Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:54 AM GMT

PDB ID : 2VAF
Title : CRYSTAL STRUCTURE OF HUMAN CARDIAC CALSEQUESTRIN
Authors : Kim, E.; Youn, B.; Kemper, L.; Campbell, C.; Milting, H.; Varsanyi, M.; Kang, C.
Deposited on : 2007-08-31
Resolution : 3.80 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 (i) symbol.

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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.80 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.
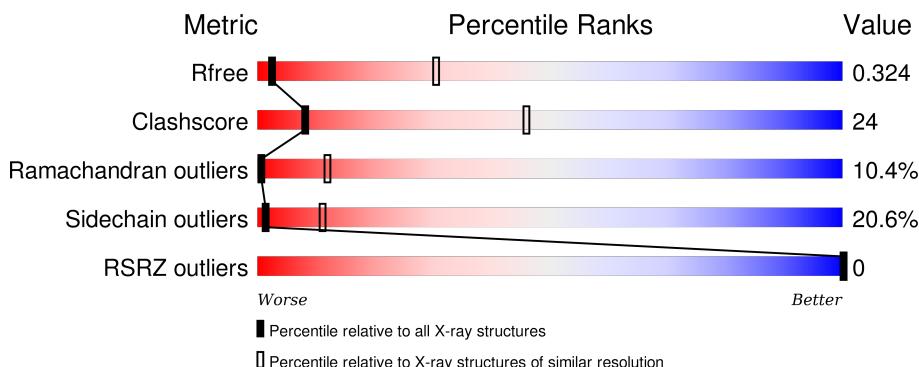
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1317 (4.10-3.50)
Clashscore	102246	1458 (4.10-3.50)
Ramachandran outliers	100387	1397 (4.10-3.50)
Sidechain outliers	100360	1392 (4.10-3.50)
RSRZ outliers	91569	1325 (4.10-3.50)

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 <=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	378	38% 37% 15% • 8%
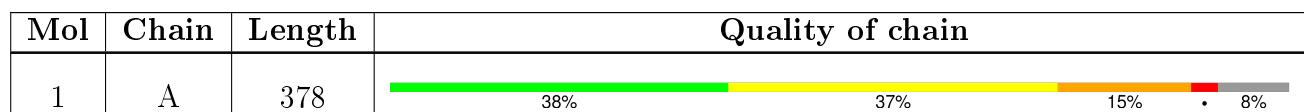
2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 2873 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 CALSEQUESTRIN-2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	349	Total	C	N	O	S	0	0	0
			2873	1868	440	559	6			

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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: CALSEQUESTRIN-2

Chain A:
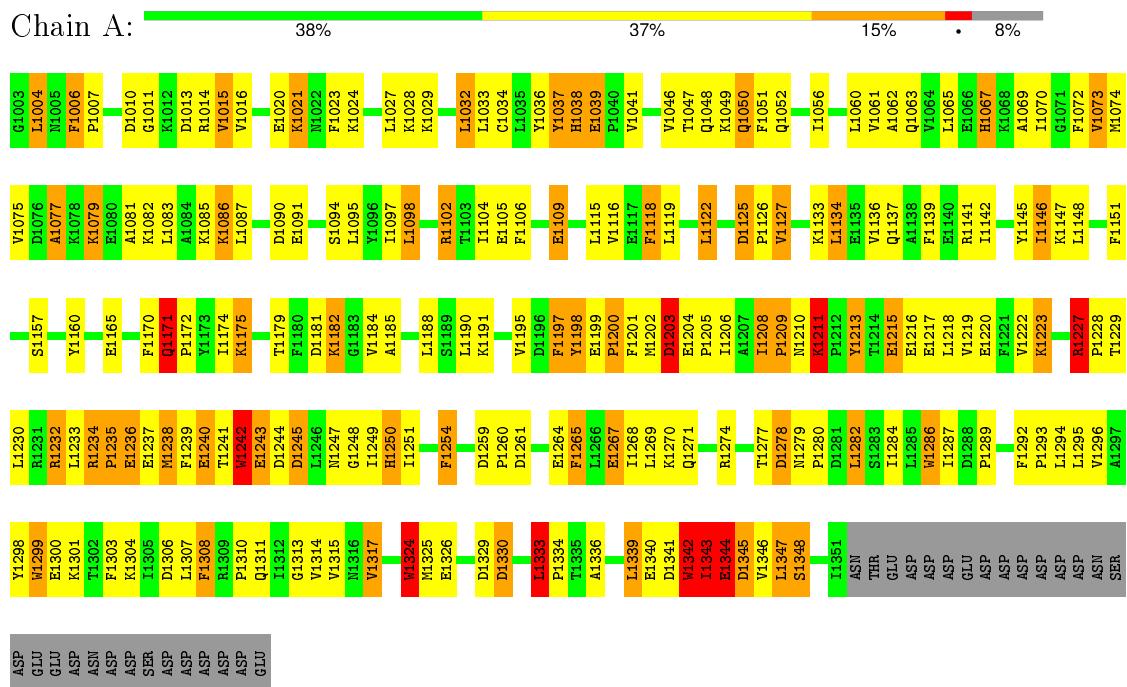
4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α, β, γ	150.65Å 150.65Å 227.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.80 14.99 – 3.80	Depositor EDS
% Data completeness (in resolution range)	88.7 (15.00-3.80) 88.6 (14.99-3.80)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.64 (at 3.77Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, R_{free}	0.274 , 0.325 0.274 , 0.324	Depositor DCC
R_{free} test set	565 reflections (4.90%)	DCC
Wilson B-factor (Å^2)	117.1	Xtriage
Anisotropy	0.193	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.03 , -5.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|> = 0.33$, $<L^2> = 0.16$	Xtriage
Outliers	0 of 11522 reflections	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	2873	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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	0.80	0/2942	1.04	18/3983 (0.5%)

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

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	1286	TRP	CD1-CG-CD2	9.34	113.77	106.30
1	A	1324	TRP	CD1-CG-CD2	9.07	113.56	106.30
1	A	1299	TRP	CD1-CG-CD2	8.65	113.22	106.30
1	A	1342	TRP	CD1-CG-CD2	8.57	113.16	106.30
1	A	1242	TRP	CD1-CG-CD2	8.37	112.99	106.30
1	A	1242	TRP	CE2-CD2-CG	-8.34	100.63	107.30
1	A	1286	TRP	CE2-CD2-CG	-7.91	100.98	107.30
1	A	1299	TRP	CE2-CD2-CG	-7.62	101.21	107.30
1	A	1342	TRP	CE2-CD2-CG	-7.49	101.31	107.30
1	A	1324	TRP	CE2-CD2-CG	-7.17	101.56	107.30
1	A	1242	TRP	CB-CG-CD1	-7.16	117.69	127.00
1	A	1242	TRP	CG-CD2-CE3	6.98	140.18	133.90
1	A	1286	TRP	CB-CG-CD1	-5.51	119.83	127.00
1	A	1299	TRP	CG-CD2-CE3	5.49	138.84	133.90
1	A	1299	TRP	CB-CG-CD1	-5.29	120.13	127.00
1	A	1342	TRP	CB-CG-CD1	-5.22	120.22	127.00
1	A	1324	TRP	CB-CG-CD1	-5.13	120.34	127.00
1	A	1342	TRP	CG-CD2-CE3	5.09	138.49	133.90

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1125	ASP	Peptide
1	A	1171	GLN	Peptide
1	A	1208	ILE	Peptide
1	A	1211	LYS	Peptide
1	A	1227	ARG	Peptide
1	A	1333	LEU	Peptide
1	A	1343	ILE	Mainchain
1	A	1344	GLU	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	2873	0	2804	139	0
All	All	2873	0	2804	139	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 24.

All (139) 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:1095:LEU:HB3	1:A:1106:PHE:HB3	1.62	0.82
1:A:1038:HIS:HB2	1:A:1074:MET:SD	2.19	0.82
1:A:1343:ILE:HG23	1:A:1344:GLU:H	1.49	0.77
1:A:1032:LEU:HD12	1:A:1070:ILE:HG22	1.67	0.75
1:A:1004:LEU:H	1:A:1004:LEU:HD13	1.52	0.75
1:A:1343:ILE:O	1:A:1345:ASP:N	2.20	0.74
1:A:1230:LEU:HD22	1:A:1270:LYS:HE3	1.69	0.74
1:A:1313:GLY:HA3	1:A:1324:TRP:HA	1.71	0.73
1:A:1148:LEU:HD13	1:A:1197:PHE:HD1	1.54	0.72
1:A:1230:LEU:HD12	1:A:1269:LEU:HD23	1.72	0.72
1:A:1268:ILE:HB	1:A:1339:LEU:HD22	1.71	0.71
1:A:1339:LEU:O	1:A:1343:ILE:HG22	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1267:GLU:O	1:A:1271:GLN:HB2	1.94	0.67
1:A:1234:ARG:HB3	1:A:1235:PRO:HD2	1.77	0.67
1:A:1015:VAL:HG22	1:A:1063:GLN:NE2	2.10	0.67
1:A:1146:ILE:H	1:A:1146:ILE:HD12	1.60	0.66
1:A:1250:HIS:HB3	1:A:1315:VAL:HB	1.78	0.66
1:A:1293:PRO:HA	1:A:1296:VAL:HB	1.79	0.65
1:A:1023:PHE:O	1:A:1027:LEU:HB2	1.97	0.65
1:A:1033:LEU:HB2	1:A:1098:LEU:HB2	1.78	0.65
1:A:1198:TYR:HA	1:A:1204:GLU:O	1.97	0.64
1:A:1198:TYR:HE1	1:A:1203:ASP:HB3	1.63	0.63
1:A:1227:ARG:H	1:A:1228:PRO:HD3	1.63	0.63
1:A:1081:ALA:HA	1:A:1087:LEU:HD13	1.81	0.63
1:A:1020:GLU:HG3	1:A:1021:LYS:H	1.65	0.61
1:A:1254:PHE:HB3	1:A:1311:GLN:HB2	1.82	0.61
1:A:1147:LYS:HA	1:A:1175:LYS:HB3	1.81	0.60
1:A:1250:HIS:O	1:A:1314:VAL:HA	2.02	0.59
1:A:1210:ASN:H	1:A:1213:TYR:HE2	1.50	0.59
1:A:1047:THR:HA	1:A:1050:GLN:HE22	1.69	0.58
1:A:1304:LYS:HD2	1:A:1324:TRP:HZ2	1.68	0.58
1:A:1118:PHE:O	1:A:1122:LEU:HB3	2.03	0.58
1:A:1340:GLU:O	1:A:1344:GLU:HB2	2.04	0.57
1:A:1217:GLU:O	1:A:1220:GLU:HB3	2.04	0.57
1:A:1170:PHE:HE1	1:A:1219:VAL:HG22	1.69	0.57
1:A:1295:LEU:HA	1:A:1298:TYR:HB3	1.87	0.56
1:A:1034:CYS:SG	1:A:1095:LEU:HD11	2.45	0.56
1:A:1048:GLN:HA	1:A:1051:PHE:HB3	1.88	0.56
1:A:1299:TRP:O	1:A:1303:PHE:HB3	2.06	0.56
1:A:1095:LEU:HG	1:A:1097:ILE:HD11	1.88	0.55
1:A:1218:LEU:O	1:A:1222:VAL:HG23	2.06	0.55
1:A:1147:LYS:HB2	1:A:1198:TYR:HB3	1.87	0.55
1:A:1145:TYR:O	1:A:1200:PRO:HA	2.07	0.55
1:A:1342:TRP:O	1:A:1346:VAL:HA	2.07	0.55
1:A:1039:GLU:HG3	1:A:1041:VAL:HG22	1.89	0.55
1:A:1284:ILE:H	1:A:1284:ILE:HD12	1.72	0.54
1:A:1307:LEU:HG	1:A:1308:PHE:H	1.72	0.54
1:A:1202:MET:HG3	1:A:1274:ARG:HA	1.90	0.54
1:A:1264:GLU:O	1:A:1268:ILE:HG12	2.08	0.54
1:A:1037:TYR:HA	1:A:1075:VAL:HB	1.89	0.54
1:A:1304:LYS:HD2	1:A:1324:TRP:CZ2	2.42	0.54
1:A:1148:LEU:HD11	1:A:1195:VAL:HG12	1.91	0.53
1:A:1343:ILE:HG23	1:A:1344:GLU:N	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1341:ASP:O	1:A:1347:LEU:HA	2.09	0.53
1:A:1073:VAL:HG12	1:A:1074:MET:N	2.24	0.53
1:A:1151:PHE:HZ	1:A:1184:VAL:HG13	1.74	0.52
1:A:1182:LYS:NZ	1:A:1182:LYS:H	2.07	0.52
1:A:1346:VAL:O	1:A:1347:LEU:HB3	2.10	0.52
1:A:1241:THR:HA	1:A:1244:ASP:HB2	1.90	0.52
1:A:1136:VAL:HG22	1:A:1184:VAL:HB	1.91	0.52
1:A:1182:LYS:HA	1:A:1185:ALA:HB3	1.92	0.51
1:A:1208:ILE:HG21	1:A:1218:LEU:CD2	2.40	0.51
1:A:1326:GLU:HA	1:A:1329:ASP:OD2	2.11	0.51
1:A:1049:LYS:O	1:A:1052:GLN:HG2	2.11	0.51
1:A:1261:ASP:O	1:A:1265:PHE:HB2	2.11	0.50
1:A:1134:LEU:HD23	1:A:1134:LEU:H	1.75	0.50
1:A:1343:ILE:O	1:A:1346:VAL:N	2.45	0.50
1:A:1065:LEU:HD12	1:A:1067:HIS:HB2	1.93	0.50
1:A:1251:ILE:HA	1:A:1314:VAL:HG12	1.94	0.50
1:A:1047:THR:HA	1:A:1050:GLN:NE2	2.27	0.50
1:A:1062:ALA:HB2	1:A:1072:PHE:CE1	2.46	0.50
1:A:1235:PRO:O	1:A:1238:MET:SD	2.70	0.49
1:A:1292:PHE:O	1:A:1296:VAL:HG23	2.12	0.49
1:A:1303:PHE:CZ	1:A:1324:TRP:HB3	2.46	0.49
1:A:1170:PHE:CE2	1:A:1223:LYS:HD2	2.46	0.49
1:A:1261:ASP:HB2	1:A:1310:PRO:HB3	1.94	0.49
1:A:1151:PHE:CZ	1:A:1184:VAL:HG13	2.47	0.49
1:A:1259:ASP:HA	1:A:1260:PRO:HD2	1.64	0.48
1:A:1251:ILE:HG22	1:A:1284:ILE:HG23	1.95	0.48
1:A:1137:GLN:O	1:A:1141:ARG:HB2	2.13	0.48
1:A:1015:VAL:HG22	1:A:1063:GLN:HE22	1.77	0.48
1:A:1215:GLU:H	1:A:1215:GLU:CD	2.17	0.48
1:A:1082:LYS:HA	1:A:1086:LYS:HA	1.96	0.48
1:A:1330:ASP:HB3	1:A:1334:PRO:HD2	1.95	0.48
1:A:1289:PRO:HB3	1:A:1296:VAL:HG21	1.94	0.48
1:A:1181:ASP:HA	1:A:1182:LYS:HZ1	1.78	0.47
1:A:1300:GLU:HG2	1:A:1307:LEU:HB3	1.97	0.47
1:A:1016:VAL:O	1:A:1073:VAL:HB	2.14	0.47
1:A:1109:GLU:OE2	1:A:1236:GLU:HA	2.13	0.47
1:A:1062:ALA:HB2	1:A:1072:PHE:CD1	2.49	0.47
1:A:1248:GLY:O	1:A:1317:VAL:HG23	2.15	0.47
1:A:1020:GLU:HG3	1:A:1021:LYS:HG3	1.97	0.47
1:A:1216:GLU:H	1:A:1216:GLU:CD	2.19	0.46
1:A:1234:ARG:HB3	1:A:1235:PRO:CD	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1341:ASP:HB3	1:A:1347:LEU:HB2	1.97	0.46
1:A:1020:GLU:HG3	1:A:1021:LYS:N	2.31	0.46
1:A:1141:ARG:HB3	1:A:1142:ILE:HD12	1.98	0.46
1:A:1006:PHE:CD1	1:A:1006:PHE:N	2.84	0.46
1:A:1345:ASP:HB3	1:A:1348:SER:HA	1.98	0.46
1:A:1336:ALA:O	1:A:1339:LEU:HB3	2.15	0.46
1:A:1239:PHE:O	1:A:1242:TRP:HB2	2.16	0.45
1:A:1170:PHE:CE1	1:A:1219:VAL:HG13	2.50	0.45
1:A:1024:LYS:O	1:A:1028:LYS:HG2	2.17	0.45
1:A:1157:SER:HB3	1:A:1160:TYR:HB2	1.99	0.45
1:A:1109:GLU:H	1:A:1236:GLU:HG2	1.80	0.45
1:A:1033:LEU:O	1:A:1097:ILE:HA	2.16	0.45
1:A:1325:MET:HA	1:A:1342:TRP:CZ2	2.52	0.45
1:A:1280:PRO:C	1:A:1282:LEU:H	2.20	0.45
1:A:1036:TYR:O	1:A:1074:MET:SD	2.75	0.44
1:A:1075:VAL:HG12	1:A:1079:LYS:NZ	2.33	0.44
1:A:1151:PHE:HE2	1:A:1188:LEU:HD23	1.83	0.44
1:A:1240:GLU:O	1:A:1243:GLU:HG3	2.18	0.44
1:A:1235:PRO:HA	1:A:1292:PHE:CZ	2.53	0.43
1:A:1036:TYR:HA	1:A:1094:SER:O	2.17	0.43
1:A:1325:MET:SD	1:A:1333:LEU:HD21	2.59	0.43
1:A:1208:ILE:HA	1:A:1209:PRO:HD3	1.76	0.43
1:A:1006:PHE:N	1:A:1006:PHE:HD1	2.17	0.42
1:A:1170:PHE:CZ	1:A:1223:LYS:HD2	2.55	0.42
1:A:1233:LEU:HD12	1:A:1287:ILE:HG13	2.01	0.42
1:A:1310:PRO:HB2	1:A:1333:LEU:HD12	2.01	0.42
1:A:1024:LYS:HD3	1:A:1024:LYS:HA	1.85	0.42
1:A:1056:ILE:O	1:A:1060:LEU:HB2	2.20	0.42
1:A:1345:ASP:H	1:A:1347:LEU:H	1.68	0.42
1:A:1061:VAL:HG13	1:A:1116:VAL:HG22	2.02	0.42
1:A:1037:TYR:HB3	1:A:1075:VAL:HB	2.03	0.41
1:A:1115:LEU:O	1:A:1119:LEU:HG	2.20	0.41
1:A:1234:ARG:O	1:A:1238:MET:SD	2.78	0.41
1:A:1204:GLU:HA	1:A:1205:PRO:HD2	1.91	0.41
1:A:1133:LYS:O	1:A:1136:VAL:HB	2.21	0.41
1:A:1232:ARG:HA	1:A:1286:TRP:HD1	1.85	0.41
1:A:1010:ASP:CG	1:A:1014:ARG:HH21	2.23	0.41
1:A:1013:ASP:HA	1:A:1063:GLN:OE1	2.21	0.41
1:A:1190:LEU:H	1:A:1190:LEU:HD23	1.86	0.41
1:A:1077:ALA:H	1:A:1079:LYS:NZ	2.19	0.40
1:A:1269:LEU:HD21	1:A:1284:ILE:HB	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1269:LEU:HD11	1:A:1284:ILE:HD13	2.02	0.40
1:A:1148:LEU:HD13	1:A:1197:PHE:CD1	2.44	0.40
1:A:1279:ASN:N	1:A:1280:PRO:HD3	2.36	0.40
1:A:1170:PHE:CE1	1:A:1219:VAL:HG22	2.52	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	347/378 (92%)	241 (70%)	70 (20%)	36 (10%)	1 12

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1073	VAL
1	A	1077	ALA
1	A	1086	LYS
1	A	1126	PRO
1	A	1171	GLN
1	A	1172	PRO
1	A	1200	PRO
1	A	1211	LYS
1	A	1227	ARG
1	A	1234	ARG
1	A	1277	THR
1	A	1317	VAL
1	A	1330	ASP
1	A	1344	GLU
1	A	1345	ASP
1	A	1085	LYS
1	A	1102	ARG

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Mol	Chain	Res	Type
1	A	1203	ASP
1	A	1229	THR
1	A	1235	PRO
1	A	1247	ASN
1	A	1343	ILE
1	A	1079	LYS
1	A	1174	ILE
1	A	1245	ASP
1	A	1069	ALA
1	A	1348	SER
1	A	1090	ASP
1	A	1215	GLU
1	A	1278	ASP
1	A	1347	LEU
1	A	1011	GLY
1	A	1282	LEU
1	A	1209	PRO
1	A	1127	VAL
1	A	1007	PRO

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 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	316/345 (92%)	251 (79%)	65 (21%)	1　11

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1004	LEU
1	A	1006	PHE
1	A	1015	VAL
1	A	1021	LYS
1	A	1029	LYS
1	A	1032	LEU
1	A	1037	TYR

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Mol	Chain	Res	Type
1	A	1038	HIS
1	A	1039	GLU
1	A	1046	VAL
1	A	1050	GLN
1	A	1067	HIS
1	A	1083	LEU
1	A	1091	GLU
1	A	1098	LEU
1	A	1102	ARG
1	A	1104	ILE
1	A	1105	GLU
1	A	1109	GLU
1	A	1118	PHE
1	A	1122	LEU
1	A	1125	ASP
1	A	1127	VAL
1	A	1134	LEU
1	A	1139	PHE
1	A	1146	ILE
1	A	1165	GLU
1	A	1171	GLN
1	A	1175	LYS
1	A	1179	THR
1	A	1182	LYS
1	A	1191	LYS
1	A	1197	PHE
1	A	1198	TYR
1	A	1199	GLU
1	A	1201	PHE
1	A	1203	ASP
1	A	1206	ILE
1	A	1211	LYS
1	A	1213	TYR
1	A	1223	LYS
1	A	1227	ARG
1	A	1232	ARG
1	A	1236	GLU
1	A	1237	GLU
1	A	1238	MET
1	A	1240	GLU
1	A	1242	TRP
1	A	1243	GLU

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Mol	Chain	Res	Type
1	A	1245	ASP
1	A	1249	ILE
1	A	1250	HIS
1	A	1254	PHE
1	A	1265	PHE
1	A	1267	GLU
1	A	1278	ASP
1	A	1294	LEU
1	A	1301	LYS
1	A	1306	ASP
1	A	1308	PHE
1	A	1324	TRP
1	A	1333	LEU
1	A	1339	LEU
1	A	1342	TRP
1	A	1343	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1050	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 carbohydrates in this entry.

5.6　Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	349/378 (92%)	-1.59	0	100	100	49, 81, 93, 97	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.