6.99	126.87	112.47
2	E	1420	ALA	CA-C-N	6.94	128.51	119.84
2	E	1420	ALA	C-N-CA	6.94	128.51	119.84
1	A	1031	GLN	CA-C-N	6.90	127.49	120.38
1	A	1031	GLN	C-N-CA	6.90	127.49	120.38
1	A	827	ALA	O-C-N	-6.89	117.30	121.71
1	D	827	ALA	O-C-N	-6.88	117.31	121.71
1	D	1042	ALA	CA-C-N	6.83	134.26	121.97
1	D	1042	ALA	C-N-CA	6.83	134.26	121.97
1	D	231	GLN	CA-C-N	-6.66	113.97	121.83
1	D	231	GLN	C-N-CA	-6.66	113.97	121.83
1	A	231	GLN	CA-C-N	-6.65	113.98	121.83
1	A	231	GLN	C-N-CA	-6.65	113.98	121.83
2	B	1408	PHE	O-C-N	6.64	129.72	122.15
1	D	1036	PRO	CA-C-N	6.63	134.21	121.54
1	D	1036	PRO	C-N-CA	6.63	134.21	121.54
1	A	408	ASP	CA-CB-CG	6.63	119.23	112.60
1	D	408	ASP	CA-CB-CG	6.63	119.23	112.60
1	A	1004	VAL	O-C-N	-6.60	113.01	122.12
1	A	1036	PRO	CA-C-N	6.57	134.09	121.54
1	A	1036	PRO	C-N-CA	6.57	134.09	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	1008	ALA	O-C-N	-6.57	113.77	121.32
1	A	95	ASN	CA-C-N	6.49	128.88	120.44
1	A	95	ASN	C-N-CA	6.49	128.88	120.44
1	D	95	ASN	CA-C-N	6.48	128.86	120.44
1	D	95	ASN	C-N-CA	6.48	128.86	120.44
1	D	1030	VAL	CA-C-N	6.45	137.55	121.80
1	D	1030	VAL	C-N-CA	6.45	137.55	121.80
1	A	723	ASP	CA-CB-CG	6.44	119.04	112.60
1	D	513	GLU	CA-C-N	6.41	128.20	120.13
1	D	513	GLU	C-N-CA	6.41	128.20	120.13
1	A	513	GLU	CA-C-N	6.41	128.20	120.13
1	A	513	GLU	C-N-CA	6.41	128.20	120.13
1	D	723	ASP	CA-CB-CG	6.39	119.00	112.60
1	A	1048	GLU	CA-C-N	6.26	133.50	121.54
1	A	1048	GLU	C-N-CA	6.26	133.50	121.54
1	D	1015	ALA	O-C-N	-6.24	114.07	122.43
1	D	903	GLN	N-CA-CB	6.17	119.38	110.06
1	A	903	GLN	N-CA-CB	6.17	119.37	110.06
2	E	1408	PHE	O-C-N	6.17	129.18	122.15
1	A	26	ASN	CA-CB-CG	6.13	118.73	112.60
1	A	723	ASP	CB-CA-C	-6.12	98.24	110.42
1	D	723	ASP	CB-CA-C	-6.09	98.31	110.42
1	D	26	ASN	CA-CB-CG	6.07	118.67	112.60
1	A	616	ASP	CA-CB-CG	6.01	118.61	112.60
1	D	616	ASP	CA-CB-CG	6.00	118.61	112.60
1	D	616	ASP	CB-CA-C	5.97	120.31	111.06
1	A	616	ASP	CB-CA-C	5.96	120.29	111.06
2	B	1428	THR	O-C-N	-5.95	114.48	121.32
2	E	138	ARG	NE-CZ-NH2	5.94	124.54	119.20
2	E	1349	TRP	CA-CB-CG	5.92	124.85	113.60
2	B	138	ARG	NE-CZ-NH2	5.92	124.53	119.20
1	A	274	ALA	CA-C-N	5.92	128.46	120.65
1	A	274	ALA	C-N-CA	5.92	128.46	120.65
1	A	100	ASP	CA-C-N	5.89	128.10	120.44
1	A	100	ASP	C-N-CA	5.89	128.10	120.44
1	D	100	ASP	CA-C-N	5.89	128.09	120.44
1	D	100	ASP	C-N-CA	5.89	128.09	120.44
1	D	274	ALA	CA-C-N	5.88	128.41	120.65
1	D	274	ALA	C-N-CA	5.88	128.41	120.65
2	E	1415	THR	O-C-N	-5.88	114.07	122.41
1	D	703	TYR	CA-C-O	-5.81	114.43	120.70
1	A	703	TYR	CA-C-O	-5.81	114.43	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	903	GLN	CB-CA-C	-5.78	99.76	109.53
1	A	903	GLN	CB-CA-C	-5.78	99.77	109.53
1	D	553	ARG	CA-C-O	-5.74	114.33	120.42
1	D	42	PRO	CB-CA-C	-5.71	103.28	111.62
1	A	42	PRO	CB-CA-C	-5.71	103.29	111.62
2	B	1415	THR	O-C-N	-5.70	114.32	122.41
1	A	553	ARG	CA-C-O	-5.67	114.41	120.42
1	A	1047	SER	CA-C-N	5.66	132.34	121.54
1	A	1047	SER	C-N-CA	5.66	132.34	121.54
1	A	722	HIS	CA-C-N	5.63	132.30	121.54
1	A	722	HIS	C-N-CA	5.63	132.30	121.54
1	D	757	ASP	CA-CB-CG	5.61	118.21	112.60
1	D	722	HIS	CA-C-N	5.60	132.24	121.54
1	D	722	HIS	C-N-CA	5.60	132.24	121.54
1	A	757	ASP	CA-CB-CG	5.60	118.20	112.60
2	B	132	ARG	NE-CZ-NH2	5.59	124.23	119.20
2	B	907	ARG	NE-CZ-NH2	5.57	124.22	119.20
1	A	1042	ALA	CA-C-N	5.57	132.00	121.97
1	A	1042	ALA	C-N-CA	5.57	132.00	121.97
2	B	384	ILE	N-CA-C	5.57	116.20	110.36
2	E	907	ARG	NE-CZ-NH2	5.57	124.21	119.20
2	E	132	ARG	NE-CZ-NH2	5.56	124.21	119.20
2	E	384	ILE	N-CA-C	5.55	116.19	110.36
1	D	950	GLY	O-C-N	5.53	127.49	122.18
1	A	1028	PRO	C-N-CD	-5.48	102.52	125.00
2	B	529	ARG	NE-CZ-NH2	5.46	124.12	119.20
2	E	529	ARG	NE-CZ-NH2	5.46	124.12	119.20
1	A	809	PHE	CA-C-O	-5.44	115.07	121.16
1	D	1048	GLU	CA-C-N	5.43	131.92	121.54
1	D	1048	GLU	C-N-CA	5.43	131.92	121.54
1	D	809	PHE	CA-C-O	-5.42	115.09	121.16
2	E	1419	ASN	O-C-N	-5.39	109.34	121.74
2	B	1419	ASN	O-C-N	-5.37	109.38	121.74
1	D	923	ILE	CA-C-N	-5.37	115.22	122.63
1	D	923	ILE	C-N-CA	-5.37	115.22	122.63
2	E	1431	LYS	C-N-CD	-5.36	103.01	125.00
2	B	1360	VAL	O-C-N	5.36	123.85	120.42
1	A	923	ILE	CA-C-N	-5.36	115.24	122.63
1	A	923	ILE	C-N-CA	-5.36	115.24	122.63
2	E	134	ASP	CA-CB-CG	5.35	117.95	112.60
2	B	1408	PHE	CA-C-N	-5.32	113.52	120.44
2	B	1408	PHE	C-N-CA	-5.32	113.52	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	134	ASP	CA-CB-CG	5.32	117.92	112.60
1	D	238	SER	CA-C-N	5.32	125.89	119.98
1	D	238	SER	C-N-CA	5.32	125.89	119.98
1	A	238	SER	CA-C-N	5.31	125.88	119.98
1	A	238	SER	C-N-CA	5.31	125.88	119.98
1	D	316	PHE	CA-C-O	-5.31	114.13	120.56
2	B	150	ASN	CB-CA-C	5.30	114.96	111.20
2	E	524	PRO	N-CA-CB	5.30	106.29	102.79
1	A	316	PHE	CA-C-O	-5.28	114.17	120.56
2	E	150	ASN	CB-CA-C	5.26	114.93	111.20
1	A	754	THR	CA-C-N	5.25	129.01	121.50
1	A	754	THR	C-N-CA	5.25	129.01	121.50
1	D	754	THR	CA-C-N	5.25	129.00	121.50
1	D	754	THR	C-N-CA	5.25	129.00	121.50
2	B	524	PRO	N-CA-CB	5.24	106.25	102.79
1	D	729	VAL	CA-C-O	-5.24	114.88	120.59
1	D	621	SER	CA-C-O	-5.23	115.25	121.32
1	A	117	SER	CA-C-O	-5.23	114.43	120.24
1	D	894	THR	CA-CB-CG2	5.23	119.39	110.50
1	A	950	GLY	O-C-N	5.22	127.19	122.18
1	D	388	ILE	CA-C-O	-5.22	116.05	120.96
1	D	117	SER	CA-C-O	-5.22	114.45	120.24
1	A	729	VAL	CA-C-O	-5.21	114.92	120.59
1	A	684	THR	CB-CA-C	5.18	117.08	110.13
1	D	684	THR	CB-CA-C	5.18	117.08	110.13
1	A	621	SER	CA-C-O	-5.17	115.32	121.32
1	D	1004	VAL	CA-C-N	5.16	129.70	121.34
1	D	1004	VAL	C-N-CA	5.16	129.70	121.34
2	E	239	ARG	NE-CZ-NH2	5.16	123.84	119.20
2	B	488	ARG	NE-CZ-NH2	5.16	123.84	119.20
1	A	388	ILE	CA-C-O	-5.16	116.11	120.96
1	A	276	GLU	CA-C-N	5.15	127.49	120.54
1	A	276	GLU	C-N-CA	5.15	127.49	120.54
1	A	699	LYS	N-CA-CB	5.14	117.43	110.59
1	D	276	GLU	CA-C-N	5.14	127.48	120.54
1	D	276	GLU	C-N-CA	5.14	127.48	120.54
2	E	1340	GLN	OE1-CD-NE2	-5.14	117.46	122.60
1	A	289	ASN	CA-C-N	5.14	127.03	120.56
1	A	289	ASN	C-N-CA	5.14	127.03	120.56
2	B	239	ARG	NE-CZ-NH2	5.13	123.82	119.20
1	D	699	LYS	N-CA-CB	5.13	117.42	110.59
2	E	488	ARG	NE-CZ-NH2	5.12	123.81	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	171	GLN	N-CA-C	-5.12	105.70	111.28
1	A	894	THR	CA-CB-CG2	5.12	119.20	110.50
1	A	839	GLY	CA-C-O	-5.11	115.93	122.01
1	A	874	ARG	CB-CA-C	5.11	119.06	109.71
1	D	171	GLN	N-CA-C	-5.11	105.71	111.28
1	D	874	ARG	CB-CA-C	5.11	119.06	109.71
1	D	289	ASN	CA-C-N	5.11	127.00	120.56
1	D	289	ASN	C-N-CA	5.11	127.00	120.56
2	B	854	ASN	CA-CB-CG	5.10	117.70	112.60
2	E	854	ASN	CA-CB-CG	5.10	117.70	112.60
1	A	1045	VAL	CA-C-N	5.08	131.24	121.54
1	A	1045	VAL	C-N-CA	5.08	131.24	121.54
2	B	1390	PHE	O-C-N	5.08	127.94	122.15
1	D	296	TYR	CA-C-O	-5.07	115.17	120.55
1	D	946	GLY	O-C-N	5.07	127.06	122.19
1	A	1051	LYS	CA-C-N	-5.07	112.57	121.70
1	A	1051	LYS	C-N-CA	-5.07	112.57	121.70
1	D	839	GLY	CA-C-O	-5.07	115.98	122.01
1	D	1032	PRO	CA-C-N	5.07	126.18	119.84
1	D	1032	PRO	C-N-CA	5.07	126.18	119.84
1	A	296	TYR	CA-C-O	-5.06	115.18	120.55
1	A	1034	SER	CA-C-N	5.06	134.14	121.80
1	A	1034	SER	C-N-CA	5.06	134.14	121.80
2	E	565	ARG	NE-CZ-NH2	5.05	123.75	119.20
1	A	1029	PRO	CA-C-N	5.05	131.07	121.97
1	A	1029	PRO	C-N-CA	5.05	131.07	121.97
2	E	1382	ASN	O-C-N	5.05	127.91	122.15
2	B	565	ARG	NE-CZ-NH2	5.04	123.73	119.20
1	D	1009	PRO	CA-C-N	-5.03	113.03	120.28
1	D	1009	PRO	C-N-CA	-5.03	113.03	120.28
2	E	1348	GLN	OE1-CD-NE2	-5.02	117.58	122.60
1	A	1031	GLN	C-N-CD	-5.01	104.45	125.00
1	D	1034	SER	CA-C-N	5.01	134.03	121.80
1	D	1034	SER	C-N-CA	5.01	134.03	121.80
1	D	1031	GLN	CA-C-N	5.00	125.53	120.38
1	D	1031	GLN	C-N-CA	5.00	125.53	120.38
2	B	1382	ASN	O-C-N	5.00	127.85	122.15

There are no chirality outliers.

All (121) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1016	ASN	Mainchain
1	A	1019	VAL	Mainchain
1	A	1020	LYS	Mainchain
1	A	1021	LYS	Mainchain
1	A	1022	PRO	Mainchain
1	A	1023	ALA	Mainchain
1	A	1024	ALA	Peptide,Mainchain
1	A	1025	PHE	Mainchain
1	A	1026	LEU	Mainchain
1	A	1027	LYS	Mainchain
1	A	1028	PRO	Mainchain
1	A	1029	PRO	Mainchain
1	A	1030	VAL	Mainchain
1	A	1031	GLN	Mainchain
1	A	1032	PRO	Mainchain
1	A	1033	PRO	Mainchain
1	A	1034	SER	Mainchain
1	A	1035	LYS	Mainchain
1	A	1036	PRO	Mainchain
1	A	1037	GLU	Mainchain
1	A	1038	GLY	Mainchain
1	A	1039	GLU	Mainchain
1	A	1040	GLN	Mainchain
1	A	1041	LYS	Mainchain
1	A	1042	ALA	Mainchain
1	A	1043	VAL	Mainchain
1	A	1044	GLU	Mainchain
1	A	1045	VAL	Mainchain
1	A	1046	LYS	Mainchain
1	A	1047	SER	Mainchain
1	A	1048	GLU	Mainchain
1	A	1049	GLU	Mainchain
1	A	1050	THR	Mainchain
1	A	1051	LYS	Mainchain
1	A	135	PRO	Peptide
1	A	178	SER	Peptide
1	A	179	GLY	Peptide
1	A	243	THR	Peptide
1	A	722	HIS	Peptide
2	B	1417	ILE	Mainchain
2	B	1418	SER	Mainchain
2	B	1419	ASN	Mainchain
2	B	1420	ALA	Mainchain

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Mol	Chain	Res	Type	Group
2	B	1421	PRO	Mainchain
2	B	1422	LYS	Mainchain
2	B	1428	THR	Mainchain
2	B	1429	PRO	Mainchain
2	B	1431	LYS	Mainchain
2	B	1432	PRO	Mainchain
2	B	1433	THR	Mainchain
2	B	1434	PRO	Mainchain
2	B	1435	LYS	Mainchain
2	B	1436	THR	Mainchain
2	B	1437	PRO	Mainchain
2	B	1438	PRO	Mainchain
2	B	1439	LYS	Mainchain
2	B	1440	PRO	Mainchain
2	B	1441	PRO	Mainchain
2	B	1442	VAL	Mainchain
2	B	1443	LYS	Mainchain
1	D	1016	ASN	Mainchain
1	D	1019	VAL	Mainchain
1	D	1020	LYS	Mainchain
1	D	1021	LYS	Mainchain
1	D	1022	PRO	Mainchain
1	D	1023	ALA	Mainchain
1	D	1024	ALA	Peptide,Mainchain
1	D	1025	PHE	Mainchain
1	D	1026	LEU	Mainchain
1	D	1027	LYS	Mainchain
1	D	1028	PRO	Mainchain
1	D	1029	PRO	Mainchain
1	D	1030	VAL	Mainchain
1	D	1031	GLN	Mainchain
1	D	1032	PRO	Mainchain
1	D	1033	PRO	Mainchain
1	D	1034	SER	Mainchain
1	D	1035	LYS	Mainchain
1	D	1036	PRO	Mainchain
1	D	1037	GLU	Mainchain
1	D	1038	GLY	Mainchain
1	D	1039	GLU	Mainchain
1	D	1040	GLN	Mainchain
1	D	1041	LYS	Mainchain
1	D	1042	ALA	Mainchain

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Mol	Chain	Res	Type	Group
1	D	1043	VAL	Mainchain
1	D	1044	GLU	Mainchain
1	D	1045	VAL	Mainchain
1	D	1046	LYS	Mainchain
1	D	1047	SER	Mainchain
1	D	1048	GLU	Mainchain
1	D	1049	GLU	Mainchain
1	D	1050	THR	Mainchain
1	D	1051	LYS	Mainchain
1	D	135	PRO	Peptide
1	D	178	SER	Peptide
1	D	179	GLY	Peptide
1	D	243	THR	Peptide
1	D	722	HIS	Peptide
2	E	1417	ILE	Mainchain
2	E	1418	SER	Mainchain
2	E	1419	ASN	Mainchain
2	E	1420	ALA	Mainchain
2	E	1421	PRO	Mainchain
2	E	1428	THR	Mainchain
2	E	1429	PRO	Mainchain
2	E	1431	LYS	Mainchain
2	E	1432	PRO	Mainchain
2	E	1433	THR	Mainchain
2	E	1434	PRO	Mainchain
2	E	1435	LYS	Mainchain
2	E	1436	THR	Mainchain
2	E	1437	PRO	Mainchain
2	E	1438	PRO	Mainchain
2	E	1439	LYS	Mainchain
2	E	1440	PRO	Mainchain
2	E	1441	PRO	Mainchain
2	E	1442	VAL	Mainchain
2	E	1443	LYS	Mainchain

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	7693	7559	7541	318	0
1	D	7693	7559	7535	335	0
2	B	10776	10558	10532	237	0
2	E	10776	10558	10536	238	0
3	C	42	37	35	1	0
3	F	42	37	35	1	0
All	All	37022	36308	36214	726	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 10.

All (726) 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:B:1210:GLU:HB3	1:D:665:ASN:CG	1.23	1.57
1:D:1001:GLN:CD	2:E:1417:ILE:HG23	1.24	1.54
1:A:1001:GLN:CD	2:B:1417:ILE:HG23	1.31	1.54
1:A:1001:GLN:OE1	2:B:1417:ILE:CG1	1.63	1.46
2:B:1038:ARG:HD3	1:D:751:GLN:NE2	1.14	1.44
1:A:994:VAL:HG11	2:B:1408:PHE:CD1	1.53	1.43
1:D:994:VAL:HG11	2:E:1408:PHE:CE1	1.51	1.43
2:B:1176:ILE:CG2	1:D:643:LYS:HG3	1.48	1.41
1:D:994:VAL:HG11	2:E:1408:PHE:CD1	1.55	1.41
1:A:665:ASN:HA	2:E:1174:ASN:ND2	1.18	1.40
1:D:966:MET:HG3	2:E:1379:MET:CE	1.49	1.40
1:A:1001:GLN:NE2	2:B:1417:ILE:CG2	1.82	1.39
1:D:1001:GLN:NE2	2:E:1417:ILE:CG2	1.85	1.38
1:D:1001:GLN:NE2	2:E:1417:ILE:HG23	1.08	1.38
2:B:1176:ILE:CD1	1:D:662:ASN:OD1	1.70	1.37
2:B:1210:GLU:CB	1:D:665:ASN:CG	1.85	1.36
1:D:1001:GLN:OE1	2:E:1417:ILE:HG12	1.23	1.33
1:A:994:VAL:HG11	2:B:1408:PHE:CE1	1.67	1.30
1:A:662:ASN:OD1	2:E:1176:ILE:CB	1.64	1.29
1:D:997:LYS:HZ1	2:E:1419:ASN:CB	1.45	1.29
1:D:997:LYS:NZ	2:E:1419:ASN:O	1.65	1.29
1:A:674:ASN:OD1	2:E:1184:GLU:HG3	1.28	1.27
2:B:1386:LEU:HA	1:D:973:GLN:NE2	1.51	1.25
1:D:966:MET:CG	2:E:1379:MET:HE3	1.68	1.23
1:D:1001:GLN:CD	2:E:1417:ILE:CG2	2.08	1.23
1:A:997:LYS:NZ	2:B:1419:ASN:O	1.67	1.23
1:A:1001:GLN:NE2	2:B:1417:ILE:HG23	0.93	1.23
1:A:966:MET:HG3	2:B:1379:MET:CE	1.69	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1038:ARG:CD	1:D:751:GLN:NE2	2.04	1.21
2:E:1427:ALA:O	2:E:1429:PRO:HD3	1.37	1.21
1:A:1001:GLN:CD	2:B:1417:ILE:CG2	2.12	1.20
1:A:754:THR:HB	2:E:1177:THR:CG2	1.69	1.20
1:A:966:MET:CB	2:B:1379:MET:HE1	1.71	1.20
1:D:966:MET:CG	2:E:1379:MET:CE	2.19	1.19
2:B:1386:LEU:CA	1:D:973:GLN:NE2	2.05	1.19
1:D:1001:GLN:OE1	2:E:1417:ILE:CG1	1.90	1.19
2:E:1412:ILE:HG23	2:E:1417:ILE:O	1.41	1.18
1:A:1001:GLN:HE22	2:B:1417:ILE:CG2	1.47	1.18
2:B:1412:ILE:HG23	2:B:1417:ILE:O	1.39	1.17
2:B:1176:ILE:HD12	1:D:662:ASN:OD1	1.27	1.17
2:B:1176:ILE:CG2	1:D:643:LYS:CG	2.23	1.17
1:A:674:ASN:OD1	2:E:1184:GLU:CG	1.93	1.16
1:A:966:MET:CG	2:B:1379:MET:HE3	1.76	1.16
1:A:973:GLN:NE2	2:E:1386:LEU:HA	1.59	1.16
1:D:997:LYS:NZ	2:E:1419:ASN:CB	2.08	1.16
1:A:973:GLN:NE2	2:E:1386:LEU:CA	2.10	1.14
2:B:1386:LEU:CA	1:D:973:GLN:HE22	1.60	1.14
1:A:997:LYS:HZ1	2:B:1419:ASN:CB	1.60	1.14
1:D:994:VAL:CG1	2:E:1408:PHE:CE1	2.31	1.14
1:A:665:ASN:CA	2:E:1174:ASN:ND2	2.10	1.12
2:B:1176:ILE:HG23	1:D:643:LYS:HG3	1.25	1.13
1:D:997:LYS:NZ	2:E:1419:ASN:HB2	1.62	1.12
2:B:1210:GLU:CG	1:D:665:ASN:OD1	1.95	1.12
1:A:997:LYS:HZ1	2:B:1419:ASN:HB2	1.10	1.11
1:A:966:MET:CA	2:B:1379:MET:CE	2.28	1.10
2:B:1177:THR:OG1	1:D:642:LYS:HG3	1.51	1.10
1:D:1001:GLN:HE22	2:E:1417:ILE:CG2	1.49	1.10
1:D:997:LYS:HZ1	2:E:1419:ASN:HB2	0.97	1.10
1:A:997:LYS:NZ	2:B:1419:ASN:CB	2.15	1.09
2:B:1176:ILE:HD11	1:D:662:ASN:OD1	1.52	1.09
1:A:966:MET:CB	2:B:1379:MET:CE	2.30	1.09
1:A:997:LYS:NZ	2:B:1419:ASN:HB2	1.65	1.08
2:B:1427:ALA:O	2:B:1429:PRO:HD3	1.51	1.08
1:A:966:MET:HB2	2:B:1379:MET:HE1	1.35	1.08
1:A:1001:GLN:OE1	2:B:1417:ILE:HG12	0.91	1.08
1:D:1001:GLN:OE1	2:E:1417:ILE:HG23	1.51	1.08
1:A:966:MET:CG	2:B:1379:MET:CE	2.31	1.06
1:D:1022:PRO:O	1:D:1024:ALA:N	1.89	1.06
1:D:966:MET:CB	2:E:1379:MET:HE1	1.85	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1210:GLU:CB	1:D:665:ASN:OD1	0.76	1.05
2:E:1391:ASP:OD1	2:E:1433:THR:HG21	1.56	1.05
1:A:1022:PRO:O	1:A:1024:ALA:N	1.90	1.04
1:A:674:ASN:ND2	2:E:1184:GLU:OE1	1.90	1.04
2:B:1210:GLU:CA	1:D:665:ASN:OD1	2.05	1.04
1:D:1001:GLN:OE1	2:E:1417:ILE:CG2	2.03	1.04
1:A:981:PHE:CE2	2:E:1392:LEU:HD23	1.92	1.03
2:B:1177:THR:OG1	1:D:642:LYS:CD	2.06	1.03
2:B:1392:LEU:HD23	1:D:981:PHE:CE2	1.92	1.03
1:A:754:THR:CB	2:E:1177:THR:HG23	1.78	1.03
1:D:966:MET:HG3	2:E:1379:MET:HE3	1.06	1.02
1:A:966:MET:CA	2:B:1379:MET:HE2	1.89	1.01
2:B:1177:THR:OG1	1:D:642:LYS:CG	2.08	1.01
1:A:662:ASN:OD1	2:E:1176:ILE:CG2	2.08	1.01
1:D:1024:ALA:HB1	1:D:1026:LEU:HG	1.39	1.01
1:A:966:MET:N	2:B:1379:MET:HE2	1.75	1.00
1:A:994:VAL:CG1	2:B:1408:PHE:CE1	2.43	1.00
1:A:966:MET:HG3	2:B:1379:MET:HE3	1.01	1.00
1:D:966:MET:CA	2:E:1379:MET:CE	2.38	1.00
2:E:1380:HIS:CE1	2:E:1384:LYS:HE3	1.97	0.99
1:A:997:LYS:HE2	2:B:1417:ILE:HG22	1.41	0.99
1:A:1001:GLN:OE1	2:B:1417:ILE:CB	2.10	0.99
1:A:973:GLN:HE22	2:E:1386:LEU:CA	1.68	0.98
2:B:1412:ILE:CG2	2:B:1417:ILE:O	2.11	0.98
2:B:1407:VAL:HG22	1:D:995:TYR:HB2	1.45	0.98
1:D:966:MET:N	2:E:1379:MET:HE2	1.79	0.98
1:A:1050:THR:OG1	2:E:1381:ARG:NH2	1.97	0.98
2:B:1367:LEU:CD1	1:D:952:LEU:CD2	2.42	0.98
2:B:1038:ARG:CD	1:D:751:GLN:HE22	1.69	0.97
2:B:1386:LEU:CB	1:D:973:GLN:HE22	1.76	0.97
2:B:1176:ILE:HG22	1:D:643:LYS:CG	1.95	0.97
2:E:1380:HIS:HE1	2:E:1384:LYS:HE3	1.28	0.96
2:B:1297:GLN:NE2	1:D:864:ASN:O	1.97	0.96
2:B:1380:HIS:HE1	2:B:1384:LYS:HE3	1.29	0.96
2:B:1210:GLU:HB2	1:D:665:ASN:OD1	1.15	0.95
1:D:966:MET:HG3	2:E:1379:MET:HE1	1.46	0.95
1:A:994:VAL:CG1	2:B:1408:PHE:CD1	2.48	0.95
2:B:1176:ILE:HG23	1:D:643:LYS:CG	1.91	0.95
1:D:966:MET:CB	2:E:1379:MET:CE	2.43	0.95
2:B:1386:LEU:HA	1:D:973:GLN:HE21	1.16	0.95
1:D:997:LYS:HZ3	2:E:1419:ASN:C	1.74	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:997:LYS:HZ1	2:E:1419:ASN:CA	1.81	0.94
1:A:997:LYS:HZ1	2:B:1419:ASN:CA	1.81	0.93
2:B:1038:ARG:HD3	1:D:751:GLN:HE21	1.28	0.93
2:B:1380:HIS:CE1	2:B:1384:LYS:HE3	2.02	0.93
1:D:994:VAL:CG1	2:E:1408:PHE:CD1	2.49	0.93
2:B:1411:ILE:HD13	2:E:1411:ILE:HD13	1.49	0.93
1:D:997:LYS:NZ	2:E:1419:ASN:C	2.26	0.92
1:A:1001:GLN:OE1	2:B:1417:ILE:CG2	2.15	0.91
1:A:995:TYR:HB2	2:E:1407:VAL:HG22	1.52	0.91
1:A:754:THR:HB	2:E:1177:THR:HG23	0.93	0.91
2:B:1178:THR:OG1	1:D:747:LEU:HD21	1.70	0.91
1:D:966:MET:CG	2:E:1379:MET:HE1	1.95	0.91
1:A:973:GLN:HE21	2:E:1386:LEU:HA	1.30	0.91
1:A:997:LYS:NZ	2:B:1419:ASN:C	2.30	0.90
1:A:966:MET:N	2:B:1379:MET:CE	2.35	0.90
1:A:662:ASN:OD1	2:E:1176:ILE:HB	1.05	0.90
2:B:1210:GLU:OE1	1:D:667:SER:CB	2.20	0.90
1:A:976:SER:HB3	2:B:1390:PHE:CG	2.07	0.90
1:D:281:LEU:H	1:D:293:GLN:HE22	1.21	0.89
1:A:281:LEU:H	1:A:293:GLN:HE22	1.21	0.88
1:D:976:SER:HB3	2:E:1390:PHE:CG	2.06	0.88
1:A:997:LYS:HZ3	2:B:1419:ASN:C	1.81	0.88
1:A:952:LEU:CD2	2:E:1367:LEU:CD1	2.52	0.88
1:A:981:PHE:HB3	2:E:1396:LYS:HE3	1.56	0.87
1:D:1001:GLN:OE1	2:E:1417:ILE:CB	2.21	0.87
2:B:1297:GLN:NE2	1:D:864:ASN:HB3	1.89	0.87
1:D:966:MET:N	2:E:1379:MET:CE	2.38	0.86
1:D:682:SER:OG	1:D:761:SER:HB3	1.76	0.86
2:B:1386:LEU:CB	1:D:973:GLN:NE2	2.37	0.86
1:D:966:MET:CA	2:E:1379:MET:HE2	2.06	0.86
1:A:966:MET:HA	2:B:1379:MET:CE	2.06	0.86
1:A:1013:LYS:HZ1	1:A:1022:PRO:HG2	1.41	0.85
1:A:665:ASN:CA	2:E:1174:ASN:HD22	1.79	0.85
1:A:754:THR:CB	2:E:1177:THR:CG2	2.24	0.85
1:A:973:GLN:HE22	2:E:1386:LEU:CB	1.89	0.85
2:E:1412:ILE:CG2	2:E:1417:ILE:O	2.23	0.85
2:B:1367:LEU:HD11	1:D:952:LEU:CD2	2.07	0.84
2:B:1396:LYS:HE3	1:D:981:PHE:HB3	1.57	0.84
1:A:682:SER:OG	1:A:761:SER:HB3	1.76	0.84
1:A:665:ASN:HA	2:E:1174:ASN:HD22	1.02	0.84
2:B:1414:ARG:NH1	1:D:999:ILE:HA	1.92	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:966:MET:HA	2:B:1379:MET:HE2	1.58	0.83
2:B:1176:ILE:HG22	1:D:643:LYS:H	1.41	0.83
1:D:1001:GLN:HE22	2:E:1417:ILE:HG22	1.42	0.83
1:A:664:GLY:CA	2:E:1175:THR:O	2.27	0.82
2:B:1386:LEU:HB2	1:D:973:GLN:HE22	1.43	0.82
1:A:665:ASN:HA	2:E:1174:ASN:HD21	1.36	0.81
2:B:1210:GLU:OE1	1:D:667:SER:HB3	1.79	0.81
1:A:986:THR:HG22	2:B:1427:ALA:HB2	1.62	0.81
2:B:1367:LEU:CD1	1:D:952:LEU:HD23	2.10	0.81
1:A:990:ALA:HB1	2:B:1424:LEU:HG	1.63	0.81
1:A:999:ILE:HD11	2:E:1410:GLU:HG2	1.61	0.81
1:A:664:GLY:HA2	2:E:1175:THR:O	1.81	0.80
1:A:973:GLN:CD	2:E:1386:LEU:HD13	2.06	0.80
1:D:997:LYS:HE2	2:E:1417:ILE:HG22	1.62	0.80
2:B:1386:LEU:HD13	1:D:973:GLN:CD	2.07	0.80
1:A:973:GLN:HE22	2:E:1386:LEU:N	1.80	0.79
1:D:1024:ALA:CB	1:D:1026:LEU:HG	2.12	0.79
2:E:1412:ILE:CD1	2:E:1420:ALA:HA	2.12	0.79
1:A:1050:THR:CG2	2:E:1381:ARG:HH22	1.96	0.79
1:D:997:LYS:NZ	2:E:1419:ASN:CA	2.44	0.79
1:D:749:GLN:N	1:D:753:THR:OG1	2.15	0.79
1:A:999:ILE:HA	2:E:1414:ARG:NH1	1.97	0.79
1:A:1001:GLN:OE1	2:B:1417:ILE:HG23	1.74	0.79
1:A:966:MET:HE1	2:E:1379:MET:HB2	1.63	0.79
1:A:662:ASN:HD22	2:E:1178:THR:HB	1.48	0.79
1:A:997:LYS:NZ	2:B:1419:ASN:CA	2.44	0.78
2:B:1210:GLU:CA	1:D:665:ASN:CG	2.56	0.78
2:B:1038:ARG:HD3	1:D:751:GLN:HE22	0.97	0.78
1:D:994:VAL:HG11	2:E:1408:PHE:HE1	1.47	0.78
2:B:1399:VAL:HG11	1:D:1040:GLN:NE2	1.99	0.77
1:A:1013:LYS:NZ	1:A:1022:PRO:HG2	1.99	0.77
2:B:1411:ILE:HD13	2:E:1411:ILE:CD1	2.13	0.77
2:B:1377:ILE:HB	2:B:1378:PRO:HD3	1.66	0.77
1:A:749:GLN:N	1:A:753:THR:OG1	2.15	0.77
1:A:973:GLN:CD	2:E:1386:LEU:CD1	2.58	0.77
2:B:1176:ILE:HG22	1:D:643:LYS:HG3	1.55	0.77
2:E:1377:ILE:HB	2:E:1378:PRO:HD3	1.65	0.77
1:D:976:SER:HB3	2:E:1390:PHE:CD1	2.19	0.77
2:B:1386:LEU:CD1	1:D:973:GLN:CD	2.58	0.76
1:D:1001:GLN:HE22	2:E:1417:ILE:HG23	1.02	0.76
2:B:1410:GLU:HG2	1:D:999:ILE:HD11	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:ASN:OD1	2:E:1184:GLU:CD	2.28	0.76
1:A:1050:THR:HG23	2:E:1381:ARG:HH22	1.50	0.76
1:A:997:LYS:HE2	2:B:1417:ILE:CG2	2.14	0.76
1:A:665:ASN:H	1:A:665:ASN:HD22	1.34	0.75
1:D:966:MET:HB2	2:E:1379:MET:HE1	1.66	0.75
1:A:976:SER:HB3	2:B:1390:PHE:CD1	2.21	0.75
1:D:665:ASN:H	1:D:665:ASN:HD22	1.34	0.75
1:A:662:ASN:HD21	2:E:1178:THR:H	1.32	0.75
1:D:1013:LYS:NZ	1:D:1022:PRO:HG2	2.01	0.75
1:A:964:ILE:HB	1:A:965:PRO:HD3	1.68	0.75
1:A:973:GLN:NE2	2:E:1386:LEU:CB	2.46	0.74
1:A:994:VAL:HG11	2:B:1408:PHE:HD1	1.45	0.74
2:B:1174:ASN:HB2	1:D:643:LYS:NZ	2.02	0.74
2:B:1176:ILE:HG21	1:D:643:LYS:HG3	1.62	0.74
1:A:665:ASN:HD21	2:E:1176:ILE:HD11	1.52	0.74
1:A:513:GLU:HG3	1:A:515:ILE:HG22	1.70	0.74
1:D:986:THR:HG22	2:E:1427:ALA:HB2	1.70	0.74
1:A:999:ILE:HA	2:E:1414:ARG:CZ	2.18	0.74
1:D:996:LYS:O	1:D:1000:THR:OG1	2.06	0.73
2:E:1427:ALA:O	2:E:1429:PRO:CD	2.27	0.73
2:B:1210:GLU:HB3	1:D:665:ASN:CB	2.19	0.73
2:B:1411:ILE:CD1	2:E:1411:ILE:HD13	2.18	0.73
1:A:662:ASN:HD22	2:E:1178:THR:CB	2.01	0.73
1:D:966:MET:HA	2:E:1379:MET:CE	2.17	0.73
2:B:1386:LEU:N	1:D:973:GLN:HE22	1.86	0.73
1:D:513:GLU:HG3	1:D:515:ILE:HG22	1.70	0.72
1:D:964:ILE:HB	1:D:965:PRO:HD3	1.68	0.72
1:A:973:GLN:HE22	2:E:1386:LEU:HB2	1.52	0.72
1:A:997:LYS:HZ2	2:B:1419:ASN:CB	2.00	0.72
2:B:1412:ILE:CD1	2:B:1420:ALA:HA	2.20	0.71
1:A:665:ASN:ND2	2:E:1176:ILE:CD1	2.53	0.71
1:D:272:LYS:NZ	1:D:276:GLU:OE2	2.24	0.71
1:A:748:ASN:ND2	2:E:1177:THR:OG1	2.18	0.71
1:A:1001:GLN:HE22	2:B:1417:ILE:HG23	0.89	0.71
1:A:1022:PRO:C	1:A:1024:ALA:N	2.47	0.71
1:D:990:ALA:HB1	2:E:1424:LEU:HG	1.71	0.71
1:A:272:LYS:NZ	1:A:276:GLU:OE2	2.24	0.70
1:D:1013:LYS:HZ1	1:D:1022:PRO:HG2	1.57	0.70
1:A:540:GLN:HG2	1:A:579:PRO:HA	1.74	0.70
2:B:1389:GLY:C	1:D:977:PHE:CE1	2.69	0.70
2:B:1386:LEU:CD1	1:D:973:GLN:NE2	2.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1410:GLU:CD	1:D:999:ILE:HD11	2.17	0.70
1:A:664:GLY:HA3	2:E:1175:THR:C	2.17	0.69
1:A:952:LEU:CD2	2:E:1367:LEU:HD11	2.22	0.69
1:A:999:ILE:HD11	2:E:1410:GLU:CG	2.22	0.69
1:A:973:GLN:NE2	2:E:1386:LEU:N	2.40	0.69
2:B:1414:ARG:NH1	1:D:999:ILE:HD13	2.08	0.69
2:B:1184:GLU:N	1:D:672:THR:HA	2.09	0.68
2:B:1174:ASN:HB2	1:D:643:LYS:HZ2	1.58	0.68
2:B:1360:VAL:HB	2:B:1361:PRO:HD3	1.76	0.68
1:D:1022:PRO:C	1:D:1024:ALA:N	2.47	0.68
1:A:999:ILE:HD11	2:E:1410:GLU:CD	2.19	0.68
1:D:540:GLN:HG2	1:D:579:PRO:HA	1.74	0.68
1:A:662:ASN:OD1	2:E:1176:ILE:HG21	1.92	0.68
1:A:966:MET:CG	2:B:1379:MET:HE1	2.10	0.68
1:A:1001:GLN:HE22	2:B:1417:ILE:HG22	1.54	0.68
2:B:1386:LEU:HD12	1:D:973:GLN:NE2	2.09	0.68
1:D:958:LEU:HD21	2:E:1372:GLY:CA	2.23	0.68
2:B:1414:ARG:CZ	1:D:999:ILE:HA	2.23	0.67
2:E:1412:ILE:HD13	2:E:1420:ALA:HA	1.77	0.67
1:D:364:GLU:HG2	1:D:367:SER:HB2	1.77	0.67
1:D:997:LYS:HZ2	2:E:1419:ASN:CB	2.04	0.67
1:A:662:ASN:ND2	2:E:1178:THR:H	1.92	0.67
1:A:977:PHE:CE1	2:E:1389:GLY:C	2.73	0.67
2:B:1412:ILE:HD13	2:B:1420:ALA:HA	1.77	0.67
1:A:954:ILE:HD13	2:B:1365:ILE:HG23	1.75	0.67
1:A:364:GLU:HG2	1:A:367:SER:HB2	1.77	0.66
2:B:1176:ILE:CG2	1:D:643:LYS:HG2	2.24	0.66
2:B:1367:LEU:HD13	1:D:952:LEU:HD23	1.78	0.66
1:D:954:ILE:HD13	2:E:1365:ILE:HG23	1.78	0.66
2:B:1430:THR:O	2:B:1432:PRO:HD3	1.95	0.66
2:B:1427:ALA:O	2:B:1429:PRO:CD	2.39	0.66
1:A:952:LEU:HD23	2:E:1367:LEU:CD1	2.23	0.66
1:A:958:LEU:HD21	2:B:1372:GLY:CA	2.24	0.66
1:D:869:LEU:C	1:D:869:LEU:HD12	2.20	0.66
2:E:1360:VAL:HB	2:E:1361:PRO:HD3	1.77	0.66
1:A:664:GLY:CA	2:E:1175:THR:C	2.69	0.66
1:A:674:ASN:CG	2:E:1184:GLU:OE1	2.39	0.65
1:A:869:LEU:HD12	1:A:869:LEU:C	2.20	0.65
1:A:959:GLY:CA	2:E:1371:LEU:HD11	2.27	0.65
2:B:1414:ARG:HH11	1:D:999:ILE:HD13	1.62	0.65
2:B:1210:GLU:CA	1:D:665:ASN:CB	2.74	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:994:VAL:CB	2:E:1408:PHE:CE1	2.80	0.65
2:B:1410:GLU:CG	1:D:999:ILE:HD11	2.25	0.65
1:A:664:GLY:HA3	2:E:1176:ILE:N	2.11	0.65
1:A:1035:LYS:O	1:A:1037:GLU:N	2.31	0.64
2:B:1210:GLU:HA	1:D:665:ASN:HB3	1.78	0.64
1:A:966:MET:HE2	2:E:1379:MET:HG3	1.79	0.64
1:D:997:LYS:NZ	2:E:1419:ASN:HB3	2.10	0.64
2:B:1297:GLN:HE21	1:D:864:ASN:HB3	1.61	0.64
2:E:1412:ILE:HD13	2:E:1420:ALA:CA	2.28	0.64
1:D:1024:ALA:C	1:D:1026:LEU:N	2.56	0.64
1:A:973:GLN:HB2	2:B:1386:LEU:HD21	1.78	0.64
1:A:67:ALA:HB2	1:A:81:LYS:HD3	1.80	0.63
1:A:966:MET:CE	2:E:1379:MET:HB2	2.28	0.63
2:B:1176:ILE:HG22	1:D:643:LYS:HG2	1.77	0.63
1:D:966:MET:HA	2:E:1379:MET:HE2	1.77	0.63
1:D:973:GLN:HB2	2:E:1386:LEU:HD21	1.81	0.63
1:D:1035:LYS:O	1:D:1037:GLU:N	2.32	0.63
1:A:138:SER:OG	1:A:565:ASP:OD1	2.17	0.63
2:B:1177:THR:HG1	1:D:642:LYS:CG	2.12	0.62
1:A:1019:VAL:O	1:A:1021:LYS:N	2.32	0.62
1:A:999:ILE:HD13	2:E:1414:ARG:NH1	2.14	0.62
2:B:1184:GLU:CD	1:D:674:ASN:HD21	2.08	0.62
1:D:67:ALA:HB2	1:D:81:LYS:HD3	1.80	0.62
1:A:665:ASN:ND2	2:E:1176:ILE:HG12	2.14	0.62
1:A:674:ASN:CG	2:E:1184:GLU:CD	2.68	0.62
2:B:1392:LEU:HD13	1:D:1043:VAL:HB	1.82	0.62
1:A:174:VAL:HG21	1:A:203:THR:HG21	1.81	0.62
1:A:1013:LYS:HZ1	1:A:1022:PRO:CG	2.12	0.62
2:B:1386:LEU:N	1:D:973:GLN:NE2	2.45	0.62
1:D:1019:VAL:O	1:D:1021:LYS:N	2.33	0.61
1:A:665:ASN:ND2	2:E:1176:ILE:HD11	2.15	0.61
2:B:1210:GLU:HA	1:D:665:ASN:CB	2.31	0.61
2:B:1414:ARG:HH11	1:D:999:ILE:CD1	2.13	0.61
2:E:1404:VAL:CG1	2:E:1408:PHE:CE2	2.83	0.61
2:B:1404:VAL:CG1	2:B:1408:PHE:CE2	2.84	0.61
1:A:149:ILE:HG22	1:A:501:LEU:HB3	1.83	0.60
1:D:149:ILE:HG22	1:D:501:LEU:HB3	1.83	0.60
1:A:958:LEU:HD11	2:B:1368:SER:O	2.01	0.60
1:D:117:SER:HB3	1:D:125:THR:HG21	1.83	0.60
1:A:117:SER:HB3	1:A:125:THR:HG21	1.83	0.60
2:B:1210:GLU:HB2	1:D:665:ASN:CG	1.88	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1177:THR:HG1	1:D:642:LYS:HG3	1.64	0.60
1:D:174:VAL:HG21	1:D:203:THR:HG21	1.81	0.60
2:B:1371:LEU:HD11	1:D:959:GLY:CA	2.32	0.60
1:A:981:PHE:CB	2:E:1396:LYS:HE3	2.31	0.60
2:B:1396:LYS:HB3	1:D:984:VAL:HG11	1.84	0.60
1:D:246:ASN:OD1	1:D:246:ASN:N	2.35	0.59
1:D:997:LYS:HZ2	2:E:1419:ASN:HB3	1.68	0.59
2:E:1412:ILE:HD11	2:E:1420:ALA:HA	1.84	0.59
1:A:976:SER:CB	2:B:1390:PHE:CG	2.83	0.59
1:A:1050:THR:CG2	2:E:1381:ARG:NH2	2.63	0.59
2:E:1404:VAL:CG1	2:E:1408:PHE:HE2	2.16	0.59
2:B:1429:PRO:C	2:B:1431:LYS:H	2.11	0.59
1:A:246:ASN:OD1	1:A:246:ASN:N	2.35	0.59
1:A:987:LEU:HD23	2:E:1400:LEU:HD21	1.84	0.59
2:B:1392:LEU:HB3	1:D:981:PHE:CZ	2.38	0.59
1:D:194:ASN:HD22	1:D:483:LYS:HD2	1.68	0.59
1:D:231:GLN:O	1:D:268:TYR:OH	2.10	0.59
1:D:994:VAL:CG1	2:E:1408:PHE:HE1	2.03	0.59
1:A:665:ASN:HD22	1:A:665:ASN:N	1.99	0.59
1:D:501:LEU:C	1:D:501:LEU:HD12	2.28	0.58
1:D:561:SER:OG	1:D:564:SER:O	2.21	0.58
1:A:999:ILE:CD1	2:E:1410:GLU:HG2	2.32	0.58
2:B:1398:ASP:OD1	2:B:1429:PRO:HD2	2.03	0.58
1:A:1013:LYS:NZ	1:A:1022:PRO:CG	2.65	0.58
2:B:1407:VAL:CG2	1:D:995:TYR:HB2	2.28	0.58
1:A:984:VAL:HG11	2:E:1396:LYS:HB3	1.86	0.58
1:A:194:ASN:ND2	1:A:483:LYS:HD2	2.19	0.58
1:A:973:GLN:OE1	2:E:1386:LEU:HD13	2.02	0.58
1:A:501:LEU:C	1:A:501:LEU:HD12	2.28	0.58
2:B:1367:LEU:CD1	1:D:952:LEU:HD21	2.33	0.58
2:B:1367:LEU:HD11	1:D:952:LEU:HD22	1.84	0.58
1:A:227:ASP:OD1	1:A:229:THR:HB	2.04	0.57
1:A:440:LYS:HB2	1:A:674:ASN:HB3	1.86	0.57
1:A:574:GLN:HE21	1:A:575:SER:H	1.51	0.57
1:A:986:THR:CG2	2:B:1427:ALA:HB2	2.34	0.57
2:B:1396:LYS:HE3	1:D:981:PHE:CB	2.32	0.57
1:D:194:ASN:ND2	1:D:483:LYS:HD2	2.19	0.57
1:A:194:ASN:HD22	1:A:483:LYS:HD2	1.68	0.57
1:A:561:SER:OG	1:A:564:SER:O	2.21	0.57
2:B:1400:LEU:HD21	1:D:987:LEU:HD23	1.86	0.57
2:E:1430:THR:O	2:E:1432:PRO:HD3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:981:PHE:CZ	2:E:1392:LEU:HB3	2.39	0.57
2:B:1176:ILE:HD11	1:D:662:ASN:CG	2.28	0.57
1:D:994:VAL:HG22	2:E:1421:PRO:HG3	1.87	0.57
1:A:470:SER:HA	1:A:482:ILE:HD13	1.86	0.57
2:B:1429:PRO:C	2:B:1431:LYS:N	2.60	0.57
2:B:1297:GLN:NE2	1:D:864:ASN:C	2.62	0.57
1:D:470:SER:HA	1:D:482:ILE:HD13	1.86	0.57
1:D:966:MET:N	2:E:1379:MET:HE1	2.19	0.57
1:A:665:ASN:C	2:E:1174:ASN:ND2	2.63	0.57
1:D:227:ASP:OD1	1:D:229:THR:HB	2.04	0.57
2:E:1432:PRO:O	2:E:1433:THR:C	2.44	0.57
1:A:665:ASN:CA	2:E:1174:ASN:HD21	2.03	0.56
1:D:574:GLN:HE21	1:D:575:SER:H	1.51	0.56
2:B:1041:TYR:OH	1:D:754:THR:HB	2.05	0.56
2:B:1386:LEU:HD12	1:D:973:GLN:CD	2.30	0.56
1:D:440:LYS:HB2	1:D:674:ASN:HB3	1.86	0.56
1:D:976:SER:CB	2:E:1390:PHE:CG	2.84	0.56
1:D:994:VAL:HG11	2:E:1408:PHE:HD1	1.52	0.56
1:A:954:ILE:HD12	2:B:1365:ILE:HG12	1.88	0.56
2:B:1297:GLN:HE22	1:D:864:ASN:C	2.08	0.56
2:B:1297:GLN:HE22	1:D:864:ASN:HB3	1.69	0.56
1:A:994:VAL:CB	2:B:1408:PHE:CE1	2.89	0.56
2:B:1386:LEU:HD11	2:E:1386:LEU:HD11	1.87	0.56
1:D:1024:ALA:C	1:D:1026:LEU:H	2.13	0.56
2:B:1396:LYS:NZ	1:D:985:ASP:OD2	2.38	0.56
1:A:1013:LYS:HZ3	1:A:1022:PRO:HD2	1.71	0.55
2:B:148:MET:HA	2:B:148:MET:HE2	1.88	0.55
1:A:1050:THR:CB	2:E:1381:ARG:HH22	2.19	0.55
1:A:555:ALA:HA	1:A:568:VAL:HG21	1.89	0.55
1:D:958:LEU:HD11	2:E:1368:SER:O	2.06	0.55
2:E:148:MET:HE2	2:E:148:MET:HA	1.88	0.55
1:A:999:ILE:CD1	2:E:1414:ARG:HH11	2.20	0.55
2:B:1410:GLU:HG2	1:D:999:ILE:CD1	2.36	0.55
1:D:665:ASN:HD22	1:D:665:ASN:N	1.99	0.55
2:B:1176:ILE:HG21	1:D:664:GLY:N	2.22	0.55
2:B:1432:PRO:O	2:B:1433:THR:C	2.43	0.55
1:D:555:ALA:HA	1:D:568:VAL:HG21	1.89	0.55
2:B:1038:ARG:CD	1:D:751:GLN:HE21	1.94	0.54
2:B:1184:GLU:HA	1:D:672:THR:O	2.06	0.54
2:B:1386:LEU:HB2	1:D:973:GLN:NE2	2.12	0.54
1:A:952:LEU:HD23	2:E:1367:LEU:HD13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:966:MET:N	2:B:1379:MET:HE1	2.17	0.54
1:D:966:MET:CA	2:E:1379:MET:HE1	2.23	0.54
1:A:1035:LYS:O	1:A:1036:PRO:C	2.47	0.54
2:B:1404:VAL:CG1	2:B:1408:PHE:HE2	2.19	0.54
1:A:973:GLN:NE2	2:E:1386:LEU:HB2	2.17	0.54
1:A:1002:THR:CB	2:E:1414:ARG:HD3	2.37	0.54
1:D:626:SER:HA	1:D:651:LEU:O	2.08	0.54
1:A:973:GLN:CD	2:E:1386:LEU:HD12	2.30	0.54
1:A:999:ILE:HG23	2:E:1414:ARG:NH1	2.23	0.54
1:D:138:SER:OG	1:D:565:ASP:OD1	2.17	0.54
1:D:281:LEU:HD11	1:D:296:TYR:CD1	2.43	0.54
1:D:734:GLY:HA3	1:D:771:SER:O	2.08	0.54
1:A:973:GLN:NE2	2:E:1386:LEU:CD1	2.70	0.53
1:A:1024:ALA:C	1:A:1026:LEU:N	2.66	0.53
1:D:317:LEU:N	1:D:317:LEU:HD23	2.23	0.53
1:A:734:GLY:HA3	1:A:771:SER:O	2.08	0.53
1:A:626:SER:HA	1:A:651:LEU:O	2.08	0.53
1:D:290:VAL:HG12	1:D:294:LEU:HD22	1.90	0.53
1:D:1022:PRO:C	1:D:1024:ALA:H	2.00	0.53
1:A:665:ASN:C	2:E:1174:ASN:HD21	2.16	0.53
2:B:1176:ILE:HG22	1:D:643:LYS:N	2.19	0.53
2:E:1404:VAL:HG12	2:E:1408:PHE:CE2	2.44	0.53
1:A:997:LYS:HZ2	2:B:1419:ASN:HB3	1.72	0.53
1:A:999:ILE:HD13	2:E:1414:ARG:HH11	1.74	0.53
1:A:281:LEU:HD11	1:A:296:TYR:CD1	2.43	0.52
1:A:966:MET:CA	2:B:1379:MET:HE1	2.12	0.52
1:A:290:VAL:HG12	1:A:294:LEU:HD22	1.90	0.52
1:A:317:LEU:N	1:A:317:LEU:HD23	2.23	0.52
1:A:341:ALA:HB1	1:A:378:PHE:HB3	1.92	0.52
1:A:1024:ALA:O	1:A:1026:LEU:N	2.40	0.52
1:D:341:ALA:HB1	1:D:378:PHE:HB3	1.92	0.52
2:B:1414:ARG:HD3	1:D:1002:THR:CB	2.39	0.52
2:B:1414:ARG:HD3	1:D:1002:THR:HG21	1.91	0.52
1:A:1016:ASN:C	1:A:1018:SER:H	2.17	0.52
1:D:997:LYS:HE2	2:E:1417:ILE:CG2	2.36	0.52
1:D:679:ILE:HD11	1:D:757:ASP:C	2.35	0.52
1:A:973:GLN:NE2	2:E:1386:LEU:HD12	2.24	0.52
1:D:965:PRO:C	2:E:1379:MET:HE2	2.34	0.52
1:D:1023:ALA:C	1:D:1025:PHE:N	2.68	0.52
1:A:665:ASN:ND2	2:E:1176:ILE:CG1	2.73	0.52
2:B:1177:THR:HG1	1:D:642:LYS:HD2	1.70	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:ASN:C	2:E:1176:ILE:HG21	2.35	0.51
2:E:1432:PRO:C	2:E:1433:THR:O	2.53	0.51
1:A:231:GLN:O	1:A:268:TYR:OH	2.10	0.51
1:A:662:ASN:ND2	2:E:1178:THR:HB	2.21	0.51
1:A:679:ILE:HD11	1:A:757:ASP:C	2.35	0.51
1:A:994:VAL:HG21	2:B:1408:PHE:CG	2.46	0.51
1:D:544:TYR:CD2	1:D:659:LEU:HD22	2.46	0.51
1:A:981:PHE:CD1	2:E:1396:LYS:HD2	2.46	0.51
2:B:1412:ILE:HD13	2:B:1420:ALA:CA	2.41	0.51
1:D:1035:LYS:O	1:D:1036:PRO:C	2.48	0.51
2:B:1177:THR:HG1	1:D:642:LYS:CD	2.21	0.51
2:E:1412:ILE:CD1	2:E:1420:ALA:CA	2.85	0.51
1:A:650:VAL:CG1	1:A:657:VAL:HG22	2.41	0.51
1:A:997:LYS:HZ1	2:B:1419:ASN:N	2.09	0.51
1:D:994:VAL:HG22	2:E:1421:PRO:CG	2.41	0.51
1:D:1013:LYS:NZ	1:D:1022:PRO:CG	2.71	0.51
1:A:966:MET:CE	2:E:1379:MET:CG	2.89	0.51
1:A:1043:VAL:HB	2:E:1392:LEU:HD22	1.92	0.51
1:D:465:PHE:HB3	1:D:515:ILE:HD13	1.93	0.51
1:A:544:TYR:CD2	1:A:659:LEU:HD22	2.46	0.50
1:A:674:ASN:HD21	2:E:1184:GLU:HB2	1.75	0.50
1:A:966:MET:HE2	2:E:1379:MET:CG	2.41	0.50
1:D:650:VAL:CG1	1:D:657:VAL:HG22	2.41	0.50
2:B:1210:GLU:HA	1:D:665:ASN:CG	2.36	0.50
2:B:1433:THR:O	2:B:1435:LYS:N	2.43	0.50
1:D:390:SER:HA	1:D:394:GLN:O	2.11	0.50
2:E:1429:PRO:C	2:E:1431:LYS:H	2.19	0.50
1:A:229:THR:HG22	1:A:230:LYS:HG3	1.93	0.50
1:D:457:PHE:CE1	3:F:3:SIA:H112	2.46	0.50
1:D:465:PHE:CB	1:D:515:ILE:HD13	2.41	0.50
1:A:554:SER:HB2	1:A:568:VAL:HG13	1.94	0.50
1:A:723:ASP:HB3	1:A:725:LYS:H	1.77	0.50
1:D:229:THR:HG22	1:D:230:LYS:HG3	1.93	0.50
1:D:650:VAL:HG12	1:D:657:VAL:HG22	1.94	0.50
1:A:390:SER:HA	1:A:394:GLN:O	2.11	0.50
1:A:650:VAL:HG12	1:A:657:VAL:HG22	1.94	0.50
1:A:985:ASP:OD2	2:E:1396:LYS:NZ	2.40	0.50
1:A:457:PHE:CE1	3:C:3:SIA:H112	2.47	0.50
1:A:904:PHE:CG	1:A:905:LEU:N	2.80	0.50
1:A:1043:VAL:CG2	2:E:1392:LEU:HD13	2.42	0.50
1:D:173:GLU:O	1:D:177:GLY:HA2	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1410:GLU:CD	1:D:999:ILE:CD1	2.85	0.49
1:D:998:ILE:O	1:D:1002:THR:OG1	2.30	0.49
1:A:754:THR:HA	2:E:1177:THR:OG1	2.13	0.49
2:E:1433:THR:O	2:E:1435:LYS:N	2.45	0.49
1:D:904:PHE:CG	1:D:905:LEU:N	2.80	0.49
1:A:173:GLU:O	1:A:177:GLY:HA2	2.12	0.49
1:A:465:PHE:CB	1:A:515:ILE:HD13	2.41	0.49
1:A:664:GLY:O	2:E:1174:ASN:HB2	2.12	0.49
2:B:1404:VAL:HG12	2:B:1408:PHE:CE2	2.48	0.49
1:D:554:SER:HB2	1:D:568:VAL:HG13	1.94	0.49
1:A:454:ASN:OD1	1:A:467:VAL:HG23	2.12	0.49
1:A:662:ASN:ND2	2:E:1178:THR:CB	2.74	0.49
1:A:998:ILE:O	1:A:1002:THR:OG1	2.30	0.49
1:D:454:ASN:OD1	1:D:467:VAL:HG23	2.12	0.49
1:A:999:ILE:CD1	2:E:1410:GLU:CD	2.85	0.49
1:A:1013:LYS:HE2	1:A:1022:PRO:CD	2.42	0.49
1:D:966:MET:HG2	2:E:1379:MET:HE3	1.78	0.49
2:B:1396:LYS:NZ	1:D:985:ASP:OD1	2.43	0.49
1:D:958:LEU:HD21	2:E:1372:GLY:HA2	1.93	0.49
1:D:1013:LYS:HZ3	1:D:1022:PRO:HG2	1.77	0.49
1:A:210:GLY:O	1:A:232:GLY:HA3	2.13	0.48
1:A:1021:LYS:O	1:A:1023:ALA:N	2.46	0.48
2:E:1380:HIS:HE1	2:E:1384:LYS:CE	2.13	0.48
2:B:1367:LEU:HD11	1:D:952:LEU:HD21	1.92	0.48
1:A:954:ILE:CD1	2:B:1365:ILE:HG23	2.41	0.48
1:D:723:ASP:HB3	1:D:725:LYS:H	1.77	0.48
1:A:1043:VAL:HG23	2:E:1392:LEU:HD13	1.95	0.48
2:B:1297:GLN:NE2	1:D:864:ASN:CB	2.71	0.48
2:B:1396:LYS:HD2	1:D:981:PHE:CD1	2.49	0.48
1:A:465:PHE:HB3	1:A:515:ILE:HD13	1.93	0.48
1:A:966:MET:CE	2:E:1379:MET:CB	2.91	0.48
1:D:210:GLY:O	1:D:232:GLY:HA3	2.13	0.48
1:D:954:ILE:HD12	2:E:1365:ILE:HG12	1.95	0.48
1:D:954:ILE:CD1	2:E:1365:ILE:HG23	2.42	0.48
2:E:1429:PRO:C	2:E:1431:LYS:N	2.66	0.48
1:A:1024:ALA:C	1:A:1025:PHE:C	2.56	0.48
1:A:94:SER:HA	1:A:96:ASN:OD1	2.14	0.47
1:D:976:SER:CB	2:E:1390:PHE:CD2	2.97	0.47
2:B:1414:ARG:NH1	1:D:999:ILE:CD1	2.75	0.47
2:B:1396:LYS:NZ	1:D:985:ASP:CG	2.73	0.47
1:D:94:SER:HA	1:D:96:ASN:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:986:THR:HG21	2:E:1427:ALA:HA	1.96	0.47
1:A:218:GLU:O	1:A:289:ASN:HA	2.14	0.47
1:A:662:ASN:O	2:E:1176:ILE:HD13	2.13	0.47
1:A:999:ILE:CD1	2:E:1414:ARG:NH1	2.77	0.47
1:D:423:GLN:HG2	1:D:424:ALA:O	2.15	0.47
1:A:959:GLY:HA3	2:E:1371:LEU:HD11	1.97	0.47
1:A:451:GLY:HA3	1:A:485:ALA:O	2.15	0.47
1:A:952:LEU:HD21	2:E:1367:LEU:CD1	2.40	0.47
1:A:977:PHE:CE2	2:B:1390:PHE:HZ	2.32	0.47
1:A:1016:ASN:C	1:A:1018:SER:N	2.72	0.47
1:D:451:GLY:HA3	1:D:485:ALA:O	2.15	0.47
1:A:440:LYS:NZ	2:E:1184:GLU:OE2	2.38	0.47
1:A:558:SER:O	1:A:561:SER:HB3	2.15	0.47
1:D:1021:LYS:O	1:D:1023:ALA:N	2.48	0.47
2:B:1176:ILE:HD12	1:D:663:PRO:HD2	1.97	0.47
1:D:172:ARG:HH21	1:D:172:ARG:HG2	1.80	0.47
1:A:158:THR:O	1:A:619:ALA:HB3	2.15	0.47
1:D:558:SER:O	1:D:561:SER:HB3	2.15	0.47
1:A:423:GLN:HG2	1:A:424:ALA:O	2.14	0.46
1:A:540:GLN:CG	1:A:579:PRO:HA	2.44	0.46
1:A:976:SER:CB	2:B:1390:PHE:CD2	2.99	0.46
1:A:172:ARG:HG2	1:A:172:ARG:HH21	1.80	0.46
1:A:1020:LYS:O	1:A:1022:PRO:N	2.48	0.46
1:A:180:GLN:O	1:A:183:GLN:HG2	2.16	0.46
1:A:964:ILE:CB	1:A:965:PRO:HD3	2.42	0.46
1:A:985:ASP:OD1	2:E:1396:LYS:NZ	2.44	0.46
1:D:180:GLN:O	1:D:183:GLN:HG2	2.16	0.46
1:A:310:VAL:HA	1:A:323:TRP:O	2.16	0.46
1:D:158:THR:O	1:D:619:ALA:HB3	2.15	0.46
1:D:218:GLU:O	1:D:289:ASN:HA	2.15	0.46
1:D:453:ILE:O	1:D:467:VAL:HG22	2.16	0.46
1:D:962:ILE:O	2:E:1379:MET:HE1	2.15	0.46
1:A:669:LEU:HD23	1:A:679:ILE:HG23	1.98	0.46
1:A:230:LYS:HB3	1:A:231:GLN:HE22	1.81	0.46
1:A:453:ILE:O	1:A:467:VAL:HG22	2.16	0.46
1:A:1040:GLN:HE21	2:E:1399:VAL:HG11	1.81	0.45
2:B:1411:ILE:HG12	1:D:998:ILE:HD13	1.98	0.45
2:B:144:ASN:HB3	2:B:148:MET:HE3	1.98	0.45
1:A:230:LYS:CB	1:A:231:GLN:NE2	2.80	0.45
2:E:144:ASN:HB3	2:E:148:MET:HE3	1.98	0.45
1:A:159:LEU:HD23	1:A:619:ALA:HB1	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:985:ASP:CG	2:E:1396:LYS:NZ	2.74	0.45
2:B:1176:ILE:CG2	1:D:664:GLY:N	2.79	0.45
2:B:1410:GLU:OE2	1:D:999:ILE:CD1	2.65	0.45
2:B:1432:PRO:C	2:B:1433:THR:O	2.57	0.45
1:D:1016:ASN:C	1:D:1018:SER:H	2.25	0.45
1:A:966:MET:HE1	2:E:1379:MET:CB	2.40	0.45
1:A:1020:LYS:O	1:A:1021:LYS:C	2.60	0.45
1:D:310:VAL:HA	1:D:323:TRP:O	2.16	0.45
1:A:1050:THR:HG23	2:E:1381:ARG:NH2	2.27	0.45
2:B:1373:LEU:O	2:B:1377:ILE:HG13	2.17	0.45
1:D:669:LEU:HD23	1:D:679:ILE:HG23	1.98	0.45
1:A:664:GLY:HA3	2:E:1175:THR:O	2.08	0.45
2:B:1428:THR:O	2:B:1430:THR:N	2.50	0.45
1:D:159:LEU:HD23	1:D:619:ALA:HB1	1.98	0.45
1:D:230:LYS:HB3	1:D:231:GLN:HE22	1.81	0.45
1:D:439:TYR:CD2	1:D:678:PRO:HD3	2.52	0.45
2:E:1391:ASP:OD1	2:E:1433:THR:CG2	2.46	0.44
1:D:230:LYS:CB	1:D:231:GLN:NE2	2.80	0.44
1:D:1020:LYS:O	1:D:1022:PRO:N	2.51	0.44
1:A:439:TYR:CD2	1:A:678:PRO:HD3	2.53	0.44
1:A:965:PRO:C	2:B:1379:MET:HE2	2.37	0.44
1:A:1013:LYS:NZ	1:A:1022:PRO:CD	2.81	0.44
1:A:558:SER:HA	1:A:566:THR:HB	2.00	0.44
2:B:1375:ILE:HG23	1:D:966:MET:SD	2.57	0.44
2:B:1400:LEU:HD21	2:E:1400:LEU:HD21	1.99	0.44
1:D:357:GLU:OE2	1:D:379:THR:OG1	2.24	0.44
2:B:1399:VAL:HG11	1:D:1040:GLN:HE22	1.81	0.44
1:A:1013:LYS:HE2	1:A:1022:PRO:HD3	1.99	0.44
1:D:540:GLN:CG	1:D:579:PRO:HA	2.44	0.44
1:A:952:LEU:HD22	2:E:1367:LEU:HD11	1.97	0.44
1:D:1013:LYS:HE2	1:D:1022:PRO:CD	2.48	0.44
2:E:1373:LEU:O	2:E:1377:ILE:HG13	2.17	0.44
1:A:132:LEU:HD22	1:A:323:TRP:CD1	2.53	0.44
2:B:1386:LEU:HD13	1:D:973:GLN:OE1	2.17	0.44
2:B:1356:LEU:O	2:B:1360:VAL:HG23	2.18	0.44
2:B:1367:LEU:HD12	1:D:952:LEU:CD2	2.43	0.44
1:D:99:PHE:CZ	1:D:108:PRO:HB3	2.53	0.44
1:D:126:MET:HE1	1:D:129:LYS:HD2	2.00	0.44
2:B:1175:THR:O	1:D:643:LYS:HG2	2.18	0.43
2:B:1176:ILE:CD1	1:D:663:PRO:N	2.81	0.43
2:E:180:TRP:HA	2:E:183:ILE:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1356:LEU:O	2:E:1360:VAL:HG23	2.18	0.43
1:A:99:PHE:CZ	1:A:108:PRO:HB3	2.53	0.43
1:A:884:ALA:HA	1:A:901:ARG:O	2.19	0.43
2:B:180:TRP:HA	2:B:183:ILE:HG22	1.99	0.43
1:D:310:VAL:HG21	1:D:395:ILE:HG13	2.00	0.43
1:A:951:ILE:HD11	2:B:1361:PRO:HB3	2.00	0.43
1:A:126:MET:HE1	1:A:129:LYS:HD2	2.00	0.43
1:A:987:LEU:HD23	2:E:1400:LEU:CD2	2.47	0.43
2:B:1432:PRO:O	2:B:1434:PRO:N	2.51	0.43
2:E:1377:ILE:CB	2:E:1378:PRO:HD3	2.39	0.43
1:A:310:VAL:HG21	1:A:395:ILE:HG13	2.00	0.43
1:A:677:ALA:O	1:A:678:PRO:C	2.62	0.43
2:B:1176:ILE:HG21	1:D:663:PRO:C	2.44	0.43
2:B:1210:GLU:OE1	1:D:667:SER:OG	2.36	0.43
1:D:132:LEU:HD22	1:D:323:TRP:CD1	2.53	0.43
1:D:558:SER:HA	1:D:566:THR:HB	2.00	0.43
1:D:884:ALA:HA	1:D:901:ARG:O	2.19	0.43
1:A:649:VAL:HA	1:A:657:VAL:O	2.18	0.43
2:B:1038:ARG:NE	1:D:751:GLN:HE22	2.15	0.42
2:B:1183:SER:C	1:D:672:THR:HA	2.43	0.42
1:D:750:ASP:O	1:D:751:GLN:C	2.62	0.42
1:A:952:LEU:CD2	2:E:1367:LEU:HD13	2.42	0.42
1:D:679:ILE:HG12	1:D:759:ALA:HB2	2.01	0.42
1:D:727:THR:O	1:D:728:PRO:C	2.62	0.42
1:D:1020:LYS:O	1:D:1021:LYS:C	2.60	0.42
1:A:357:GLU:OE2	1:A:379:THR:OG1	2.24	0.42
1:A:364:GLU:HG2	1:A:367:SER:CB	2.47	0.42
1:A:667:SER:OG	2:E:1176:ILE:HD11	2.20	0.42
1:A:750:ASP:O	1:A:751:GLN:C	2.62	0.42
2:B:1377:ILE:CB	2:B:1378:PRO:HD3	2.40	0.42
1:D:649:VAL:HA	1:D:657:VAL:O	2.19	0.42
1:A:405:VAL:HG22	1:A:501:LEU:HD11	2.02	0.42
1:D:1020:LYS:C	1:D:1021:LYS:O	2.63	0.42
1:D:405:VAL:HG22	1:D:501:LEU:HD11	2.02	0.42
1:D:574:GLN:HE21	1:D:575:SER:N	2.16	0.42
1:A:138:SER:CB	1:A:565:ASP:OD1	2.68	0.42
1:A:674:ASN:CG	2:E:1184:GLU:CG	2.83	0.42
1:A:727:THR:O	1:A:728:PRO:C	2.62	0.42
1:A:866:PRO:HA	1:A:869:LEU:HG	2.02	0.42
1:A:665:ASN:ND2	1:A:667:SER:OG	2.50	0.42
1:A:679:ILE:HG12	1:A:759:ALA:HB2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:999:ILE:CD1	2:E:1410:GLU:OE2	2.67	0.42
2:B:1210:GLU:CD	1:D:665:ASN:OD1	2.60	0.42
2:B:1411:ILE:CD1	2:E:1411:ILE:CD1	2.88	0.42
1:D:138:SER:CB	1:D:565:ASP:OD1	2.68	0.42
1:D:977:PHE:CE2	2:E:1390:PHE:HZ	2.38	0.42
1:D:1024:ALA:C	1:D:1025:PHE:C	2.53	0.42
1:A:44:ALA:HB3	1:A:799:ILE:HD13	2.01	0.42
1:D:210:GLY:H	1:D:232:GLY:HA3	1.85	0.42
1:D:364:GLU:HG2	1:D:367:SER:CB	2.46	0.42
1:D:398:SER:HA	1:D:544:TYR:HA	2.02	0.42
1:A:1013:LYS:NZ	1:A:1022:PRO:HD2	2.34	0.42
1:D:58:ALA:O	1:D:129:LYS:NZ	2.45	0.42
1:A:210:GLY:H	1:A:232:GLY:HA3	1.85	0.42
1:A:658:ARG:NH1	1:A:746:GLU:OE2	2.47	0.42
1:A:792:LYS:HA	1:A:796:GLN:O	2.20	0.42
1:A:958:LEU:HD21	2:B:1372:GLY:HA2	1.99	0.42
2:B:1361:PRO:O	2:B:1365:ILE:HG13	2.20	0.42
2:B:1436:THR:O	2:B:1437:PRO:C	2.60	0.42
1:D:391:VAL:CG2	1:D:631:ALA:HB1	2.50	0.42
1:D:792:LYS:HA	1:D:796:GLN:O	2.20	0.42
1:A:156:LYS:HE2	1:A:696:THR:OG1	2.20	0.41
1:A:317:LEU:N	1:A:317:LEU:CD2	2.82	0.41
1:A:997:LYS:HG2	2:B:1417:ILE:HG21	2.01	0.41
1:D:120:ILE:HD13	1:D:918:GLY:O	2.20	0.41
1:A:999:ILE:HD13	2:E:1414:ARG:CZ	2.50	0.41
2:B:1360:VAL:O	2:B:1364:VAL:HG23	2.20	0.41
1:A:554:SER:O	1:A:557:SER:HB3	2.20	0.41
2:B:1297:GLN:HE22	1:D:864:ASN:CB	2.33	0.41
1:D:866:PRO:HA	1:D:869:LEU:HG	2.02	0.41
1:D:156:LYS:HE2	1:D:696:THR:OG1	2.20	0.41
1:A:546:ILE:O	1:A:572:ASN:HB2	2.21	0.41
1:A:668:LEU:HB3	1:A:680:SER:HB3	2.03	0.41
1:D:453:ILE:HG12	1:D:467:VAL:HG21	2.02	0.41
1:D:658:ARG:NH1	1:D:746:GLU:OE2	2.47	0.41
1:D:677:ALA:O	1:D:678:PRO:C	2.62	0.41
1:D:964:ILE:CB	1:D:965:PRO:HD3	2.42	0.41
1:D:973:GLN:CB	2:E:1386:LEU:HD21	2.50	0.41
1:A:1020:LYS:C	1:A:1021:LYS:O	2.62	0.41
2:B:1174:ASN:HB2	1:D:643:LYS:HZ1	1.81	0.41
1:D:317:LEU:N	1:D:317:LEU:CD2	2.82	0.41
1:D:994:VAL:HG21	2:E:1408:PHE:CD1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:391:VAL:CG2	1:A:631:ALA:HB1	2.50	0.41
1:A:995:TYR:HB2	2:E:1407:VAL:CG2	2.36	0.41
1:A:999:ILE:CD1	2:E:1410:GLU:CG	2.95	0.41
1:D:645:ASN:ND2	1:D:747:LEU:O	2.37	0.41
1:A:398:SER:HA	1:A:544:TYR:HA	2.02	0.41
1:A:962:ILE:O	2:B:1379:MET:HE1	2.20	0.41
1:D:132:LEU:HD22	1:D:323:TRP:CG	2.55	0.41
1:A:47:ILE:HG22	1:A:50:SER:HB3	2.03	0.41
1:A:994:VAL:HG21	2:B:1408:PHE:CD1	2.56	0.41
2:B:1400:LEU:CD2	1:D:987:LEU:HD23	2.50	0.41
1:D:117:SER:HB3	1:D:125:THR:CG2	2.49	0.41
1:D:434:ASP:CG	1:D:469:TYR:HA	2.46	0.41
1:D:997:LYS:CE	2:E:1419:ASN:HB2	2.45	0.41
1:D:1016:ASN:C	1:D:1018:SER:N	2.79	0.41
2:E:1361:PRO:O	2:E:1365:ILE:HG13	2.21	0.41
1:A:120:ILE:HD13	1:A:918:GLY:O	2.20	0.41
1:D:44:ALA:HB3	1:D:799:ILE:HD13	2.01	0.41
1:A:434:ASP:CG	1:A:469:TYR:HA	2.46	0.40
1:A:750:ASP:O	1:A:752:ALA:N	2.54	0.40
1:A:958:LEU:HD21	2:B:1372:GLY:N	2.36	0.40
1:A:1002:THR:OG1	2:E:1414:ARG:HD3	2.21	0.40
1:A:574:GLN:HE21	1:A:575:SER:N	2.16	0.40
2:B:1210:GLU:N	1:D:665:ASN:HB2	2.35	0.40
1:D:47:ILE:HG22	1:D:50:SER:HB3	2.03	0.40
1:D:230:LYS:CB	1:D:231:GLN:HE22	2.35	0.40
1:D:546:ILE:O	1:D:572:ASN:HB2	2.21	0.40
1:D:750:ASP:O	1:D:752:ALA:N	2.54	0.40
1:D:994:VAL:HG21	2:E:1408:PHE:CG	2.56	0.40
1:A:117:SER:HB3	1:A:125:THR:CG2	2.49	0.40
1:A:453:ILE:HG12	1:A:467:VAL:HG21	2.02	0.40
1:D:163:LEU:HD23	1:D:622:ILE:HD11	2.03	0.40
1:D:986:THR:CG2	2:E:1427:ALA:HB2	2.47	0.40
1:D:994:VAL:HB	2:E:1408:PHE:CE1	2.55	0.40
2:E:1360:VAL:O	2:E:1364:VAL:HG23	2.21	0.40
1:A:77:PHE:CE2	1:A:113:GLU:HB2	2.56	0.40
1:A:132:LEU:HD22	1:A:323:TRP:CG	2.55	0.40
1:A:869:LEU:C	1:A:869:LEU:CD1	2.94	0.40
2:B:1377:ILE:N	2:B:1378:PRO:CD	2.84	0.40
1:D:77:PHE:CE2	1:D:113:GLU:HB2	2.56	0.40
1:D:554:SER:O	1:D:557:SER:HB3	2.20	0.40
1:D:965:PRO:O	1:D:969:VAL:HG23	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:1433:THR:O	2:E:1434:PRO:C	2.63	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	993/1053 (94%)	887 (89%)	64 (6%)	42 (4%)	2	17
1	D	993/1053 (94%)	887 (89%)	64 (6%)	42 (4%)	2	17
2	B	1376/1444 (95%)	1251 (91%)	102 (7%)	23 (2%)	7	36
2	E	1376/1444 (95%)	1249 (91%)	104 (8%)	23 (2%)	7	36
All	All	4738/4994 (95%)	4274 (90%)	334 (7%)	130 (3%)	6	25

All (130) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	262	SER
1	A	723	ASP
1	A	1020	LYS
1	A	1022	PRO
1	A	1023	ALA
1	A	1024	ALA
1	A	1025	PHE
1	A	1026	LEU
1	A	1029	PRO
1	A	1030	VAL
1	A	1036	PRO
1	A	1037	GLU
1	A	1039	GLU
1	A	1040	GLN

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Mol	Chain	Res	Type
1	A	1041	LYS
1	A	1042	ALA
1	A	1043	VAL
1	A	1044	GLU
1	A	1045	VAL
1	A	1046	LYS
1	A	1047	SER
1	A	1048	GLU
1	A	1049	GLU
1	A	1050	THR
1	A	1051	LYS
2	B	1430	THR
2	B	1434	PRO
2	B	1435	LYS
2	B	1442	VAL
2	B	1443	LYS
1	D	262	SER
1	D	723	ASP
1	D	1020	LYS
1	D	1023	ALA
1	D	1024	ALA
1	D	1025	PHE
1	D	1029	PRO
1	D	1030	VAL
1	D	1033	PRO
1	D	1036	PRO
1	D	1037	GLU
1	D	1039	GLU
1	D	1040	GLN
1	D	1041	LYS
1	D	1042	ALA
1	D	1043	VAL
1	D	1044	GLU
1	D	1045	VAL
1	D	1046	LYS
1	D	1047	SER
1	D	1048	GLU
1	D	1049	GLU
1	D	1050	THR
1	D	1051	LYS
2	E	1434	PRO
2	E	1435	LYS

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Mol	Chain	Res	Type
2	E	1442	VAL
2	E	1443	LYS
1	A	460	GLN
1	A	748	ASN
1	A	1033	PRO
1	A	1034	SER
2	B	1418	SER
2	B	1432	PRO
2	B	1441	PRO
1	D	460	GLN
1	D	748	ASN
1	D	1022	PRO
1	D	1028	PRO
1	D	1031	GLN
1	D	1034	SER
2	E	1418	SER
2	E	1430	THR
2	E	1441	PRO
1	A	156	LYS
1	A	164	ALA
1	A	237	SER
1	A	529	SER
1	A	561	SER
1	A	937	PRO
1	A	1017	PRO
1	A	1028	PRO
1	A	1031	GLN
2	B	643	SER
2	B	1092	THR
2	B	1429	PRO
2	B	1438	PRO
1	D	156	LYS
1	D	164	ALA
1	D	237	SER
1	D	529	SER
1	D	561	SER
1	D	937	PRO
2	E	643	SER
2	E	1092	THR
2	E	1351	ASP
2	E	1429	PRO
2	E	1432	PRO

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Mol	Chain	Res	Type
2	E	1438	PRO
1	A	453	ILE
1	A	1032	PRO
2	B	833	GLY
2	B	1433	THR
2	B	1437	PRO
1	D	453	ILE
1	D	1026	LEU
2	E	833	GLY
2	E	1428	THR
1	A	1021	LYS
1	A	1035	LYS
2	B	1187	LYS
2	B	1436	THR
1	D	1021	LYS
1	D	1032	PRO
2	E	1187	LYS
2	E	1433	THR
2	E	1436	THR
2	E	1437	PRO
2	B	641	ILE
2	B	822	PRO
1	D	1017	PRO
1	D	1035	LYS
2	E	641	ILE
2	E	822	PRO
2	B	1428	THR
2	B	593	THR
2	B	1440	PRO
2	E	593	THR
2	B	857	THR
2	E	857	THR

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	873/914 (96%)	790 (90%)	83 (10%)	8	25
1	D	873/914 (96%)	790 (90%)	83 (10%)	8	25
2	B	1207/1267 (95%)	1182 (98%)	25 (2%)	47	65
2	E	1207/1267 (95%)	1180 (98%)	27 (2%)	45	64
All	All	4160/4362 (95%)	3942 (95%)	218 (5%)	22	42

All (218) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	52	SER
1	A	69	GLN
1	A	79	LEU
1	A	81	LYS
1	A	90	GLU
1	A	104	GLN
1	A	106	GLU
1	A	125	THR
1	A	149	ILE
1	A	163	LEU
1	A	169	LYS
1	A	172	ARG
1	A	180	GLN
1	A	182	ASN
1	A	186	SER
1	A	190	GLN
1	A	229	THR
1	A	231	GLN
1	A	237	SER
1	A	241	SER
1	A	246	ASN
1	A	249	LYS
1	A	264	THR
1	A	275	LEU
1	A	277	SER
1	A	286	THR
1	A	294	LEU
1	A	302	LEU
1	A	317	LEU
1	A	364	GLU
1	A	368	THR
1	A	376	LYS

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Mol	Chain	Res	Type
1	A	377	SER
1	A	390	SER
1	A	393	ASP
1	A	409	SER
1	A	421	LYS
1	A	437	THR
1	A	441	ASP
1	A	459	ILE
1	A	466	VAL
1	A	469	TYR
1	A	470	SER
1	A	492	GLN
1	A	493	LYS
1	A	495	THR
1	A	500	SER
1	A	521	LEU
1	A	528	LYS
1	A	530	ASN
1	A	533	ARG
1	A	536	SER
1	A	537	ARG
1	A	540	GLN
1	A	543	VAL
1	A	561	SER
1	A	574	GLN
1	A	576	ARG
1	A	643	LYS
1	A	657	VAL
1	A	665	ASN
1	A	676	ILE
1	A	679	ILE
1	A	680	SER
1	A	684	THR
1	A	725	LYS
1	A	765	VAL
1	A	766	GLN
1	A	792	LYS
1	A	793	ASP
1	A	863	ILE
1	A	869	LEU
1	A	898	VAL
1	A	956	LEU

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Mol	Chain	Res	Type
1	A	958	LEU
1	A	966	MET
1	A	1012	LEU
1	A	1018	SER
1	A	1030	VAL
1	A	1034	SER
1	A	1050	THR
1	A	1052	SER
2	B	243	ASP
2	B	251	LYS
2	B	401	ASN
2	B	503	TRP
2	B	622	PHE
2	B	638	GLU
2	B	650	LEU
2	B	725	ARG
2	B	752	THR
2	B	778	SER
2	B	819	VAL
2	B	876	LYS
2	B	887	ILE
2	B	890	THR
2	B	1030	THR
2	B	1231	THR
2	B	1312	GLN
2	B	1356	LEU
2	B	1371	LEU
2	B	1418	SER
2	B	1424	LEU
2	B	1428	THR
2	B	1430	THR
2	B	1433	THR
2	B	1436	THR
1	D	26	ASN
1	D	52	SER
1	D	69	GLN
1	D	79	LEU
1	D	81	LYS
1	D	90	GLU
1	D	104	GLN
1	D	106	GLU
1	D	125	THR

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Mol	Chain	Res	Type
1	D	149	ILE
1	D	163	LEU
1	D	169	LYS
1	D	172	ARG
1	D	180	GLN
1	D	182	ASN
1	D	186	SER
1	D	190	GLN
1	D	229	THR
1	D	231	GLN
1	D	237	SER
1	D	241	SER
1	D	246	ASN
1	D	249	LYS
1	D	264	THR
1	D	275	LEU
1	D	277	SER
1	D	286	THR
1	D	294	LEU
1	D	302	LEU
1	D	317	LEU
1	D	364	GLU
1	D	368	THR
1	D	376	LYS
1	D	377	SER
1	D	390	SER
1	D	393	ASP
1	D	409	SER
1	D	421	LYS
1	D	437	THR
1	D	441	ASP
1	D	459	ILE
1	D	466	VAL
1	D	469	TYR
1	D	470	SER
1	D	492	GLN
1	D	493	LYS
1	D	495	THR
1	D	500	SER
1	D	521	LEU
1	D	528	LYS
1	D	530	ASN

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Mol	Chain	Res	Type
1	D	533	ARG
1	D	536	SER
1	D	537	ARG
1	D	540	GLN
1	D	543	VAL
1	D	561	SER
1	D	574	GLN
1	D	576	ARG
1	D	643	LYS
1	D	657	VAL
1	D	665	ASN
1	D	676	ILE
1	D	679	ILE
1	D	680	SER
1	D	684	THR
1	D	725	LYS
1	D	765	VAL
1	D	766	GLN
1	D	792	LYS
1	D	793	ASP
1	D	863	ILE
1	D	869	LEU
1	D	898	VAL
1	D	956	LEU
1	D	958	LEU
1	D	1000	THR
1	D	1012	LEU
1	D	1018	SER
1	D	1030	VAL
1	D	1034	SER
1	D	1050	THR
1	D	1052	SER
2	E	243	ASP
2	E	251	LYS
2	E	401	ASN
2	E	503	TRP
2	E	622	PHE
2	E	638	GLU
2	E	650	LEU
2	E	725	ARG
2	E	752	THR
2	E	778	SER

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Mol	Chain	Res	Type
2	E	819	VAL
2	E	876	LYS
2	E	887	ILE
2	E	890	THR
2	E	1030	THR
2	E	1231	THR
2	E	1266	THR
2	E	1349	TRP
2	E	1356	LEU
2	E	1371	LEU
2	E	1418	SER
2	E	1424	LEU
2	E	1428	THR
2	E	1430	THR
2	E	1433	THR
2	E	1436	THR
2	E	1442	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (98) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	ASN
1	A	182	ASN
1	A	183	GLN
1	A	187	GLN
1	A	189	ASN
1	A	194	ASN
1	A	200	ASN
1	A	231	GLN
1	A	250	ASN
1	A	285	GLN
1	A	293	GLN
1	A	330	GLN
1	A	352	GLN
1	A	369	ASN
1	A	492	GLN
1	A	499	ASN
1	A	574	GLN
1	A	662	ASN
1	A	665	ASN
1	A	748	ASN
1	A	770	GLN

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Mol	Chain	Res	Type
1	A	850	GLN
1	A	973	GLN
1	A	1040	GLN
2	B	199	ASN
2	B	215	ASN
2	B	462	ASN
2	B	631	ASN
2	B	633	ASN
2	B	634	ASN
2	B	665	GLN
2	B	675	ASN
2	B	716	ASN
2	B	727	ASN
2	B	735	ASN
2	B	745	ASN
2	B	779	ASN
2	B	815	ASN
2	B	837	GLN
2	B	849	GLN
2	B	862	ASN
2	B	908	ASN
2	B	967	HIS
2	B	1003	ASN
2	B	1207	ASN
2	B	1235	ASN
2	B	1240	GLN
2	B	1262	ASN
2	B	1297	GLN
2	B	1344	GLN
2	B	1380	HIS
1	D	73	ASN
1	D	183	GLN
1	D	187	GLN
1	D	189	ASN
1	D	194	ASN
1	D	200	ASN
1	D	231	GLN
1	D	250	ASN
1	D	285	GLN
1	D	293	GLN
1	D	330	GLN
1	D	352	GLN

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Mol	Chain	Res	Type
1	D	369	ASN
1	D	492	GLN
1	D	499	ASN
1	D	574	GLN
1	D	674	ASN
1	D	751	GLN
1	D	770	GLN
1	D	850	GLN
1	D	973	GLN
1	D	1040	GLN
2	E	199	ASN
2	E	215	ASN
2	E	462	ASN
2	E	631	ASN
2	E	633	ASN
2	E	634	ASN
2	E	652	HIS
2	E	665	GLN
2	E	668	ASN
2	E	716	ASN
2	E	727	ASN
2	E	735	ASN
2	E	745	ASN
2	E	779	ASN
2	E	815	ASN
2	E	840	ASN
2	E	849	GLN
2	E	862	ASN
2	E	908	ASN
2	E	967	HIS
2	E	1003	ASN
2	E	1174	ASN
2	E	1235	ASN
2	E	1240	GLN
2	E	1380	HIS

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 ⓘ

6 monosaccharides 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	BGC	C	1	3	11,11,12	1.51	3 (27%)	15,15,17	0.82	0
3	GAL	C	2	3	11,11,12	1.35	2 (18%)	15,15,17	0.79	0
3	SIA	C	3	3	20,20,21	2.03	2 (10%)	21,28,31	1.34	3 (14%)
3	BGC	F	1	3	11,11,12	1.50	3 (27%)	15,15,17	0.83	0
3	GAL	F	2	3	11,11,12	1.34	2 (18%)	15,15,17	0.79	0
3	SIA	F	3	3	20,20,21	2.03	2 (10%)	21,28,31	1.35	3 (14%)

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	BGC	C	1	3	-	0/2/19/22	0/1/1/1
3	GAL	C	2	3	-	0/2/19/22	0/1/1/1
3	SIA	C	3	3	-	0/18/34/38	0/1/1/1
3	BGC	F	1	3	-	0/2/19/22	0/1/1/1
3	GAL	F	2	3	-	0/2/19/22	0/1/1/1
3	SIA	F	3	3	-	0/18/34/38	0/1/1/1

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	3	SIA	C2-C1	7.47	1.61	1.52
3	F	3	SIA	C2-C1	7.45	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	3	SIA	C4-C5	2.80	1.55	1.53
3	C	3	SIA	C4-C5	2.78	1.55	1.53
3	C	1	BGC	O5-C1	2.71	1.48	1.43
3	F	1	BGC	O5-C1	2.71	1.48	1.43
3	C	2	GAL	O5-C5	2.70	1.48	1.43
3	F	2	GAL	O5-C5	2.68	1.48	1.43
3	C	1	BGC	O5-C5	2.60	1.48	1.43
3	F	1	BGC	O5-C5	2.55	1.48	1.43
3	F	1	BGC	O4-C4	2.45	1.49	1.43
3	C	1	BGC	O4-C4	2.44	1.49	1.43
3	C	2	GAL	O5-C1	2.08	1.47	1.43
3	F	2	GAL	O5-C1	2.03	1.47	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	3	SIA	O6-C2-C1	3.27	113.89	107.72
3	F	3	SIA	O6-C2-C1	3.26	113.86	107.72
3	F	3	SIA	O6-C2-C3	-2.64	107.01	110.56
3	C	3	SIA	O6-C2-C3	-2.62	107.03	110.56
3	F	3	SIA	O1B-C1-C2	2.32	118.73	112.71
3	C	3	SIA	O1B-C1-C2	2.29	118.67	112.71

There are no chirality outliers.

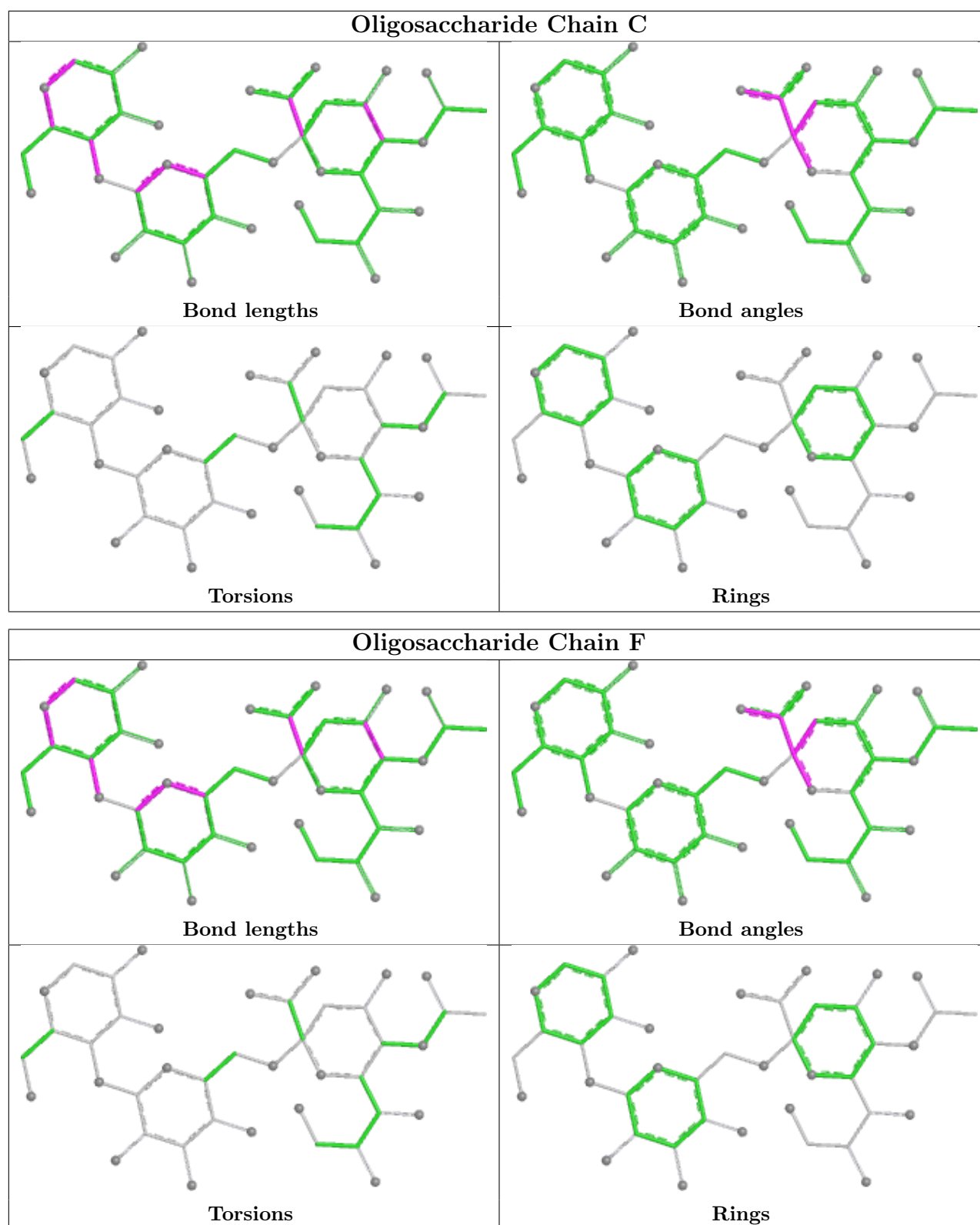
There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	3	SIA	1	0
3	F	3	SIA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	17
1	D	16
2	E	7
2	B	5

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	1040:GLN	C	1041:LYS	N	1.20
1	D	1040:GLN	C	1041:LYS	N	1.20
1	A	1013:LYS	C	1014:ALA	N	1.19
1	A	1048:GLU	C	1049:GLU	N	1.19
1	D	1047:SER	C	1048:GLU	N	1.19
1	E	1420:ALA	C	1421:PRO	N	1.19
1	A	1002:THR	C	1003:GLY	N	1.18
1	A	1041:LYS	C	1042:ALA	N	1.18
1	B	1427:ALA	C	1428:THR	N	1.18
1	D	1035:LYS	C	1036:PRO	N	1.18
1	D	1041:LYS	C	1042:ALA	N	1.18
1	E	1428:THR	C	1429:PRO	N	1.18
1	E	1433:THR	C	1434:PRO	N	1.18
1	A	1035:LYS	C	1036:PRO	N	1.17
1	A	1047:SER	C	1048:GLU	N	1.17
1	D	1013:LYS	C	1014:ALA	N	1.17
1	D	1016:ASN	C	1017:PRO	N	1.17
1	A	1016:ASN	C	1017:PRO	N	1.16
1	A	1038:GLY	C	1039:GLU	N	1.16
1	B	1420:ALA	C	1421:PRO	N	1.16
1	D	1002:THR	C	1003:GLY	N	1.16
1	D	1038:GLY	C	1039:GLU	N	1.16
1	A	1049:GLU	C	1050:THR	N	1.15
1	D	1029:PRO	C	1030:VAL	N	1.15
1	E	1427:ALA	C	1428:THR	N	1.15
1	A	1029:PRO	C	1030:VAL	N	1.14
1	D	1021:LYS	C	1022:PRO	N	1.14

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	1048:GLU	C	1049:GLU	N	1.14
1	A	1036:PRO	C	1037:GLU	N	1.13
1	D	1042:ALA	C	1043:VAL	N	1.13
1	A	1021:LYS	C	1022:PRO	N	1.12
1	A	1039:GLU	C	1040:GLN	N	1.12
1	D	1022:PRO	C	1023:ALA	N	1.12
1	E	1431:LYS	C	1432:PRO	N	1.12
1	E	1434:PRO	C	1435:LYS	N	1.12
1	D	1036:PRO	C	1037:GLU	N	1.11
1	A	1022:PRO	C	1023:ALA	N	1.10
1	A	1042:ALA	C	1043:VAL	N	1.10
1	D	1039:GLU	C	1040:GLN	N	1.10
1	B	1431:LYS	C	1432:PRO	N	1.05
1	B	1434:PRO	C	1435:LYS	N	1.05
1	B	1429:PRO	C	1430:THR	N	1.02
1	E	1429:PRO	C	1430:THR	N	0.98
1	D	1024:ALA	C	1025:PHE	N	0.77
1	A	1024:ALA	C	1025:PHE	N	0.76

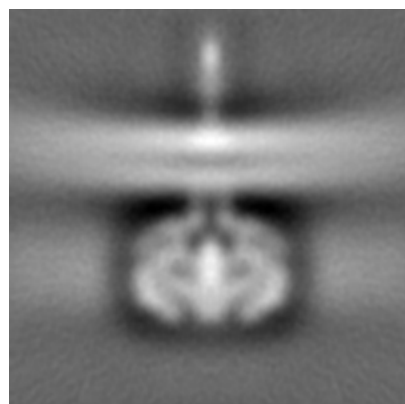
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-17591. These allow visual inspection of the internal detail of the map and identification of artifacts.

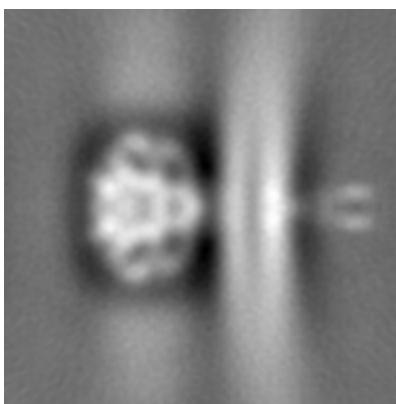
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

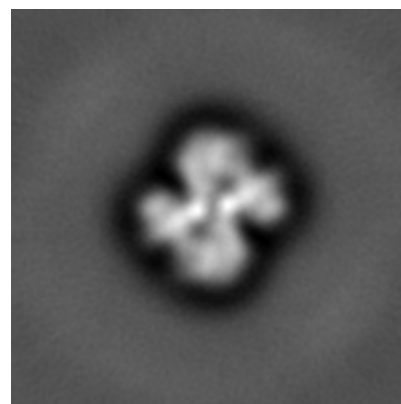
6.1.1 Primary map



X

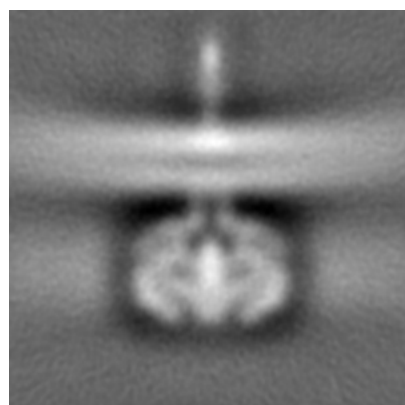


Y

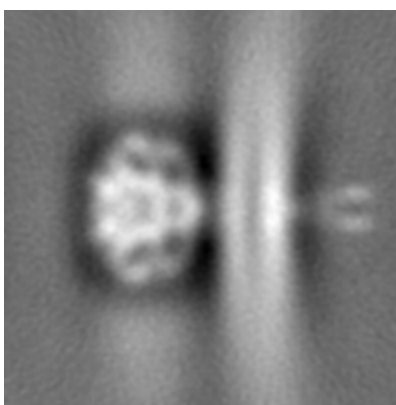


Z

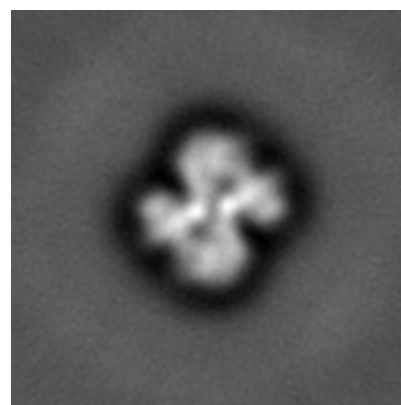
6.1.2 Raw map



X



Y

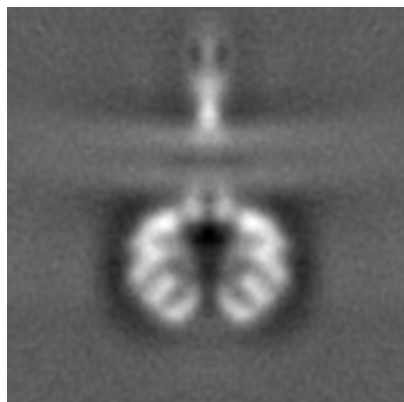


Z

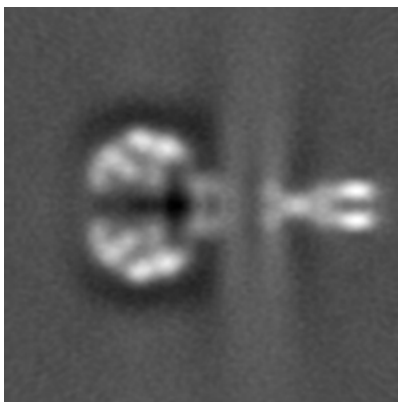
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

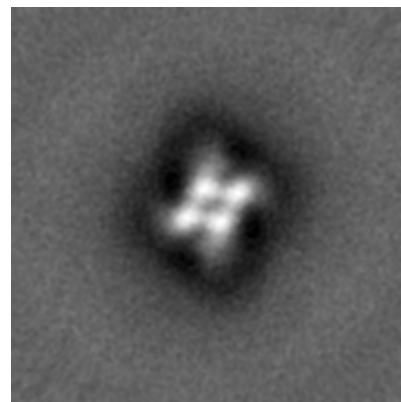
6.2.1 Primary map



X Index: 64

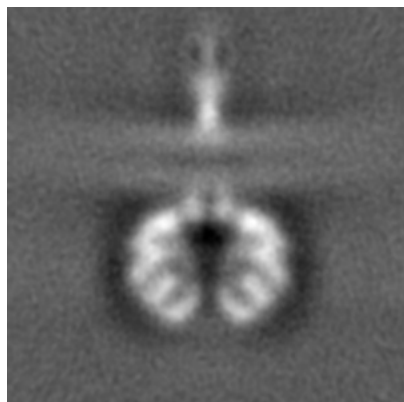


Y Index: 64

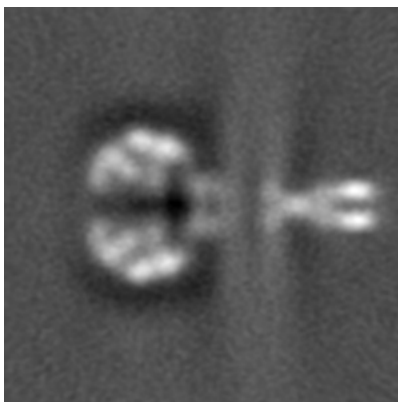


Z Index: 64

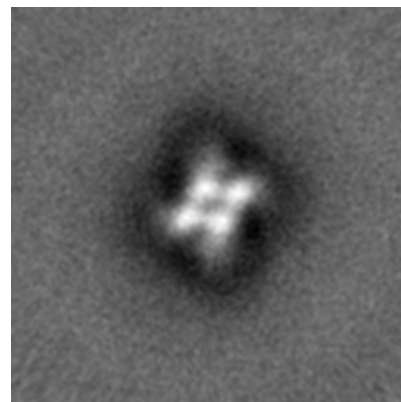
6.2.2 Raw map



X Index: 64



Y Index: 64

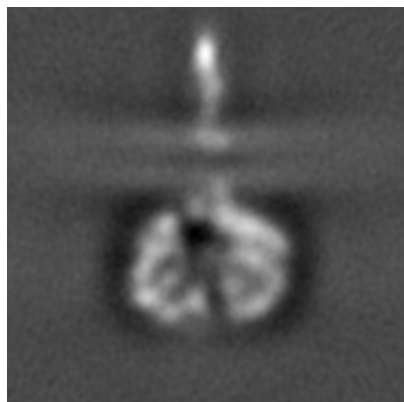


Z Index: 64

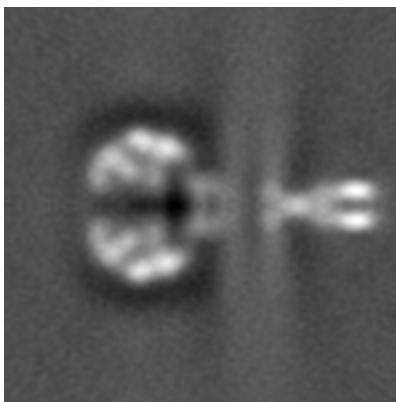
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

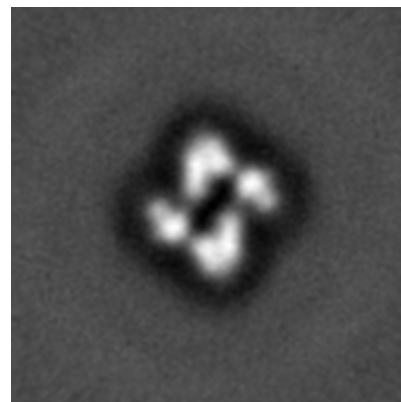
6.3.1 Primary map



X Index: 60

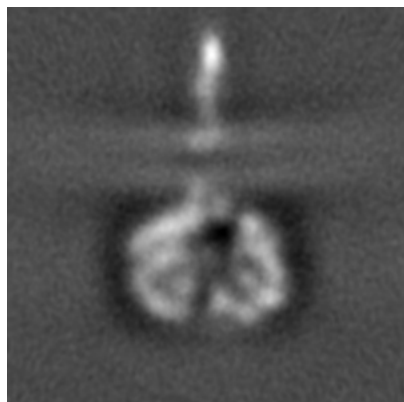


Y Index: 64

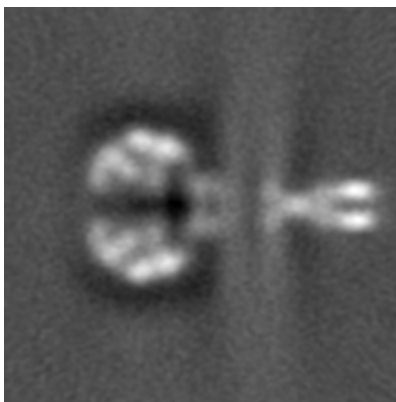


Z Index: 57

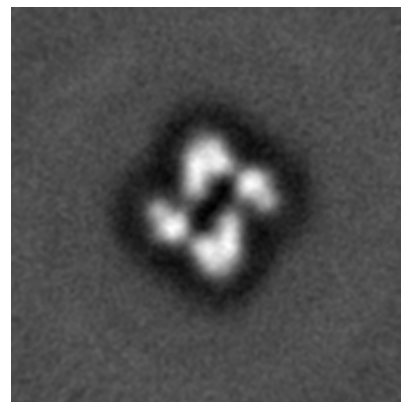
6.3.2 Raw map



X Index: 68



Y Index: 64

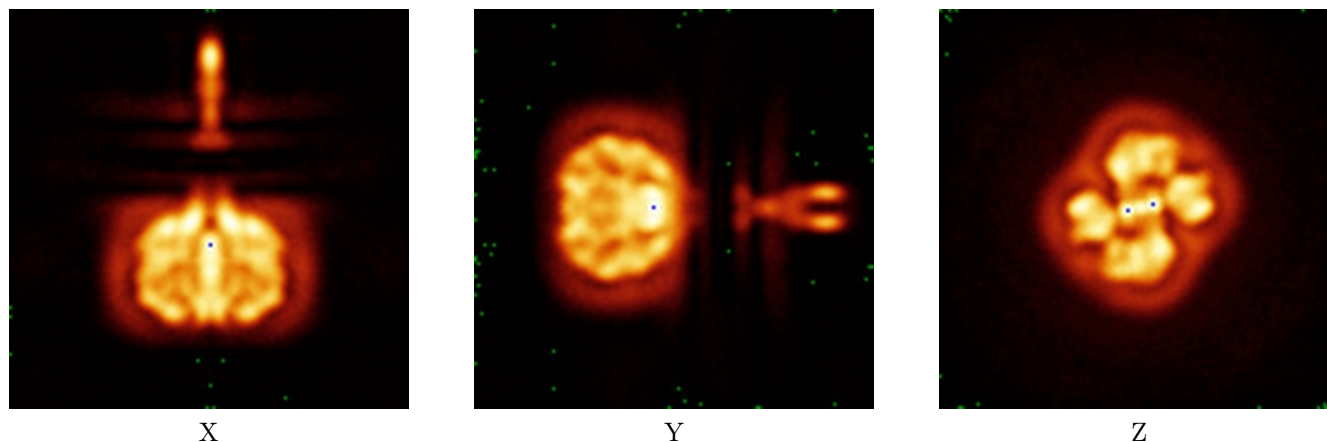


Z Index: 57

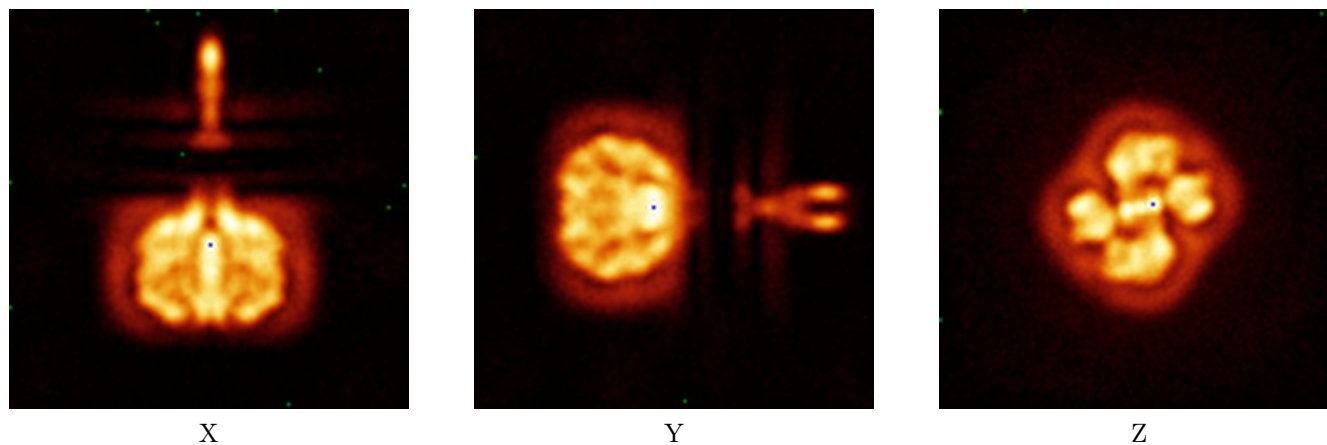
The images above show the largest variance slices of the map in three orthogonal directions.

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

6.4.1 Primary map



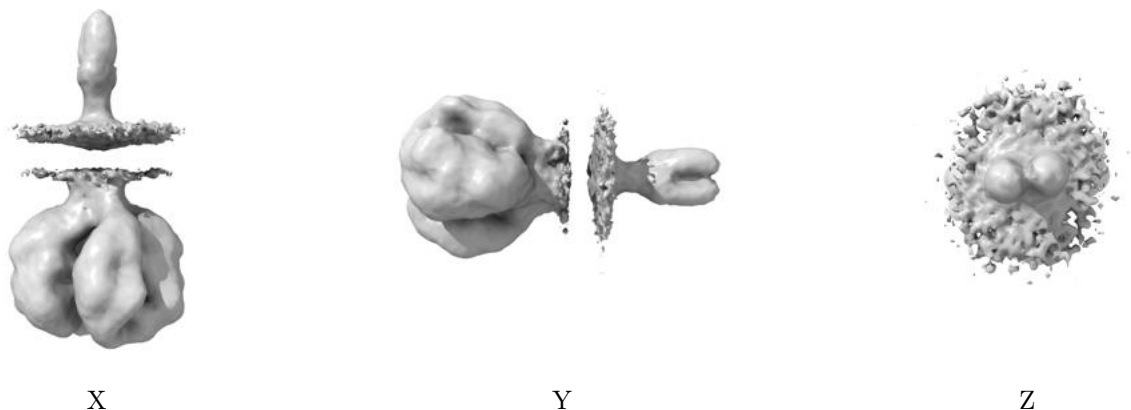
6.4.2 Raw map



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

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 1.66. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

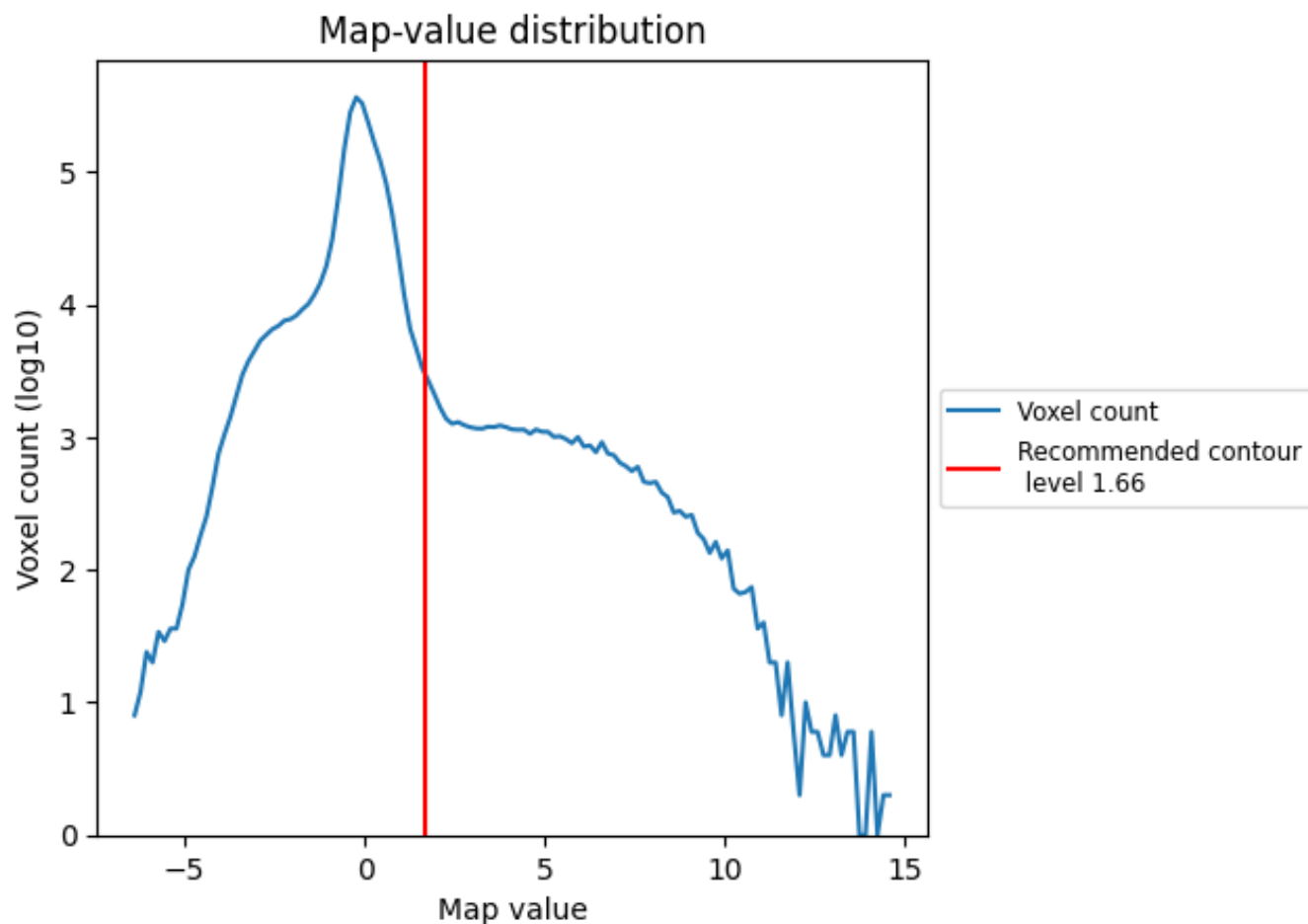
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

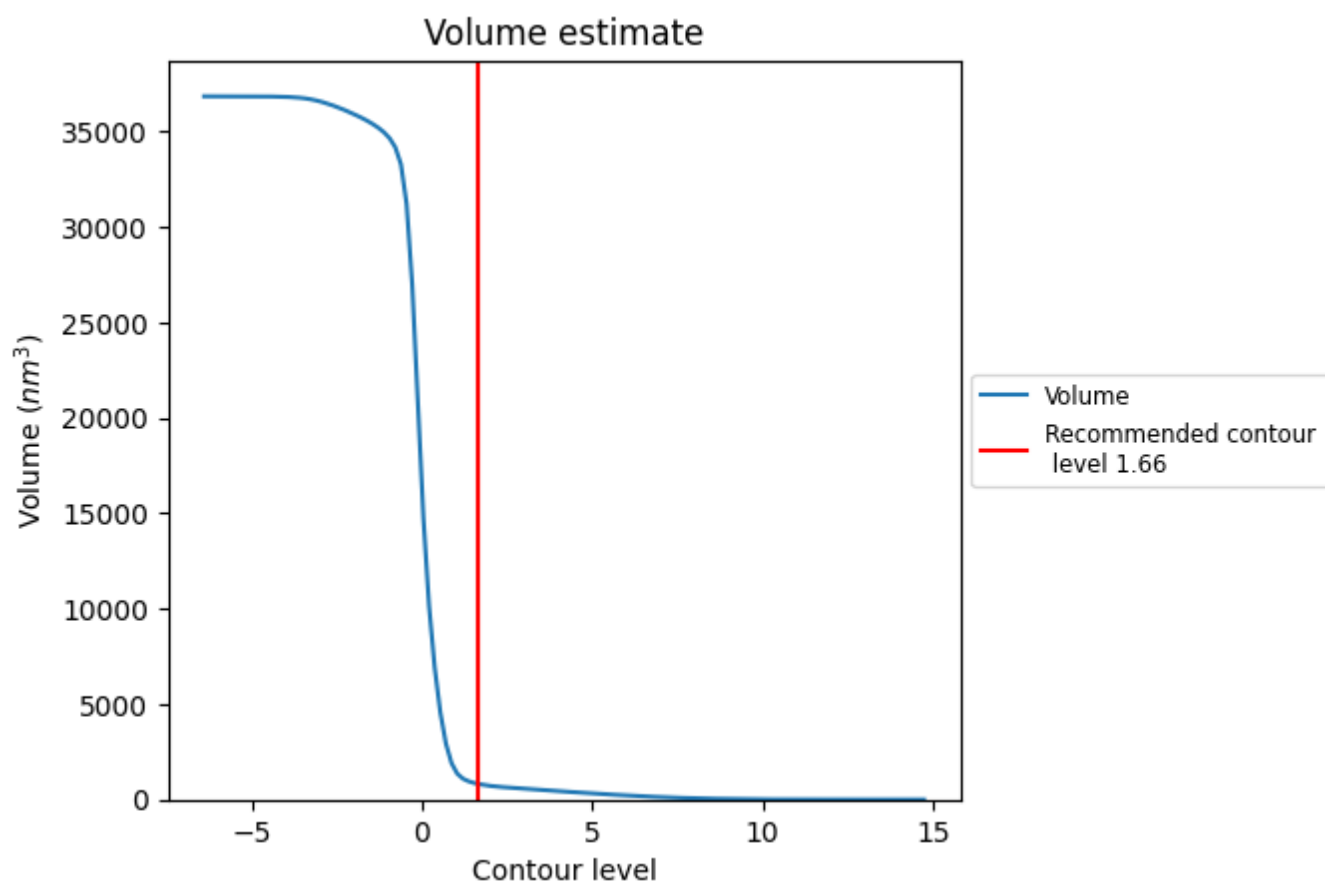
This section contains the results of statistical analysis of the map.

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.

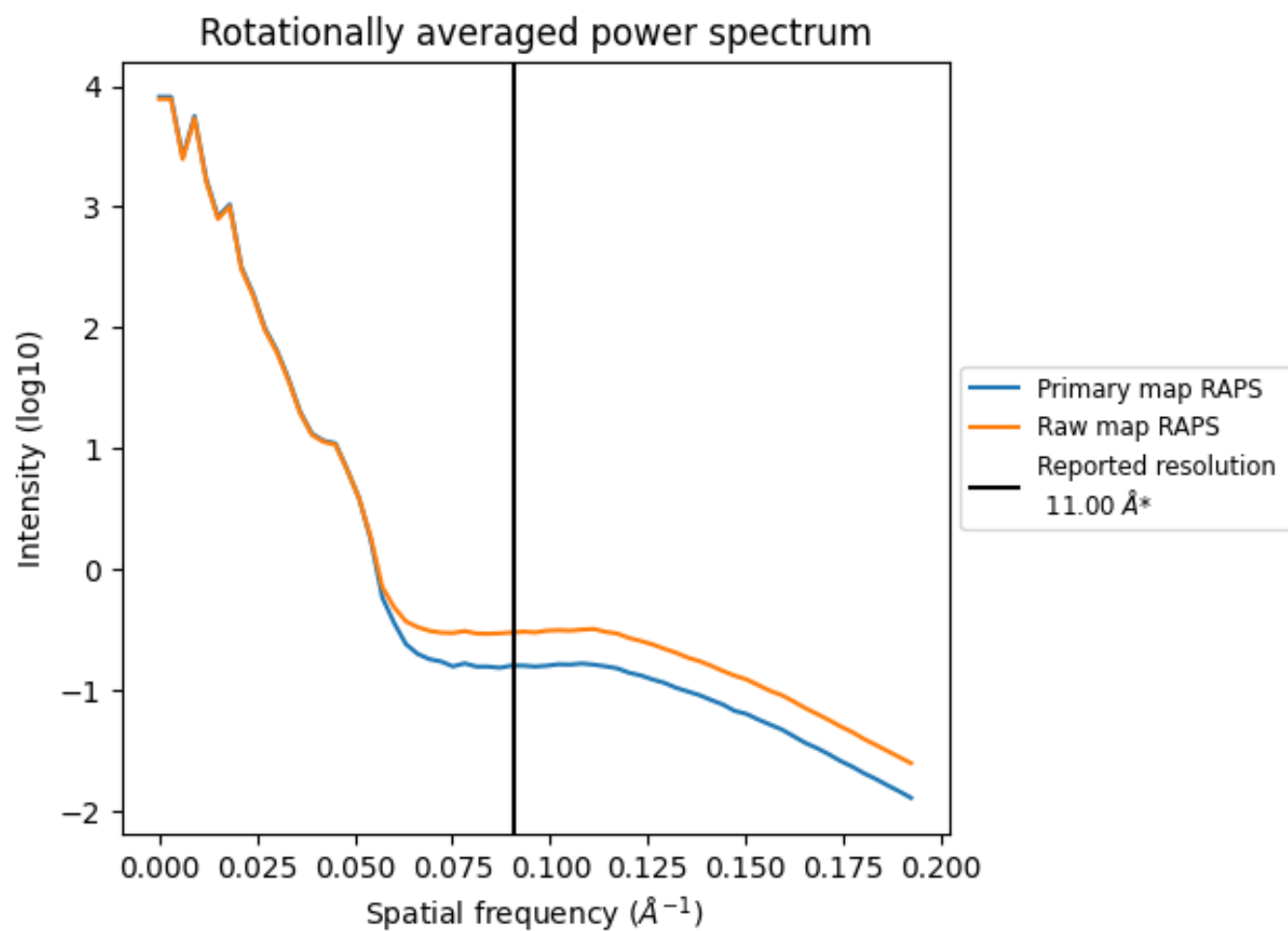
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 819 nm³; this corresponds to an approximate mass of 740 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](#)

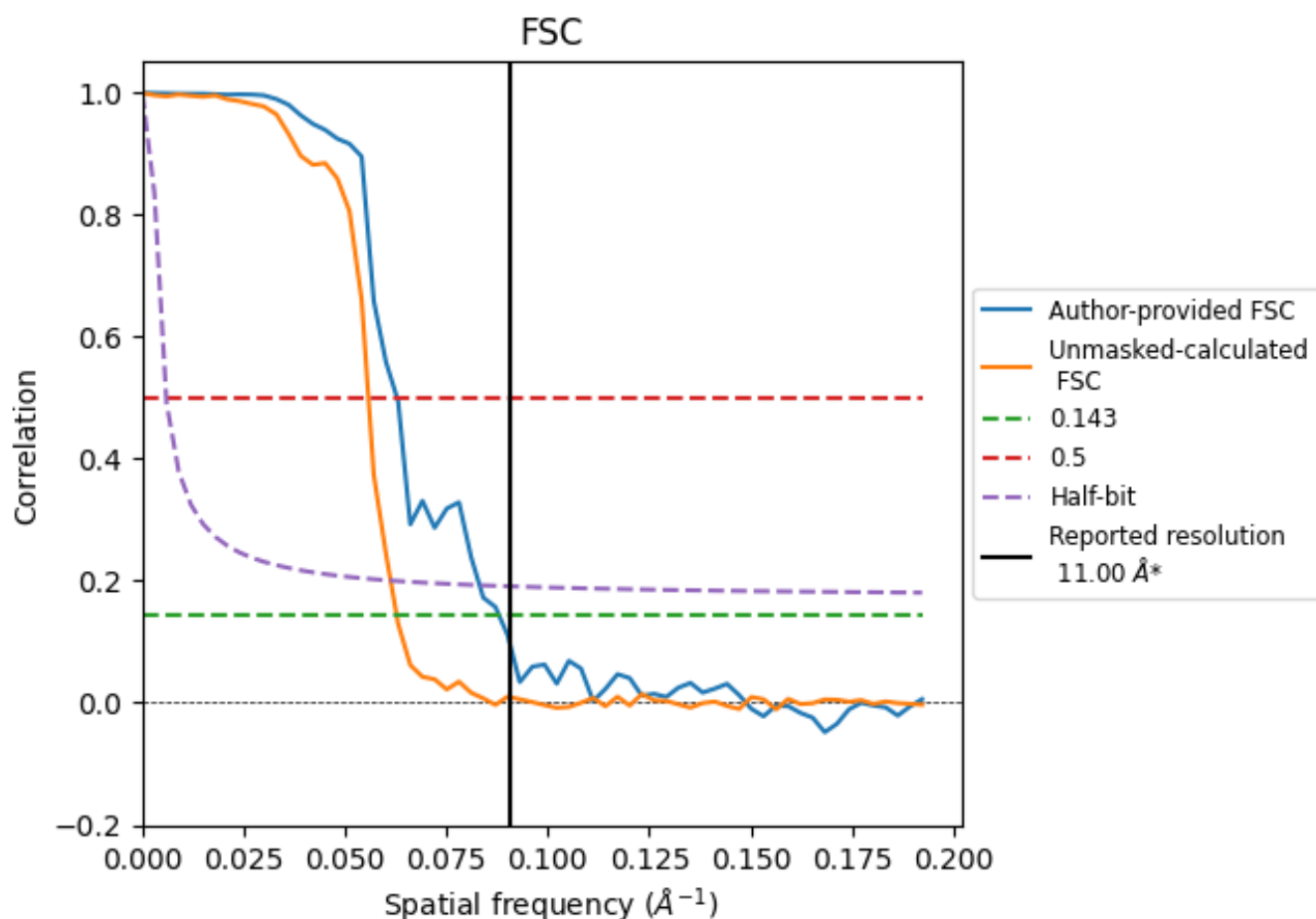


*Reported resolution corresponds to spatial frequency of 0.091 $\text{\AA}^{-1}$

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.091 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

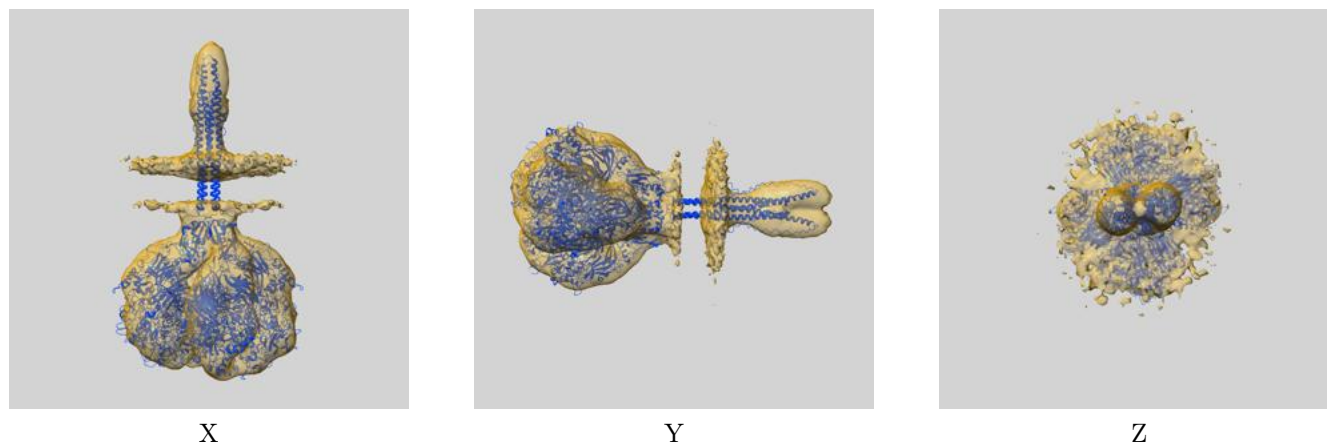
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	11.00	-	-
Author-provided FSC curve	11.35	15.90	12.02
Unmasked-calculated*	15.92	17.92	16.34

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 15.92 differs from the reported value 11.0 by more than 10 %

9 Map-model fit [i](#)

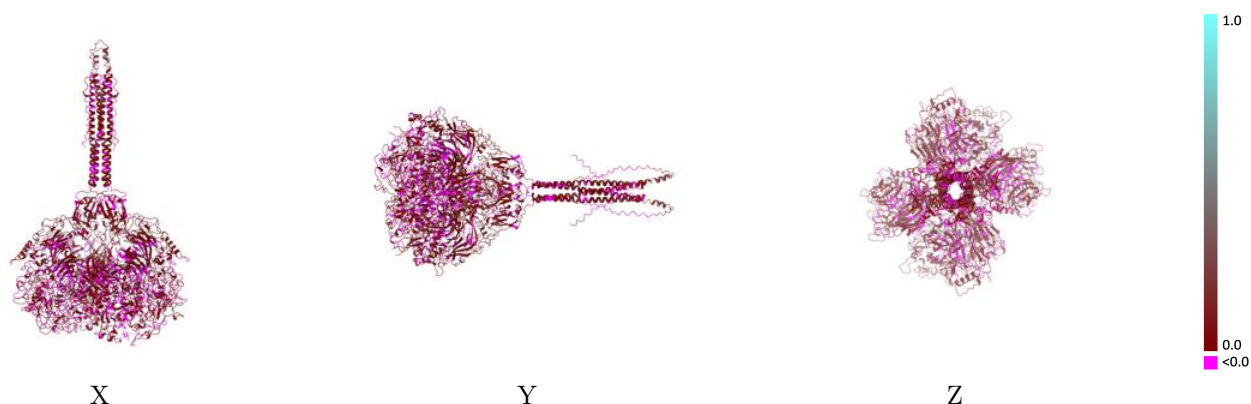
This section contains information regarding the fit between EMDB map EMD-17591 and PDB model 8PBZ. Per-residue inclusion information can be found in section [3](#) on page [5](#).

9.1 Map-model overlay [i](#)



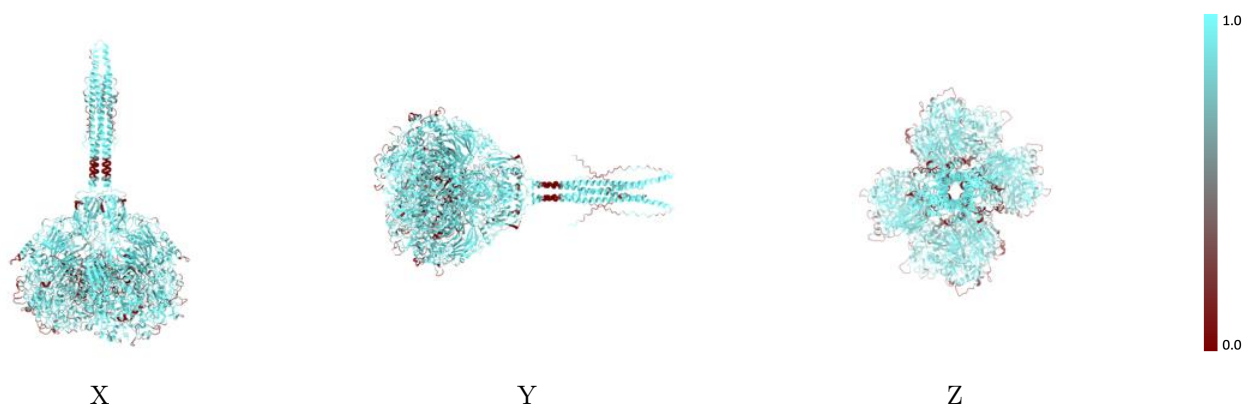
The images above show the 3D surface view of the map at the recommended contour level 1.66 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



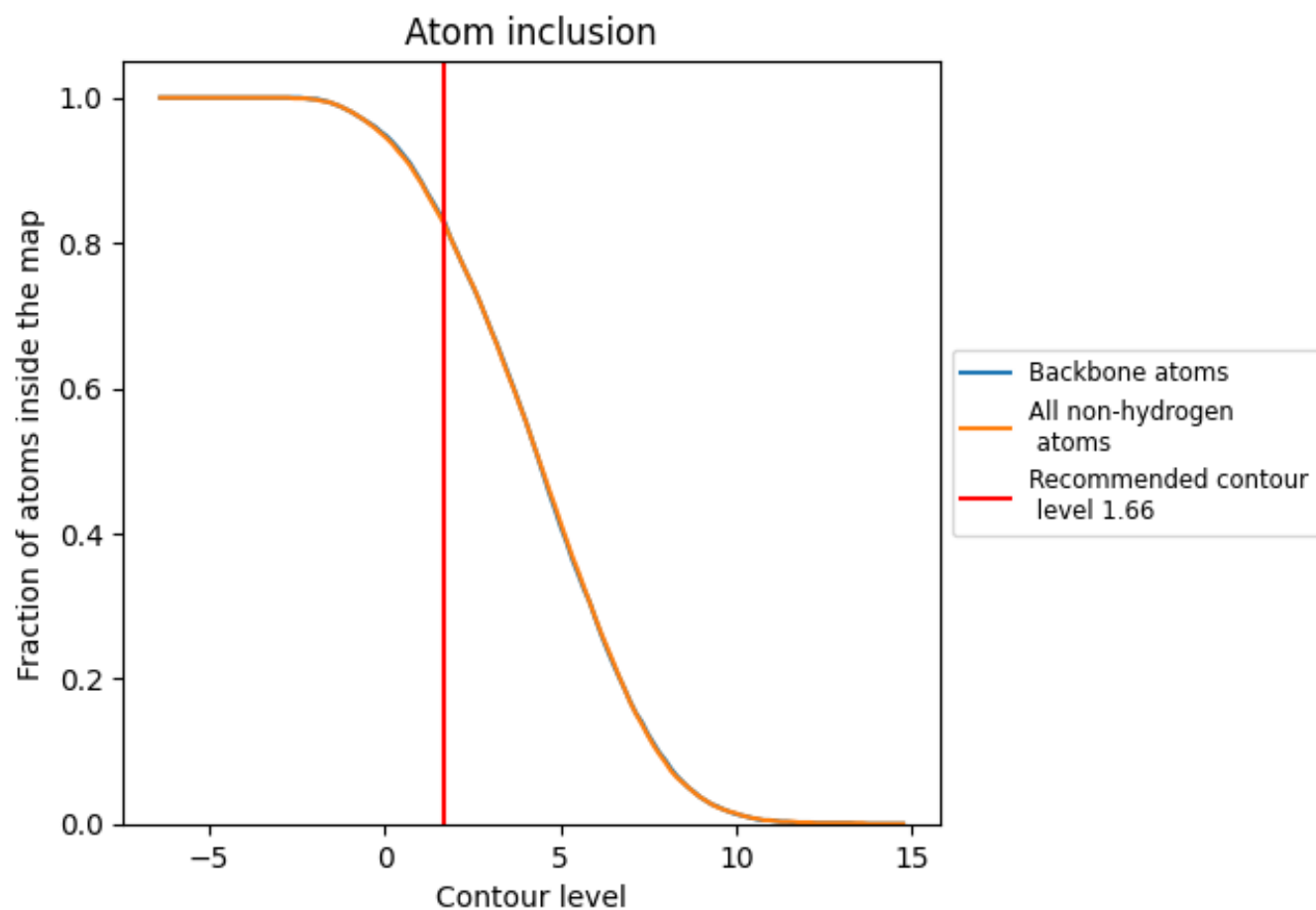
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (1.66).

9.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 83% 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 (1.66) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8280	0.0440
A	0.8530	0.0480
B	0.8180	0.0420
C	0.9760	-0.0310
D	0.8390	0.0450
E	0.8110	0.0410
F	0.9050	-0.0170

