



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 02:12 am GMT

PDB ID : 4BM5
Title : Chloroplast inner membrane protein TIC110
Authors : Tsai, J.-Y.; Chu, C.-C.; Yeh, Y.-H.; Chen, L.-J.; Li, H.-m.; Hsiao, C.-D.
Deposited on : 2013-05-06
Resolution : 4.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

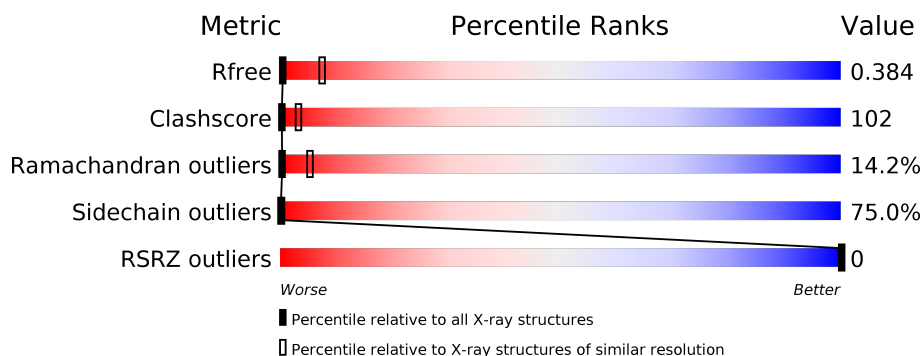
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1177 (4.80-3.60)
Clashscore	112137	1025 (4.72-3.66)
Ramachandran outliers	110173	1024 (4.76-3.62)
Sidechain outliers	110143	1008 (4.76-3.62)
RSRZ outliers	101464	1188 (4.80-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	348	

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 1350 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 SIMILAR TO CHLOROPLAST INNER MEMBRANE PROTEIN TIC110.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	268	Total	C	N	O	S	0	0	0
			1350	806	268	268	8			

4 Data and refinement statistics

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	121.10Å 121.10Å 242.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.37 – 4.20 27.37 – 4.20	Depositor EDS
% Data completeness (in resolution range)	81.8 (27.37-4.20) 94.0 (27.37-4.20)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.89 (at 4.25Å)	Xtriage
Refinement program	CNS 1.3	Depositor
R, R_{free}	0.350 , 0.366 0.360 , 0.384	Depositor DCC
R_{free} test set	811 reflections (10.59%)	DCC
Wilson B-factor (Å ²)	153.7	Xtriage
Anisotropy	0.057	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 2077.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.85	EDS
Total number of atoms	1350	wwPDB-VP
Average B, all atoms (Å ²)	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.54	0/1343	1.07	9/1855 (0.5%)

There are no bond length outliers.

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1143	ARG	N-CA-C	6.58	128.75	111.00
1	A	1005	GLU	N-CA-C	-6.57	93.26	111.00
1	A	1144	GLN	N-CA-C	6.34	128.12	111.00
1	A	1002	ARG	N-CA-C	-6.22	94.20	111.00
1	A	917	MET	N-CA-C	-5.78	95.40	111.00
1	A	904	ASN	N-CA-C	-5.66	95.71	111.00
1	A	910	ILE	N-CA-C	-5.54	96.05	111.00
1	A	1004	GLU	N-CA-C	5.43	125.67	111.00
1	A	1213	LEU	N-CA-C	-5.25	96.82	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1350	0	682	208	0
All	All	1350	0	682	208	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 102.

All (208) 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:949:PHE:O	1:A:1017:MET:HG3	1.63	0.99
1:A:937:LEU:O	1:A:940:MET:HB2	1.74	0.88
1:A:1154:LEU:O	1:A:1157:ALA:HB3	1.73	0.88
1:A:1025:CYS:O	1:A:1027:THR:N	2.11	0.84
1:A:1025:CYS:C	1:A:1027:THR:H	1.80	0.84
1:A:1190:LEU:HA	1:A:1193:ALA:HB3	1.59	0.83
1:A:1004:GLU:CB	1:A:1006:LYS:H	1.96	0.79
1:A:1211:GLU:O	1:A:1215:ILE:N	2.17	0.78
1:A:1141:SER:CB	1:A:1148:GLU:HA	2.15	0.77
1:A:903:SER:O	1:A:907:ASP:N	2.18	0.76
1:A:1011:LEU:O	1:A:1014:ILE:N	2.19	0.76
1:A:1029:LEU:O	1:A:1033:LYS:N	2.13	0.75
1:A:1061:VAL:C	1:A:1063:ARG:H	1.89	0.75
1:A:1185:TYR:O	1:A:1189:ALA:N	2.16	0.74
1:A:994:ALA:O	1:A:997:ALA:HB3	1.87	0.74
1:A:1058:PHE:O	1:A:1062:CYS:N	2.21	0.74
1:A:996:GLN:O	1:A:999:THR:CB	2.36	0.74
1:A:1194:ARG:O	1:A:1196:ASN:N	2.20	0.73
1:A:962:ASN:O	1:A:965:ALA:HB3	1.91	0.71
1:A:961:PHE:HA	1:A:964:LEU:CB	2.21	0.70
1:A:993:TYR:O	1:A:995:SER:N	2.24	0.70
1:A:1135:ILE:O	1:A:1138:ALA:N	2.25	0.69
1:A:1054:ALA:O	1:A:1057:GLU:N	2.28	0.66
1:A:1054:ALA:HA	1:A:1057:GLU:CB	2.25	0.66
1:A:1212:MET:O	1:A:1216:GLN:N	2.18	0.64
1:A:1007:ASP:O	1:A:1008:ILE:C	2.37	0.64
1:A:1025:CYS:C	1:A:1027:THR:N	2.46	0.64
1:A:910:ILE:O	1:A:913:GLY:N	2.30	0.64
1:A:927:ASN:O	1:A:929:ARG:N	2.31	0.64
1:A:958:GLU:O	1:A:962:ASN:CB	2.46	0.63
1:A:1029:LEU:O	1:A:1030:GLN:C	2.37	0.63
1:A:948:SER:C	1:A:950:ALA:H	2.03	0.62
1:A:906:ILE:HA	1:A:909:TYR:CB	2.28	0.62
1:A:965:ALA:C	1:A:967:LEU:H	2.04	0.61
1:A:1051:MET:O	1:A:1053:GLU:N	2.33	0.61
1:A:989:ILE:C	1:A:991:LYS:N	2.53	0.60
1:A:1011:LEU:O	1:A:1012:ARG:C	2.39	0.60
1:A:927:ASN:O	1:A:928:LEU:C	2.40	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:903:SER:C	1:A:905:LEU:N	2.50	0.60
1:A:917:MET:O	1:A:918:GLU:O	2.19	0.60
1:A:982:HIS:C	1:A:984:ASN:H	2.03	0.60
1:A:1054:ALA:C	1:A:1056:ALA:N	2.54	0.60
1:A:995:SER:C	1:A:997:ALA:N	2.55	0.60
1:A:1061:VAL:O	1:A:1063:ARG:N	2.34	0.59
1:A:1032:THR:O	1:A:1035:ALA:HB3	2.03	0.59
1:A:1084:PHE:O	1:A:1088:ILE:N	2.36	0.59
1:A:911:ARG:O	1:A:915:LEU:N	2.29	0.58
1:A:991:LYS:O	1:A:995:SER:N	2.32	0.58
1:A:993:TYR:C	1:A:995:SER:N	2.55	0.58
1:A:965:ALA:O	1:A:967:LEU:N	2.36	0.58
1:A:991:LYS:O	1:A:993:TYR:N	2.36	0.58
1:A:1137:GLN:CB	1:A:1151:ALA:HB1	2.34	0.58
1:A:953:SER:O	1:A:955:THR:N	2.37	0.57
1:A:1042:ASP:C	1:A:1044:ILE:H	2.08	0.57
1:A:970:ILE:O	1:A:971:LEU:C	2.42	0.57
1:A:1003:LEU:O	1:A:1007:ASP:CB	2.52	0.57
1:A:1108:SER:O	1:A:1112:LEU:N	2.38	0.57
1:A:989:ILE:C	1:A:991:LYS:H	2.08	0.56
1:A:917:MET:O	1:A:921:GLN:CB	2.53	0.56
1:A:991:LYS:O	1:A:992:THR:C	2.42	0.56
1:A:935:ASN:O	1:A:938:GLN:N	2.38	0.56
1:A:995:SER:C	1:A:997:ALA:H	2.08	0.56
1:A:1023:ALA:O	1:A:1024:THR:C	2.44	0.56
1:A:1025:CYS:HA	1:A:1028:LEU:CB	2.35	0.56
1:A:965:ALA:C	1:A:967:LEU:N	2.59	0.56
1:A:1051:MET:HE1	1:A:1052:ALA:HB2	1.87	0.56
1:A:997:ALA:C	1:A:999:THR:H	2.08	0.56
1:A:1061:VAL:C	1:A:1063:ARG:N	2.57	0.56
1:A:1021:ASP:O	1:A:1023:ALA:N	2.39	0.55
1:A:917:MET:O	1:A:921:GLN:N	2.36	0.55
1:A:986:GLY:O	1:A:987:SER:C	2.44	0.55
1:A:1027:THR:O	1:A:1028:LEU:C	2.45	0.55
1:A:1027:THR:HA	1:A:1030:GLN:CB	2.37	0.55
1:A:966:HIS:HA	1:A:969:ASN:CB	2.37	0.55
1:A:1051:MET:CE	1:A:1052:ALA:H	2.20	0.54
1:A:923:VAL:O	1:A:926:VAL:N	2.40	0.54
1:A:967:LEU:O	1:A:970:ILE:N	2.40	0.54
1:A:1183:LEU:C	1:A:1185:TYR:H	2.10	0.54
1:A:958:GLU:O	1:A:962:ASN:N	2.36	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:935:ASN:O	1:A:936:ILE:C	2.46	0.53
1:A:1029:LEU:O	1:A:1031:GLU:N	2.40	0.53
1:A:1039:PHE:O	1:A:1041:PHE:N	2.41	0.53
1:A:1158:LEU:O	1:A:1159:ARG:CB	2.55	0.53
1:A:948:SER:C	1:A:950:ALA:N	2.62	0.53
1:A:1051:MET:CG	1:A:1052:ALA:N	2.72	0.53
1:A:1036:ARG:O	1:A:1038:GLY:N	2.42	0.53
1:A:923:VAL:O	1:A:924:TYR:C	2.47	0.53
1:A:1034:GLU:O	1:A:1037:ALA:N	2.43	0.52
1:A:1029:LEU:C	1:A:1031:GLU:N	2.63	0.52
1:A:1109:GLN:HA	1:A:1112:LEU:CB	2.39	0.52
1:A:1155:SER:C	1:A:1157:ALA:H	2.12	0.52
1:A:1209:LEU:C	1:A:1211:GLU:H	2.13	0.52
1:A:917:MET:CG	1:A:918:GLU:H	2.23	0.52
1:A:1152:ARG:O	1:A:1156:ARG:N	2.35	0.52
1:A:993:TYR:C	1:A:995:SER:H	2.13	0.52
1:A:1065:LEU:C	1:A:1067:VAL:H	2.14	0.51
1:A:1217:ALA:O	1:A:1218:ALA:HB3	2.09	0.51
1:A:903:SER:N	1:A:906:ILE:CB	2.73	0.51
1:A:1141:SER:CB	1:A:1151:ALA:HB3	2.40	0.51
1:A:916:GLU:O	1:A:920:GLU:CB	2.58	0.51
1:A:1061:VAL:O	1:A:1064:GLU:N	2.44	0.51
1:A:967:LEU:C	1:A:969:ASN:N	2.62	0.50
1:A:927:ASN:C	1:A:929:ARG:N	2.63	0.50
1:A:1037:ALA:O	1:A:1041:PHE:CB	2.60	0.50
1:A:1113:GLY:O	1:A:1116:ALA:HB3	2.12	0.50
1:A:963:ASN:C	1:A:965:ALA:N	2.62	0.49
1:A:1190:LEU:O	1:A:1191:GLY:C	2.49	0.49
1:A:971:LEU:O	1:A:972:GLY:C	2.50	0.49
1:A:1051:MET:CE	1:A:1052:ALA:HB2	2.42	0.49
1:A:903:SER:O	1:A:907:ASP:CB	2.61	0.49
1:A:910:ILE:C	1:A:912:ASN:N	2.65	0.49
1:A:993:TYR:O	1:A:994:ALA:C	2.49	0.49
1:A:1012:ARG:O	1:A:1013:ASN:C	2.52	0.49
1:A:941:TYR:O	1:A:942:ARG:C	2.52	0.49
1:A:1058:PHE:C	1:A:1060:ARG:N	2.66	0.49
1:A:903:SER:N	1:A:906:ILE:H	2.11	0.48
1:A:986:GLY:O	1:A:988:VAL:N	2.45	0.48
1:A:903:SER:C	1:A:905:LEU:H	2.14	0.48
1:A:921:GLN:O	1:A:922:ALA:C	2.51	0.48
1:A:1011:LEU:O	1:A:1014:ILE:CB	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:908:PHE:O	1:A:911:ARG:CB	2.62	0.48
1:A:910:ILE:C	1:A:913:GLY:H	2.16	0.48
1:A:987:SER:HA	1:A:990:TYR:CB	2.44	0.48
1:A:1194:ARG:C	1:A:1196:ASN:N	2.68	0.48
1:A:982:HIS:C	1:A:984:ASN:N	2.67	0.47
1:A:1190:LEU:O	1:A:1194:ARG:N	2.33	0.47
1:A:1183:LEU:C	1:A:1185:TYR:N	2.66	0.47
1:A:1058:PHE:O	1:A:1060:ARG:N	2.48	0.47
1:A:999:THR:O	1:A:1001:ASN:N	2.47	0.47
1:A:1036:ARG:C	1:A:1038:GLY:H	2.17	0.47
1:A:938:GLN:O	1:A:939:GLU:C	2.51	0.47
1:A:1190:LEU:O	1:A:1192:THR:N	2.48	0.47
1:A:936:ILE:O	1:A:940:MET:HG2	2.16	0.47
1:A:1179:GLN:HA	1:A:1182:TYR:CB	2.45	0.46
1:A:1125:ASP:O	1:A:1129:ASP:CB	2.64	0.46
1:A:1208:LEU:O	1:A:1211:GLU:CB	2.63	0.46
1:A:1103:SER:O	1:A:1107:GLU:N	2.49	0.46
1:A:1209:LEU:C	1:A:1211:GLU:N	2.69	0.46
1:A:1009:GLU:O	1:A:1010:PHE:C	2.54	0.46
1:A:1027:THR:O	1:A:1029:LEU:N	2.48	0.46
1:A:1126:CYS:O	1:A:1130:ARG:N	2.49	0.46
1:A:1152:ARG:O	1:A:1156:ARG:CB	2.63	0.46
1:A:995:SER:O	1:A:997:ALA:N	2.49	0.46
1:A:1036:ARG:C	1:A:1038:GLY:N	2.70	0.45
1:A:987:SER:O	1:A:991:LYS:N	2.49	0.45
1:A:1201:GLN:O	1:A:1204:GLU:N	2.50	0.45
1:A:1212:MET:C	1:A:1214:GLY:N	2.67	0.45
1:A:921:GLN:O	1:A:925:PRO:CB	2.63	0.45
1:A:944:TYR:O	1:A:947:GLN:CB	2.65	0.45
1:A:986:GLY:C	1:A:988:VAL:N	2.68	0.45
1:A:1022:GLU:O	1:A:1024:THR:N	2.49	0.45
1:A:1182:TYR:O	1:A:1185:TYR:CB	2.64	0.45
1:A:958:GLU:O	1:A:959:ARG:C	2.55	0.45
1:A:1021:ASP:C	1:A:1023:ALA:N	2.70	0.45
1:A:1022:GLU:C	1:A:1024:THR:N	2.68	0.45
1:A:1058:PHE:C	1:A:1060:ARG:H	2.19	0.45
1:A:939:GLU:O	1:A:940:MET:C	2.55	0.45
1:A:994:ALA:HA	1:A:997:ALA:HB2	1.99	0.44
1:A:1201:GLN:C	1:A:1203:LYS:N	2.70	0.44
1:A:907:ASP:C	1:A:910:ILE:H	2.20	0.44
1:A:1051:MET:HG2	1:A:1052:ALA:N	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1093:GLU:O	1:A:1094:ASN:C	2.55	0.44
1:A:1151:ALA:O	1:A:1155:SER:CB	2.65	0.44
1:A:942:ARG:O	1:A:943:GLN:C	2.56	0.44
1:A:1034:GLU:C	1:A:1036:ARG:N	2.69	0.43
1:A:1185:TYR:C	1:A:1188:TYR:H	2.21	0.43
1:A:913:GLY:O	1:A:914:ILE:C	2.56	0.43
1:A:921:GLN:O	1:A:925:PRO:N	2.50	0.43
1:A:1033:LYS:C	1:A:1035:ALA:N	2.71	0.43
1:A:1033:LYS:O	1:A:1035:ALA:N	2.51	0.43
1:A:1029:LEU:O	1:A:1033:LYS:CB	2.66	0.43
1:A:911:ARG:C	1:A:913:GLY:N	2.71	0.43
1:A:922:ALA:O	1:A:926:VAL:N	2.47	0.43
1:A:1056:ALA:O	1:A:1059:ARG:N	2.51	0.43
1:A:1042:ASP:C	1:A:1044:ILE:N	2.71	0.43
1:A:1034:GLU:O	1:A:1036:ARG:N	2.52	0.43
1:A:984:ASN:C	1:A:986:GLY:N	2.68	0.43
1:A:1056:ALA:C	1:A:1058:PHE:N	2.69	0.43
1:A:1201:GLN:O	1:A:1202:VAL:C	2.57	0.43
1:A:1034:GLU:O	1:A:1035:ALA:C	2.57	0.42
1:A:1051:MET:CG	1:A:1052:ALA:H	2.32	0.42
1:A:1212:MET:C	1:A:1215:ILE:H	2.22	0.42
1:A:1058:PHE:C	1:A:1062:CYS:SG	2.98	0.42
1:A:941:TYR:O	1:A:942:ARG:O	2.37	0.42
1:A:1185:TYR:HA	1:A:1188:TYR:CB	2.50	0.42
1:A:912:ASN:O	1:A:915:LEU:CB	2.67	0.42
1:A:996:GLN:O	1:A:999:THR:N	2.49	0.42
1:A:1031:GLU:O	1:A:1032:THR:C	2.58	0.42
1:A:989:ILE:O	1:A:991:LYS:N	2.53	0.42
1:A:935:ASN:C	1:A:937:LEU:N	2.73	0.41
1:A:1054:ALA:C	1:A:1056:ALA:H	2.23	0.41
1:A:944:TYR:O	1:A:947:GLN:N	2.52	0.41
1:A:987:SER:O	1:A:990:TYR:N	2.52	0.41
1:A:1141:SER:CB	1:A:1151:ALA:CB	2.99	0.41
1:A:1205:ASP:O	1:A:1209:LEU:CB	2.69	0.41
1:A:1084:PHE:O	1:A:1087:GLU:N	2.52	0.41
1:A:997:ALA:C	1:A:999:THR:N	2.71	0.41
1:A:1012:ARG:O	1:A:1014:ILE:N	2.54	0.40
1:A:927:ASN:O	1:A:930:GLY:N	2.54	0.40
1:A:1031:GLU:C	1:A:1033:LYS:N	2.71	0.40
1:A:1039:PHE:C	1:A:1041:PHE:H	2.25	0.40
1:A:950:ALA:O	1:A:1017:MET:HE3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1181:LEU:O	1:A:1184:VAL:CB	2.70	0.40
1:A:1023:ALA:O	1:A:1026:ARG:N	2.55	0.40
1:A:1051:MET:SD	1:A:1052:ALA:N	2.83	0.40
1:A:1135:ILE:O	1:A:1138:ALA:HB3	2.22	0.40
1:A:1031:GLU:O	1:A:1033:LYS:N	2.55	0.40
1:A:903:SER:C	1:A:906:ILE:H	2.25	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 X-ray entries followed by that with respect to entries of similar resolution.

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	254/348 (73%)	148 (58%)	70 (28%)	36 (14%)	0 5

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	918	GLU
1	A	942	ARG
1	A	954	ARG
1	A	960	LEU
1	A	993	TYR
1	A	999	THR
1	A	1000	ASN
1	A	1009	GLU
1	A	1011	LEU
1	A	1020	MET
1	A	1026	ARG
1	A	1033	LYS
1	A	1039	PHE
1	A	1052	ALA
1	A	923	VAL

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Mol	Chain	Res	Type
1	A	928	LEU
1	A	966	HIS
1	A	992	THR
1	A	994	ALA
1	A	995	SER
1	A	1001	ASN
1	A	1008	ILE
1	A	1022	GLU
1	A	1037	ALA
1	A	1040	LEU
1	A	1117	GLU
1	A	1195	SER
1	A	1197	ALA
1	A	1023	ALA
1	A	1062	CYS
1	A	938	GLN
1	A	986	GLY
1	A	1012	ARG
1	A	949	PHE
1	A	1066	ASP
1	A	1191	GLY

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 X-ray entries followed by that with respect to entries of similar resolution.

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	8/292 (3%)	2 (25%)	6 (75%)	0 0

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	917	MET
1	A	1017	MET
1	A	1020	MET
1	A	1051	MET
1	A	1062	CYS

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Mol	Chain	Res	Type
1	A	1212	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates 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 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	268/348 (77%)	-0.93	0 100 100	3, 67, 153, 185	0

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.