



## Full wwPDB EM Validation Report ⓘ

Oct 21, 2024 – 09:48 PM JST

PDB ID : 7W7G  
EMDB ID : EMD-32344  
Title : Structure of Mammalian NALCN-FAM155A-UNC79-UNC80 quaternary complex  
Authors : Chen, L.; Kang, Y.  
Deposited on : 2021-12-04  
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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev113  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
MapQ : 1.9.13  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

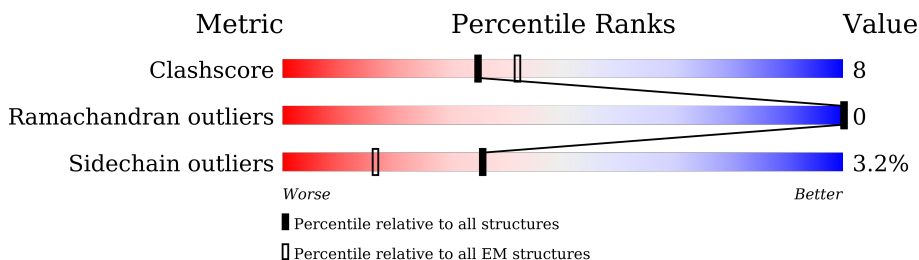
# 1 Overall quality at a glance

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)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	2654	
2	B	3326	
3	C	1738	
4	D	467	

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 38143 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 Protein unc-79 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1528	Total	C	N	O	S	0	0
			12097	7833	1998	2161	105		

- Molecule 2 is a protein called Protein unc-80 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	1711	Total	C	N	O	S	0	0
			13777	8900	2351	2430	96		

- Molecule 3 is a protein called Sodium leak channel non-selective protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	1346	Total	C	N	O	S	0	0
			10847	7164	1777	1821	85		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	52	SER	PRO	conflict	UNP Q6Q760
C	748	ALA	THR	conflict	UNP Q6Q760

- Molecule 4 is a protein called Transmembrane protein FAM155A.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	173	Total	C	N	O	S	0	0
			1378	875	212	275	16		

- Molecule 5 is ZINC ION (three-letter code: ZN) (formula: Zn) (labeled as "Ligand of Interest" by depositor).

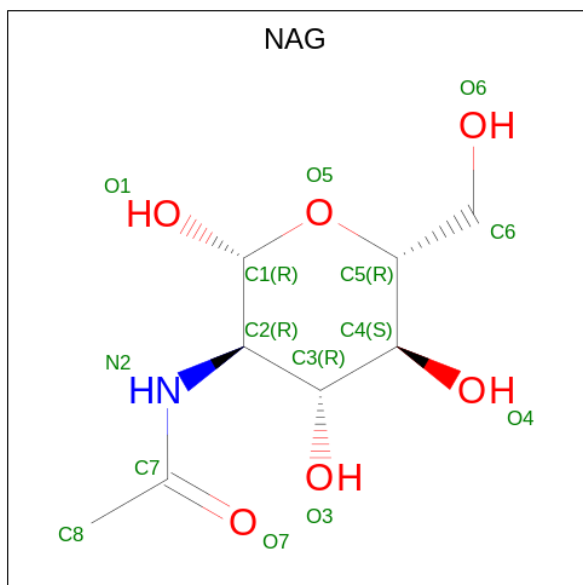
Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	

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Mol	Chain	Residues	Atoms		AltConf
5	B	1	Total	Zn	0
			1	1	

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ) (labeled as "Ligand of Interest" by depositor).



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



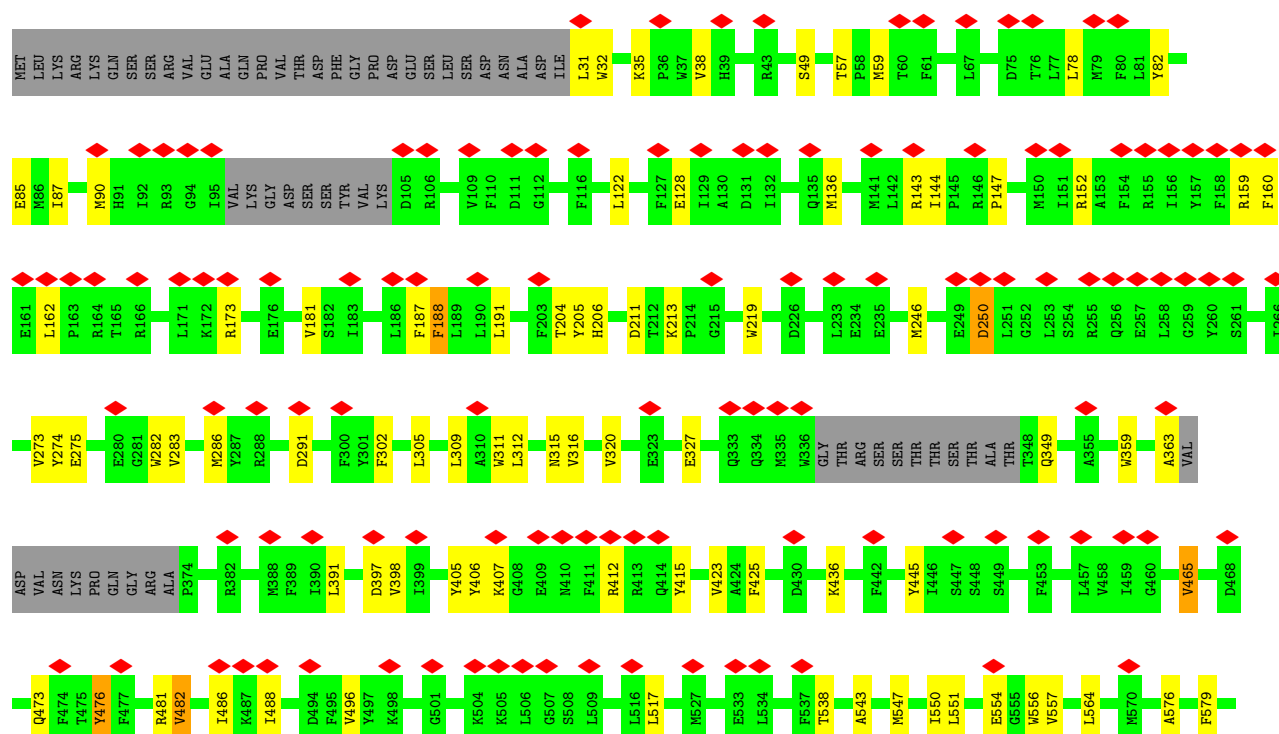
ASN	PHE	GLY	HIS	PRO	PRO	GLY	GLY	ARG	THR	ILE	ASP	PHE	ASP	ASP	CYS	GLU	D740	Q758	Q762	D763	D764	G765	I766	L774	S775	I779	S780	I781	W790	GLY	GLY	SER	HIS	SER	CYS	GLN	ALA	LYS	LYS	LYS	ALA	THR	THR	GLU	ARG	C905	P927	R932	L933	V934	E935	P936	THR	ASP	SER
GLU	ASP	SER	LEU	LEU	LEU	SER	SER	ARG	PRO	PRO	GLU	ARG	PRO	GLU	GLY	GLU	D740	Q758	Q762	D763	D764	G765	I766	L774	S775	I779	S780	I781	W790	GLY	GLY	SER	HIS	SER	CYS	GLN	ALA	LYS	LYS	LYS	ALA	THR	THR	GLU	ARG	C905	P927	R932	L933	V934	E935	P936	THR	ASP	SER
W910	D917	I918	L919	H922	L926	C930	H932	L931	E934	C935	L936	Y937	I950	M954	L955	V962	Q969	L984	G997	S1001	F1008	E1009	A1010	V1011	E1012	V1016	R1019	K1028	L1032	H1038	F1043	T1045	D1049	V1050	R1057	L1060																			
L1061	R1067	L1070	D1087	T1090	L1096	Q1103	D1104	I1105	F1112	F1113	V1114	N1115	R1116	F1117	E1118	T1119	L1122	E1123	C1130	P1135	F1136	I1140	T1141	R1144	T1145	N1146	V1147	A1148	N1149	L1150	T1158	R1162	R1165	R1172	S1173	S1177	V1178	P1181	ALA	GLU															
LYS	ARG	ALA	LEU	SER	LEU	PRO	GLU	THR	THR	LYS	ILE	PRO	VAL	ARG	LEU	THR	ARG	GLY	GLY	THR	PRO	GLU	GLN	THR	PRO	GLY	GLN	GLN	SER	PRO	ASN	T1230	I1231	K1232	D1233	D1238	I1241	D1242	H1243	Q1244	T1245	V1246	I1250												
M1284	K1285	R1289	D1280	E1281	E1285	S1286	D1267	T1276	R1279	L1285	F1294	M1301	R1302	M1318	V1335	C1339	H1346	Q1350	P1351	P1352	R1353	C1354	S1355	L1356	I1363	R1364	Q1365	M1366	L1372	L1375	Y1376	K1377	Y1378	R1381	D1382	L1389	I1393	N1398																	
Q1403	K1408	PRO	HIS	ALA	THR	ALA	GLY	PRO	GLY	LEU	TYR	THR	ASP	ASN	ASN	ILE	SER	ARG	TYR	ALA	SER	GLU	LYS	GLU	LYS	GLY	GLU	ASP	VAL	PHE	ASP	ASP	GLU	VAL	GLN	GLY	THR	PHE	PHE	ALA	ARG	LEU	LEU	ASP	ILE	ARG	ILE	GLY	ASN	GLY					
GLY	SER	ARG	MET	LYS	GLY	GLN	VAL	PRO	GLY	VAL	MET	TYR	ASN	VAL	GLN	SER	ILE	GLY	GLU	TYR	ALA	GLU	LYS	GLU	LYS	GLY	GLU	ASP	VAL	PHE	ASP	ASP	GLU	VAL	GLN	GLY	THR	PHE	PHE	ALA	ARG	LEU	LEU	ASP	ILE	ARG	ILE	GLY	ASN	GLY					
ALA	ASP	SER	LEU	PHE	THR	LEU	ASP	HIS	ARG	LYS	ARG	CYS	ASP	ILE	ASP	ARG	CYS	GLY	ILE	ASP	ILE	ASN	GLY	ALA	GLN	ALA	GLY	ALA	TYR	ILE	ASP	ILE	GLN	TYR	ALA	GLY	ASP	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN	GLN					
GLY	THR	GLY	PHE	GLN	ILE	ARG	ARG	PRO	VAL	PRO	ILE	PRO	GLY	VAL	GLY	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL	VAL					
THR	SER	ASP	SER	ASP	SER	VAL	PHE	GLY	PRO	PRO	VAL	ARG	GLY	ILE	ARG	VAL	ASN	GLY	SER	ASP	GLY	GLU	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY				
GLN	VAL	SER	VAL	GLY	ASP	CYS	SER	LYS	ASP	LYS	ASP	GLY	ASP	GLY	ASN	HIS	GLN	SER	GLY	THR	ALA	GLY	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA	ALA				
LYS	ARG	ASP	LEU	GLN	LYS	SER	GLY	ASN	PRO	GLY	THR	ASN	PRO	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY				
ALA	GLY	SER	THR	GLN	ASN	PRO	GLY	LEU	THR	ASN	GLY	SER	GLY	THR	ILE	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY				
LYS	ASP	PRO	ASP	PRO	GLY	LEU	THR	ASN	THR	ILE	GLY	SER	GLY	THR	TRP	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY			
ARG	GLN	LEU	HIS	GLN	SER	ALA	PRO	HIS	ASN	ILE	SER	GLY	THR	TRP	THR	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY	GLY		

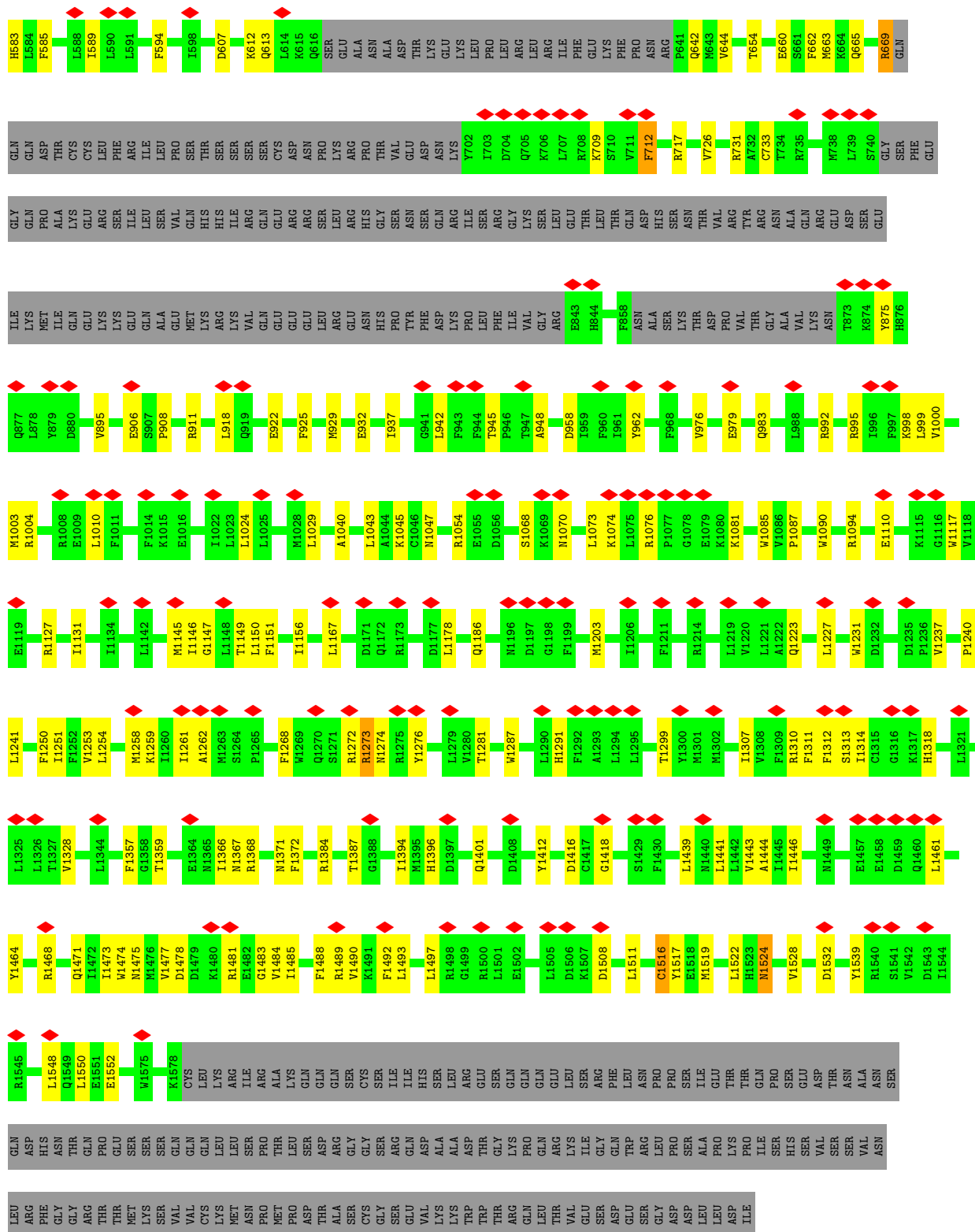






SER	ALA	GLU	PRO	SER	ILE	GLU	PRO	GLY	LEU	ASN	THR	GLY	ALA	ASN	GLU	THR	ARG	LEU	THR	PRO	THR	ASN	VAL	ASN	VAL	ASP	GLY	ASP	SER	VAL	ASP	SER	LEU	ARG	GLU	SER	ASN	HIS	ILE	SER		





● Molecule 4: Transmembrane protein FAM155A



[illegible]

## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	275170	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	50	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	Not provided	
Image detector	GATAN K2 QUANTUM (4k x 4k)	Depositor
Maximum map value	8.606	Depositor
Minimum map value	-0.139	Depositor
Average map value	0.087	Depositor
Map value standard deviation	0.155	Depositor
Recommended contour level	0.95	Depositor
Map size ( $\text{\AA}$ )	370.72, 370.72, 370.72	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	1.324, 1.324, 1.324	Depositor

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 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	0.27	0/12360	0.43	0/16769
2	B	0.28	0/14084	0.46	0/19082
3	C	0.26	0/11121	0.43	0/15080
4	D	0.25	0/1410	0.41	0/1913
All	All	0.27	0/38975	0.44	0/52844

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12097	0	12285	230	0
2	B	13777	0	14013	239	0
3	C	10847	0	10959	138	0
4	D	1378	0	1253	23	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
6	C	42	0	39	1	0
All	All	38143	0	38549	596	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 8.

All (596) 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:1545:HIS:HE1	2:B:1553:CYS:SG	1.88	0.97
1:A:1162:ARG:HE	1:A:1231:ILE:HG23	1.49	0.77
3:C:173:ARG:HH21	3:C:327:GLU:HB2	1.54	0.73
2:B:1214:ALA:O	2:B:1219:ARG:NH1	2.22	0.72
3:C:205:TYR:HA	3:C:246:MET:O	1.90	0.71
1:A:218:PRO:HG3	1:A:447:LEU:HD21	1.73	0.70
2:B:2314:SER:HA	3:C:709:LYS:HE2	1.73	0.70
2:B:1732:GLU:HG2	2:B:1734:GLY:H	1.56	0.70
2:B:38:LEU:HB2	2:B:98:LYS:HE3	1.73	0.70
1:A:2512:THR:HG1	1:A:2521:SER:N	1.88	0.69
3:C:398:VAL:HG11	3:C:482:VAL:HG12	1.75	0.69
2:B:2238:GLU:OE2	2:B:2284:ASN:ND2	2.26	0.69
1:A:2344:VAL:HG21	1:A:2391:GLU:HG3	1.73	0.69
3:C:613:GLN:HB3	3:C:1550:LEU:HD21	1.73	0.69
1:A:656:SER:HB3	1:A:781:ILE:HD11	1.75	0.68
1:A:646:VAL:O	1:A:762:GLN:NE2	2.26	0.68
1:A:2258:VAL:HG12	1:A:2306:PHE:HD1	1.56	0.68
1:A:1067:ARG:HG3	1:A:1105:ILE:HG22	1.76	0.67
2:B:2569:THR:HG22	2:B:2635:MET:HB2	1.76	0.67
2:B:360:LEU:HD12	2:B:680:ILE:HD11	1.76	0.67
1:A:1165:ARG:NH2	1:A:1242:ASP:OD1	2.28	0.67
1:A:1244:GLN:NE2	2:B:1930:GLU:OE1	2.28	0.67
2:B:2910:ARG:HB3	2:B:2955:ARG:HD3	1.78	0.66
3:C:188:PHE:HB3	3:C:309:LEU:HD21	1.76	0.66
1:A:225:PHE:O	1:A:232:LYS:NZ	2.28	0.65
1:A:834:VAL:HG11	1:A:1032:LEU:HD11	1.77	0.65
2:B:2554:ARG:NH1	2:B:2619:ASP:OD1	2.29	0.65
1:A:233:PRO:HD3	1:A:457:SER:HB3	1.79	0.65
2:B:1746:ILE:HD13	2:B:1959:ARG:HH22	1.62	0.64
2:B:1826:PRO:HB2	2:B:1829:GLN:HB2	1.78	0.64
3:C:906:GLU:HG2	3:C:918:LEU:HD13	1.77	0.64
3:C:1024:LEU:HD21	3:C:1147:GLY:HA3	1.78	0.64
3:C:1054:ARG:NH2	4:D:375:GLU:OE1	2.30	0.64
2:B:669:ILE:HA	2:B:673:ILE:HD11	1.79	0.64
3:C:1508:ASP:HB3	3:C:1511:LEU:HB3	1.79	0.64
3:C:1401:GLN:NE2	3:C:1418:GLY:O	2.31	0.64
1:A:2119:GLN:OE1	1:A:2157:LYS:NZ	2.32	0.63
2:B:97:ASN:HA	2:B:102:GLN:HE21	1.62	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:99:LEU:HD12	2:B:101:HIS:H	1.63	0.63
1:A:393:VAL:HG13	1:A:473:LEU:HD23	1.79	0.63
2:B:2432:LEU:HD13	2:B:2559:ARG:HG2	1.80	0.63
2:B:2453:THR:HG21	2:B:2465:GLU:HB2	1.80	0.63
1:A:110:LEU:HD23	1:A:147:SER:HB3	1.81	0.63
2:B:1721:TRP:O	2:B:1724:ARG:NH1	2.32	0.63
3:C:406:TYR:HB2	3:C:1040:ALA:HB1	1.80	0.63
1:A:2530:GLU:OE2	2:B:35:ARG:NH1	2.31	0.62
3:C:908:PRO:O	3:C:911:ARG:NH1	2.32	0.62
1:A:934:GLU:HB3	1:A:937:TYR:HB2	1.81	0.62
2:B:2295:LEU:O	3:C:665:GLN:NE2	2.31	0.62
2:B:1969:ASN:OD1	2:B:1971:GLN:NE2	2.33	0.62
1:A:1141:THR:O	1:A:1144:ARG:NH2	2.31	0.62
2:B:2105:GLN:HB3	2:B:2108:HIS:HB2	1.82	0.62
3:C:397:ASP:OD2	3:C:481:ARG:NH2	2.33	0.62
2:B:1344:MET:HB3	2:B:1637:LEU:HB3	1.81	0.61
2:B:1710:ARG:NH1	2:B:1928:ASP:OD2	2.33	0.61
1:A:1070:LEU:HB3	1:A:1105:ILE:HD13	1.81	0.61
1:A:1259:ARG:HH21	2:B:1987:ASP:HB2	1.65	0.61
2:B:951:ARG:HD2	2:B:1028:ARG:HD3	1.81	0.61
2:B:1667:LEU:HD13	2:B:1675:MET:HE1	1.82	0.61
1:A:445:ARG:HH12	1:A:490:ASP:HB3	1.64	0.61
4:D:237:SER:O	4:D:330:GLN:NE2	2.34	0.61
1:A:2233:ARG:HH21	1:A:2272:ARG:HH22	1.47	0.60
1:A:2409:TRP:HA	1:A:2412:HIS:HB3	1.83	0.60
2:B:357:LEU:HA	2:B:680:ILE:HD13	1.82	0.60
1:A:555:LEU:HD13	1:A:598:MET:HG2	1.83	0.60
1:A:2243:LEU:HD12	1:A:2277:LEU:HD12	1.84	0.60
2:B:361:ARG:NH1	2:B:683:CYS:SG	2.74	0.60
3:C:1045:LYS:HE3	3:C:1127:ARG:HG2	1.84	0.60
2:B:1920:LEU:HD23	2:B:1977:MET:HG3	1.84	0.60
2:B:2453:THR:OG1	2:B:2578:ARG:NH2	2.35	0.60
3:C:1471:GLN:O	3:C:1475:ASN:ND2	2.31	0.60
3:C:1010:LEU:HD13	3:C:1441:LEU:HD11	1.84	0.60
1:A:445:ARG:NH2	1:A:488:MET:SD	2.75	0.59
2:B:1724:ARG:NH2	2:B:1952:GLU:OE2	2.34	0.59
3:C:59:MET:HG3	3:C:538:THR:HB	1.83	0.59
1:A:2439:LEU:HD21	1:A:2634:GLN:HB2	1.84	0.59
1:A:133:PRO:HD2	1:A:136:LEU:HD12	1.84	0.59
1:A:2207:LEU:HD13	1:A:2213:LEU:HD12	1.84	0.59
2:B:2003:LEU:HD22	2:B:2022:THR:HG21	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2202:PRO:O	2:B:2206:ILE:HB	2.03	0.59
1:A:394:GLU:HB2	2:B:2952:PHE:HZ	1.68	0.59
1:A:2541:GLN:O	1:A:2545:HIS:ND1	2.36	0.59
4:D:335:LYS:HB2	4:D:387:ASP:HB3	1.85	0.58
2:B:2644:GLU:OE2	2:B:2647:ARG:NH1	2.37	0.58
3:C:283:VAL:HG13	3:C:1384:ARG:HD2	1.84	0.58
1:A:397:ILE:HG23	1:A:476:MET:HG3	1.86	0.58
2:B:1803:LEU:HD13	2:B:1806:LEU:HD12	1.84	0.58
3:C:1477:VAL:O	3:C:1489:ARG:NH2	2.36	0.58
1:A:1352:PRO:O	1:A:1398:ASN:ND2	2.37	0.58
1:A:1363:ILE:HA	1:A:1366:MET:HE2	1.86	0.58
1:A:624:TYR:O	1:A:629:GLN:NE2	2.37	0.58
3:C:412:ARG:NH2	3:C:415:TYR:O	2.37	0.58
3:C:1539:TYR:HE1	3:C:1548:LEU:HD21	1.68	0.58
4:D:278:GLN:O	4:D:282:HIS:ND1	2.37	0.58
3:C:998:LYS:O	3:C:1004:ARG:NH1	2.37	0.58
3:C:1186:GLN:O	3:C:1471:GLN:NE2	2.36	0.58
1:A:2469:HIS:O	1:A:2472:VAL:HG22	2.04	0.57
3:C:312:LEU:HD22	3:C:1446:ILE:HD11	1.86	0.57
1:A:2396:ASN:ND2	1:A:2457:PRO:O	2.37	0.57
2:B:1178:LEU:HD21	2:B:1326:LEU:HD22	1.86	0.57
1:A:2065:LEU:HA	1:A:2068:MET:HE2	1.86	0.57
2:B:2809:LEU:HD11	2:B:2884:LEU:HD21	1.85	0.57
3:C:1357:PHE:HB2	3:C:1372:PHE:HD2	1.69	0.57
1:A:617:ILE:HG12	1:A:635:TRP:HE1	1.70	0.57
1:A:184:PRO:HA	1:A:187:HIS:CE1	2.39	0.57
2:B:2334:ARG:HH11	2:B:2397:SER:HB3	1.70	0.57
2:B:2791:GLY:HA3	2:B:2872:CYS:HB3	1.84	0.57
3:C:585:PHE:O	3:C:589:ILE:HB	2.04	0.57
2:B:2109:TYR:HB3	2:B:2142:LEU:HD22	1.87	0.57
1:A:1376:TYR:OH	2:B:1763:PHE:O	2.20	0.57
1:A:2223:LEU:HD13	1:A:2235:LEU:HD21	1.86	0.57
1:A:2564:LEU:HB3	1:A:2572:PHE:HB2	1.86	0.57
1:A:2348:LEU:HD22	1:A:2433:LEU:HD11	1.85	0.57
3:C:311:TRP:O	3:C:315:ASN:ND2	2.38	0.57
2:B:2234:ILE:HG22	2:B:2281:THR:HG21	1.86	0.56
3:C:1287:TRP:NE1	3:C:1299:THR:O	2.38	0.56
2:B:1561:CYS:HB3	2:B:1637:LEU:HB2	1.87	0.56
1:A:576:LEU:HB3	1:A:635:TRP:HB2	1.88	0.56
1:A:2574:LYS:HE2	2:B:191:LEU:HD11	1.86	0.56
2:B:1525:ASN:O	2:B:1525:ASN:ND2	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1926:MET:HE2	2:B:1943:GLN:HG2	1.86	0.56
2:B:2555:GLU:HG2	2:B:2558:ARG:HH22	1.70	0.56
2:B:1634:VAL:C	2:B:1636:SER:H	2.09	0.56
3:C:181:VAL:HG21	3:C:320:VAL:HG21	1.87	0.56
2:B:1320:ASP:O	2:B:1563:ARG:NH1	2.35	0.56
1:A:2431:ILE:HD11	1:A:2469:HIS:HB3	1.88	0.56
1:A:775:SER:O	1:A:779:ILE:HG12	2.06	0.56
1:A:2379:HIS:ND1	1:A:2634:GLN:OE1	2.30	0.56
2:B:359:ARG:O	2:B:362:HIS:ND1	2.38	0.56
2:B:1919:VAL:HB	2:B:1961:PHE:HZ	1.71	0.56
1:A:1119:THR:O	1:A:1123:GLU:HG2	2.06	0.55
2:B:2089:GLU:HB2	2:B:2122:ASN:HB3	1.88	0.55
2:B:2270:GLU:HG2	2:B:2315:ASN:HD22	1.72	0.55
2:B:2946:ASP:HB3	2:B:2951:ARG:HH21	1.70	0.55
1:A:1250:ILE:O	1:A:1254:MET:HG2	2.07	0.55
3:C:275:GLU:HG3	3:C:557:VAL:HG21	1.89	0.55
2:B:2415:ILE:HG23	2:B:2438:LEU:HD21	1.89	0.55
1:A:181:THR:HB	1:A:186:TYR:HD2	1.72	0.55
2:B:1231:HIS:HE1	2:B:1235:ARG:HE	1.55	0.55
3:C:958:ASP:OD2	3:C:995:ARG:NH2	2.37	0.55
1:A:490:ASP:O	1:A:494:SER:N	2.31	0.55
1:A:1135:PRO:HB2	1:A:1246:VAL:HG21	1.87	0.55
1:A:88:VAL:HG13	1:A:89:PRO:HD3	1.89	0.54
1:A:1302:ARG:NH1	1:A:1339:CYS:O	2.36	0.54
1:A:2403:VAL:HG13	1:A:2410:LEU:HD23	1.88	0.54
3:C:1478:ASP:O	3:C:1481:ARG:NH2	2.39	0.54
1:A:617:ILE:HG21	1:A:636:LEU:HD22	1.89	0.54
2:B:2313:GLU:HG2	3:C:709:LYS:HE3	1.89	0.54
2:B:1201:PRO:HG2	2:B:1206:LEU:HD13	1.88	0.54
3:C:391:LEU:HD13	3:C:488:ILE:HG22	1.88	0.54
1:A:1130:CYS:HB3	1:A:1232:LYS:HE2	1.88	0.54
2:B:665:LEU:HD22	2:B:795:MET:HG3	1.89	0.54
3:C:128:GLU:OE2	3:C:143:ARG:NH2	2.40	0.54
1:A:779:ILE:HG23	1:A:902:LEU:HD22	1.90	0.54
1:A:2174:ALA:O	1:A:2178:GLU:HG2	2.08	0.54
2:B:2477:GLN:HE21	2:B:2597:LEU:H	1.55	0.54
1:A:551:LEU:HB3	1:A:594:VAL:HG11	1.90	0.54
1:A:2574:LYS:HE3	2:B:87:HIS:CE1	2.43	0.54
2:B:2008:VAL:HG21	2:B:2053:LYS:HG3	1.90	0.54
2:B:2781:ASN:OD1	2:B:2974:LYS:NZ	2.35	0.54
3:C:159:ARG:NH1	3:C:162:LEU:O	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:473:GLN:O	3:C:476:TYR:HB2	2.08	0.54
1:A:39:LEU:HD12	1:A:105:THR:HG21	1.90	0.54
1:A:2526:LEU:HB3	2:B:36:PRO:HB3	1.89	0.54
2:B:2763:SER:HB3	2:B:2807:LEU:HD23	1.88	0.54
3:C:1548:LEU:HD23	3:C:1552:GLU:HG2	1.90	0.53
1:A:1114:VAL:O	1:A:1118:GLU:HG2	2.08	0.53
1:A:1285:LEU:HD13	1:A:1335:VAL:HG21	1.89	0.53
1:A:1238:ASP:HB2	1:A:1241:ILE:HG12	1.90	0.53
2:B:1332:ASN:HB3	2:B:1333:PRO:HD3	1.90	0.53
2:B:2313:GLU:HA	2:B:2319:ARG:HD2	1.89	0.53
1:A:43:SER:HB2	1:A:105:THR:HG22	1.91	0.53
2:B:1721:TRP:NE1	2:B:1952:GLU:OE1	2.35	0.53
3:C:305:LEU:HG	3:C:309:LEU:HD12	1.90	0.53
1:A:758:GLN:HE21	1:A:762:GLN:HE21	1.57	0.53
3:C:1464:TYR:OH	3:C:1468:ARG:NH2	2.42	0.53
3:C:1367:ASN:O	3:C:1371:ASN:ND2	2.40	0.53
2:B:2179:ILE:HG13	2:B:2187:HIS:CD2	2.43	0.53
1:A:1267:ASP:N	1:A:1267:ASP:OD1	2.41	0.53
1:A:497:GLU:OE2	1:A:560:TYR:OH	2.27	0.53
1:A:836:PRO:HB3	1:A:1028:LYS:HB3	1.91	0.52
3:C:564:LEU:HD21	3:C:576:ALA:HB2	1.90	0.52
4:D:312:ASP:OD1	4:D:312:ASP:N	2.42	0.52
1:A:2487:HIS:O	1:A:2490:SER:OG	2.24	0.52
3:C:1259:LYS:HE3	3:C:1268:PHE:HE1	1.73	0.52
1:A:1356:LEU:O	1:A:1364:ARG:NE	2.42	0.52
1:A:1375:LEU:HD21	1:A:1389:LEU:HD21	1.90	0.52
2:B:2588:GLU:HG3	2:B:2590:ARG:H	1.74	0.52
2:B:332:ASP:O	2:B:356:TYR:OH	2.26	0.52
2:B:2947:GLN:HA	2:B:2951:ARG:HD2	1.92	0.52
1:A:496:VAL:HG13	1:A:500:LYS:HD3	1.91	0.52
2:B:2297:GLY:HA2	2:B:2300:TRP:HD1	1.74	0.52
3:C:144:ILE:O	3:C:147:PRO:HD2	2.10	0.52
2:B:189:VAL:HG11	2:B:335:VAL:HA	1.92	0.52
1:A:85:LEU:HD13	1:A:128:THR:HG22	1.92	0.52
2:B:1732:GLU:HB3	2:B:1735:ALA:HB2	1.91	0.52
2:B:1961:PHE:HB3	2:B:1974:LEU:HD13	1.91	0.52
2:B:336:LEU:HD12	2:B:339:LEU:HD12	1.91	0.52
2:B:1711:LEU:HD21	2:B:1941:VAL:HG21	1.91	0.52
2:B:2021:ALA:O	2:B:2024:THR:OG1	2.28	0.52
1:A:636:LEU:HD11	1:A:646:VAL:HG21	1.91	0.51
2:B:2366:GLN:NE2	2:B:2370:ASP:OD1	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:227:LEU:HA	4:D:230:PHE:HE2	1.75	0.51
1:A:2577:PRO:HG2	2:B:187:LEU:HD22	1.93	0.51
2:B:1543:CYS:SG	2:B:1550:HIS:ND1	2.83	0.51
1:A:1381:ARG:NH2	1:A:2058:ASP:OD1	2.42	0.51
2:B:1757:MET:HG2	2:B:2035:GLY:HA3	1.91	0.51
3:C:273:VAL:HG13	3:C:305:LEU:HD11	1.93	0.51
3:C:945:THR:HB	3:C:948:ALA:HB2	1.92	0.51
1:A:2543:MET:SD	1:A:2586:ASN:ND2	2.83	0.51
1:A:918:ILE:O	1:A:922:MET:HG3	2.10	0.51
2:B:2409:PHE:CZ	2:B:2414:ALA:HB2	2.46	0.51
3:C:1522:LEU:HD23	3:C:1532:ASP:HB3	1.93	0.51
1:A:116:ASP:OD1	1:A:116:ASP:N	2.43	0.51
1:A:175:MET:HE1	1:A:212:GLY:HA3	1.92	0.51
1:A:2594:LEU:H	1:A:2594:LEU:HD12	1.76	0.51
1:A:517:ASP:N	1:A:517:ASP:OD1	2.41	0.51
1:A:1382:ASP:N	1:A:1382:ASP:OD1	2.44	0.51
1:A:2468:ASP:O	1:A:2471:ILE:HG12	2.10	0.51
1:A:2533:SER:HB3	2:B:34:LEU:HD12	1.91	0.51
2:B:1646:ILE:HG22	2:B:1731:MET:HA	1.92	0.51
2:B:2293:PHE:HA	2:B:2296:SER:O	2.11	0.51
1:A:2049:LEU:HD13	1:A:2067:ILE:HG23	1.93	0.50
1:A:2526:LEU:HD23	2:B:36:PRO:HA	1.92	0.50
3:C:1081:LYS:NZ	6:C:2002:NAG:O5	2.38	0.50
1:A:1049:ASP:OD1	1:A:1050:VAL:N	2.44	0.50
2:B:2334:ARG:HH22	2:B:2407:LEU:HD13	1.75	0.50
1:A:1259:ARG:NH2	2:B:1987:ASP:HB2	2.25	0.50
1:A:2389:ALA:O	1:A:2393:SER:N	2.42	0.50
2:B:1681:ALA:HA	2:B:1727:VAL:HG22	1.94	0.50
2:B:2596:LEU:H	2:B:2596:LEU:HD23	1.77	0.50
2:B:1811:GLU:OE2	2:B:1814:ARG:NH2	2.44	0.50
3:C:612:LYS:HZ1	3:C:1167:LEU:HB3	1.76	0.50
2:B:53:LEU:O	2:B:74:ARG:NH2	2.42	0.50
2:B:841:ASP:HB3	2:B:844:GLN:HB2	1.94	0.50
4:D:227:LEU:HB2	4:D:241:TRP:HE3	1.77	0.50
1:A:2247:ILE:HD13	1:A:2303:LEU:HD21	1.93	0.50
3:C:204:THR:O	3:C:206:HIS:ND1	2.40	0.50
4:D:360:VAL:HG13	4:D:362:TYR:HE1	1.77	0.50
3:C:644:VAL:HG21	3:C:663:MET:HG3	1.94	0.50
3:C:1223:GLN:OE1	3:C:1310:ARG:NH1	2.45	0.50
1:A:1011:VAL:HG12	1:A:1061:LEU:HD12	1.93	0.49
2:B:216:GLN:HA	2:B:219:TRP:CE3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:CYS:O	1:A:559:PRO:HD2	2.12	0.49
1:A:2213:LEU:HD21	1:A:2246:VAL:HG13	1.93	0.49
2:B:218:MET:O	2:B:351:TRP:NE1	2.35	0.49
2:B:2313:GLU:HA	2:B:2319:ARG:HH11	1.78	0.49
2:B:2664:ILE:HG12	2:B:2671:ARG:HG3	1.95	0.49
2:B:1985:ILE:HG22	2:B:1987:ASP:H	1.76	0.49
3:C:1485:ILE:HB	3:C:1489:ARG:HB2	1.95	0.49
1:A:2237:GLU:HB3	1:A:2238:PRO:HD3	1.94	0.49
3:C:1473:ILE:HG21	3:C:1497:LEU:HD23	1.95	0.49
1:A:2495:PHE:CG	1:A:2556:HIS:HB3	2.47	0.49
1:A:2558:ILE:O	1:A:2561:MET:HG2	2.13	0.49
2:B:2417:LEU:O	2:B:2421:VAL:HG23	2.12	0.49
2:B:2045:MET:HB3	2:B:2051:GLU:HA	1.93	0.49
3:C:32:TRP:O	3:C:35:LYS:NZ	2.40	0.49
3:C:486:ILE:HD11	3:C:496:VAL:HG21	1.95	0.49
3:C:1253:VAL:HG22	3:C:1281:THR:HB	1.95	0.49
1:A:2275:PHE:HB2	1:A:2278:SER:HB3	1.94	0.49
2:B:2308:VAL:HG12	2:B:2318:LEU:HD21	1.93	0.49
2:B:2802:GLN:NE2	2:B:2876:GLN:O	2.38	0.49
3:C:922:GLU:OE1	3:C:992:ARG:NH1	2.36	0.49
3:C:937:ILE:HG12	3:C:942:LEU:HD13	1.94	0.48
1:A:629:GLN:NE2	1:A:661:SER:OG	2.46	0.48
1:A:2557:VAL:O	1:A:2560:LEU:HB3	2.13	0.48
3:C:405:TYR:CZ	3:C:407:LYS:HE3	2.49	0.48
3:C:1273:ARG:H	3:C:1273:ARG:HE	1.61	0.48
2:B:1926:MET:SD	2:B:1946:LEU:HD12	2.53	0.48
2:B:2109:TYR:CE2	2:B:2144:HIS:HB2	2.48	0.48
2:B:2487:THR:O	2:B:2611:SER:OG	2.30	0.48
3:C:159:ARG:NH1	3:C:160:PHE:O	2.45	0.48
1:A:1060:LEU:HD21	2:B:2170:LEU:HD11	1.95	0.48
2:B:2068:VAL:HG22	2:B:2140:LEU:HB2	1.94	0.48
1:A:910:MET:HG3	1:A:919:LEU:HD22	1.95	0.48
1:A:2064:LEU:HD21	1:A:2108:LEU:HD13	1.96	0.48
2:B:2372:LEU:HG	2:B:2409:PHE:HE2	1.79	0.48
1:A:2546:ASN:HB3	1:A:2549:MET:HG2	1.95	0.48
3:C:211:ASP:OD1	3:C:211:ASP:N	2.42	0.48
3:C:517:LEU:HD21	3:C:551:LEU:HD22	1.96	0.48
3:C:250:ASP:OD1	3:C:250:ASP:N	2.47	0.48
2:B:1228:ARG:HD2	2:B:1626:MET:SD	2.53	0.48
2:B:2633:MET:SD	2:B:2681:SER:OG	2.64	0.48
1:A:897:PRO:HG2	1:A:900:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:49:SER:HB2	3:C:78:LEU:HD13	1.96	0.47
1:A:904:TYR:CD1	1:A:954:MET:HE1	2.49	0.47
1:A:2384:LEU:O	1:A:2387:ILE:HG12	2.13	0.47
2:B:2562:GLU:HG3	2:B:2627:GLY:HA3	1.96	0.47
3:C:82:TYR:HA	3:C:85:GLU:HG3	1.97	0.47
3:C:191:LEU:HB2	3:C:1311:PHE:HE2	1.79	0.47
2:B:2547:GLU:OE2	2:B:2551:ARG:NE	2.47	0.47
4:D:347:GLN:OE1	4:D:370:CYS:N	2.47	0.47
1:A:997:GLY:O	1:A:1001:SER:OG	2.28	0.47
1:A:2246:VAL:HA	1:A:2250:ALA:HB3	1.97	0.47
1:A:2574:LYS:HZ3	2:B:187:LEU:HD11	1.79	0.47
3:C:1490:VAL:HG11	3:C:1519:MET:HG3	1.96	0.47
2:B:2573:LYS:HD3	2:B:2634:GLU:HB3	1.96	0.47
2:B:2788:LEU:O	2:B:2792:SER:OG	2.23	0.47
3:C:1146:ILE:O	3:C:1150:LEU:N	2.40	0.47
2:B:866:HIS:NE2	2:B:872:CYS:HB3	2.29	0.47
3:C:1047:ASN:OD1	3:C:1047:ASN:N	2.46	0.47
3:C:1484:VAL:HA	3:C:1528:VAL:O	2.15	0.47
2:B:2096:LEU:HD23	2:B:2142:LEU:HD11	1.97	0.47
3:C:87:ILE:HA	3:C:90:MET:HG2	1.96	0.47
3:C:979:GLU:N	3:C:983:GLN:OE1	2.42	0.47
3:C:1068:SER:OG	3:C:1070:ASN:OD1	2.31	0.47
3:C:1110:GLU:OE2	3:C:1396:HIS:NE2	2.47	0.47
1:A:2597:ARG:O	1:A:2601:ILE:HG12	2.15	0.47
2:B:1572:TYR:CZ	2:B:1626:MET:HG2	2.50	0.47
1:A:2058:ASP:OD1	1:A:2058:ASP:N	2.46	0.47
2:B:336:LEU:HB2	2:B:356:TYR:OH	2.14	0.47
2:B:1950:LEU:O	2:B:1954:PRO:HG3	2.15	0.47
3:C:312:LEU:O	3:C:316:VAL:HG23	2.14	0.47
1:A:175:MET:HE3	2:B:2917:VAL:HG21	1.97	0.46
2:B:2738:PRO:HB2	2:B:2740:PRO:HD2	1.97	0.46
1:A:1012:GLU:O	1:A:1016:VAL:HG23	2.15	0.46
2:B:2456:VAL:HG12	2:B:2457:GLU:H	1.80	0.46
1:A:452:ILE:HG13	1:A:500:LYS:HE3	1.98	0.46
1:A:2396:ASN:O	1:A:2397:HIS:ND1	2.48	0.46
4:D:361:ILE:HG22	4:D:363:GLY:H	1.80	0.46
1:A:2353:ASP:HB2	1:A:2356:THR:HG23	1.97	0.46
1:A:1165:ARG:HD3	1:A:1165:ARG:HA	1.68	0.46
2:B:96:ARG:NH2	2:B:102:GLN:O	2.49	0.46
2:B:2179:ILE:HG13	2:B:2187:HIS:HD2	1.80	0.46
2:B:2554:ARG:HD3	2:B:2619:ASP:OD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:642:GLN:HG2	3:C:660:GLU:HG3	1.96	0.46
1:A:211:TYR:OH	2:B:2912:ARG:NH1	2.48	0.46
1:A:1276:THR:HG23	1:A:1279:ARG:NH2	2.31	0.46
1:A:2491:LEU:HB3	1:A:2556:HIS:CD2	2.51	0.46
2:B:353:LEU:HD11	2:B:664:VAL:HG11	1.97	0.46
2:B:1316:LEU:HD23	2:B:1548:TYR:HD2	1.81	0.46
3:C:1258:MET:O	3:C:1261:ILE:HG13	2.15	0.46
4:D:342:TYR:O	4:D:345:GLU:HB2	2.16	0.46
2:B:2913:ILE:HG22	2:B:2915:ILE:HG12	1.97	0.46
3:C:1043:LEU:O	3:C:1127:ARG:NH1	2.40	0.46
2:B:2176:THR:HG22	2:B:2187:HIS:NE2	2.31	0.45
2:B:2657:LEU:HA	2:B:2660:MET:HG2	1.98	0.45
4:D:230:PHE:O	4:D:239:THR:HA	2.16	0.45
1:A:1375:LEU:HD11	1:A:1393:ILE:HD11	1.98	0.45
1:A:2468:ASP:O	1:A:2472:VAL:HG13	2.16	0.45
2:B:2626:ARG:CZ	2:B:2630:ARG:HH22	2.30	0.45
1:A:136:LEU:O	1:A:140:ILE:HG12	2.17	0.45
1:A:1158:ILE:HG22	1:A:1162:ARG:HH12	1.81	0.45
1:A:1318:MET:O	1:A:1378:TYR:OH	2.26	0.45
2:B:85:VAL:HG21	2:B:119:MET:SD	2.57	0.45
2:B:2230:LYS:O	2:B:2234:ILE:HG13	2.16	0.45
2:B:2306:LEU:HD21	2:B:2341:LEU:HD11	1.98	0.45
2:B:2466:ILE:HD13	2:B:2591:VAL:HG11	1.97	0.45
4:D:354:LEU:HD12	4:D:355:PRO:HD2	1.98	0.45
1:A:2182:MET:O	1:A:2226:ILE:HA	2.16	0.45
1:A:2590:LEU:HD13	1:A:2594:LEU:HB2	1.98	0.45
2:B:690:VAL:HG23	2:B:788:ASN:HB2	1.99	0.45
2:B:1034:LYS:HD3	2:B:1212:LEU:HD23	1.98	0.45
2:B:2041:LEU:HD11	2:B:2171:PHE:HZ	1.82	0.45
2:B:2264:ALA:HB1	2:B:2274:LEU:HD11	1.98	0.45
1:A:456:VAL:HG21	1:A:503:PHE:HB3	1.99	0.45
2:B:2087:GLN:HA	2:B:2125:TYR:HA	1.99	0.45
3:C:1273:ARG:H	3:C:1273:ARG:NE	2.14	0.45
1:A:128:THR:HB	1:A:132:PHE:CE2	2.52	0.45
1:A:2310:ASP:OD2	1:A:2336:ALA:N	2.50	0.45
2:B:1962:LEU:HD13	2:B:1999:TYR:CD1	2.52	0.45
1:A:149:LEU:HB2	1:A:150:PRO:HD3	1.99	0.45
1:A:2035:GLU:OE1	1:A:2037:TYR:OH	2.30	0.45
1:A:2463:GLY:O	1:A:2466:ILE:HG12	2.17	0.45
2:B:2792:SER:HB3	2:B:2963:ILE:HG12	1.98	0.45
4:D:195:SER:HB2	4:D:198:ALA:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1087:ASP:OD1	1:A:1173:SER:HB2	2.17	0.45
1:A:2354:MET:SD	1:A:2354:MET:N	2.74	0.45
1:A:2529:LEU:HD21	2:B:87:HIS:CE1	2.52	0.45
1:A:2552:MET:O	1:A:2555:LEU:HB2	2.16	0.45
2:B:1545:HIS:CE1	2:B:1555:LEU:HB2	2.52	0.45
3:C:1516:CYS:SG	3:C:1517:TYR:N	2.90	0.45
1:A:555:LEU:HD21	1:A:597:LYS:HD3	1.98	0.44
1:A:919:LEU:HD13	1:A:962:VAL:HG23	1.99	0.44
1:A:2144:ILE:HD13	1:A:2180:LEU:HD13	1.99	0.44
2:B:2952:PHE:HD2	2:B:2954:PRO:HD3	1.82	0.44
1:A:461:PRO:HD3	1:A:507:TRP:HE1	1.82	0.44
1:A:464:ASN:OD1	1:A:464:ASN:N	2.51	0.44
1:A:2542:LEU:HA	1:A:2545:HIS:HD1	1.82	0.44
2:B:2066:LEU:HA	2:B:2137:SER:HB2	1.99	0.44
3:C:594:PHE:HB3	3:C:1149:THR:HG21	2.00	0.44
1:A:168:LEU:HD12	1:A:168:LEU:H	1.82	0.44
2:B:93:LEU:HD11	2:B:113:LEU:HD21	1.99	0.44
2:B:2339:LEU:HD12	3:C:662:PHE:HE2	1.81	0.44
2:B:2626:ARG:NH1	2:B:2630:ARG:HH22	2.16	0.44
4:D:304:TYR:CG	4:D:351:PRO:HB3	2.52	0.44
1:A:1103:GLN:NE2	1:A:1261:GLU:OE1	2.50	0.44
2:B:26:LEU:HB3	2:B:84:HIS:CD2	2.53	0.44
2:B:928:LEU:HD13	2:B:929:GLY:H	1.83	0.44
2:B:2335:LYS:HG3	2:B:2417:LEU:HD11	1.99	0.44
2:B:2453:THR:HG22	2:B:2461:ALA:HB1	2.00	0.44
3:C:665:GLN:O	3:C:669:ARG:HG2	2.17	0.44
1:A:80:THR:O	1:A:84:LEU:HG	2.17	0.44
1:A:1294:PHE:CD1	1:A:1301:MET:HE1	2.53	0.44
1:A:2409:TRP:CZ3	1:A:2430:HIS:HB3	2.53	0.44
3:C:1311:PHE:O	3:C:1314:ILE:HG22	2.16	0.44
1:A:123:TYR:O	1:A:127:SER:N	2.49	0.44
1:A:2395:GLY:HA3	1:A:2402:ALA:HB2	1.99	0.44
1:A:103:PHE:HE2	1:A:125:MET:HE3	1.83	0.44
1:A:110:LEU:HB3	1:A:111:PRO:HD3	2.00	0.44
1:A:779:ILE:HG22	1:A:898:VAL:HG12	2.00	0.44
1:A:1008:PHE:CZ	1:A:1057:ARG:HD2	2.53	0.44
1:A:1096:LEU:HD21	1:A:1255:LYS:HD2	1.99	0.44
2:B:1224:LEU:HB3	2:B:1626:MET:HE1	1.99	0.44
2:B:2582:LEU:O	2:B:2586:ALA:N	2.51	0.44
3:C:1268:PHE:CE2	3:C:1274:ASN:HB3	2.53	0.44
1:A:2099:GLN:HG2	2:B:1833:TYR:HB3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:976:VAL:O	3:C:1412:TYR:N	2.51	0.44
1:A:827:PRO:HD2	1:A:932:HIS:O	2.18	0.43
1:A:1011:VAL:HG13	1:A:1043:PHE:CE1	2.53	0.43
2:B:2020:SER:HA	2:B:2164:GLU:HG2	1.99	0.43
2:B:2267:LEU:HD21	3:C:726:VAL:HG21	2.00	0.43
2:B:2923:ILE:HA	2:B:2927:LEU:HB3	1.99	0.43
1:A:523:LEU:HD22	1:A:554:ILE:HG12	2.00	0.43
1:A:649:GLN:HG3	1:A:774:LEU:HD11	2.00	0.43
2:B:2718:GLY:HA2	2:B:2719:PRO:HD3	1.85	0.43
3:C:1203:MET:HG2	3:C:1261:ILE:HD11	1.99	0.43
2:B:1946:LEU:HD23	2:B:1946:LEU:HA	1.75	0.43
1:A:491:GLU:H	1:A:491:GLU:HG3	1.66	0.43
2:B:1951:ILE:HD13	2:B:1951:ILE:HA	1.81	0.43
2:B:2656:ARG:HD2	2:B:2656:ARG:HA	1.76	0.43
2:B:2923:ILE:HG22	2:B:2948:LEU:HD11	1.98	0.43
3:C:291:ASP:OD1	3:C:1368:ARG:NH2	2.47	0.43
1:A:187:HIS:CD2	1:A:187:HIS:H	2.35	0.43
2:B:1533:ILE:O	2:B:1537:ASN:HB2	2.19	0.43
2:B:2639:THR:HB	2:B:2641:TRP:CE2	2.53	0.43
1:A:455:LEU:O	1:A:459:CYS:HB3	2.18	0.43
1:A:595:LEU:HD23	1:A:598:MET:HE2	2.01	0.43
1:A:832:ARG:H	1:A:832:ARG:HG3	1.56	0.43
2:B:2463:ARG:HH22	2:B:2588:GLU:HB3	1.84	0.43
2:B:2666:LYS:HB3	2:B:2668:PRO:HD2	2.01	0.43
4:D:334:ARG:NH1	4:D:334:ARG:HA	2.34	0.43
2:B:204:LEU:HD11	2:B:215:TRP:HD1	1.83	0.43
1:A:2150:LEU:HD21	1:A:2173:ILE:HG12	2.00	0.43
1:A:2529:LEU:HD21	2:B:87:HIS:NE2	2.33	0.43
1:A:2564:LEU:HD13	1:A:2572:PHE:HB2	2.01	0.43
2:B:1647:LYS:HA	2:B:1731:MET:O	2.19	0.43
2:B:1687:ALA:HB2	2:B:1694:VAL:HG11	2.01	0.43
1:A:46:LEU:HD23	1:A:109:LEU:HD13	2.01	0.43
1:A:177:ALA:O	1:A:181:THR:OG1	2.36	0.43
1:A:620:ARG:HG3	1:A:632:ALA:HB2	1.99	0.43
1:A:2574:LYS:HE2	2:B:191:LEU:HD21	2.00	0.43
2:B:1920:LEU:HB2	2:B:1921:PRO:HD3	2.01	0.43
2:B:2557:PHE:O	2:B:2561:ARG:NH1	2.52	0.43
3:C:349:GLN:HA	3:C:363:ALA:HA	2.00	0.43
2:B:2051:GLU:HG3	2:B:2055:LEU:HD12	2.00	0.43
2:B:2333:HIS:HE2	2:B:2398:LEU:HD12	1.84	0.43
3:C:895:VAL:HG12	3:C:925:PHE:HD1	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2354:MET:HB3	1:A:2432:ARG:NH1	2.33	0.42
2:B:118:TRP:NE1	2:B:122:GLU:OE1	2.52	0.42
2:B:1206:LEU:HD12	2:B:1206:LEU:HA	1.76	0.42
2:B:1912:PRO:HG2	2:B:1915:ILE:HG12	2.01	0.42
2:B:2311:ASP:HA	3:C:712:PHE:HD2	1.84	0.42
2:B:2430:ARG:NH2	3:C:669:ARG:HB2	2.34	0.42
3:C:995:ARG:HH12	3:C:999:LEU:HD11	1.83	0.42
3:C:1087:PRO:HD3	4:D:320:TRP:CZ2	2.54	0.42
3:C:1272:ARG:HB2	3:C:1273:ARG:HH21	1.83	0.42
3:C:1524:ASN:OD1	3:C:1524:ASN:N	2.52	0.42
2:B:677:ALA:HB1	2:B:795:MET:HE3	2.01	0.42
1:A:633:LEU:HD23	1:A:633:LEU:HA	1.85	0.42
1:A:1060:LEU:HD12	2:B:2228:LEU:HD13	2.02	0.42
1:A:2270:LYS:O	1:A:2274:LYS:HG3	2.20	0.42
2:B:2060:MET:HB2	2:B:2131:PRO:HB2	2.01	0.42
2:B:2647:ARG:N	2:B:2648:PRO:HD2	2.34	0.42
3:C:274:TYR:OH	3:C:583:HIS:ND1	2.33	0.42
3:C:397:ASP:HB2	3:C:425:PHE:CG	2.55	0.42
3:C:1251:ILE:O	3:C:1254:LEU:HG	2.18	0.42
2:B:2689:THR:HG22	2:B:2696:ILE:HD13	2.02	0.42
3:C:550:ILE:HA	3:C:556:TRP:HB3	2.00	0.42
1:A:2419:GLN:HB3	1:A:2480:GLN:HE22	1.84	0.42
1:A:2435:SER:HB3	1:A:2497:PHE:HB2	2.02	0.42
2:B:1219:ARG:HE	2:B:1342:LEU:HD21	1.83	0.42
2:B:2158:VAL:HG12	2:B:2222:LEU:HD21	2.01	0.42
1:A:452:ILE:HG21	1:A:500:LYS:NZ	2.34	0.42
1:A:1038:HIS:CD2	1:A:1177:SER:HG	2.37	0.42
1:A:2151:LEU:HD21	1:A:2196:PHE:CD2	2.54	0.42
1:A:2584:GLN:O	1:A:2587:THR:OG1	2.32	0.42
3:C:1156:ILE:HG12	3:C:1444:ALA:HB2	2.02	0.42
2:B:852:TYR:CE2	2:B:861:VAL:HG12	2.55	0.42
2:B:1752:SER:OG	2:B:1753:PRO:HD3	2.20	0.42
3:C:1359:THR:O	3:C:1416:ASP:HA	2.19	0.42
4:D:191:PHE:H	4:D:231:TYR:HD2	1.67	0.42
4:D:252:THR:O	4:D:254:ASN:N	2.45	0.42
1:A:147:SER:O	1:A:150:PRO:HD2	2.19	0.42
1:A:2197:GLN:HG3	1:A:2238:PRO:HG2	2.01	0.42
1:A:2209:LEU:O	1:A:2250:ALA:HA	2.20	0.42
3:C:1074:LYS:HA	3:C:1076:ARG:NH1	2.34	0.42
2:B:1200:ILE:HA	2:B:1201:PRO:HA	1.73	0.42
2:B:1647:LYS:HD3	2:B:1731:MET:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2064:LYS:HD3	2:B:2133:ARG:HH21	1.84	0.42
1:A:103:PHE:HZ	1:A:128:THR:HG21	1.84	0.42
1:A:461:PRO:HD3	1:A:507:TRP:NE1	2.35	0.42
1:A:1350:GLN:HB2	1:A:1351:PRO:HD3	2.02	0.42
1:A:2463:GLY:HA2	1:A:2466:ILE:HD13	2.02	0.42
2:B:2324:PHE:O	2:B:2328:GLN:HG2	2.20	0.42
2:B:2566:ASN:OD1	2:B:2627:GLY:HA2	2.20	0.42
3:C:1178:LEU:HD22	3:C:1461:LEU:HG	2.02	0.42
1:A:2247:ILE:O	1:A:2299:ASN:ND2	2.38	0.41
2:B:947:ASN:OD1	2:B:1032:TRP:NE1	2.52	0.41
2:B:2399:ASP:HB3	2:B:2402:TYR:HD2	1.85	0.41
3:C:35:LYS:O	3:C:38:VAL:HG12	2.20	0.41
1:A:936:LEU:HD23	1:A:936:LEU:HA	1.87	0.41
1:A:936:LEU:HB3	1:A:984:LEU:HD11	2.02	0.41
1:A:1112:PHE:O	1:A:1116:ARG:HD2	2.20	0.41
1:A:2065:LEU:HD13	3:C:359:TRP:CZ2	2.55	0.41
1:A:2257:LEU:HD11	1:A:2281:VAL:HG21	2.02	0.41
2:B:33:PHE:HE2	2:B:92:LEU:HD22	1.84	0.41
2:B:1317:ARG:NH1	2:B:1547:ASP:OD1	2.53	0.41
2:B:2342:PHE:CZ	2:B:2414:ALA:HB1	2.55	0.41
4:D:289:GLU:HA	4:D:292:GLU:HG2	2.02	0.41
1:A:2233:ARG:HH21	1:A:2272:ARG:NH2	2.16	0.41
2:B:1704:HIS:CE1	2:B:1709:GLN:HG3	2.56	0.41
2:B:2195:LEU:HD22	2:B:2201:PHE:CD1	2.55	0.41
3:C:219:TRP:NE1	3:C:1073:LEU:HB3	2.36	0.41
3:C:423:VAL:HG22	3:C:465:VAL:HG22	2.02	0.41
3:C:929:MET:HE2	3:C:962:TYR:HB2	2.01	0.41
3:C:1085:TRP:O	4:D:317:TYR:OH	2.30	0.41
3:C:1314:ILE:HD12	3:C:1314:ILE:HA	1.85	0.41
3:C:1474:TRP:HZ2	3:C:1483:GLY:HA2	1.85	0.41
1:A:2532:TRP:HA	1:A:2535:VAL:HG22	2.02	0.41
2:B:2330:TYR:CZ	2:B:2409:PHE:HB2	2.55	0.41
3:C:1000:VAL:HB	3:C:1003:MET:HG2	2.01	0.41
1:A:74:TYR:HB2	1:A:75:GLN:H	1.75	0.41
1:A:129:LEU:HD12	1:A:137:HIS:CD2	2.55	0.41
1:A:2564:LEU:O	1:A:2568:ASN:N	2.50	0.41
2:B:2677:GLU:HB2	2:B:2678:PRO:HD3	2.01	0.41
3:C:1227:LEU:HD21	3:C:1307:ILE:HD12	2.03	0.41
1:A:2555:LEU:O	1:A:2558:ILE:HG12	2.20	0.41
2:B:799:ILE:O	2:B:802:SER:OG	2.27	0.41
2:B:2639:THR:O	2:B:2693:GLN:NE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2687:CYS:SG	2:B:2748:LEU:HB2	2.61	0.41
4:D:298:TYR:CE2	4:D:300:GLN:HB2	2.56	0.41
1:A:926:LEU:O	1:A:930:CYS:N	2.43	0.41
1:A:1241:ILE:O	1:A:1245:THR:HG23	2.20	0.41
1:A:2173:ILE:O	1:A:2177:MET:HG2	2.21	0.41
2:B:1343:LYS:HD3	2:B:1535:LEU:HD21	2.03	0.41
2:B:2783:LEU:O	2:B:2787:VAL:HG23	2.21	0.41
2:B:2864:LEU:O	2:B:2868:VAL:HG23	2.21	0.41
3:C:473:GLN:HE21	3:C:1131:ILE:HG13	1.86	0.41
3:C:1237:VAL:O	3:C:1240:PRO:HD2	2.20	0.41
1:A:445:ARG:HG2	1:A:487:MET:HE1	2.03	0.41
1:A:567:VAL:HG12	1:A:571:ILE:HD13	2.02	0.41
1:A:1012:GLU:HB2	1:A:1057:ARG:CZ	2.50	0.41
1:A:1117:PHE:HB3	1:A:1140:ILE:HG21	2.03	0.41
2:B:1745:SER:OG	2:B:1963:GLU:OE2	2.38	0.41
2:B:2009:ARG:NH2	2:B:2048:GLU:OE1	2.38	0.41
2:B:2209:GLU:N	2:B:2209:GLU:OE1	2.54	0.41
2:B:2452:GLN:O	2:B:2456:VAL:HG23	2.21	0.41
2:B:2948:LEU:HD23	2:B:2948:LEU:HA	1.94	0.41
3:C:286:MET:HA	3:C:302:PHE:CE2	2.56	0.41
3:C:579:PHE:HD1	3:C:579:PHE:HA	1.76	0.41
3:C:1439:LEU:O	3:C:1443:VAL:HG23	2.21	0.41
1:A:616:PHE:CE2	1:A:617:ILE:HG13	2.56	0.41
1:A:1045:THR:HG21	1:A:1178:VAL:HG13	2.03	0.41
1:A:1112:PHE:CE1	1:A:1116:ARG:HD3	2.56	0.41
1:A:2355:HIS:O	1:A:2359:LYS:HG2	2.21	0.41
2:B:1763:PHE:HE1	2:B:1813:LYS:HA	1.86	0.41
2:B:2756:LEU:HG	2:B:2759:ASP:HB3	2.02	0.41
1:A:2419:GLN:OE1	1:A:2475:ILE:HG22	2.21	0.40
2:B:1231:HIS:HB2	2:B:1352:GLU:OE1	2.21	0.40
2:B:1922:ILE:O	2:B:1926:MET:HG3	2.21	0.40
2:B:2143:VAL:HG12	2:B:2145:MET:HG3	2.03	0.40
2:B:2157:GLN:O	2:B:2161:ARG:HG3	2.21	0.40
2:B:2302:LEU:N	2:B:2303:PRO:HD2	2.36	0.40
3:C:282:TRP:NE1	3:C:1387:THR:O	2.45	0.40
3:C:1045:LYS:HA	3:C:1090:TRP:CE2	2.56	0.40
1:A:2157:LYS:HE3	1:A:2157:LYS:HB2	1.87	0.40
1:A:2446:ALA:O	1:A:2627:ARG:NH2	2.53	0.40
2:B:344:TRP:HD1	2:B:345:SER:H	1.69	0.40
2:B:680:ILE:HD12	2:B:680:ILE:HA	1.94	0.40
2:B:2814:ASN:O	2:B:2818:PRO:HD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:543:ALA:O	3:C:547:MET:HG2	2.21	0.40
3:C:1203:MET:HB3	3:C:1262:ALA:HB2	2.03	0.40
3:C:1231:TRP:HE1	3:C:1241:LEU:HD13	1.86	0.40
1:A:633:LEU:HD21	1:A:655:PHE:CE1	2.56	0.40
1:A:1011:VAL:HG13	1:A:1043:PHE:HE1	1.85	0.40
1:A:1346:HIS:HB3	1:A:1354:CYS:SG	2.62	0.40
1:A:2546:ASN:O	1:A:2550:VAL:HG13	2.20	0.40
2:B:2763:SER:HA	2:B:2766:ILE:HG12	2.03	0.40
3:C:213:LYS:HA	3:C:213:LYS:HD3	1.93	0.40
3:C:607:ASP:OD1	3:C:607:ASP:N	2.53	0.40
3:C:1276:TYR:CE1	3:C:1313:SER:HB2	2.56	0.40
1:A:1019:ARG:NH2	1:A:1061:LEU:HD22	2.37	0.40
1:A:1045:THR:HG21	1:A:1178:VAL:O	2.21	0.40
2:B:216:GLN:HB3	2:B:217:PRO:HD3	2.03	0.40
2:B:793:LEU:HD11	2:B:845:PHE:CD1	2.56	0.40
2:B:2104:SER:OG	2:B:2105:GLN:OE1	2.27	0.40
3:C:312:LEU:HD13	3:C:1328:VAL:HG13	2.03	0.40
3:C:554:GLU:HB3	3:C:1117:TRP:HE1	1.86	0.40
1:A:917:ASP:OD1	3:C:717:ARG:NH2	2.53	0.40
1:A:2590:LEU:HD12	1:A:2595:GLN:HG2	2.04	0.40
2:B:2172:LEU:O	2:B:2176:THR:HG23	2.22	0.40
2:B:2409:PHE:HZ	2:B:2414:ALA:HB2	1.87	0.40
3:C:436:LYS:HE3	3:C:445:TYR:HE1	1.86	0.40
3:C:1094:ARG:HD2	4:D:364:GLY:O	2.22	0.40
3:C:1366:ILE:HD11	3:C:1394:ILE:HG23	2.03	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	1492/2654 (56%)	1441 (97%)	51 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	B	1671/3326 (50%)	1586 (95%)	85 (5%)	0	100	100
3	C	1330/1738 (76%)	1294 (97%)	36 (3%)	0	100	100
4	D	167/467 (36%)	157 (94%)	10 (6%)	0	100	100
All	All	4660/8185 (57%)	4478 (96%)	182 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1363/2366 (58%)	1315 (96%)	48 (4%)	31	63
2	B	1529/2916 (52%)	1478 (97%)	51 (3%)	33	64
3	C	1174/1572 (75%)	1143 (97%)	31 (3%)	41	70
4	D	157/409 (38%)	150 (96%)	7 (4%)	23	56
All	All	4223/7263 (58%)	4086 (97%)	137 (3%)	36	65

All (137) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	85	LEU
1	A	88	VAL
1	A	120	THR
1	A	129	LEU
1	A	202	TRP
1	A	464	ASN
1	A	473	LEU
1	A	481	PHE
1	A	488	MET
1	A	491	GLU
1	A	500	LYS
1	A	517	ASP
1	A	602	GLU

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Mol	Chain	Res	Type
1	A	635	TRP
1	A	645	THR
1	A	832	ARG
1	A	950	ILE
1	A	955	LEU
1	A	962	VAL
1	A	969	GLN
1	A	1009	GLU
1	A	1090	THR
1	A	1104	ASP
1	A	1116	ARG
1	A	1122	LEU
1	A	1136	PHE
1	A	1172	ARG
1	A	1233	ASP
1	A	1238	ASP
1	A	1259	ARG
1	A	1354	CYS
1	A	1372	LEU
1	A	1382	ASP
1	A	1403	GLN
1	A	2138	PHE
1	A	2188	LEU
1	A	2196	PHE
1	A	2213	LEU
1	A	2243	LEU
1	A	2275	PHE
1	A	2276	TYR
1	A	2394	ARG
1	A	2436	TRP
1	A	2466	ILE
1	A	2469	HIS
1	A	2477	PHE
1	A	2522	PHE
1	A	2634	GLN
2	B	87	HIS
2	B	107	VAL
2	B	206	PHE
2	B	793	LEU
2	B	849	MET
2	B	868	LEU
2	B	928	LEU

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Mol	Chain	Res	Type
2	B	1029	LYS
2	B	1031	PHE
2	B	1034	LYS
2	B	1196	GLU
2	B	1206	LEU
2	B	1224	LEU
2	B	1331	VAL
2	B	1537	ASN
2	B	1685	LEU
2	B	1752	SER
2	B	1833	TYR
2	B	1914	CYS
2	B	1920	LEU
2	B	1934	ASP
2	B	1965	LEU
2	B	1971	GLN
2	B	1988	PHE
2	B	1991	GLN
2	B	2041	LEU
2	B	2052	VAL
2	B	2056	VAL
2	B	2063	THR
2	B	2066	LEU
2	B	2075	ASP
2	B	2142	LEU
2	B	2206	ILE
2	B	2207	ASP
2	B	2223	PHE
2	B	2274	LEU
2	B	2277	GLN
2	B	2320	ARG
2	B	2335	LYS
2	B	2427	GLU
2	B	2432	LEU
2	B	2547	GLU
2	B	2559	ARG
2	B	2596	LEU
2	B	2601	SER
2	B	2630	ARG
2	B	2663	LYS
2	B	2807	LEU
2	B	2913	ILE

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Mol	Chain	Res	Type
2	B	2926	LYS
2	B	2938	LEU
3	C	31	LEU
3	C	57	THR
3	C	122	LEU
3	C	136	MET
3	C	152	ARG
3	C	187	PHE
3	C	188	PHE
3	C	250	ASP
3	C	465	VAL
3	C	476	TYR
3	C	482	VAL
3	C	654	THR
3	C	669	ARG
3	C	712	PHE
3	C	731	ARG
3	C	733	CYS
3	C	875	TYR
3	C	932	GLU
3	C	1029	LEU
3	C	1145	MET
3	C	1151	PHE
3	C	1250	PHE
3	C	1273	ARG
3	C	1291	HIS
3	C	1312	PHE
3	C	1318	HIS
3	C	1488	PHE
3	C	1492	PHE
3	C	1493	LEU
3	C	1516	CYS
3	C	1524	ASN
4	D	252	THR
4	D	279	ASP
4	D	280	TYR
4	D	312	ASP
4	D	313	CYS
4	D	348	THR
4	D	349	ARG

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

Mol	Chain	Res	Type
1	A	758	GLN
2	B	1545	HIS
2	B	2477	GLN
3	C	63	HIS
3	C	315	ASN
3	C	1471	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 for Mogul analysis.

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	$\# Z  > 2$
6	NAG	C	2001	3	14,14,15	0.19	0	17,19,21	0.41	0
6	NAG	C	2003	3	14,14,15	0.21	0	17,19,21	0.45	0
6	NAG	C	2002	3	14,14,15	0.21	0	17,19,21	0.46	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
6	NAG	C	2001	3	-	4/6/23/26	0/1/1/1
6	NAG	C	2003	3	-	0/6/23/26	0/1/1/1
6	NAG	C	2002	3	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

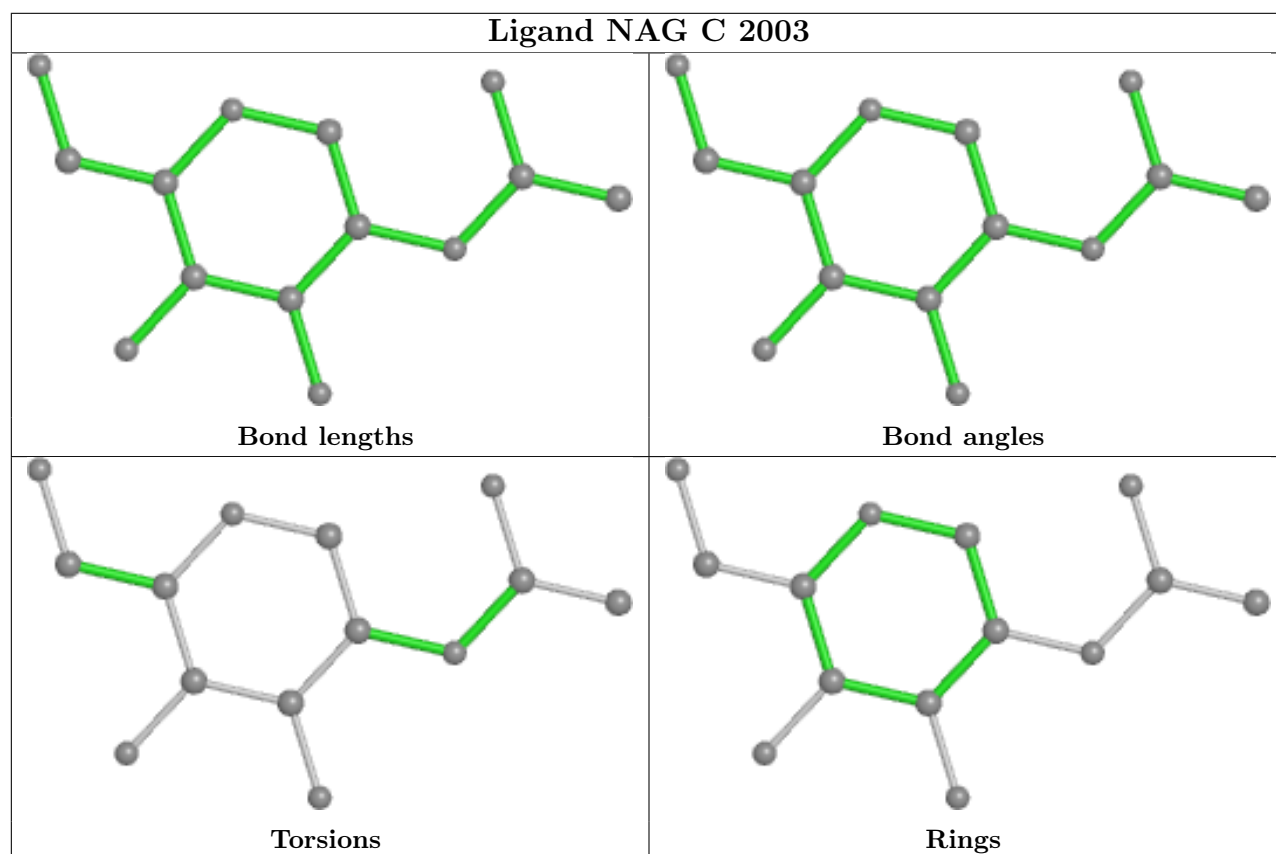
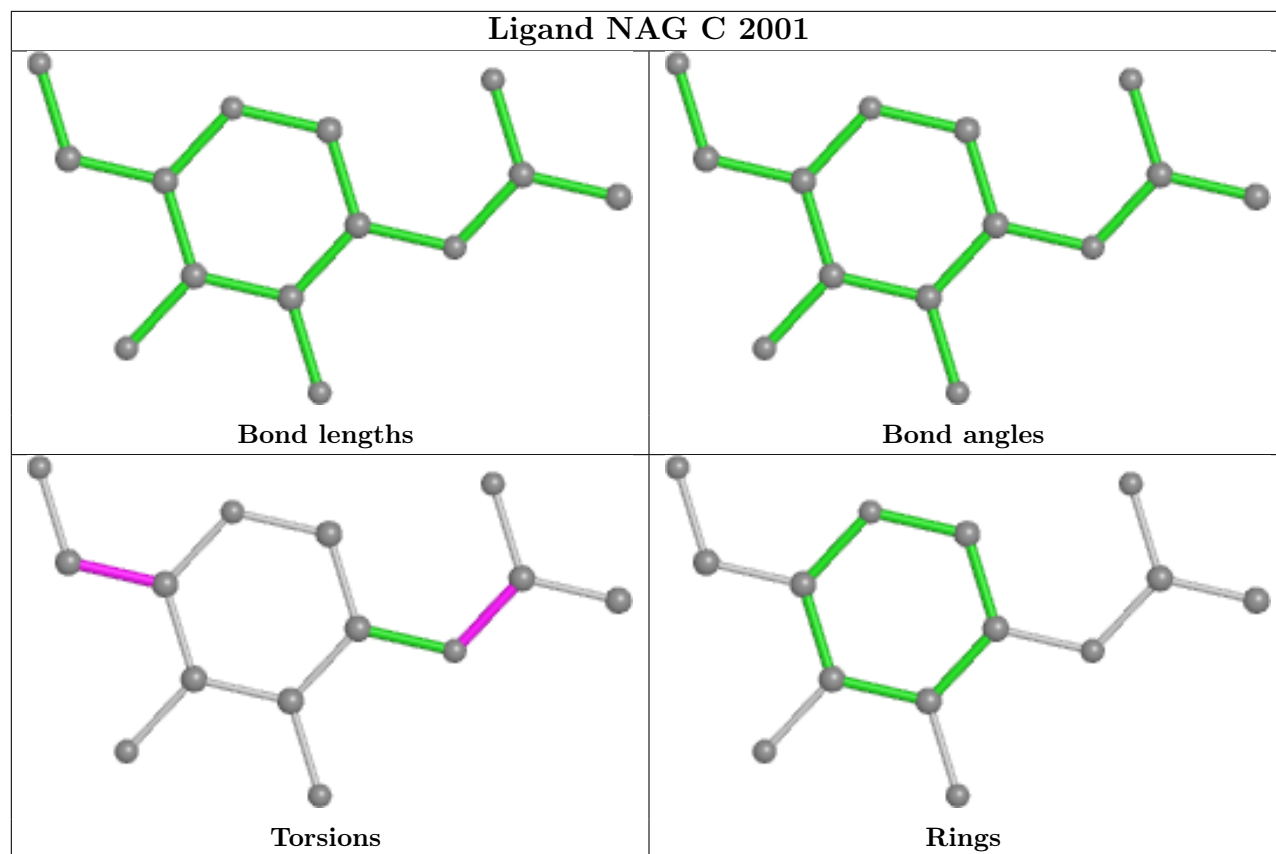
Mol	Chain	Res	Type	Atoms
6	C	2001	NAG	C4-C5-C6-O6
6	C	2001	NAG	O5-C5-C6-O6
6	C	2001	NAG	C8-C7-N2-C2
6	C	2001	NAG	O7-C7-N2-C2

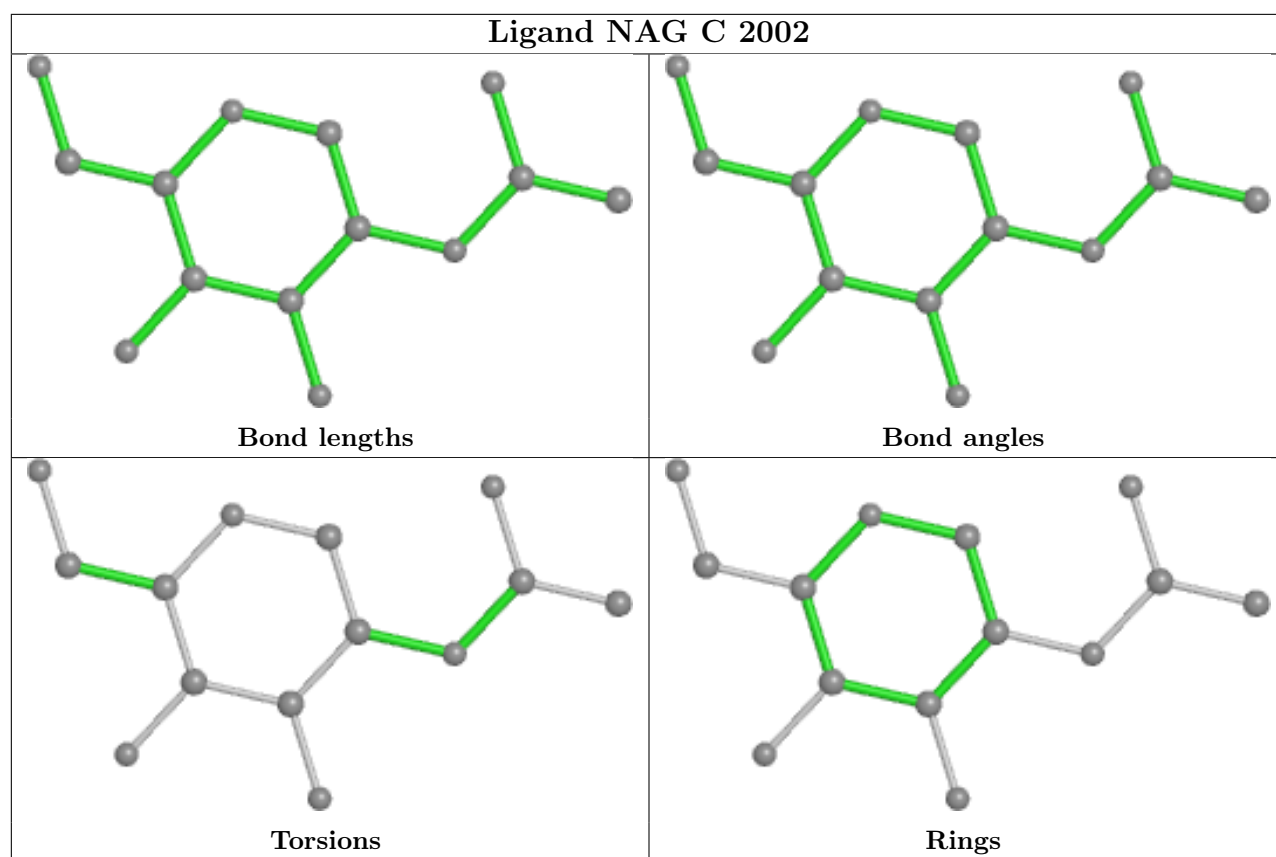
There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	2002	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 [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

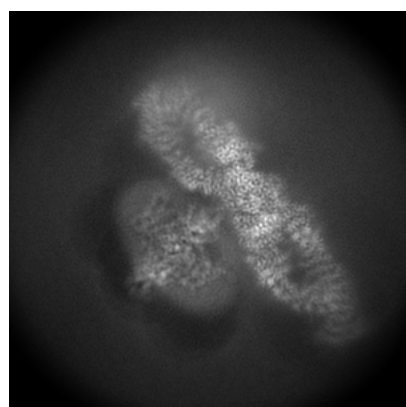
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-32344. These allow visual inspection of the internal detail of the map and identification of artifacts.

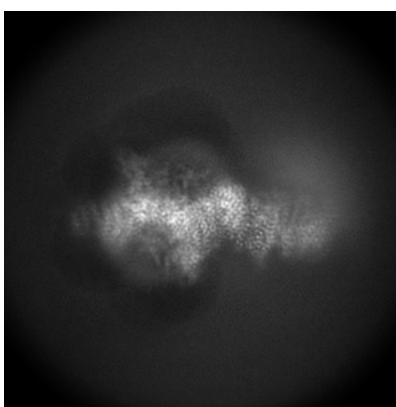
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

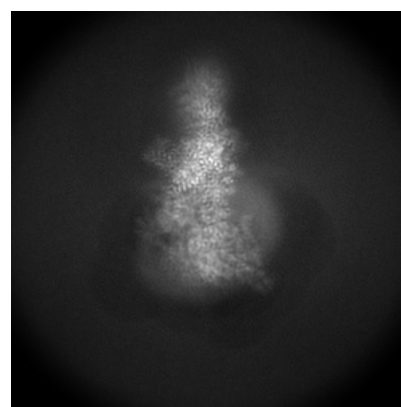
#### 6.1.1 Primary map



X



Y

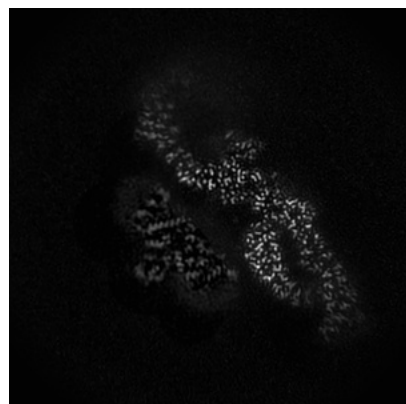


Z

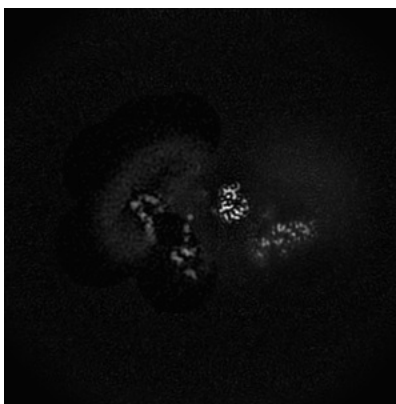
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

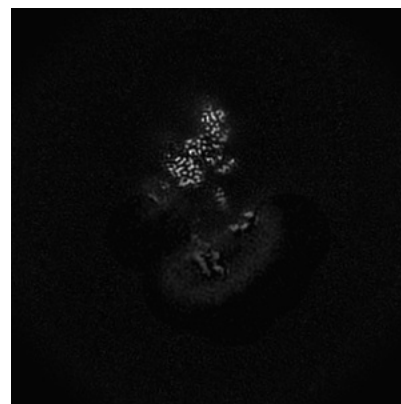
#### 6.2.1 Primary map



X Index: 140



Y Index: 140

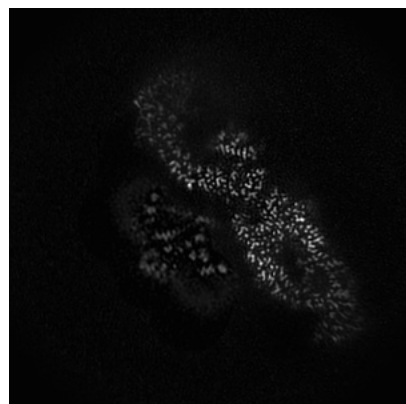


Z Index: 140

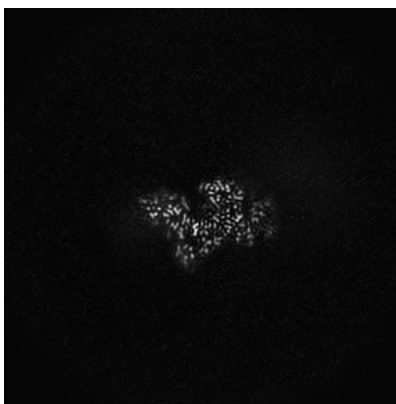
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

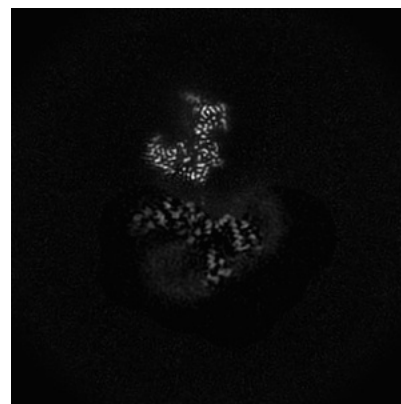
### 6.3.1 Primary map



X Index: 135



Y Index: 170

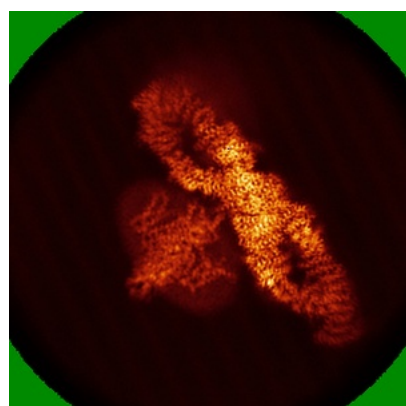


Z Index: 126

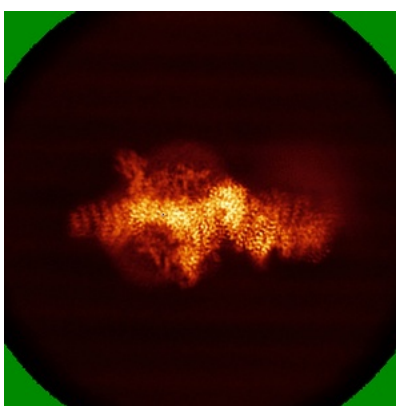
The images above show the largest variance slices of the map in three orthogonal directions.

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

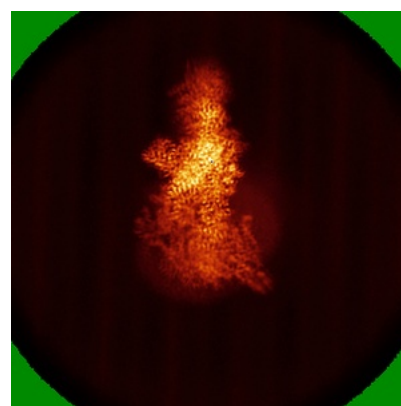
### 6.4.1 Primary map



X



Y

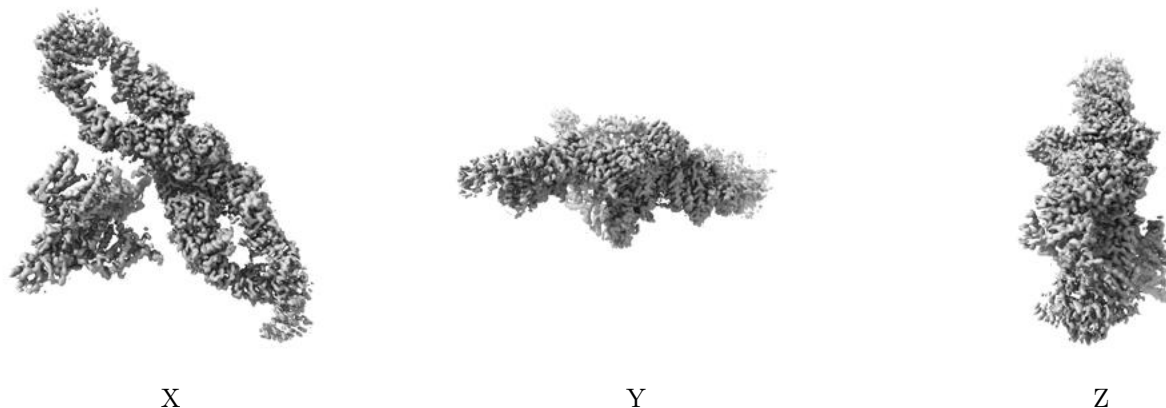


Z

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

## 6.5 Orthogonal surface views [i](#)

### 6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.95. 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](#)

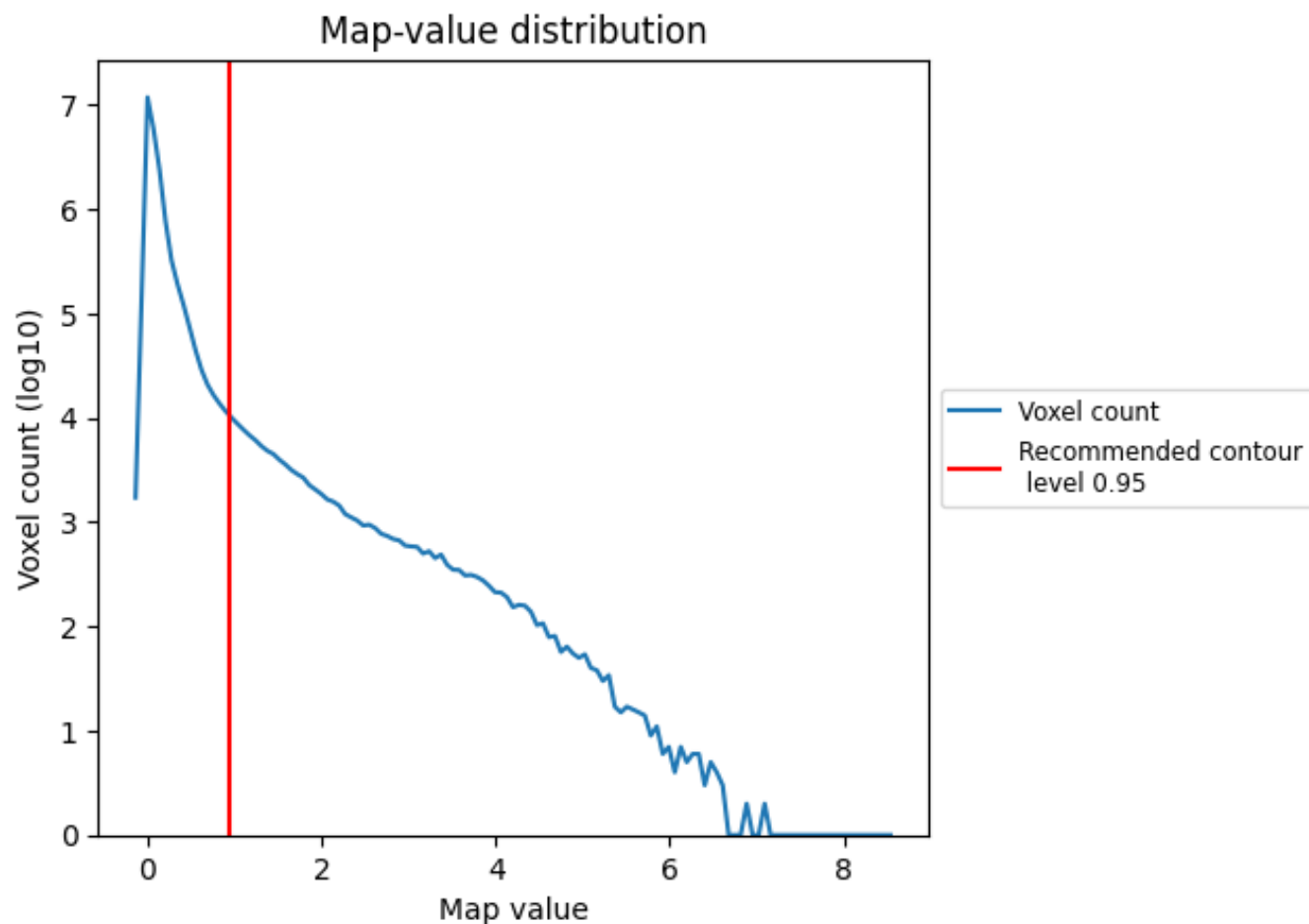
This section was not generated. No masks/segmentation were deposited.



## 7 Map analysis [i](#)

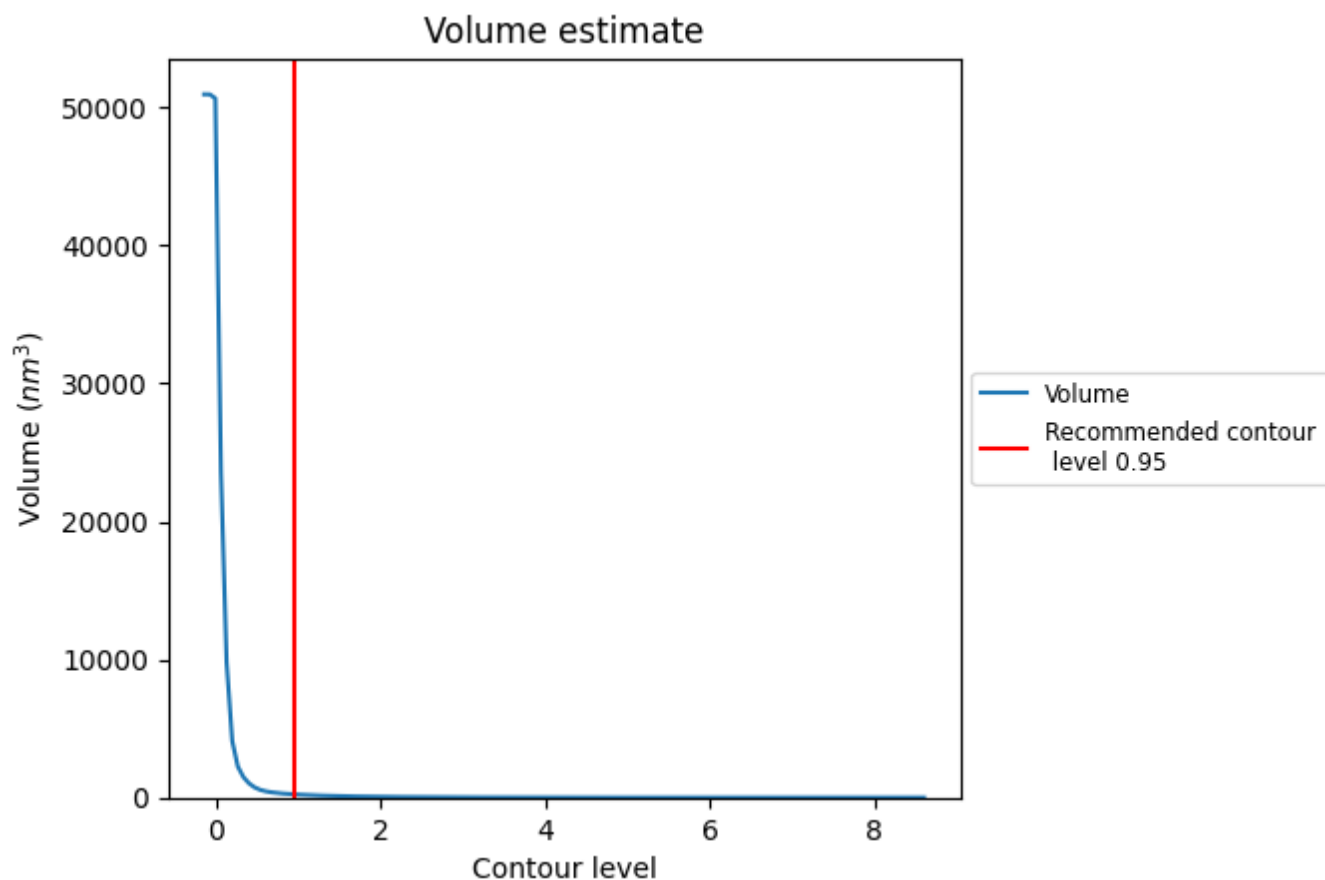
This section contains the results of statistical analysis of the map.

### 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.

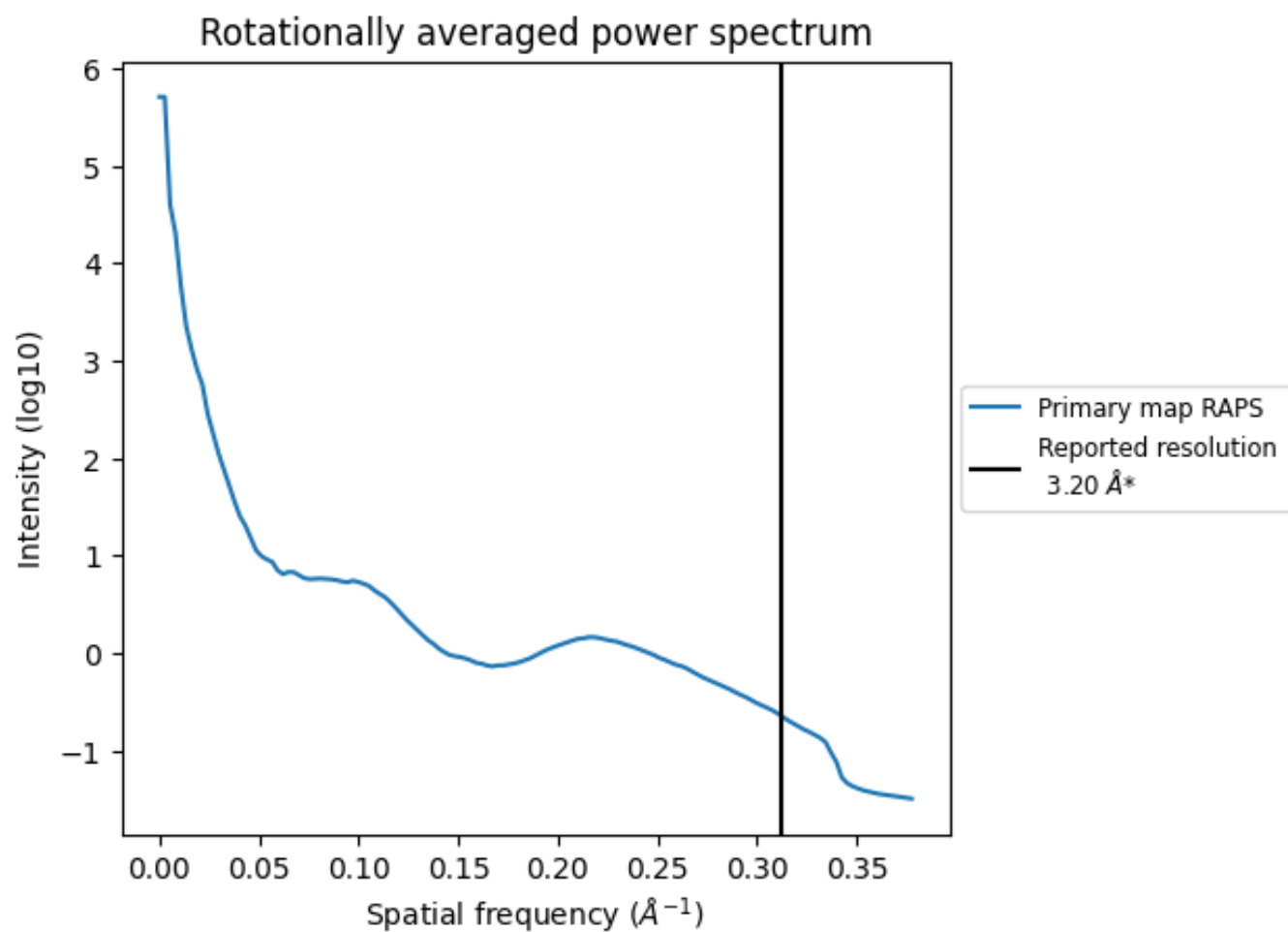
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 234 nm<sup>3</sup>; this corresponds to an approximate mass of 211 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<sup>-1</sup>

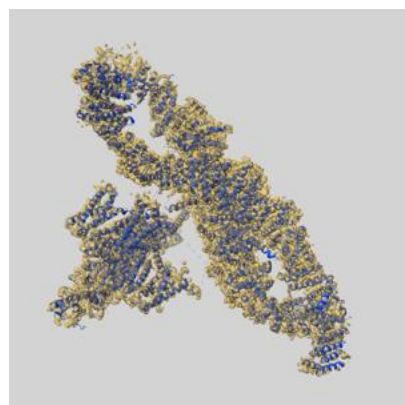
## 8 Fourier-Shell correlation

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

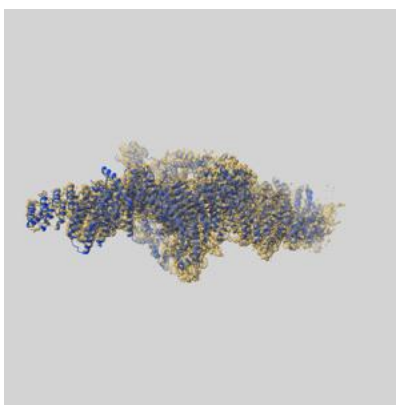
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-32344 and PDB model 7W7G. Per-residue inclusion information can be found in [section 3](#) on [page 5](#).

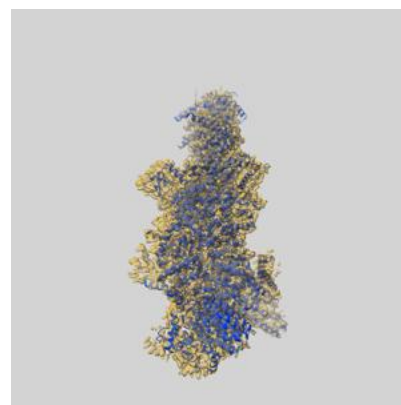
### 9.1 Map-model overlay [i](#)



X



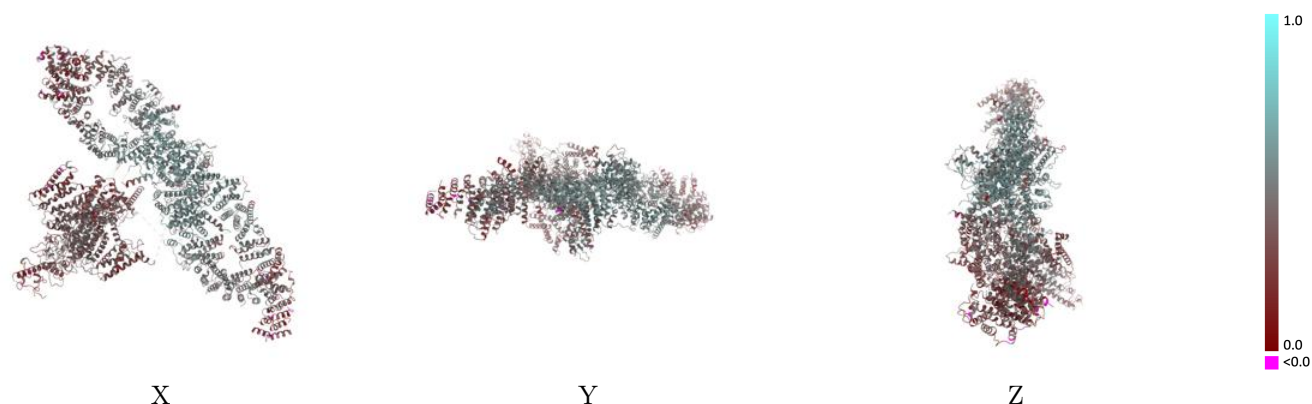
Y



Z

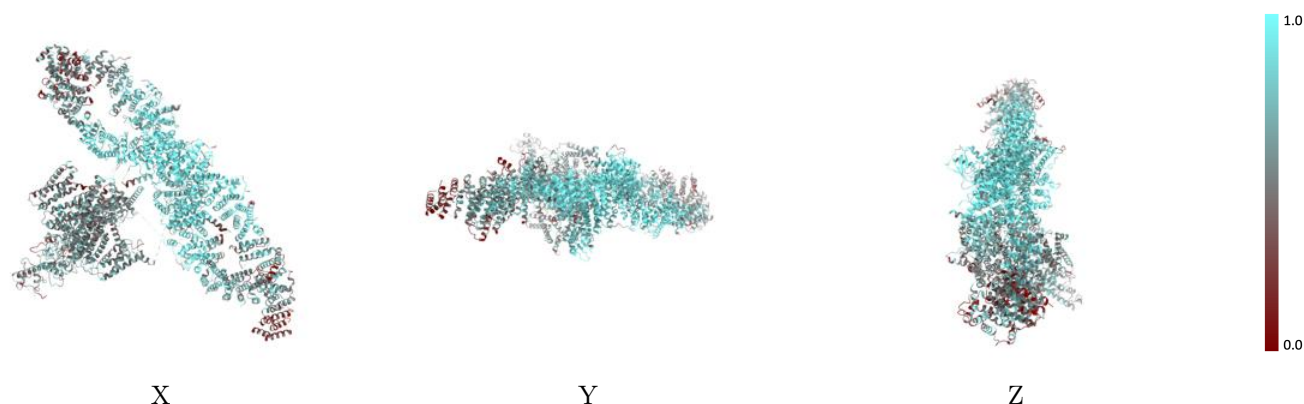
The images above show the 3D surface view of the map at the recommended contour level 0.95 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



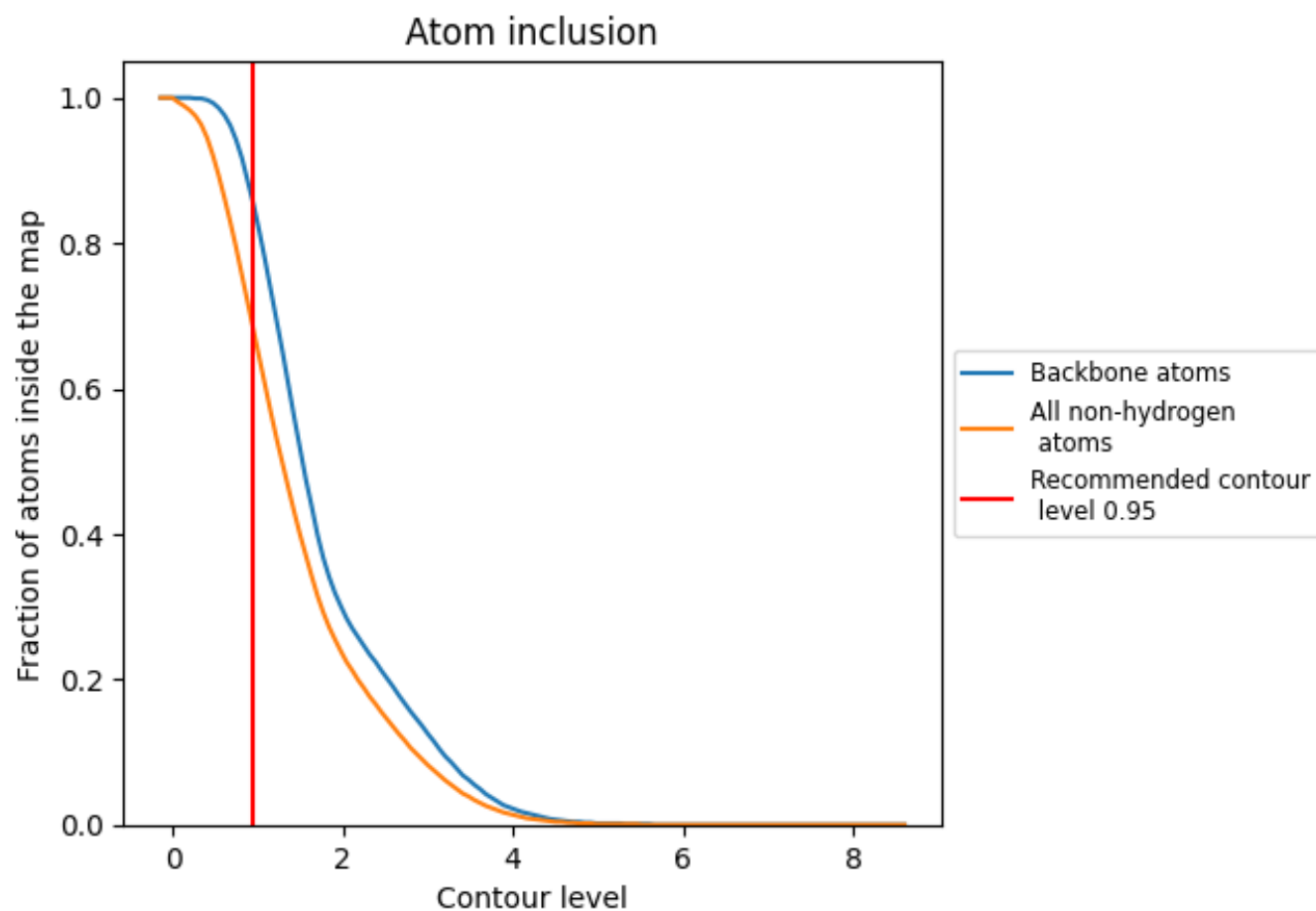
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.95).

## 9.4 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 68% 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 (0.95) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.6820	<div></div> 0.4200
A	<div></div> 0.7210	<div></div> 0.4400
B	<div></div> 0.7710	<div></div> 0.4660
C	<div></div> 0.5450	<div></div> 0.3520
D	<div></div> 0.5240	<div></div> 0.3220

