



Full wwPDB EM Validation Report ⓘ

Oct 6, 2024 – 05:54 AM JST

PDB ID : 7FG7
EMDB ID : EMD-31578
Title : Cryo-EM structure of S protein trimer of SARS-CoV2
Authors : Song, C.; Murata, K.; Katayama, K.
Deposited on : 2021-07-26
Resolution : 6.90 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 ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev113
MolProbity : 4.02b-467
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

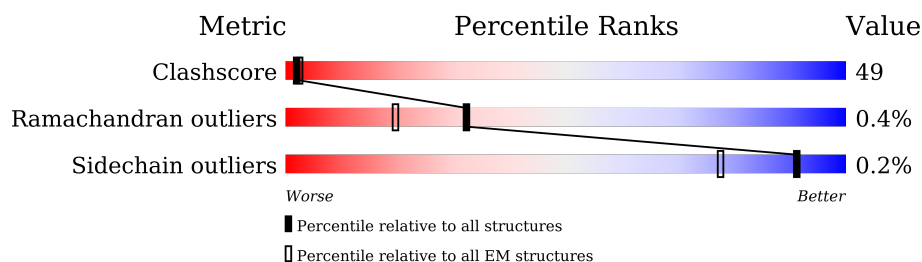
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.90 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	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 ≥ 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	1273	<div> <div>33%</div> <div>30%</div> <div>57%</div> <div>•</div> <div>12%</div> </div>

2 Entry composition [i](#)

There is only 1 type of molecule in this entry. The entry contains 8690 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

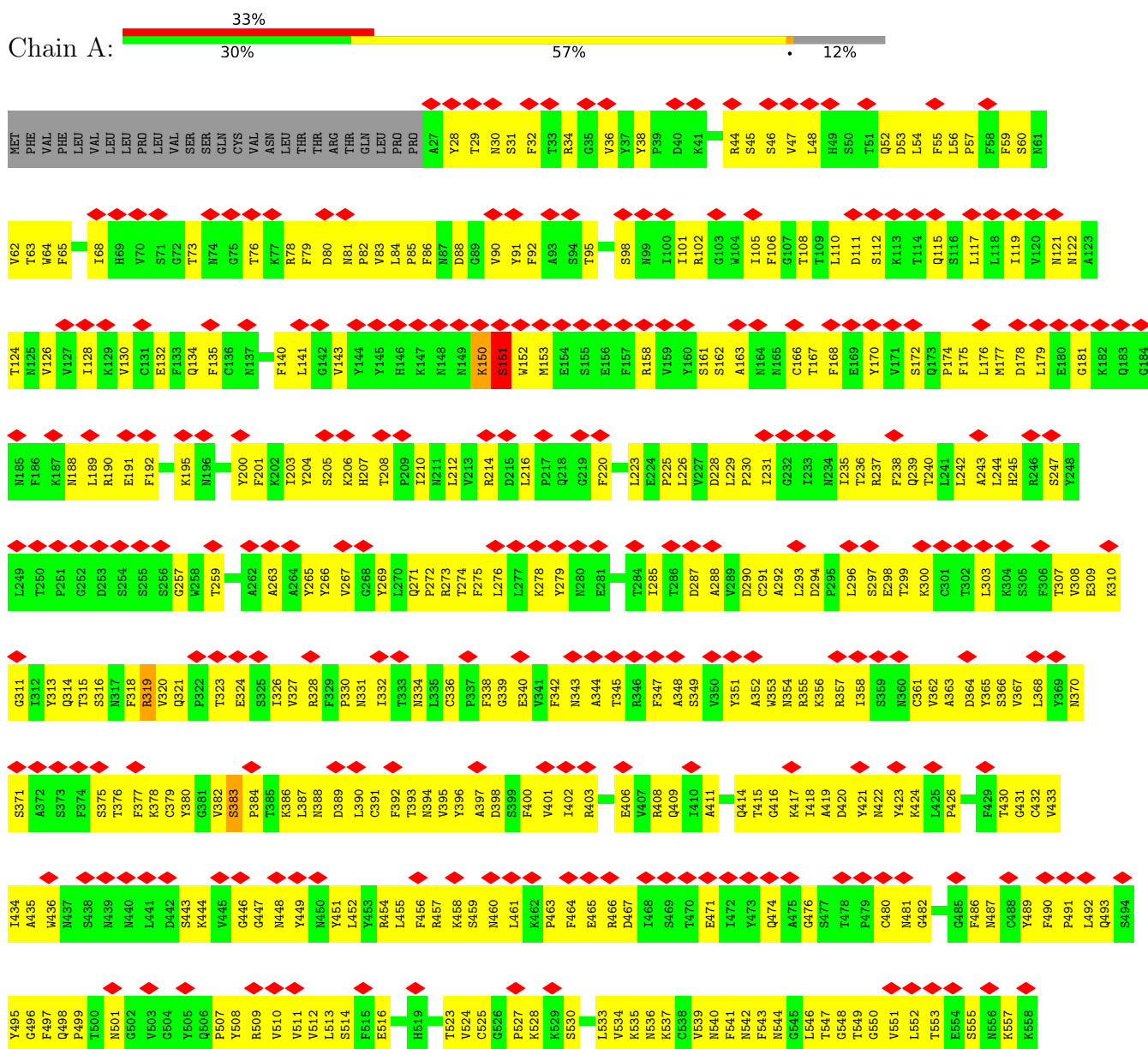
- Molecule 1 is a protein called Spike glycoprotein.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1114	8690	5534	1460	1657	39	0	0

3 Residue-property plots

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

• Molecule 1: Spike glycoprotein



Lys	Arg	His125	L1063	R1000	T934	Q872	P812	L752	R685	I624	F559
Gly	Leu	C1126	H1064	L1001	Q935	Y873	S813	L753	R686	H625	
Cys	Asn	D1127	V1065	L1002	D936	T874	K814	L754	V687	A826	P561
Cys	Val	V1128	T1066	S1003	S937	S875	R815	Q755	A888	D627	
Cys	Ala	V1129	V1067	L1005	L938	A876	S816	Q756	S689	Q628	Q564
Gly	Lys	I1130	V1068	T1006	S939	L877	F817	G757	Q690	L629	F565
Ser	Asn	G1131	V1069	Y1007	S940	A878	T818	S758	S691	T629	
Cys	Leu	I1132	A1070	T1008	T941	G880	E819	F759	T630	L630	G566
Cys	Asn	V1133	T1009	T881	A944	G881	D820	Q760	I692	P631	R567
Lys	Glu	H1134	Q1071	Q1010	A945	I882	L821	T761	I693	T632	D568
Phe	Ser	N1135	E1072	Q1011	Q946	T883	L822	Q762	A694	G633	I569
Asp	Leu	T1136	K1073	I1012	K947	S884	F823	L763	T696	M634	A570
Glu	Ile			I1013	L948	K925	M824	T64	R697	V635	D571
Asp	Asp	V1137	T1077	R1014	Q949	G885	V826	A765	S698	G636	T572
Asp	Ala15	A1015	A1078	A1016	D950	M886	T827	L767	L699	T638	T573
Ser	Gln	D1138	A1078	A1016	V951	L828	L828	Q769		G639	D574
Glu	Glu	D1139	P1079	E1017	V952	F888	A829	T770	V705	S640	A575
Pro	Leu	P1140	A1060	I1018	V953	Q889	D830	I771	A706	G639	V576
Val	Gly	Leu	I1081	R1019	Q954	Q891	A831	A771	A707	M641	R577
Leu	Gln	Leu	H1083	A1020	N955	G892	G832	V772	S708	V642	D578
Lys	Gln	Glu	G1082	L1024	Q957	A893	F833	V773	N709	Q643	P579
Lys	Leu	Leu	G1085	L1025	Q958	A894	K935	D775	S711	T645	Q580
Ser	Ser	Asp	A1026	A1025	Q895	Q895	K936	K776	I712	R646	T581
Ile	Phe	Ser	K1086	A1026	I896	I896	Q836	T777	A713	L582	L582
Lys	Thr	Lys	A1087	T1027	T961	T961	G837	T778	I714	C649	E584
Thr	Thr	Lys	H1088	K1028	L962	P897	Y838	Q779	P715	L650	L585
Thr	Glu	Glu	F1089	M1028	V963	F898	G838	E780	T716	G852	D586
Trp	Glu	Leu	P1090	S1030	K964	A999	D839	I781	N717	E654	T588
Leu	Leu	Leu	E1091	E1031	K964	N900	C940	F782	F718	H655	P589
Asp	Ile	Asp	E1092	C1032	Q966	Q901	L841	A783	I720	V656	C590
Lys	Thr	Leu	G1093	V1033	F970	N902	G842	Q784		R657	S591
Phe	Gly	Leu	V1094	G1035		A903	D843	K786	E725	N658	F592
Phe	Phe	Lys	F1095	Q1036	I973	Y904	I844	I788	I726	S659	V595
Ala	Ala	Asn	V1096	S1037	S974	R905	A845	V789	I727	V660	V597
Thr	Gly	Thr	S1097	K1038	V976	F906	A946	K790	P728	E661	I598
Ser	Ser	Leu	N1098	R1039	L977	N907	R947	T791	C662	C662	T599
Pro	Ile	Pro	G1099	V1040	L978	Q908	D848	F792	D663	D663	G601
Ala	Ala	Asp	H1100	D1041	N978	I909	L849	P792	I664	I664	T602
Val	Ile	Val	H101	I1041	D979	G910	I850	P793	P665	P665	G603
Val	Met	Asp	V1102	F1042	V911	V911	C851	I794	I666	G667	T604
Met	Leu	Leu	F1103	C1043	T912	G913		F797	A668	G667	
Val	Val	Gly	V1104		Q913			G798	G668	G669	
Thr	Thr	Asp	T1105		L916			G799	D737	I670	
Ile	Ile	Ser	Q1066	H1048	Y917	Y917	N856	C738	C738	C571	
Leu	Gly	Leu	R1107	L1049	E988	E918	G857	F800	T739	C571	
Ser	Ser	Gly	F1108	M1050	V987	N919	L858	N801	M740	A672	Q607
Cys	Cys	Asn	Y1109	S1051	E988	N919	L858	F800	M740	A672	Q608
Cys	Met	Ala	E1111	F1052	V991	Q920	T859	N801	Y741	G674	A609
Thr	Ser	Val	P1112	P1053	G991	K921	V860	F802	I742	Y674	V610
Val	Ser	Val	Q1113	Q1054	Q992	L922	L861	S803	T676	Q675	L611
Cys	Cys	Val	T1114	S1055	Q993	Q923	P862	Q804	I742	Q675	Y612
Val	Val	Val	I1115	A1056	D994	T923	P863	I805	C743	T676	Q613
Val	Val	Val	P1116	P1057	V991	A924	L864	L806	G744	Q677	
Val	Val	Val	H1058	H1058	G995	A924	L864	L806	G744	Q677	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	
Val	Val	Val	T1117	G1059	Q997	N928	T866	D808	D745	T678	</

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14235	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	JEOL 2200FS	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1578.3	Depositor
Maximum defocus (nm)	4967.2	Depositor
Magnification	45065	Depositor
Image detector	DIRECT ELECTRON DE-20 (5k x 3k)	Depositor
Maximum map value	0.213	Depositor
Minimum map value	-0.145	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.02	Depositor
Map size (\AA)	363.52, 363.52, 363.52	wwPDB
Map dimensions	256, 256, 256	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.42, 1.42, 1.42	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.43	2/8893 (0.0%)	0.63	4/12105 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	590	CYS	C-N	6.64	1.49	1.34
1	A	274	THR	C-N	6.34	1.48	1.34

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1050	MET	CG-SD-CE	6.62	110.78	100.20
1	A	763	LEU	CA-CB-CG	-6.05	101.39	115.30
1	A	1001	LEU	CB-CG-CD2	-5.58	101.51	111.00
1	A	1014	ARG	NE-CZ-NH1	-5.21	117.69	120.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	151	SER	Peptide
1	A	383	SER	Peptide
1	A	590	CYS	Peptide
1	A	837	TYR	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	845	ALA	Peptide
1	A	847	ARG	Peptide
1	A	849	LEU	Peptide
1	A	851	CYS	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	8690	0	8483	833	0
All	All	8690	0	8483	833	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 49.

All (833) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:VAL:HG11	1:A:623:ALA:HB2	1.44	1.00
1:A:781:VAL:HG12	1:A:1026:ALA:HB2	1.48	0.96
1:A:1010:GLN:HB3	1:A:1014:ARG:HH12	1.30	0.94
1:A:448:ASN:HB3	1:A:497:PHE:HB3	1.51	0.93
1:A:739:THR:O	1:A:743:CYS:N	2.01	0.92
1:A:620:VAL:HG13	1:A:627:ASP:HB2	1.52	0.91
1:A:833:PHE:HB3	1:A:852:ALA:H	1.39	0.88
1:A:121:ASN:HD21	1:A:175:PHE:H	1.21	0.88
1:A:115:GLN:HA	1:A:132:GLU:HG3	1.56	0.86
1:A:190:ARG:HE	1:A:192:PHE:HZ	1.22	0.86
1:A:945:LEU:HB3	1:A:948:LEU:HD12	1.57	0.86
1:A:498:GLN:HB2	1:A:501:ASN:HB2	1.55	0.86
1:A:576:VAL:HB	1:A:587:ILE:HD11	1.58	0.85
1:A:731:MET:HG3	1:A:732:THR:H	1.38	0.85
1:A:906:PHE:HB3	1:A:911:VAL:HB	1.57	0.85
1:A:903:ALA:HB1	1:A:913:GLN:HB3	1.59	0.83
1:A:310:LYS:HD2	1:A:685:ARG:HE	1.42	0.83
1:A:734:THR:HA	1:A:860:VAL:HA	1.60	0.83

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:833:PHE:CB	1:A:852:ALA:H	1.92	0.81
1:A:811:LYS:HD2	1:A:812:PRO:HD2	1.62	0.81
1:A:780:GLU:O	1:A:784:GLN:NE2	2.14	0.81
1:A:646:ARG:HH11	1:A:668:ALA:HB2	1.46	0.81
1:A:386:LYS:HG2	1:A:389:ASP:HB3	1.62	0.80
1:A:655:HIS:HA	1:A:694:ALA:HB3	1.63	0.80
1:A:378:LYS:HG3	1:A:380:TYR:HE1	1.47	0.80
1:A:951:VAL:O	1:A:955:ASN:ND2	2.15	0.79
1:A:1049:LEU:N	1:A:1065:VAL:O	2.13	0.79
1:A:1128:VAL:HG23	1:A:1129:VAL:HG23	1.63	0.78
1:A:742:ILE:HG23	1:A:1000:ARG:HD2	1.66	0.78
1:A:598:ILE:HG23	1:A:664:ILE:HG21	1.64	0.78
1:A:1009:THR:HA	1:A:1012:LEU:HD12	1.66	0.77
1:A:126:VAL:HG13	1:A:174:PRO:HA	1.67	0.77
1:A:564:GLN:OE1	1:A:577:ARG:NH2	2.18	0.77
1:A:935:GLN:NE2	1:A:936:ASP:OD1	2.18	0.77
1:A:1010:GLN:HB3	1:A:1014:ARG:NH1	2.00	0.76
1:A:1114:ILE:O	1:A:1119:ASN:ND2	2.16	0.76
1:A:307:THR:HG23	1:A:602:THR:HB	1.67	0.76
1:A:201:PHE:N	1:A:229:LEU:O	2.19	0.76
1:A:807:PRO:HA	1:A:816:SER:HA	1.68	0.76
1:A:331:ASN:HB2	1:A:580:GLN:HA	1.68	0.76
1:A:112:SER:HA	1:A:132:GLU:HB3	1.68	0.75
1:A:674:TYR:O	1:A:677:GLN:NE2	2.18	0.75
1:A:416:GLY:O	1:A:420:ASP:N	2.18	0.75
1:A:431:GLY:H	1:A:514:SER:HA	1.51	0.75
1:A:330:PRO:HA	1:A:579:PRO:HB2	1.68	0.75
1:A:392:PHE:O	1:A:523:THR:N	2.18	0.75
1:A:807:PRO:HB2	1:A:814:LYS:HB3	1.69	0.75
1:A:388:ASN:HB3	1:A:527:PRO:HD2	1.69	0.75
1:A:720:ILE:HG22	1:A:1067:TYR:HA	1.69	0.75
1:A:802:PHE:HB3	1:A:806:LEU:HD13	1.67	0.75
1:A:355:ARG:NE	1:A:396:TYR:HB3	2.01	0.74
1:A:769:GLY:O	1:A:773:GLU:HB2	1.87	0.74
1:A:345:THR:HA	1:A:509:ARG:HH22	1.52	0.74
1:A:457:ARG:HD3	1:A:489:TYR:HE1	1.52	0.74
1:A:815:ARG:HD3	1:A:823:PHE:HE2	1.53	0.74
1:A:961:THR:HA	1:A:964:LYS:HE2	1.70	0.74
1:A:786:LYS:NZ	1:A:891:GLY:O	2.19	0.74
1:A:1117:THR:N	1:A:1138:TYR:O	2.20	0.74
1:A:1052:PHE:HB2	1:A:1063:LEU:HB2	1.70	0.74

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:995:ARG:O	1:A:998:THR:OG1	2.06	0.73
1:A:206:LYS:NZ	1:A:207:HIS:O	2.20	0.73
1:A:1054:GLN:O	1:A:1061:VAL:N	2.15	0.73
1:A:386:LYS:HE3	1:A:390:LEU:HD12	1.69	0.73
1:A:401:VAL:HG22	1:A:509:ARG:HG2	1.69	0.73
1:A:804:GLN:HB3	1:A:817:PHE:CD2	2.24	0.72
1:A:461:LEU:HD12	1:A:465:GLU:HB3	1.71	0.72
1:A:56:LEU:O	1:A:273:ARG:NH2	2.22	0.72
1:A:924:ALA:O	1:A:928:ASN:ND2	2.23	0.72
1:A:1047:TYR:HB2	1:A:1067:TYR:HB3	1.69	0.72
1:A:314:GLN:NE2	1:A:315:THR:O	2.23	0.71
1:A:330:PRO:O	1:A:580:GLN:NE2	2.22	0.71
1:A:952:VAL:HA	1:A:955:ASN:HD21	1.55	0.71
1:A:44:ARG:HG2	1:A:44:ARG:HH11	1.56	0.71
1:A:712:ILE:HG12	1:A:1077:THR:HG21	1.73	0.71
1:A:1116:THR:HG22	1:A:1138:TYR:HB2	1.73	0.71
1:A:119:ILE:HG12	1:A:128:ILE:HG23	1.72	0.71
1:A:931:ILE:HA	1:A:934:ILE:HD12	1.71	0.71
1:A:242:LEU:HD11	1:A:263:ALA:HB3	1.73	0.70
1:A:1048:HIS:NE2	1:A:1051:SER:OG	2.24	0.70
1:A:725:GLU:OE1	1:A:1064:HIS:NE2	2.23	0.70
1:A:430:THR:HG23	1:A:514:SER:HB3	1.74	0.70
1:A:46:SER:H	1:A:279:TYR:HB2	1.57	0.70
1:A:451:TYR:HB2	1:A:495:TYR:HD2	1.56	0.70
1:A:357:ARG:HD2	1:A:394:ASN:HD21	1.56	0.70
1:A:1010:GLN:HA	1:A:1013:ILE:HD12	1.72	0.70
1:A:610:VAL:HB	1:A:651:ILE:HG22	1.72	0.70
1:A:363:ALA:N	1:A:525:CYS:O	2.26	0.69
1:A:609:ALA:HB2	1:A:692:ILE:HG21	1.73	0.69
1:A:1028:LYS:NZ	1:A:1042:PHE:O	2.22	0.69
1:A:376:THR:HB	1:A:435:ALA:H	1.58	0.69
1:A:976:VAL:HG22	1:A:978:ASN:H	1.56	0.69
1:A:1006:THR:C	1:A:1010:GLN:HE22	1.96	0.69
1:A:102:ARG:NH1	1:A:121:ASN:O	2.22	0.68
1:A:177:MET:O	1:A:188:ASN:ND2	2.26	0.68
1:A:682:ARG:CZ	1:A:690:GLN:HA	2.22	0.68
1:A:787:GLN:NE2	1:A:788:ILE:O	2.27	0.68
1:A:364:ASP:HA	1:A:527:PRO:HD3	1.74	0.68
1:A:833:PHE:HA	1:A:836:GLN:OE1	1.94	0.68
1:A:731:MET:HA	1:A:1058:HIS:HD2	1.57	0.68
1:A:1006:THR:HG22	1:A:1010:GLN:HE22	1.58	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:776:LYS:O	1:A:779:GLN:NE2	2.26	0.68
1:A:92:PHE:HB3	1:A:192:PHE:HB2	1.74	0.67
1:A:319:ARG:HH12	1:A:540:ASN:N	1.92	0.67
1:A:866:THR:HG23	1:A:868:GLU:H	1.58	0.67
1:A:386:LYS:NZ	1:A:389:ASP:O	2.26	0.67
1:A:902:MET:SD	1:A:905:ARG:NH1	2.67	0.67
1:A:658:ASN:O	1:A:674:TYR:OH	2.11	0.67
1:A:378:LYS:HG3	1:A:380:TYR:CE1	2.27	0.67
1:A:725:GLU:HB3	1:A:1062:PHE:HB2	1.76	0.67
1:A:673:SER:H	1:A:695:TYR:HE1	1.41	0.67
1:A:815:ARG:HD3	1:A:823:PHE:CE2	2.30	0.67
1:A:1024:LEU:O	1:A:1028:LYS:HG2	1.95	0.67
1:A:331:ASN:N	1:A:579:PRO:O	2.24	0.66
1:A:370:ASN:OD1	1:A:371:SER:N	2.28	0.66
1:A:451:TYR:HB2	1:A:495:TYR:CD2	2.31	0.66
1:A:315:THR:HG22	1:A:316:SER:H	1.60	0.65
1:A:432:CYS:HB2	1:A:513:LEU:HB2	1.79	0.65
1:A:1083:HIS:HB3	1:A:1088:HIS:CD2	2.31	0.65
1:A:1056:ALA:N	1:A:1059:GLY:O	2.22	0.65
1:A:898:PHE:HA	1:A:901:GLN:HB3	1.78	0.65
1:A:354:ASN:O	1:A:398:ASP:HA	1.97	0.65
1:A:733:LYS:HE2	1:A:861:LEU:HB3	1.77	0.65
1:A:829:ALA:HB1	1:A:832:GLY:HA2	1.78	0.65
1:A:890:ALA:HB2	1:A:1034:LEU:HD21	1.77	0.65
1:A:57:PRO:HA	1:A:273:ARG:CZ	2.26	0.65
1:A:763:LEU:HD13	1:A:1005:GLN:HG2	1.79	0.65
1:A:598:ILE:HB	1:A:609:ALA:HB3	1.78	0.65
1:A:1089:PHE:O	1:A:1121:PHE:N	2.28	0.65
1:A:351:TYR:O	1:A:466:ARG:NH1	2.27	0.65
1:A:365:TYR:HA	1:A:368:LEU:HB2	1.79	0.65
1:A:57:PRO:HD3	1:A:271:GLN:OE1	1.96	0.64
1:A:1006:THR:O	1:A:1010:GLN:NE2	2.30	0.64
1:A:576:VAL:O	1:A:585:LEU:N	2.31	0.64
1:A:708:SER:OG	1:A:710:ASN:OD1	2.14	0.64
1:A:762:GLN:O	1:A:765:ARG:NH2	2.31	0.64
1:A:823:PHE:HB3	1:A:828:LEU:HD11	1.78	0.64
1:A:92:PHE:O	1:A:192:PHE:N	2.30	0.64
1:A:319:ARG:NH2	1:A:320:VAL:HG22	2.13	0.64
1:A:598:ILE:HG21	1:A:672:ALA:HB3	1.80	0.64
1:A:819:GLU:HA	1:A:822:LEU:HD12	1.80	0.64
1:A:993:ILE:O	1:A:997:ILE:HG13	1.98	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:ARG:NH1	1:A:457:ARG:HB3	2.13	0.63
1:A:1016:ALA:O	1:A:1019:ARG:HG2	1.98	0.63
1:A:623:ALA:HA	1:A:633:TRP:HE1	1.62	0.63
1:A:641:ASN:HA	1:A:654:GLU:OE2	1.97	0.63
1:A:973:ILE:HG12	1:A:983:ARG:HH22	1.63	0.63
1:A:73:THR:HB	1:A:78:ARG:HA	1.81	0.63
1:A:348:ALA:O	1:A:401:VAL:N	2.31	0.63
1:A:821:LEU:HD23	1:A:939:SER:HB3	1.80	0.63
1:A:953:ASN:O	1:A:956:ALA:HB3	1.98	0.63
1:A:53:ASP:OD1	1:A:195:LYS:NZ	2.32	0.63
1:A:1116:THR:HA	1:A:1138:TYR:H	1.63	0.63
1:A:850:ILE:HG13	1:A:851:CYS:H	1.63	0.62
1:A:643:PHE:O	1:A:650:LEU:N	2.28	0.62
1:A:869:MET:HA	1:A:872:GLN:HE21	1.64	0.62
1:A:128:ILE:HD13	1:A:170:TYR:HD2	1.63	0.62
1:A:930:ALA:O	1:A:934:ILE:HG13	2.00	0.62
1:A:960:ASN:O	1:A:963:VAL:HB	1.99	0.62
1:A:1011:GLN:HE21	1:A:1014:ARG:NH2	1.97	0.62
1:A:565:PHE:HE2	1:A:567:ARG:HE	1.46	0.62
1:A:901:GLN:HG2	1:A:905:ARG:HE	1.64	0.62
1:A:275:PHE:HA	1:A:291:CYS:H	1.64	0.62
1:A:321:GLN:OE1	1:A:625:HIS:HE1	1.81	0.62
1:A:1037:SER:HB3	1:A:1048:HIS:CG	2.35	0.62
1:A:201:PHE:HB3	1:A:229:LEU:HB2	1.81	0.62
1:A:426:PRO:HD3	1:A:464:PHE:HE2	1.65	0.62
1:A:542:ASN:HA	1:A:547:THR:HA	1.80	0.62
1:A:345:THR:O	1:A:509:ARG:NH1	2.32	0.62
1:A:44:ARG:HD2	1:A:47:VAL:HB	1.82	0.61
1:A:353:TRP:HA	1:A:400:PHE:HB3	1.80	0.61
1:A:424:LYS:NZ	1:A:460:ASN:OD1	2.33	0.61
1:A:424:LYS:HB2	1:A:463:PRO:HA	1.83	0.61
1:A:376:THR:HB	1:A:435:ALA:N	2.15	0.61
1:A:905:ARG:HD3	1:A:1050:MET:HE3	1.83	0.61
1:A:729:VAL:N	1:A:1058:HIS:O	2.29	0.61
1:A:294:ASP:OD1	1:A:296:LEU:N	2.32	0.60
1:A:392:PHE:N	1:A:524:VAL:O	2.26	0.60
1:A:789:TYR:O	1:A:790:LYS:HD3	2.01	0.60
1:A:1009:THR:O	1:A:1012:LEU:HB2	2.01	0.60
1:A:48:LEU:HB3	1:A:276:LEU:HD21	1.82	0.60
1:A:336:CYS:N	1:A:362:VAL:O	2.32	0.60
1:A:785:VAL:HG12	1:A:787:GLN:H	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:495:TYR:CZ	1:A:497:PHE:HB2	2.36	0.60
1:A:628:GLN:HB2	1:A:633:TRP:HB3	1.83	0.60
1:A:177:MET:SD	1:A:190:ARG:HD3	2.42	0.60
1:A:726:ILE:HA	1:A:1061:VAL:HG22	1.83	0.60
1:A:970:PHE:HB2	1:A:996:LEU:HD23	1.84	0.60
1:A:294:ASP:O	1:A:298:GLU:HG2	2.02	0.60
1:A:426:PRO:HD3	1:A:464:PHE:CE2	2.36	0.60
1:A:681:PRO:HD2	1:A:689:SER:HB2	1.84	0.60
1:A:737:ASP:N	1:A:857:GLY:O	2.33	0.60
1:A:909:ILE:HD13	1:A:1049:LEU:HD21	1.83	0.60
1:A:448:ASN:O	1:A:497:PHE:N	2.26	0.60
1:A:960:ASN:C	1:A:964:LYS:HZ3	2.05	0.60
1:A:351:TYR:CE1	1:A:454:ARG:HB2	2.37	0.59
1:A:349:SER:HB2	1:A:452:LEU:H	1.67	0.59
1:A:539:VAL:HG12	1:A:540:ASN:O	2.01	0.59
1:A:465:GLU:HG2	1:A:467:ASP:HB2	1.82	0.59
1:A:600:PRO:O	1:A:685:ARG:NH1	2.35	0.59
1:A:937:SER:OG	1:A:938:LEU:N	2.36	0.59
1:A:551:VAL:HG22	1:A:590:CYS:HA	1.85	0.59
1:A:950:ASP:O	1:A:954:GLN:HG3	2.03	0.59
1:A:609:ALA:HB2	1:A:692:ILE:HG13	1.85	0.59
1:A:747:THR:OG1	1:A:748:GLU:OE2	2.21	0.59
1:A:866:THR:HG22	1:A:869:MET:CE	2.32	0.59
1:A:391:CYS:HA	1:A:525:CYS:HA	1.85	0.59
1:A:1086:LYS:HB3	1:A:1122:VAL:HG21	1.84	0.59
1:A:635:VAL:HB	1:A:651:ILE:HD13	1.84	0.59
1:A:719:THR:O	1:A:1068:VAL:HB	2.03	0.59
1:A:739:THR:O	1:A:742:ILE:N	2.36	0.59
1:A:191:GLU:HG3	1:A:223:LEU:HD11	1.85	0.59
1:A:393:THR:OG1	1:A:516:GLU:HG3	2.03	0.58
1:A:421:TYR:OH	1:A:459:SER:N	2.36	0.58
1:A:474:GLN:HG3	1:A:481:ASN:HB3	1.85	0.58
1:A:68:ILE:HG21	1:A:259:THR:HB	1.85	0.58
1:A:86:PHE:HB2	1:A:235:ILE:HG22	1.83	0.58
1:A:454:ARG:NH1	1:A:471:GLU:OE1	2.35	0.58
1:A:290:ASP:OD1	1:A:292:ALA:N	2.24	0.58
1:A:850:ILE:HG13	1:A:851:CYS:N	2.17	0.58
1:A:348:ALA:HB1	1:A:352:ALA:HB3	1.85	0.58
1:A:920:GLN:N	1:A:920:GLN:OE1	2.36	0.58
1:A:906:PHE:O	1:A:911:VAL:N	2.32	0.58
1:A:1050:MET:H	1:A:1065:VAL:HB	1.69	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:774:GLN:HA	1:A:777:ASN:OD1	2.04	0.58
1:A:406:GLU:HB3	1:A:418:ILE:HD13	1.84	0.57
1:A:544:ASN:HD21	1:A:579:PRO:HB3	1.68	0.57
1:A:869:MET:HA	1:A:872:GLN:NE2	2.19	0.57
1:A:1037:SER:O	1:A:1048:HIS:HB3	2.04	0.57
1:A:328:ARG:HH21	1:A:533:LEU:HB2	1.68	0.57
1:A:729:VAL:N	1:A:1059:GLY:HA2	2.19	0.57
1:A:435:ALA:CB	1:A:510:VAL:HG22	2.35	0.57
1:A:600:PRO:HB3	1:A:685:ARG:HB2	1.86	0.57
1:A:734:THR:HG22	1:A:860:VAL:HB	1.86	0.57
1:A:961:THR:O	1:A:964:LYS:N	2.37	0.57
1:A:906:PHE:O	1:A:910:GLY:N	2.37	0.57
1:A:36:VAL:HG11	1:A:220:PHE:CZ	2.40	0.57
1:A:398:ASP:O	1:A:511:VAL:HA	2.04	0.57
1:A:1032:CYS:SG	1:A:1037:SER:HB2	2.45	0.57
1:A:457:ARG:NH2	1:A:486:PHE:HE1	2.02	0.57
1:A:756:TYR:OH	1:A:994:ASP:OD1	2.22	0.57
1:A:801:ASN:N	1:A:928:ASN:OD1	2.36	0.57
1:A:375:SER:HB2	1:A:436:TRP:HA	1.87	0.56
1:A:778:THR:HA	1:A:781:VAL:HG22	1.86	0.56
1:A:633:TRP:O	1:A:635:VAL:HG22	2.05	0.56
1:A:906:PHE:HA	1:A:909:ILE:HG12	1.88	0.56
1:A:52:GLN:HG3	1:A:273:ARG:C	2.25	0.56
1:A:417:LYS:O	1:A:422:ASN:ND2	2.37	0.56
1:A:1006:THR:HG22	1:A:1010:GLN:NE2	2.20	0.56
1:A:190:ARG:HD2	1:A:207:HIS:NE2	2.20	0.56
1:A:415:THR:HB	1:A:420:ASP:OD2	2.04	0.56
1:A:741:TYR:OH	1:A:962:LEU:O	2.22	0.56
1:A:119:ILE:HG23	1:A:128:ILE:HG13	1.87	0.56
1:A:303:LEU:HD23	1:A:308:VAL:HG12	1.88	0.56
1:A:566:GLY:O	1:A:574:ASP:N	2.39	0.56
1:A:992:GLN:O	1:A:995:ARG:HG2	2.05	0.56
1:A:1098:ASN:OD1	1:A:1101:HIS:N	2.32	0.56
1:A:589:PRO:HG2	1:A:592:PHE:CD1	2.41	0.56
1:A:1091:ARG:HG3	1:A:1092:GLU:H	1.71	0.56
1:A:727:LEU:O	1:A:1060:VAL:N	2.30	0.56
1:A:1101:HIS:HB3	1:A:1103:PHE:HE2	1.71	0.56
1:A:203:ILE:O	1:A:226:LEU:N	2.29	0.55
1:A:344:ALA:HB3	1:A:347:PHE:HE1	1.70	0.55
1:A:411:ALA:O	1:A:414:GLN:HG2	2.06	0.55
1:A:497:PHE:CD2	1:A:507:PRO:HD3	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:713:ALA:HA	1:A:1073:LYS:O	2.06	0.55
1:A:802:PHE:CB	1:A:806:LEU:HD13	2.36	0.55
1:A:310:LYS:HB2	1:A:685:ARG:HH11	1.71	0.55
1:A:330:PRO:HB2	1:A:332:ILE:HB	1.88	0.55
1:A:833:PHE:O	1:A:853:GLN:N	2.40	0.55
1:A:838:GLY:O	1:A:839:ASP:HB2	2.06	0.55
1:A:152:TRP:HH2	1:A:244:LEU:HD23	1.70	0.55
1:A:607:GLN:HG2	1:A:682:ARG:NH1	2.22	0.55
1:A:941:THR:OG1	1:A:944:ALA:HB2	2.06	0.55
1:A:356:LYS:HB3	1:A:397:ALA:HB3	1.89	0.55
1:A:996:LEU:HB3	1:A:1000:ARG:NH2	2.22	0.55
1:A:739:THR:HG22	1:A:753:LEU:HD11	1.87	0.55
1:A:34:ARG:HB3	1:A:91:TYR:OH	2.07	0.55
1:A:86:PHE:HB3	1:A:236:THR:HA	1.89	0.55
1:A:353:TRP:HB2	1:A:398:ASP:OD1	2.07	0.55
1:A:408:ARG:HE	1:A:409:GLN:NE2	2.05	0.55
1:A:1097:SER:HA	1:A:1101:HIS:O	2.06	0.55
1:A:418:ILE:HA	1:A:422:ASN:HB2	1.87	0.55
1:A:768:THR:O	1:A:772:VAL:HG12	2.07	0.55
1:A:959:LEU:O	1:A:962:LEU:HB3	2.07	0.55
1:A:1100:THR:HG23	1:A:1101:HIS:ND1	2.22	0.55
1:A:541:PHE:N	1:A:548:GLY:O	2.37	0.54
1:A:733:LYS:HB2	1:A:771:ALA:HB1	1.88	0.54
1:A:659:SER:OG	1:A:696:THR:O	2.19	0.54
1:A:778:THR:O	1:A:781:VAL:N	2.39	0.54
1:A:872:GLN:HA	1:A:875:SER:OG	2.06	0.54
1:A:31:SER:N	1:A:60:SER:O	2.39	0.54
1:A:567:ARG:HA	1:A:572:THR:O	2.08	0.54
1:A:53:ASP:O	1:A:272:PRO:HA	2.08	0.54
1:A:476:GLY:HA2	1:A:482:GLY:HA3	1.89	0.54
1:A:927:PHE:CE2	1:A:931:ILE:HD11	2.43	0.54
1:A:778:THR:O	1:A:781:VAL:HG22	2.06	0.54
1:A:540:ASN:HA	1:A:549:THR:HA	1.89	0.54
1:A:865:LEU:HD12	1:A:873:TYR:HE2	1.73	0.54
1:A:45:SER:HA	1:A:279:TYR:HD2	1.73	0.54
1:A:364:ASP:CG	1:A:527:PRO:HG3	2.28	0.54
1:A:574:ASP:O	1:A:587:ILE:N	2.39	0.54
1:A:1017:GLU:OE2	1:A:1018:ILE:HG13	2.08	0.54
1:A:110:LEU:HD11	1:A:239:GLN:HE22	1.73	0.54
1:A:534:VAL:O	1:A:535:LYS:HE2	2.08	0.54
1:A:973:ILE:N	1:A:992:GLN:OE1	2.36	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:379:CYS:HA	1:A:432:CYS:HA	1.90	0.53
1:A:418:ILE:HA	1:A:422:ASN:ND2	2.23	0.53
1:A:578:ASP:OD1	1:A:583:GLU:N	2.39	0.53
1:A:715:PRO:O	1:A:1109:PHE:HA	2.08	0.53
1:A:98:SER:HA	1:A:178:ASP:OD2	2.08	0.53
1:A:106:PHE:O	1:A:117:LEU:N	2.36	0.53
1:A:378:LYS:HD2	1:A:379:CYS:H	1.72	0.53
1:A:771:ALA:O	1:A:774:GLN:HG2	2.07	0.53
1:A:1091:ARG:CZ	1:A:1119:ASN:HA	2.37	0.53
1:A:663:ASP:HB2	1:A:673:SER:OG	2.08	0.53
1:A:809:PRO:HD3	1:A:814:LYS:HZ2	1.74	0.53
1:A:996:LEU:HB3	1:A:1000:ARG:CZ	2.39	0.53
1:A:1089:PHE:N	1:A:1121:PHE:O	2.22	0.53
1:A:314:GLN:HA	1:A:596:SER:HA	1.91	0.53
1:A:746:SER:O	1:A:749:CYS:HB3	2.07	0.53
1:A:772:VAL:HG13	1:A:776:LYS:NZ	2.23	0.53
1:A:759:PHE:HA	1:A:762:GLN:OE1	2.09	0.53
1:A:760:CYS:SG	1:A:761:THR:N	2.82	0.53
1:A:122:ASN:C	1:A:124:THR:H	2.12	0.53
1:A:770:ILE:O	1:A:773:GLU:HB3	2.09	0.53
1:A:906:PHE:CE2	1:A:916:LEU:HB2	2.43	0.53
1:A:919:ASN:OD1	1:A:922:LEU:HB3	2.09	0.53
1:A:299:THR:HG21	1:A:597:VAL:HG21	1.89	0.53
1:A:800:PHE:CE2	1:A:924:ALA:HA	2.43	0.53
1:A:994:ASP:O	1:A:997:ILE:N	2.42	0.53
1:A:421:TYR:CD2	1:A:456:PHE:HA	2.44	0.53
1:A:827:THR:HB	1:A:831:ALA:H	1.73	0.53
1:A:356:LYS:NZ	1:A:358:ILE:HG12	2.24	0.53
1:A:729:VAL:HG13	1:A:1059:GLY:HA2	1.89	0.53
1:A:773:GLU:OE2	1:A:1019:ARG:NH1	2.42	0.53
1:A:1080:ALA:HB2	1:A:1089:PHE:CE1	2.43	0.53
1:A:652:GLY:O	1:A:692:ILE:HB	2.09	0.52
1:A:718:PHE:CD2	1:A:720:ILE:HG23	2.44	0.52
1:A:903:ALA:HB1	1:A:913:GLN:CB	2.36	0.52
1:A:1091:ARG:HD2	1:A:1092:GLU:HG2	1.89	0.52
1:A:376:THR:N	1:A:435:ALA:O	2.36	0.52
1:A:1104:VAL:HB	1:A:1113:GLN:HB2	1.91	0.52
1:A:319:ARG:HD3	1:A:320:VAL:O	2.10	0.52
1:A:688:ALA:N	1:A:691:SER:O	2.42	0.52
1:A:874:THR:O	1:A:877:LEU:HB2	2.08	0.52
1:A:1007:TYR:O	1:A:1011:GLN:NE2	2.42	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1014:ARG:HA	1:A:1017:GLU:HG3	1.91	0.52
1:A:730:SER:O	1:A:1058:HIS:HB3	2.08	0.52
1:A:56:LEU:HD12	1:A:57:PRO:HD2	1.91	0.52
1:A:1030:SER:OG	1:A:1031:GLU:OE1	2.28	0.52
1:A:676:THR:HB	1:A:683:ARG:HH12	1.74	0.52
1:A:733:LYS:NZ	1:A:863:PRO:HA	2.24	0.52
1:A:766:ALA:O	1:A:770:ILE:HG12	2.09	0.52
1:A:916:LEU:O	1:A:920:GLN:N	2.42	0.52
1:A:1036:GLN:NE2	1:A:1048:HIS:O	2.32	0.52
1:A:882:ILE:O	1:A:901:GLN:NE2	2.36	0.52
1:A:961:THR:O	1:A:965:GLN:HG2	2.09	0.52
1:A:44:ARG:NH1	1:A:47:VAL:H	2.07	0.52
1:A:52:GLN:HE21	1:A:272:PRO:C	2.12	0.51
1:A:110:LEU:HD11	1:A:239:GLN:NE2	2.25	0.51
1:A:319:ARG:HH21	1:A:320:VAL:HG22	1.74	0.51
1:A:731:MET:HA	1:A:1058:HIS:CD2	2.43	0.51
1:A:792:PRO:HG2	1:A:797:PHE:HZ	1.75	0.51
1:A:1105:THR:HG21	1:A:1110:TYR:HD1	1.75	0.51
1:A:86:PHE:N	1:A:236:THR:O	2.35	0.51
1:A:454:ARG:NH2	1:A:455:LEU:O	2.43	0.51
1:A:1004:LEU:O	1:A:1007:TYR:N	2.43	0.51
1:A:457:ARG:CD	1:A:489:TYR:HE1	2.21	0.51
1:A:852:ALA:O	1:A:854:LYS:HD2	2.10	0.51
1:A:932:GLY:O	1:A:935:GLN:HG3	2.11	0.51
1:A:339:GLY:O	1:A:343:ASN:N	2.33	0.51
1:A:677:GLN:HG2	1:A:688:ALA:HB2	1.92	0.51
1:A:733:LYS:NZ	1:A:862:PRO:O	2.41	0.51
1:A:418:ILE:HG13	1:A:419:ALA:N	2.25	0.51
1:A:534:VAL:O	1:A:552:LEU:HD12	2.09	0.51
1:A:811:LYS:CD	1:A:812:PRO:HD2	2.37	0.51
1:A:278:LYS:HE2	1:A:287:ASP:HB3	1.92	0.51
1:A:527:PRO:C	1:A:528:LYS:HD2	2.31	0.51
1:A:278:LYS:O	1:A:285:ILE:HA	2.11	0.51
1:A:338:PHE:CD2	1:A:368:LEU:HD21	2.46	0.51
1:A:423:TYR:CE2	1:A:512:VAL:HG21	2.45	0.50
1:A:880:GLY:HA3	1:A:888:PHE:CG	2.46	0.50
1:A:130:VAL:HG13	1:A:167:THR:HB	1.92	0.50
1:A:1102:TRP:CZ2	1:A:1133:VAL:HG11	2.46	0.50
1:A:212:LEU:HD11	1:A:214:ARG:HB2	1.93	0.50
1:A:444:LYS:HG2	1:A:446:GLY:H	1.77	0.50
1:A:660:TYR:HD2	1:A:674:TYR:CZ	2.29	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:TYR:HD1	1:A:422:ASN:OD1	1.95	0.50
1:A:353:TRP:NE1	1:A:422:ASN:O	2.44	0.50
1:A:686:SER:O	1:A:692:ILE:HA	2.12	0.50
1:A:947:LYS:O	1:A:951:VAL:HG23	2.12	0.50
1:A:759:PHE:O	1:A:763:LEU:HG	2.12	0.50
1:A:772:VAL:C	1:A:776:LYS:HZ3	2.15	0.50
1:A:85:PRO:HA	1:A:236:THR:O	2.12	0.50
1:A:111:ASP:OD2	1:A:135:PHE:HB2	2.11	0.50
1:A:909:ILE:HG21	1:A:1049:LEU:HD22	1.94	0.50
1:A:1003:SER:O	1:A:1006:THR:HB	2.12	0.50
1:A:1081:ILE:N	1:A:1088:HIS:O	2.27	0.50
1:A:339:GLY:HA2	1:A:342:PHE:HB2	1.94	0.50
1:A:758:SER:O	1:A:762:GLN:N	2.28	0.50
1:A:38:TYR:HB2	1:A:225:PRO:HD3	1.94	0.50
1:A:749:CYS:HB2	1:A:977:LEU:HD21	1.93	0.50
1:A:867:ASP:HA	1:A:870:ILE:HD12	1.92	0.50
1:A:765:ARG:HH22	1:A:766:ALA:HB2	1.76	0.49
1:A:901:GLN:HG2	1:A:905:ARG:HH21	1.76	0.49
1:A:189:LEU:HD22	1:A:210:ILE:HG23	1.95	0.49
1:A:327:VAL:HG11	1:A:542:ASN:H	1.77	0.49
1:A:340:GLU:O	1:A:344:ALA:HB2	2.12	0.49
1:A:28:TYR:CE1	1:A:63:THR:HA	2.47	0.49
1:A:57:PRO:O	1:A:60:SER:OG	2.29	0.49
1:A:388:ASN:CB	1:A:527:PRO:HD2	2.41	0.49
1:A:976:VAL:HG13	1:A:979:ASP:H	1.76	0.49
1:A:29:THR:O	1:A:62:VAL:HG22	2.13	0.49
1:A:32:PHE:CD1	1:A:216:LEU:HB3	2.47	0.49
1:A:361:CYS:O	1:A:524:VAL:HA	2.13	0.49
1:A:763:LEU:CD1	1:A:1005:GLN:HG2	2.41	0.49
1:A:866:THR:O	1:A:869:MET:HG2	2.13	0.49
1:A:1048:HIS:HA	1:A:1066:THR:HG22	1.94	0.49
1:A:65:PHE:CD2	1:A:82:PRO:HD2	2.46	0.49
1:A:352:ALA:HA	1:A:466:ARG:HH22	1.77	0.49
1:A:402:ILE:HG22	1:A:508:TYR:O	2.13	0.49
1:A:418:ILE:HA	1:A:422:ASN:HD22	1.77	0.49
1:A:38:TYR:N	1:A:223:LEU:O	2.44	0.49
1:A:115:GLN:HG3	1:A:132:GLU:OE2	2.13	0.49
1:A:204:TYR:HD1	1:A:225:PRO:HA	1.77	0.49
1:A:357:ARG:NH1	1:A:394:ASN:OD1	2.44	0.49
1:A:420:ASP:HA	1:A:424:LYS:HE2	1.94	0.49
1:A:679:ASN:HB3	1:A:689:SER:HB2	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:ILE:HG12	1:A:1077:THR:CG2	2.40	0.49
1:A:189:LEU:HD23	1:A:208:THR:O	2.13	0.49
1:A:394:ASN:HB3	1:A:516:GLU:OE2	2.13	0.49
1:A:457:ARG:HG3	1:A:457:ARG:O	2.12	0.49
1:A:533:LEU:HD21	1:A:552:LEU:HD13	1.95	0.49
1:A:953:ASN:O	1:A:957:GLN:OE1	2.30	0.49
1:A:299:THR:OG1	1:A:308:VAL:HG11	2.12	0.49
1:A:423:TYR:HE2	1:A:512:VAL:HG21	1.78	0.49
1:A:457:ARG:HD3	1:A:489:TYR:CE1	2.39	0.49
1:A:652:GLY:C	1:A:692:ILE:HB	2.33	0.49
1:A:752:LEU:HD11	1:A:990:GLU:OE1	2.13	0.49
1:A:804:GLN:O	1:A:817:PHE:HB3	2.13	0.49
1:A:353:TRP:CE2	1:A:466:ARG:HD2	2.48	0.49
1:A:398:ASP:HB3	1:A:512:VAL:HB	1.94	0.49
1:A:1052:PHE:O	1:A:1062:PHE:HA	2.13	0.49
1:A:28:TYR:CE1	1:A:63:THR:HG22	2.48	0.48
1:A:80:ASP:OD1	1:A:81:ASN:N	2.46	0.48
1:A:247:SER:H	1:A:257:GLY:HA2	1.78	0.48
1:A:376:THR:O	1:A:434:ILE:HA	2.13	0.48
1:A:725:GLU:O	1:A:1061:VAL:HA	2.13	0.48
1:A:808:ASP:O	1:A:814:LYS:HA	2.12	0.48
1:A:1126:CYS:O	1:A:1132:ILE:HD13	2.12	0.48
1:A:46:SER:N	1:A:279:TYR:HB2	2.26	0.48
1:A:110:LEU:HD22	1:A:135:PHE:CD1	2.47	0.48
1:A:315:THR:HG22	1:A:316:SER:N	2.26	0.48
1:A:557:LYS:HD2	1:A:557:LYS:N	2.28	0.48
1:A:309:GLU:N	1:A:309:GLU:OE1	2.45	0.48
1:A:1014:ARG:O	1:A:1015:ALA:C	2.51	0.48
1:A:866:THR:HG22	1:A:869:MET:HE3	1.95	0.48
1:A:1055:SER:HA	1:A:1060:VAL:HA	1.95	0.48
1:A:298:GLU:HB3	1:A:315:THR:HG21	1.95	0.48
1:A:364:ASP:OD1	1:A:366:SER:N	2.37	0.48
1:A:613:GLN:O	1:A:615:VAL:HG23	2.14	0.48
1:A:825:LYS:HD3	1:A:939:SER:O	2.14	0.48
1:A:758:SER:OG	1:A:761:THR:HB	2.13	0.48
1:A:1054:GLN:NE2	1:A:1063:LEU:HD13	2.29	0.48
1:A:30:ASN:HB3	1:A:59:PHE:HA	1.95	0.48
1:A:105:ILE:HB	1:A:239:GLN:NE2	2.28	0.48
1:A:364:ASP:OD2	1:A:367:VAL:HG22	2.14	0.48
1:A:636:TYR:O	1:A:640:SER:HB2	2.14	0.48
1:A:796:ASP:OD1	1:A:796:ASP:N	2.43	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1081:ILE:HG12	1:A:1095:PHE:CE2	2.48	0.48
1:A:153:MET:SD	1:A:243:ALA:HB1	2.54	0.48
1:A:725:GLU:OE2	1:A:1028:LYS:HE2	2.14	0.48
1:A:727:LEU:HD12	1:A:1062:PHE:CE2	2.48	0.48
1:A:729:VAL:HG22	1:A:1058:HIS:C	2.34	0.48
1:A:729:VAL:H	1:A:1059:GLY:HA2	1.77	0.48
1:A:31:SER:OG	1:A:60:SER:OG	2.31	0.48
1:A:101:ILE:HA	1:A:242:LEU:HD21	1.96	0.48
1:A:572:THR:O	1:A:574:ASP:N	2.47	0.48
1:A:1110:TYR:CZ	1:A:1112:PRO:HB3	2.49	0.48
1:A:32:PHE:HD1	1:A:216:LEU:HD23	1.79	0.48
1:A:176:LEU:HD12	1:A:179:LEU:HD22	1.96	0.48
1:A:200:TYR:CE1	1:A:230:PRO:HB3	2.49	0.48
1:A:715:PRO:HG2	1:A:1108:ASN:O	2.14	0.48
1:A:996:LEU:HD13	1:A:1000:ARG:HH22	1.79	0.48
1:A:1090:PRO:HA	1:A:1120:THR:HA	1.95	0.48
1:A:229:LEU:HB3	1:A:231:ILE:HG13	1.95	0.47
1:A:576:VAL:N	1:A:585:LEU:O	2.40	0.47
1:A:610:VAL:HB	1:A:651:ILE:CG2	2.40	0.47
1:A:623:ALA:HA	1:A:633:TRP:NE1	2.29	0.47
1:A:1083:HIS:O	1:A:1088:HIS:NE2	2.38	0.47
1:A:334:ASN:O	1:A:362:VAL:N	2.27	0.47
1:A:375:SER:H	1:A:436:TRP:HB3	1.80	0.47
1:A:106:PHE:HB2	1:A:117:LEU:HB2	1.94	0.47
1:A:455:LEU:N	1:A:491:PRO:O	2.46	0.47
1:A:1008:VAL:O	1:A:1012:LEU:HG	2.14	0.47
1:A:1014:ARG:HB3	1:A:1018:ILE:HD11	1.97	0.47
1:A:1083:HIS:HB3	1:A:1088:HIS:NE2	2.29	0.47
1:A:55:PHE:C	1:A:271:GLN:H	2.18	0.47
1:A:772:VAL:HG22	1:A:776:LYS:NZ	2.28	0.47
1:A:840:CYS:SG	1:A:843:ASP:HB3	2.55	0.47
1:A:993:ILE:HG22	1:A:997:ILE:HD11	1.96	0.47
1:A:728:PRO:HA	1:A:1059:GLY:CA	2.44	0.47
1:A:712:ILE:HG22	1:A:713:ALA:N	2.30	0.47
1:A:823:PHE:HA	1:A:828:LEU:HD21	1.96	0.47
1:A:1007:TYR:HA	1:A:1010:GLN:NE2	2.30	0.47
1:A:1087:ALA:HB2	1:A:1126:CYS:N	2.30	0.47
1:A:1117:THR:HB	1:A:1139:ASP:HA	1.95	0.47
1:A:377:PHE:CD2	1:A:434:ILE:HD12	2.50	0.47
1:A:604:THR:HG21	1:A:685:ARG:NH1	2.30	0.47
1:A:677:GLN:HB2	1:A:683:ARG:HG3	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:832:GLY:O	1:A:835:LYS:N	2.43	0.47
1:A:871:ALA:O	1:A:874:THR:N	2.47	0.47
1:A:909:ILE:HB	1:A:1047:TYR:HB3	1.97	0.47
1:A:380:TYR:HB2	1:A:430:THR:O	2.15	0.47
1:A:578:ASP:OD2	1:A:581:THR:HB	2.14	0.47
1:A:1107:ARG:NH2	1:A:1108:ASN:OD1	2.48	0.47
1:A:577:ARG:NH1	1:A:579:PRO:HA	2.30	0.47
1:A:682:ARG:NH2	1:A:690:GLN:HG3	2.30	0.47
1:A:1091:ARG:HA	1:A:1121:PHE:CD1	2.50	0.47
1:A:1105:THR:OG1	1:A:1109:PHE:O	2.31	0.47
1:A:444:LYS:O	1:A:447:GLY:N	2.33	0.47
1:A:622:VAL:O	1:A:633:TRP:NE1	2.48	0.47
1:A:682:ARG:HG2	1:A:687:VAL:HG21	1.97	0.47
1:A:763:LEU:O	1:A:766:ALA:HB3	2.15	0.47
1:A:770:ILE:HG13	1:A:771:ALA:N	2.30	0.47
1:A:805:ILE:HA	1:A:818:ILE:HD13	1.96	0.47
1:A:946:GLY:HA2	1:A:949:GLN:NE2	2.29	0.47
1:A:996:LEU:O	1:A:1000:ARG:HG2	2.15	0.47
1:A:1078:ALA:O	1:A:1095:PHE:HB2	2.15	0.47
1:A:1115:ILE:HG23	1:A:1120:THR:HG21	1.95	0.47
1:A:92:PHE:HZ	1:A:240:THR:HG1	1.59	0.46
1:A:776:LYS:O	1:A:780:GLU:HB2	2.15	0.46
1:A:958:ALA:HB1	1:A:1007:TYR:HE1	1.79	0.46
1:A:825:LYS:NZ	1:A:939:SER:O	2.38	0.46
1:A:847:ARG:HH12	1:A:850:ILE:HG23	1.80	0.46
1:A:1101:HIS:HB3	1:A:1103:PHE:CE2	2.51	0.46
1:A:383:SER:HA	1:A:384:PRO:HD3	1.70	0.46
1:A:731:MET:HG3	1:A:732:THR:N	2.18	0.46
1:A:189:LEU:HD22	1:A:210:ILE:CG2	2.45	0.46
1:A:386:LYS:HE3	1:A:390:LEU:CD1	2.42	0.46
1:A:497:PHE:CE2	1:A:507:PRO:HD3	2.50	0.46
1:A:76:THR:HB	1:A:79:PHE:HB3	1.98	0.46
1:A:616:ASN:OD1	1:A:644:GLN:NE2	2.48	0.46
1:A:869:MET:O	1:A:870:ILE:C	2.53	0.46
1:A:355:ARG:HD3	1:A:396:TYR:HD2	1.81	0.46
1:A:436:TRP:NE1	1:A:509:ARG:HB2	2.30	0.46
1:A:726:ILE:HD13	1:A:945:LEU:HD23	1.96	0.46
1:A:140:PHE:HB2	1:A:244:LEU:H	1.81	0.46
1:A:664:ILE:H	1:A:673:SER:HB2	1.80	0.46
1:A:669:GLY:O	1:A:696:THR:HA	2.15	0.46
1:A:868:GLU:O	1:A:872:GLN:HG3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:961:THR:O	1:A:962:LEU:C	2.54	0.46
1:A:1090:PRO:HD3	1:A:1095:PHE:CE2	2.51	0.46
1:A:674:TYR:CD2	1:A:693:ILE:HD13	2.50	0.46
1:A:64:TRP:CD1	1:A:266:TYR:HD2	2.34	0.46
1:A:189:LEU:HD21	1:A:208:THR:HB	1.98	0.46
1:A:735:SER:OG	1:A:736:VAL:N	2.49	0.46
1:A:1018:ILE:O	1:A:1021:SER:OG	2.17	0.46
1:A:365:TYR:HB2	1:A:387:LEU:HB3	1.98	0.46
1:A:763:LEU:HG	1:A:763:LEU:H	1.42	0.46
1:A:823:PHE:O	1:A:828:LEU:HG	2.16	0.46
1:A:130:VAL:HG12	1:A:168:PHE:HB3	1.98	0.45
1:A:630:THR:OG1	1:A:631:PRO:HD3	2.15	0.45
1:A:684:ALA:H	1:A:687:VAL:HG23	1.81	0.45
1:A:728:PRO:HB3	1:A:948:LEU:HD23	1.98	0.45
1:A:818:ILE:HG13	1:A:819:GLU:N	2.32	0.45
1:A:843:ASP:CG	1:A:844:ILE:H	2.20	0.45
1:A:90:VAL:HG12	1:A:269:TYR:CE1	2.51	0.45
1:A:106:PHE:CE2	1:A:119:ILE:HD12	2.52	0.45
1:A:152:TRP:CH2	1:A:244:LEU:HD23	2.50	0.45
1:A:457:ARG:NE	1:A:481:ASN:OD1	2.49	0.45
1:A:487:ASN:O	1:A:489:TYR:N	2.49	0.45
1:A:661:GLU:HA	1:A:697:MET:SD	2.56	0.45
1:A:816:SER:OG	1:A:819:GLU:HG2	2.16	0.45
1:A:952:VAL:CA	1:A:955:ASN:HD21	2.25	0.45
1:A:541:PHE:O	1:A:547:THR:HA	2.16	0.45
1:A:627:ASP:HA	1:A:633:TRP:CD1	2.52	0.45
1:A:697:MET:HG3	1:A:699:LEU:HD23	1.98	0.45
1:A:994:ASP:HA	1:A:997:ILE:HD12	1.98	0.45
1:A:490:PHE:CE1	1:A:492:LEU:HD23	2.51	0.45
1:A:622:VAL:HG13	1:A:635:VAL:HG21	1.98	0.45
1:A:682:ARG:HD3	1:A:690:GLN:NE2	2.32	0.45
1:A:865:LEU:HD12	1:A:869:MET:HG3	1.97	0.45
1:A:1139:ASP:OD1	1:A:1140:PRO:HD2	2.17	0.45
1:A:90:VAL:HG11	1:A:238:PHE:CZ	2.52	0.45
1:A:128:ILE:HD13	1:A:170:TYR:CD2	2.48	0.45
1:A:358:ILE:HB	1:A:395:VAL:HB	1.96	0.45
1:A:726:ILE:HG21	1:A:945:LEU:HA	1.98	0.45
1:A:865:LEU:HD11	1:A:873:TYR:OH	2.16	0.45
1:A:1048:HIS:NE2	1:A:1050:MET:C	2.70	0.45
1:A:447:GLY:HA2	1:A:499:PRO:HD3	1.97	0.45
1:A:866:THR:HG22	1:A:869:MET:HE2	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:870:ILE:O	1:A:873:TYR:HB2	2.17	0.45
1:A:732:THR:OG1	1:A:734:THR:HG23	2.16	0.45
1:A:902:MET:HG3	1:A:906:PHE:CE2	2.51	0.45
1:A:433:VAL:O	1:A:434:ILE:HD13	2.17	0.45
1:A:607:GLN:HG2	1:A:682:ARG:HH12	1.81	0.45
1:A:684:ALA:H	1:A:687:VAL:CG2	2.30	0.45
1:A:733:LYS:HE2	1:A:861:LEU:CB	2.44	0.45
1:A:795:LYS:HG2	1:A:797:PHE:HE2	1.81	0.45
1:A:833:PHE:HB2	1:A:852:ALA:H	1.79	0.45
1:A:869:MET:HA	1:A:872:GLN:HG3	1.98	0.45
1:A:909:ILE:HG23	1:A:1036:GLN:NE2	2.32	0.45
1:A:1104:VAL:H	1:A:1113:GLN:H	1.64	0.45
1:A:655:HIS:CA	1:A:694:ALA:HB3	2.42	0.44
1:A:660:TYR:HD2	1:A:674:TYR:CE1	2.35	0.44
1:A:727:LEU:HD12	1:A:1062:PHE:HE2	1.82	0.44
1:A:905:ARG:HD2	1:A:1050:MET:HG2	1.98	0.44
1:A:1014:ARG:HB3	1:A:1018:ILE:CD1	2.47	0.44
1:A:1080:ALA:HB2	1:A:1089:PHE:CZ	2.52	0.44
1:A:81:ASN:HB3	1:A:265:TYR:CE1	2.52	0.44
1:A:101:ILE:H	1:A:101:ILE:HD12	1.83	0.44
1:A:170:TYR:CZ	1:A:172:SER:HB2	2.52	0.44
1:A:323:THR:O	1:A:324:GLU:HB2	2.17	0.44
1:A:767:LEU:HA	1:A:770:ILE:HD11	1.99	0.44
1:A:802:PHE:HB3	1:A:806:LEU:CD1	2.44	0.44
1:A:388:ASN:O	1:A:528:LYS:HD3	2.18	0.44
1:A:409:GLN:C	1:A:414:GLN:HG3	2.38	0.44
1:A:787:GLN:O	1:A:788:ILE:HD13	2.16	0.44
1:A:931:ILE:O	1:A:934:ILE:HB	2.17	0.44
1:A:424:LYS:HE3	1:A:461:LEU:HD23	1.98	0.44
1:A:313:TYR:O	1:A:597:VAL:HG22	2.17	0.44
1:A:364:ASP:OD1	1:A:365:TYR:N	2.51	0.44
1:A:461:LEU:CD1	1:A:465:GLU:HB3	2.43	0.44
1:A:661:GLU:N	1:A:661:GLU:OE2	2.51	0.44
1:A:817:PHE:CE1	1:A:821:LEU:HD11	2.53	0.44
1:A:31:SER:OG	1:A:57:PRO:O	2.32	0.44
1:A:536:ASN:OD1	1:A:536:ASN:O	2.36	0.44
1:A:1010:GLN:O	1:A:1013:ILE:HB	2.17	0.44
1:A:1078:ALA:HB1	1:A:1132:ILE:HA	2.00	0.44
1:A:294:ASP:H	1:A:297:SER:HB2	1.83	0.44
1:A:356:LYS:HZ2	1:A:358:ILE:HG12	1.82	0.44
1:A:1088:HIS:CG	1:A:1137:VAL:HG21	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1096:VAL:HG21	1:A:1110:TYR:HE1	1.82	0.44
1:A:63:THR:HG1	1:A:267:VAL:HB	1.82	0.44
1:A:153:MET:HG3	1:A:245:HIS:ND1	2.33	0.44
1:A:400:PHE:CE1	1:A:510:VAL:HB	2.52	0.44
1:A:641:ASN:O	1:A:651:ILE:HA	2.18	0.44
1:A:710:ASN:O	1:A:1077:THR:N	2.39	0.44
1:A:300:LYS:HG2	1:A:308:VAL:HG13	2.00	0.44
1:A:408:ARG:NE	1:A:409:GLN:NE2	2.66	0.44
1:A:455:LEU:HB2	1:A:491:PRO:HA	1.99	0.44
1:A:482:GLY:H	1:A:486:PHE:HE2	1.66	0.44
1:A:543:PHE:O	1:A:546:LEU:HB2	2.18	0.44
1:A:807:PRO:HB2	1:A:814:LYS:HE3	2.00	0.44
1:A:1111:GLU:O	1:A:1113:GLN:HG3	2.18	0.44
1:A:81:ASN:HB3	1:A:265:TYR:HE1	1.83	0.43
1:A:434:ILE:HB	1:A:511:VAL:HG12	1.99	0.43
1:A:537:LYS:C	1:A:551:VAL:HG12	2.39	0.43
1:A:741:TYR:HD2	1:A:742:ILE:HG13	1.84	0.43
1:A:800:PHE:CD2	1:A:924:ALA:HA	2.52	0.43
1:A:130:VAL:CG1	1:A:167:THR:HB	2.48	0.43
1:A:565:PHE:HE2	1:A:567:ARG:NE	2.13	0.43
1:A:697:MET:HE3	1:A:698:SER:O	2.18	0.43
1:A:134:GLN:H	1:A:161:SER:HG	1.67	0.43
1:A:228:ASP:C	1:A:229:LEU:HD12	2.37	0.43
1:A:887:THR:HB	1:A:892:ALA:O	2.17	0.43
1:A:894:LEU:HD13	1:A:894:LEU:HA	1.76	0.43
1:A:1091:ARG:HG3	1:A:1092:GLU:N	2.33	0.43
1:A:65:PHE:HB2	1:A:265:TYR:CZ	2.53	0.43
1:A:555:SER:HA	1:A:586:ASP:CG	2.39	0.43
1:A:624:ILE:O	1:A:625:HIS:HB3	2.18	0.43
1:A:656:VAL:HG11	1:A:693:ILE:HD11	2.00	0.43
1:A:986:LYS:HA	1:A:989:ALA:HB3	2.00	0.43
1:A:386:LYS:CG	1:A:389:ASP:HB3	2.41	0.43
1:A:541:PHE:O	1:A:548:GLY:N	2.52	0.43
1:A:905:ARG:CD	1:A:1050:MET:HE3	2.49	0.43
1:A:959:LEU:O	1:A:963:VAL:HG23	2.19	0.43
1:A:977:LEU:O	1:A:980:ILE:HG22	2.18	0.43
1:A:1011:GLN:HE21	1:A:1014:ARG:HH21	1.66	0.43
1:A:454:ARG:HG2	1:A:455:LEU:O	2.18	0.43
1:A:870:ILE:HA	1:A:873:TYR:HD2	1.84	0.43
1:A:319:ARG:HH12	1:A:540:ASN:H	1.65	0.43
1:A:355:ARG:HA	1:A:397:ALA:O	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:LEU:HB3	1:A:143:VAL:HG12	1.99	0.43
1:A:415:THR:C	1:A:419:ALA:HB3	2.39	0.43
1:A:551:VAL:HG23	1:A:588:THR:HB	2.01	0.43
1:A:573:THR:O	1:A:587:ILE:HD13	2.18	0.43
1:A:807:PRO:HB3	1:A:814:LYS:O	2.18	0.43
1:A:1037:SER:HB3	1:A:1048:HIS:ND1	2.34	0.43
1:A:1081:ILE:HD12	1:A:1135:ASN:CB	2.48	0.43
1:A:56:LEU:HD22	1:A:91:TYR:HB3	2.00	0.43
1:A:308:VAL:N	1:A:602:THR:OG1	2.48	0.43
1:A:887:THR:OG1	1:A:893:ALA:HA	2.19	0.43
1:A:1091:ARG:NE	1:A:1119:ASN:HA	2.34	0.43
1:A:52:GLN:HG3	1:A:273:ARG:O	2.18	0.43
1:A:152:TRP:HA	1:A:152:TRP:CE3	2.53	0.43
1:A:163:ALA:HB1	1:A:166:CYS:SG	2.59	0.43
1:A:375:SER:CB	1:A:436:TRP:HA	2.48	0.43
1:A:436:TRP:O	1:A:508:TYR:HA	2.19	0.43
1:A:550:GLY:HA2	1:A:590:CYS:H	1.84	0.43
1:A:555:SER:HA	1:A:586:ASP:OD2	2.19	0.43
1:A:421:TYR:HE2	1:A:456:PHE:CG	2.37	0.42
1:A:443:SER:HA	1:A:497:PHE:CE1	2.53	0.42
1:A:674:TYR:HD2	1:A:693:ILE:HD13	1.83	0.42
1:A:727:LEU:N	1:A:1060:VAL:O	2.48	0.42
1:A:57:PRO:HB2	1:A:60:SER:HB3	2.00	0.42
1:A:200:TYR:HB3	1:A:228:ASP:OD1	2.18	0.42
1:A:310:LYS:HG3	1:A:664:ILE:HD11	2.01	0.42
1:A:391:CYS:HB2	1:A:544:ASN:O	2.19	0.42
1:A:451:TYR:O	1:A:495:TYR:N	2.32	0.42
1:A:28:TYR:CD1	1:A:63:THR:HA	2.55	0.42
1:A:44:ARG:NH1	1:A:47:VAL:N	2.67	0.42
1:A:117:LEU:HD12	1:A:235:ILE:HD11	2.02	0.42
1:A:140:PHE:HB3	1:A:243:ALA:HA	2.01	0.42
1:A:1007:TYR:HA	1:A:1010:GLN:HE21	1.82	0.42
1:A:108:THR:O	1:A:237:ARG:NH1	2.52	0.42
1:A:884:SER:OG	1:A:888:PHE:HB3	2.19	0.42
1:A:1000:ARG:HG3	1:A:1001:LEU:N	2.35	0.42
1:A:134:GLN:OE1	1:A:134:GLN:N	2.45	0.42
1:A:319:ARG:HD3	1:A:320:VAL:N	2.35	0.42
1:A:762:GLN:O	1:A:765:ARG:CZ	2.67	0.42
1:A:854:LYS:HZ1	1:A:859:THR:N	2.18	0.42
1:A:1050:MET:O	1:A:1065:VAL:N	2.26	0.42
1:A:191:GLU:HG2	1:A:206:LYS:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:LEU:HD23	1:A:392:PHE:CE1	2.55	0.42
1:A:660:TYR:HA	1:A:698:SER:OG	2.18	0.42
1:A:827:THR:O	1:A:830:ASP:N	2.49	0.42
1:A:101:ILE:HG13	1:A:263:ALA:HB1	2.01	0.42
1:A:328:ARG:HG3	1:A:579:PRO:HD2	2.01	0.42
1:A:661:GLU:HG3	1:A:697:MET:CE	2.50	0.42
1:A:718:PHE:HE2	1:A:720:ILE:HG12	1.84	0.42
1:A:728:PRO:HA	1:A:1059:GLY:HA3	2.01	0.42
1:A:998:THR:OG1	1:A:999:GLY:N	2.53	0.42
1:A:1091:ARG:HG3	1:A:1091:ARG:HH11	1.84	0.42
1:A:1096:VAL:HG11	1:A:1105:THR:HG22	2.00	0.42
1:A:775:ASP:O	1:A:779:GLN:HG3	2.20	0.42
1:A:878:LEU:O	1:A:881:THR:HG22	2.19	0.42
1:A:32:PHE:CE1	1:A:216:LEU:HB3	2.55	0.42
1:A:508:TYR:O	1:A:510:VAL:HG23	2.20	0.42
1:A:732:THR:HB	1:A:860:VAL:CG2	2.50	0.42
1:A:996:LEU:HB3	1:A:1000:ARG:NH1	2.33	0.42
1:A:1056:ALA:HB3	1:A:1059:GLY:CA	2.50	0.42
1:A:143:VAL:O	1:A:158:ARG:HG2	2.20	0.42
1:A:178:ASP:HA	1:A:188:ASN:ND2	2.35	0.42
1:A:273:ARG:HB2	1:A:292:ALA:CB	2.49	0.42
1:A:287:ASP:OD1	1:A:288:ALA:N	2.49	0.42
1:A:311:GLY:CA	1:A:664:ILE:HG12	2.50	0.42
1:A:379:CYS:HB3	1:A:382:VAL:HG23	2.02	0.42
1:A:434:ILE:O	1:A:510:VAL:HA	2.19	0.42
1:A:454:ARG:HH12	1:A:457:ARG:HB3	1.80	0.42
1:A:495:TYR:OH	1:A:497:PHE:HB2	2.20	0.42
1:A:764:ASN:OD1	1:A:767:LEU:HD12	2.20	0.42
1:A:785:VAL:HG22	1:A:889:GLY:HA2	2.01	0.42
1:A:873:TYR:O	1:A:876:ALA:N	2.53	0.42
1:A:948:LEU:CD2	1:A:1059:GLY:HA3	2.50	0.42
1:A:29:THR:HB	1:A:64:TRP:HE1	1.84	0.41
1:A:378:LYS:HD2	1:A:378:LYS:HA	1.77	0.41
1:A:733:LYS:HD3	1:A:775:ASP:OD2	2.20	0.41
1:A:736:VAL:HG22	1:A:737:ASP:C	2.39	0.41
1:A:741:TYR:CE1	1:A:966:LEU:HD21	2.55	0.41
1:A:1028:LYS:NZ	1:A:1043:CYS:SG	2.83	0.41
1:A:1048:HIS:HE2	1:A:1050:MET:C	2.23	0.41
1:A:190:ARG:HB3	1:A:192:PHE:CZ	2.55	0.41
1:A:293:LEU:O	1:A:624:ILE:HG13	2.20	0.41
1:A:449:TYR:HA	1:A:496:GLY:HA2	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:PRO:O	1:A:528:LYS:HD2	2.20	0.41
1:A:565:PHE:CD2	1:A:573:THR:HG22	2.56	0.41
1:A:677:GLN:O	1:A:683:ARG:NH1	2.53	0.41
1:A:758:SER:HG	1:A:761:THR:HB	1.86	0.41
1:A:825:LYS:HZ1	1:A:941:THR:C	2.23	0.41
1:A:1088:HIS:ND1	1:A:1122:VAL:HB	2.35	0.41
1:A:206:LYS:HA	1:A:206:LYS:HD2	1.82	0.41
1:A:310:LYS:HD2	1:A:685:ARG:NE	2.22	0.41
1:A:818:ILE:O	1:A:822:LEU:HG	2.20	0.41
1:A:874:THR:HA	1:A:877:LEU:HD13	2.02	0.41
1:A:1061:VAL:HG12	1:A:1062:PHE:N	2.36	0.41
1:A:205:SER:HB2	1:A:226:LEU:HD11	2.02	0.41
1:A:330:PRO:C	1:A:332:ILE:N	2.74	0.41
1:A:357:ARG:HH11	1:A:394:ASN:CG	2.22	0.41
1:A:759:PHE:HA	1:A:762:GLN:CD	2.40	0.41
1:A:958:ALA:HB1	1:A:1007:TYR:CE1	2.55	0.41
1:A:1010:GLN:HB3	1:A:1014:ARG:HH22	1.86	0.41
1:A:150:LYS:HB2	1:A:151:SER:H	1.67	0.41
1:A:731:MET:CG	1:A:732:THR:H	2.19	0.41
1:A:827:THR:CB	1:A:831:ALA:H	2.33	0.41
1:A:298:GLU:CD	1:A:318:PHE:HZ	2.24	0.41
1:A:659:SER:C	1:A:698:SER:HB3	2.41	0.41
1:A:790:LYS:HD3	1:A:790:LYS:HA	1.80	0.41
1:A:832:GLY:O	1:A:836:GLN:N	2.54	0.41
1:A:833:PHE:HB3	1:A:852:ALA:N	2.20	0.41
1:A:134:GLN:HB2	1:A:161:SER:HB2	2.03	0.41
1:A:636:TYR:H	1:A:640:SER:CB	2.34	0.41
1:A:816:SER:O	1:A:819:GLU:HG2	2.20	0.41
1:A:328:ARG:CG	1:A:579:PRO:HD2	2.51	0.41
1:A:714:ILE:HG23	1:A:1107:ARG:O	2.20	0.41
1:A:1027:THR:O	1:A:1028:LYS:C	2.59	0.41
1:A:1102:TRP:CE2	1:A:1133:VAL:HG21	2.56	0.41
1:A:134:GLN:NE2	1:A:162:SER:HB3	2.36	0.41
1:A:458:LYS:HB2	1:A:481:ASN:HD21	1.85	0.41
1:A:540:ASN:N	1:A:540:ASN:OD1	2.54	0.41
1:A:577:ARG:HH12	1:A:579:PRO:HA	1.85	0.41
1:A:856:ASN:OD1	1:A:856:ASN:N	2.54	0.41
1:A:935:GLN:HA	1:A:938:LEU:HG	2.03	0.41
1:A:976:VAL:HG22	1:A:978:ASN:N	2.28	0.41
1:A:1083:HIS:HB2	1:A:1135:ASN:O	2.20	0.41
1:A:1119:ASN:OD1	1:A:1120:THR:HG23	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:LEU:HD22	1:A:88:ASP:OD2	2.21	0.41
1:A:55:PHE:N	1:A:271:GLN:O	2.30	0.41
1:A:95:THR:HA	1:A:177:MET:HE1	2.03	0.41
1:A:203:ILE:O	1:A:225:PRO:HA	2.21	0.41
1:A:326:ILE:HD13	1:A:528:LYS:HB3	2.03	0.41
1:A:551:VAL:HG13	1:A:590:CYS:HB2	2.02	0.41
1:A:553:THR:O	1:A:586:ASP:N	2.54	0.41
1:A:560:LEU:HA	1:A:561:PRO:HD3	1.90	0.41
1:A:777:ASN:O	1:A:780:GLU:HB3	2.21	0.41
1:A:1083:HIS:CG	1:A:1136:THR:HA	2.56	0.41
1:A:1089:PHE:HB2	1:A:1121:PHE:CE2	2.56	0.41
1:A:106:PHE:HB3	1:A:235:ILE:HD12	2.02	0.40
1:A:421:TYR:CG	1:A:454:ARG:NH2	2.89	0.40
1:A:1054:GLN:N	1:A:1061:VAL:O	2.53	0.40
1:A:178:ASP:O	1:A:181:GLY:N	2.54	0.40
1:A:334:ASN:OD1	1:A:361:CYS:HA	2.21	0.40
1:A:458:LYS:HD2	1:A:480:CYS:HB3	2.03	0.40
1:A:624:ILE:HG12	1:A:633:TRP:CH2	2.56	0.40
1:A:833:PHE:O	1:A:852:ALA:N	2.55	0.40
1:A:83:VAL:O	1:A:84:LEU:HD23	2.20	0.40
1:A:836:GLN:O	1:A:838:GLY:HA2	2.21	0.40
1:A:955:ASN:OD1	1:A:956:ALA:N	2.54	0.40
1:A:1010:GLN:HB3	1:A:1014:ARG:CZ	2.50	0.40
1:A:52:GLN:NE2	1:A:272:PRO:O	2.47	0.40
1:A:461:LEU:HD12	1:A:465:GLU:CB	2.45	0.40
1:A:834:ILE:HD11	1:A:835:LYS:NZ	2.36	0.40
1:A:1012:LEU:HD23	1:A:1012:LEU:HA	1.89	0.40
1:A:326:ILE:O	1:A:530:SER:HA	2.20	0.40
1:A:330:PRO:HB2	1:A:332:ILE:H	1.86	0.40
1:A:364:ASP:O	1:A:368:LEU:HD13	2.21	0.40
1:A:403:ARG:HB2	1:A:406:GLU:HG3	2.02	0.40
1:A:452:LEU:HG	1:A:493:GLN:O	2.22	0.40
1:A:746:SER:HB3	1:A:749:CYS:CB	2.52	0.40
1:A:772:VAL:HG13	1:A:776:LYS:HZ1	1.85	0.40
1:A:924:ALA:O	1:A:927:PHE:HB3	2.22	0.40
1:A:1088:HIS:HA	1:A:1122:VAL:HA	2.02	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	1112/1273 (87%)	927 (83%)	180 (16%)	5 (0%)	30 68

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	838	GLY
1	A	839	ASP
1	A	150	LYS
1	A	151	SER
1	A	836	GLN

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	965/1112 (87%)	963 (100%)	2 (0%)	92 94

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	319	ARG
1	A	847	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	121	ASN
1	A	409	GLN
1	A	625	HIS
1	A	655	HIS
1	A	955	ASN
1	A	1010	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](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-31578. These allow visual inspection of the internal detail of the map and identification of artifacts.

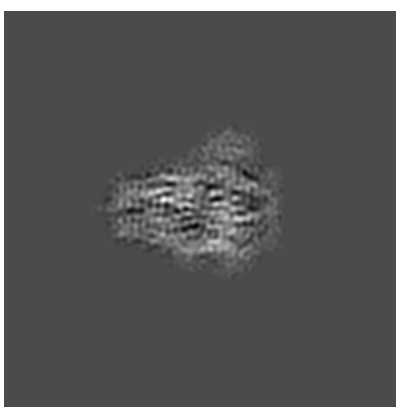
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

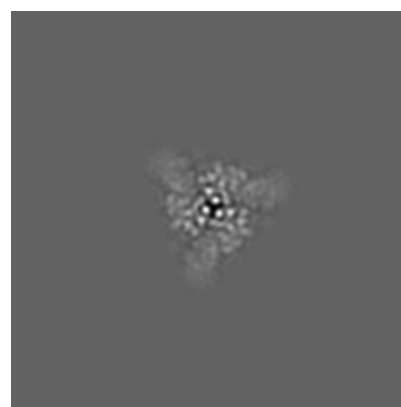
6.1.1 Primary map



X



Y



Z

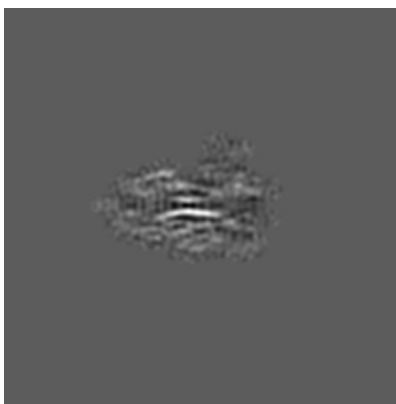
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

6.2.1 Primary map



X Index: 128



Y Index: 128



Z Index: 128

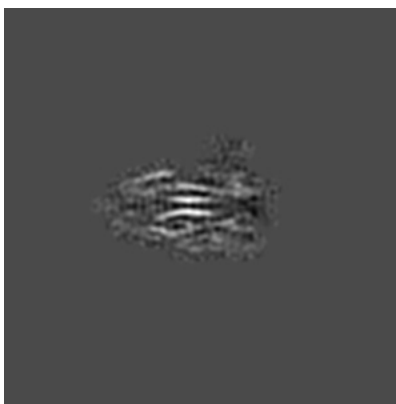
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

6.3.1 Primary map



X Index: 133



Y Index: 127

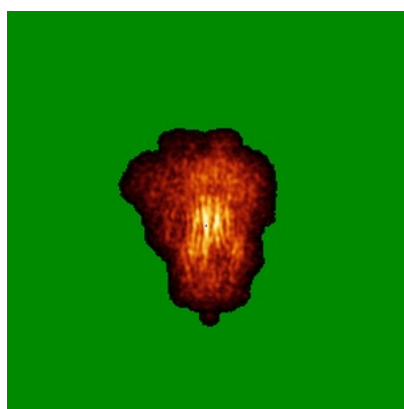


Z Index: 124

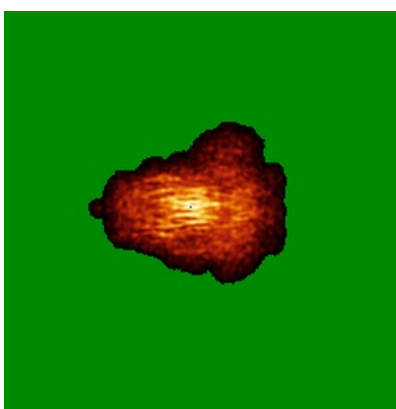
The images above show the largest variance slices of the map in three orthogonal directions.

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

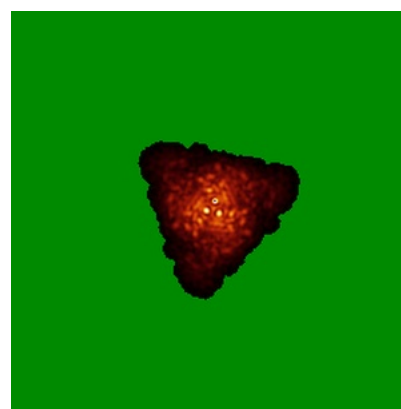
6.4.1 Primary map



X



Y

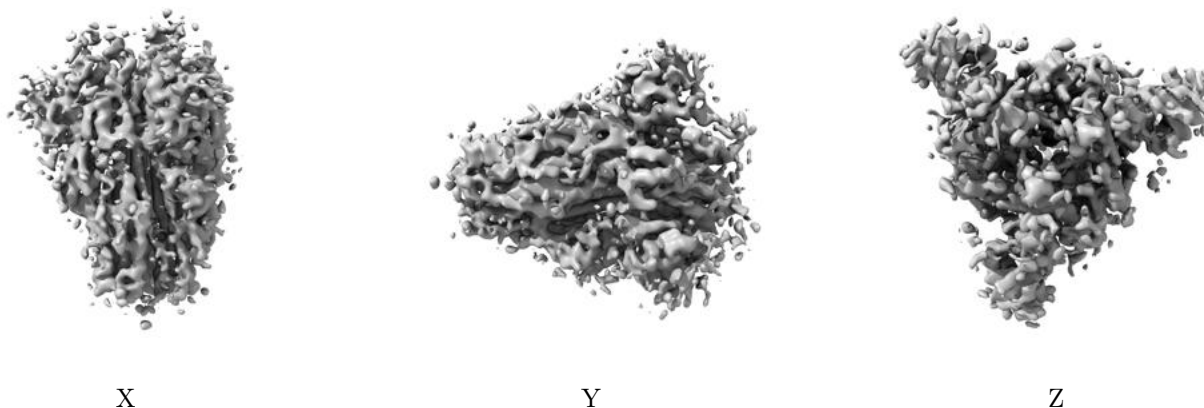


Z

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 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

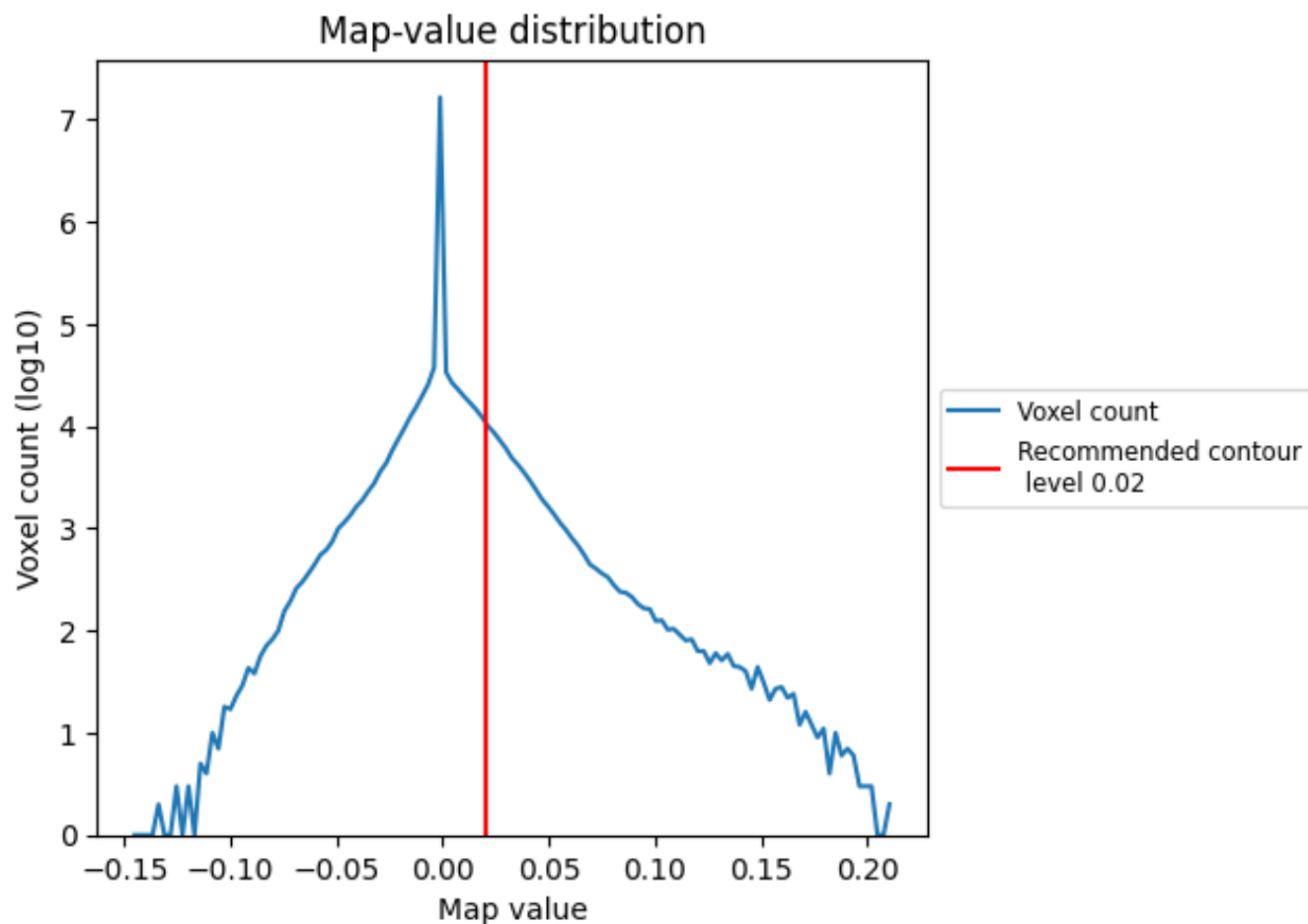
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

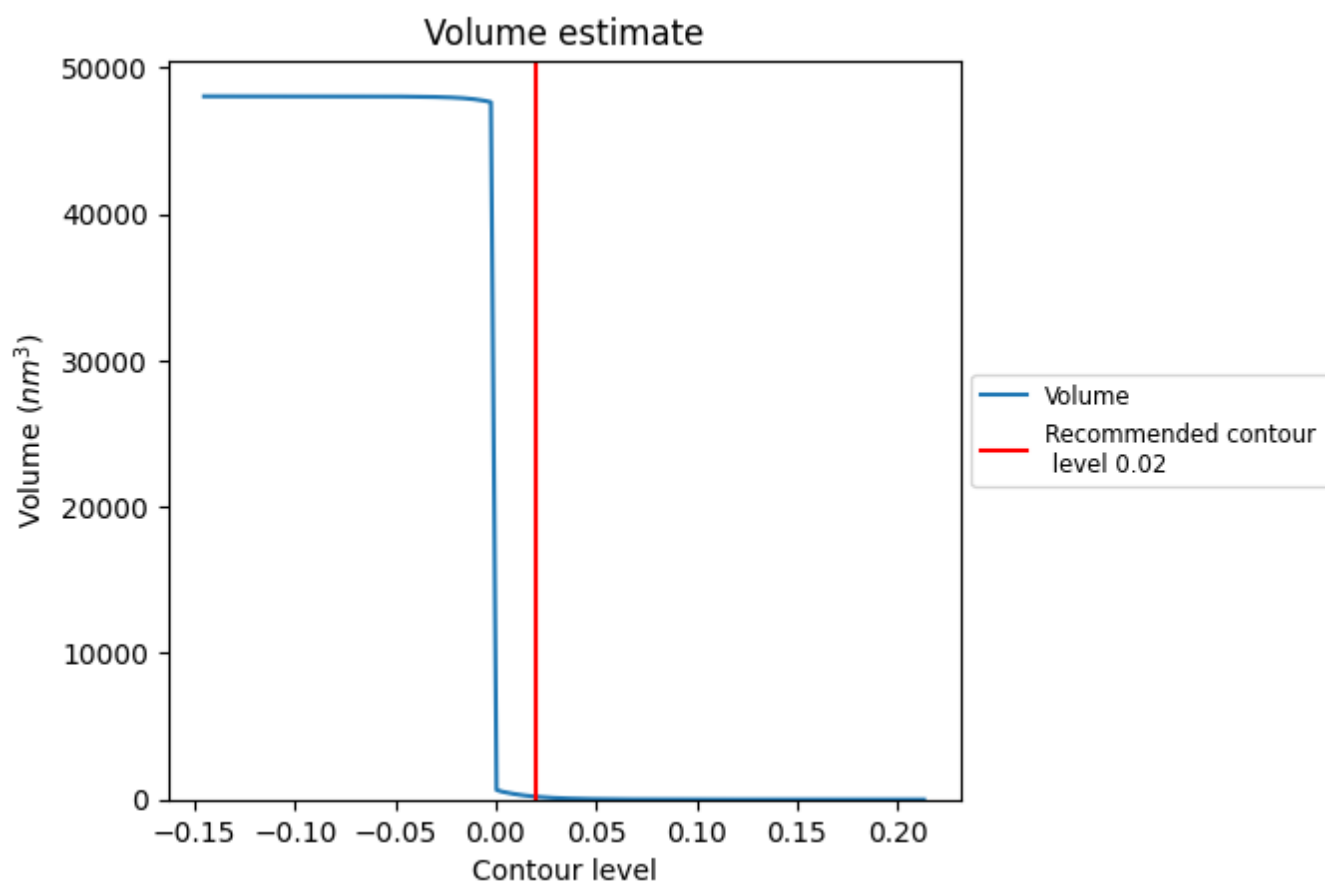
This section contains the results of statistical analysis of the map.

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.

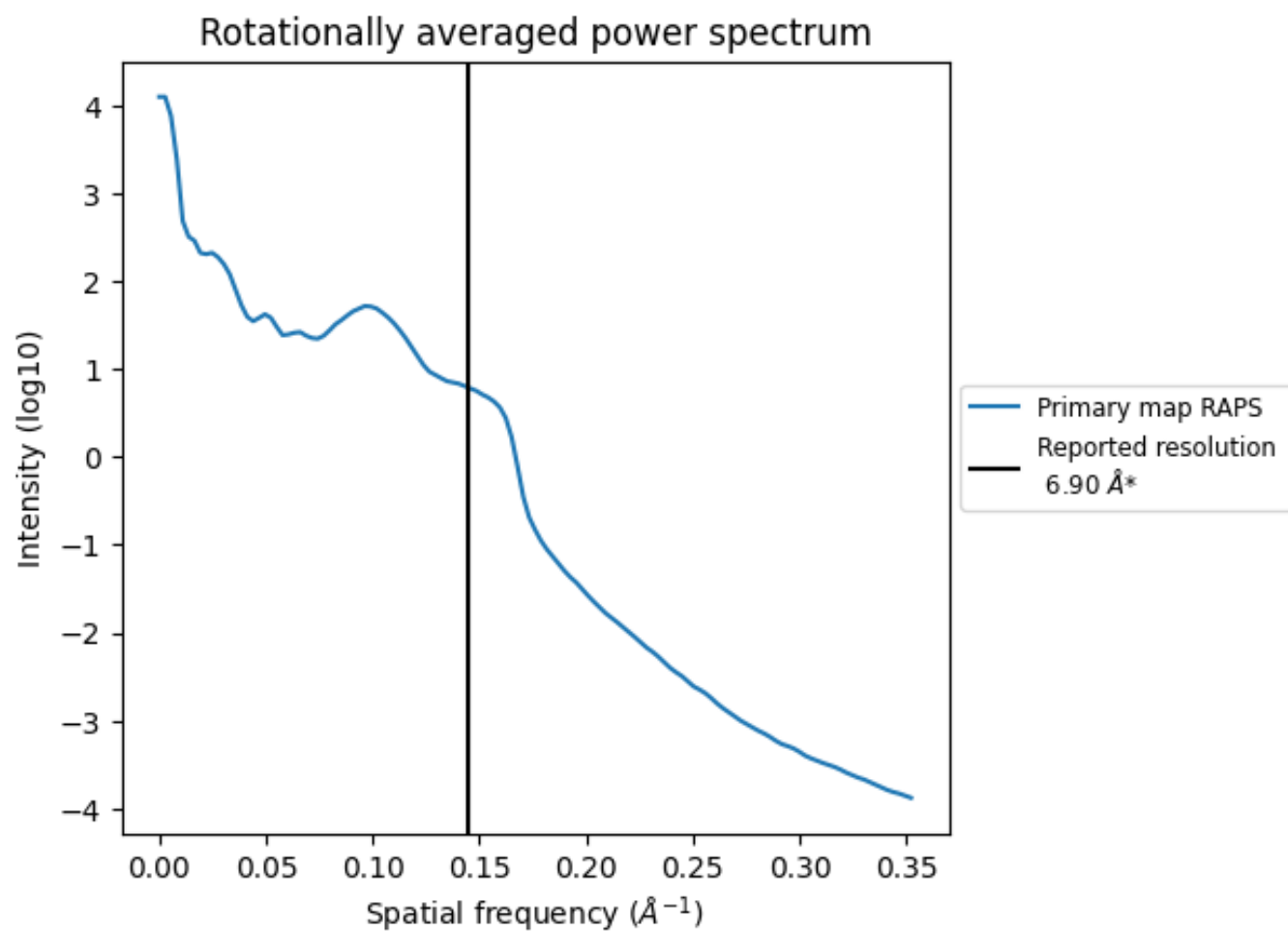
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 197 nm³; this corresponds to an approximate mass of 178 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 ⓘ

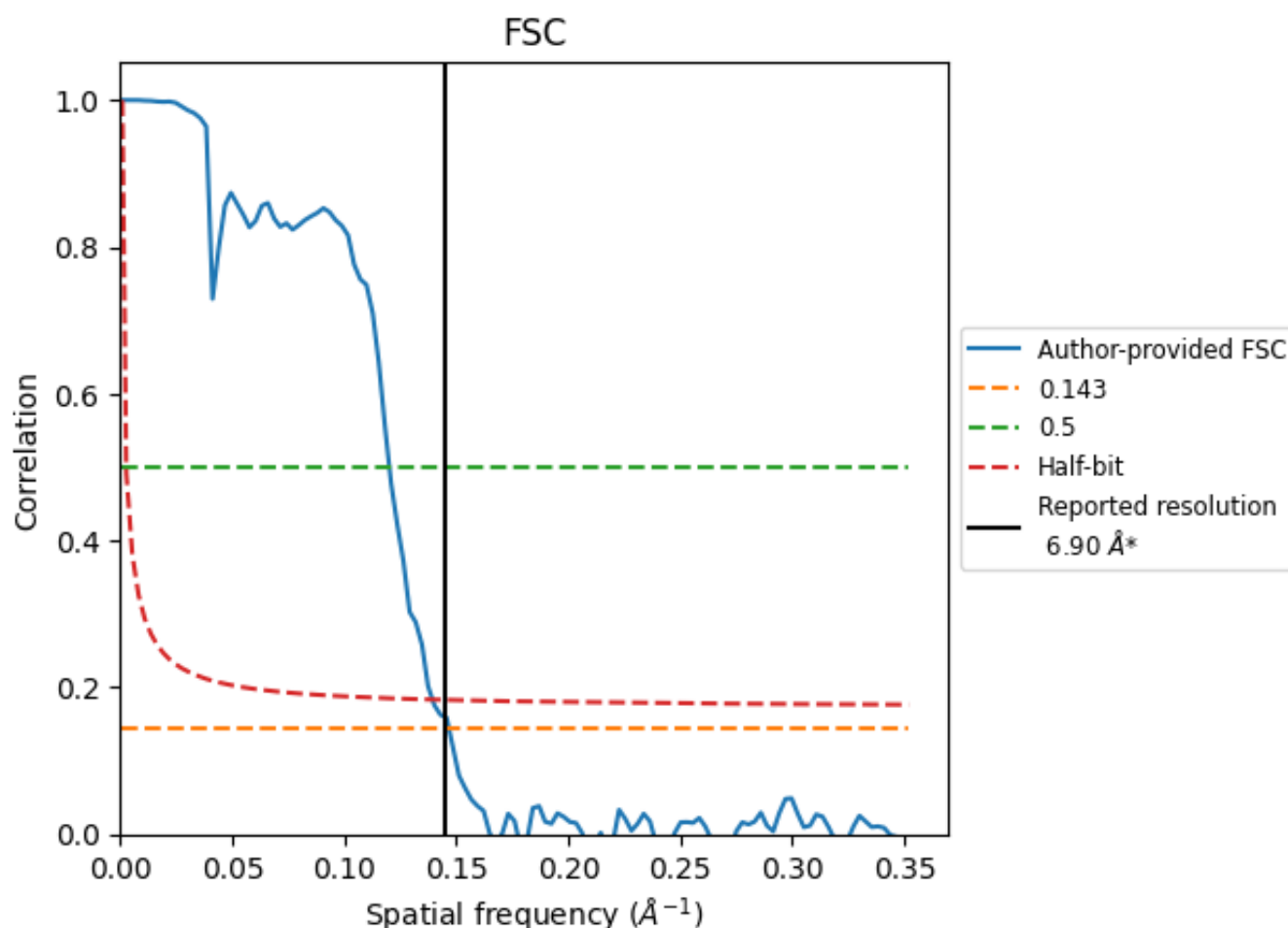


*Reported resolution corresponds to spatial frequency of 0.145 \AA^{-1}

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.145 \AA^{-1}

8.2 Resolution estimates [i](#)

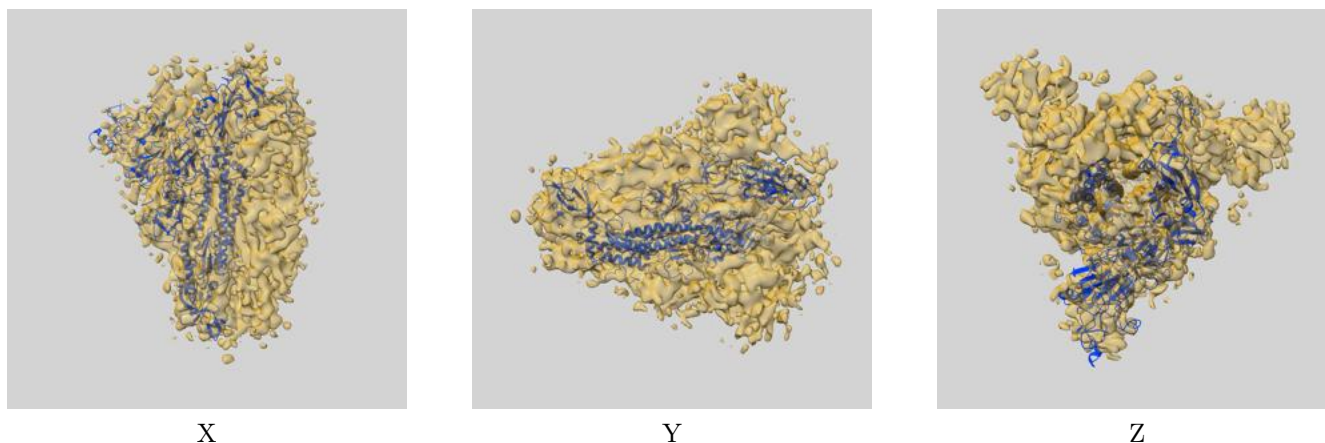
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.90	-	-
Author-provided FSC curve	6.81	8.32	7.17
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

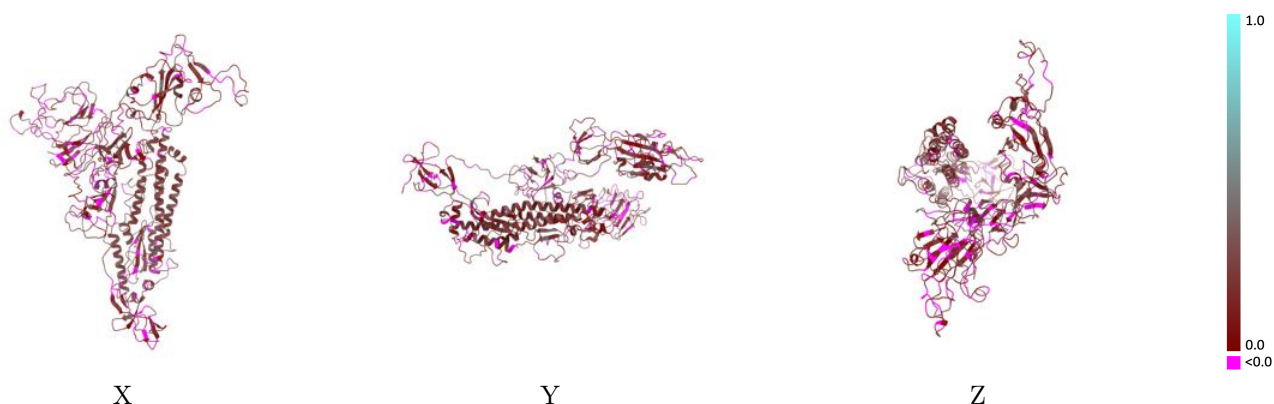
This section contains information regarding the fit between EMDB map EMD-31578 and PDB model 7FG7. Per-residue inclusion information can be found in section [3](#) on page [4](#).

9.1 Map-model overlay [i](#)



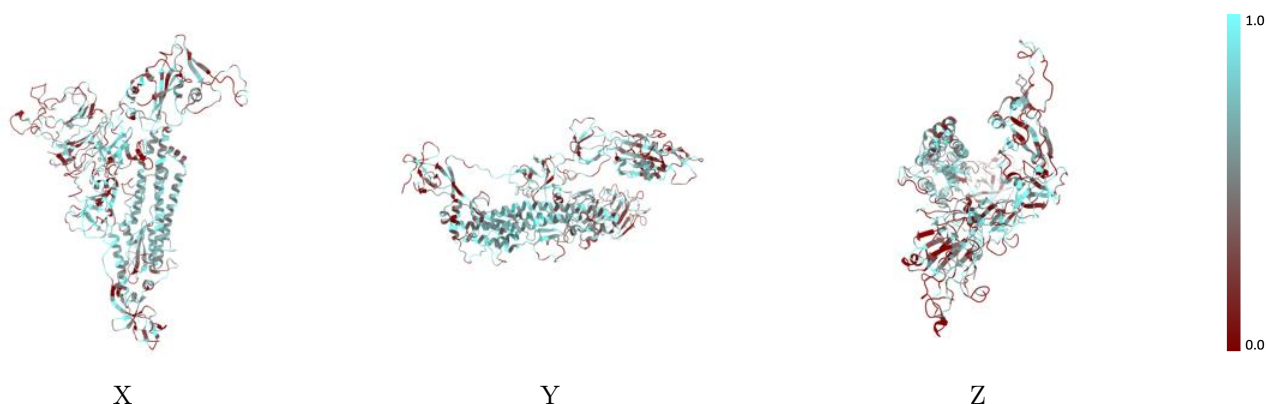
The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



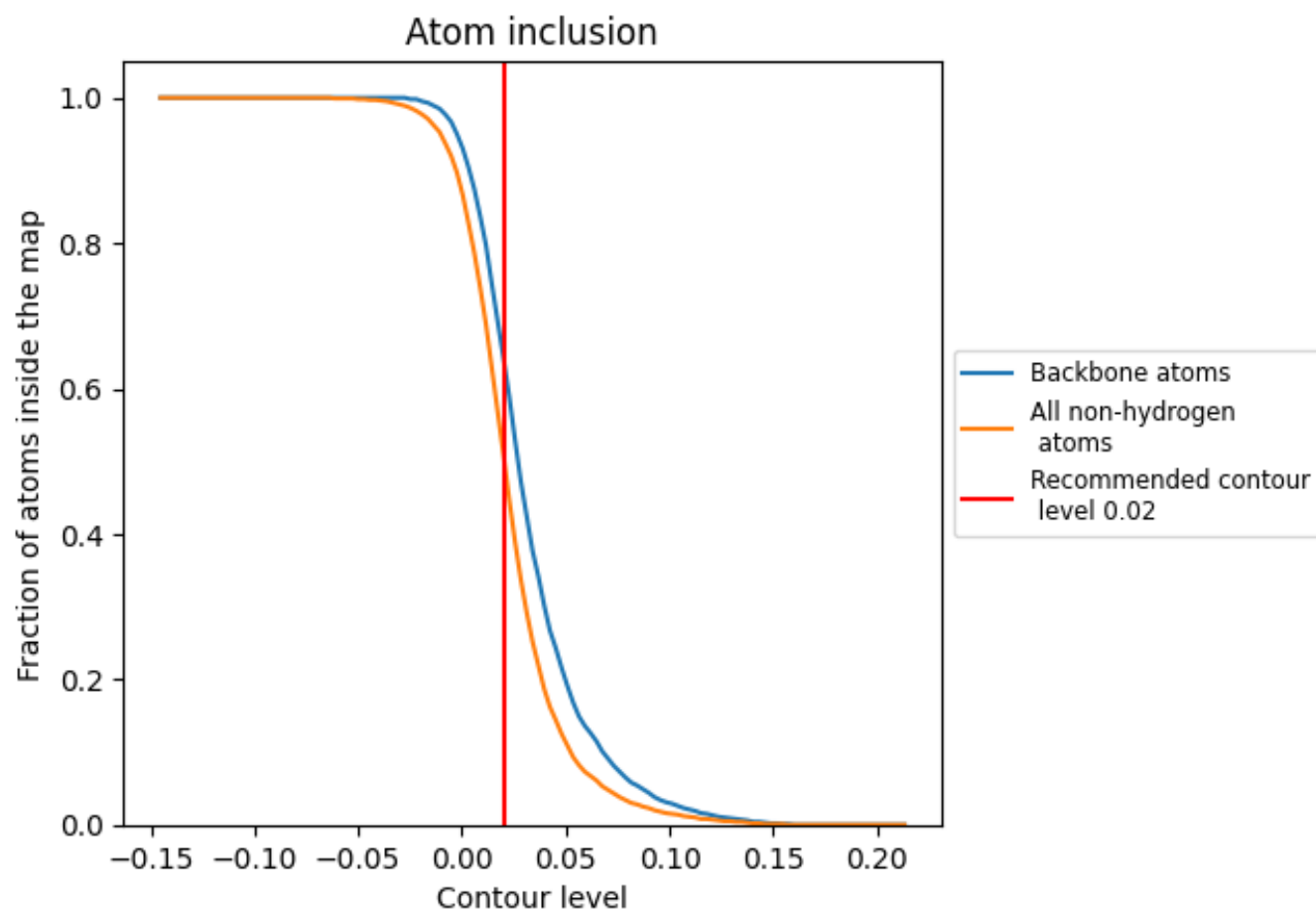
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.02).

9.4 Atom inclusion [i](#)



At the recommended contour level, 64% of all backbone atoms, 51% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.5100	<div></div> 0.1530
A	<div></div> 0.5100	<div></div> 0.1530

