Full wwPDB EM Validation Report (i)

Nov 23, 2022 – 08:01 AM EST

PDB ID	:	7S1X
EMDB ID	:	EMD-24807
Title	:	Cryo-EM structure of human NKCC1 K289NA492EL671C bound with bumetanide
Authors	:	Zhao, Y.X.; Cao, E.H.
Deposited on	:	2021-09-02
Resolution	:	2.90 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 (i) 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 (1)) were used in the production of this report:

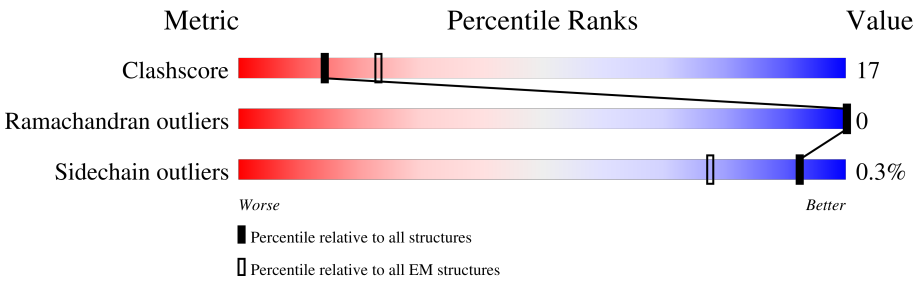
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.5 (274361), CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 Å.

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



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

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	1216	47% 25% 28%
1	B	1216	47% 24% 28%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CL	A	1303	-	-	X	-
4	CL	B	1303	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 12658 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.

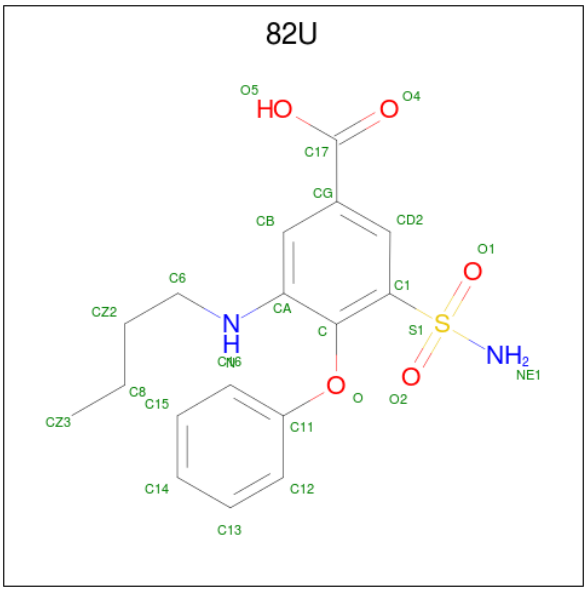
- Molecule 1 is a protein called Solute carrier family 12 member 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	B	871	6302	4115	1063	1088	36	0	0
1	A	871	6302	4115	1063	1088	36	0	0

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-3	GLY	-	expression tag	UNP P55011
B	-2	ALA	-	expression tag	UNP P55011
B	-1	MET	-	expression tag	UNP P55011
B	0	GLY	-	expression tag	UNP P55011
B	1	SER	-	expression tag	UNP P55011
B	289	ASN	LYS	engineered mutation	UNP P55011
B	492	GLU	ALA	engineered mutation	UNP P55011
B	671	CYS	LEU	engineered mutation	UNP P55011
A	-3	GLY	-	expression tag	UNP P55011
A	-2	ALA	-	expression tag	UNP P55011
A	-1	MET	-	expression tag	UNP P55011
A	0	GLY	-	expression tag	UNP P55011
A	1	SER	-	expression tag	UNP P55011
A	289	ASN	LYS	engineered mutation	UNP P55011
A	492	GLU	ALA	engineered mutation	UNP P55011
A	671	CYS	LEU	engineered mutation	UNP P55011

- Molecule 2 is 3-(butylamino)-4-phenoxy-5-sulfamoylbenzoic acid (three-letter code: 82U) (formula: $C_{17}H_{20}N_2O_5S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	S	
2	B	1	25	17	2	5	1	0
2	A	1	25	17	2	5	1	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		AltConf
			Total	K	
3	B	1	1	1	0
3	A	1	1	1	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl) (labeled as "Ligand of Interest" by depositor).

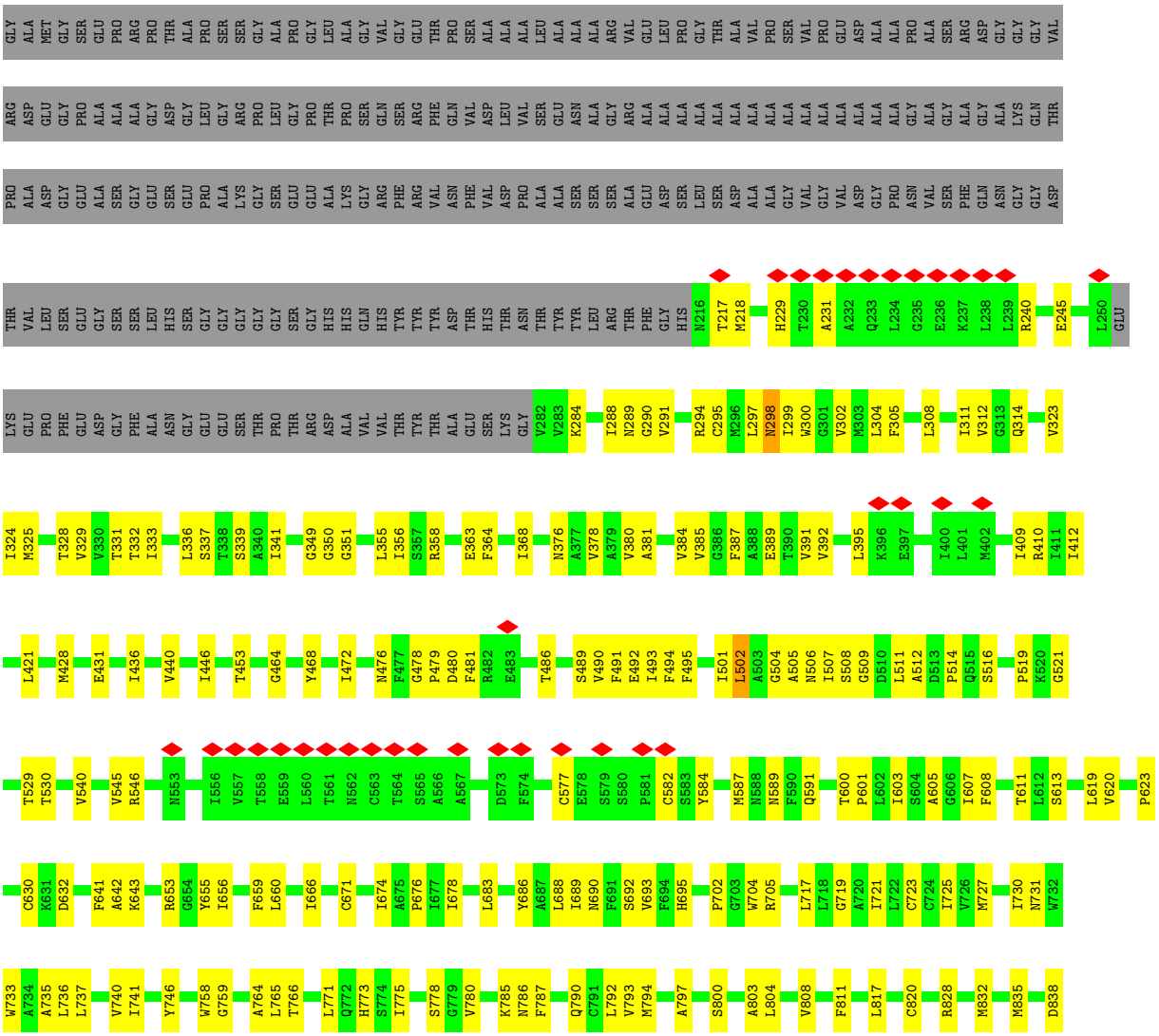
Mol	Chain	Residues	Atoms		AltConf
			Total	Cl	
4	B	1	1	1	0
4	A	1	1	1	0

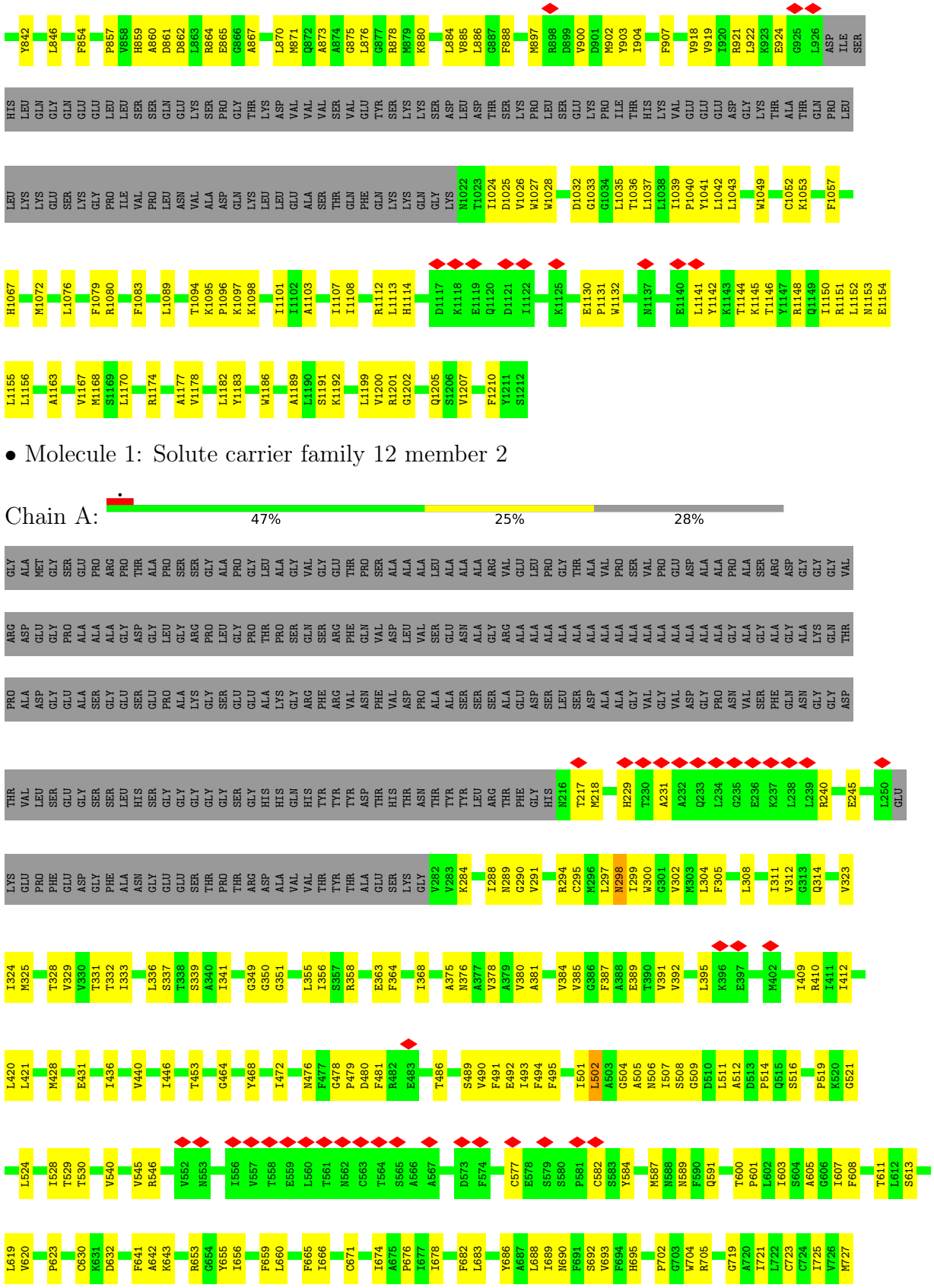
3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

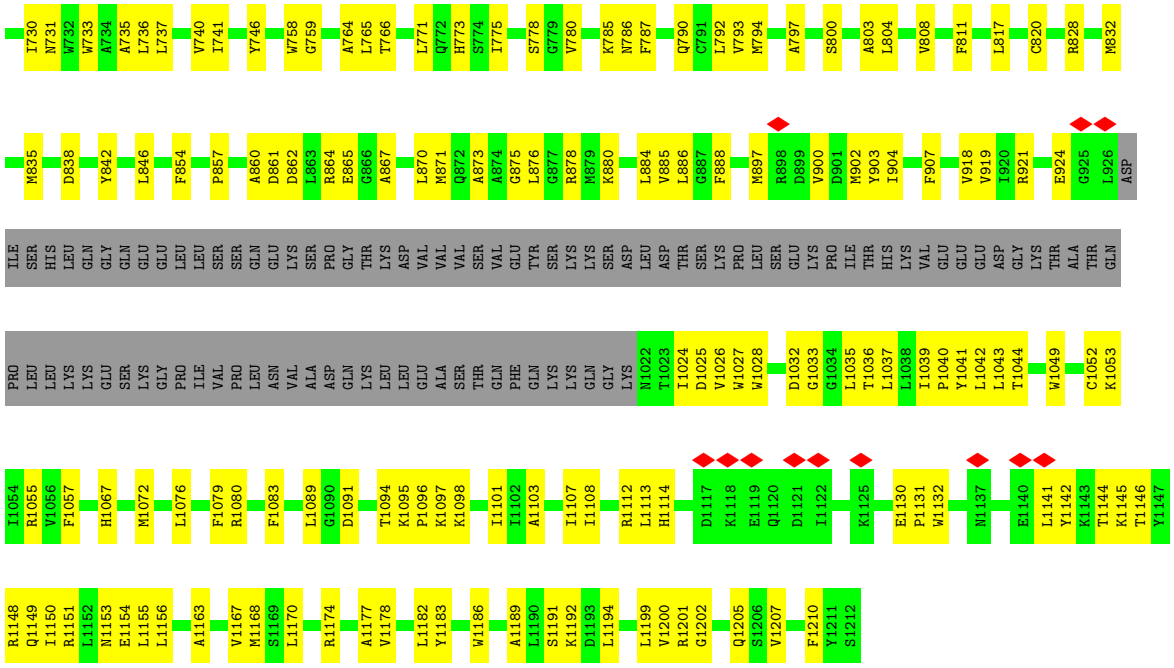
- Molecule 1: Solute carrier family 12 member 2

Chain B:





- Molecule 1: Solute carrier family 12 member 2


I730 N731 W732 W733 A734 A735 L736 L737 V740 I741 Y746 W758 G759 A764 L765 T766 L771 Q772 H773 S774 I775 S778 G779 V780 K785 N786 F787 Q790 C791 L792 V793 M794 A797 S800 A803 L804 V808 F811 L817 C820 R828 M832
M835 D838 Y842 L846 F854 P857 A860 D861 D862 L863 R864 E865 G866 A867 L870 M871 Q872 A873 A874 G875 L876 G877 R878 M879 K880 L884 V885 L886 G887 F888 M897 R898 D899 V900 D901 M902 Y903 I904 F907 V918 V919 I920 R921 E924 G925 L926 ASP
ILE SER HIS LEU GLN GLY GLN GLU GLU LEU LEU SER SER GLN GLU LYS SER PRO GLY THR LYS ASP VAL VAL VAL SER VAL GLU TYR SER LYS LYS SER ASP LEU ASP THR SER LYS PRO LEU SER GLU LYS PRO ILE THR HIS LYS VAL GLU GLU GLU ASP GLY LYS THR ALA THR GLN
PRO LEU LEU LYS LYS GLU SER LYS GLY PRO ILE VAL PRO LEU ASN VAL ALA ASP GLN LYS LEU LEU GLU ALA SER THR GLN PHE GLN LYS LYS GLN GLY LYS N1022 T1023 I1024 D1025 V1026 W1027 W1028 D1032 G1033 G1034 L1035 T1036 L1037 L1038 I1039 P1040 Y1041 L1042 L1043 T1044 W1049 C1052 K1053
I1054 R1055 V1056 F1057 H1067 M1072 L1076 F1079 R1080 F1083 L1089 G1090 D1091 T1094 K1095 P1096 K1097 K1098 I1101 I1102 A1103 I1107 I1108 R1112 L1113 H1114 D1117 K1118 E1119 Q1120 D1121 I1122 K1125 E1130 P1131 W1132 N1137 E1140 L1141 Y1142 K1143 T1144 K1145 T1146 Y1147
R1148 Q1149 I1150 R1151 L1152 N1153 E1154 L1155 L1156 A1163 V1167 M1168 S1169 L1170 R1174 A1177 V1178 L1182 Y1183 W1186 A1189 L1190 S1191 K1192 D1193 L1194 L1199 V1200 R1201 G1202 Q1205 S1206 V1207 F1210 Y1211 S1212

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	504481	Depositor
Resolution determination method	DIFFRACTION PATTERN/LAYERLINES	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	1.175	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	5.478	Depositor
Minimum map value	-3.239	Depositor
Average map value	0.009	Depositor
Map value standard deviation	0.148	Depositor
Recommended contour level	0.6	Depositor
Map size (Å)	271.36, 271.36, 271.36	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.06, 1.06, 1.06	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: 82U, CL, K

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	0.31	0/6451	0.51	1/8796 (0.0%)
1	B	0.31	0/6451	0.51	1/8796 (0.0%)
All	All	0.31	0/12902	0.51	2/17592 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	502	LEU	CA-CB-CG	5.12	127.08	115.30
1	A	502	LEU	CA-CB-CG	5.11	127.05	115.30

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	6302	0	6014	228	0
1	B	6302	0	6014	225	0
2	A	25	0	0	0	0
2	B	25	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	1	0	0	2	0
All	All	12658	0	12028	429	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 17.

All (429) 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:B:686:TYR:OH	4:B:1303:CL:CL	2.06	1.10
1:A:686:TYR:OH	4:A:1303:CL:CL	2.06	1.07
1:B:1079:PHE:O	1:A:705:ARG:NH1	2.05	0.88
1:B:705:ARG:NH1	1:A:1079:PHE:O	2.05	0.88
1:B:476:ASN:HA	1:B:546:ARG:HH12	1.42	0.83
1:A:476:ASN:HA	1:A:546:ARG:HH12	1.42	0.83
1:B:584:TYR:HB2	1:B:589:ASN:HB2	1.63	0.79
1:B:1153:ASN:ND2	1:B:1189:ALA:O	2.15	0.79
1:A:1153:ASN:ND2	1:A:1189:ALA:O	2.15	0.79
1:A:1028:TRP:CE2	1:A:1037:LEU:HD21	2.18	0.79
1:B:1146:THR:HG22	1:B:1186:TRP:HE1	1.48	0.78
1:A:584:TYR:HB2	1:A:589:ASN:HB2	1.63	0.78
1:B:1028:TRP:CE2	1:B:1037:LEU:HD21	2.18	0.78
1:A:1146:THR:HG22	1:A:1186:TRP:HE1	1.48	0.77
1:A:1032:ASP:HB2	1:A:1202:GLY:H	1.50	0.77
1:B:1032:ASP:HB2	1:B:1202:GLY:H	1.50	0.76
1:B:363:GLU:HG2	1:B:364:PHE:H	1.51	0.76
1:A:363:GLU:HG2	1:A:364:PHE:H	1.51	0.75
1:B:1094:THR:OG1	1:B:1151:ARG:NH1	2.21	0.74
1:B:1027:TRP:CD1	1:B:1057:PHE:HB2	2.24	0.73
1:A:1027:TRP:CD1	1:A:1057:PHE:HB2	2.24	0.73
1:A:1094:THR:OG1	1:A:1151:ARG:NH1	2.21	0.72
1:A:297:LEU:HG	1:A:613:SER:HB2	1.71	0.71
1:B:297:LEU:HG	1:B:613:SER:HB2	1.71	0.71
1:B:1170:LEU:HB3	1:B:1201:ARG:HB2	1.74	0.70
1:A:1170:LEU:HB3	1:A:1201:ARG:HB2	1.74	0.69
1:B:873:ALA:HB3	1:A:873:ALA:HB3	1.74	0.69
1:B:1205:GLN:O	1:A:240:ARG:NH1	2.27	0.68
1:A:472:ILE:O	1:A:476:ASN:ND2	2.27	0.68
1:B:1042:LEU:HD21	1:A:702:PRO:HB3	1.76	0.68
1:B:305:PHE:HB3	1:B:607:ILE:HG13	1.77	0.67
1:B:421:LEU:HD13	1:B:659:PHE:HB2	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:472:ILE:O	1:B:476:ASN:ND2	2.27	0.67
1:B:240:ARG:NH1	1:A:1205:GLN:O	2.27	0.67
1:B:702:PRO:HB3	1:A:1042:LEU:HD21	1.76	0.67
1:A:305:PHE:HB3	1:A:607:ILE:HG13	1.76	0.67
1:B:864:ARG:HB2	1:B:902:MET:HG2	1.77	0.67
1:B:785:LYS:NZ	1:A:759:GLY:O	2.28	0.67
1:A:864:ARG:HB2	1:A:902:MET:HG2	1.77	0.67
1:A:421:LEU:HD13	1:A:659:PHE:HB2	1.75	0.66
1:B:480:ASP:HB3	1:B:546:ARG:HE	1.60	0.66
1:B:759:GLY:O	1:A:785:LYS:NZ	2.28	0.66
1:B:603:ILE:O	1:B:607:ILE:HD12	1.96	0.65
1:A:603:ILE:O	1:A:607:ILE:HD12	1.96	0.65
1:B:323:VAL:HG13	1:B:491:PHE:HD1	1.62	0.65
1:A:480:ASP:HB3	1:A:546:ARG:HE	1.60	0.65
1:A:323:VAL:HG13	1:A:491:PHE:HD1	1.62	0.65
1:A:492:GLU:HG2	1:A:730:ILE:HG23	1.78	0.64
1:B:350:GLY:O	1:B:508:SER:OG	2.15	0.64
1:B:897:MET:HG3	1:B:1131:PRO:HB2	1.79	0.64
1:A:897:MET:HG3	1:A:1131:PRO:HB2	1.79	0.64
1:B:1156:LEU:HD11	1:B:1168:MET:SD	2.38	0.64
1:A:350:GLY:O	1:A:508:SER:OG	2.15	0.64
1:B:492:GLU:HG2	1:B:730:ILE:HG23	1.78	0.63
1:A:298:ASN:C	1:A:298:ASN:HD22	2.01	0.63
1:B:605:ALA:HA	1:B:608:PHE:HD2	1.64	0.62
1:A:1156:LEU:HD11	1:A:1168:MET:SD	2.38	0.62
1:B:351:GLY:HA3	1:B:506:ASN:HA	1.81	0.62
1:B:368:ILE:HB	1:B:688:LEU:HD22	1.82	0.62
1:A:351:GLY:HA3	1:A:506:ASN:HA	1.81	0.62
1:A:888:PHE:CD1	1:A:921:ARG:HD2	2.35	0.62
1:B:888:PHE:CD1	1:B:921:ARG:HD2	2.35	0.62
1:B:1033:GLY:HA2	1:A:240:ARG:NH1	2.15	0.61
1:B:835:MET:HG2	1:B:857:PRO:HB2	1.82	0.61
1:A:363:GLU:HG2	1:A:364:PHE:N	2.15	0.61
1:A:368:ILE:HB	1:A:688:LEU:HD22	1.81	0.61
1:A:489:SER:O	1:A:493:ILE:HG12	2.01	0.61
1:B:793:VAL:HG21	1:B:808:VAL:HG11	1.82	0.61
1:B:643:LYS:HB3	1:B:653:ARG:HH12	1.66	0.61
1:A:835:MET:HG2	1:A:857:PRO:HB2	1.82	0.61
1:A:605:ALA:HA	1:A:608:PHE:HD2	1.64	0.60
1:A:641:PHE:HD2	1:A:653:ARG:HB3	1.65	0.60
1:A:793:VAL:HG21	1:A:808:VAL:HG11	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:643:LYS:HB3	1:A:653:ARG:HH12	1.66	0.60
1:B:489:SER:O	1:B:493:ILE:HG12	2.01	0.60
1:B:641:PHE:HD2	1:B:653:ARG:HB3	1.65	0.60
1:A:508:SER:HA	1:A:511:LEU:HD12	1.84	0.60
1:B:363:GLU:HG2	1:B:364:PHE:N	2.15	0.60
1:B:240:ARG:NH1	1:A:1033:GLY:HA2	2.15	0.60
1:A:502:LEU:HB2	1:A:505:ALA:HB3	1.84	0.59
1:B:502:LEU:HB2	1:B:505:ALA:HB3	1.84	0.59
1:B:508:SER:HA	1:B:511:LEU:HD12	1.84	0.59
1:B:298:ASN:C	1:B:298:ASN:HD22	2.01	0.59
1:A:384:VAL:HG11	1:A:666:ILE:HD11	1.85	0.58
1:A:803:ALA:HB3	1:A:924:GLU:OE1	2.03	0.58
1:A:797:ALA:O	1:A:800:SER:OG	2.19	0.58
1:B:1142:TYR:O	1:B:1146:THR:HG23	2.03	0.58
1:B:331:THR:HG23	1:B:501:ILE:HD13	1.86	0.58
1:B:623:PRO:HG2	1:B:655:TYR:CD1	2.39	0.58
1:B:1027:TRP:CZ3	1:B:1156:LEU:HD12	2.39	0.58
1:B:1089:LEU:HD13	1:B:1155:LEU:HD23	1.85	0.58
1:A:1142:TYR:O	1:A:1146:THR:HG23	2.03	0.58
1:A:331:THR:HG23	1:A:501:ILE:HD13	1.86	0.57
1:A:1146:THR:HG22	1:A:1186:TRP:NE1	2.19	0.57
1:B:797:ALA:O	1:B:800:SER:OG	2.19	0.57
1:B:384:VAL:HG11	1:B:666:ILE:HD11	1.85	0.57
1:A:1089:LEU:HD13	1:A:1155:LEU:HD23	1.85	0.57
1:B:1146:THR:HG22	1:B:1186:TRP:NE1	2.19	0.57
1:A:623:PRO:HG2	1:A:655:TYR:CD1	2.39	0.56
1:A:886:LEU:HD23	1:A:903:TYR:CE1	2.40	0.56
1:B:803:ALA:HB3	1:B:924:GLU:OE1	2.03	0.56
1:A:1027:TRP:CZ3	1:A:1156:LEU:HD12	2.39	0.56
1:A:793:VAL:HG22	1:A:885:VAL:HB	1.88	0.56
1:B:793:VAL:HG22	1:B:885:VAL:HB	1.88	0.56
1:A:300:TRP:NE1	1:A:529:THR:HG23	2.20	0.56
1:B:300:TRP:NE1	1:B:529:THR:HG23	2.20	0.55
1:B:867:ALA:O	1:B:871:MET:HG3	2.06	0.55
1:B:1032:ASP:OD2	1:B:1036:THR:OG1	2.14	0.55
1:B:886:LEU:HD23	1:B:903:TYR:CE1	2.40	0.55
1:A:867:ALA:O	1:A:871:MET:HG3	2.06	0.55
1:A:1027:TRP:CH2	1:A:1155:LEU:HB3	2.42	0.55
1:B:689:ILE:O	1:B:692:SER:HB2	2.07	0.55
1:A:363:GLU:HG3	1:A:746:TYR:HE1	1.72	0.55
1:A:778:SER:O	1:A:878:ARG:NH1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:363:GLU:HG3	1:B:746:TYR:HE1	1.72	0.55
1:B:1024:ILE:HG13	1:B:1052:CYS:SG	2.47	0.54
1:A:689:ILE:O	1:A:692:SER:HB2	2.07	0.54
1:B:385:VAL:O	1:B:389:GLU:HG3	2.08	0.54
1:A:1024:ILE:HG13	1:A:1052:CYS:SG	2.47	0.54
1:B:778:SER:O	1:B:878:ARG:NH1	2.37	0.54
1:A:294:ARG:HH22	1:A:620:VAL:HB	1.73	0.54
1:B:1027:TRP:CH2	1:B:1155:LEU:HB3	2.42	0.54
1:A:1025:ASP:OD2	1:A:1163:ALA:HB2	2.08	0.54
1:A:1026:VAL:HG21	1:A:1040:PRO:HG3	1.90	0.54
1:B:773:HIS:CE1	1:A:773:HIS:CE1	2.96	0.53
1:B:294:ARG:HH22	1:B:620:VAL:HB	1.73	0.53
1:B:325:MET:O	1:B:329:VAL:HG23	2.08	0.53
1:B:1025:ASP:OD2	1:B:1163:ALA:HB2	2.08	0.53
1:B:476:ASN:OD1	1:B:546:ARG:NH1	2.42	0.53
1:B:786:ASN:OD1	1:A:764:ALA:HB2	2.08	0.53
1:A:476:ASN:OD1	1:A:546:ARG:NH1	2.42	0.53
1:A:1146:THR:O	1:A:1150:ILE:HG13	2.09	0.53
1:B:428:MET:HA	1:B:431:GLU:HG3	1.90	0.53
1:A:325:MET:O	1:A:329:VAL:HG23	2.08	0.53
1:A:385:VAL:O	1:A:389:GLU:HG3	2.07	0.53
1:B:1026:VAL:HG21	1:B:1040:PRO:HG3	1.90	0.53
1:A:291:VAL:HG23	1:A:504:GLY:HA3	1.91	0.53
1:A:312:VAL:HG11	1:A:540:VAL:HG13	1.91	0.53
1:B:339:SER:OG	1:B:519:PRO:HB3	2.09	0.53
1:B:312:VAL:HG11	1:B:540:VAL:HG13	1.91	0.53
1:B:764:ALA:HB2	1:A:786:ASN:OD1	2.08	0.53
1:A:339:SER:OG	1:A:519:PRO:HB3	2.09	0.53
1:A:686:TYR:CZ	4:A:1303:CL:CL	2.99	0.53
1:A:1153:ASN:HD21	1:A:1192:LYS:HG2	1.74	0.53
1:B:1153:ASN:HD21	1:B:1192:LYS:HG2	1.74	0.52
1:A:861:ASP:N	1:A:865:GLU:OE2	2.40	0.52
1:A:428:MET:HA	1:A:431:GLU:HG3	1.90	0.52
1:B:291:VAL:HG23	1:B:504:GLY:HA3	1.91	0.52
1:A:686:TYR:O	1:A:690:ASN:ND2	2.42	0.52
1:B:686:TYR:O	1:B:690:ASN:ND2	2.42	0.52
1:B:771:LEU:O	1:B:775:ILE:HG12	2.10	0.52
1:B:861:ASP:N	1:B:865:GLU:OE2	2.40	0.52
1:B:1146:THR:O	1:B:1150:ILE:HG13	2.09	0.52
1:A:514:PRO:C	1:A:516:SER:H	2.13	0.52
1:B:671:CYS:HA	1:B:674:ILE:HG22	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:514:PRO:C	1:B:516:SER:H	2.14	0.51
1:A:328:THR:HG21	1:A:530:THR:HG21	1.91	0.51
1:B:299:ILE:CG2	1:B:529:THR:HG21	2.40	0.51
1:B:686:TYR:CZ	4:B:1303:CL:CL	2.99	0.51
1:B:1072:MET:HE3	1:B:1076:LEU:HD23	1.92	0.51
1:A:299:ILE:HG21	1:A:529:THR:HG21	1.93	0.51
1:B:328:THR:HG21	1:B:530:THR:HG21	1.91	0.51
1:A:589:ASN:OD1	1:A:591:GLN:N	2.44	0.51
1:A:671:CYS:HA	1:A:674:ILE:HG22	1.92	0.51
1:B:299:ILE:HG21	1:B:529:THR:HG21	1.93	0.51
1:A:771:LEU:O	1:A:775:ILE:HG12	2.10	0.51
1:B:589:ASN:OD1	1:B:591:GLN:N	2.44	0.51
1:A:1072:MET:HE3	1:A:1076:LEU:HD23	1.92	0.51
1:B:481:PHE:HE1	1:B:490:VAL:HG21	1.76	0.51
1:B:1027:TRP:HH2	1:B:1155:LEU:HB3	1.76	0.51
1:B:245:GLU:O	1:A:1174:ARG:NH1	2.33	0.50
1:B:1141:LEU:HD23	1:B:1141:LEU:H	1.76	0.50
1:A:299:ILE:CG2	1:A:529:THR:HG21	2.40	0.50
1:A:1141:LEU:O	1:A:1144:THR:HG22	2.11	0.50
1:B:1026:VAL:HG22	1:B:1167:VAL:HB	1.93	0.50
1:B:1036:THR:HG23	1:B:1167:VAL:HG12	1.94	0.50
1:A:337:SER:HA	1:A:693:VAL:HG21	1.93	0.50
1:B:775:ILE:O	1:B:778:SER:OG	2.22	0.50
1:B:1112:ARG:HD3	1:B:1114:HIS:CE1	2.47	0.50
1:A:862:ASP:OD1	1:A:865:GLU:HG3	2.12	0.50
1:A:1027:TRP:HH2	1:A:1155:LEU:HB3	1.76	0.50
1:B:304:LEU:HD21	1:B:446:ILE:HD11	1.93	0.50
1:B:358:ARG:HA	1:B:758:TRP:CD1	2.47	0.50
1:B:854:PHE:HE2	1:A:778:SER:HB3	1.77	0.50
1:A:1026:VAL:HG22	1:A:1167:VAL:HB	1.93	0.50
1:B:1145:LYS:HE2	1:B:1148:ARG:HH22	1.77	0.50
1:A:304:LEU:HD21	1:A:446:ILE:HD11	1.93	0.50
1:A:1141:LEU:H	1:A:1141:LEU:HD23	1.76	0.50
1:B:298:ASN:C	1:B:298:ASN:ND2	2.65	0.50
1:A:436:ILE:O	1:A:440:VAL:HG23	2.12	0.50
1:B:298:ASN:ND2	1:B:298:ASN:O	2.40	0.49
1:B:778:SER:HB3	1:A:854:PHE:HE2	1.77	0.49
1:B:862:ASP:OD1	1:B:865:GLU:HG3	2.12	0.49
1:A:358:ARG:HA	1:A:758:TRP:CD1	2.47	0.49
1:B:1141:LEU:O	1:B:1144:THR:HG22	2.11	0.49
1:A:875:GLY:HA3	1:A:880:LYS:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1032:ASP:OD2	1:A:1036:THR:OG1	2.14	0.49
1:A:1112:ARG:HD3	1:A:1114:HIS:CE1	2.47	0.49
1:B:436:ILE:O	1:B:440:VAL:HG23	2.12	0.49
1:A:1145:LYS:HE2	1:A:1148:ARG:HH22	1.77	0.49
1:B:337:SER:HA	1:B:693:VAL:HG21	1.93	0.49
1:B:897:MET:CG	1:B:1131:PRO:HB2	2.42	0.49
1:A:298:ASN:C	1:A:298:ASN:ND2	2.65	0.49
1:A:481:PHE:HE1	1:A:490:VAL:HG21	1.76	0.49
1:A:897:MET:CG	1:A:1131:PRO:HB2	2.42	0.49
1:B:1174:ARG:NH1	1:A:245:GLU:O	2.34	0.49
1:A:363:GLU:HG3	1:A:746:TYR:CE1	2.47	0.49
1:A:683:LEU:HD11	1:A:730:ILE:HD12	1.94	0.49
1:A:302:VAL:HG22	1:A:611:THR:HG22	1.95	0.49
1:B:363:GLU:HG3	1:B:746:TYR:CE1	2.47	0.49
1:B:302:VAL:HG22	1:B:611:THR:HG22	1.95	0.49
1:B:875:GLY:HA3	1:B:880:LYS:HA	1.93	0.49
1:A:723:CYS:O	1:A:727:MET:HG2	2.13	0.49
1:B:683:LEU:HD11	1:B:730:ILE:HD12	1.94	0.48
1:B:308:LEU:O	1:B:312:VAL:HG12	2.12	0.48
1:B:391:VAL:HG11	1:B:412:ILE:HG12	1.95	0.48
1:B:723:CYS:O	1:B:727:MET:HG2	2.13	0.48
1:A:1091:ASP:O	1:A:1094:THR:OG1	2.26	0.48
1:A:918:VAL:HG13	1:A:1200:VAL:HG22	1.96	0.48
1:B:1097:LYS:NZ	1:B:1154:GLU:HG2	2.28	0.48
1:A:308:LEU:O	1:A:312:VAL:HG12	2.12	0.48
1:A:1036:THR:HG23	1:A:1167:VAL:HG12	1.94	0.48
1:A:341:ILE:HD13	1:A:704:TRP:HH2	1.78	0.48
1:A:792:LEU:HD11	1:A:870:LEU:HD13	1.96	0.48
1:A:1097:LYS:NZ	1:A:1154:GLU:HG2	2.28	0.48
1:B:378:VAL:HG11	1:B:678:ILE:HD12	1.96	0.48
1:B:828:ARG:O	1:B:832:MET:HG2	2.14	0.48
1:A:378:VAL:HG11	1:A:678:ILE:CD1	2.44	0.48
1:B:341:ILE:HD13	1:B:704:TRP:HH2	1.78	0.47
1:B:378:VAL:HG11	1:B:678:ILE:CD1	2.44	0.47
1:A:288:ILE:HG13	1:A:289:ASN:N	2.29	0.47
1:B:392:VAL:HA	1:B:395:LEU:HG	1.97	0.47
1:B:918:VAL:HG13	1:B:1200:VAL:HG22	1.96	0.47
1:A:507:ILE:HG22	1:A:507:ILE:O	2.14	0.47
1:A:1043:LEU:O	1:A:1049:TRP:HB2	2.15	0.47
1:B:385:VAL:HG11	1:B:671:CYS:SG	2.54	0.47
1:B:705:ARG:HB3	1:A:1041:TYR:OH	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1024:ILE:N	1:B:1053:LYS:O	2.35	0.47
1:A:385:VAL:HG11	1:A:671:CYS:SG	2.54	0.47
1:A:391:VAL:HG11	1:A:412:ILE:HG12	1.95	0.47
1:A:392:VAL:HA	1:A:395:LEU:HG	1.97	0.47
1:A:828:ARG:O	1:A:832:MET:HG2	2.14	0.47
1:B:311:ILE:HG13	1:B:490:VAL:HG13	1.97	0.47
1:B:1035:LEU:O	1:B:1039:ILE:HG12	2.15	0.47
1:B:288:ILE:HG13	1:B:289:ASN:N	2.29	0.47
1:A:298:ASN:ND2	1:A:298:ASN:O	2.40	0.47
1:B:792:LEU:HD11	1:B:870:LEU:HD13	1.96	0.47
1:A:308:LEU:O	1:A:311:ILE:HG22	2.15	0.47
1:A:378:VAL:HG11	1:A:678:ILE:HD12	1.96	0.47
1:A:1095:LYS:HD3	1:A:1096:PRO:O	2.15	0.47
1:B:308:LEU:O	1:B:311:ILE:HG22	2.15	0.47
1:A:311:ILE:HG13	1:A:490:VAL:HG13	1.96	0.47
1:A:907:PHE:CZ	1:A:919:VAL:HG21	2.50	0.47
1:B:453:THR:HG22	1:B:468:TYR:CE2	2.50	0.47
1:B:507:ILE:HG22	1:B:507:ILE:O	2.14	0.47
1:B:790:GLN:HB2	1:B:817:LEU:HB3	1.97	0.47
1:A:295:CYS:O	1:A:299:ILE:HG12	2.15	0.47
1:A:453:THR:HG22	1:A:468:TYR:CE2	2.50	0.47
1:B:295:CYS:O	1:B:299:ILE:HG12	2.15	0.46
1:B:1041:TYR:OH	1:A:705:ARG:HB3	2.15	0.46
1:B:1043:LEU:O	1:B:1049:TRP:HB2	2.15	0.46
1:A:333:ILE:HG21	1:A:719:GLY:HA3	1.97	0.46
1:A:842:TYR:O	1:A:846:LEU:HG	2.15	0.46
1:B:314:GLN:HG2	1:B:587:MET:HG2	1.98	0.46
1:B:643:LYS:HD3	1:B:653:ARG:HH22	1.80	0.46
1:B:904:ILE:O	1:B:907:PHE:HB2	2.15	0.46
1:B:1095:LYS:HD3	1:B:1096:PRO:O	2.15	0.46
1:A:904:ILE:O	1:A:907:PHE:HB2	2.15	0.46
1:A:1035:LEU:O	1:A:1039:ILE:HG12	2.15	0.46
1:B:333:ILE:HG21	1:B:719:GLY:HA3	1.97	0.46
1:B:907:PHE:CZ	1:B:919:VAL:HG21	2.50	0.46
1:A:1130:GLU:O	1:A:1132:TRP:N	2.45	0.46
1:A:1080:ARG:HH12	1:A:1210:PHE:HA	1.80	0.46
1:A:790:GLN:HB2	1:A:817:LEU:HB3	1.97	0.46
1:B:1103:ALA:O	1:B:1107:ILE:HG12	2.16	0.46
1:B:376:ASN:O	1:B:380:VAL:HG23	2.16	0.45
1:A:314:GLN:HG2	1:A:587:MET:HG2	1.98	0.45
1:A:676:PRO:HB2	1:A:731:ASN:HD22	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1178:VAL:HG13	1:A:1182:LEU:HD23	1.98	0.45
1:A:376:ASN:O	1:A:380:VAL:HG23	2.16	0.45
1:B:1035:LEU:HD23	1:B:1200:VAL:HG13	1.98	0.45
1:A:643:LYS:HD3	1:A:653:ARG:HH22	1.81	0.45
1:A:1028:TRP:CD2	1:A:1037:LEU:HD21	2.51	0.45
1:B:842:TYR:O	1:B:846:LEU:HG	2.15	0.45
1:A:1103:ALA:O	1:A:1107:ILE:HG12	2.16	0.45
1:B:332:THR:O	1:B:336:LEU:HG	2.17	0.45
1:B:1080:ARG:HH12	1:B:1210:PHE:HA	1.80	0.45
1:A:478:GLY:O	1:A:546:ARG:NH2	2.49	0.45
1:A:860:ALA:HB1	1:A:865:GLU:OE2	2.17	0.45
1:A:381:ALA:HA	1:A:384:VAL:HG12	1.97	0.45
1:A:478:GLY:HA2	1:A:479:PRO:HD3	1.79	0.45
1:B:381:ALA:HA	1:B:384:VAL:HG12	1.97	0.45
1:B:478:GLY:O	1:B:546:ARG:NH2	2.49	0.45
1:B:676:PRO:HB2	1:B:731:ASN:HD22	1.80	0.45
1:B:1113:LEU:HD12	1:B:1132:TRP:HB2	1.99	0.45
1:B:907:PHE:HZ	1:B:919:VAL:HG21	1.82	0.44
1:A:311:ILE:CD1	1:A:494:PHE:HB2	2.47	0.44
1:A:332:THR:O	1:A:336:LEU:HG	2.17	0.44
1:B:311:ILE:CD1	1:B:494:PHE:HB2	2.47	0.44
1:B:1178:VAL:HG13	1:B:1182:LEU:HD23	1.99	0.44
1:A:297:LEU:HG	1:A:613:SER:CB	2.45	0.44
1:A:656:ILE:O	1:A:660:LEU:HG	2.18	0.44
1:B:1028:TRP:CD2	1:B:1037:LEU:HD21	2.51	0.44
1:A:919:VAL:HB	1:A:1199:LEU:HB2	2.00	0.44
1:B:291:VAL:HG13	1:B:521:GLY:HA3	1.99	0.44
1:B:656:ILE:O	1:B:660:LEU:HG	2.18	0.44
1:A:775:ILE:O	1:A:778:SER:OG	2.22	0.44
1:A:1035:LEU:HD23	1:A:1200:VAL:HG13	1.98	0.44
1:A:1113:LEU:HD12	1:A:1132:TRP:HB2	1.99	0.44
1:B:305:PHE:CB	1:B:607:ILE:HG13	2.46	0.44
1:B:324:ILE:HG12	1:B:494:PHE:CE2	2.53	0.44
1:B:731:ASN:OD1	1:B:733:TRP:NE1	2.51	0.44
1:B:860:ALA:HB1	1:B:865:GLU:OE2	2.17	0.44
1:A:727:MET:O	1:A:735:ALA:HB2	2.18	0.44
1:B:546:ARG:HD2	1:B:587:MET:SD	2.58	0.44
1:B:577:CYS:HB2	1:B:582:CYS:HB3	1.50	0.44
1:B:790:GLN:HA	1:B:817:LEU:H	1.83	0.44
1:B:904:ILE:HD12	1:B:1183:TYR:HD2	1.83	0.44
1:B:229:HIS:C	1:B:231:ALA:H	2.21	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:464:GLY:HA2	1:B:545:VAL:HG22	2.00	0.43
1:A:737:LEU:O	1:A:741:ILE:HG12	2.18	0.43
1:B:492:GLU:CG	1:B:730:ILE:HG23	2.46	0.43
1:B:1108:ILE:O	1:B:1108:ILE:HG13	2.18	0.43
1:A:349:GLY:HA2	1:A:509:GLY:CA	2.48	0.43
1:A:380:VAL:HG11	1:A:619:LEU:HD12	2.00	0.43
1:B:727:MET:O	1:B:735:ALA:HB2	2.18	0.43
1:A:464:GLY:HA2	1:A:545:VAL:HG22	2.00	0.43
1:B:737:LEU:O	1:B:741:ILE:HG12	2.18	0.43
1:B:919:VAL:HB	1:B:1199:LEU:HB2	2.00	0.43
1:A:420:LEU:HD23	1:A:420:LEU:HA	1.83	0.43
1:A:486:THR:O	1:A:490:VAL:HG23	2.19	0.43
1:A:577:CYS:HB2	1:A:582:CYS:HB3	1.50	0.43
1:A:731:ASN:OD1	1:A:733:TRP:NE1	2.51	0.43
1:A:907:PHE:HZ	1:A:919:VAL:HG21	1.82	0.43
1:A:1024:ILE:N	1:A:1053:LYS:O	2.35	0.43
1:B:349:GLY:HA2	1:B:509:GLY:CA	2.48	0.43
1:A:1108:ILE:HG13	1:A:1108:ILE:O	2.18	0.43
1:B:409:ILE:HG13	1:B:410:ARG:N	2.34	0.43
1:A:291:VAL:HG13	1:A:521:GLY:HA3	1.99	0.43
1:A:546:ARG:HD2	1:A:587:MET:SD	2.58	0.43
1:B:380:VAL:HG11	1:B:619:LEU:HD12	2.00	0.43
1:B:835:MET:HE1	1:B:859:HIS:HB2	1.99	0.43
1:A:356:ILE:HD13	1:A:368:ILE:HG21	2.01	0.43
1:A:808:VAL:HA	1:A:811:PHE:CE2	2.54	0.43
1:B:1080:ARG:NH1	1:B:1210:PHE:HA	2.34	0.43
1:B:284:LYS:HB3	1:B:512:ALA:HA	2.01	0.42
1:B:341:ILE:HG21	1:B:355:LEU:HB3	2.01	0.42
1:B:780:VAL:HG21	1:A:766:THR:HG21	2.01	0.42
1:A:324:ILE:HG12	1:A:494:PHE:CE2	2.53	0.42
1:B:356:ILE:HD13	1:B:368:ILE:HG21	2.01	0.42
1:B:808:VAL:HA	1:B:811:PHE:CE2	2.54	0.42
1:A:790:GLN:HA	1:A:817:LEU:H	1.83	0.42
1:A:838:ASP:HB3	1:A:842:TYR:CE2	2.54	0.42
1:A:1097:LYS:HZ1	1:A:1154:GLU:HG2	1.84	0.42
1:B:1076:LEU:HD11	1:B:1083:PHE:CD1	2.54	0.42
1:B:1130:GLU:O	1:B:1132:TRP:N	2.45	0.42
1:A:229:HIS:C	1:A:231:ALA:H	2.21	0.42
1:A:409:ILE:HG13	1:A:410:ARG:N	2.34	0.42
1:A:787:PHE:CD2	1:A:1207:VAL:HG13	2.55	0.42
1:A:1080:ARG:NH1	1:A:1210:PHE:HA	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:PHE:CE2	1:B:608:PHE:HD1	2.38	0.42
1:B:897:MET:HA	1:B:900:VAL:HG22	2.01	0.42
1:B:922:LEU:HD11	1:B:924:GLU:OE1	2.20	0.42
1:A:794:MET:HG2	1:A:884:LEU:HD11	2.02	0.42
1:A:1076:LEU:HD11	1:A:1083:PHE:CD1	2.54	0.42
1:B:217:THR:HG23	1:B:218:MET:N	2.34	0.42
1:B:695:HIS:NE2	1:B:765:LEU:HD22	2.34	0.42
1:B:766:THR:HG21	1:A:780:VAL:HG21	2.01	0.42
1:B:838:ASP:HB3	1:B:842:TYR:CE2	2.54	0.42
1:B:1028:TRP:CZ2	1:B:1037:LEU:HD21	2.54	0.42
1:A:904:ILE:HD12	1:A:1183:TYR:HD2	1.83	0.42
1:B:478:GLY:HA2	1:B:479:PRO:HD3	1.79	0.42
1:A:284:LYS:HB3	1:A:512:ALA:HA	2.01	0.42
1:A:387:PHE:CE2	1:A:608:PHE:HD1	2.38	0.42
1:A:1098:LYS:HA	1:A:1101:ILE:HG22	2.01	0.42
1:B:486:THR:O	1:B:490:VAL:HG23	2.19	0.42
1:B:1174:ARG:HB3	1:B:1177:ALA:HB3	2.02	0.42
1:A:217:THR:HG23	1:A:218:MET:N	2.34	0.42
1:B:804:LEU:O	1:B:808:VAL:HG23	2.20	0.42
1:B:1098:LYS:HA	1:B:1101:ILE:HG22	2.01	0.42
1:B:290:GLY:O	1:B:294:ARG:HD3	2.20	0.41
1:B:721:ILE:O	1:B:725:ILE:HG12	2.20	0.41
1:A:341:ILE:HG21	1:A:355:LEU:HB3	2.01	0.41
1:A:492:GLU:CG	1:A:730:ILE:HG23	2.46	0.41
1:A:897:MET:HA	1:A:900:VAL:HG22	2.01	0.41
1:A:1025:ASP:OD1	1:A:1055:ARG:NE	2.31	0.41
1:B:368:ILE:HD12	1:B:368:ILE:HA	1.96	0.41
1:A:297:LEU:HD12	1:A:297:LEU:HA	1.87	0.41
1:B:787:PHE:CD2	1:B:1207:VAL:HG13	2.55	0.41
1:B:794:MET:HG2	1:B:884:LEU:HD11	2.02	0.41
1:A:290:GLY:O	1:A:294:ARG:HD3	2.20	0.41
1:A:305:PHE:CB	1:A:607:ILE:HG13	2.46	0.41
1:A:721:ILE:O	1:A:725:ILE:HG12	2.20	0.41
1:A:1028:TRP:CZ2	1:A:1037:LEU:HD21	2.54	0.41
1:B:229:HIS:O	1:B:231:ALA:N	2.49	0.41
1:A:695:HIS:NE2	1:A:765:LEU:HD22	2.34	0.41
1:B:389:GLU:HA	1:B:392:VAL:HG12	2.03	0.41
1:A:524:LEU:O	1:A:528:ILE:HG12	2.21	0.41
1:A:736:LEU:O	1:A:740:VAL:HG23	2.21	0.41
1:A:1194:LEU:HD23	1:A:1194:LEU:HA	1.90	0.41
1:B:297:LEU:HG	1:B:613:SER:CB	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:PHE:CZ	1:B:683:LEU:HD21	2.56	0.41
1:B:870:LEU:HD23	1:B:870:LEU:HA	1.88	0.41
1:B:876:LEU:HD11	1:A:854:PHE:CD1	2.56	0.41
1:B:1148:ARG:O	1:B:1152:LEU:HG	2.21	0.41
1:B:1191:SER:OG	1:B:1199:LEU:HD11	2.21	0.41
1:A:389:GLU:HA	1:A:392:VAL:HG12	2.03	0.41
1:A:820:CYS:N	1:A:854:PHE:O	2.44	0.41
1:A:1040:PRO:O	1:A:1044:THR:HG23	2.21	0.41
1:A:1145:LYS:O	1:A:1149:GLN:HG2	2.21	0.41
1:A:375:ALA:HB1	1:A:682:PHE:CE2	2.56	0.41
1:A:804:LEU:O	1:A:808:VAL:HG23	2.20	0.41
1:B:600:THR:N	1:B:601:PRO:HD2	2.36	0.40
1:B:717:LEU:O	1:B:721:ILE:HG12	2.22	0.40
1:B:736:LEU:O	1:B:740:VAL:HG23	2.21	0.40
1:B:854:PHE:CD1	1:A:876:LEU:HD11	2.56	0.40
1:A:501:ILE:O	1:A:502:LEU:HG	2.21	0.40
1:A:1174:ARG:HB3	1:A:1177:ALA:HB3	2.02	0.40
1:B:358:ARG:NH1	1:B:632:ASP:OD2	2.35	0.40
1:B:480:ASP:HB3	1:B:546:ARG:NE	2.34	0.40
1:B:501:ILE:O	1:B:502:LEU:HG	2.21	0.40
1:A:358:ARG:NH1	1:A:632:ASP:OD2	2.35	0.40
1:A:495:PHE:CZ	1:A:683:LEU:HD21	2.56	0.40
1:A:630:CYS:HB2	1:A:642:ALA:HB2	2.03	0.40
1:A:665:PHE:HE1	1:A:674:ILE:HG12	1.87	0.40
1:A:1191:SER:OG	1:A:1199:LEU:HD11	2.21	0.40
1:B:630:CYS:HB2	1:B:642:ALA:HB2	2.03	0.40
1:B:820:CYS:N	1:B:854:PHE:O	2.44	0.40
1:A:600:THR:N	1:A:601:PRO:HD2	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	865/1216 (71%)	779 (90%)	86 (10%)	0	100	100
1	B	865/1216 (71%)	780 (90%)	85 (10%)	0	100	100
All	All	1730/2432 (71%)	1559 (90%)	171 (10%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	592/985 (60%)	590 (100%)	2 (0%)	92	98
1	B	592/985 (60%)	590 (100%)	2 (0%)	92	98
All	All	1184/1970 (60%)	1180 (100%)	4 (0%)	92	98

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	298	ASN
1	B	1067	HIS
1	A	298	ASN
1	A	1067	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	731	ASN
1	B	773	HIS
1	B	1153	ASN
1	A	731	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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	$\#\|Z\| > 2$
2	82U	B	1301	3	26,26,26	1.48	5 (19%)	32,36,36	1.31	1 (3%)
2	82U	A	1301	3	26,26,26	1.48	5 (19%)	32,36,36	1.31	1 (3%)

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	82U	B	1301	3	-	1/19/19/19	0/2/2/2
2	82U	A	1301	3	-	1/19/19/19	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1301	82U	S1-NE1	5.32	1.70	1.60
2	A	1301	82U	S1-NE1	5.28	1.70	1.60
2	A	1301	82U	CA-N	2.64	1.44	1.37
2	B	1301	82U	CA-N	2.61	1.44	1.37
2	B	1301	82U	O4-C17	2.39	1.29	1.22
2	A	1301	82U	O4-C17	2.39	1.29	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1301	82U	C1-S1	-2.34	1.74	1.77
2	B	1301	82U	C1-S1	-2.26	1.74	1.77
2	B	1301	82U	O5-C17	-2.16	1.23	1.30
2	A	1301	82U	O5-C17	-2.14	1.24	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1301	82U	O2-S1-O1	-5.79	109.25	118.76
2	B	1301	82U	O2-S1-O1	-5.78	109.25	118.76

There are no chirality outliers.

All (2) torsion outliers are listed below:

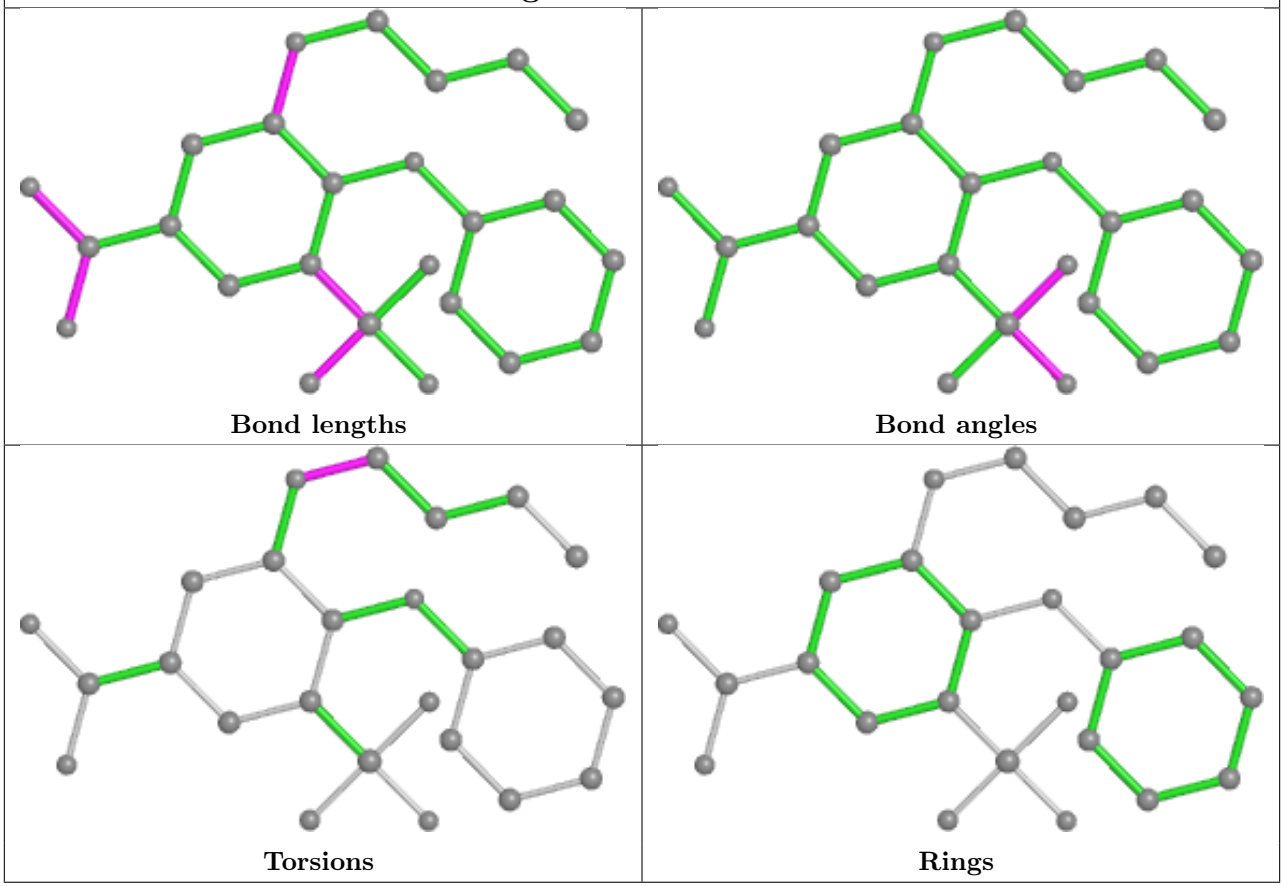
Mol	Chain	Res	Type	Atoms
2	B	1301	82U	CZ2-C6-N-CA
2	A	1301	82U	CZ2-C6-N-CA

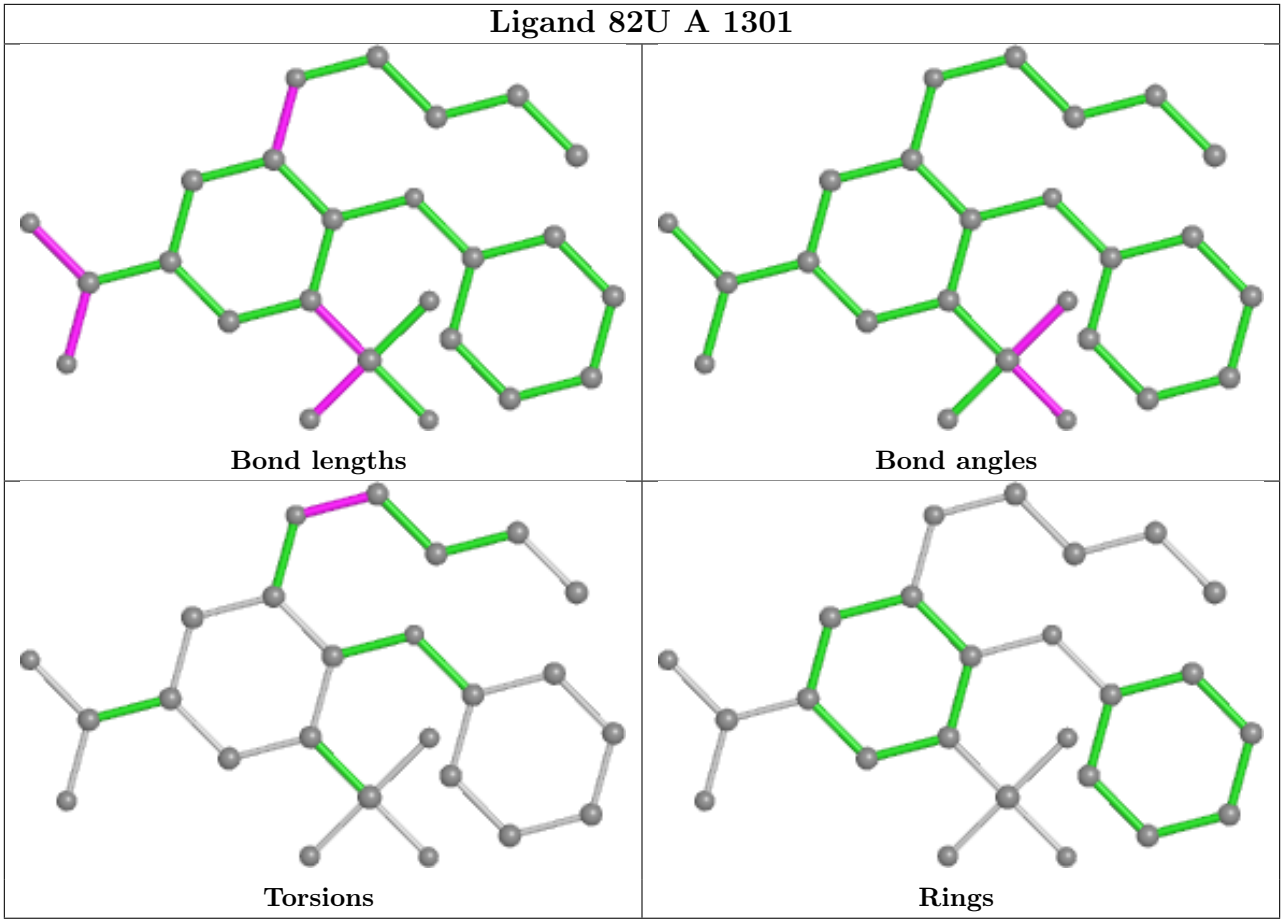
There are no ring outliers.

No monomer is involved in short contacts.

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 then 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.

Ligand 82U B 1301





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)

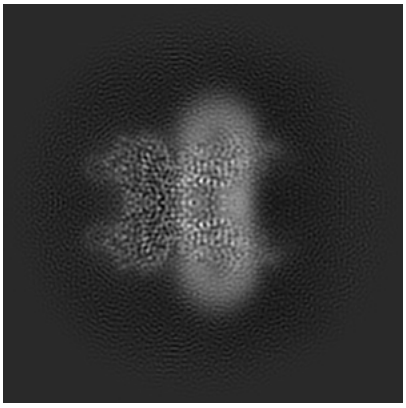
This section contains visualisations of the EMDB entry EMD-24807. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

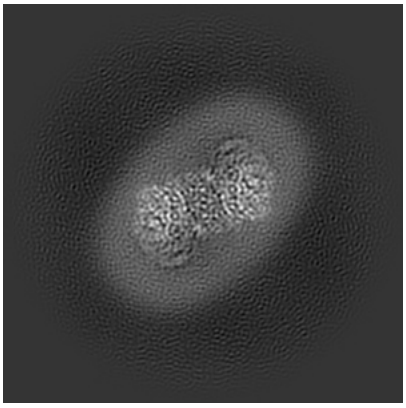
6.1 Orthogonal projections (i)

6.1.1 Primary map

X



Y

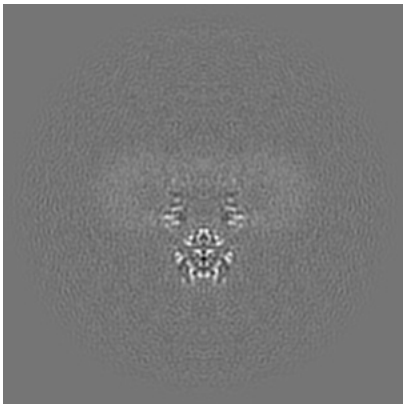


Z

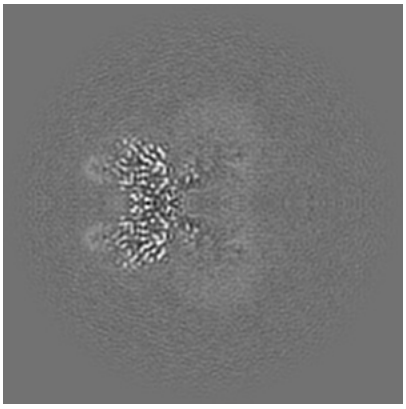
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

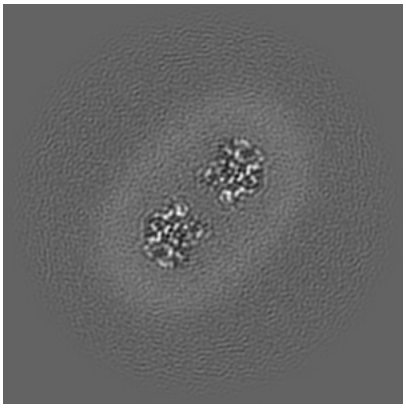
6.2.1 Primary map



X Index: 128



Y Index: 128

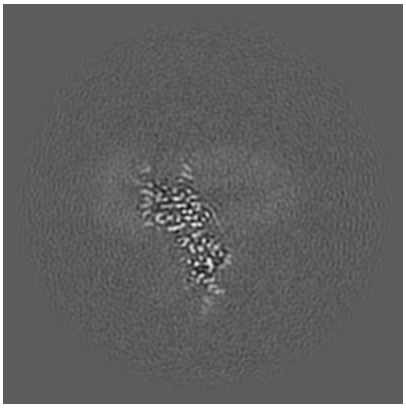


Z Index: 128

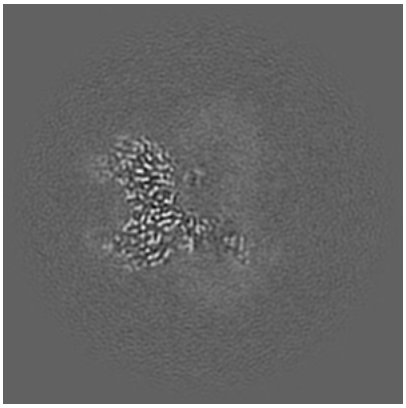
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

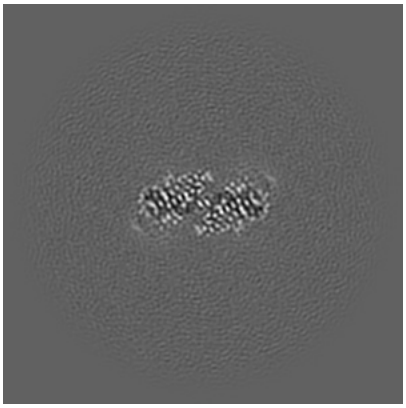
6.3.1 Primary map



X Index: 113



Y Index: 124



Z Index: 91

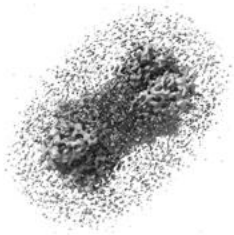
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

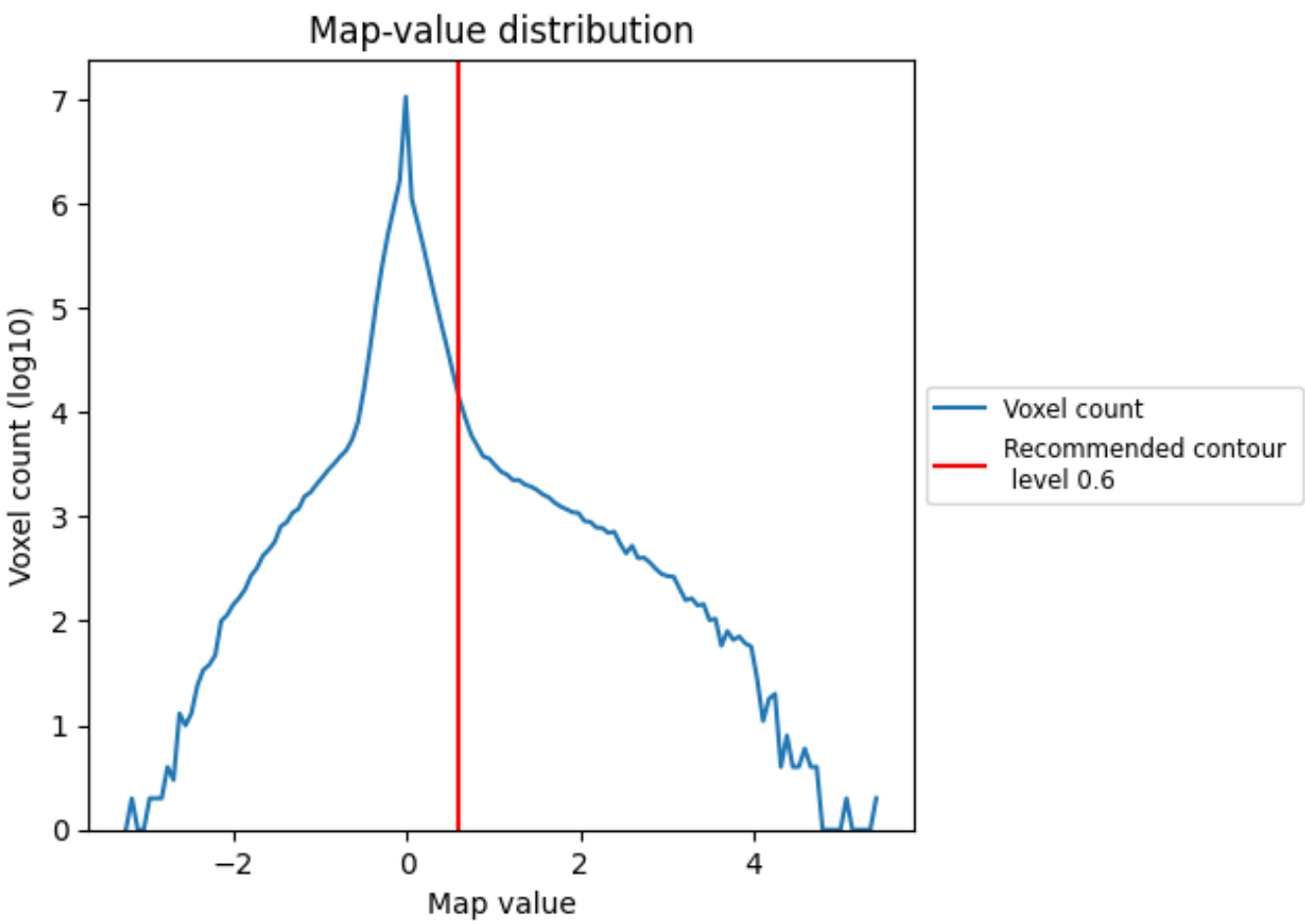
6.5 Mask visualisation (i)

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

7 Map analysis (i)

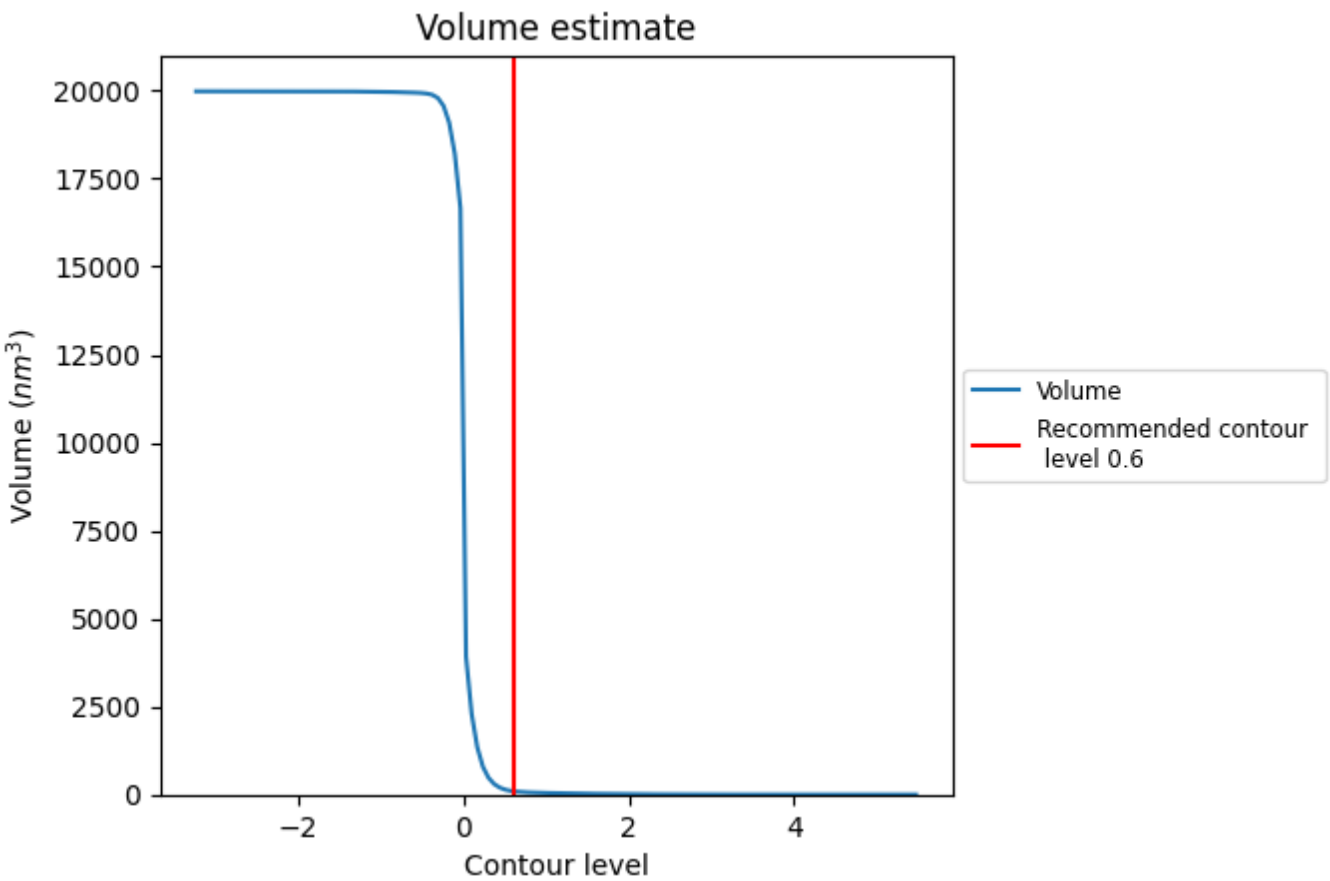
This section contains the results of statistical analysis of the map.

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.

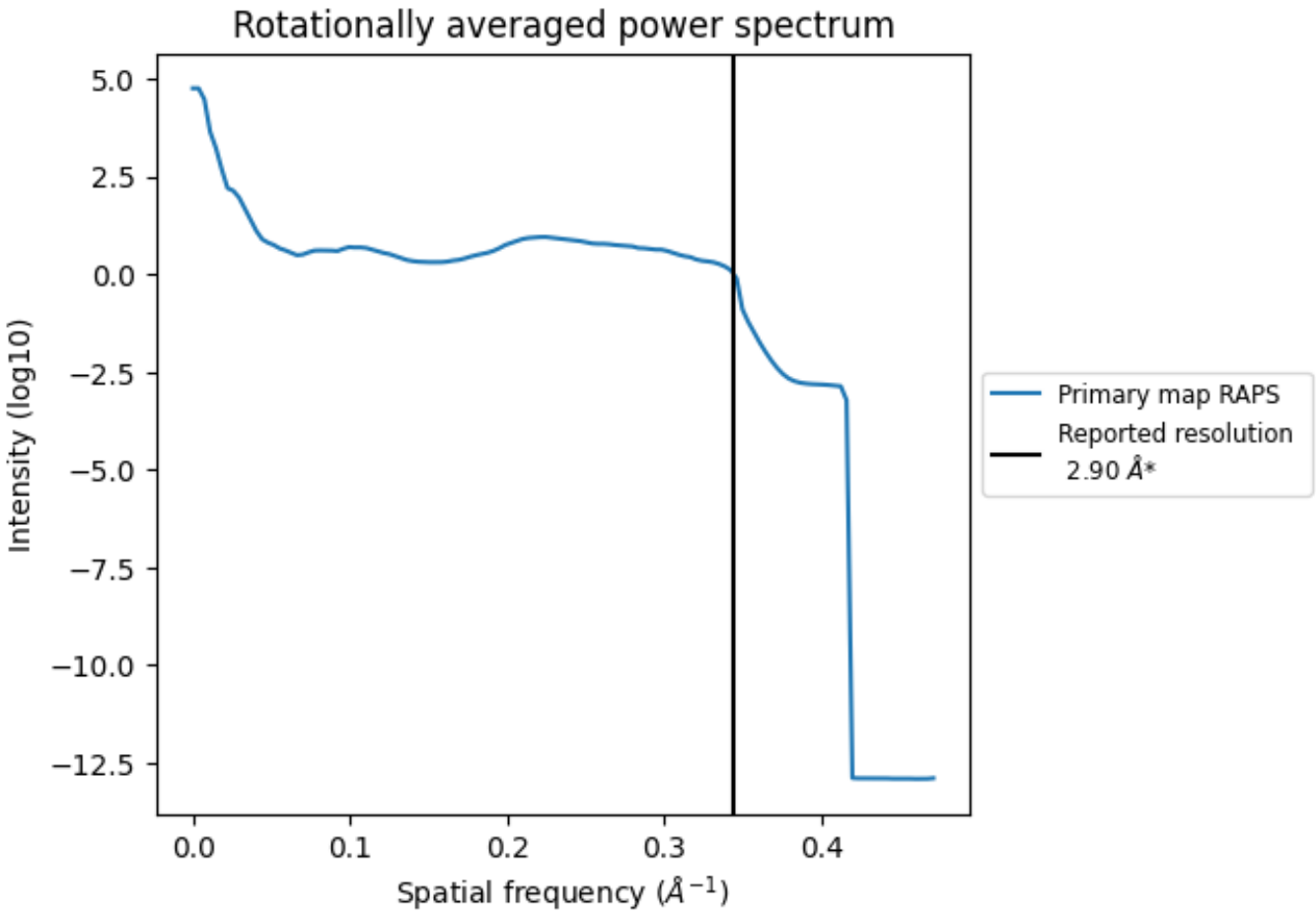
7.2 Volume estimate (i)



The volume at the recommended contour level is 96 nm^3; this corresponds to an approximate mass of 87 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.345 Å^{-1}

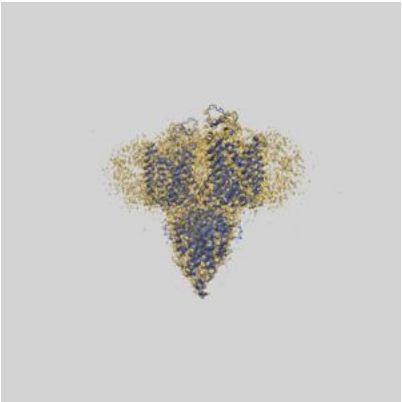
8 Fourier-Shell correlation (i)

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

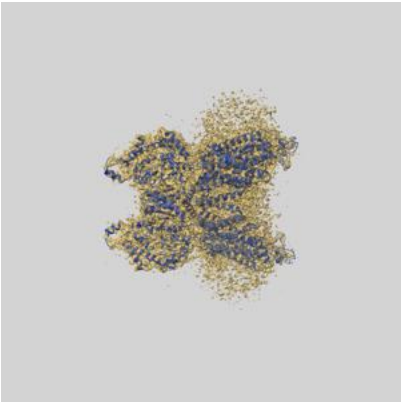
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-24807 and PDB model 7S1X. Per-residue inclusion information can be found in section 3 on page 5.

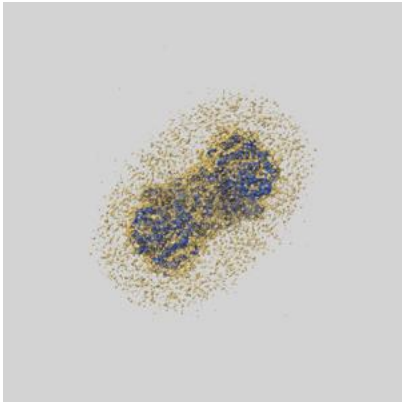
9.1 Map-model overlay (i)



X



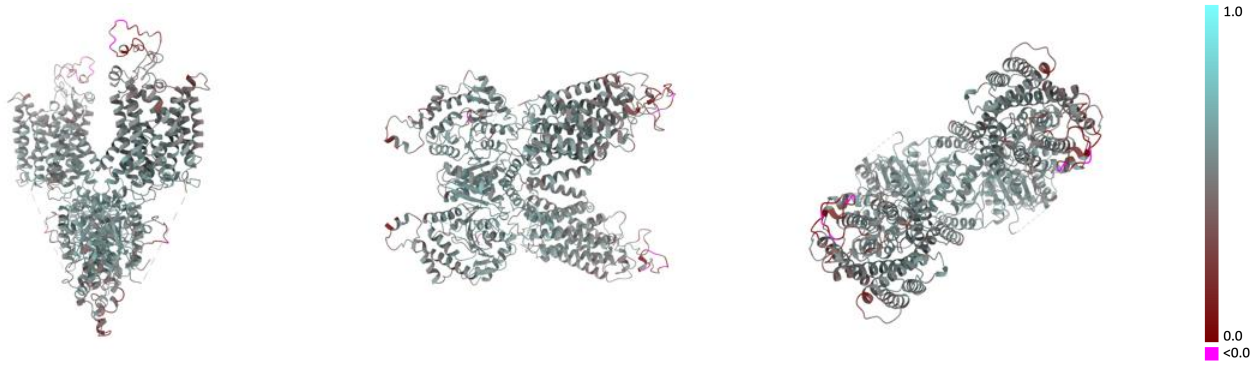
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.6 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.

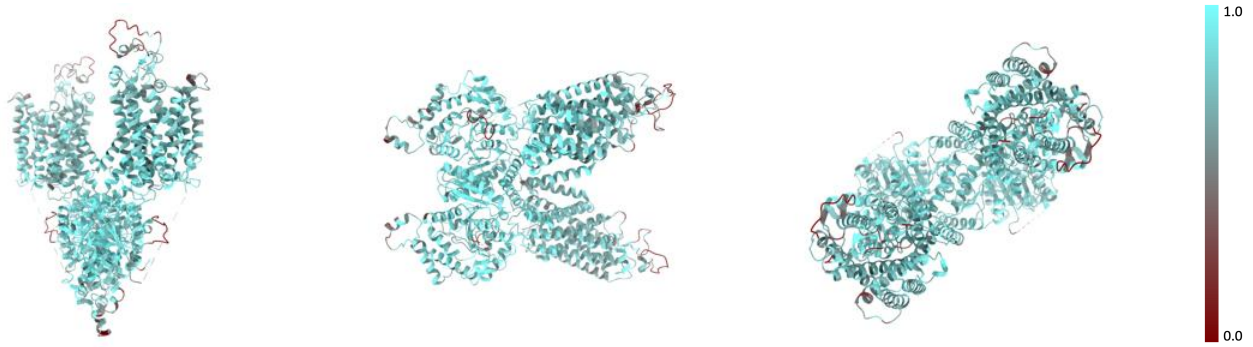
9.2 Q-score mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according 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.

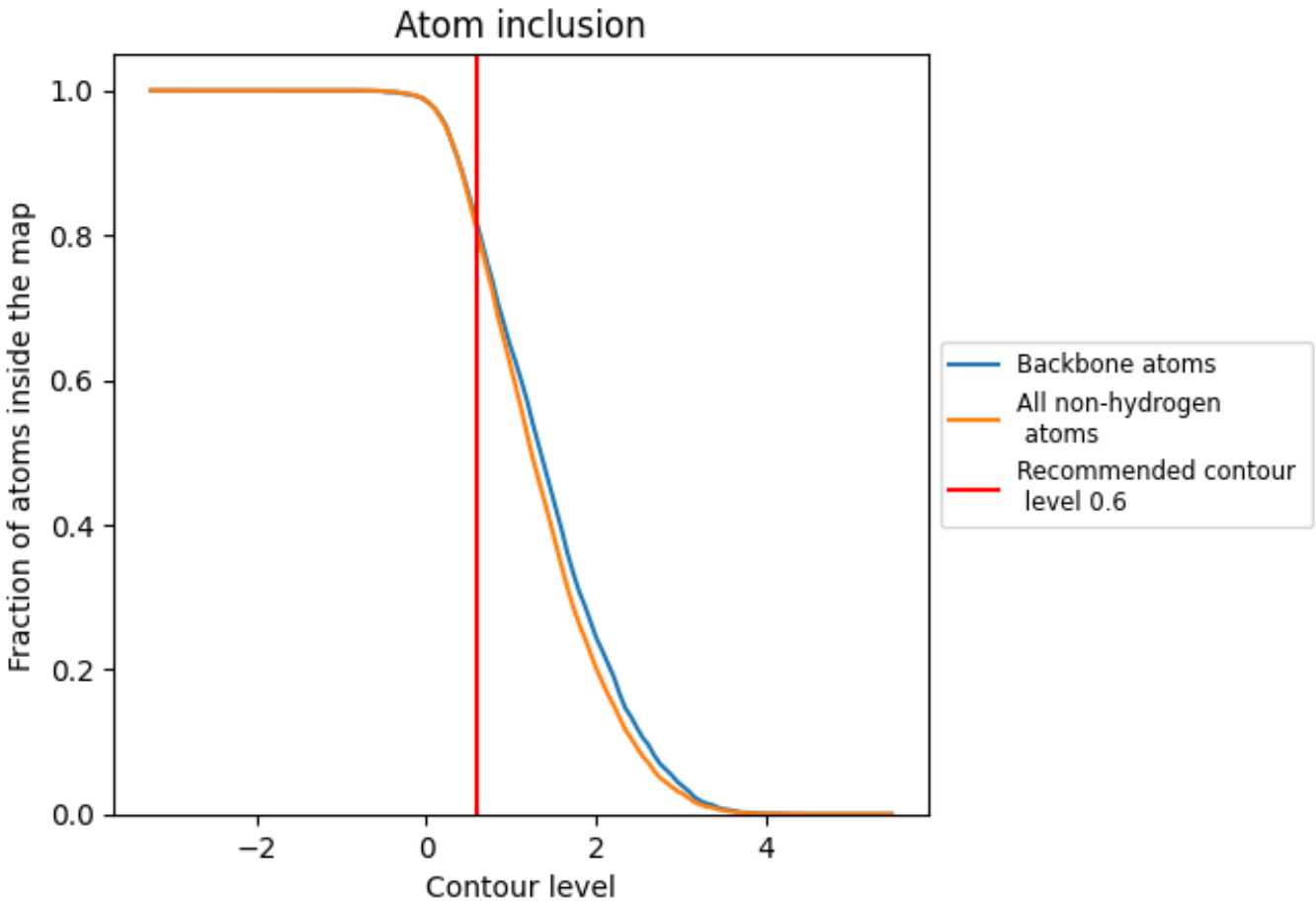
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

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 (0.6).

9.4 Atom inclusion (i)



At the recommended contour level, 81% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.6) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8059	0.5150
A	0.8061	0.5150
B	0.8056	0.5150