



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 06:33 AM UTC

PDB ID : 8XUT / pdb_00008xut
EMDB ID : EMD-38683
Title : XBB.1.5 Spike Trimer in complex with heparan sulfate
Authors : Yue, C.; Liu, P.; Mao, X.
Deposited on : 2024-01-14
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

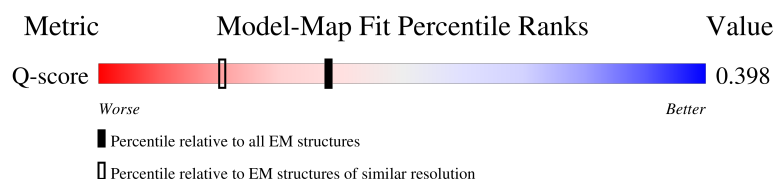
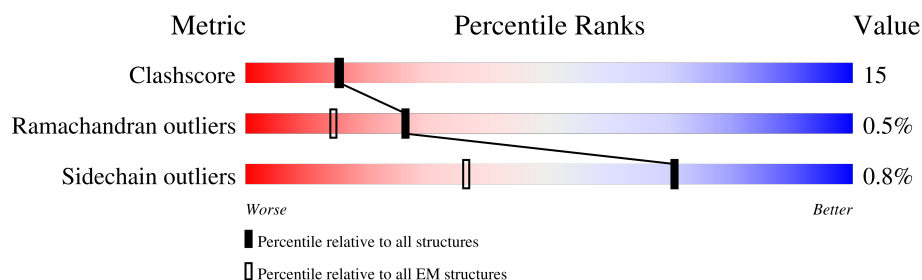
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data 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 3.20 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	15020 (2.70 - 3.70)

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	1269	
1	B	1269	
1	C	1269	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25149 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	B	1042	Total	C	N	O	S	0	0
			8154	5216	1359	1542	37		
1	A	1042	Total	C	N	O	S	0	0
			8154	5216	1359	1542	37		
1	C	1042	Total	C	N	O	S	0	0
			8154	5216	1359	1542	37		

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	22	ILE	THR	variant	UNP P0DTC2
B	?	-	LEU	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	?	-	PRO	deletion	UNP P0DTC2
B	27	SER	ALA	variant	UNP P0DTC2
B	83	ALA	VAL	variant	UNP P0DTC2
B	142	ASP	GLY	variant	UNP P0DTC2
B	?	-	TYR	deletion	UNP P0DTC2
B	146	GLN	HIS	variant	UNP P0DTC2
B	183	GLU	GLN	variant	UNP P0DTC2
B	213	GLU	VAL	variant	UNP P0DTC2
B	252	VAL	GLY	variant	UNP P0DTC2
B	339	HIS	GLY	variant	UNP P0DTC2
B	346	THR	ARG	variant	UNP P0DTC2
B	368	ILE	LEU	variant	UNP P0DTC2
B	371	PHE	SER	variant	UNP P0DTC2
B	373	PRO	SER	variant	UNP P0DTC2
B	375	PHE	SER	variant	UNP P0DTC2
B	376	ALA	THR	variant	UNP P0DTC2
B	405	ASN	ASP	variant	UNP P0DTC2
B	408	SER	ARG	variant	UNP P0DTC2
B	417	ASN	LYS	variant	UNP P0DTC2
B	440	LYS	ASN	variant	UNP P0DTC2
B	445	PRO	VAL	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	446	SER	GLY	variant	UNP P0DTC2
B	460	LYS	ASN	variant	UNP P0DTC2
B	477	ASN	SER	variant	UNP P0DTC2
B	478	LYS	THR	variant	UNP P0DTC2
B	484	ALA	GLU	variant	UNP P0DTC2
B	486	PRO	PHE	variant	UNP P0DTC2
B	490	SER	PHE	variant	UNP P0DTC2
B	498	ARG	GLN	variant	UNP P0DTC2
B	501	TYR	ASN	variant	UNP P0DTC2
B	505	HIS	TYR	variant	UNP P0DTC2
B	614	GLY	ASP	variant	UNP P0DTC2
B	655	TYR	HIS	variant	UNP P0DTC2
B	679	LYS	ASN	variant	UNP P0DTC2
B	681	HIS	PRO	variant	UNP P0DTC2
B	764	LYS	ASN	variant	UNP P0DTC2
B	796	TYR	ASP	variant	UNP P0DTC2
B	954	HIS	GLN	variant	UNP P0DTC2
B	969	LYS	ASN	variant	UNP P0DTC2
A	22	ILE	THR	variant	UNP P0DTC2
A	?	-	LEU	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	?	-	PRO	deletion	UNP P0DTC2
A	27	SER	ALA	variant	UNP P0DTC2
A	83	ALA	VAL	variant	UNP P0DTC2
A	142	ASP	GLY	variant	UNP P0DTC2
A	?	-	TYR	deletion	UNP P0DTC2
A	146	GLN	HIS	variant	UNP P0DTC2
A	183	GLU	GLN	variant	UNP P0DTC2
A	213	GLU	VAL	variant	UNP P0DTC2
A	252	VAL	GLY	variant	UNP P0DTC2
A	339	HIS	GLY	variant	UNP P0DTC2
A	346	THR	ARG	variant	UNP P0DTC2
A	368	ILE	LEU	variant	UNP P0DTC2
A	371	PHE	SER	variant	UNP P0DTC2
A	373	PRO	SER	variant	UNP P0DTC2
A	375	PHE	SER	variant	UNP P0DTC2
A	376	ALA	THR	variant	UNP P0DTC2
A	405	ASN	ASP	variant	UNP P0DTC2
A	408	SER	ARG	variant	UNP P0DTC2
A	417	ASN	LYS	variant	UNP P0DTC2
A	440	LYS	ASN	variant	UNP P0DTC2
A	445	PRO	VAL	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
A	446	SER	GLY	variant	UNP P0DTC2
A	460	LYS	ASN	variant	UNP P0DTC2
A	477	ASN	SER	variant	UNP P0DTC2
A	478	LYS	THR	variant	UNP P0DTC2
A	484	ALA	GLU	variant	UNP P0DTC2
A	486	PRO	PHE	variant	UNP P0DTC2
A	490	SER	PHE	variant	UNP P0DTC2
A	498	ARG	GLN	variant	UNP P0DTC2
A	501	TYR	ASN	variant	UNP P0DTC2
A	505	HIS	TYR	variant	UNP P0DTC2
A	614	GLY	ASP	variant	UNP P0DTC2
A	655	TYR	HIS	variant	UNP P0DTC2
A	679	LYS	ASN	variant	UNP P0DTC2
A	681	HIS	PRO	variant	UNP P0DTC2
A	764	LYS	ASN	variant	UNP P0DTC2
A	796	TYR	ASP	variant	UNP P0DTC2
A	954	HIS	GLN	variant	UNP P0DTC2
A	969	LYS	ASN	variant	UNP P0DTC2
C	22	ILE	THR	variant	UNP P0DTC2
C	?	-	LEU	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	?	-	PRO	deletion	UNP P0DTC2
C	27	SER	ALA	variant	UNP P0DTC2
C	83	ALA	VAL	variant	UNP P0DTC2
C	142	ASP	GLY	variant	UNP P0DTC2
C	?	-	TYR	deletion	UNP P0DTC2
C	146	GLN	HIS	variant	UNP P0DTC2
C	183	GLU	GLN	variant	UNP P0DTC2
C	213	GLU	VAL	variant	UNP P0DTC2
C	252	VAL	GLY	variant	UNP P0DTC2
C	339	HIS	GLY	variant	UNP P0DTC2
C	346	THR	ARG	variant	UNP P0DTC2
C	368	ILE	LEU	variant	UNP P0DTC2
C	371	PHE	SER	variant	UNP P0DTC2
C	373	PRO	SER	variant	UNP P0DTC2
C	375	PHE	SER	variant	UNP P0DTC2
C	376	ALA	THR	variant	UNP P0DTC2
C	405	ASN	ASP	variant	UNP P0DTC2
C	408	SER	ARG	variant	UNP P0DTC2
C	417	ASN	LYS	variant	UNP P0DTC2
C	440	LYS	ASN	variant	UNP P0DTC2
C	445	PRO	VAL	variant	UNP P0DTC2

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
C	446	SER	GLY	variant	UNP P0DTC2
C	460	LYS	ASN	variant	UNP P0DTC2
C	477	ASN	SER	variant	UNP P0DTC2
C	478	LYS	THR	variant	UNP P0DTC2
C	484	ALA	GLU	variant	UNP P0DTC2
C	486	PRO	PHE	variant	UNP P0DTC2
C	490	SER	PHE	variant	UNP P0DTC2
C	498	ARG	GLN	variant	UNP P0DTC2
C	501	TYR	ASN	variant	UNP P0DTC2
C	505	HIS	TYR	variant	UNP P0DTC2
C	614	GLY	ASP	variant	UNP P0DTC2
C	655	TYR	HIS	variant	UNP P0DTC2
C	679	LYS	ASN	variant	UNP P0DTC2
C	681	HIS	PRO	variant	UNP P0DTC2
C	764	LYS	ASN	variant	UNP P0DTC2
C	796	TYR	ASP	variant	UNP P0DTC2
C	954	HIS	GLN	variant	UNP P0DTC2
C	969	LYS	ASN	variant	UNP P0DTC2

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



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

Continued on next page...

Continued from previous page...

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

Continued on next page...

Continued from previous page...

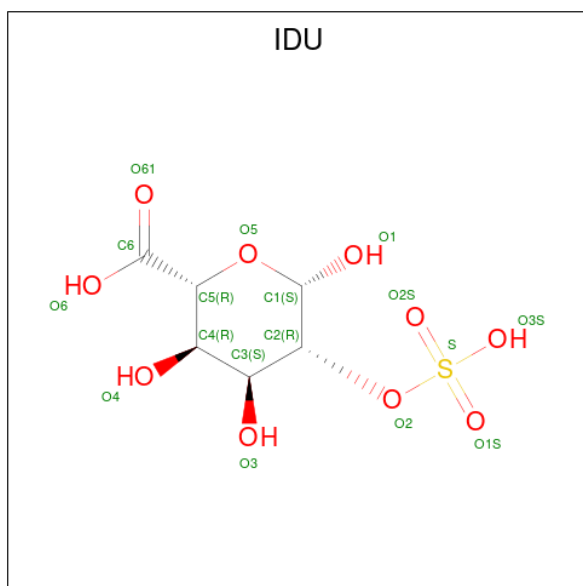
Mol	Chain	Residues	Atoms				AltConf
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	A	1	Total	C	N	O	0
			14	8	1	5	
2	C	1	Total	C	N	O	0
			14	8	1	5	
2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

Continued on next page...

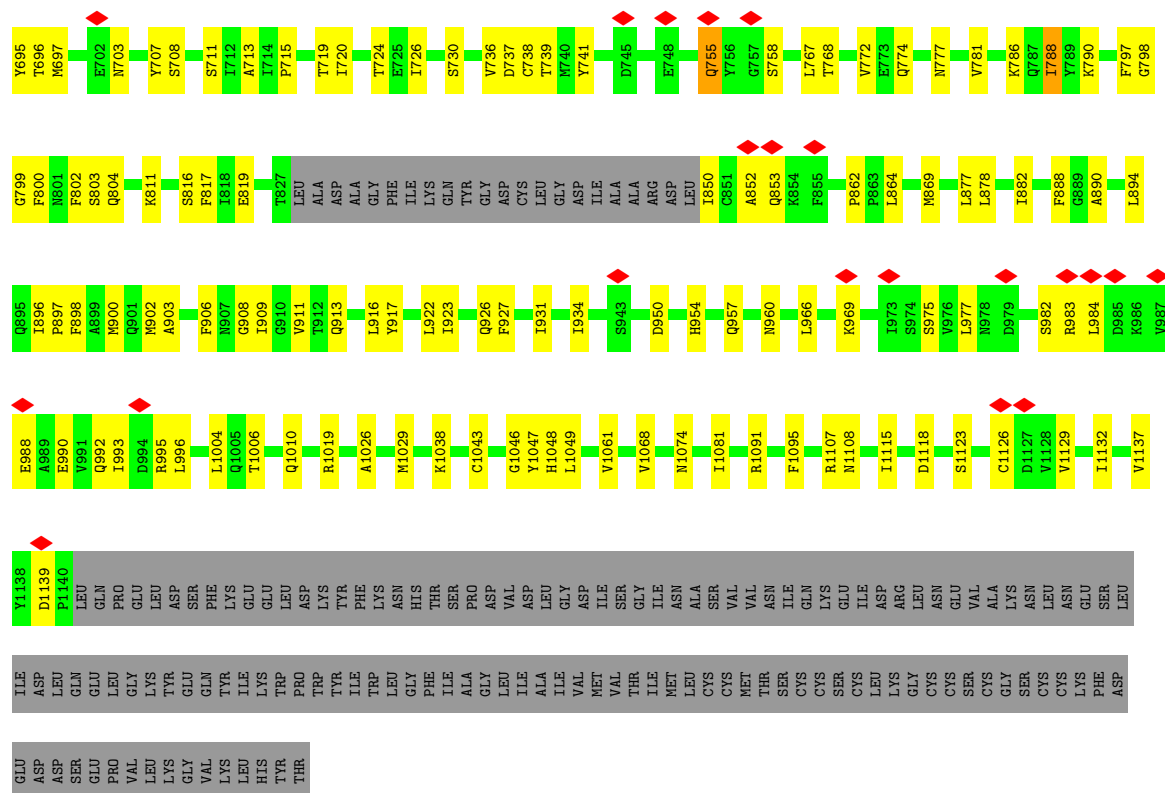
Continued from previous page...

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

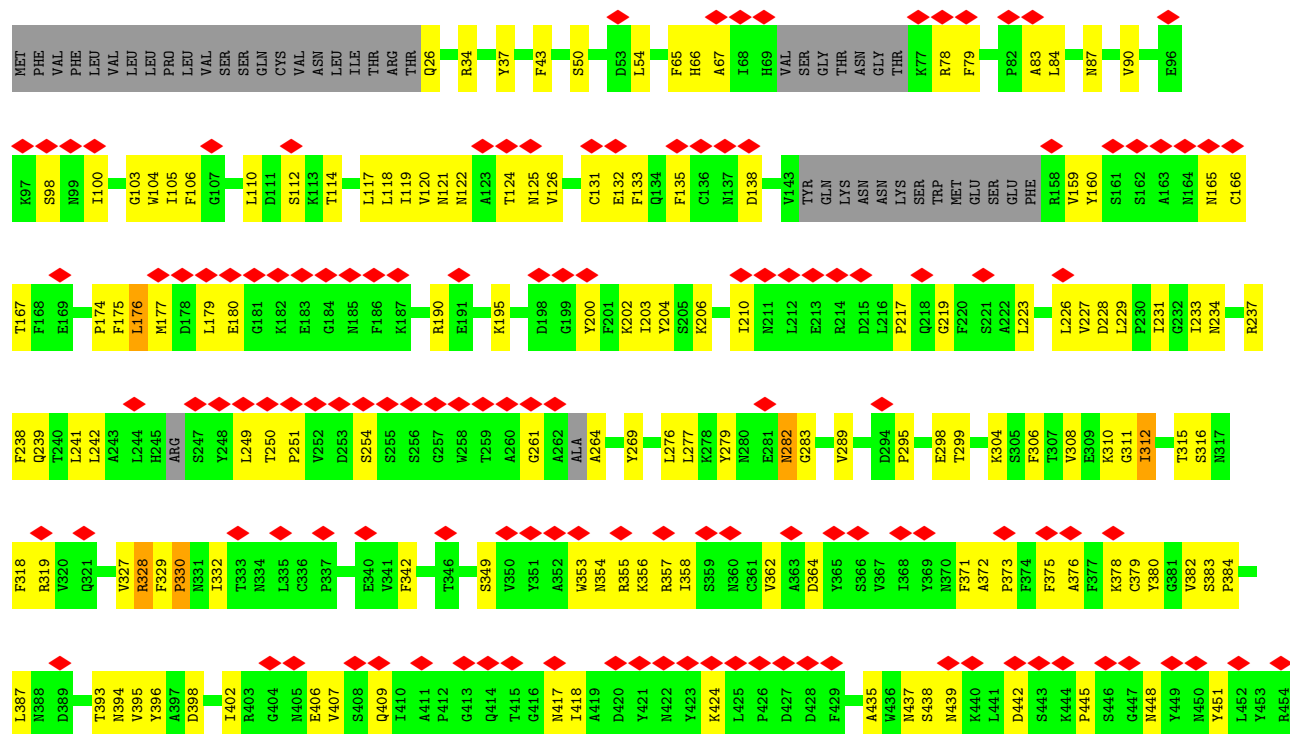
- Molecule 3 is 2-O-sulfo-beta-L-altropyranuronic acid (CCD ID: IDU) (formula: $C_6H_{10}O_{10}S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				AltConf
3	A	1	Total	C	O	S	0
			15	6	8	1	



• Molecule 1: Spike glycoprotein



PHE	THR	G1046	F906	F812	N709	ILE	N544	S469	F392	F318	F220
ILE	SER	Y1047	I909	S813	N710	HIS	G545	T470	T393	R319	S221
ALA	PRO	H1048	I909	K814	I712	ALA	L546	E471	N394		A222
GLY	ASP	L1049	A924	R815	I713	GLN	T547	I472	N405		L223
LEU	VAL	S816	F927	F817	I714	LEU	G548	Y473			L226
ILE	ASP	F1052	N928	I818	T724	THR	V551	Q474	S408		V227
ALA	GLY	S1055	I931	E819	E725	PRO	L552	A475	Q409		D228
VAL	ASP	V1061	I931	N830	I726	THR	T553	G476	I410		I231
VAL	SER	T1076	I934	L821	V635	THR	E554	N477	A411		G232
THR	GLY	Q935	Q935	L822	V635	THR	S555	K478	P412		I233
ILE	ILE	K1086	T827	T827	V636	THR	N556	N479	Q413		H234
MET	ASN	S939	LEU	ALA	S637	THR	K557	C480	Q414		R237
LEU	ALA	S940	ALA	ASP	T638	THR	K558	N481	T415		F238
CYS	SER	T941	ASP	ASP	F559	THR	F559	G482	G416		Q239
CYS	VAL	A942	ALA	ALA	L560	THR	G639	V483	N417		T240
THR	ASN	F1094	GLY	PHE	Q663	THR	Q663	A484	I418		L241
SER	ILE	F1095	GLY	GLY	V642	THR	Q664	G485	A419		L242
SER	ILE	V1096	ILE	ILE	F643	THR	Q644	P486	T345		A243
CYS	GLN	S1097	LYS	LYS	Q644	THR	V651	N487	T346		L244
CYS	LYS	N1098	GLN	GLN	Q644	THR	D661	C488	F347		H245
SER	GLY	G946	TYR	TYR	V651	THR	D662	A489	N343		S247
CYS	ILE	K947	ASP	ASP	D662	THR	D663	S490	A344		Y248
LEU	ASP	L966	CYS	CYS	T664	THR	A570	P491	T345		L249
LYS	ARG	K969	GLY	GLY	P665	THR	D571	L492	Y351		T250
CYS	ASN	A972	LEU	LEU	A672	THR	A575	Q493	R357		P251
CYS	ASN	S975	GLY	ILE	Q669	THR	V576	S494	N360		V252
CYS	ASN	D979	ILE	ALA	C671	THR	R577	T434	C361		D253
LYS	GLY	I980	ALA	ALA	A672	THR	D578	A436	V362		S254
PHE	SER	D1127	ASP	ASP	Q675	THR	F579		D364		S255
ASP	ILE	V1128	LEU	LEU	Q675	THR	Q880	R498	Y365		S256
ASP	ILE	V1129	C851	C851	L763	THR	T581	P499	Y369		G257
ASP	ILE	V1137	A852	A852	K764	THR	L582	T500	N370		W258
ASP	LEU	F1140	Q853	Q853	L767	THR	E883	Y501	F371		T259
GLN	GLN	LEU	K854	K854	I770	SER	L585	G502	A372		A260
PRO	PRO	PRO	F855	F855	D776	SER	D586	V503	P373		G261
VAL	GLY	GLY	T859	T859	K776	ARG	C590	G504	F374		A262
LEU	GLY	LEU	W860	W860	N777	ARG	S591	H505	A264		ALA
LYS	TYR	ASP	L861	L861	V781	VAL	F592	R509	F375		A264
GLY	GLY	SER	L864	L864	V788	ALA	G593	V510	A376		ALA
VAL	GLN	PHE	E868	E868	I788	SER	S596	V511	F377		L276
LYS	TYR	LYS	L878	L878	I794	THR	V597	E516	K378		L276
THR	THR	THR	L878	L878	L794	THR	L598	L517	C379		N280
THR	THR	THR	A890	A890	G798	THR	A609	L518	Y380		N280
THR	THR	THR	L894	L894	G799	THR	Q613	H519	G381		T284
THR	THR	THR	N801	N801	F800	THR	C617	A520	V382		T284
THR	THR	THR	F802	F802	L699	THR	T618	K459	S383		D290
THR	THR	THR	Y904	Y904	S704	THR	GLU	V524	T385		S297
GLY	GLY	GLY	R905	R905	Y707	THR	VAL	C525	K386		S297
					S708	THR	PRO	K528	L387		C301
						THR	VAL	K529	N388		C301
						THR	ALA	N532	D389		K304
						THR		K537	L390		I312
						THR		F541	C391		I312
						THR					N317

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	257757	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	1.838	Depositor
Minimum map value	-1.122	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.057	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	310.80002, 310.80002, 310.80002	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.036, 1.036, 1.036	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: IDU, 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	0.36	0/8345	0.51	0/11349
1	B	0.33	0/8345	0.47	1/11349 (0.0%)
1	C	0.28	0/8345	0.43	0/11349
All	All	0.33	0/25035	0.47	1/34047 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	862	PRO	O-C-N	-5.04	118.78	121.15

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	328	ARG	Sidechain
1	B	158	ARG	Sidechain
1	B	328	ARG	Sidechain

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	8154	0	7959	278	0
1	B	8154	0	7959	278	0
1	C	8154	0	7959	238	0
2	A	224	0	208	2	0
2	B	224	0	208	5	0
2	C	224	0	208	4	0
3	A	15	0	4	0	0
All	All	25149	0	24505	732	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 15.

All (732) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:277:LEU:HD11	1:A:279:TYR:CE1	1.76	1.20
1:A:126:VAL:HG21	1:A:175:PHE:HE2	0.99	1.12
1:A:126:VAL:HG21	1:A:175:PHE:CE2	1.86	1.10
1:B:121:ASN:HD22	1:B:176:LEU:HD23	1.07	1.07
1:B:697:MET:HE2	1:B:697:MET:HA	1.38	1.04
1:B:121:ASN:HD22	1:B:176:LEU:CD2	1.72	1.02
1:A:342:PHE:HD1	1:A:371:PHE:HE1	1.09	0.98
1:C:738:CYS:SG	1:C:753:LEU:HD21	2.06	0.95
1:B:121:ASN:ND2	1:B:176:LEU:CD2	2.31	0.92
1:A:460:LYS:HD3	1:A:461:LEU:H	1.32	0.92
1:A:342:PHE:CD1	1:A:371:PHE:HE1	1.90	0.90
1:B:121:ASN:ND2	1:B:176:LEU:HD23	1.86	0.90
1:A:342:PHE:HD1	1:A:371:PHE:CE1	1.89	0.90
1:B:984:LEU:HD12	1:B:988:GLU:CG	2.03	0.89
1:A:126:VAL:CG2	1:A:175:PHE:HE2	1.87	0.85
1:A:277:LEU:CD1	1:A:279:TYR:CE1	2.58	0.85
1:A:477:ASN:O	1:A:478:LYS:HG3	1.77	0.84
1:B:477:ASN:O	1:B:478:LYS:HG3	1.79	0.82
1:C:106:PHE:HB2	1:C:117:LEU:HB3	1.60	0.82
1:B:560:LEU:H	1:B:563:GLN:HB3	1.46	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:477:ASN:O	1:C:478:LYS:HG3	1.81	0.80
1:B:131:CYS:HA	1:B:166:CYS:HB3	1.63	0.79
1:A:330:PRO:HD3	1:A:544:ASN:HD21	1.47	0.79
1:B:984:LEU:HD12	1:B:988:GLU:HG3	1.65	0.77
1:A:106:PHE:HB2	1:A:117:LEU:HB3	1.66	0.77
1:B:984:LEU:HD12	1:B:988:GLU:HG2	1.65	0.77
1:B:697:MET:HA	1:B:697:MET:CE	2.11	0.76
1:C:448:ASN:HB2	1:C:497:PHE:HB2	1.69	0.75
1:B:909:ILE:HD11	1:B:1047:TYR:HB3	1.68	0.75
1:B:456:PHE:H	1:B:491:PRO:HB3	1.51	0.75
1:B:121:ASN:ND2	1:B:176:LEU:HD22	2.00	0.73
1:B:708:SER:HB3	1:B:711:SER:HB3	1.70	0.73
1:A:780:GLU:OE1	1:A:780:GLU:N	2.19	0.73
1:B:206:LYS:HE2	1:B:221:SER:HB2	1.72	0.72
1:C:821:LEU:HD11	1:C:939:SER:HB2	1.72	0.72
1:A:566:GLY:HA3	1:A:575:ALA:HB3	1.72	0.71
1:C:115:GLN:HA	1:C:132:GLU:HG2	1.72	0.71
1:C:226:LEU:HG	1:C:227:VAL:HG13	1.72	0.71
1:C:442:ASP:O	1:C:448:ASN:ND2	2.24	0.71
1:C:724:THR:HG22	1:C:934:ILE:HD11	1.72	0.71
1:B:448:ASN:HB2	1:B:497:PHE:HB2	1.71	0.70
1:B:570:ALA:HB2	1:A:852:ALA:HB1	1.73	0.70
1:B:852:ALA:HB1	1:C:570:ALA:HB2	1.74	0.70
1:A:112:SER:HA	1:A:132:GLU:HG2	1.73	0.70
1:C:697:MET:HE2	1:C:697:MET:HA	1.73	0.70
1:A:442:ASP:O	1:A:448:ASN:ND2	2.25	0.70
1:B:100:ILE:HG22	1:B:242:LEU:HD12	1.73	0.69
1:A:277:LEU:HD11	1:A:279:TYR:HE1	1.47	0.69
1:B:124:THR:HB	2:B:1302:NAG:H62	1.75	0.69
1:B:419:ALA:O	1:B:424:LYS:NZ	2.26	0.69
1:C:189:LEU:HD22	1:C:210:ILE:HG12	1.75	0.69
1:A:456:PHE:H	1:A:491:PRO:HB3	1.57	0.68
1:A:318:PHE:HB3	1:A:593:GLY:HA3	1.75	0.68
1:B:580:GLN:HB3	2:B:1306:NAG:H82	1.76	0.68
1:A:806:LEU:HD23	1:A:878:LEU:HD23	1.76	0.67
1:B:878:LEU:O	1:B:882:ILE:HD12	1.94	0.67
1:A:118:LEU:HD21	1:A:120:VAL:HG23	1.74	0.67
1:C:81:ASN:HB3	1:C:138:ASP:HB2	1.76	0.67
1:A:354:ASN:O	1:A:356:LYS:NZ	2.27	0.67
1:C:67:ALA:HA	1:C:264:ALA:HB2	1.76	0.67
1:B:402:ILE:HG21	1:B:418:ILE:HD11	1.77	0.67

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:CYS:HB3	1:A:384:PRO:HG3	1.75	0.67
1:C:330:PRO:HB2	1:C:332:ILE:HG12	1.77	0.67
1:A:1094:VAL:N	1:A:1105:THR:O	2.27	0.66
1:C:391:CYS:HA	1:C:525:CYS:HB3	1.77	0.66
1:A:435:ALA:HB2	1:A:510:VAL:HG13	1.77	0.66
1:A:643:PHE:HD1	1:A:644:GLN:H	1.40	0.66
1:A:490:SER:O	1:A:493:GLN:NE2	2.29	0.66
1:C:330:PRO:HD3	1:C:544:ASN:HD21	1.61	0.66
1:B:1126:CYS:HB2	1:B:1132:ILE:HG21	1.78	0.66
1:C:139:PRO:HB3	1:C:159:VAL:HA	1.77	0.66
1:C:924:ALA:O	1:C:928:ASN:ND2	2.29	0.66
1:A:448:ASN:HB2	1:A:497:PHE:HB2	1.78	0.65
1:C:419:ALA:O	1:C:424:LYS:NZ	2.30	0.65
1:B:106:PHE:HB2	1:B:117:LEU:HB3	1.77	0.65
1:A:100:ILE:HG22	1:A:242:LEU:HD12	1.79	0.65
1:B:358:ILE:HB	1:B:395:VAL:HG13	1.79	0.65
1:B:703:ASN:HD22	1:A:787:GLN:HE21	1.44	0.65
1:A:591:SER:OG	1:A:634:ARG:NH2	2.30	0.65
1:B:984:LEU:HD22	1:C:381:GLY:O	1.97	0.65
1:B:566:GLY:HA3	1:B:575:ALA:HB3	1.80	0.64
1:B:917:TYR:HB3	1:C:1129:VAL:HG23	1.80	0.64
1:B:289:VAL:HG23	1:B:306:PHE:HE1	1.63	0.64
1:C:969:LYS:HZ1	1:C:975:SER:H	1.46	0.64
1:C:516:GLU:OE2	1:C:516:GLU:N	2.31	0.64
1:A:598:ILE:HB	1:A:609:ALA:HB3	1.78	0.63
1:B:697:MET:HE2	1:B:697:MET:CA	2.24	0.63
1:A:457:ARG:HH12	1:A:461:LEU:HD13	1.62	0.63
1:A:78:ARG:HE	1:A:261:GLY:HA3	1.63	0.63
1:C:710:ASN:ND2	1:C:1076:THR:OG1	2.31	0.63
1:B:560:LEU:HB2	1:B:563:GLN:HB2	1.80	0.63
1:C:212:LEU:HD12	1:C:214:ARG:H	1.63	0.63
1:B:98:SER:HA	1:B:180:GLU:H	1.63	0.63
1:A:731:MET:H	1:A:774:GLN:HE21	1.47	0.63
1:A:457:ARG:HH22	1:A:461:LEU:HB2	1.64	0.63
1:A:574:ASP:O	1:A:587:ILE:N	2.30	0.62
1:C:102:ARG:HE	1:C:243:ALA:HB3	1.64	0.62
1:A:358:ILE:HB	1:A:395:VAL:HG23	1.80	0.62
1:C:492:LEU:HD12	1:C:492:LEU:O	1.98	0.62
1:B:353:TRP:CZ2	1:B:466:ARG:HD2	2.33	0.62
1:C:34:ARG:NH1	1:C:219:GLY:O	2.32	0.62
1:B:404:GLY:HA2	1:B:508:TYR:HE1	1.64	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:LEU:HD23	1:A:119:ILE:N	2.14	0.62
1:A:383:SER:N	1:C:983:ARG:O	2.32	0.62
1:A:560:LEU:H	1:A:563:GLN:HB3	1.63	0.62
1:A:555:SER:HB2	1:A:584:ILE:HB	1.81	0.62
1:A:249:LEU:HG	1:A:251:PRO:HD2	1.81	0.62
1:B:376:ALA:HB3	1:B:435:ALA:HB3	1.82	0.62
1:B:755:GLN:OE1	1:C:969:LYS:HB2	2.00	0.62
1:B:1123:SER:OG	1:A:914:ASN:ND2	2.32	0.62
1:A:357:ARG:NH1	1:A:396:TYR:OH	2.33	0.61
1:A:1046:GLY:HA2	1:C:890:ALA:HA	1.82	0.61
1:A:104:TRP:O	1:A:105:ILE:HD13	2.01	0.61
1:A:460:LYS:HD3	1:A:461:LEU:N	2.09	0.61
1:B:908:GLY:O	1:B:1038:LYS:NZ	2.26	0.61
1:C:261:GLY:O	1:C:262:ALA:C	2.43	0.61
1:B:29:THR:HG23	1:B:62:VAL:HG23	1.83	0.61
1:B:909:ILE:HG23	1:B:911:VAL:HG23	1.83	0.61
1:A:34:ARG:HH22	1:A:217:PRO:HB2	1.66	0.60
1:B:442:ASP:O	1:B:448:ASN:ND2	2.34	0.60
1:B:409:GLN:O	1:B:414:GLN:NE2	2.34	0.60
1:B:673:SER:HB3	1:B:695:TYR:HE2	1.66	0.60
1:B:897:PRO:HA	1:C:707:TYR:CE1	2.37	0.60
1:B:433:VAL:HG22	1:B:512:VAL:HG23	1.83	0.60
1:B:696:THR:O	1:B:697:MET:HE2	2.01	0.60
1:A:643:PHE:HE2	1:A:655:TYR:CG	2.20	0.60
1:C:159:VAL:HG13	1:C:160:TYR:HD1	1.67	0.60
1:B:247:SER:O	1:B:248:TYR:HB3	2.02	0.60
1:A:804:GLN:NE2	1:A:935:GLN:OE1	2.33	0.60
1:C:477:ASN:O	1:C:478:LYS:CG	2.49	0.59
1:B:289:VAL:HG23	1:B:306:PHE:CE1	2.37	0.59
1:B:992:GLN:HE21	1:B:995:ARG:HH21	1.49	0.59
1:C:204:TYR:HB3	1:C:223:LEU:HG	1.82	0.59
1:A:237:ARG:NH1	1:A:239:GLN:OE1	2.35	0.59
1:A:780:GLU:H	1:A:780:GLU:CD	2.10	0.59
1:C:200:TYR:HB3	1:C:202:LYS:HE2	1.85	0.59
1:C:566:GLY:HA3	1:C:575:ALA:HB3	1.84	0.59
1:A:1041:ASP:OD1	1:A:1041:ASP:O	2.19	0.59
1:B:473:TYR:O	1:B:474:GLN:NE2	2.35	0.59
1:B:488:CYS:O	1:B:489:TYR:C	2.46	0.59
1:A:316:SER:O	1:A:595:VAL:HG12	2.02	0.59
1:B:1107:ARG:HD2	1:A:904:TYR:CE2	2.38	0.59
1:B:558:LYS:HG3	1:A:282:ASN:HA	1.84	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:ILE:HD11	1:A:1012:LEU:HD23	1.85	0.58
1:B:406:GLU:HB3	1:B:418:ILE:HD12	1.85	0.58
1:A:439:ASN:ND2	1:A:506:GLN:OE1	2.36	0.58
1:A:1115:ILE:HG22	1:A:1137:VAL:HG23	1.85	0.58
1:C:318:PHE:HZ	1:C:635:VAL:HA	1.68	0.58
1:B:897:PRO:HA	1:C:707:TYR:HE1	1.66	0.58
1:A:477:ASN:O	1:A:478:LYS:CG	2.47	0.58
1:C:523:THR:HG22	1:C:524:VAL:HG13	1.85	0.58
1:B:78:ARG:HH11	1:B:261:GLY:HA3	1.68	0.58
1:A:729:VAL:O	1:A:777:ASN:ND2	2.36	0.58
1:C:966:LEU:O	1:C:975:SER:OG	2.20	0.58
1:B:663:ASP:OD1	1:B:663:ASP:N	2.35	0.58
1:A:315:THR:HG22	1:A:316:SER:H	1.68	0.58
1:A:457:ARG:NE	1:A:459:SER:O	2.37	0.58
1:B:502:GLY:O	1:B:506:GLN:NE2	2.36	0.57
1:B:724:THR:HG23	1:B:934:ILE:HD11	1.86	0.57
1:B:903:ALA:HB1	1:B:913:GLN:HG3	1.85	0.57
1:C:391:CYS:SG	1:C:544:ASN:ND2	2.75	0.57
1:C:564:GLN:HB2	1:C:577:ARG:HG2	1.86	0.57
1:B:139:PRO:HB2	1:B:241:LEU:HD21	1.86	0.57
1:A:617:CYS:N	1:A:644:GLN:OE1	2.37	0.57
1:A:896:ILE:HD11	1:A:900:MET:HG2	1.87	0.57
1:B:477:ASN:O	1:B:478:LYS:CG	2.48	0.57
1:B:439:ASN:ND2	1:B:506:GLN:OE1	2.37	0.57
1:A:564:GLN:HG2	1:A:565:PHE:HD1	1.69	0.57
1:A:990:GLU:HA	1:A:993:ILE:HG22	1.86	0.57
1:A:37:TYR:HB3	1:A:223:LEU:HD23	1.86	0.57
1:A:724:THR:CG2	1:A:725:GLU:N	2.68	0.57
1:C:98:SER:HA	1:C:180:GLU:H	1.69	0.57
1:C:379:CYS:HB3	1:C:384:PRO:HG3	1.87	0.57
1:C:726:ILE:HD11	1:C:947:LYS:HB3	1.87	0.57
1:A:731:MET:HG2	1:A:774:GLN:NE2	2.20	0.57
1:C:770:ILE:HD12	1:C:1015:ALA:HB2	1.87	0.57
1:C:488:CYS:O	1:C:489:TYR:C	2.48	0.57
1:B:328:ARG:HD2	1:B:580:GLN:HG3	1.86	0.57
1:A:1077:THR:OG1	1:A:1078:ALA:N	2.38	0.56
1:C:190:ARG:HH11	1:C:207:HIS:HD2	1.52	0.56
1:B:117:LEU:HA	1:B:130:VAL:HA	1.87	0.56
1:A:226:LEU:HG	1:A:227:VAL:HG12	1.86	0.56
1:A:973:ILE:HD11	1:A:980:ILE:HG13	1.86	0.56
1:B:69:HIS:HB2	1:B:77:LYS:HD2	1.88	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:758:SER:O	1:B:758:SER:OG	2.21	0.56
1:B:738:CYS:SG	1:B:739:THR:N	2.79	0.56
1:A:445:PRO:O	1:A:498:ARG:NH1	2.39	0.56
1:B:555:SER:HB2	1:B:584:ILE:HB	1.88	0.56
1:A:708:SER:HB3	1:A:711:SER:HB3	1.87	0.56
1:C:343:ASN:HB3	1:C:371:PHE:HZ	1.69	0.56
1:A:250:THR:O	1:A:254:SER:OG	2.20	0.56
1:C:133:PHE:HB2	1:C:135:PHE:CZ	2.40	0.56
1:A:550:GLY:HA3	1:A:589:PRO:HA	1.88	0.55
1:C:212:LEU:HD21	1:C:217:PRO:HB3	1.88	0.55
1:C:473:TYR:O	1:C:474:GLN:NE2	2.39	0.55
1:C:735:SER:HG	1:C:859:THR:HG1	1.46	0.55
1:C:817:PHE:CE2	1:C:935:GLN:HG3	2.41	0.55
1:B:435:ALA:HB2	1:B:510:VAL:HG13	1.87	0.55
1:B:445:PRO:O	1:B:498:ARG:NH1	2.40	0.55
1:A:712:ILE:HD13	1:A:1094:VAL:HG11	1.89	0.55
1:B:210:ILE:HD13	1:B:217:PRO:HG3	1.88	0.55
1:B:487:ASN:HA	1:B:489:TYR:CE1	2.41	0.55
1:C:708:SER:HB3	1:C:711:SER:HB3	1.88	0.55
1:A:488:CYS:O	1:A:489:TYR:C	2.49	0.55
1:C:726:ILE:HG22	1:C:1061:VAL:HG13	1.89	0.55
1:C:456:PHE:H	1:C:491:PRO:HB3	1.71	0.55
1:B:327:VAL:HB	1:B:528:LYS:HD2	1.88	0.55
1:A:904:TYR:HE1	1:A:913:GLN:HE22	1.53	0.55
1:A:735:SER:HG	1:A:859:THR:HG1	1.50	0.55
1:C:553:THR:HB	1:C:586:ASP:HB3	1.88	0.55
1:B:720:ILE:H	1:B:926:GLN:NE2	2.05	0.54
1:A:282:ASN:N	1:A:282:ASN:OD1	2.40	0.54
1:C:758:SER:O	1:C:758:SER:OG	2.21	0.54
1:A:206:LYS:HB2	1:A:223:LEU:HD12	1.90	0.54
1:A:719:THR:HA	1:A:926:GLN:HE22	1.72	0.54
1:B:416:GLY:H	1:B:419:ALA:HB3	1.71	0.54
1:A:289:VAL:HB	1:A:306:PHE:CE1	2.42	0.54
1:B:353:TRP:CH2	1:B:466:ARG:HA	2.43	0.54
1:B:647:ALA:HA	1:A:862:PRO:HG3	1.89	0.54
1:A:104:TRP:C	1:A:105:ILE:HD13	2.33	0.54
1:A:707:TYR:HE1	1:C:897:PRO:HA	1.72	0.54
1:A:741:TYR:CD2	1:A:1004:LEU:HD22	2.42	0.54
1:A:1116:THR:HG22	1:A:1118:ASP:H	1.73	0.54
1:C:124:THR:HB	2:C:1302:NAG:H62	1.90	0.54
1:C:318:PHE:HB2	1:C:593:GLY:HA3	1.89	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:360:ASN:H	1:C:523:THR:HG23	1.73	0.54
1:B:755:GLN:HG3	1:C:969:LYS:O	2.07	0.53
1:A:329:PHE:HB3	1:A:330:PRO:CD	2.38	0.53
1:A:311:GLY:HA2	1:A:664:ILE:HG23	1.91	0.53
1:C:393:THR:OG1	1:C:516:GLU:O	2.20	0.53
1:B:78:ARG:HD2	1:B:261:GLY:HA3	1.91	0.53
1:B:318:PHE:HZ	1:B:635:VAL:HA	1.72	0.53
1:A:906:PHE:HE1	1:A:1049:LEU:HD11	1.73	0.53
1:B:662:CYS:HB2	1:B:697:MET:SD	2.49	0.53
1:B:707:TYR:HE1	1:A:897:PRO:HA	1.73	0.53
1:B:1043:CYS:HB3	1:B:1048:HIS:CD2	2.43	0.53
1:A:310:LYS:HE2	1:A:664:ILE:HD11	1.90	0.53
1:A:731:MET:H	1:A:774:GLN:NE2	2.07	0.53
1:C:906:PHE:HE1	1:C:1049:LEU:HD11	1.74	0.53
1:B:206:LYS:HE2	1:B:221:SER:CB	2.38	0.53
1:B:890:ALA:HA	1:C:1046:GLY:HA2	1.90	0.53
1:C:329:PHE:HB3	1:C:330:PRO:CD	2.38	0.53
1:A:67:ALA:HA	1:A:264:ALA:HB2	1.91	0.53
1:C:617:CYS:HA	1:C:633:TRP:HB2	1.91	0.53
1:B:386:LYS:O	1:B:390:LEU:HD21	2.09	0.53
1:A:200:TYR:O	1:A:202:LYS:HG3	2.08	0.53
1:A:553:THR:HB	1:A:586:ASP:HB2	1.91	0.53
1:A:851:CYS:O	1:A:855:PHE:CE2	2.62	0.53
1:C:487:ASN:HA	1:C:489:TYR:CE2	2.44	0.53
1:C:591:SER:O	1:C:634:ARG:NH2	2.32	0.53
1:C:596:SER:HB2	1:C:613:GLN:HE22	1.74	0.53
1:B:249:LEU:HG	1:B:251:PRO:HG2	1.91	0.52
1:C:374:PHE:HD1	1:C:436:TRP:HB3	1.74	0.52
1:B:523:THR:HG22	1:B:524:VAL:HG12	1.90	0.52
1:C:128:ILE:HB	1:C:170:TYR:HB3	1.91	0.52
1:B:226:LEU:HG	1:B:227:VAL:HG13	1.92	0.52
1:A:175:PHE:HE1	1:A:203:ILE:HD11	1.75	0.52
1:B:984:LEU:CD1	1:B:988:GLU:HG3	2.36	0.52
1:A:1026:ALA:O	1:A:1030:SER:OG	2.21	0.52
1:C:456:PHE:HB3	1:C:473:TYR:HE2	1.73	0.52
1:B:1006:THR:HG21	1:A:762:GLN:HE22	1.73	0.52
1:B:804:GLN:HA	1:B:817:PHE:CD2	2.44	0.52
1:B:252:VAL:O	1:B:253:ASP:C	2.53	0.52
1:B:437:ASN:HA	1:B:508:TYR:HD2	1.73	0.52
1:C:37:TYR:HB3	1:C:223:LEU:HB3	1.92	0.52
1:C:344:ALA:HB3	1:C:347:PHE:HE1	1.75	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:798:GLY:C	1:C:800:PHE:H	2.17	0.52
1:B:483:VAL:O	1:B:484:ALA:C	2.53	0.52
1:B:1107:ARG:HG2	1:A:904:TYR:HE2	1.75	0.52
1:C:357:ARG:NE	1:C:357:ARG:O	2.43	0.52
1:C:435:ALA:HB2	1:C:510:VAL:HG13	1.92	0.52
1:A:277:LEU:C	1:A:277:LEU:HD12	2.35	0.51
1:A:644:GLN:HE21	2:A:1309:NAG:H82	1.75	0.51
1:A:103:GLY:HA3	1:A:241:LEU:HB2	1.91	0.51
1:C:40:ASP:N	1:C:40:ASP:OD1	2.41	0.51
1:C:931:ILE:O	1:C:934:ILE:HG22	2.10	0.51
1:A:118:LEU:HD23	1:A:118:LEU:C	2.36	0.51
1:B:34:ARG:NH1	1:B:219:GLY:O	2.44	0.51
1:C:767:LEU:HD21	1:C:1008:VAL:HG22	1.91	0.51
1:B:906:PHE:HE1	1:B:1049:LEU:HD11	1.76	0.51
1:A:79:PHE:CE2	1:A:138:ASP:HB2	2.46	0.51
1:C:822:LEU:HD23	1:C:945:LEU:HD11	1.93	0.51
1:C:909:ILE:HG21	1:C:1047:TYR:HB3	1.90	0.51
1:B:1091:ARG:NH1	1:B:1118:ASP:O	2.44	0.51
1:A:312:ILE:HG23	1:A:596:SER:OG	2.11	0.51
1:A:487:ASN:HA	1:A:489:TYR:CE2	2.46	0.51
1:A:574:ASP:HA	1:A:587:ILE:HB	1.93	0.51
1:C:312:ILE:HG23	1:C:596:SER:OG	2.11	0.51
1:A:78:ARG:HH21	1:A:261:GLY:HA3	1.77	0.50
1:A:724:THR:HG22	1:A:725:GLU:N	2.25	0.50
1:C:364:ASP:N	1:C:364:ASP:OD1	2.44	0.50
1:B:982:SER:HA	1:C:386:LYS:HE2	1.93	0.50
1:C:421:TYR:HD1	1:C:460:LYS:HA	1.76	0.50
1:B:280:ASN:OD1	1:B:284:THR:N	2.45	0.50
1:A:78:ARG:HB3	1:A:261:GLY:C	2.37	0.50
1:B:43:PHE:N	1:C:565:PHE:O	2.41	0.50
1:A:175:PHE:H	1:A:175:PHE:HD2	1.60	0.50
1:A:502:GLY:O	1:A:506:GLN:NE2	2.45	0.50
1:B:96:GLU:O	1:B:190:ARG:NH2	2.36	0.50
1:B:204:TYR:HB3	1:B:223:LEU:HG	1.94	0.50
1:B:911:VAL:HG22	1:B:1108:ASN:HB2	1.92	0.50
1:A:437:ASN:HB3	1:A:508:TYR:CZ	2.47	0.50
1:C:301:CYS:O	1:C:304:LYS:NZ	2.44	0.50
1:B:87:ASN:N	1:B:87:ASN:OD1	2.45	0.50
1:B:877:LEU:HD23	1:B:888:PHE:HE2	1.77	0.50
1:A:328:ARG:CG	1:A:579:PRO:HD2	2.42	0.50
1:C:327:VAL:HG21	1:C:528:LYS:HD3	1.93	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:761:THR:O	1:A:765:ARG:HB2	2.12	0.50
1:A:909:ILE:HG21	1:A:1047:TYR:HB3	1.93	0.50
1:A:393:THR:OG1	1:A:394:ASN:OD1	2.28	0.49
1:A:642:VAL:HG22	1:A:651:ILE:HG22	1.93	0.49
1:A:822:LEU:HD21	1:A:938:LEU:HD21	1.94	0.49
1:A:916:LEU:HD12	1:A:923:ILE:HG13	1.93	0.49
1:A:1006:THR:HG21	1:C:762:GLN:HE22	1.76	0.49
1:B:250:THR:N	1:B:251:PRO:HD2	2.27	0.49
1:B:708:SER:HB3	1:B:711:SER:CB	2.41	0.49
1:A:589:PRO:HD2	1:C:855:PHE:CE1	2.48	0.49
1:B:741:TYR:CD2	1:B:1004:LEU:HD22	2.48	0.49
1:A:327:VAL:HG11	1:A:528:LYS:HG2	1.93	0.49
1:A:394:ASN:OD1	1:A:394:ASN:N	2.45	0.49
1:C:815:ARG:HB2	1:C:819:GLU:HB2	1.94	0.49
1:B:565:PHE:O	1:A:43:PHE:HB3	2.13	0.49
1:C:79:PHE:HB2	1:C:258:TRP:CE3	2.47	0.49
1:B:505:HIS:CE1	1:A:503:VAL:HG11	2.48	0.49
1:B:737:ASP:OD2	1:C:317:ASN:ND2	2.46	0.49
1:B:781:VAL:HG22	1:B:1026:ALA:HB2	1.95	0.49
1:A:977:LEU:O	1:A:980:ILE:HG22	2.13	0.49
1:C:190:ARG:HD2	1:C:207:HIS:CD2	2.48	0.49
1:C:1105:THR:HG22	1:C:1112:PRO:HA	1.94	0.49
1:B:311:GLY:HA2	1:B:664:ILE:HG22	1.95	0.49
1:B:741:TYR:CE1	1:B:966:LEU:HD11	2.48	0.49
1:A:643:PHE:HD1	1:A:644:GLN:N	2.08	0.49
1:C:598:ILE:HB	1:C:609:ALA:HB3	1.95	0.49
1:B:330:PRO:O	1:B:331:ASN:HB2	2.12	0.49
1:B:724:THR:CG2	1:B:934:ILE:HD11	2.42	0.49
1:A:724:THR:HG23	1:A:1061:VAL:HG13	1.95	0.49
1:B:343:ASN:HB3	1:B:371:PHE:HZ	1.78	0.48
1:B:797:PHE:O	1:B:799:GLY:N	2.46	0.48
1:A:665:PRO:HB3	1:C:864:LEU:HD11	1.95	0.48
1:C:104:TRP:HB2	1:C:119:ILE:HB	1.94	0.48
1:B:249:LEU:HB3	1:B:252:VAL:HG22	1.96	0.48
1:B:1139:ASP:OD1	1:B:1139:ASP:N	2.39	0.48
1:A:409:GLN:OE1	1:A:417:ASN:N	2.46	0.48
1:C:560:LEU:H	1:C:563:GLN:HB3	1.78	0.48
1:B:138:ASP:OD1	1:B:138:ASP:N	2.47	0.48
1:B:1126:CYS:HB3	1:B:1132:ILE:HD13	1.95	0.48
1:A:881:THR:HA	1:A:885:GLY:O	2.13	0.48
1:B:48:LEU:HB3	1:B:276:LEU:HD11	1.95	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:715:PRO:HD3	1:A:894:LEU:HD13	1.96	0.48
1:A:822:LEU:HD22	1:A:945:LEU:HD11	1.95	0.48
1:C:372:ALA:N	1:C:373:PRO:HD2	2.28	0.48
1:B:977:LEU:HD21	1:B:996:LEU:HD22	1.95	0.48
1:B:343:ASN:HB3	1:B:371:PHE:CZ	2.48	0.48
1:B:1115:ILE:HG22	1:B:1137:VAL:HG13	1.96	0.48
1:A:330:PRO:CD	1:A:544:ASN:HD21	2.22	0.48
1:A:713:ALA:HB3	1:C:894:LEU:HB3	1.95	0.48
1:C:735:SER:HB3	1:C:861:LEU:HD11	1.96	0.48
1:B:37:TYR:HA	1:B:223:LEU:HB3	1.95	0.48
1:A:233:ILE:HG12	1:A:234:ASN:H	1.79	0.48
1:C:738:CYS:SG	1:C:753:LEU:CD2	2.94	0.48
1:B:657:ASN:OD1	2:B:1310:NAG:N2	2.47	0.48
1:A:487:ASN:HA	1:A:489:TYR:CZ	2.49	0.48
1:A:560:LEU:HB2	1:A:563:GLN:HB2	1.96	0.48
1:A:805:ILE:HD12	1:A:878:LEU:HD11	1.96	0.48
1:C:378:LYS:HD3	1:C:380:TYR:CZ	2.48	0.48
1:B:736:VAL:HG22	1:B:767:LEU:HD12	1.96	0.48
1:A:98:SER:HA	1:A:179:LEU:HB2	1.95	0.48
1:A:372:ALA:N	1:A:373:PRO:HD2	2.29	0.48
1:A:856:ASN:HD22	1:A:966:LEU:HD12	1.79	0.48
1:A:858:LEU:HD22	1:A:959:LEU:HD22	1.95	0.48
1:B:80:ASP:HA	1:B:260:ALA:HA	1.95	0.47
1:B:617:CYS:SG	1:B:635:VAL:HG21	2.54	0.47
1:B:864:LEU:HD22	1:C:665:PRO:HB3	1.96	0.47
1:A:537:LYS:HA	1:A:537:LYS:HD3	1.58	0.47
1:A:552:LEU:HD12	1:A:585:LEU:HB3	1.96	0.47
1:C:477:ASN:C	1:C:478:LYS:HG3	2.38	0.47
1:B:50:SER:HA	1:B:276:LEU:HA	1.96	0.47
1:B:1081:ILE:HG13	1:B:1095:PHE:CD2	2.49	0.47
1:C:318:PHE:CZ	1:C:635:VAL:HA	2.48	0.47
1:B:200:TYR:O	1:B:202:LYS:HG3	2.13	0.47
1:B:421:TYR:O	1:B:457:ARG:NH1	2.35	0.47
1:A:175:PHE:N	1:A:175:PHE:CD2	2.82	0.47
1:A:733:LYS:HD2	1:A:771:ALA:HB1	1.95	0.47
1:C:280:ASN:OD1	1:C:284:THR:N	2.46	0.47
1:A:125:ASN:HA	1:A:174:PRO:HD3	1.95	0.47
1:C:714:ILE:HD11	1:C:1094:VAL:HG21	1.97	0.47
1:A:114:THR:O	1:A:132:GLU:HG3	2.14	0.47
1:C:131:CYS:HB3	1:C:166:CYS:HB3	1.74	0.47
1:C:742:ILE:HD11	1:C:1004:LEU:HD12	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:VAL:HG21	1:B:238:PHE:CZ	2.49	0.47
1:A:50:SER:HA	1:A:276:LEU:HA	1.95	0.47
1:A:662:CYS:HB2	1:A:697:MET:HE3	1.96	0.47
1:A:663:ASP:OD1	1:A:663:ASP:N	2.47	0.47
1:A:1043:CYS:HB3	1:A:1048:HIS:CD2	2.49	0.47
1:C:330:PRO:HD3	1:C:544:ASN:ND2	2.30	0.47
1:C:777:ASN:O	1:C:781:VAL:HG23	2.15	0.47
1:B:233:ILE:HD13	1:B:235:ILE:HD11	1.96	0.47
1:C:664:ILE:O	1:C:664:ILE:HG13	2.14	0.47
1:B:797:PHE:O	1:B:800:PHE:HD1	1.98	0.47
1:A:1094:VAL:HG22	1:C:904:TYR:OH	2.15	0.47
1:C:1097:SER:HB2	1:C:1102:TRP:CD2	2.50	0.47
1:B:113:LYS:HB3	1:B:113:LYS:HE3	1.78	0.47
1:C:560:LEU:HB2	1:C:563:GLN:HB2	1.97	0.47
1:B:106:PHE:HB3	1:B:235:ILE:HD12	1.96	0.46
1:B:328:ARG:HG2	1:B:579:PRO:HD2	1.98	0.46
1:B:730:SER:HB2	1:B:774:GLN:HG3	1.98	0.46
1:A:467:ASP:N	1:A:467:ASP:OD1	2.47	0.46
1:C:474:GLN:HE22	1:C:482:GLY:H	1.62	0.46
1:C:665:PRO:HA	1:C:671:CYS:SG	2.55	0.46
1:B:477:ASN:C	1:B:478:LYS:HG3	2.39	0.46
1:B:517:LEU:HD12	1:A:983:ARG:HD3	1.96	0.46
1:C:434:ILE:HB	1:C:511:VAL:HG23	1.97	0.46
1:B:79:PHE:HB2	1:B:258:TRP:HB3	1.96	0.46
1:A:713:ALA:HA	1:A:1074:ASN:HA	1.97	0.46
1:A:722:VAL:HG22	1:A:1065:VAL:HG22	1.97	0.46
1:A:741:TYR:CE1	1:A:966:LEU:HD21	2.50	0.46
1:A:1082:CYS:HB2	1:A:1132:ILE:HG12	1.97	0.46
1:B:129:LYS:HB3	1:B:131:CYS:SG	2.55	0.46
1:B:983:ARG:HD3	1:C:517:LEU:HD12	1.97	0.46
1:C:330:PRO:CD	1:C:544:ASN:HD21	2.27	0.46
1:A:50:SER:HB2	1:A:276:LEU:HD12	1.96	0.46
1:A:781:VAL:O	1:A:1029:MET:HG2	2.16	0.46
1:B:36:VAL:HG11	1:B:220:PHE:HZ	1.81	0.46
1:B:442:ASP:HB2	1:B:509:ARG:HH21	1.80	0.46
1:B:605:SER:OG	1:B:606:ASN:N	2.49	0.46
1:B:950:ASP:O	1:B:954:HIS:HB2	2.15	0.46
1:A:402:ILE:HD11	1:A:510:VAL:HG21	1.96	0.46
1:C:249:LEU:HG	1:C:251:PRO:HD2	1.97	0.46
1:C:537:LYS:C	1:C:551:VAL:HG12	2.41	0.46
1:A:970:PHE:HE1	1:C:756:TYR:HA	1.81	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1009:THR:O	1:A:1013:ILE:HD12	2.15	0.46
1:C:190:ARG:HH11	1:C:207:HIS:CD2	2.32	0.46
1:C:662:CYS:SG	1:C:697:MET:HE1	2.56	0.46
1:A:210:ILE:HG21	1:A:217:PRO:HG2	1.97	0.46
1:C:77:LYS:HG3	1:C:78:ARG:HG2	1.97	0.46
1:C:726:ILE:C	1:C:726:ILE:HD12	2.41	0.46
1:B:537:LYS:C	1:B:551:VAL:HG12	2.40	0.46
1:B:894:LEU:HB3	1:C:713:ALA:HB3	1.96	0.46
1:B:969:LYS:HZ3	1:B:975:SER:H	1.63	0.46
1:B:1046:GLY:HA2	1:A:890:ALA:HA	1.98	0.46
1:A:229:LEU:HB3	1:A:231:ILE:HD11	1.98	0.46
1:B:897:PRO:HB2	1:B:900:MET:HG2	1.97	0.46
1:B:931:ILE:O	1:B:934:ILE:HG22	2.16	0.46
1:A:993:ILE:O	1:A:997:ILE:HG12	2.15	0.46
1:B:54:LEU:HD12	1:B:195:LYS:HD3	1.98	0.45
1:B:797:PHE:CD2	1:B:802:PHE:HD2	2.35	0.45
1:A:533:LEU:HD22	1:A:585:LEU:HD11	1.97	0.45
1:A:596:SER:HB2	1:A:613:GLN:HE22	1.81	0.45
1:C:445:PRO:O	1:C:498:ARG:NH1	2.49	0.45
1:C:483:VAL:O	1:C:484:ALA:C	2.58	0.45
1:B:121:ASN:HD21	1:B:176:LEU:H	1.64	0.45
1:B:26:GLN:HG3	1:B:65:PHE:HA	1.99	0.45
1:B:786:LYS:HB2	1:B:786:LYS:HE2	1.77	0.45
1:B:864:LEU:O	1:C:669:GLY:N	2.43	0.45
1:A:456:PHE:HB3	1:A:473:TYR:HE2	1.81	0.45
1:B:81:ASN:N	1:B:81:ASN:OD1	2.48	0.45
1:B:327:VAL:HG13	1:B:542:ASN:HB3	1.98	0.45
1:A:483:VAL:O	1:A:484:ALA:C	2.59	0.45
1:A:1110:TYR:CZ	1:A:1112:PRO:HG3	2.52	0.45
1:C:343:ASN:HB3	1:C:371:PHE:CZ	2.50	0.45
1:C:598:ILE:HD12	1:C:664:ILE:HD12	1.97	0.45
1:C:642:VAL:HG12	1:C:651:ILE:HG22	1.99	0.45
1:B:118:LEU:N	1:B:129:LYS:O	2.49	0.45
1:B:384:PRO:HA	1:B:387:LEU:HD13	1.99	0.45
1:B:398:ASP:HB3	1:B:512:VAL:HG12	1.99	0.45
1:B:439:ASN:HA	1:B:507:PRO:HG2	1.98	0.45
1:A:43:PHE:HE1	1:A:283:GLY:HA3	1.82	0.45
1:A:175:PHE:CE1	1:A:203:ILE:HD11	2.51	0.45
1:A:804:GLN:HA	1:A:817:PHE:CD2	2.51	0.45
1:B:490:SER:O	1:B:493:GLN:NE2	2.49	0.45
1:B:541:PHE:CZ	1:B:587:ILE:HD13	2.51	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LEU:HD12	1:A:190:ARG:HH11	1.82	0.45
1:C:736:VAL:HG11	1:C:1004:LEU:HD21	1.98	0.45
1:C:752:LEU:HD11	1:C:990:GLU:OE2	2.15	0.45
1:B:34:ARG:HH22	1:B:217:PRO:HB2	1.82	0.45
1:B:755:GLN:OE1	1:C:969:LYS:CB	2.64	0.45
1:B:850:ILE:O	1:B:853:GLN:HG2	2.17	0.45
1:A:79:PHE:HE2	1:A:138:ASP:HB2	1.79	0.45
1:B:777:ASN:HD21	1:B:1019:ARG:HA	1.81	0.45
1:A:87:ASN:OD1	1:A:87:ASN:N	2.47	0.45
1:A:896:ILE:HD12	1:A:897:PRO:HD2	1.98	0.45
1:A:382:VAL:HG21	1:A:387:LEU:HD11	1.98	0.45
1:A:550:GLY:CA	1:A:589:PRO:HA	2.46	0.45
1:B:104:TRP:CZ3	1:B:238:PHE:HD2	2.35	0.45
1:B:388:ASN:OD1	1:B:526:GLY:HA3	2.17	0.45
1:B:788:ILE:HD11	1:C:699:LEU:HB3	1.99	0.45
1:A:797:PHE:HD2	1:A:802:PHE:HD2	1.65	0.45
1:A:817:PHE:N	1:A:817:PHE:CD1	2.82	0.45
1:C:87:ASN:OD1	1:C:87:ASN:N	2.48	0.45
1:C:591:SER:H	1:C:634:ARG:HH12	1.64	0.45
1:C:664:ILE:HD11	1:C:672:ALA:HB3	1.98	0.45
1:C:394:ASN:OD1	1:C:394:ASN:O	2.35	0.44
1:A:26:GLN:OE1	1:A:66:HIS:NE2	2.50	0.44
1:B:328:ARG:HB3	1:B:543:PHE:CE1	2.53	0.44
1:A:565:PHE:O	1:C:43:PHE:N	2.46	0.44
1:C:452:LEU:HD11	1:C:492:LEU:HB2	1.98	0.44
1:B:719:THR:HA	1:B:926:GLN:HE22	1.83	0.44
1:B:811:LYS:H	1:B:811:LYS:HG2	1.53	0.44
1:A:353:TRP:HH2	1:A:418:ILE:HD11	1.81	0.44
1:A:505:HIS:HE2	1:C:503:VAL:HG11	1.82	0.44
1:A:858:LEU:HD21	1:A:962:LEU:HD23	1.98	0.44
1:B:882:ILE:HG23	1:B:898:PHE:CD2	2.52	0.44
1:A:228:ASP:C	1:A:229:LEU:HD12	2.42	0.44
1:C:34:ARG:HA	1:C:34:ARG:HD3	1.74	0.44
1:C:101:ILE:HD11	1:C:240:THR:OG1	2.18	0.44
1:C:662:CYS:HB2	1:C:671:CYS:HB3	1.69	0.44
1:B:434:ILE:HB	1:B:511:VAL:HG23	1.99	0.44
1:B:803:SER:OG	1:B:804:GLN:NE2	2.49	0.44
1:C:237:ARG:HG2	1:C:239:GLN:NE2	2.33	0.44
1:C:1027:THR:O	1:C:1031:GLU:HG3	2.18	0.44
1:B:29:THR:OG1	1:B:30:ASN:N	2.50	0.44
1:B:534:VAL:HG21	1:B:539:VAL:HG11	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1129:VAL:HG22	1:A:917:TYR:HB3	1.99	0.44
1:A:328:ARG:HG3	1:A:579:PRO:HD2	2.00	0.44
1:A:905:ARG:HD2	1:A:1049:LEU:O	2.18	0.44
1:C:409:GLN:O	1:C:414:GLN:NE2	2.50	0.44
1:C:578:ASP:C	1:C:580:GLN:H	2.26	0.44
1:B:391:CYS:HA	1:B:525:CYS:HB3	2.00	0.44
1:B:635:VAL:HG12	1:B:635:VAL:O	2.18	0.44
1:B:1010:GLN:OE1	1:B:1010:GLN:HA	2.18	0.44
1:A:477:ASN:C	1:A:478:LYS:HG3	2.41	0.44
1:A:887:THR:C	1:A:889:GLY:H	2.26	0.44
1:A:1028:LYS:HB2	1:A:1028:LYS:HE3	1.62	0.44
1:C:994:ASP:O	1:C:998:THR:HG23	2.18	0.44
1:B:347:PHE:CD1	1:B:509:ARG:HD2	2.53	0.44
1:B:379:CYS:HB2	1:B:384:PRO:HG3	1.99	0.44
1:B:591:SER:H	1:B:634:ARG:HH12	1.66	0.44
1:B:922:LEU:HD11	2:B:1312:NAG:H3	1.99	0.44
1:A:886:TRP:HZ3	1:A:901:GLN:HG3	1.83	0.44
1:C:80:ASP:HB2	1:C:262:ALA:H	1.83	0.44
1:C:546:LEU:HD21	1:C:565:PHE:HZ	1.83	0.44
1:C:802:PHE:CD1	1:C:805:ILE:HD11	2.53	0.44
1:C:1091:ARG:NH1	1:C:1118:ASP:O	2.50	0.44
1:B:669:GLY:N	1:A:864:LEU:O	2.46	0.43
1:C:1115:ILE:HG22	1:C:1137:VAL:HG23	2.00	0.43
1:B:133:PHE:HB2	1:B:135:PHE:CZ	2.53	0.43
1:B:294:ASP:O	1:B:297:SER:OG	2.35	0.43
1:B:666:ILE:HB	1:B:670:ILE:O	2.18	0.43
1:B:708:SER:HA	2:B:1311:NAG:H82	1.99	0.43
1:B:896:ILE:HD12	1:B:897:PRO:HD2	1.99	0.43
1:B:990:GLU:HA	1:B:993:ILE:HG22	2.00	0.43
1:A:110:LEU:HD12	1:A:135:PHE:HD2	1.83	0.43
1:A:517:LEU:HD12	1:C:983:ARG:NH1	2.33	0.43
1:C:80:ASP:H	1:C:262:ALA:HB2	1.83	0.43
1:A:319:ARG:HH12	1:C:740:MET:HB2	1.82	0.43
1:A:536:ASN:O	1:A:537:LYS:HD3	2.18	0.43
1:C:591:SER:N	1:C:634:ARG:HH12	2.16	0.43
1:B:421:TYR:CD1	1:B:460:LYS:HD2	2.54	0.43
1:A:54:LEU:HB2	1:A:195:LYS:HE3	2.01	0.43
1:B:126:VAL:HB	1:B:174:PRO:HA	2.01	0.43
1:B:869:MET:H	1:B:869:MET:HG2	1.57	0.43
1:A:98:SER:HA	1:A:180:GLU:H	1.83	0.43
1:A:276:LEU:HD11	1:A:304:LYS:HD3	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:ASP:O	1:A:940:SER:N	2.51	0.43
1:C:34:ARG:HH21	1:C:217:PRO:HG2	1.84	0.43
1:C:318:PHE:O	1:C:319:ARG:HG3	2.19	0.43
1:C:708:SER:HA	2:C:1311:NAG:H82	1.99	0.43
1:C:969:LYS:NZ	1:C:975:SER:H	2.16	0.43
1:A:166:CYS:HB2	1:A:167:THR:H	1.60	0.43
1:C:206:LYS:HB2	1:C:223:LEU:HD13	2.01	0.43
1:C:240:THR:O	1:C:241:LEU:HD22	2.17	0.43
1:C:733:LYS:NZ	1:C:775:ASP:OD2	2.34	0.43
1:C:801:ASN:N	1:C:928:ASN:OD1	2.41	0.43
1:C:1098:ASN:OD1	1:C:1098:ASN:N	2.52	0.43
1:B:416:GLY:N	1:B:419:ALA:HB3	2.33	0.43
1:B:528:LYS:HD3	1:B:529:LYS:N	2.34	0.43
1:B:595:VAL:HG22	1:B:612:TYR:CE1	2.53	0.43
1:B:902:MET:HE3	1:B:902:MET:HB3	1.73	0.43
1:B:1029:MET:HE2	1:B:1029:MET:HB2	1.88	0.43
1:A:83:ALA:HA	1:A:237:ARG:HH21	1.84	0.43
1:A:378:LYS:HD3	1:A:380:TYR:CZ	2.54	0.43
1:B:767:LEU:HD23	1:B:767:LEU:HA	1.83	0.43
1:A:570:ALA:HB2	1:C:852:ALA:HB1	2.01	0.43
1:C:457:ARG:HH22	1:C:461:LEU:HB2	1.82	0.43
1:B:278:LYS:HB2	1:B:306:PHE:CE2	2.53	0.43
1:B:342:PHE:HE1	1:B:511:VAL:HG21	1.83	0.43
1:B:392:PHE:HD1	1:B:517:LEU:HD21	1.84	0.43
1:A:355:ARG:CZ	1:A:396:TYR:HB3	2.49	0.43
1:C:378:LYS:HD3	1:C:380:TYR:CE2	2.54	0.43
1:B:162:SER:O	1:B:163:ALA:C	2.62	0.43
1:B:353:TRP:HD1	1:B:398:ASP:OD1	2.02	0.43
1:B:719:THR:O	1:B:1068:VAL:HG22	2.19	0.43
1:B:737:ASP:OD1	1:B:737:ASP:N	2.51	0.43
1:A:289:VAL:HB	1:A:306:PHE:HE1	1.84	0.43
1:C:127:VAL:C	1:C:128:ILE:HD13	2.44	0.43
1:C:487:ASN:HA	1:C:489:TYR:CZ	2.54	0.43
1:C:739:THR:HG22	1:C:753:LEU:HD23	2.01	0.43
1:C:800:PHE:HD2	1:C:927:PHE:CD2	2.37	0.43
1:C:819:GLU:OE1	1:C:1055:SER:HB2	2.19	0.43
1:B:720:ILE:HD12	1:B:923:ILE:HG23	2.00	0.42
1:A:406:GLU:OE1	1:A:495:TYR:OH	2.37	0.42
1:A:552:LEU:HD12	1:A:585:LEU:HD22	2.01	0.42
1:C:129:LYS:HA	1:C:129:LYS:HE2	2.01	0.42
1:B:233:ILE:HG12	1:B:234:ASN:H	1.83	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ASN:OD1	1:A:175:PHE:HD2	2.02	0.42
1:A:505:HIS:NE2	1:C:503:VAL:HG11	2.33	0.42
1:A:1107:ARG:HD3	1:C:904:TYR:CD2	2.54	0.42
1:C:117:LEU:HA	1:C:130:VAL:HA	2.01	0.42
1:C:643:PHE:HD1	1:C:644:GLN:H	1.66	0.42
1:A:34:ARG:NH1	1:A:217:PRO:O	2.52	0.42
1:A:396:TYR:O	1:A:513:LEU:HA	2.20	0.42
1:A:707:TYR:CE1	1:C:897:PRO:HA	2.53	0.42
1:A:986:LYS:HA	1:A:986:LYS:HD3	1.88	0.42
1:C:81:ASN:OD1	1:C:81:ASN:N	2.53	0.42
1:B:382:VAL:HG13	1:A:983:ARG:HH11	1.85	0.42
1:A:357:ARG:NE	1:C:231:ILE:O	2.52	0.42
1:A:1106:GLN:H	1:A:1106:GLN:HG3	1.56	0.42
1:C:128:ILE:HG12	1:C:170:TYR:CD1	2.55	0.42
1:A:931:ILE:O	1:A:934:ILE:HG22	2.20	0.42
1:C:81:ASN:HB3	1:C:138:ASP:CB	2.49	0.42
1:C:131:CYS:HB2	1:C:133:PHE:CZ	2.54	0.42
1:C:878:LEU:HD11	1:C:1052:PHE:HB3	2.01	0.42
1:B:424:LYS:HD3	1:B:424:LYS:HA	1.86	0.42
1:A:90:VAL:HG21	1:A:238:PHE:CE1	2.54	0.42
1:A:328:ARG:HG2	1:A:579:PRO:HD2	2.01	0.42
1:A:376:ALA:HB3	1:A:435:ALA:HB3	2.00	0.42
1:A:617:CYS:HA	1:A:633:TRP:N	2.35	0.42
1:C:34:ARG:NH2	1:C:217:PRO:HG2	2.34	0.42
1:C:854:LYS:HE3	1:C:854:LYS:HB3	1.90	0.42
1:B:178:ASP:OD1	1:B:178:ASP:N	2.53	0.42
1:B:768:THR:O	1:B:772:VAL:HG13	2.19	0.42
1:A:118:LEU:CD2	1:A:120:VAL:HG23	2.46	0.42
1:B:78:ARG:HB3	1:B:261:GLY:C	2.44	0.42
1:B:497:PHE:CE2	1:B:507:PRO:HB3	2.55	0.42
1:A:126:VAL:HB	1:A:174:PRO:HA	2.02	0.42
1:A:159:VAL:HG23	1:A:160:TYR:H	1.83	0.42
1:A:438:SER:HB3	1:A:509:ARG:HG2	2.02	0.42
1:A:536:ASN:O	1:A:537:LYS:CD	2.68	0.42
1:A:1028:LYS:O	1:A:1032:CYS:HB2	2.19	0.42
1:B:707:TYR:CE1	1:A:897:PRO:HA	2.53	0.42
1:A:34:ARG:NH1	1:A:219:GLY:O	2.52	0.42
1:A:122:ASN:O	1:A:124:THR:N	2.52	0.42
1:A:295:PRO:HA	1:A:298:GLU:HB3	2.02	0.42
1:C:50:SER:HA	1:C:276:LEU:HA	2.02	0.42
1:C:159:VAL:HG13	1:C:160:TYR:CD1	2.51	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:TRP:CD1	1:C:258:TRP:N	2.88	0.42
1:B:247:SER:O	1:B:248:TYR:CB	2.68	0.42
1:A:131:CYS:HB2	1:A:133:PHE:CZ	2.54	0.42
1:A:299:THR:HG22	1:A:308:VAL:HG11	2.02	0.42
1:A:332:ILE:HG23	1:A:362:VAL:HG23	2.01	0.42
1:A:349:SER:HB2	1:A:451:TYR:CD1	2.54	0.42
1:A:355:ARG:HD3	1:A:398:ASP:OD1	2.20	0.42
1:A:804:GLN:HG3	1:A:931:ILE:HG23	2.02	0.42
1:A:950:ASP:OD1	1:A:950:ASP:C	2.62	0.42
1:B:429:PHE:CE1	1:B:431:GLY:C	2.98	0.41
1:B:902:MET:HE1	1:B:1049:LEU:HD13	2.01	0.41
1:C:557:LYS:HE2	1:C:557:LYS:HB3	1.88	0.41
1:C:726:ILE:HG22	1:C:1061:VAL:HG22	2.01	0.41
1:C:739:THR:O	1:C:740:MET:C	2.63	0.41
1:B:992:GLN:NE2	1:B:995:ARG:HH21	2.17	0.41
1:C:541:PHE:CZ	1:C:548:GLY:HA3	2.56	0.41
1:C:1094:VAL:HG23	1:C:1096:VAL:HG23	2.01	0.41
1:B:140:PHE:HA	1:B:241:LEU:HD11	2.02	0.41
1:B:715:PRO:HD3	1:A:894:LEU:CD1	2.50	0.41
1:B:816:SER:OG	1:B:819:GLU:HG3	2.20	0.41
1:B:983:ARG:O	1:C:383:SER:N	2.53	0.41
1:A:565:PHE:HD2	1:A:567:ARG:HH21	1.66	0.41
1:A:813:SER:OG	1:A:868:GLU:OE2	2.30	0.41
1:C:28:TYR:CE2	2:C:1301:NAG:H62	2.56	0.41
1:B:133:PHE:HB3	1:B:160:TYR:HB3	2.02	0.41
1:B:428:ASP:OD1	1:B:429:PHE:N	2.53	0.41
1:B:557:LYS:HB3	1:B:557:LYS:HE2	1.83	0.41
1:B:560:LEU:N	1:B:563:GLN:HB3	2.26	0.41
1:B:713:ALA:HA	1:B:1074:ASN:HA	2.01	0.41
1:A:869:MET:H	1:A:869:MET:HG2	1.70	0.41
1:B:359:SER:HA	1:B:523:THR:HG23	2.02	0.41
1:B:446:SER:O	1:B:498:ARG:NH2	2.53	0.41
1:B:633:TRP:O	1:B:634:ARG:HG3	2.20	0.41
1:B:121:ASN:OD1	1:B:174:PRO:HB3	2.21	0.41
1:B:790:LYS:HE2	1:C:704:SER:HB3	2.01	0.41
1:A:269:TYR:CD1	1:A:269:TYR:N	2.88	0.41
1:C:177:MET:H	1:C:190:ARG:HH12	1.68	0.41
1:C:798:GLY:C	1:C:800:PHE:N	2.78	0.41
1:B:43:PHE:CE2	1:C:557:LYS:HD3	2.55	0.41
1:B:877:LEU:HD23	1:B:888:PHE:CE2	2.55	0.41
1:A:356:LYS:HE2	1:A:356:LYS:HB2	1.77	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:ASP:N	1:A:364:ASP:OD1	2.54	0.41
1:A:1083:HIS:CG	1:A:1137:VAL:HG12	2.55	0.41
1:C:1023:ASN:O	1:C:1027:THR:HG23	2.21	0.41
1:C:1086:LYS:HA	1:C:1086:LYS:HD2	1.90	0.41
1:B:804:GLN:HA	1:B:817:PHE:HD2	1.86	0.41
1:A:65:PHE:CZ	1:A:84:LEU:HD21	2.55	0.41
1:A:644:GLN:HG3	2:A:1309:NAG:HN2	1.86	0.41
1:C:349:SER:HB3	1:C:351:TYR:CD1	2.56	0.41
1:C:726:ILE:CD1	1:C:947:LYS:HB3	2.49	0.41
1:B:304:LYS:HE3	1:B:304:LYS:HB3	1.89	0.41
1:B:349:SER:OG	1:B:350:VAL:N	2.54	0.41
1:B:487:ASN:HA	1:B:489:TYR:CZ	2.55	0.41
1:B:503:VAL:HG11	1:C:505:HIS:NE2	2.36	0.41
1:B:642:VAL:HG22	1:B:651:ILE:HG22	2.03	0.41
1:B:916:LEU:HD12	1:B:923:ILE:HG13	2.02	0.41
1:A:138:ASP:OD1	1:A:138:ASP:N	2.53	0.41
1:A:394:ASN:ND2	1:C:200:TYR:OH	2.53	0.41
1:A:424:LYS:HD3	1:A:424:LYS:HA	1.89	0.41
1:C:290:ASP:O	1:C:297:SER:OG	2.28	0.41
1:C:559:PHE:HD1	1:C:563:GLN:HG3	1.85	0.41
1:B:431:GLY:HA3	1:B:513:LEU:O	2.21	0.41
1:B:726:ILE:HG13	1:B:1061:VAL:HG22	2.02	0.41
1:B:969:LYS:O	1:A:755:GLN:HB3	2.21	0.41
1:C:424:LYS:HD3	1:C:424:LYS:HA	1.94	0.41
1:C:802:PHE:HD1	1:C:805:ILE:HD11	1.86	0.41
1:C:817:PHE:CZ	1:C:821:LEU:HD12	2.56	0.41
1:B:558:LYS:O	1:B:559:PHE:HB2	2.21	0.40
1:B:564:GLN:HG2	1:B:565:PHE:HD1	1.86	0.40
1:B:664:ILE:O	1:B:671:CYS:HB3	2.21	0.40
1:B:1006:THR:HG23	1:A:1005:GLN:HE22	1.86	0.40
1:B:1095:PHE:HD1	1:B:1095:PHE:HA	1.80	0.40
1:A:135:PHE:HE1	1:A:159:VAL:HB	1.86	0.40
1:A:204:TYR:HB2	1:A:223:LEU:HD21	2.03	0.40
1:C:304:LYS:HA	1:C:304:LYS:HD3	1.93	0.40
1:C:336:CYS:HB2	1:C:361:CYS:HB2	1.95	0.40
1:C:555:SER:HB2	1:C:584:ILE:HB	2.04	0.40
1:C:559:PHE:CD1	1:C:563:GLN:HG3	2.56	0.40
1:B:390:LEU:O	1:B:525:CYS:HB3	2.20	0.40
1:B:695:TYR:HD1	1:B:696:THR:O	2.04	0.40
1:A:797:PHE:HE2	1:A:806:LEU:HD11	1.87	0.40
1:C:347:PHE:CD2	1:C:509:ARG:HD2	2.56	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:380:TYR:HE2	1:C:412:PRO:HD3	1.87	0.40
1:C:714:ILE:HD12	1:C:1096:VAL:HG21	2.02	0.40
1:C:764:LYS:HB3	1:C:764:LYS:HE3	1.87	0.40
1:C:984:LEU:HD22	1:C:988:GLU:HG3	2.03	0.40
1:B:220:PHE:HE2	1:B:285:ILE:HG22	1.86	0.40
1:B:800:PHE:HD2	1:B:927:PHE:CD2	2.40	0.40
1:B:456:PHE:CE1	1:A:372:ALA:HB1	2.56	0.40
1:B:957:GLN:HA	1:B:960:ASN:HB3	2.03	0.40
1:A:375:PHE:CE2	1:A:407:VAL:HG11	2.57	0.40
1:A:375:PHE:HE2	1:A:407:VAL:HG11	1.86	0.40
1:A:636:TYR:HB3	1:A:637:SER:H	1.69	0.40
1:C:28:TYR:CD2	2:C:1301:NAG:H62	2.57	0.40
1:B:409:GLN:OE1	1:B:417:ASN:N	2.55	0.40
1:A:105:ILE:HB	1:A:239:GLN:HG2	2.04	0.40
1:C:741:TYR:CE1	1:C:966:LEU:HD11	2.55	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	1026/1269 (81%)	911 (89%)	109 (11%)	6 (1%)	21	56
1	B	1026/1269 (81%)	923 (90%)	96 (9%)	7 (1%)	18	52
1	C	1026/1269 (81%)	936 (91%)	87 (8%)	3 (0%)	36	68
All	All	3078/3807 (81%)	2770 (90%)	292 (10%)	16 (0%)	26	59

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	331	ASN
1	B	253	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	788	ILE
1	B	798	GLY
1	A	788	ILE
1	C	788	ILE
1	B	330	PRO
1	B	489	TYR
1	A	177	MET
1	A	738	CYS
1	C	489	TYR
1	B	254	SER
1	A	330	PRO
1	A	489	TYR
1	A	888	PHE
1	C	166	CYS

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	908/1109 (82%)	901 (99%)	7 (1%)	73	82
1	B	908/1109 (82%)	898 (99%)	10 (1%)	65	79
1	C	908/1109 (82%)	904 (100%)	4 (0%)	84	86
All	All	2724/3327 (82%)	2703 (99%)	21 (1%)	70	82

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	81	ASN
1	B	84	LEU
1	B	118	LEU
1	B	241	LEU
1	B	312	ILE
1	B	390	LEU
1	B	525	CYS
1	B	560	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	664	ILE
1	B	755	GLN
1	A	165	ASN
1	A	176	LEU
1	A	282	ASN
1	A	312	ILE
1	A	525	CYS
1	A	534	VAL
1	A	546	LEU
1	C	203	ILE
1	C	693	ILE
1	C	775	ASP
1	C	1104	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	115	GLN
1	B	121	ASN
1	B	211	ASN
1	B	317	ASN
1	B	493	GLN
1	B	675	GLN
1	B	774	GLN
1	B	779	GLN
1	B	787	GLN
1	B	853	GLN
1	B	926	GLN
1	B	1005	GLN
1	B	1011	GLN
1	B	1106	GLN
1	A	211	ASN
1	A	354	ASN
1	A	360	ASN
1	A	370	ASN
1	A	439	ASN
1	A	544	ASN
1	A	762	GLN
1	A	774	GLN
1	A	787	GLN
1	A	856	ASN
1	A	907	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	913	GLN
1	A	926	GLN
1	A	1010	GLN
1	A	1011	GLN
1	A	1023	ASN
1	A	1048	HIS
1	A	1135	ASN
1	C	30	ASN
1	C	207	HIS
1	C	339	HIS
1	C	394	ASN
1	C	487	ASN
1	C	544	ASN
1	C	613	GLN
1	C	710	ASN
1	C	751	ASN
1	C	755	GLN
1	C	762	GLN
1	C	774	GLN
1	C	777	ASN
1	C	872	GLN
1	C	901	GLN
1	C	926	GLN
1	C	935	GLN
1	C	1011	GLN
1	C	1048	HIS
1	C	1106	GLN
1	C	1135	ASN

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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

49 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1311	1	14,14,15	0.41	0	17,19,21	0.53	0
2	NAG	B	1301	1	14,14,15	0.23	0	17,19,21	0.48	0
2	NAG	A	1314	1	14,14,15	0.25	0	17,19,21	0.51	0
2	NAG	B	1305	1	14,14,15	0.33	0	17,19,21	0.44	0
2	NAG	B	1311	1	14,14,15	0.39	0	17,19,21	0.45	0
2	NAG	A	1311	1	14,14,15	0.41	0	17,19,21	0.52	0
2	NAG	A	1312	1	14,14,15	0.22	0	17,19,21	0.51	0
2	NAG	C	1315	1	14,14,15	0.21	0	17,19,21	0.49	0
3	IDU	A	1317	-	15,15,17	0.94	1 (6%)	14,22,26	1.14	1 (7%)
2	NAG	C	1303	1	14,14,15	0.39	0	17,19,21	0.52	0
2	NAG	C	1314	1	14,14,15	0.25	0	17,19,21	0.54	0
2	NAG	B	1302	1	14,14,15	0.19	0	17,19,21	0.48	0
2	NAG	B	1315	1	14,14,15	0.22	0	17,19,21	0.49	0
2	NAG	B	1314	1	14,14,15	0.37	0	17,19,21	0.67	0
2	NAG	C	1306	1	14,14,15	0.34	0	17,19,21	0.45	0
2	NAG	C	1307	1	14,14,15	0.27	0	17,19,21	0.50	0
2	NAG	A	1316	1	14,14,15	0.20	0	17,19,21	0.44	0
2	NAG	A	1306	1	14,14,15	0.28	0	17,19,21	0.47	0
2	NAG	A	1308	1	14,14,15	0.22	0	17,19,21	0.44	0
2	NAG	A	1301	1	14,14,15	0.23	0	17,19,21	0.44	0
2	NAG	A	1310	1	14,14,15	0.39	0	17,19,21	0.37	0
2	NAG	B	1308	1	14,14,15	0.18	0	17,19,21	0.45	0
2	NAG	C	1305	1	14,14,15	0.53	0	17,19,21	0.45	0
2	NAG	A	1304	1	14,14,15	0.25	0	17,19,21	0.46	0
2	NAG	C	1301	1	14,14,15	0.32	0	17,19,21	0.48	0
2	NAG	B	1306	1	14,14,15	0.35	0	17,19,21	0.42	0
2	NAG	A	1302	1	14,14,15	0.28	0	17,19,21	0.51	0
2	NAG	A	1309	1	14,14,15	0.22	0	17,19,21	0.42	0
2	NAG	C	1312	1	14,14,15	0.20	0	17,19,21	0.48	0
2	NAG	C	1316	1	14,14,15	0.23	0	17,19,21	0.47	0
2	NAG	B	1313	1	14,14,15	0.23	0	17,19,21	0.48	0
2	NAG	A	1305	1	14,14,15	0.40	0	17,19,21	0.42	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	C	1313	1	14,14,15	0.25	0	17,19,21	0.51	0
2	NAG	B	1309	1	14,14,15	0.21	0	17,19,21	0.42	0
2	NAG	B	1312	1	14,14,15	0.24	0	17,19,21	0.47	0
2	NAG	A	1303	1	14,14,15	0.38	0	17,19,21	0.40	0
2	NAG	A	1313	1	14,14,15	0.24	0	17,19,21	0.50	0
2	NAG	C	1310	1	14,14,15	0.27	0	17,19,21	0.50	0
2	NAG	B	1316	1	14,14,15	0.23	0	17,19,21	0.46	0
2	NAG	C	1304	1	14,14,15	0.25	0	17,19,21	0.45	0
2	NAG	A	1307	1	14,14,15	0.26	0	17,19,21	0.49	0
2	NAG	B	1303	1	14,14,15	0.99	1 (7%)	17,19,21	1.30	1 (5%)
2	NAG	B	1307	1	14,14,15	0.22	0	17,19,21	0.50	0
2	NAG	B	1304	1	14,14,15	0.25	0	17,19,21	0.48	0
2	NAG	B	1310	1	14,14,15	0.36	0	17,19,21	0.52	0
2	NAG	C	1302	1	14,14,15	0.20	0	17,19,21	0.48	0
2	NAG	C	1308	1	14,14,15	0.23	0	17,19,21	0.43	0
2	NAG	C	1309	1	14,14,15	0.23	0	17,19,21	0.42	0
2	NAG	A	1315	1	14,14,15	0.21	0	17,19,21	0.51	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	1311	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1301	1	-	1/6/23/26	0/1/1/1
2	NAG	A	1314	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1305	1	-	3/6/23/26	0/1/1/1
2	NAG	B	1311	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1311	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1312	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1315	1	-	2/6/23/26	0/1/1/1
3	IDU	A	1317	-	-	4/9/22/29	1/1/1/1
2	NAG	C	1303	1	-	1/6/23/26	0/1/1/1
2	NAG	C	1314	1	-	4/6/23/26	0/1/1/1
2	NAG	B	1302	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1315	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1314	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1306	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1307	1	-	3/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1316	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1306	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1308	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1310	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1308	1	-	1/6/23/26	0/1/1/1
2	NAG	C	1305	1	-	3/6/23/26	0/1/1/1
2	NAG	A	1304	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1301	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1306	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1302	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1309	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1312	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1316	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1313	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1305	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1313	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1309	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1312	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1303	1	-	0/6/23/26	0/1/1/1
2	NAG	A	1313	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1310	1	-	0/6/23/26	0/1/1/1
2	NAG	B	1316	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1304	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1307	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1303	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1307	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1304	1	-	2/6/23/26	0/1/1/1
2	NAG	B	1310	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1302	1	-	2/6/23/26	0/1/1/1
2	NAG	C	1308	1	-	0/6/23/26	0/1/1/1
2	NAG	C	1309	1	-	2/6/23/26	0/1/1/1
2	NAG	A	1315	1	-	2/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1303	NAG	O5-C1	3.55	1.49	1.43

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1317	IDU	O6-C6	-2.99	1.21	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1303	NAG	C1-O5-C5	5.13	119.06	112.19
3	A	1317	IDU	O6-C6-C5	2.61	119.49	112.71

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1317	IDU	C1-C2-O2-S
3	A	1317	IDU	C3-C2-O2-S
2	C	1307	NAG	C4-C5-C6-O6
2	B	1307	NAG	C4-C5-C6-O6
2	C	1314	NAG	O5-C5-C6-O6
2	B	1315	NAG	O5-C5-C6-O6
2	A	1307	NAG	C4-C5-C6-O6
2	B	1304	NAG	O5-C5-C6-O6
2	A	1315	NAG	O5-C5-C6-O6
2	C	1315	NAG	O5-C5-C6-O6
2	C	1307	NAG	O5-C5-C6-O6
2	C	1313	NAG	O5-C5-C6-O6
2	B	1315	NAG	C4-C5-C6-O6
2	A	1308	NAG	C4-C5-C6-O6
2	B	1303	NAG	O5-C5-C6-O6
2	C	1314	NAG	C4-C5-C6-O6
2	A	1307	NAG	O5-C5-C6-O6
2	B	1307	NAG	O5-C5-C6-O6
2	A	1306	NAG	O5-C5-C6-O6
2	B	1304	NAG	C4-C5-C6-O6
2	C	1315	NAG	C4-C5-C6-O6
2	B	1306	NAG	O5-C5-C6-O6
2	A	1315	NAG	C4-C5-C6-O6
2	A	1306	NAG	C4-C5-C6-O6
2	A	1311	NAG	C8-C7-N2-C2
2	B	1306	NAG	C4-C5-C6-O6
2	C	1313	NAG	C4-C5-C6-O6
2	A	1308	NAG	O5-C5-C6-O6
2	C	1304	NAG	O5-C5-C6-O6
2	B	1305	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	B	1305	NAG	O7-C7-N2-C2
2	A	1305	NAG	C8-C7-N2-C2
2	A	1305	NAG	O7-C7-N2-C2
2	A	1311	NAG	O7-C7-N2-C2
2	C	1305	NAG	C8-C7-N2-C2
2	C	1305	NAG	O7-C7-N2-C2
2	C	1311	NAG	C8-C7-N2-C2
2	B	1313	NAG	O5-C5-C6-O6
2	C	1304	NAG	C4-C5-C6-O6
2	B	1313	NAG	C4-C5-C6-O6
2	C	1306	NAG	C4-C5-C6-O6
2	B	1303	NAG	C4-C5-C6-O6
2	A	1316	NAG	O5-C5-C6-O6
2	A	1316	NAG	C4-C5-C6-O6
2	C	1311	NAG	O7-C7-N2-C2
2	C	1306	NAG	O5-C5-C6-O6
2	B	1310	NAG	C4-C5-C6-O6
2	A	1311	NAG	O5-C5-C6-O6
2	C	1303	NAG	O5-C5-C6-O6
2	C	1302	NAG	C4-C5-C6-O6
2	B	1310	NAG	O5-C5-C6-O6
2	C	1309	NAG	C4-C5-C6-O6
2	A	1309	NAG	C4-C5-C6-O6
2	B	1314	NAG	C1-C2-N2-C7
2	A	1314	NAG	C1-C2-N2-C7
2	C	1302	NAG	O5-C5-C6-O6
2	A	1309	NAG	O5-C5-C6-O6
2	B	1314	NAG	C3-C2-N2-C7
2	A	1314	NAG	C3-C2-N2-C7
2	C	1314	NAG	C3-C2-N2-C7
3	A	1317	IDU	O5-C5-C6-O61
2	C	1309	NAG	O5-C5-C6-O6
2	B	1305	NAG	C4-C5-C6-O6
2	C	1305	NAG	C4-C5-C6-O6
2	B	1301	NAG	C1-C2-N2-C7
2	B	1308	NAG	C1-C2-N2-C7
2	C	1307	NAG	C1-C2-N2-C7
2	C	1314	NAG	C1-C2-N2-C7
3	A	1317	IDU	C4-C5-C6-O61

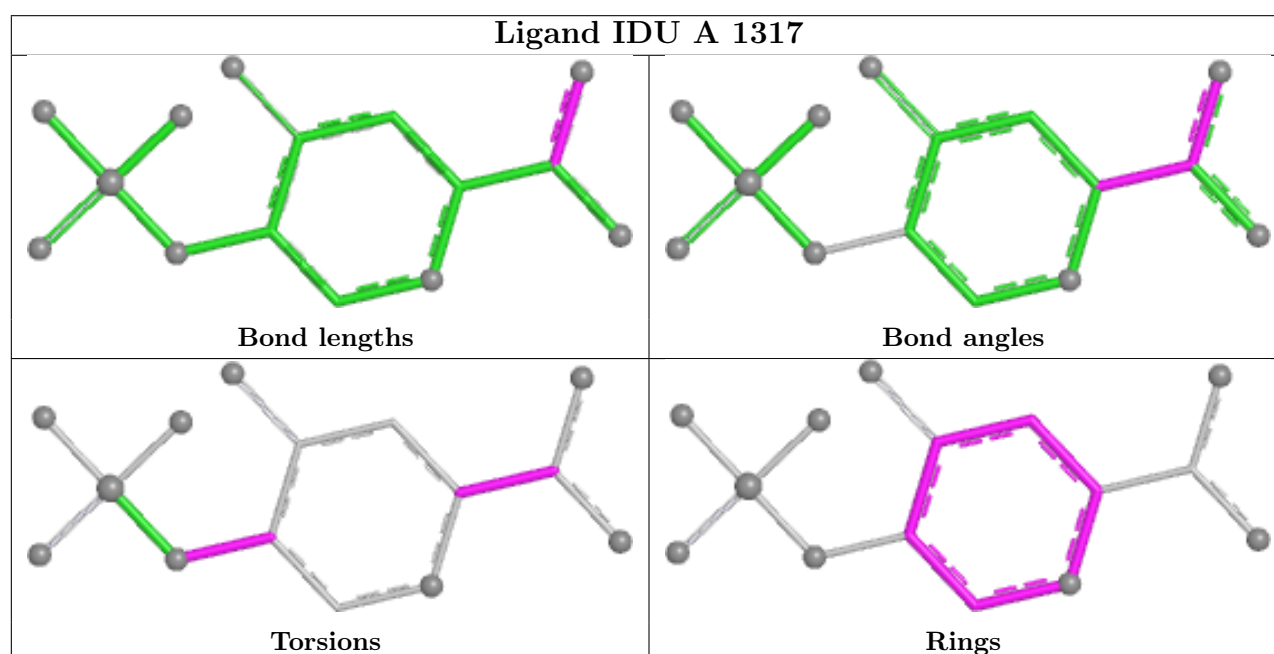
All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1317	IDU	C1-C2-C3-C4-C5-O5

9 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1311	NAG	1	0
2	B	1311	NAG	1	0
2	B	1302	NAG	1	0
2	C	1301	NAG	2	0
2	B	1306	NAG	1	0
2	A	1309	NAG	2	0
2	B	1312	NAG	1	0
2	B	1310	NAG	1	0
2	C	1302	NAG	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 all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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.

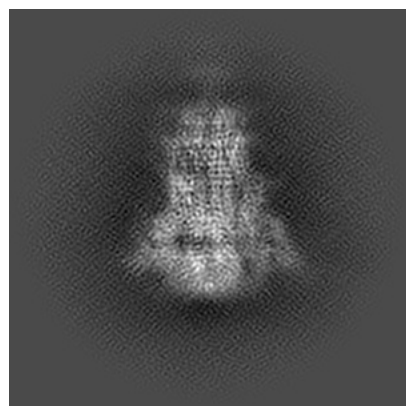
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-38683. These allow visual inspection of the internal detail of the map and identification of artifacts.

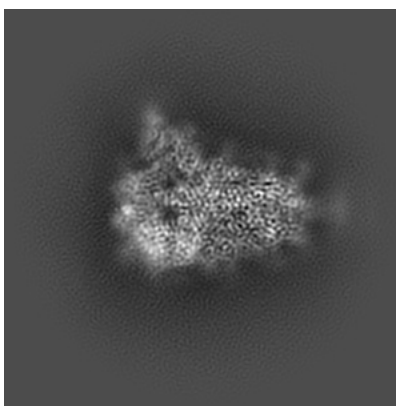
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

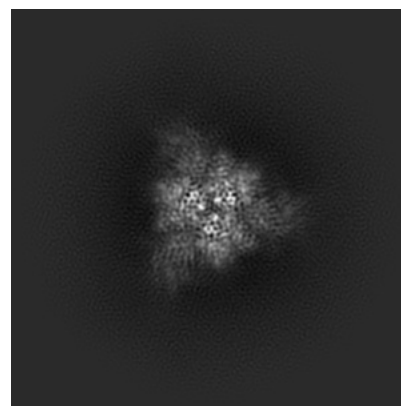
6.1.1 Primary map



X

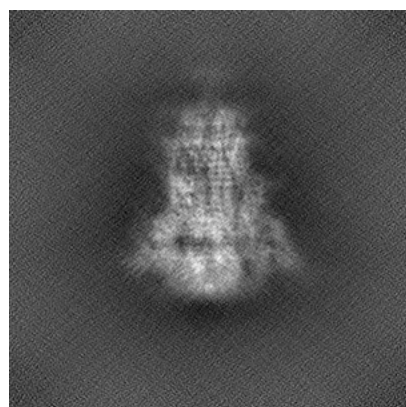


Y

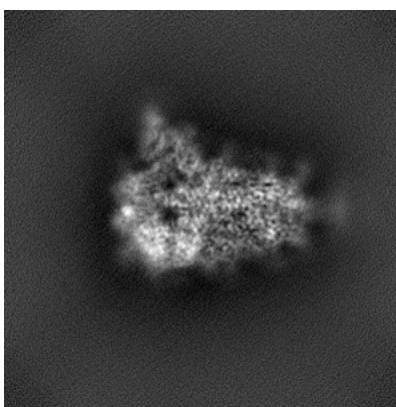


Z

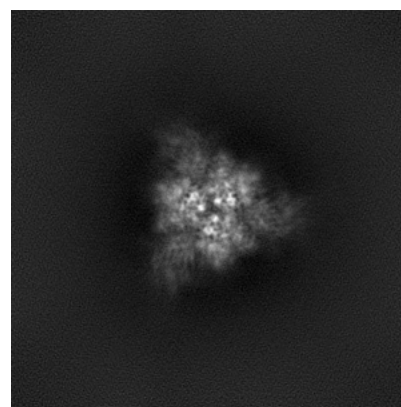
6.1.2 Raw map



X



Y

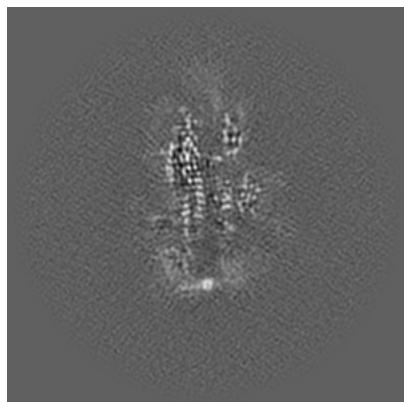


Z

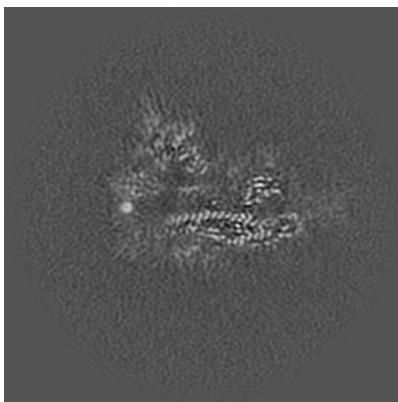
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

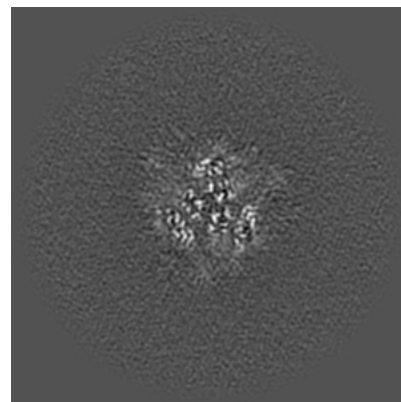
6.2.1 Primary map



X Index: 150

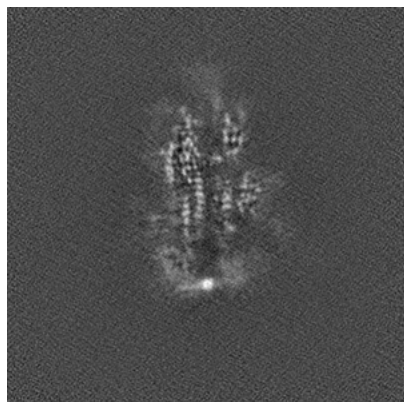


Y Index: 150



Z Index: 150

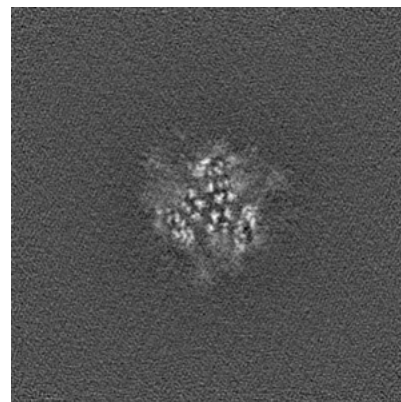
6.2.2 Raw map



X Index: 150



Y Index: 150

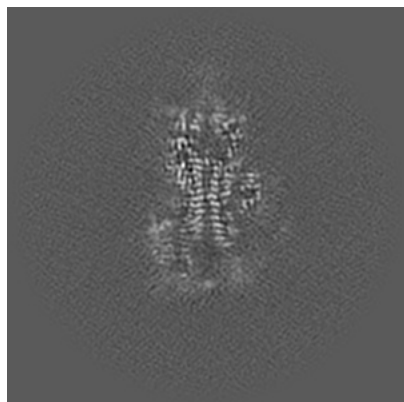


Z Index: 150

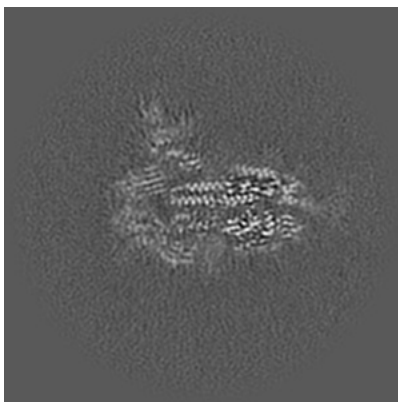
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

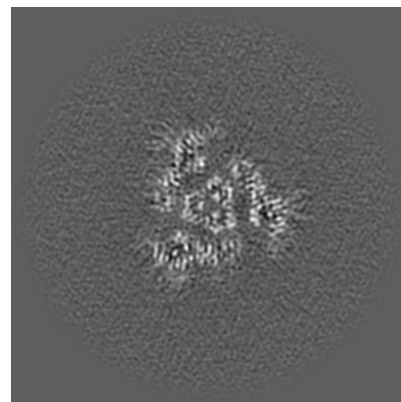
6.3.1 Primary map



X Index: 153

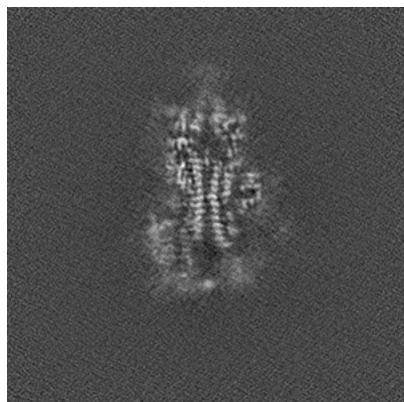


Y Index: 157

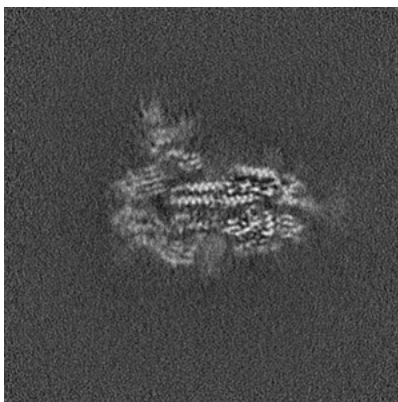


Z Index: 132

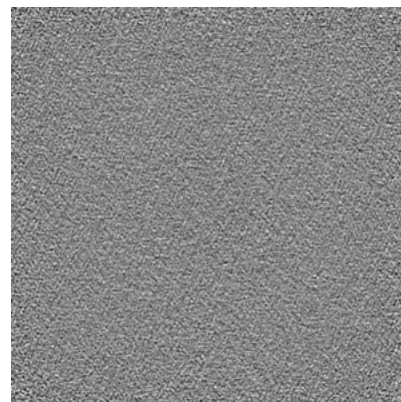
6.3.2 Raw map



X Index: 153



Y Index: 157

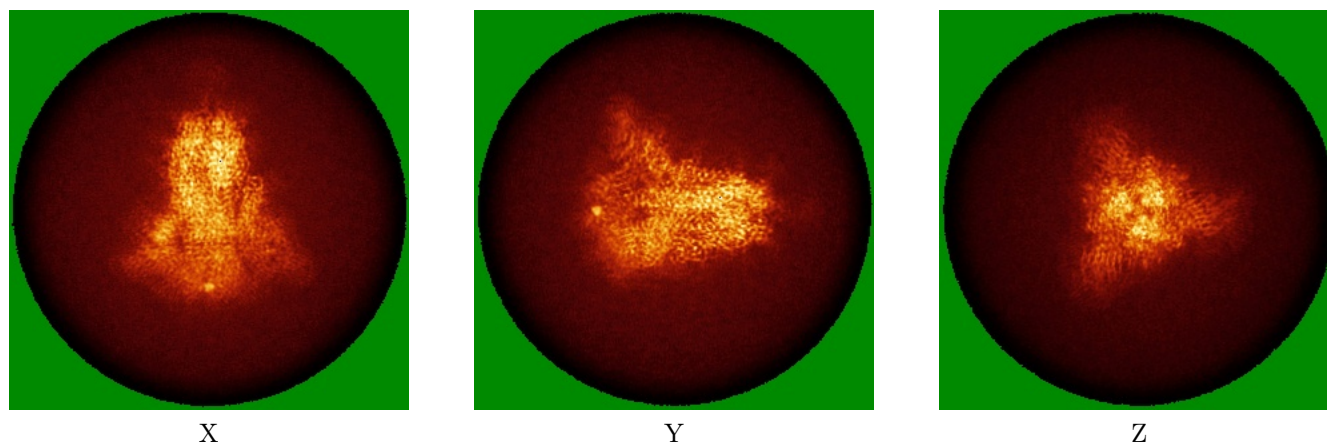


Z Index: 0

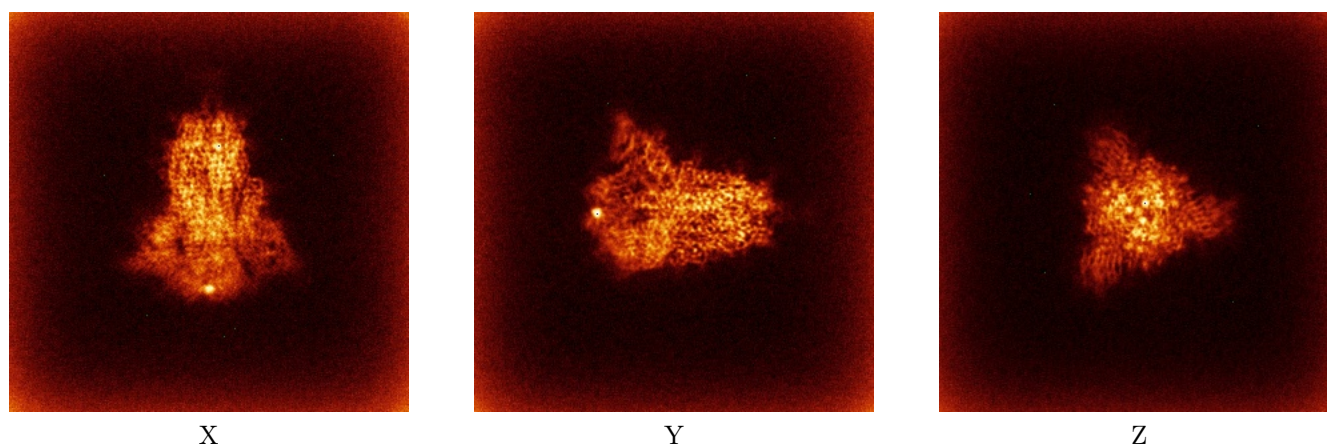
The images above show the largest variance slices of the map in three orthogonal directions.

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](#)

This section was not generated.

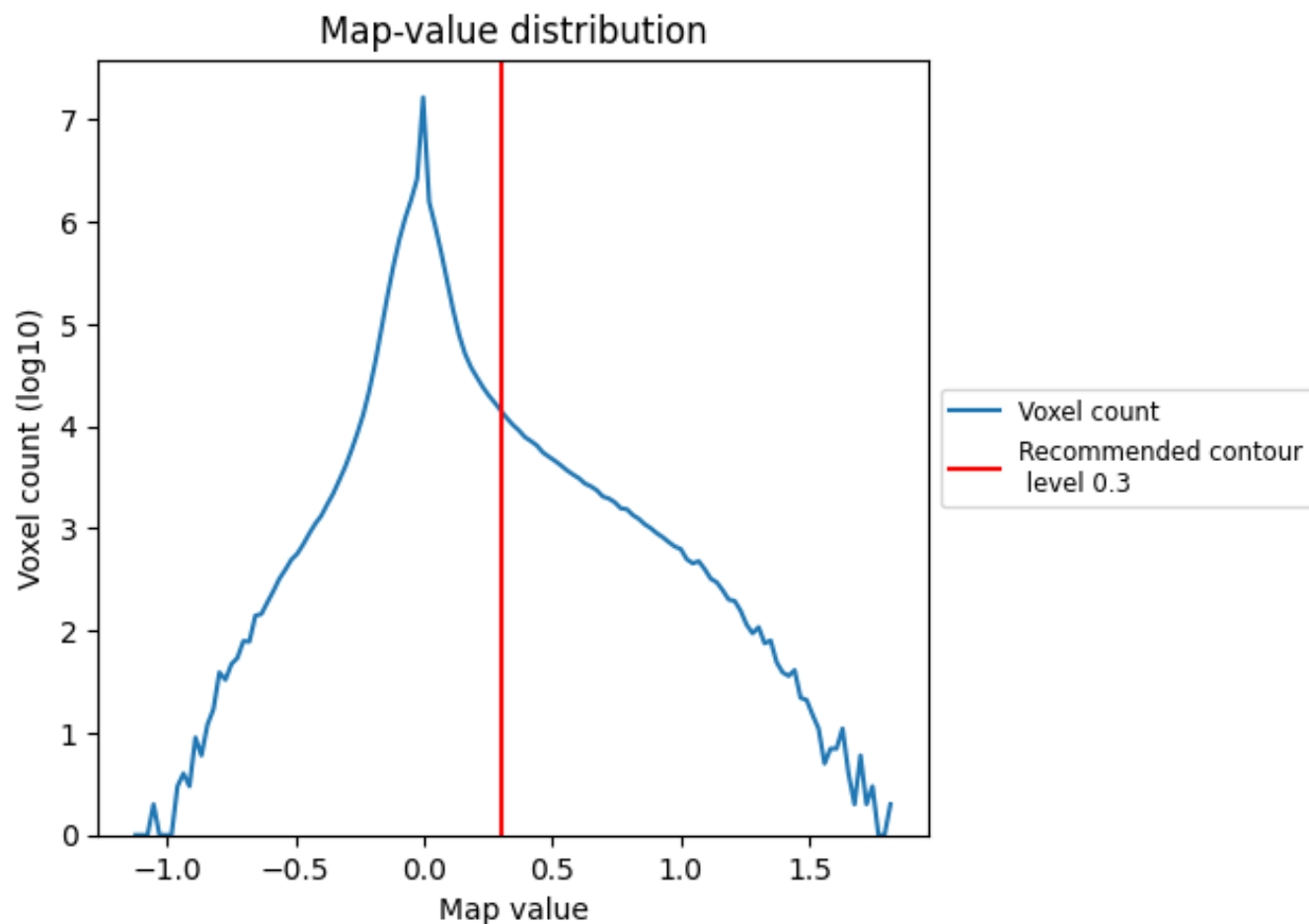
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

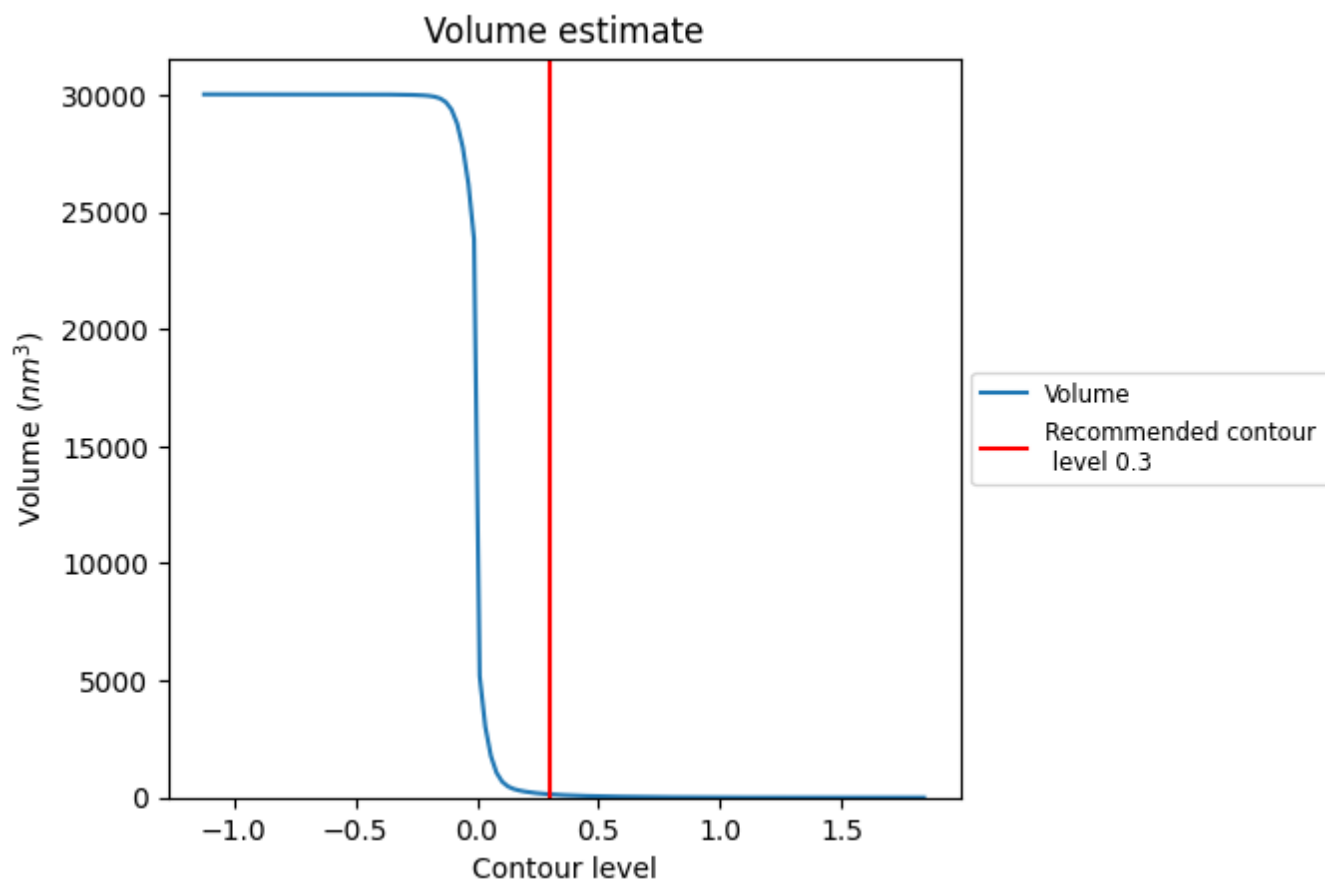
This section contains the results of statistical analysis of the map.

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.

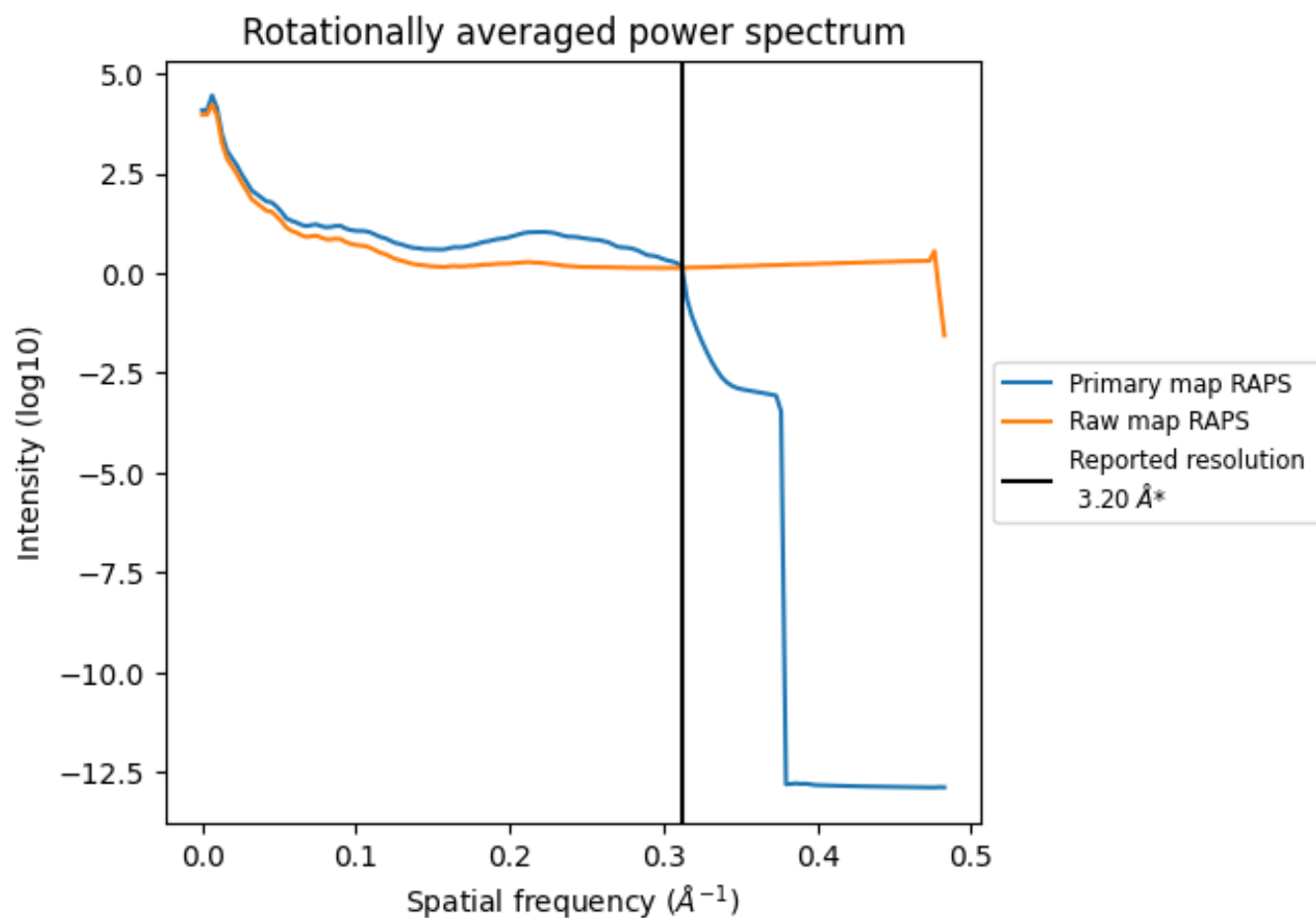
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 139 nm³; this corresponds to an approximate mass of 126 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 ⓘ

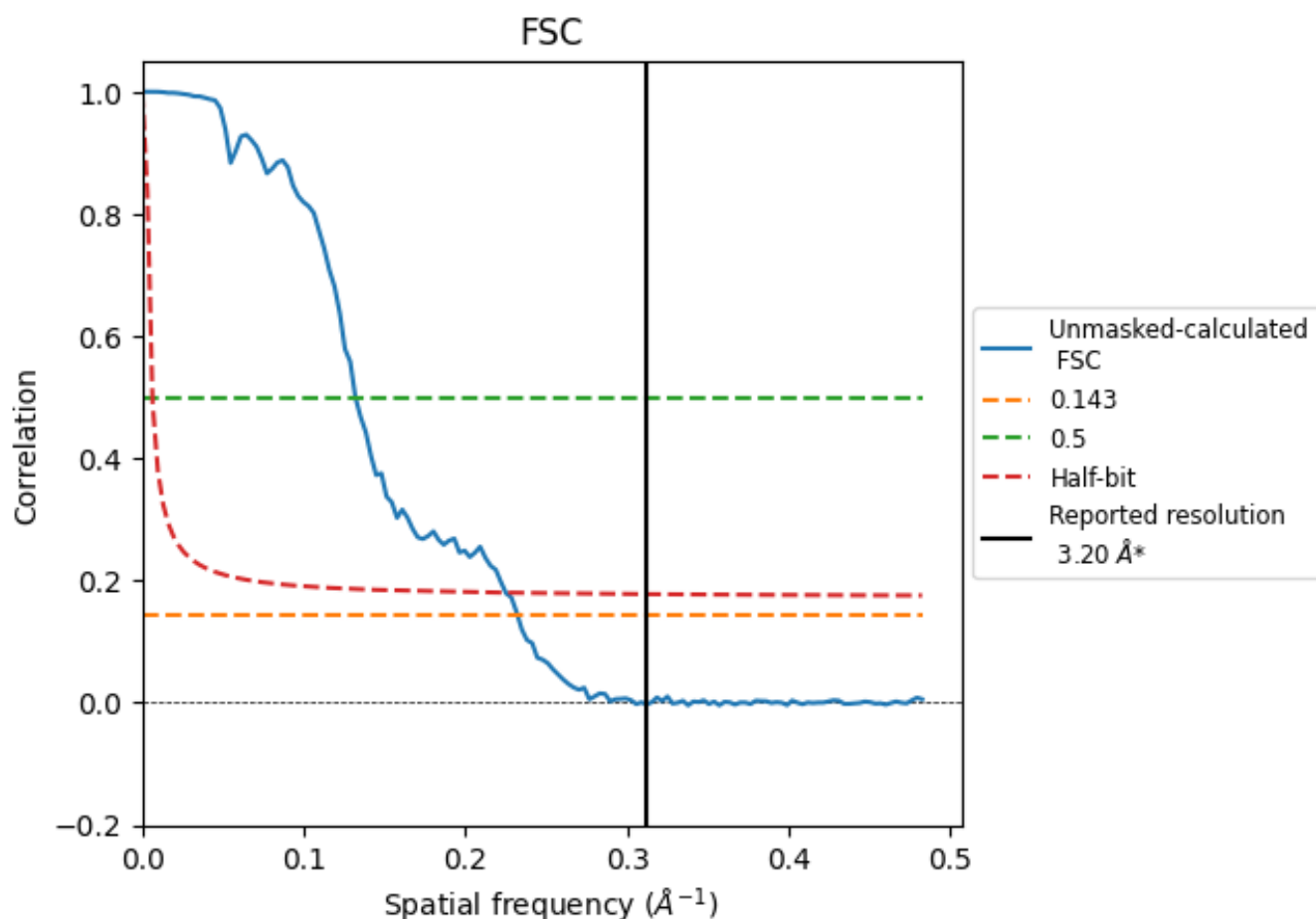


*Reported resolution corresponds to spatial frequency of 0.312 Å⁻¹

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 0.312 Å⁻¹

8.2 Resolution estimates [i](#)

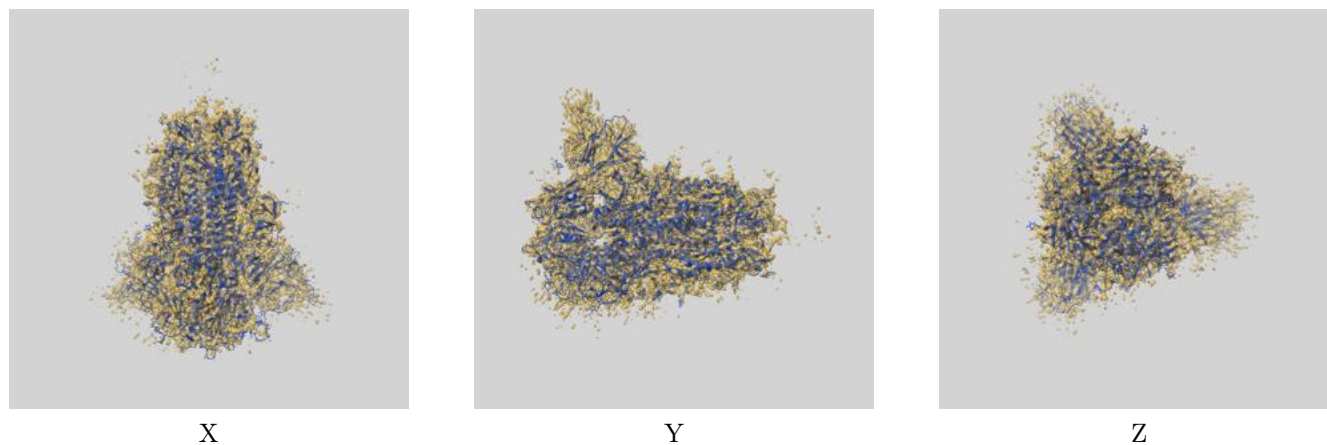
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.20	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	4.31	7.58	4.44

*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 4.31 differs from the reported value 3.2 by more than 10 %

9 Map-model fit [i](#)

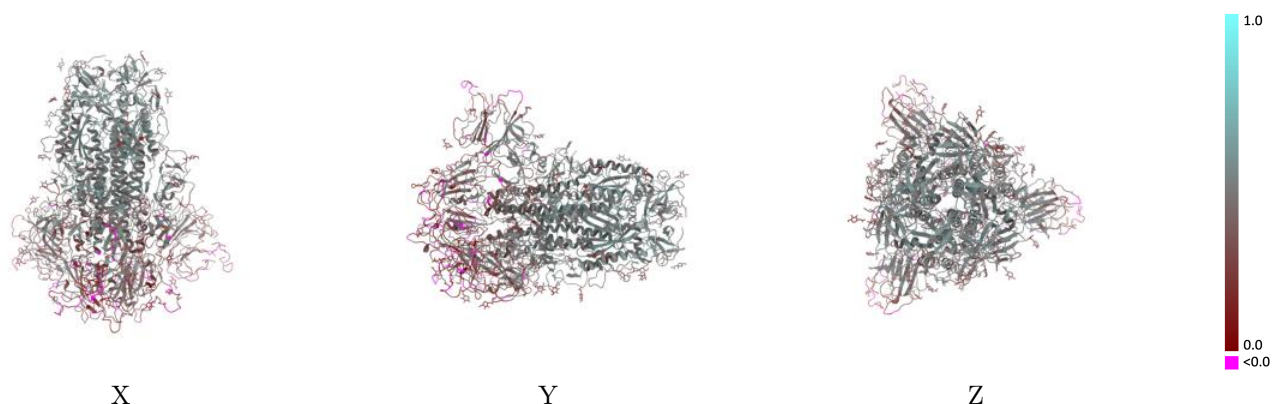
This section contains information regarding the fit between EMDB map EMD-38683 and PDB model 8XUT. Per-residue inclusion information can be found in section [3](#) on page [10](#).

9.1 Map-model overlay [i](#)



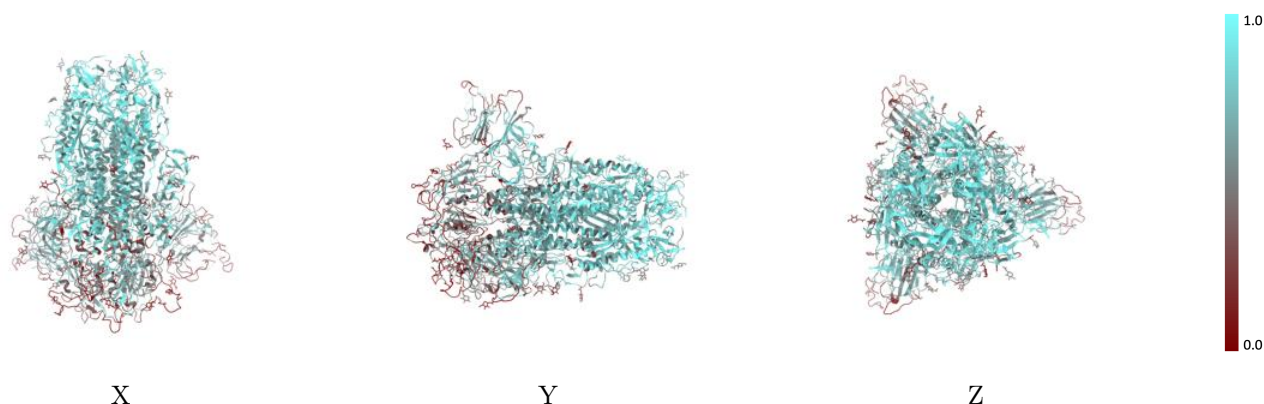
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



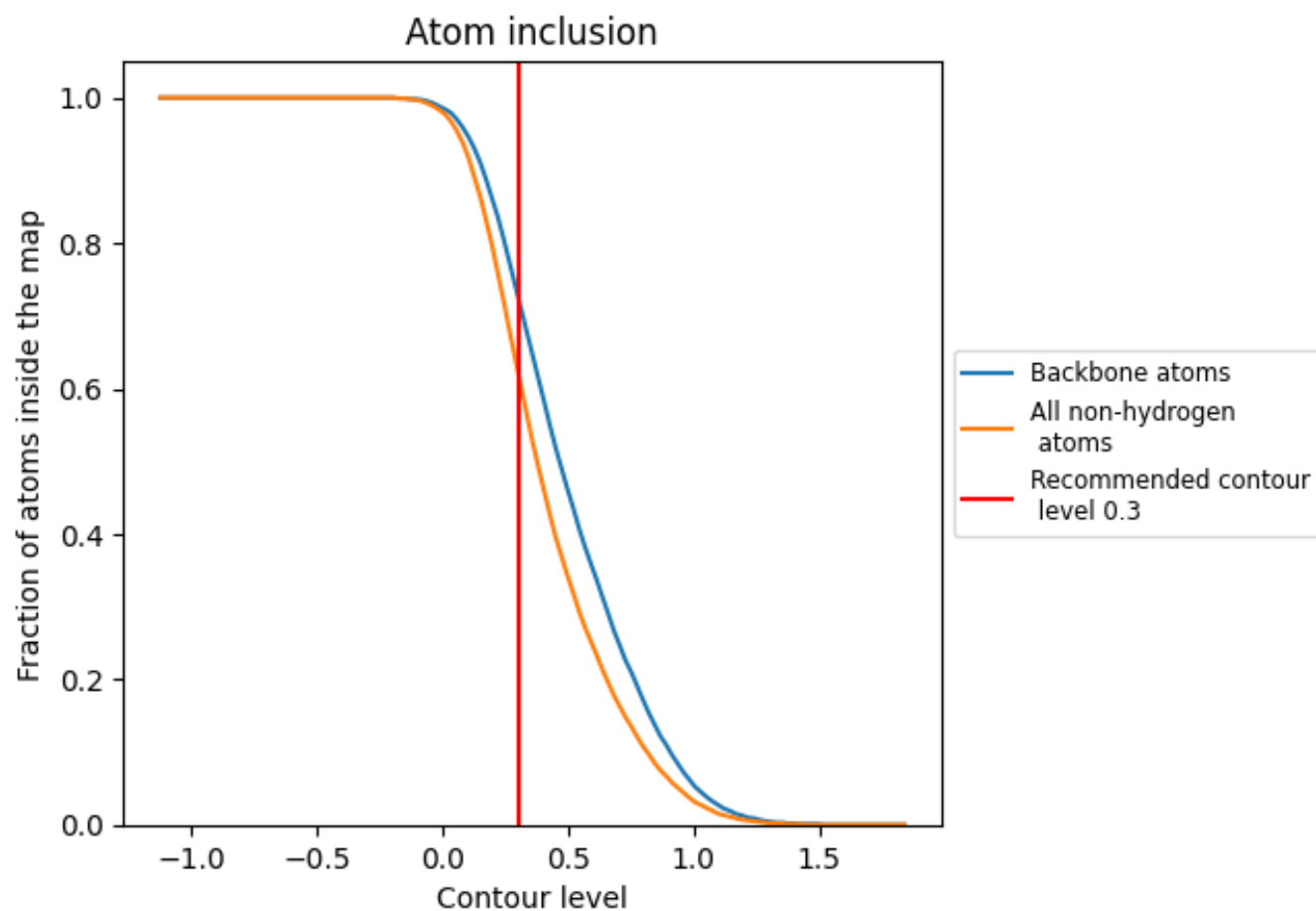
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.3).

9.4 Atom inclusion [i](#)



At the recommended contour level, 73% of all backbone atoms, 62% 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 (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6230	0.3980
A	0.6180	0.3930
B	0.6410	0.4040
C	0.6120	0.3960

