



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 02:39 PM UTC

PDB ID : 8JQH / pdb_00008jqh
EMDB ID : EMD-36572
Title : Cryo EM map of full length PLC gamma 2 in autoinhibition state
Authors : Shin, Y.-C.; Liao, M.
Deposited on : 2023-06-14
Resolution : 4.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

EMDB validation analysis : 0.0.1.dev132
MolProbity : 4-5-2 with Phenix2.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

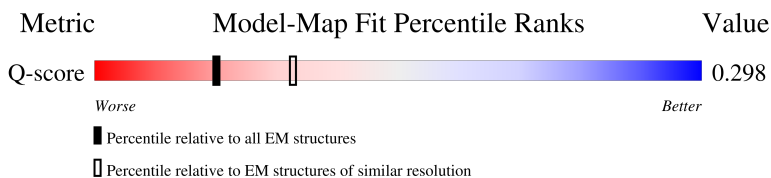
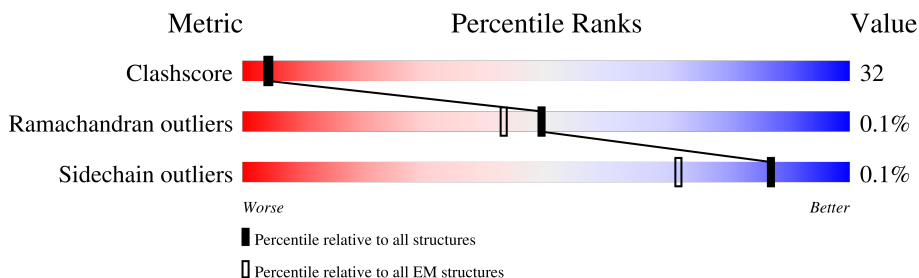
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 4.20 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	5410 (3.70 - 4.70)

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

Mol	Chain	Length	Quality of chain
1	A	1265	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 9920 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.

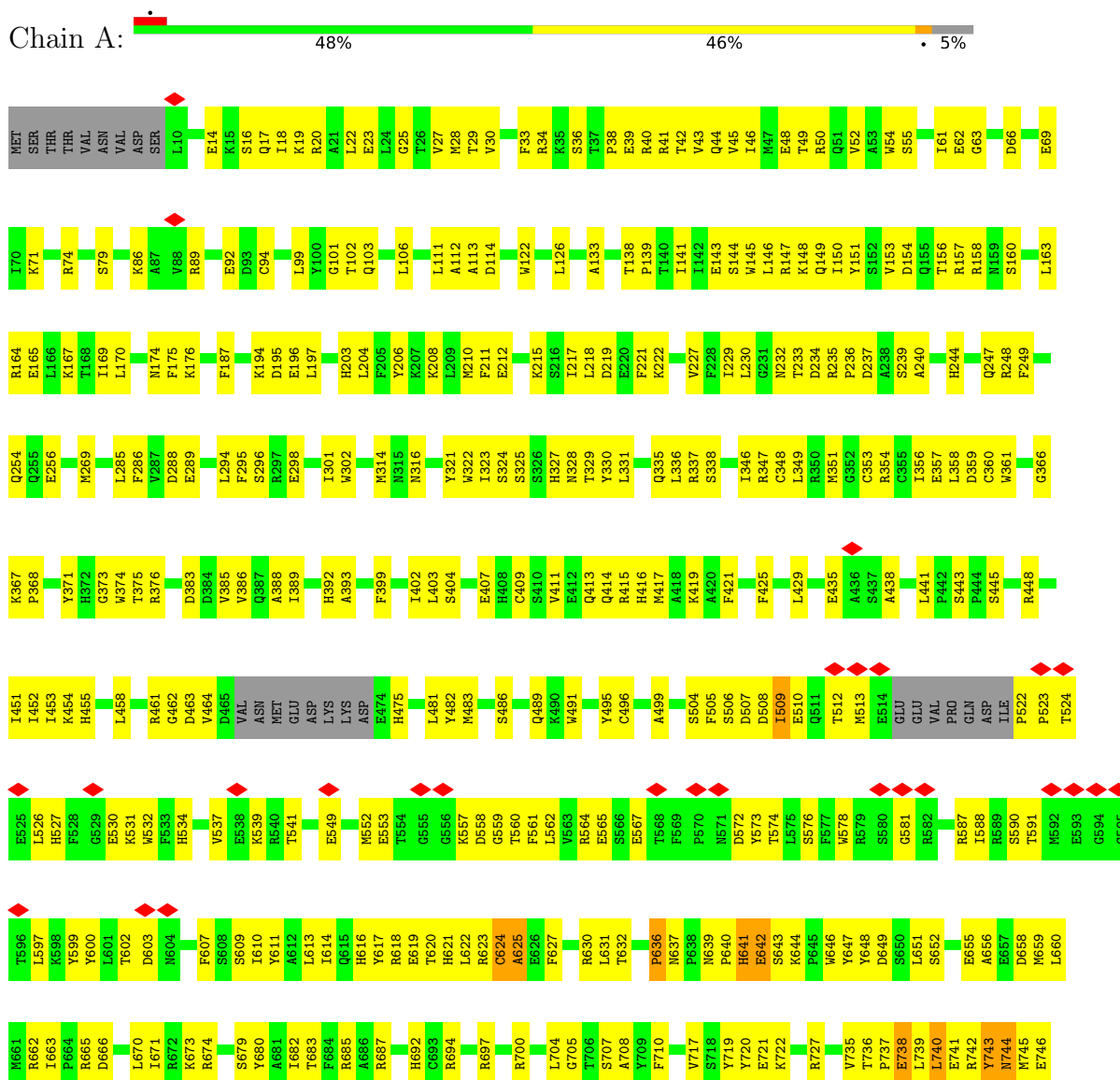
- Molecule 1 is a protein called 1-phosphatidylinositol 4,5-bisphosphate phosphodiesterase gamma-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1206	9920	6299	1710	1862	49	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: 1-phosphatidylinositol 4,5-bisphosphate phosphodiesterase gamma-2



L1210	L1211	Q1213	L1214	F1215	L1216	Y1217	D1218	L1223	R1224	N1225	A1226	N1227	R1228	D1229	A1230	L1231	V1232	K1233	E1234	F1235	S1236	V1237	N1238	E1239	N1240	Q1241	L1242	Q1243	L1244	Y1245	Q1246	E1247	K1248	C1249	N1250	K1251	R1252	L1253	ARG	GLU	LYS	ARG	VAL	SER	ASN	SER	LYS	PHE	TYR	SER					
F1131	L1132	R1133	F1134	V1135	V1136	Y1137	E1138	M1141	P1145	M1146	F1147	L1148	A1149	H1150	A1151	T1152	Y1153	P1154	T1155	V1158	R1163	S1164	M1169	G1170	Y1171	I1175	E1176	L1177	A1178	L1181	V1182	M1186	R1187	P1188	V1189	L1190	E1193	E1194	E1195	L1196	Y1197	C1200	R1201	Q1202	L1203	R1204	R1205	L1206	Q1207						
P1050	E1054	R1057	K1058	I1059	L1060	M1061	T1062	K1066	V1067	L1068	G1069	A1070	R1071	H1072	L1073	R1078	A1081	C1082	P1083	F1084	V1085	E1086	I1089	E1093	Y1094	D1095	N1096	N1097	K1098	F1099	K1100	T1101	T1102	N1105	D1106	L1109	S1110	P1111	Q1117	E1118	K1119	V1120	Y1125	D1126	P1127	N1128	L1129	A1130							
V972	D973	L974	L975	K976	Y977	N978	G981	L982	T983	R984	V985	Y986	P987	K988	G989	Q990	S994	F1000	R1001	L1002	V1003	L1004	C1005	G1006	S1007	Q1008	M1009	V1010	A1011	L1012	N1013	F1014	Q1015	T1016	A1017	D1018	K1019	Y1020	M1021	Q1022	F1028	N1031	Y1036	V1037	L1038	Q1039	P1040	E1041	T1045	E1046					
V886	E887	F888	A889	R892	E895	W899	I903	T906	K909	ILE	ASP	THR	LYS	GLU	ASN	ASN	F1000	R1001	L1002	V1003	L1004	C1005	G1006	S1007	Q1008	M1009	V1010	A1011	L1012	N1013	F1014	Q1015	T1016	A1017	D1018	K1019	Y1020	M1021	Q1022	F1028	N1031	Y1036	V1037	L1038	Q1039	P1040	E1041	T1045	E1046						
I815	Q816	Q817	P820	S821	N822	Y823	V824	E825	D826	I827	S828	T829	A830	D831	F832	E833	E834	L835	E836	K837	Q838	I839	I840	E841	D842	N843	P844	L845	G846	S847	L848	C849	R850	G851	I852	L853	D854	L855	N856	T857	Y858	P864	K867	K870	I875	L876	E877	P878	K879	D883	P884	P885			
R747	D748	I749	N750	S751	L752	Y753	D754	V755	SER	ARG	MET	TYR	VAL	ASP	PRO	SER	GLU	ILE	ASN	P767	S768	M769	P770	Q771	R772	T773	V774	K775	A776	L777	Y778	D779	Y780	K781	R784	S785	D786	E787	L788	R792	G793	A794	L795	I796	H797	N798	K801	E802	P803	G804	G805	W806	W807	D810	Y811

4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	24761	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	53.0932	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	2.062	Depositor
Minimum map value	-1.125	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.070	Depositor
Recommended contour level	0.3	Depositor
Map size ($\text{\AA}$)	237.6, 237.6, 237.6	wwPDB
Map dimensions	216, 216, 216	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing ($\text{\AA}$)	1.1, 1.1, 1.1	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	0.38	6/10148 (0.1%)	0.65	28/13694 (0.2%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1240	ASN	CA-C	-7.08	1.44	1.52
1	A	1244	LEU	CA-C	-6.78	1.44	1.52
1	A	642	GLU	CA-C	-5.48	1.45	1.52
1	A	743	TYR	CA-C	-5.35	1.45	1.52
1	A	1242	LEU	CA-C	-5.23	1.46	1.53
1	A	1250	ASN	CA-C	-5.06	1.46	1.52

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	744	ASN	N-CA-C	-10.36	99.80	111.71
1	A	1233	LYS	N-CA-C	-9.68	100.41	110.97
1	A	1247	GLU	N-CA-C	-9.61	101.57	113.20
1	A	743	TYR	N-CA-C	-9.45	101.94	112.72
1	A	641	HIS	N-CA-C	-7.58	102.04	111.75
1	A	1251	LYS	N-CA-C	-7.45	103.14	111.71
1	A	1232	VAL	N-CA-C	-7.39	101.85	111.09
1	A	1237	VAL	N-CA-C	-7.21	103.50	110.42
1	A	735	VAL	CB-CA-C	-7.20	104.47	112.68
1	A	1249	CYS	N-CA-C	-7.00	104.61	113.01
1	A	1250	ASN	N-CA-C	-6.69	103.24	111.40
1	A	642	GLU	CA-C-N	-6.49	114.25	123.20
1	A	642	GLU	C-N-CA	-6.49	114.25	123.20
1	A	625	ALA	N-CA-C	-6.28	103.73	111.33
1	A	624	CYS	N-CA-C	-6.12	99.22	108.52
1	A	735	VAL	N-CA-C	6.10	115.40	106.55
1	A	636	PRO	CA-N-CD	-6.08	103.48	112.00
1	A	740	LEU	N-CA-C	-5.72	104.40	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	738	GLU	N-CA-C	-5.62	104.53	111.33
1	A	1105	ASN	N-CA-C	5.58	117.83	108.96
1	A	1241	GLN	CA-C-N	-5.50	109.92	121.80
1	A	1241	GLN	C-N-CA	-5.50	109.92	121.80
1	A	509	ILE	N-CA-C	-5.29	105.97	111.58
1	A	1242	LEU	CA-CB-CG	-5.28	97.83	116.30
1	A	768	SER	CA-C-N	-5.22	117.05	122.89
1	A	768	SER	C-N-CA	-5.22	117.05	122.89
1	A	1072	HIS	CA-C-N	-5.09	113.85	120.67
1	A	1072	HIS	C-N-CA	-5.09	113.85	120.67

There are no chirality outliers.

There are no planarity outliers.

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	9920	0	9758	620	0
All	All	9920	0	9758	620	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 32.

All (620) 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:617:TYR:HE1	1:A:622:LEU:HD11	1.01	1.12
1:A:1203:LEU:HD22	1:A:1242:LEU:HG	1.32	1.07
1:A:617:TYR:CE1	1:A:622:LEU:HD11	1.91	1.06
1:A:752:LEU:HD22	1:A:852:ILE:H	1.26	0.98
1:A:28:MET:SD	1:A:113:ALA:HA	2.07	0.94
1:A:656:ALA:HB1	1:A:683:THR:HG21	1.49	0.92
1:A:641:HIS:HA	1:A:644:LYS:HB2	1.49	0.92
1:A:1089:ILE:O	1:A:1096:ASN:HA	1.69	0.91
1:A:620:THR:HG22	1:A:622:LEU:H	1.31	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1203:LEU:HD13	1:A:1242:LEU:HB2	1.54	0.89
1:A:752:LEU:HD21	1:A:852:ILE:HD12	1.56	0.87
1:A:1234:GLU:O	1:A:1237:VAL:HG22	1.75	0.86
1:A:746:GLU:H	1:A:747:ARG:HH11	1.23	0.86
1:A:1085:VAL:HG12	1:A:1136:VAL:HG12	1.57	0.86
1:A:649:ASP:HA	1:A:673:LYS:HB3	1.57	0.85
1:A:1231:LEU:HG	1:A:1234:GLU:HG3	1.58	0.85
1:A:878:PRO:HG2	1:A:883:ASP:HB3	1.59	0.84
1:A:402:ILE:HG22	1:A:452:ILE:HB	1.59	0.84
1:A:323:ILE:HG22	1:A:1036:TYR:CE1	2.14	0.83
1:A:559:GLY:HA2	1:A:631:LEU:HB2	1.60	0.83
1:A:617:TYR:HE1	1:A:622:LEU:CD1	1.89	0.83
1:A:1233:LYS:O	1:A:1237:VAL:HG13	1.79	0.82
1:A:613:LEU:HA	1:A:616:HIS:CE1	2.15	0.81
1:A:621:HIS:HB2	1:A:623:ARG:HG3	1.63	0.80
1:A:499:ALA:HB3	1:A:844:PRO:HG3	1.62	0.79
1:A:752:LEU:CD2	1:A:852:ILE:HD12	2.13	0.79
1:A:354:ARG:HG3	1:A:1036:TYR:CE2	2.17	0.78
1:A:671:ILE:HG12	1:A:682:ILE:HG22	1.65	0.78
1:A:553:GLU:CD	1:A:700:ARG:HH21	1.92	0.77
1:A:877:GLU:HG2	1:A:885:PRO:HG3	1.66	0.77
1:A:1203:LEU:CD2	1:A:1242:LEU:HG	2.13	0.76
1:A:1223:LEU:HD23	1:A:1228:ARG:HD3	1.66	0.76
1:A:1061:MET:HE1	1:A:1186:MET:HA	1.67	0.76
1:A:705:GLY:HA2	1:A:1141:MET:SD	2.26	0.75
1:A:624:CYS:N	1:A:627:PHE:O	2.20	0.75
1:A:28:MET:HE3	1:A:28:MET:HA	1.69	0.75
1:A:1203:LEU:HD13	1:A:1242:LEU:CB	2.16	0.75
1:A:218:LEU:HD13	1:A:234:ASP:HB2	1.69	0.75
1:A:240:ALA:HB2	1:A:286:PHE:CD1	2.21	0.75
1:A:942:LYS:HG3	1:A:943:THR:HG23	1.68	0.74
1:A:1242:LEU:O	1:A:1243:GLN:C	2.28	0.74
1:A:1189:VAL:HG21	1:A:1194:GLU:OE1	1.88	0.74
1:A:1014:PHE:HA	1:A:1021:MET:HE3	1.69	0.73
1:A:710:PHE:HE1	1:A:1078:ARG:HG2	1.52	0.73
1:A:429:LEU:HA	1:A:451:ILE:HB	1.69	0.73
1:A:229:ILE:HD12	1:A:229:ILE:H	1.53	0.72
1:A:1059:ILE:HD13	1:A:1197:TYR:HB3	1.69	0.72
1:A:458:LEU:HG	1:A:461:ARG:HA	1.70	0.72
1:A:522:PRO:HD2	1:A:526:LEU:HD22	1.71	0.72
1:A:240:ALA:HA	1:A:286:PHE:HA	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:561:PHE:HB3	1:A:631:LEU:HD11	1.71	0.72
1:A:532:TRP:CZ3	1:A:614:ILE:HG21	2.25	0.72
1:A:1239:GLU:O	1:A:1243:GLN:HG2	1.90	0.72
1:A:637:ASN:HB3	1:A:640:PRO:HG3	1.72	0.71
1:A:532:TRP:CH2	1:A:614:ILE:HG21	2.26	0.71
1:A:510:GLU:HA	1:A:513:MET:HE2	1.73	0.71
1:A:983:THR:O	1:A:1009:MET:HB3	1.91	0.71
1:A:164:ARG:O	1:A:167:LYS:N	2.24	0.70
1:A:323:ILE:CG2	1:A:1036:TYR:CE1	2.74	0.70
1:A:1022:GLN:OE1	1:A:1133:ARG:NH2	2.24	0.70
1:A:507:ASP:HA	1:A:850:ARG:HD3	1.72	0.70
1:A:1150:HIS:NE2	1:A:1169:ASN:O	2.24	0.70
1:A:658:ASP:OD2	1:A:662:ARG:NH1	2.25	0.70
1:A:163:LEU:HD13	1:A:195:ASP:HB2	1.74	0.70
1:A:736:THR:H	1:A:739:LEU:HD12	1.56	0.70
1:A:984:ARG:HG2	1:A:1009:MET:HE3	1.74	0.70
1:A:784:ARG:HD3	1:A:786:ASP:H	1.57	0.69
1:A:741:GLU:HA	1:A:744:ASN:CG	2.16	0.69
1:A:530:GLU:HG2	1:A:532:TRP:CE3	2.27	0.69
1:A:835:LEU:O	1:A:839:ILE:HG13	1.92	0.69
1:A:752:LEU:HD22	1:A:852:ILE:N	2.06	0.69
1:A:323:ILE:HG22	1:A:1036:TYR:CD1	2.27	0.69
1:A:623:ARG:HA	1:A:627:PHE:O	1.93	0.68
1:A:649:ASP:HA	1:A:673:LYS:CB	2.22	0.68
1:A:50:ARG:HH12	1:A:133:ALA:HA	1.58	0.68
1:A:644:LYS:HG2	1:A:646:TRP:CZ2	2.30	0.67
1:A:153:VAL:HG11	1:A:169:ILE:HG13	1.76	0.67
1:A:507:ASP:OD1	1:A:508:ASP:N	2.27	0.67
1:A:739:LEU:O	1:A:740:LEU:C	2.36	0.66
1:A:752:LEU:HD21	1:A:852:ILE:CD1	2.25	0.66
1:A:158:ARG:HG2	1:A:160:SER:H	1.61	0.66
1:A:256:GLU:OE2	1:A:1163:ARG:NH2	2.28	0.66
1:A:785:SER:O	1:A:817:GLN:NE2	2.28	0.66
1:A:176:LYS:HE2	1:A:707:SER:OG	1.96	0.66
1:A:736:THR:O	1:A:739:LEU:HB2	1.96	0.66
1:A:489:GLN:HG2	1:A:742:ARG:NH1	2.10	0.65
1:A:878:PRO:HG2	1:A:883:ASP:CB	2.25	0.65
1:A:830:ALA:HB1	1:A:833:GLU:HB2	1.79	0.65
1:A:1215:PHE:HA	1:A:1218:ASP:HB2	1.78	0.65
1:A:176:LYS:HD2	1:A:1106:ASP:HB3	1.77	0.65
1:A:784:ARG:HH11	1:A:786:ASP:HB2	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:346:ILE:HD11	1:A:388:ALA:HB1	1.78	0.64
1:A:441:LEU:HG	1:A:952:PHE:HB2	1.79	0.64
1:A:530:GLU:HG2	1:A:532:TRP:CZ3	2.32	0.64
1:A:27:VAL:HG22	1:A:42:THR:HG22	1.79	0.64
1:A:705:GLY:HA2	1:A:1141:MET:HG3	1.78	0.64
1:A:705:GLY:CA	1:A:1141:MET:SD	2.85	0.64
1:A:206:TYR:OH	1:A:1072:HIS:HE1	1.81	0.64
1:A:616:HIS:HA	1:A:619:GLU:HG2	1.80	0.64
1:A:1231:LEU:HG	1:A:1234:GLU:CG	2.26	0.64
1:A:1136:VAL:HG23	1:A:1148:LEU:HB2	1.79	0.64
1:A:482:TYR:HB2	1:A:889:ALA:HB3	1.79	0.64
1:A:772:ARG:HH22	1:A:801:LYS:HB2	1.62	0.64
1:A:687:ARG:NH1	1:A:727:ARG:HH12	1.95	0.63
1:A:1204:ARG:HA	1:A:1207:GLN:HG3	1.79	0.63
1:A:407:GLU:OE2	1:A:414:GLN:NE2	2.32	0.63
1:A:1247:GLU:O	1:A:1251:LYS:HG3	1.99	0.62
1:A:1223:LEU:HG	1:A:1224:ARG:N	2.12	0.62
1:A:27:VAL:HG12	1:A:40:ARG:HE	1.64	0.62
1:A:1240:ASN:O	1:A:1241:GLN:C	2.42	0.62
1:A:710:PHE:CE1	1:A:1078:ARG:HG2	2.35	0.62
1:A:721:GLU:OE2	1:A:722:LYS:NZ	2.31	0.62
1:A:524:THR:CG2	1:A:597:LEU:HD13	2.30	0.62
1:A:176:LYS:HD2	1:A:1106:ASP:CG	2.25	0.62
1:A:233:THR:O	1:A:236:PRO:HD2	2.00	0.62
1:A:752:LEU:HD23	1:A:851:GLY:HA2	1.82	0.61
1:A:164:ARG:O	1:A:165:GLU:C	2.41	0.61
1:A:165:GLU:O	1:A:169:ILE:HD12	2.00	0.61
1:A:648:TYR:HB3	1:A:651:LEU:HB2	1.81	0.61
1:A:659:MET:HB3	1:A:662:ARG:NH2	2.14	0.61
1:A:978:ASN:ND2	1:A:1006:GLY:O	2.34	0.61
1:A:335:GLN:N	1:A:335:GLN:OE1	2.33	0.61
1:A:532:TRP:CZ2	1:A:614:ILE:HB	2.35	0.61
1:A:792:ARG:HD3	1:A:1204:ARG:NH2	2.15	0.61
1:A:646:TRP:CE2	1:A:717:VAL:HG21	2.35	0.61
1:A:985:VAL:HG21	1:A:1002:LEU:HD13	1.83	0.61
1:A:331:LEU:HD13	1:A:335:GLN:HA	1.83	0.61
1:A:777:LEU:HD13	1:A:1099:PHE:HA	1.83	0.61
1:A:1206:ARG:O	1:A:1206:ARG:HD3	2.00	0.60
1:A:741:GLU:HA	1:A:744:ASN:OD1	2.00	0.60
1:A:374:TRP:CG	1:A:475:HIS:HB3	2.37	0.60
1:A:737:PRO:O	1:A:738:GLU:C	2.44	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1000:PHE:CE2	1:A:1004:LEU:HD11	2.37	0.60
1:A:1070:ALA:HB3	1:A:1111:PRO:HG2	1.84	0.60
1:A:1216:LEU:HG	1:A:1223:LEU:CD2	2.31	0.60
1:A:705:GLY:HA2	1:A:1141:MET:CG	2.31	0.59
1:A:219:ASP:HA	1:A:222:LYS:HB3	1.83	0.59
1:A:1203:LEU:HD13	1:A:1242:LEU:CG	2.32	0.59
1:A:621:HIS:HB2	1:A:623:ARG:CG	2.30	0.59
1:A:403:LEU:HD23	1:A:451:ILE:HG23	1.85	0.59
1:A:705:GLY:CA	1:A:1141:MET:HG3	2.33	0.59
1:A:923:ASN:OD1	1:A:924:GLN:N	2.35	0.59
1:A:89:ARG:O	1:A:89:ARG:NH1	2.34	0.59
1:A:641:HIS:CA	1:A:644:LYS:HB2	2.27	0.59
1:A:640:PRO:C	1:A:642:GLU:N	2.54	0.59
1:A:40:ARG:O	1:A:41:ARG:NH1	2.35	0.58
1:A:887:GLU:OE1	1:A:887:GLU:N	2.36	0.58
1:A:389:ILE:O	1:A:393:ALA:HB2	2.03	0.58
1:A:146:LEU:HD21	1:A:206:TYR:CD2	2.39	0.58
1:A:327:HIS:CG	1:A:987:PRO:HD2	2.38	0.58
1:A:314:MET:SD	1:A:1031:ASN:ND2	2.77	0.58
1:A:641:HIS:O	1:A:642:GLU:C	2.44	0.58
1:A:674:ARG:HH11	1:A:694:ARG:HG2	1.67	0.58
1:A:738:GLU:O	1:A:741:GLU:HB2	2.03	0.58
1:A:1134:PHE:CE2	1:A:1182:VAL:HG11	2.38	0.58
1:A:204:LEU:O	1:A:208:LYS:HG2	2.04	0.58
1:A:754:ASP:O	1:A:755:VAL:C	2.44	0.58
1:A:687:ARG:HH12	1:A:727:ARG:HH12	1.48	0.58
1:A:624:CYS:HB2	1:A:627:PHE:H	1.67	0.58
1:A:984:ARG:CG	1:A:1009:MET:HE3	2.34	0.58
1:A:1137:TYR:HD1	1:A:1147:PHE:HA	1.69	0.58
1:A:741:GLU:O	1:A:744:ASN:HB2	2.03	0.58
1:A:975:LEU:HD22	1:A:1050:PRO:HG3	1.85	0.58
1:A:564:ARG:NH1	1:A:567:GLU:OE1	2.37	0.57
1:A:66:ASP:HB3	1:A:69:GLU:HB2	1.85	0.57
1:A:44:GLN:HE22	1:A:46:ILE:HG12	1.68	0.57
1:A:174:ASN:HD21	1:A:1081:ALA:H	1.52	0.57
1:A:620:THR:CG2	1:A:622:LEU:H	2.10	0.57
1:A:335:GLN:HE22	1:A:994:SER:HA	1.70	0.57
1:A:323:ILE:HD11	1:A:1009:MET:SD	2.44	0.57
1:A:512:THR:HG23	1:A:513:MET:SD	2.45	0.57
1:A:158:ARG:NE	1:A:160:SER:O	2.38	0.57
1:A:797:HIS:NE2	1:A:1218:ASP:OD1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:LYS:HD2	1:A:1106:ASP:CB	2.35	0.57
1:A:523:PRO:HB2	1:A:597:LEU:HD21	1.87	0.56
1:A:680:TYR:OH	1:A:697:ARG:NH1	2.37	0.56
1:A:483:MET:HG2	1:A:888:PHE:HE1	1.70	0.56
1:A:982:LEU:HB3	1:A:1008:GLN:HE22	1.70	0.56
1:A:1057:ARG:HB2	1:A:1201:ARG:HH12	1.70	0.56
1:A:1193:GLU:O	1:A:1197:TYR:N	2.39	0.56
1:A:298:GLU:OE1	1:A:298:GLU:N	2.34	0.56
1:A:509:ILE:O	1:A:512:THR:HG22	2.05	0.56
1:A:1242:LEU:HD12	1:A:1246:GLN:HG3	1.88	0.56
1:A:288:ASP:OD1	1:A:289:GLU:N	2.38	0.56
1:A:346:ILE:HD12	1:A:392:HIS:CD2	2.41	0.56
1:A:530:GLU:CG	1:A:532:TRP:CE3	2.89	0.56
1:A:106:LEU:HG	1:A:347:ARG:HD3	1.87	0.56
1:A:646:TRP:CE3	1:A:671:ILE:HD12	2.40	0.56
1:A:1246:GLN:C	1:A:1248:LYS:H	2.13	0.56
1:A:1233:LYS:O	1:A:1234:GLU:C	2.44	0.56
1:A:322:TRP:HD1	1:A:1008:GLN:HA	1.70	0.55
1:A:331:LEU:HD22	1:A:338:SER:HB3	1.88	0.55
1:A:839:ILE:HG22	1:A:843:ASN:ND2	2.21	0.55
1:A:1128:ASN:OD1	1:A:1129:LEU:N	2.38	0.55
1:A:210:MET:HE1	1:A:1109:LEU:HD21	1.86	0.55
1:A:644:LYS:HG2	1:A:646:TRP:CH2	2.42	0.55
1:A:534:HIS:CG	1:A:637:ASN:HB2	2.41	0.55
1:A:102:THR:HB	1:A:1169:ASN:ND2	2.21	0.55
1:A:772:ARG:HH12	1:A:801:LYS:HB2	1.71	0.55
1:A:802:GLU:HG3	1:A:803:PRO:HD2	1.88	0.55
1:A:1017:ALA:HB2	1:A:1171:TYR:CE1	2.41	0.55
1:A:145:TRP:HA	1:A:148:LYS:NZ	2.21	0.55
1:A:206:TYR:CE1	1:A:210:MET:HG3	2.41	0.55
1:A:69:GLU:HG3	1:A:101:GLY:H	1.71	0.55
1:A:496:CYS:HA	1:A:504:SER:O	2.05	0.55
1:A:527:HIS:HB2	1:A:610:ILE:HB	1.89	0.55
1:A:1210:LEU:O	1:A:1213:GLN:HG3	2.06	0.55
1:A:1242:LEU:O	1:A:1244:LEU:N	2.40	0.55
1:A:229:ILE:HG12	1:A:249:PHE:HD1	1.71	0.54
1:A:486:SER:O	1:A:489:GLN:NE2	2.40	0.54
1:A:504:SER:HB2	1:A:849:CYS:SG	2.47	0.54
1:A:48:GLU:OE2	1:A:48:GLU:N	2.28	0.54
1:A:705:GLY:CA	1:A:1141:MET:CG	2.85	0.54
1:A:892:ARG:HB2	1:A:895:GLU:HG2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:741:GLU:O	1:A:744:ASN:N	2.31	0.54
1:A:794:ALA:HB1	1:A:811:TYR:HE2	1.71	0.54
1:A:1084:PHE:HZ	1:A:1145:PRO:HB3	1.72	0.54
1:A:778:TYR:HA	1:A:792:ARG:HG2	1.88	0.54
1:A:23:GLU:HG2	1:A:45:VAL:HG23	1.90	0.54
1:A:45:VAL:HG12	1:A:52:VAL:HG22	1.89	0.54
1:A:368:PRO:HG3	1:A:413:GLN:HB3	1.89	0.54
1:A:46:ILE:HD11	1:A:157:ARG:HH11	1.73	0.54
1:A:621:HIS:O	1:A:622:LEU:C	2.49	0.54
1:A:746:GLU:H	1:A:747:ARG:NH1	2.01	0.54
1:A:532:TRP:CE3	1:A:614:ILE:HG21	2.43	0.54
1:A:28:MET:HG3	1:A:29:THR:N	2.22	0.54
1:A:187:PHE:CE1	1:A:197:LEU:HG	2.44	0.54
1:A:776:ALA:HB3	1:A:794:ALA:H	1.72	0.53
1:A:1190:LEU:HB2	1:A:1193:GLU:HG3	1.90	0.53
1:A:74:ARG:NH2	1:A:79:SER:OG	2.41	0.53
1:A:527:HIS:H	1:A:610:ILE:HD12	1.71	0.53
1:A:640:PRO:O	1:A:641:HIS:C	2.45	0.53
1:A:1189:VAL:CG2	1:A:1194:GLU:OE1	2.56	0.53
1:A:1203:LEU:CD1	1:A:1242:LEU:HB2	2.34	0.53
1:A:646:TRP:CZ3	1:A:671:ILE:HD12	2.44	0.53
1:A:792:ARG:HD3	1:A:1204:ARG:HH21	1.73	0.53
1:A:876:LEU:HD21	1:A:903:ILE:HD12	1.91	0.53
1:A:1066:LYS:HB2	1:A:1119:LYS:HD3	1.89	0.53
1:A:347:ARG:NH1	1:A:351:MET:HE2	2.24	0.53
1:A:532:TRP:CZ2	1:A:614:ILE:HG21	2.44	0.53
1:A:743:TYR:C	1:A:745:MET:N	2.57	0.53
1:A:29:THR:OG1	1:A:112:ALA:O	2.25	0.53
1:A:1231:LEU:O	1:A:1235:PHE:N	2.31	0.53
1:A:1054:GLU:O	1:A:1201:ARG:NH1	2.41	0.53
1:A:537:VAL:HG21	1:A:565:GLU:H	1.74	0.53
1:A:659:MET:CB	1:A:662:ARG:NH2	2.72	0.52
1:A:960:GLU:OE1	1:A:988:LYS:NZ	2.42	0.52
1:A:737:PRO:O	1:A:740:LEU:N	2.42	0.52
1:A:222:LYS:HZ3	1:A:232:ASN:HA	1.73	0.52
1:A:557:LYS:HE2	1:A:581:GLY:HA2	1.92	0.52
1:A:1246:GLN:C	1:A:1248:LYS:N	2.67	0.52
1:A:578:TRP:HE1	1:A:581:GLY:H	1.56	0.52
1:A:244:HIS:O	1:A:248:ARG:HG3	2.10	0.52
1:A:621:HIS:CB	1:A:623:ARG:HG3	2.36	0.52
1:A:1210:LEU:HD21	1:A:1235:PHE:HD1	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:322:TRP:N	1:A:1039:GLN:OE1	2.39	0.52
1:A:1133:ARG:HD2	1:A:1152:THR:HG22	1.92	0.52
1:A:506:SER:O	1:A:850:ARG:NH1	2.43	0.51
1:A:524:THR:CG2	1:A:597:LEU:CD1	2.88	0.51
1:A:532:TRP:CE2	1:A:614:ILE:CG2	2.94	0.51
1:A:943:THR:HB	1:A:946:ASN:HB2	1.92	0.51
1:A:878:PRO:HG2	1:A:883:ASP:CG	2.35	0.51
1:A:354:ARG:CG	1:A:1036:TYR:CE2	2.90	0.51
1:A:530:GLU:HG3	1:A:531:LYS:H	1.75	0.51
1:A:943:THR:OG1	1:A:956:ARG:NH2	2.43	0.51
1:A:429:LEU:HD21	1:A:933:LEU:HD22	1.93	0.51
1:A:1200:CYS:O	1:A:1203:LEU:HB3	2.11	0.51
1:A:1216:LEU:HG	1:A:1223:LEU:HD22	1.91	0.51
1:A:235:ARG:HB3	1:A:236:PRO:HD3	1.91	0.51
1:A:539:LYS:HA	1:A:567:GLU:HG2	1.92	0.51
1:A:411:VAL:O	1:A:415:ARG:HG3	2.10	0.51
1:A:899:TRP:O	1:A:903:ILE:HG12	2.10	0.51
1:A:572:ASP:OD1	1:A:590:SER:OG	2.23	0.51
1:A:206:TYR:O	1:A:210:MET:HG2	2.10	0.51
1:A:221:PHE:HE2	1:A:294:LEU:HD11	1.75	0.51
1:A:687:ARG:HD3	1:A:753:TYR:HE1	1.74	0.51
1:A:752:LEU:CD2	1:A:852:ILE:H	2.12	0.51
1:A:839:ILE:O	1:A:843:ASN:HB2	2.11	0.51
1:A:853:LEU:HB2	1:A:858:TYR:HE2	1.75	0.51
1:A:984:ARG:HD2	1:A:1009:MET:HE3	1.92	0.51
1:A:562:LEU:O	1:A:576:SER:N	2.43	0.50
1:A:648:TYR:CE2	1:A:670:LEU:HB2	2.46	0.50
1:A:1066:LYS:HZ1	1:A:1117:GLN:C	2.19	0.50
1:A:801:LYS:HG2	1:A:807:TRP:NE1	2.26	0.50
1:A:17:GLN:HA	1:A:20:ARG:HG2	1.93	0.50
1:A:482:TYR:HB3	1:A:491:TRP:HB3	1.92	0.50
1:A:651:LEU:HD11	1:A:659:MET:SD	2.52	0.50
1:A:984:ARG:CD	1:A:1009:MET:HE3	2.41	0.50
1:A:531:LYS:HA	1:A:534:HIS:NE2	2.26	0.50
1:A:784:ARG:NH1	1:A:786:ASP:HB2	2.26	0.50
1:A:847:SER:O	1:A:848:LEU:HB2	2.12	0.50
1:A:611:TYR:O	1:A:614:ILE:HG13	2.11	0.50
1:A:1250:ASN:O	1:A:1251:LYS:C	2.53	0.50
1:A:988:LYS:HE2	1:A:990:GLN:HB2	1.94	0.50
1:A:346:ILE:HD12	1:A:392:HIS:HD2	1.76	0.50
1:A:656:ALA:HA	1:A:659:MET:HG2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1216:LEU:HG	1:A:1223:LEU:HD21	1.93	0.50
1:A:781:LYS:HE2	1:A:1243:GLN:HG3	1.94	0.49
1:A:417:MET:HE3	1:A:421:PHE:CE2	2.47	0.49
1:A:458:LEU:HG	1:A:461:ARG:CA	2.39	0.49
1:A:506:SER:HB3	1:A:845:LEU:HD13	1.94	0.49
1:A:665:ARG:HH21	1:A:749:ILE:HB	1.77	0.49
1:A:1073:LEU:HD12	1:A:1111:PRO:HG3	1.95	0.49
1:A:176:LYS:HE2	1:A:707:SER:HG	1.76	0.49
1:A:824:VAL:O	1:A:1100:LYS:NZ	2.35	0.49
1:A:323:ILE:CG2	1:A:1036:TYR:HE1	2.26	0.49
1:A:302:TRP:HZ3	1:A:1154:PRO:HD2	1.78	0.49
1:A:322:TRP:HA	1:A:1008:GLN:HB2	1.95	0.49
1:A:1203:LEU:HD22	1:A:1242:LEU:CG	2.22	0.49
1:A:153:VAL:HG21	1:A:169:ILE:HD11	1.93	0.49
1:A:530:GLU:CG	1:A:532:TRP:HE3	2.25	0.49
1:A:649:ASP:CA	1:A:673:LYS:HB3	2.37	0.49
1:A:704:LEU:O	1:A:708:ALA:HB3	2.13	0.49
1:A:752:LEU:CD2	1:A:851:GLY:HA2	2.43	0.49
1:A:1019:LYS:HG3	1:A:1133:ARG:NH1	2.28	0.49
1:A:163:LEU:HD12	1:A:187:PHE:CE2	2.47	0.49
1:A:43:VAL:HG11	1:A:111:LEU:HD11	1.93	0.49
1:A:683:THR:OG1	1:A:692:HIS:NE2	2.44	0.49
1:A:741:GLU:C	1:A:744:ASN:H	2.18	0.49
1:A:1242:LEU:C	1:A:1244:LEU:N	2.62	0.49
1:A:1001:ARG:HD3	1:A:1093:GLU:OE2	2.13	0.49
1:A:28:MET:HE1	1:A:114:ASP:CG	2.37	0.48
1:A:1196:LEU:HD11	1:A:1248:LYS:HD2	1.95	0.48
1:A:1134:PHE:HB2	1:A:1151:ALA:HB3	1.95	0.48
1:A:560:THR:N	1:A:631:LEU:HD13	2.28	0.48
1:A:235:ARG:HD3	1:A:235:ARG:C	2.38	0.48
1:A:743:TYR:O	1:A:744:ASN:C	2.53	0.48
1:A:1133:ARG:HG2	1:A:1135:VAL:HG13	1.95	0.48
1:A:361:TRP:CE2	1:A:373:GLY:HA3	2.48	0.48
1:A:495:TYR:HB2	1:A:509:ILE:HD11	1.96	0.48
1:A:549:GLU:HA	1:A:552:MET:HE3	1.96	0.48
1:A:641:HIS:O	1:A:644:LYS:N	2.47	0.48
1:A:1203:LEU:HG	1:A:1204:ARG:NH1	2.28	0.48
1:A:25:GLY:HA2	1:A:43:VAL:O	2.13	0.48
1:A:348:CYS:HA	1:A:351:MET:HE3	1.96	0.48
1:A:499:ALA:CB	1:A:844:PRO:HG3	2.39	0.48
1:A:578:TRP:NE1	1:A:581:GLY:H	2.11	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:940:THR:HG23	1:A:956:ARG:HH22	1.77	0.48
1:A:984:ARG:HG3	1:A:984:ARG:HH11	1.78	0.48
1:A:141:ILE:HG23	1:A:1177:LEU:HD21	1.96	0.48
1:A:943:THR:O	1:A:956:ARG:NH2	2.46	0.48
1:A:1247:GLU:HA	1:A:1250:ASN:HB2	1.95	0.48
1:A:674:ARG:NH1	1:A:679:SER:OG	2.47	0.48
1:A:1203:LEU:HB2	1:A:1242:LEU:CD2	2.44	0.48
1:A:25:GLY:HA3	1:A:44:GLN:HB3	1.95	0.48
1:A:29:THR:OG1	1:A:112:ALA:HB3	2.13	0.48
1:A:366:GLY:HA2	1:A:413:GLN:HE21	1.79	0.48
1:A:704:LEU:HB3	1:A:708:ALA:HB3	1.96	0.48
1:A:145:TRP:HA	1:A:148:LYS:HZ2	1.79	0.48
1:A:375:THR:HG22	1:A:376:ARG:H	1.78	0.48
1:A:769:MET:N	1:A:770:PRO:HD3	2.28	0.48
1:A:1154:PRO:O	1:A:1158:VAL:HG23	2.13	0.48
1:A:145:TRP:HZ3	1:A:206:TYR:HE2	1.61	0.47
1:A:530:GLU:HG2	1:A:532:TRP:HE3	1.77	0.47
1:A:705:GLY:HA2	1:A:1141:MET:HE2	1.96	0.47
1:A:1225:ASN:HA	1:A:1228:ARG:HE	1.79	0.47
1:A:719:TYR:HD1	1:A:720:TYR:CD1	2.32	0.47
1:A:741:GLU:O	1:A:744:ASN:CB	2.62	0.47
1:A:875:ILE:HG12	1:A:887:GLU:HG3	1.95	0.47
1:A:978:ASN:ND2	1:A:1007:SER:HA	2.29	0.47
1:A:99:LEU:HB3	1:A:106:LEU:HD13	1.96	0.47
1:A:739:LEU:C	1:A:741:GLU:N	2.67	0.47
1:A:870:LYS:HG2	1:A:889:ALA:HB1	1.97	0.47
1:A:984:ARG:HD2	1:A:1009:MET:HG2	1.95	0.47
1:A:222:LYS:NZ	1:A:232:ASN:HA	2.30	0.47
1:A:659:MET:O	1:A:663:ILE:HG22	2.15	0.47
1:A:795:LEU:HB3	1:A:797:HIS:NE2	2.30	0.47
1:A:963:ALA:O	1:A:967:ILE:HG12	2.15	0.47
1:A:301:ILE:HD11	1:A:1158:VAL:HG13	1.97	0.47
1:A:417:MET:HE3	1:A:421:PHE:HE2	1.80	0.47
1:A:54:TRP:CZ2	1:A:63:GLY:HA3	2.50	0.47
1:A:349:LEU:HD22	1:A:393:ALA:HA	1.97	0.47
1:A:1248:LYS:HD3	1:A:1248:LYS:C	2.40	0.47
1:A:212:GLU:O	1:A:215:LYS:NZ	2.33	0.47
1:A:656:ALA:O	1:A:660:LEU:HD23	2.15	0.47
1:A:772:ARG:NH2	1:A:801:LYS:HB2	2.30	0.47
1:A:532:TRP:CZ2	1:A:614:ILE:CB	2.98	0.46
1:A:532:TRP:HE1	1:A:618:ARG:NH2	2.13	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:753:TYR:CG	1:A:754:ASP:N	2.82	0.46
1:A:815:ILE:HG22	1:A:816:GLN:HG2	1.96	0.46
1:A:145:TRP:O	1:A:149:GLN:HG2	2.15	0.46
1:A:532:TRP:CZ2	1:A:614:ILE:CG2	2.98	0.46
1:A:746:GLU:N	1:A:747:ARG:HH11	2.02	0.46
1:A:793:GLY:O	1:A:1211:ASN:ND2	2.40	0.46
1:A:978:ASN:HD22	1:A:1007:SER:HA	1.79	0.46
1:A:1084:PHE:CZ	1:A:1145:PRO:HB3	2.49	0.46
1:A:324:SER:HB3	1:A:1028:PHE:CG	2.50	0.46
1:A:324:SER:OG	1:A:353:CYS:HA	2.15	0.46
1:A:486:SER:O	1:A:742:ARG:HD3	2.15	0.46
1:A:622:LEU:O	1:A:627:PHE:O	2.34	0.46
1:A:772:ARG:O	1:A:774:VAL:HG13	2.16	0.46
1:A:176:LYS:HD2	1:A:1106:ASP:OD2	2.15	0.46
1:A:621:HIS:HB2	1:A:623:ARG:CD	2.45	0.46
1:A:55:SER:HA	1:A:62:GLU:H	1.80	0.46
1:A:853:LEU:HB2	1:A:858:TYR:CE2	2.49	0.46
1:A:1060:LEU:HA	1:A:1189:VAL:HG11	1.98	0.46
1:A:1243:GLN:N	1:A:1243:GLN:CD	2.72	0.46
1:A:652:SER:H	1:A:655:GLU:CD	2.23	0.46
1:A:843:ASN:HD21	1:A:852:ILE:HD11	1.81	0.46
1:A:1223:LEU:CG	1:A:1224:ARG:N	2.78	0.46
1:A:146:LEU:O	1:A:150:ILE:HG12	2.15	0.46
1:A:404:SER:HB2	1:A:454:LYS:HE3	1.96	0.46
1:A:1054:GLU:HB2	1:A:1201:ARG:HH22	1.79	0.46
1:A:336:LEU:HD22	1:A:495:TYR:CE2	2.50	0.46
1:A:822:ASN:HD22	1:A:1102:THR:N	2.14	0.46
1:A:1040:PRO:HG2	1:A:1128:ASN:ND2	2.31	0.46
1:A:211:PHE:CD2	1:A:237:ASP:HB3	2.51	0.46
1:A:1060:LEU:HB2	1:A:1127:PRO:HD3	1.98	0.46
1:A:560:THR:HB	1:A:578:TRP:HB2	1.98	0.45
1:A:796:ILE:HG12	1:A:811:TYR:HD2	1.82	0.45
1:A:837:LYS:O	1:A:841:GLU:HG3	2.15	0.45
1:A:50:ARG:NH1	1:A:133:ALA:HA	2.28	0.45
1:A:102:THR:HB	1:A:1169:ASN:HD21	1.81	0.45
1:A:1225:ASN:HB3	1:A:1228:ARG:HH21	1.81	0.45
1:A:55:SER:HB2	1:A:61:ILE:HA	1.98	0.45
1:A:316:ASN:H	1:A:443:SER:HB2	1.81	0.45
1:A:877:GLU:HG2	1:A:885:PRO:CG	2.41	0.45
1:A:1186:MET:SD	1:A:1187:ARG:N	2.90	0.45
1:A:42:THR:OG1	1:A:55:SER:OG	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:GLU:OE2	1:A:102:THR:HG23	2.17	0.45
1:A:462:GLY:O	1:A:463:ASP:C	2.59	0.45
1:A:176:LYS:HE3	1:A:1106:ASP:OD2	2.17	0.45
1:A:254:GLN:HE21	1:A:1163:ARG:NH1	2.14	0.45
1:A:302:TRP:HE3	1:A:1153:TYR:HD2	1.65	0.45
1:A:143:GLU:HG2	1:A:203:HIS:HE2	1.81	0.45
1:A:504:SER:OG	1:A:845:LEU:HG	2.16	0.45
1:A:1057:ARG:HB3	1:A:1125:TYR:CD2	2.51	0.45
1:A:1155:ILE:HA	1:A:1158:VAL:HG23	1.98	0.45
1:A:367:LYS:HE2	1:A:416:HIS:CE1	2.52	0.45
1:A:389:ILE:HD13	1:A:403:LEU:HD11	1.98	0.45
1:A:746:GLU:C	1:A:747:ARG:HE	2.25	0.45
1:A:780:TYR:HB2	1:A:823:TYR:CD2	2.52	0.45
1:A:624:CYS:O	1:A:625:ALA:C	2.59	0.45
1:A:930:LEU:HD12	1:A:933:LEU:HD12	1.98	0.45
1:A:28:MET:HE2	1:A:29:THR:H	1.81	0.45
1:A:194:LYS:O	1:A:196:GLU:HG2	2.16	0.45
1:A:234:ASP:O	1:A:235:ARG:C	2.59	0.45
1:A:92:GLU:OE1	1:A:92:GLU:N	2.38	0.45
1:A:244:HIS:O	1:A:247:GLN:HG3	2.16	0.45
1:A:784:ARG:HD3	1:A:785:SER:N	2.32	0.45
1:A:354:ARG:NH1	1:A:399:PHE:O	2.49	0.44
1:A:855:LEU:HB3	1:A:906:ILE:HG21	1.99	0.44
1:A:867:LYS:HD3	1:A:867:LYS:HA	1.76	0.44
1:A:505:PHE:CZ	1:A:851:GLY:HA3	2.52	0.44
1:A:857:THR:O	1:A:858:TYR:HD1	2.00	0.44
1:A:1099:PHE:CE2	1:A:1120:VAL:HG21	2.52	0.44
1:A:1137:TYR:CD1	1:A:1147:PHE:HA	2.52	0.44
1:A:495:TYR:HD2	1:A:845:LEU:HD22	1.83	0.44
1:A:617:TYR:O	1:A:620:THR:HB	2.17	0.44
1:A:771:GLN:HG3	1:A:798:ASN:H	1.83	0.44
1:A:977:TYR:O	1:A:981:GLY:N	2.41	0.44
1:A:1242:LEU:HD13	1:A:1242:LEU:HA	1.67	0.44
1:A:607:PHE:HD2	1:A:609:SER:H	1.64	0.44
1:A:647:TYR:OH	1:A:673:LYS:HD2	2.17	0.44
1:A:624:CYS:CB	1:A:627:PHE:H	2.29	0.44
1:A:705:GLY:HA2	1:A:1141:MET:CE	2.47	0.44
1:A:644:LYS:HB3	1:A:647:TYR:HB3	1.98	0.44
1:A:1013:ASN:O	1:A:1016:THR:HG22	2.17	0.44
1:A:1175:ILE:HG23	1:A:1178:ALA:HB3	2.00	0.44
1:A:481:LEU:HD21	1:A:899:TRP:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:670:LEU:HD23	1:A:683:THR:O	2.18	0.44
1:A:792:ARG:CZ	1:A:1097:ASN:HD21	2.30	0.44
1:A:613:LEU:HA	1:A:616:HIS:HE1	1.76	0.44
1:A:660:LEU:HD13	1:A:663:ILE:HG23	2.00	0.44
1:A:895:GLU:O	1:A:899:TRP:HD1	2.01	0.44
1:A:1094:TYR:CE1	1:A:1125:TYR:HB2	2.53	0.44
1:A:539:LYS:HG3	1:A:541:THR:H	1.83	0.44
1:A:1131:PHE:HE1	1:A:1154:PRO:HG3	1.83	0.44
1:A:1138:GLU:HB3	1:A:1148:LEU:HD11	2.00	0.44
1:A:354:ARG:HG3	1:A:1036:TYR:CD2	2.51	0.43
1:A:404:SER:CB	1:A:454:LYS:HE3	2.48	0.43
1:A:522:PRO:HG2	1:A:526:LEU:HB2	2.00	0.43
1:A:122:TRP:O	1:A:126:LEU:HD23	2.17	0.43
1:A:138:THR:OG1	1:A:139:PRO:HD3	2.18	0.43
1:A:298:GLU:H	1:A:298:GLU:CD	2.25	0.43
1:A:329:THR:HG21	1:A:356:ILE:HG22	2.00	0.43
1:A:599:TYR:CZ	1:A:613:LEU:HD12	2.53	0.43
1:A:857:THR:O	1:A:879:LYS:HG2	2.18	0.43
1:A:1204:ARG:HA	1:A:1207:GLN:CG	2.46	0.43
1:A:103:GLN:HA	1:A:1171:TYR:CD2	2.54	0.43
1:A:407:GLU:HB2	1:A:455:HIS:CD2	2.54	0.43
1:A:523:PRO:C	1:A:524:THR:HG23	2.43	0.43
1:A:574:THR:HA	1:A:588:ILE:H	1.83	0.43
1:A:777:LEU:HD11	1:A:1100:LYS:HZ2	1.83	0.43
1:A:18:ILE:O	1:A:22:LEU:HD23	2.18	0.43
1:A:28:MET:HE2	1:A:112:ALA:O	2.18	0.43
1:A:151:TYR:CD1	1:A:157:ARG:HA	2.53	0.43
1:A:639:ASN:O	1:A:642:GLU:CB	2.66	0.43
1:A:836:GLU:HA	1:A:839:ILE:HD12	2.01	0.43
1:A:1188:PRO:HG2	1:A:1190:LEU:HD21	1.99	0.43
1:A:1234:GLU:C	1:A:1237:VAL:HG22	2.43	0.43
1:A:170:LEU:HD12	1:A:175:PHE:CD2	2.54	0.43
1:A:321:TYR:CZ	1:A:1038:LEU:HD13	2.54	0.43
1:A:323:ILE:HG21	1:A:1036:TYR:HE1	1.84	0.43
1:A:573:TYR:O	1:A:587:ARG:HG2	2.18	0.43
1:A:751:SER:O	1:A:752:LEU:C	2.61	0.43
1:A:1002:LEU:HB3	1:A:1007:SER:HB2	2.01	0.43
1:A:294:LEU:HB3	1:A:1181:LEU:HD12	2.00	0.43
1:A:928:ILE:HD12	1:A:931:SER:OG	2.18	0.43
1:A:982:LEU:HB3	1:A:1008:GLN:NE2	2.31	0.43
1:A:983:THR:H	1:A:1008:GLN:HE22	1.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1248:LYS:HD3	1:A:1249:CYS:N	2.32	0.43
1:A:938:LYS:HG2	1:A:953:ARG:O	2.18	0.43
1:A:982:LEU:HD22	1:A:1008:GLN:NE2	2.34	0.43
1:A:375:THR:HG22	1:A:376:ARG:N	2.34	0.43
1:A:602:THR:HG22	1:A:603:ASP:N	2.34	0.43
1:A:1071:ARG:O	1:A:1178:ALA:HA	2.18	0.43
1:A:86:LYS:HA	1:A:86:LYS:HD2	1.93	0.42
1:A:337:ARG:NH1	1:A:509:ILE:HG21	2.34	0.42
1:A:599:TYR:OH	1:A:609:SER:O	2.36	0.42
1:A:662:ARG:HE	1:A:740:LEU:CD2	2.32	0.42
1:A:217:ILE:HD12	1:A:1068:LEU:HB3	2.01	0.42
1:A:416:HIS:HA	1:A:419:LYS:HE3	2.00	0.42
1:A:591:THR:HG23	1:A:600:TYR:HE1	1.84	0.42
1:A:640:PRO:O	1:A:643:SER:N	2.48	0.42
1:A:665:ARG:NH1	1:A:665:ARG:HB2	2.34	0.42
1:A:1062:THR:HG23	1:A:1062:THR:O	2.19	0.42
1:A:1223:LEU:CD2	1:A:1228:ARG:HD3	2.43	0.42
1:A:1245:TYR:C	1:A:1248:LYS:HB3	2.44	0.42
1:A:235:ARG:HD3	1:A:236:PRO:N	2.33	0.42
1:A:662:ARG:HB3	1:A:740:LEU:HD21	2.00	0.42
1:A:810:ASP:OD1	1:A:816:GLN:N	2.50	0.42
1:A:830:ALA:O	1:A:834:GLU:HG3	2.19	0.42
1:A:830:ALA:CB	1:A:833:GLU:HB2	2.46	0.42
1:A:932:ASP:OD1	1:A:933:LEU:N	2.53	0.42
1:A:1201:ARG:HA	1:A:1201:ARG:HD2	1.79	0.42
1:A:662:ARG:HE	1:A:740:LEU:HD21	1.84	0.42
1:A:752:LEU:CD2	1:A:852:ILE:N	2.79	0.42
1:A:1022:GLN:HG2	1:A:1150:HIS:NE2	2.35	0.42
1:A:1067:VAL:HG21	1:A:1101:THR:HG21	2.02	0.42
1:A:69:GLU:O	1:A:71:LYS:HD3	2.19	0.42
1:A:358:LEU:HD11	1:A:385:VAL:HG11	2.01	0.42
1:A:666:ASP:HA	1:A:685:ARG:HB3	2.01	0.42
1:A:778:TYR:CG	1:A:779:ASP:N	2.86	0.42
1:A:836:GLU:O	1:A:840:ILE:HG13	2.19	0.42
1:A:838:GLN:HA	1:A:841:GLU:CD	2.44	0.42
1:A:1086:GLU:HA	1:A:1100:LYS:HA	2.02	0.42
1:A:49:THR:HG22	1:A:147:ARG:HB3	2.02	0.42
1:A:210:MET:SD	1:A:1110:SER:OG	2.77	0.42
1:A:652:SER:OG	1:A:655:GLU:HG3	2.19	0.42
1:A:383:ASP:HA	1:A:386:VAL:HG12	2.01	0.42
1:A:138:THR:O	1:A:141:ILE:HG22	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154:ASP:OD1	1:A:156:THR:HG22	2.19	0.42
1:A:227:VAL:O	1:A:230:LEU:N	2.52	0.42
1:A:269:MET:CE	1:A:285:LEU:HD22	2.49	0.42
1:A:830:ALA:HB1	1:A:833:GLU:CB	2.48	0.42
1:A:984:ARG:HH21	1:A:1011:ALA:CB	2.33	0.42
1:A:1248:LYS:C	1:A:1250:ASN:N	2.72	0.42
1:A:46:ILE:HG22	1:A:49:THR:H	1.85	0.42
1:A:86:LYS:HZ2	1:A:89:ARG:HB3	1.85	0.42
1:A:414:GLN:O	1:A:417:MET:HB2	2.20	0.42
1:A:445:SER:O	1:A:448:ARG:HG2	2.20	0.42
1:A:972:VAL:O	1:A:976:LYS:HG2	2.20	0.42
1:A:1041:GLU:O	1:A:1045:THR:HG23	2.20	0.42
1:A:1136:VAL:O	1:A:1148:LEU:HB2	2.20	0.42
1:A:1147:PHE:HZ	1:A:1150:HIS:HD2	1.68	0.42
1:A:1241:GLN:HG3	1:A:1242:LEU:HD22	2.01	0.42
1:A:94:CYS:HB2	1:A:113:ALA:HB3	2.01	0.42
1:A:269:MET:HE1	1:A:285:LEU:HD22	2.01	0.41
1:A:1245:TYR:HA	1:A:1248:LYS:HB3	2.02	0.41
1:A:463:ASP:O	1:A:464:VAL:HB	2.20	0.41
1:A:1203:LEU:CG	1:A:1242:LEU:HG	2.50	0.41
1:A:48:GLU:O	1:A:144:SER:HA	2.20	0.41
1:A:170:LEU:HD12	1:A:175:PHE:HD2	1.86	0.41
1:A:229:ILE:HD12	1:A:229:ILE:N	2.29	0.41
1:A:296:SER:O	1:A:1164:SER:OG	2.36	0.41
1:A:328:ASN:N	1:A:357:GLU:OE1	2.39	0.41
1:A:330:TYR:OH	1:A:359:ASP:OD2	2.31	0.41
1:A:623:ARG:CA	1:A:627:PHE:O	2.67	0.41
1:A:357:GLU:HA	1:A:404:SER:HB3	2.01	0.41
1:A:435:GLU:OE2	1:A:438:ALA:HA	2.21	0.41
1:A:648:TYR:CD2	1:A:670:LEU:HD12	2.56	0.41
1:A:325:SER:OG	1:A:1009:MET:HG3	2.21	0.41
1:A:360:CYS:SG	1:A:407:GLU:HA	2.61	0.41
1:A:532:TRP:CE2	1:A:614:ILE:HG21	2.55	0.41
1:A:621:HIS:HA	1:A:630:ARG:HB3	2.03	0.41
1:A:705:GLY:HA3	1:A:1141:MET:CG	2.50	0.41
1:A:14:GLU:O	1:A:18:ILE:HG12	2.21	0.41
1:A:46:ILE:HD11	1:A:157:ARG:NH1	2.34	0.41
1:A:163:LEU:O	1:A:164:ARG:C	2.59	0.41
1:A:558:ASP:HA	1:A:578:TRP:CD1	2.55	0.41
1:A:773:THR:HG22	1:A:797:HIS:ND1	2.35	0.41
1:A:831:ASP:OD1	1:A:831:ASP:N	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1019:LYS:HA	1:A:1133:ARG:HH22	1.86	0.41
1:A:138:THR:HA	1:A:141:ILE:HG22	2.03	0.41
1:A:641:HIS:C	1:A:643:SER:N	2.71	0.41
1:A:649:ASP:O	1:A:673:LYS:HB3	2.21	0.41
1:A:651:LEU:HA	1:A:655:GLU:OE1	2.20	0.41
1:A:655:GLU:O	1:A:659:MET:HG2	2.21	0.41
1:A:839:ILE:HG22	1:A:843:ASN:CG	2.45	0.41
1:A:940:THR:HG23	1:A:940:THR:O	2.21	0.41
1:A:229:ILE:H	1:A:229:ILE:CD1	2.28	0.41
1:A:295:PHE:CE1	1:A:1181:LEU:HB2	2.56	0.41
1:A:674:ARG:HD2	1:A:694:ARG:NE	2.36	0.41
1:A:968:ARG:HB2	1:A:968:ARG:NH1	2.36	0.41
1:A:1213:GLN:NE2	1:A:1214:LEU:HD22	2.36	0.41
1:A:682:ILE:O	1:A:692:HIS:HA	2.21	0.41
1:A:883:ASP:O	1:A:884:PRO:C	2.63	0.41
1:A:33:PHE:CE1	1:A:34:ARG:HG3	2.56	0.40
1:A:234:ASP:HA	1:A:239:SER:CB	2.51	0.40
1:A:371:TYR:CE2	1:A:373:GLY:HA2	2.57	0.40
1:A:740:LEU:HD22	1:A:740:LEU:HA	1.72	0.40
1:A:820:PRO:HB2	1:A:822:ASN:OD1	2.21	0.40
1:A:1083:PRO:HA	1:A:1137:TYR:O	2.21	0.40
1:A:610:ILE:O	1:A:613:LEU:HB3	2.20	0.40
1:A:769:MET:SD	1:A:772:ARG:HG2	2.60	0.40
1:A:788:LEU:HD11	1:A:811:TYR:HB3	2.02	0.40
1:A:1093:GLU:OE2	1:A:1093:GLU:N	2.52	0.40
1:A:16:SER:HA	1:A:19:LYS:HG2	2.02	0.40
1:A:30:VAL:HG12	1:A:39:GLU:O	2.22	0.40
1:A:36:SER:O	1:A:38:PRO:HD3	2.21	0.40
1:A:74:ARG:HH21	1:A:79:SER:HG	1.69	0.40
1:A:358:LEU:N	1:A:404:SER:O	2.49	0.40
1:A:409:CYS:SG	1:A:414:GLN:HG3	2.61	0.40
1:A:425:PHE:CD2	1:A:451:ILE:HG21	2.56	0.40
1:A:962:LYS:HD2	1:A:962:LYS:HA	1.85	0.40
1:A:974:LEU:HB3	1:A:1005:CYS:SG	2.61	0.40
1:A:316:ASN:HB3	1:A:321:TYR:CE2	2.56	0.40
1:A:403:LEU:HB2	1:A:453:ILE:HD13	2.03	0.40
1:A:631:LEU:HD12	1:A:632:THR:N	2.36	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1196/1265 (94%)	1130 (94%)	65 (5%)	1 (0%)	48	82

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	636	PRO

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1099/1158 (95%)	1098 (100%)	1 (0%)	88	88

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1242	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	HIS
1	A	131	GLN
1	A	174	ASN
1	A	478	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	489	GLN
1	A	771	GLN
1	A	978	ASN
1	A	1072	HIS
1	A	1243	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.

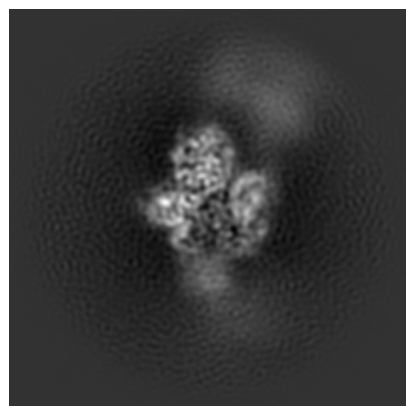
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-36572. These allow visual inspection of the internal detail of the map and identification of artifacts.

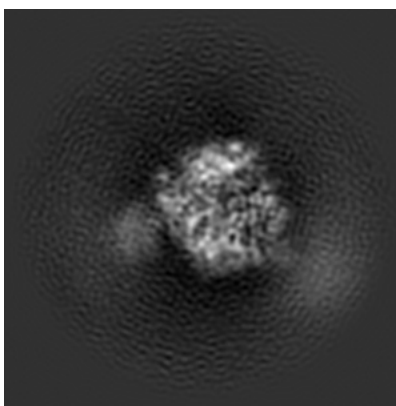
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

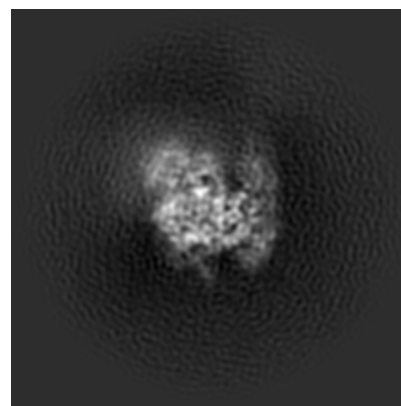
6.1.1 Primary map



X

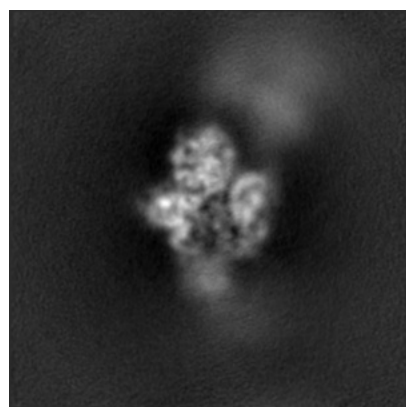


Y

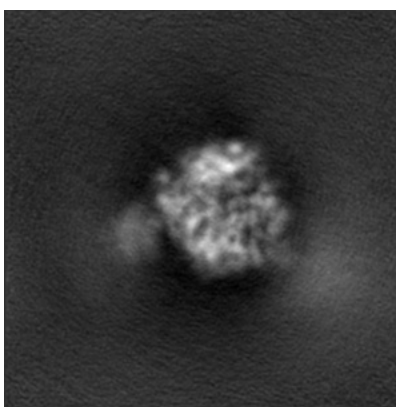


Z

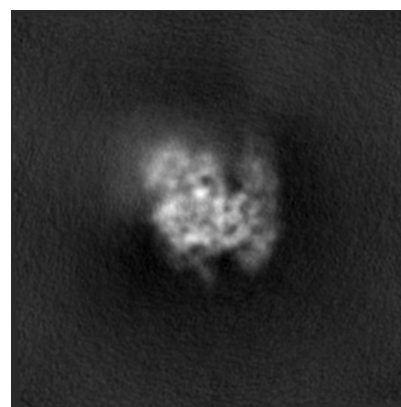
6.1.2 Raw map



X



Y

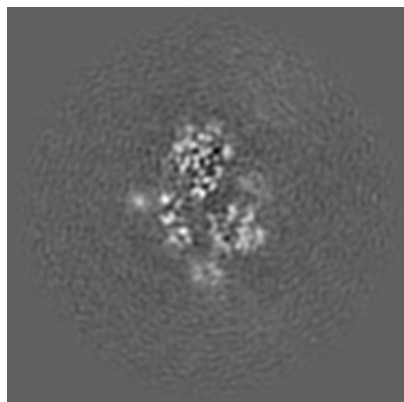


Z

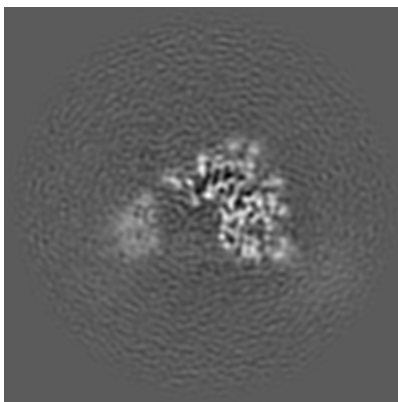
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

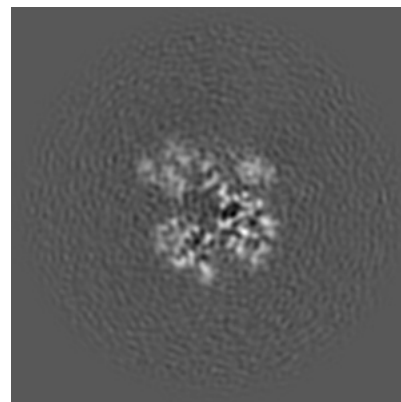
6.2.1 Primary map



X Index: 108

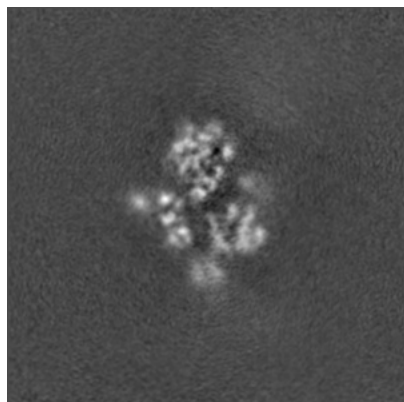


Y Index: 108

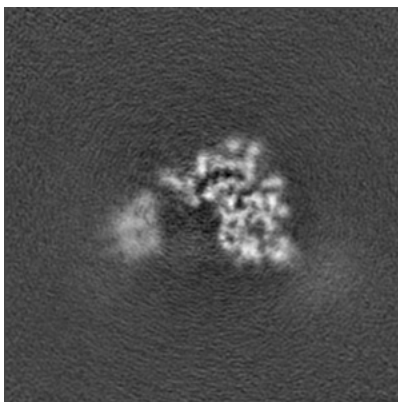


Z Index: 108

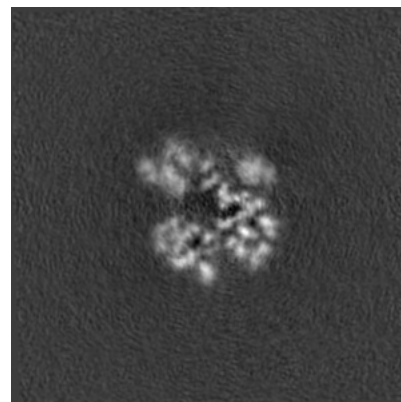
6.2.2 Raw map



X Index: 108



Y Index: 108

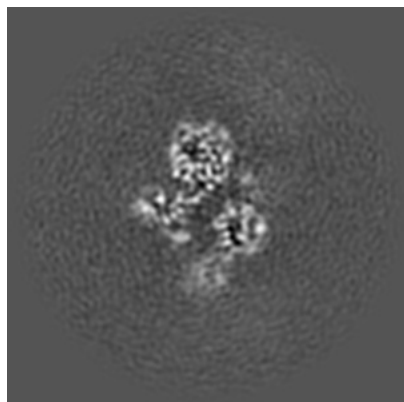


Z Index: 108

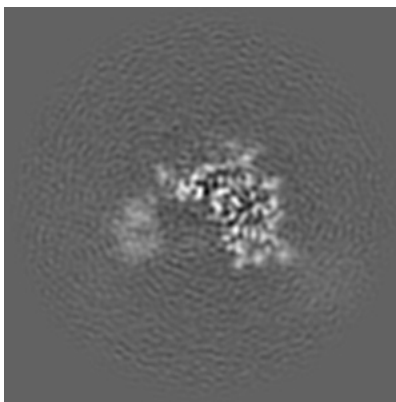
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

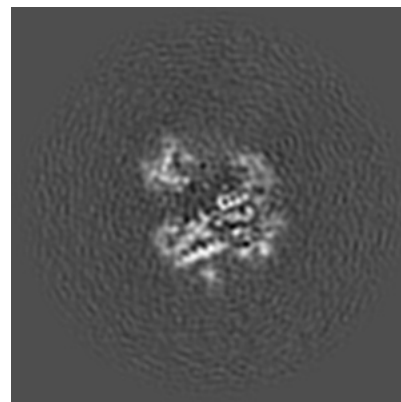
6.3.1 Primary map



X Index: 104

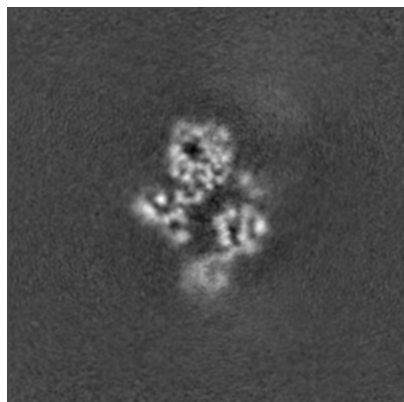


Y Index: 105

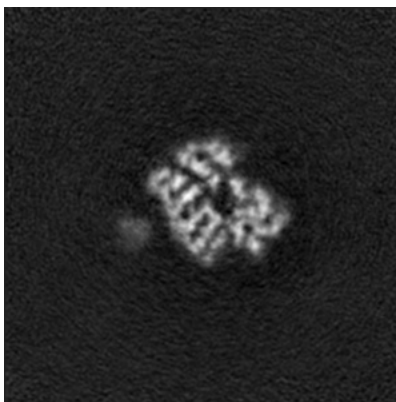


Z Index: 111

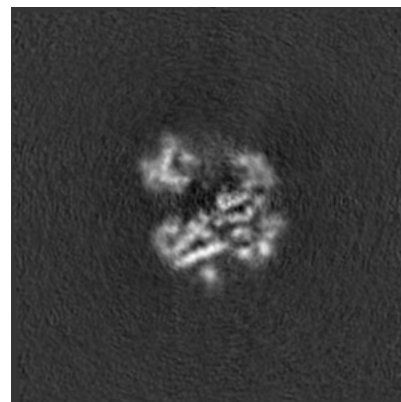
6.3.2 Raw map



X Index: 103



Y Index: 92

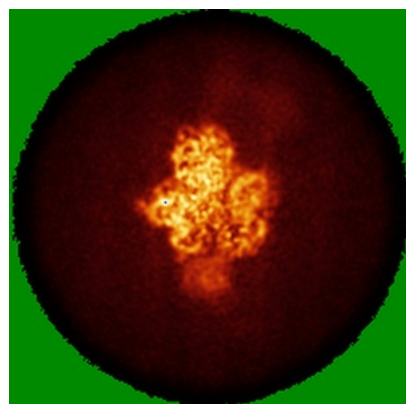


Z Index: 111

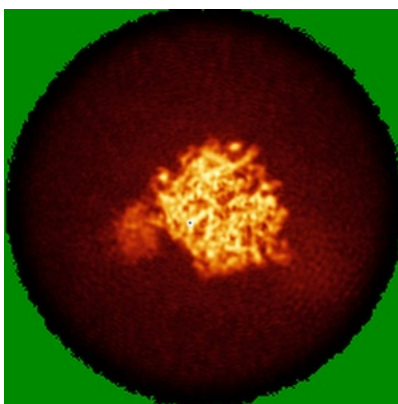
The images above show the largest variance slices of the map in three orthogonal directions.

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

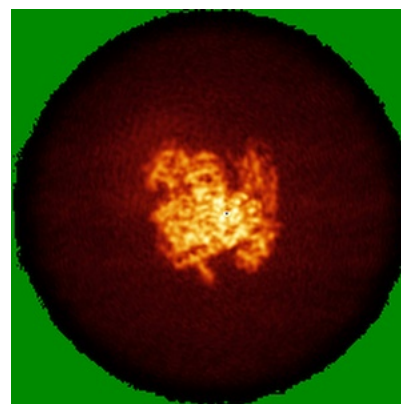
6.4.1 Primary map



X

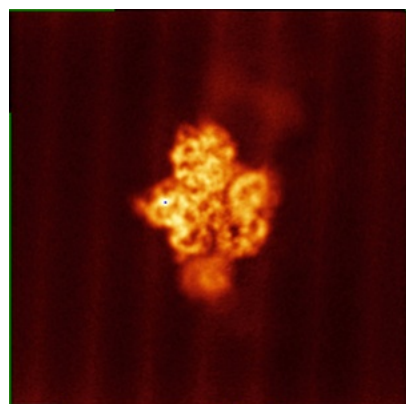


Y

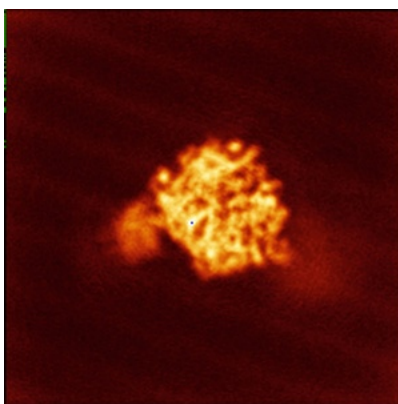


Z

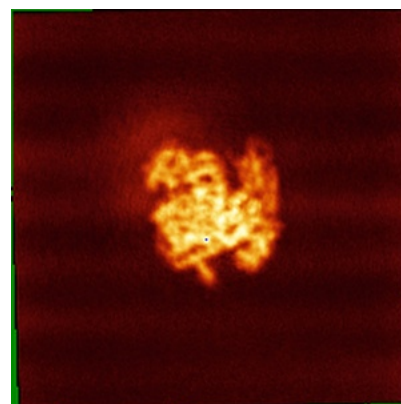
6.4.2 Raw map



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.

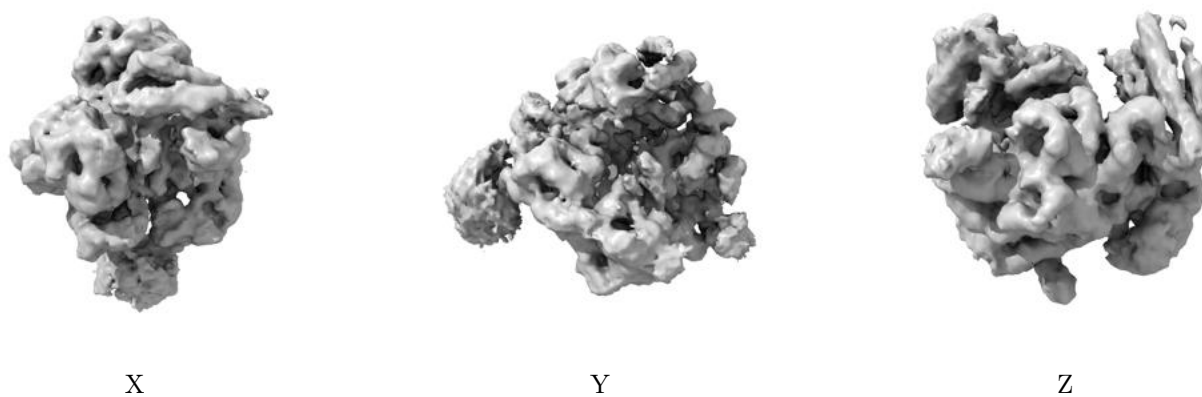
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.3. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

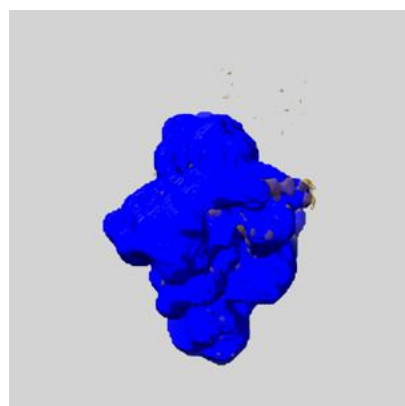
6.6 Mask visualisation [i](#)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

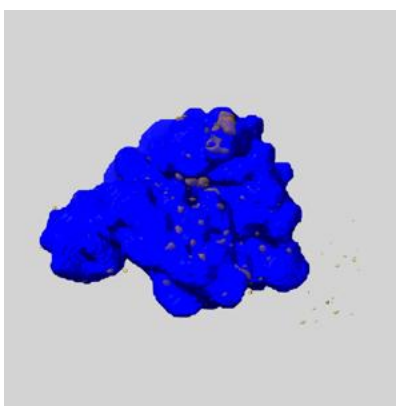
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

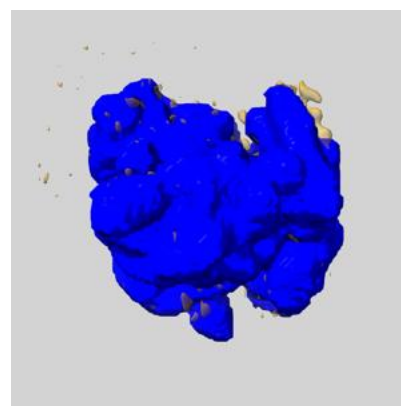
6.6.1 emd_36572_msk_1.map [i](#)



X



Y

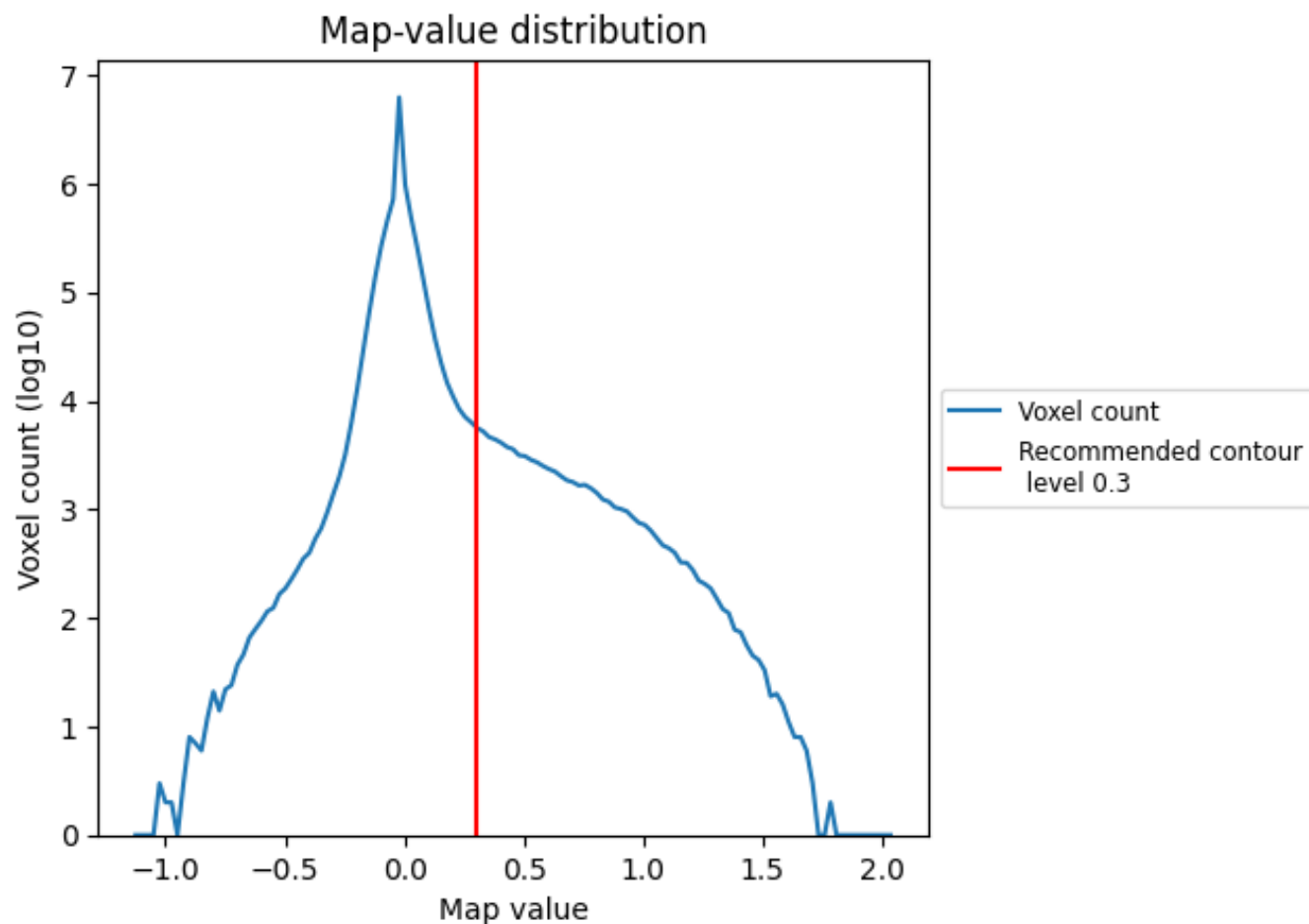


Z

7 Map analysis [i](#)

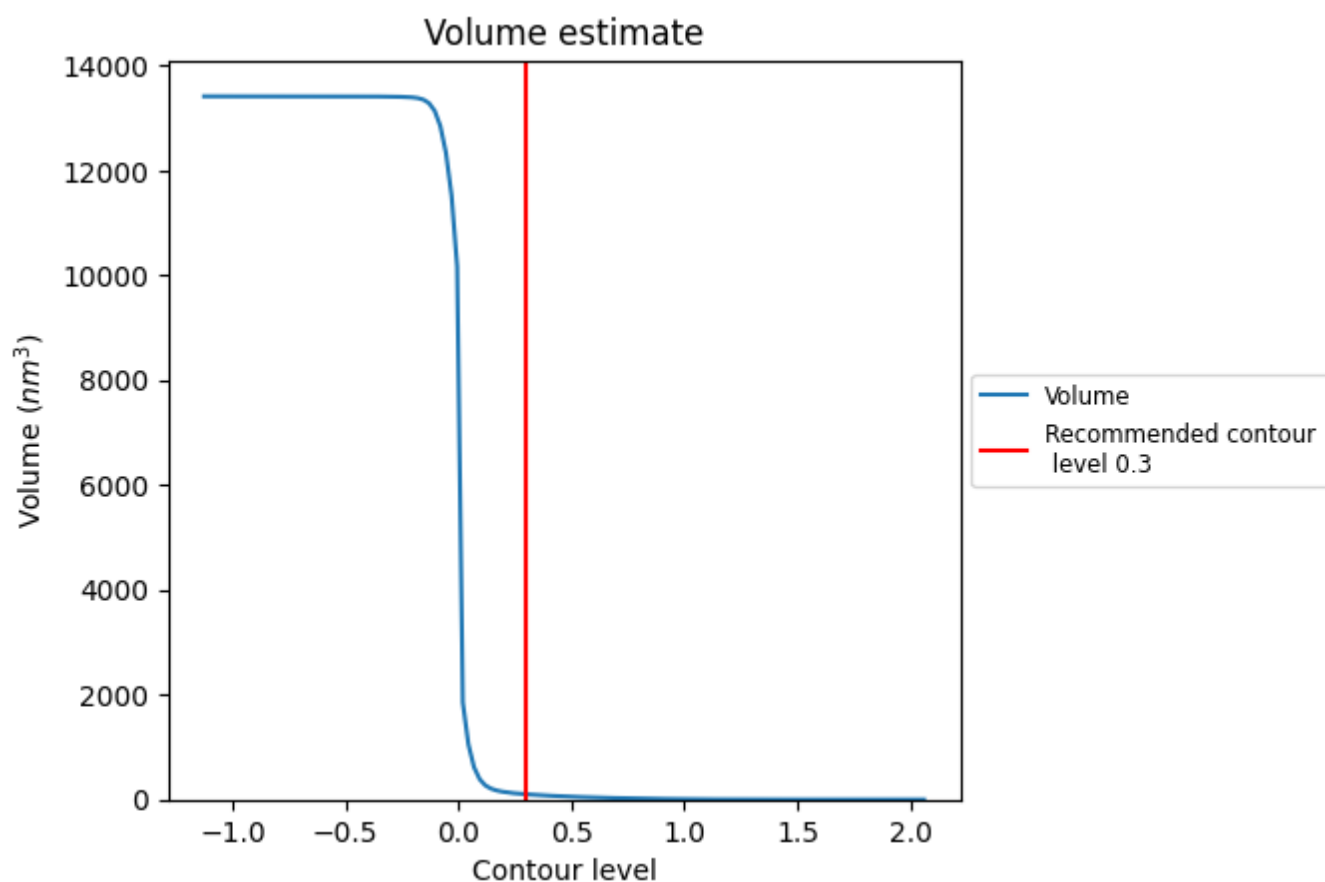
This section contains the results of statistical analysis of the map.

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.

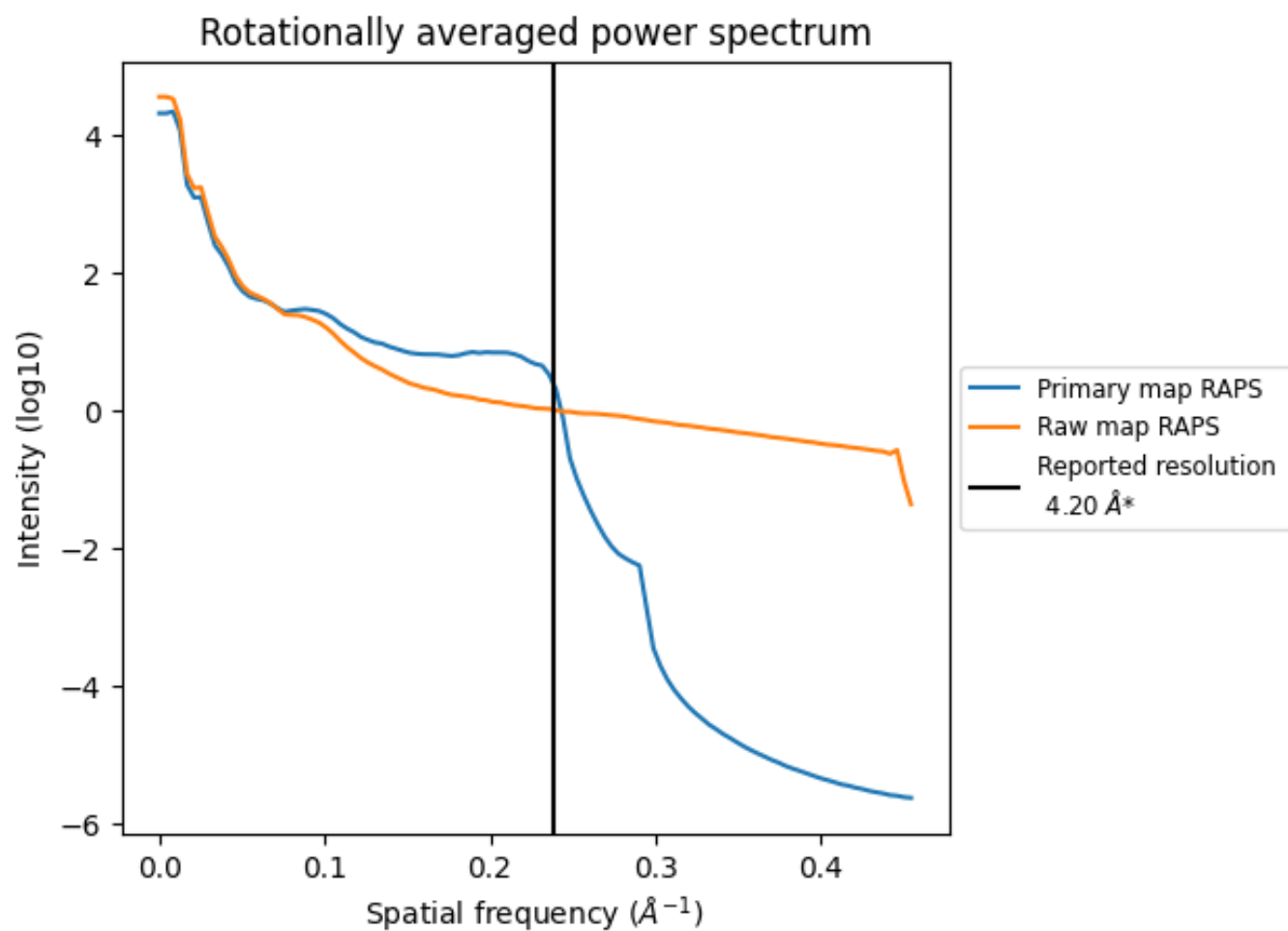
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 101 nm³; this corresponds to an approximate mass of 92 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 ⓘ

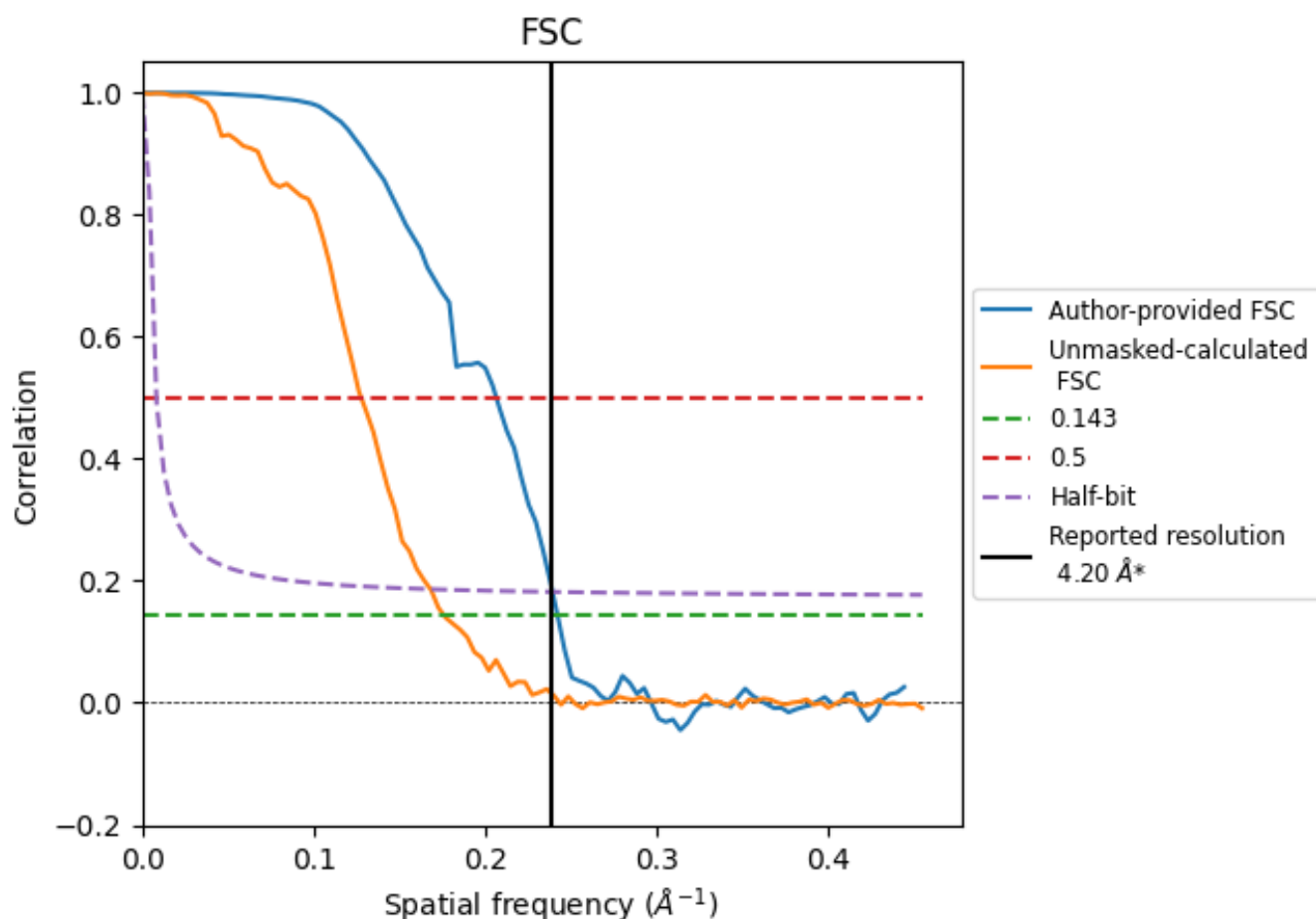


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8 Fourier-Shell correlation [i](#)

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

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.238 $\text{\AA}^{-1}$

8.2 Resolution estimates [i](#)

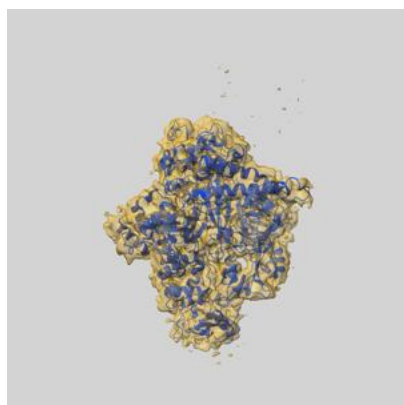
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.13	4.84	4.18
Unmasked-calculated*	5.69	7.84	5.95

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 5.69 differs from the reported value 4.2 by more than 10 %

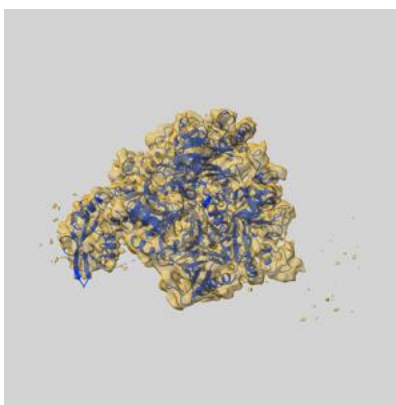
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-36572 and PDB model 8JQH. Per-residue inclusion information can be found in [section 3](#) on [page 4](#).

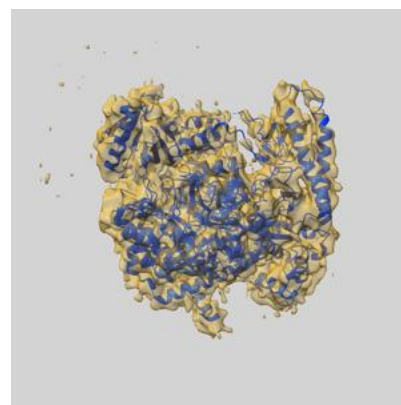
9.1 Map-model overlay [i](#)



X



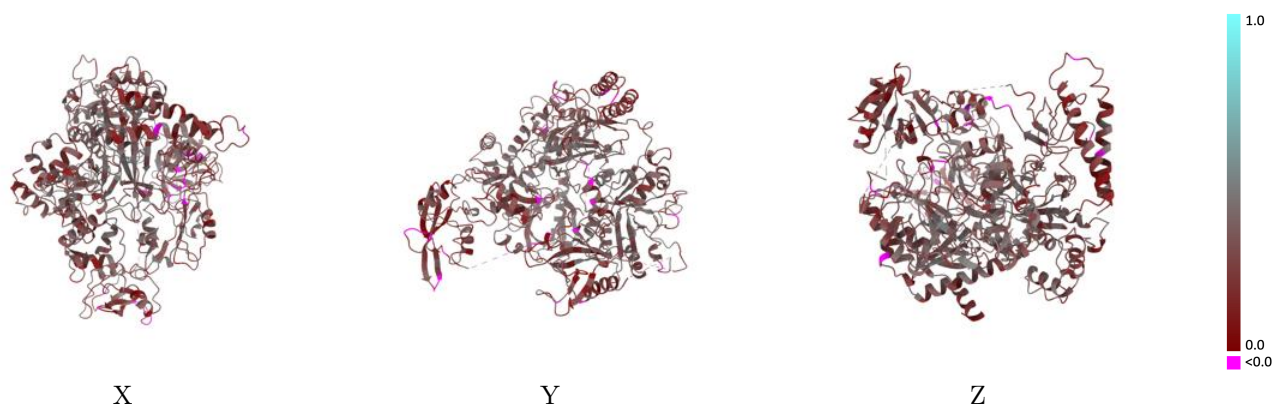
Y



Z

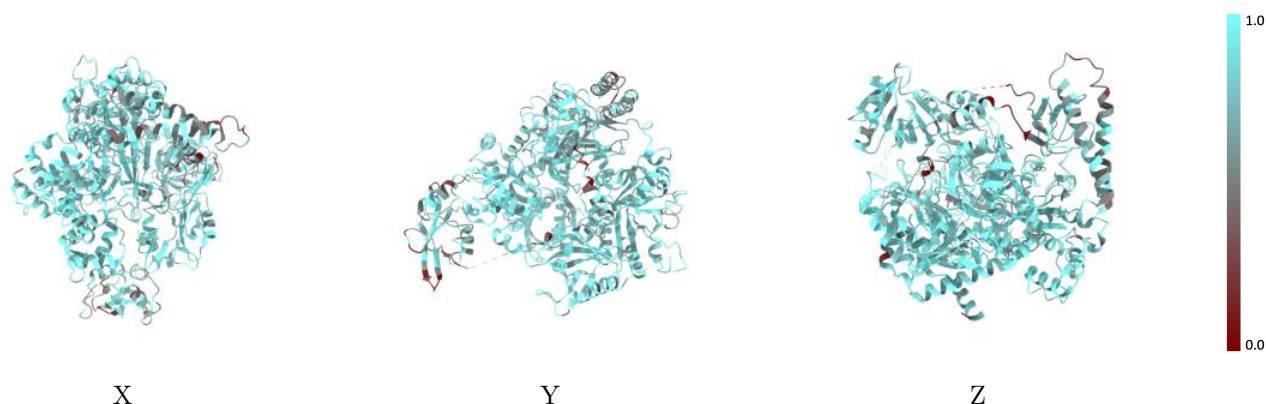
The images above show the 3D surface view of the map at the recommended contour level 0.3 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



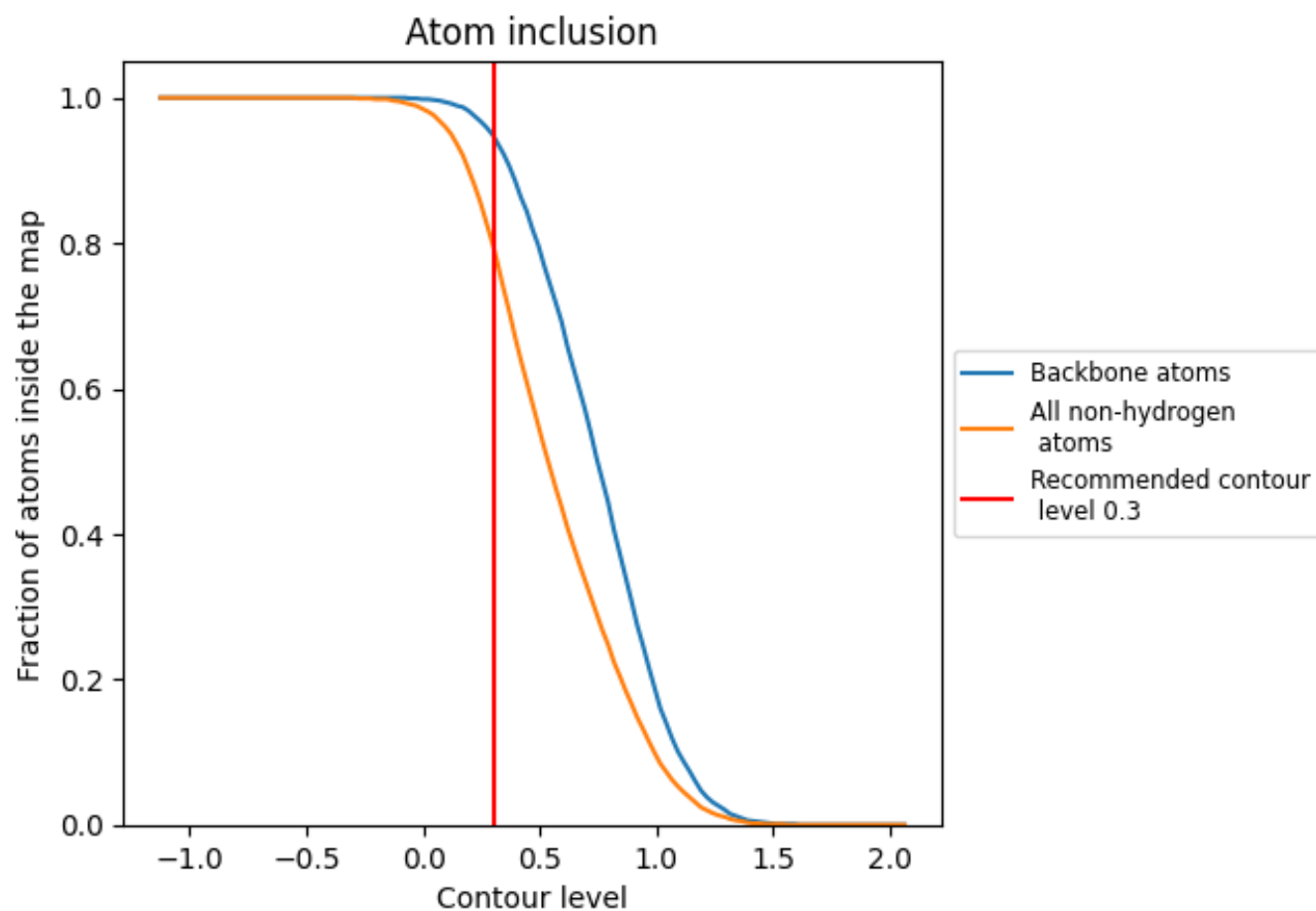
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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



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

9.4 Atom inclusion [i](#)



At the recommended contour level, 95% of all backbone atoms, 80% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7960	0.2980
A	0.7960	0.2980

