



wwPDB EM Validation Summary Report ⓘ

Mar 5, 2026 – 10:04 AM UTC

PDB ID : 6ZTS / pdb_00006zts
EMDB ID : EMD-22165
Title : Assembly intermediates of orthoreovirus captured in the cell
Authors : Sutton, G.C.; Stuart, D.I.
Deposited on : 2020-07-20
Resolution : 6.60 Å(reported)

This is a wwPDB EM Validation Summary 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

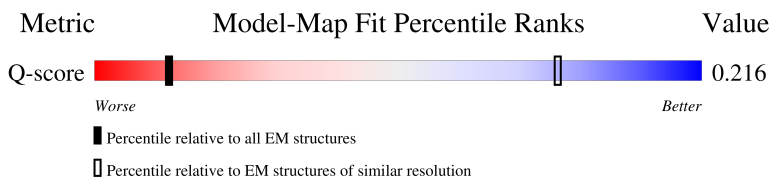
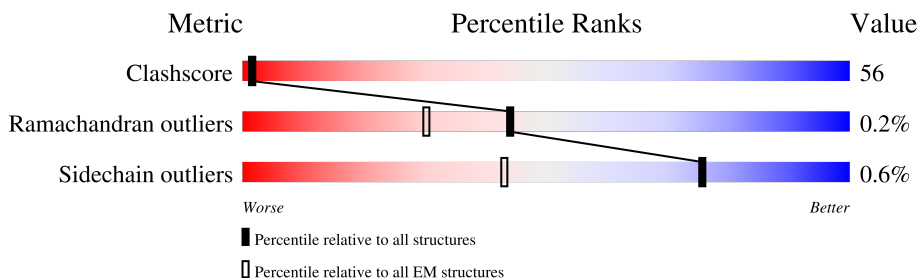
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

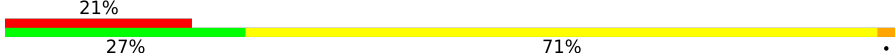
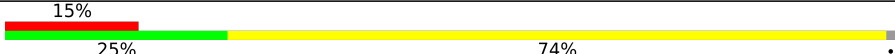
The reported resolution of this entry is 6.60 Å.

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	531 (6.10 - 7.10)

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	975	
1	B	975	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 15341 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 Lambda-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	974	Total	C	N	O	S	0	0
			7696	4911	1304	1432	49		
1	B	967	Total	C	N	O	S	0	0
			7645	4883	1296	1417	49		

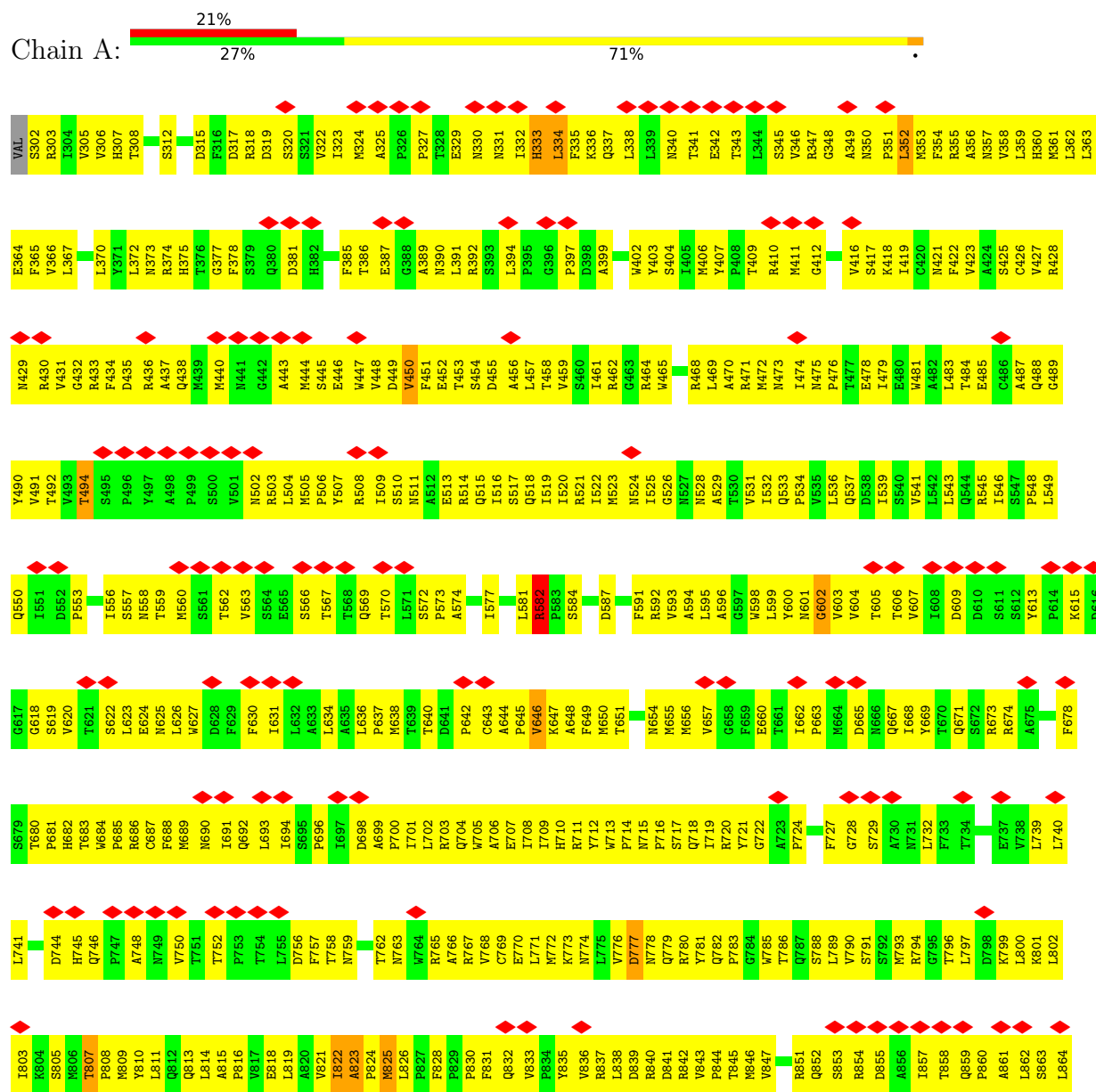
There are 10 discrepancies between the modelled and reference sequences:

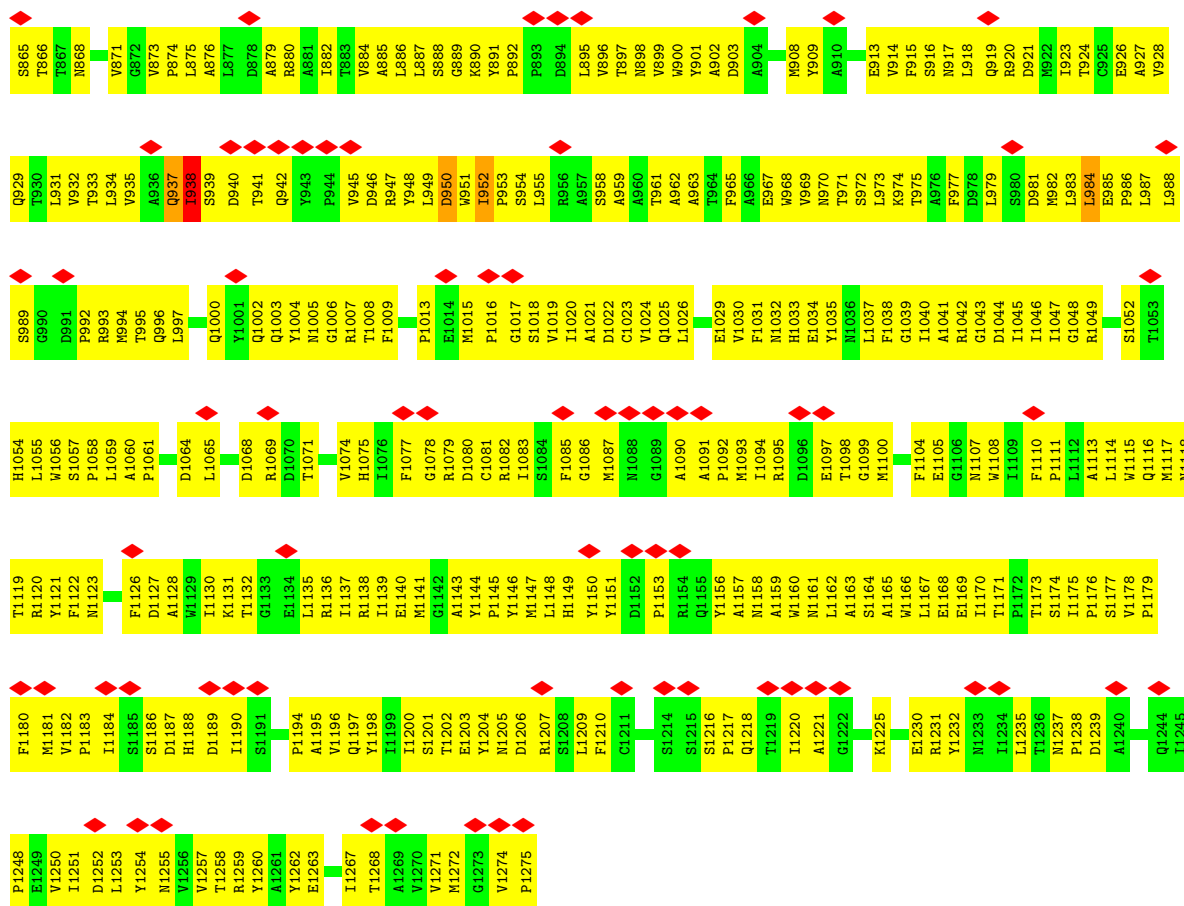
Chain	Residue	Modelled	Actual	Comment	Reference
A	336	LYS	ARG	conflict	UNP A0A023VYS9
A	507	TYR	ARG	conflict	UNP A0A023VYS9
A	973	LEU	MET	conflict	UNP A0A023VYS9
A	1010	ASP	ASN	conflict	UNP A0A023VYS9
A	1163	ALA	THR	conflict	UNP A0A023VYS9
B	336	LYS	ARG	conflict	UNP A0A023VYS9
B	507	TYR	ARG	conflict	UNP A0A023VYS9
B	973	LEU	MET	conflict	UNP A0A023VYS9
B	1010	ASP	ASN	conflict	UNP A0A023VYS9
B	1163	ALA	THR	conflict	UNP A0A023VYS9

3 Residue-property plots

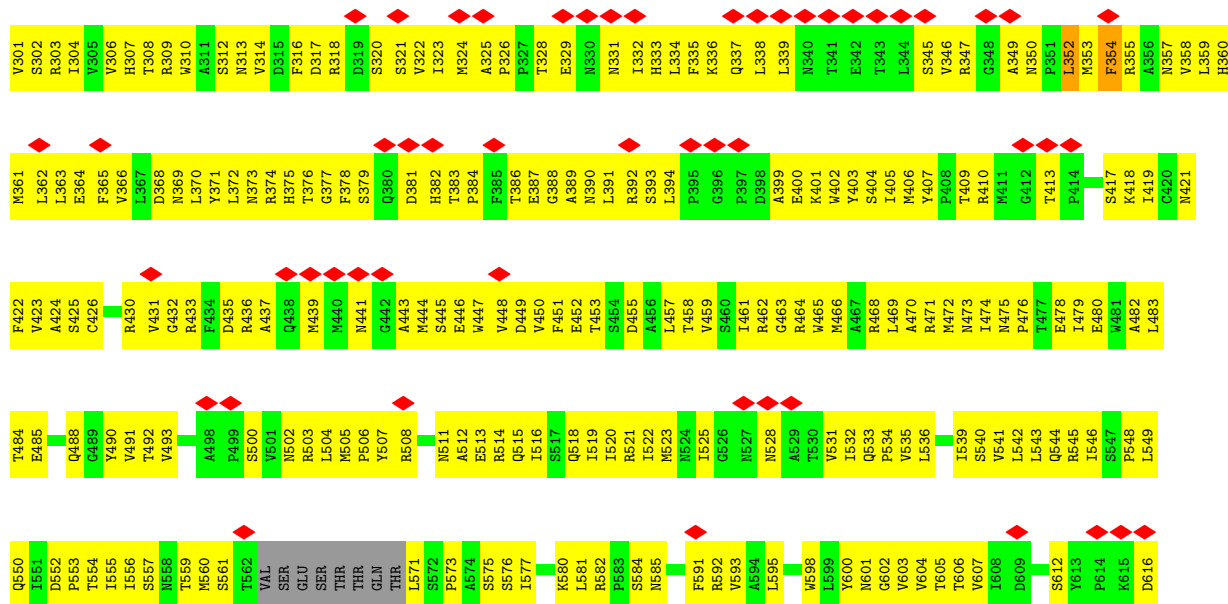
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Lambda-1





• Molecule 1: Lambda-1



Y1254	H1188	D1127	L1065	Y1001	D940	G872	Q812	T751	P885	G817
N1255	D1189	A1128	V1066	Q1002	T941	V873	Q813	T752	R886	G818
V1256	F1067	W1129	F1068	Q1003	Q942	P874	L814	P753	C887	S819
T1258	R1069	K1131	R1069	N1005	Y943	L875	A815	T754	F688	V620
R1269	D1070	T1132	G1066	G1006	P944	L877	V817	T757	M889	T621
A1195	T1071	G1133	R1007	R1007	V945	D878	E818	F758	N690	S622
V1196	P1072	E1134	T1008	T1008	D946	A879	L819	T759	I691	L623
Q1197	P1072	L1135	F1072	F1009	R947	R880	A820	E760	Q692	E824
Y1198	H1075	R1136	H1075	V1011	Y948	A881	V821	E760	L693	N625
I1199	I1076	I1137	I1076	V1011	D1010	T882	I822	L761	I694	L626
I1200	I1077	R1138	I1077	E1014	D949	T883	A823	T762	D628	D628
S1201	G1078	E1139	G1078	M1015	D950	V884	P824	N763	F629	F629
T1202	R1079	E1140	R1079	M1016	W951	A885	M825	W764	F700	F700
E1203	D1080	M1141	D1080	G1017	P952	L886	L825	F655	I701	F630
Y1204	C1081	G1142	C1081	P1016	P953	L887	P827	A766	L702	I631
R1205	R1082	A1143	R1082	S1018	S954	S888	F828	R767	R703	L632
D1206	I1083	Y1144	I1083	V1019	L955	G899	P829	V768	Q704	A833
R1207	S1084	Y1145	S1084	I1020	R956	K890	P830	C769	W705	L634
S1208	F1085	Y1146	F1085	A1021	A957	Y891	F831	E770	A706	A635
L1209	G1086	M1147	G1086	D1022	S958	P892	Q832	L771	E707	L636
F1210	M1087	L1148	M1087	C1023	A959	P893	V833	M772	I708	P637
C1211	N1088	Y1150	N1088	Q1025	A960	D894	P834	K773	I709	M638
T1212	G1089	Y1151	G1089	L1026	T961	L895	Y835	N774	H710	T639
N1213	A1090	D1152	A1090	T1027	A962	V896	V836	L775	R711	T640
S1214	A1091	P1153	A1091	E1029	R963	T897	L838	L776	Y712	M650
S1215	P1092	R1154	P1092	F1030	F965	N898	D839	D777	W713	T951
S1216	M1093	Q1155	M1093	F1031	A966	V899	R840	D778	P714	L652
P1217	I1094	Y1156	I1094	M1032	E967	W900	D841	Q779	N715	A653
Q1218	R1095	A1157	R1095	H1033	W968	A902	R842	R780	M654	N654
T1219	D1096	M1158	D1096	E1034	P969	I905	V843	Y781	M655	M656
A1221	G1099	W1160	G1099	Y1035	N970	Y906	P844	Q782	V657	G658
G1222	M1100	L1162	M1100	M1036	T971	E913	T845	G784	F659	G659
P1223	M1101	W1163	M1101	L1037	L973	V914	N846	W785	E860	E860
D1224	V1102	A1163	V1102	F1038	K974	F915	V847	T786	T661	T661
K1225	P1103	S1164	P1103	G1039	F977	S916	G848	Q787	I662	I662
H1226	E1104	A1165	E1104	I1040	D978	N917	T850	S788	P663	P663
P1228	F1105	L1166	F1105	R1042	L979	Q919	R851	L789	M664	M664
H1228	G1106	L1167	G1106	G1043	S980	R920	Q852	S791	D665	D665
E1230	M1107	E1168	M1107	D1044	D981	D921	R854	S792	N666	N666
R1231	W1108	F1169	W1108	I1045	M982	N922	D955	R794	Q667	Q667
Y1232	F1110	T1170	F1110	I1046	L983	T923	A856	Q795	I668	I668
N1233	P1111	T1171	P1111	I1047	L984	T924	I857	T796	Y669	Y669
I1234	L1112	P1172	L1112	G1048	E965	T924	T858	L797	T670	T670
L1235	A1113	T1175	A1113	R1049	P986	V928	Q859	D798	Q671	Q671
T1236	L1114	P1176	L1114	V1050	L987	Q929	P860	K799	R672	R672
N1237	W1115	S1177	N1237	Q1051	L988	T930	A861	L800	R673	R673
D1238	M1116	V1178	D1238	W1056	S989	L931	L862	L740	R674	R674
D1239	M1117	F1179	D1239	S1057	G990	V932	S863	L741	A675	A675
A1240	M1118	F1180	A1240	P1058	D991	T933	S863	L742	A677	A677
L1247	T1119	M1181	L1247	L1059	P992	L934	L864	I743	F678	F678
P1248	R1120	V1182	P1248	A1060	R993	V935	S865	D744	S679	S679
E1249	Y1121	F1183	E1249	M994	M994	A936	T866	Q745	T680	T680
V1250	Y1122	Y1184	V1250	P1061	T995	Q937	T867	H745	P681	P681
I1251	P1062	I1185	I1251	P1063	Q996	I938	N868	Q746	H682	H682
D1252	M1123	Q1124	D1252	D1064	L997	S939	T869	Y750	T683	T683
L1253	Q1125	F1126	L1253		I999		W871		W684	W684

4 Experimental information

Property	Value	Source
EM reconstruction method	TOMOGRAPHY	Depositor
Imposed symmetry	POINT, Not provided	
Number of tilted images used	41	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	2	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum voxel value	10.927	Depositor
Minimum voxel value	-5.906	Depositor
Average voxel value	0.059	Depositor
Voxel value standard deviation	0.498	Depositor
Recommended contour level	3	Depositor
Tomogram size ($\text{\AA}$)	696.6, 696.6, 696.6	wwPDB
Tomogram dimensions	387, 387, 387	wwPDB
Tomogram angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Grid spacing ($\text{\AA}$)	1.8, 1.8, 1.8	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	0.37	0/7902	0.71	8/10819 (0.1%)
1	B	0.37	0/7850	0.64	0/10746
All	All	0.37	0/15752	0.68	8/21565 (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	7
1	B	0	1
All	All	0	8

There are no bond length outliers.

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	825	MET	CA-C-N	10.45	147.29	121.80
1	A	825	MET	C-N-CA	10.45	147.29	121.80
1	A	306	VAL	N-CA-C	-8.11	105.58	113.53
1	A	602	GLY	N-CA-C	-6.63	105.32	115.66
1	A	950	ASP	N-CA-C	-6.15	105.48	114.39

There are no chirality outliers.

5 of 8 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	334	LEU	Peptide
1	A	352	LEU	Peptide
1	A	582	ARG	Peptide
1	A	822	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	A	823	ALA	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7696	0	7605	857	0
1	B	7645	0	7559	860	0
All	All	15341	0	15164	1711	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 56.

The worst 5 of 1711 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:446:GLU:HA	1:B:1261:ALA:H	1.24	1.02
1:B:511:ASN:HA	1:B:514:ARG:HH21	1.25	1.00
1:A:847:VAL:H	1:A:871:VAL:HG11	1.23	0.98
1:A:929:GLN:HB2	1:A:1015:MET:HG2	1.43	0.97
1:A:449:ASP:HA	1:A:1257:VAL:O	1.67	0.95

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	972/975 (100%)	783 (81%)	187 (19%)	2 (0%)	43	78
1	B	963/975 (99%)	806 (84%)	156 (16%)	1 (0%)	48	83
All	All	1935/1950 (99%)	1589 (82%)	343 (18%)	3 (0%)	44	78

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1111	PRO
1	A	1161	ASN
1	A	582	ARG

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	861/862 (100%)	854 (99%)	7 (1%)	73	80
1	B	854/862 (99%)	850 (100%)	4 (0%)	81	83
All	All	1715/1724 (100%)	1704 (99%)	11 (1%)	76	83

5 of 11 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	352	LEU
1	B	354	PHE
1	B	1227	ILE
1	B	1212	THR
1	A	777	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 44 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	710	HIS
1	B	942	GLN
1	B	715	ASN

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Mol	Chain	Res	Type
1	B	852	GLN
1	B	1051	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.

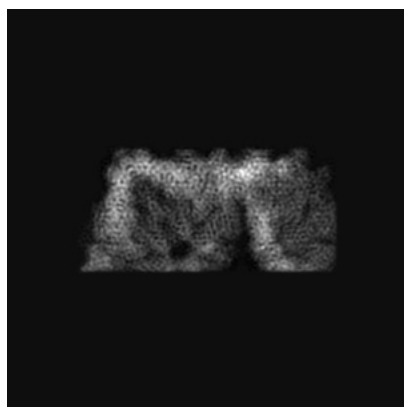
5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

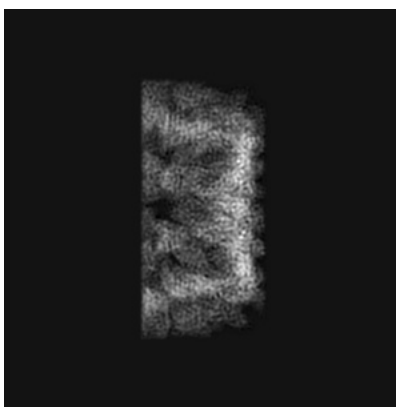
6 Tomogram visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-22165. These allow visual inspection of the internal detail of the tomogram and identification of artifacts.

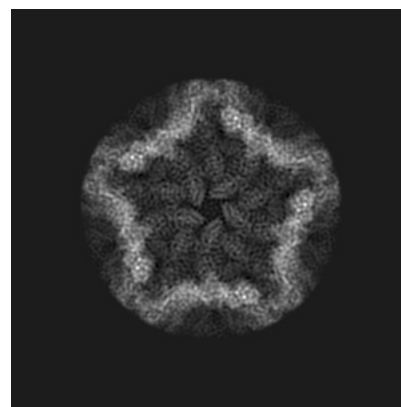
6.1 Orthogonal projections [i](#)



X



Y



Z

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

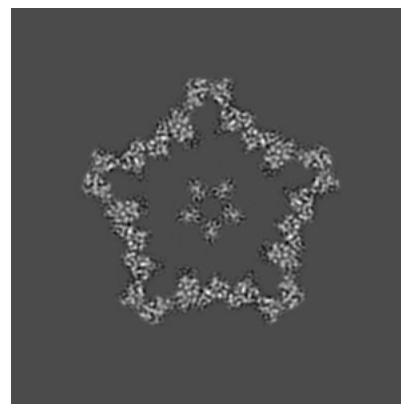
6.2 Central slices [i](#)



X Index: 193



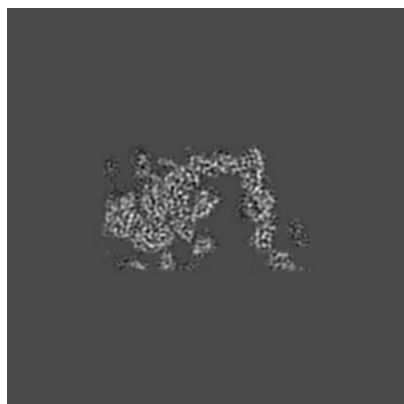
Y Index: 193



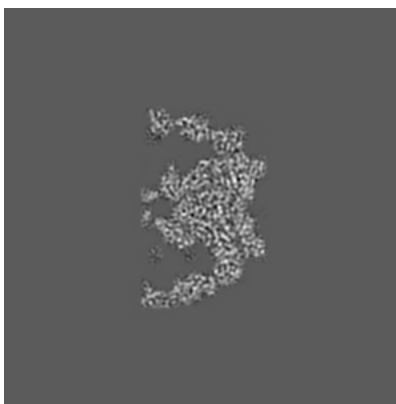
Z Index: 193

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

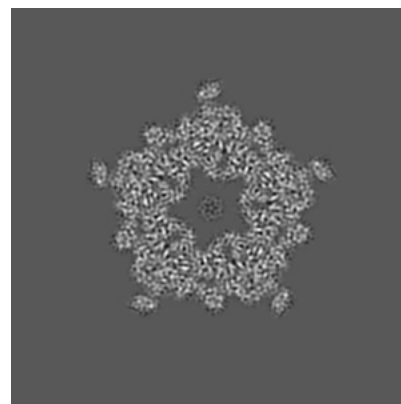
6.3 Largest variance slices [i](#)



X Index: 117



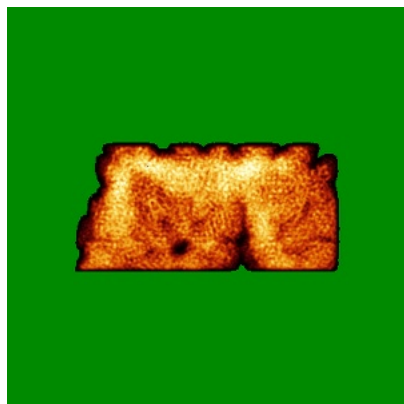
Y Index: 112



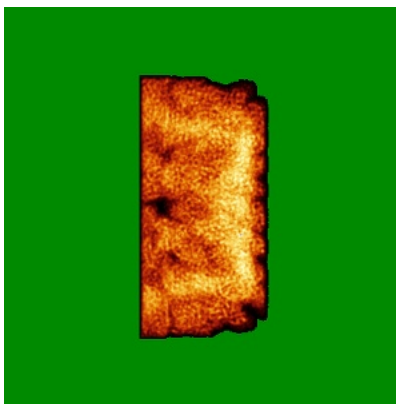
Z Index: 230

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

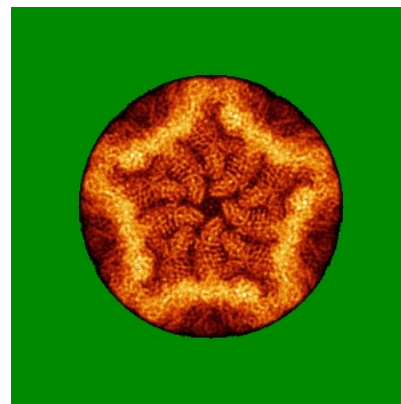
6.4 Orthogonal standard-deviation projections (False-color) [i](#)



X



Y



Z

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

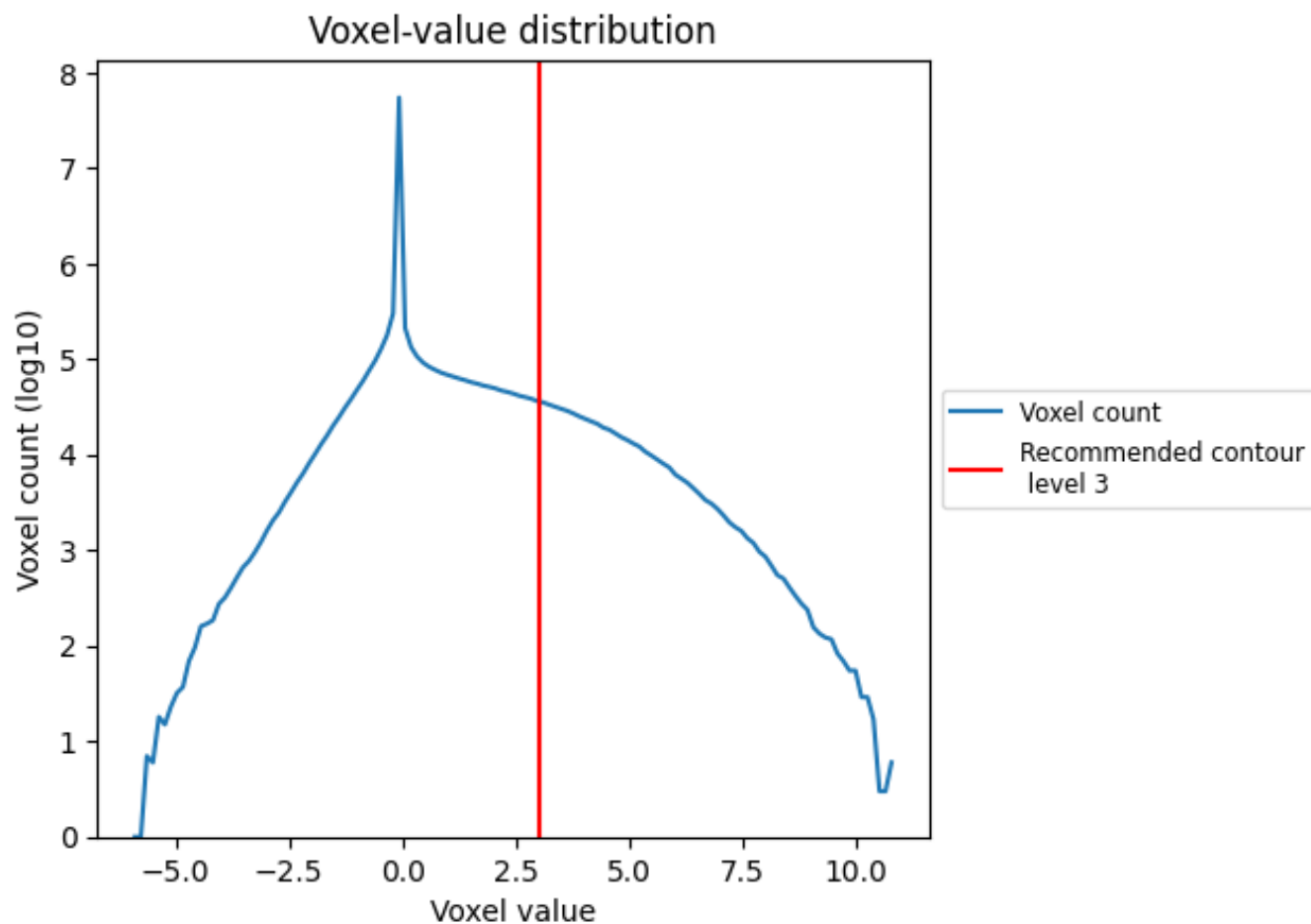
6.5 Mask visualisation [i](#)

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

7 Tomogram analysis [i](#)

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

7.1 Voxel-value distribution [i](#)



The voxel-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic.

8 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-22165 and PDB model 6ZTS. Per-residue inclusion information can be found in section 3 on page 4.

8.1 Map-model overlay [i](#)

This section was not generated.

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

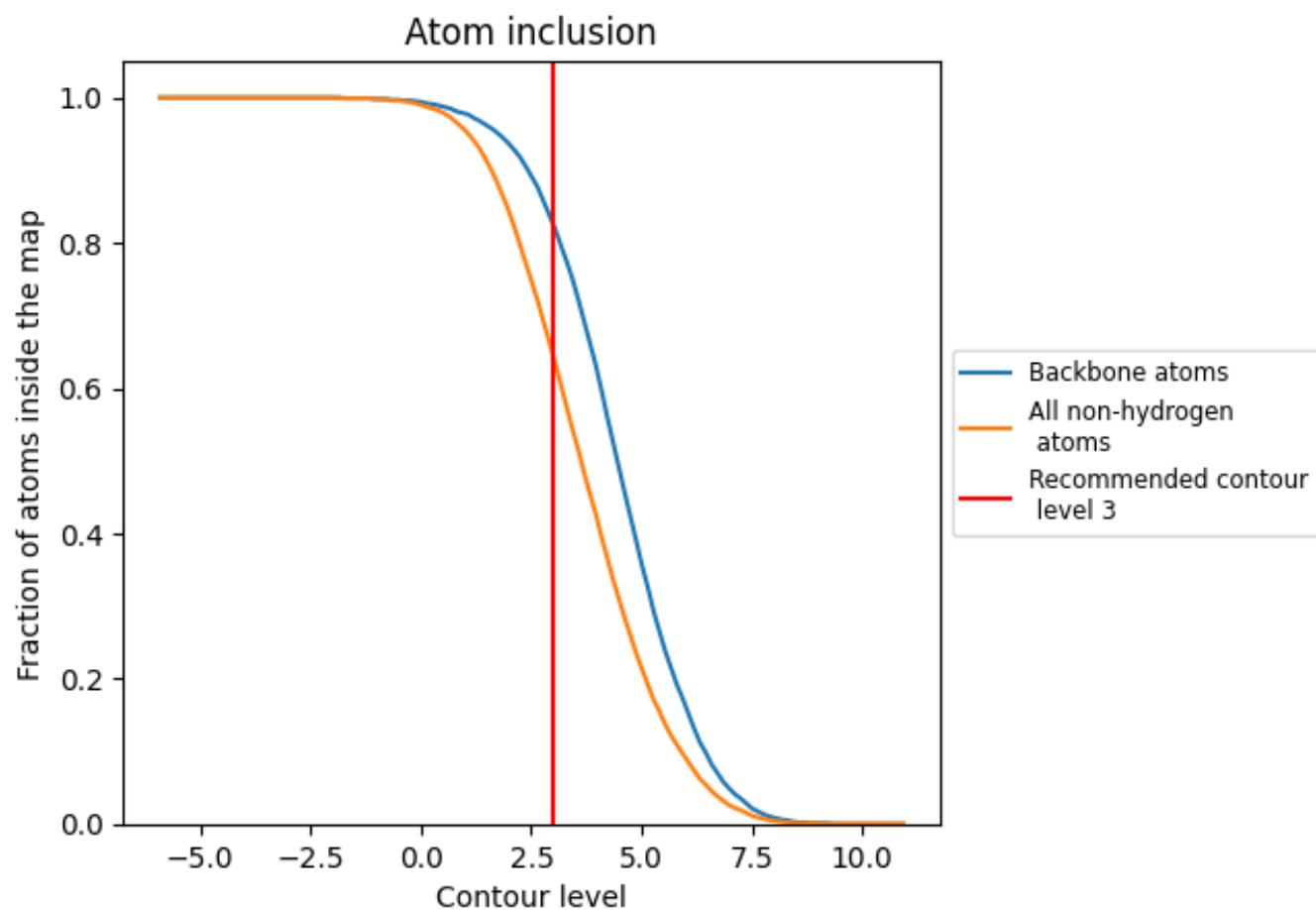


The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions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

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

This section was not generated.

8.4 Atom inclusion [i](#)



At the recommended contour level, 83% of all backbone atoms, 64% of all non-hydrogen atoms, are inside the map.

8.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (3) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6450	0.2160
A	0.6350	0.2110
B	0.6550	0.2220

