Full wwPDB X-ray Structure Validation Report (i)

May 21, 2020 – 06:47 pm BST

PDB ID	:	3KG7
Title	:	Dehydratase domain from CurH module of Curacin polyketide synthase
Authors	:	Akey, D.L.; Smith, J.L.
Deposited on	:	2009-10-28
Resolution	:	2.77 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
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

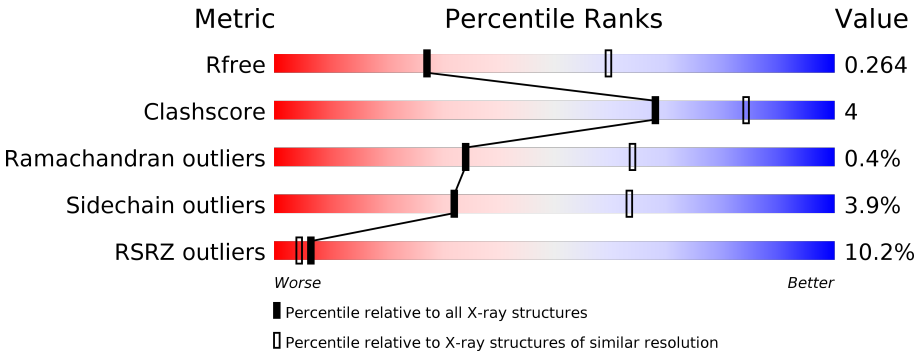
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.77 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}	130704	4107 (2.80-2.76)
Clashscore	141614	4575 (2.80-2.76)
Ramachandran outliers	138981	4487 (2.80-2.76)
Sidechain outliers	138945	4489 (2.80-2.76)
RSRZ outliers	127900	4027 (2.80-2.76)

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 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 <=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	293	6% 87% 10%
1	B	293	4% 84% 12%
1	C	293	13% 83% 14%
1	D	293	16% 83% 14%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9076 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 CurH.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	Se	0	0	0
			2259	1440	381	431	2	5			
1	B	285	Total	C	N	O	S	Se	0	0	0
			2252	1435	380	430	2	5			
1	C	287	Total	C	N	O	S	Se	0	0	0
			2268	1445	383	433	2	5			
1	D	285	Total	C	N	O	S	Se	0	0	0
			2252	1435	380	430	2	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	931	SER	-	EXPRESSION TAG	UNP Q6DNE5
A	932	ASN	-	EXPRESSION TAG	UNP Q6DNE5
A	933	ALA	-	EXPRESSION TAG	UNP Q6DNE5
B	931	SER	-	EXPRESSION TAG	UNP Q6DNE5
B	932	ASN	-	EXPRESSION TAG	UNP Q6DNE5
B	933	ALA	-	EXPRESSION TAG	UNP Q6DNE5
C	931	SER	-	EXPRESSION TAG	UNP Q6DNE5
C	932	ASN	-	EXPRESSION TAG	UNP Q6DNE5
C	933	ALA	-	EXPRESSION TAG	UNP Q6DNE5
D	931	SER	-	EXPRESSION TAG	UNP Q6DNE5
D	932	ASN	-	EXPRESSION TAG	UNP Q6DNE5
D	933	ALA	-	EXPRESSION TAG	UNP Q6DNE5

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	17	Total	O	0	0
			17	17		
2	B	9	Total	O	0	0
			9	9		

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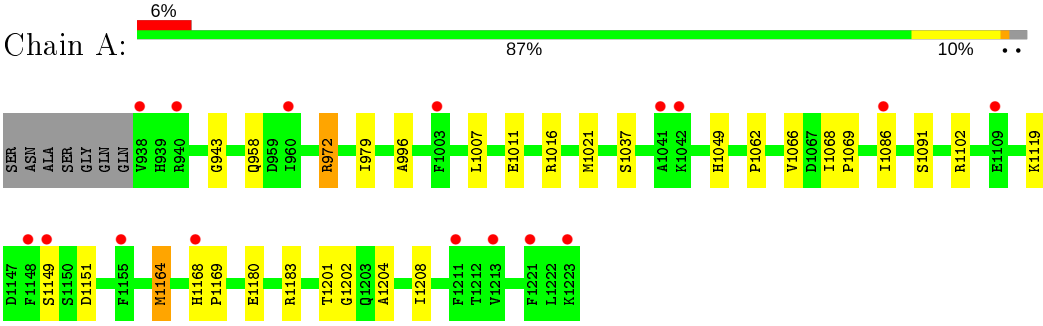
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	C	9	Total O 9 9	0	0
2	D	10	Total O 10 10	0	0

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 the various outlier classes 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.

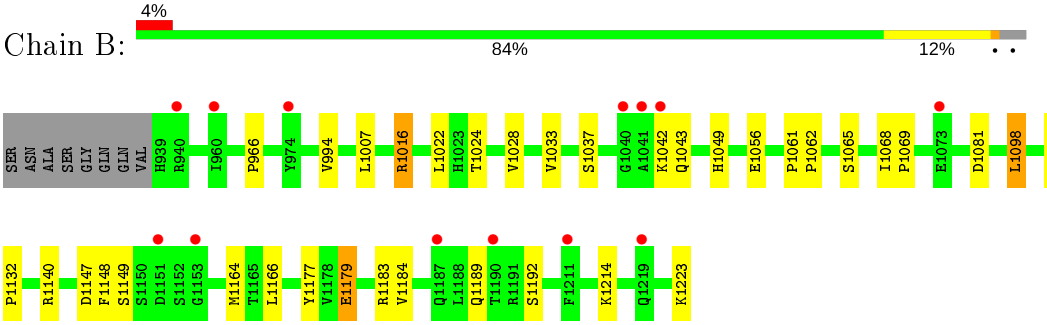
- Molecule 1: CurH

Chain A:



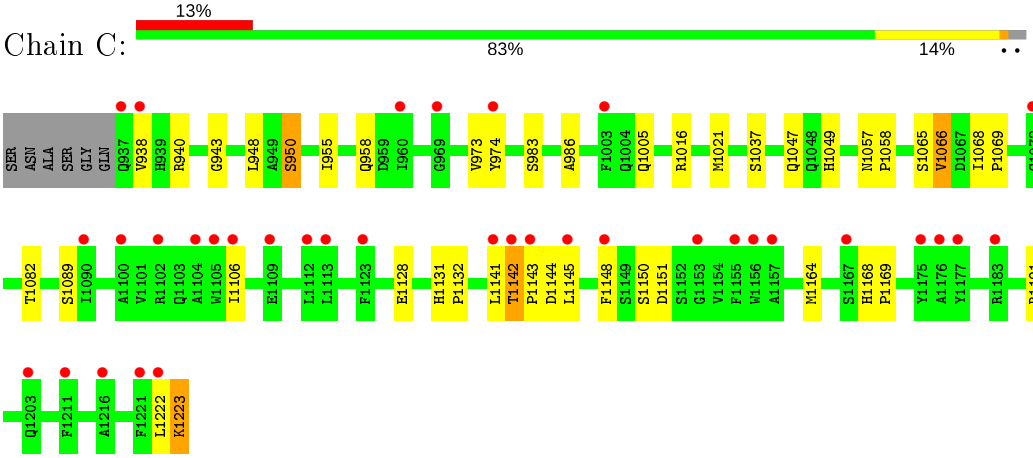
- Molecule 1: CurH

Chain B:



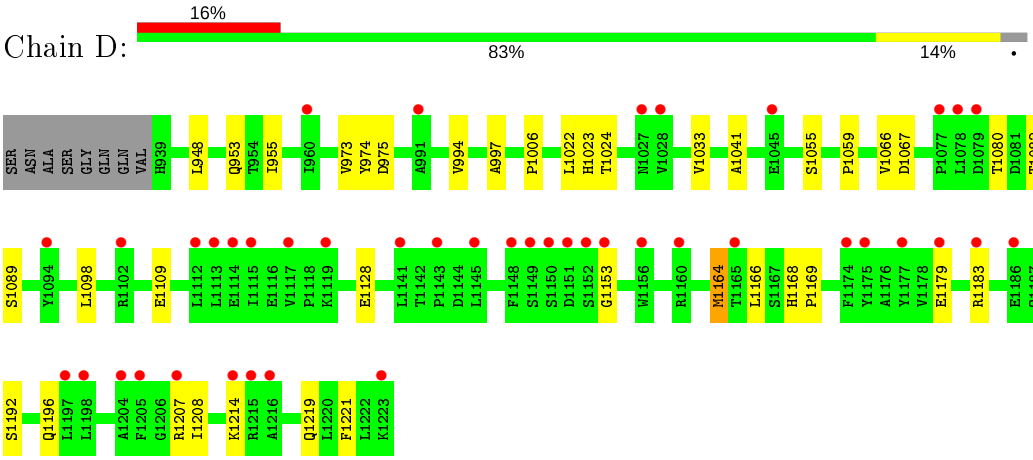
- Molecule 1: CurH

Chain C:



- Molecule 1: CurH

Chain D:


16%
83%
14%
SER ASN ALA SER GLY GLN GLN VAL H939 L948 Q953 T954 I955 I960 V973 Y974 D975 A991 V994 A997 P1006 L1022 H1023 T1024 N1027 V1028 V1033 A1041 E1045 S1055 P1059 V1066 D1067 P1077 L1078 D1079 T1080 D1081 T1082 L1083 I1086
S1089 Y1094 L1098 R1102 E1109 L1112 L1113 E1114 I1115 E1116 V1117 P1118 K1119 E1128 L1141 T1142 P1143 D1144 L1145 F1148 S1149 S1150 D1151 S1152 G1153 W1156 R1160 M1164 T1165 L1166 S1167 H1168 P1169 F1174 Y1175 A1176 Y1177 V1178 E1179 R1183 E1186 Q1187 L1188 Q1189 T1190 R1191
S1192 Q1196 L1197 L1198 A1204 F1205 G1206 R1207 I1208 K1214 R1215 A1216 Q1219 L1220 F1221 L1222 K1223

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	82.16Å 74.45Å 103.48Å 90.00° 108.84° 90.00°	Depositor
Resolution (Å)	48.97 – 2.77 48.97 – 2.77	Depositor EDS
% Data completeness (in resolution range)	98.8 (48.97-2.77) 98.8 (48.97-2.77)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	3.26 (at 2.77Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.203 , 0.269 0.200 , 0.264	Depositor DCC
R_{free} test set	1996 reflections (6.69%)	wwPDB-VP
Wilson B-factor (Å^2)	73.1	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 76.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9076	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.43	0/2313	0.56	0/3154
1	B	0.40	0/2306	0.55	0/3144
1	C	0.48	2/2322 (0.1%)	0.58	2/3166 (0.1%)
1	D	0.39	0/2306	0.54	0/3144
All	All	0.43	2/9247 (0.0%)	0.56	2/12608 (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	C	0	1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	1076	ARG	CZ-NH1	6.76	1.41	1.33
1	C	1076	ARG	NE-CZ	5.77	1.40	1.33

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1076	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	1076	ARG	NE-CZ-NH2	-5.26	117.67	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	1222	LEU	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	2259	0	2209	14	0
1	B	2252	0	2200	17	0
1	C	2268	0	2217	20	0
1	D	2252	0	2200	18	0
2	A	17	0	0	2	0
2	B	9	0	0	0	0
2	C	9	0	0	0	0
2	D	10	0	0	1	0
All	All	9076	0	8826	68	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 4.

All (68) 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:1016:ARG:NH1	1:B:1037:SER:OG	2.23	0.70
1:B:1028:VAL:HG12	1:B:1056:GLU:OE1	1.93	0.68
1:D:1168:HIS:HB2	1:D:1169:PRO:HD2	1.79	0.63
1:D:994:VAL:HG11	1:D:1166:LEU:HD23	1.81	0.63
1:A:979:ILE:HD12	1:A:1007:LEU:HD22	1.80	0.62
1:C:1047:GLN:OE1	1:C:1223:LYS:HD2	1.99	0.61
1:B:1183:ARG:HG3	1:B:1192:SER:HB3	1.83	0.59
1:D:953:GLN:HG2	1:D:1023:HIS:HA	1.85	0.58
1:D:997:ALA:HB2	1:D:1059:PRO:HB3	1.88	0.55
1:C:1142:THR:HG22	1:C:1143:PRO:HD2	1.88	0.55
1:C:1037:SER:OG	1:C:1049:HIS:NE2	2.36	0.54
1:C:1089:SER:HB3	1:C:1150:SER:HB2	1.88	0.53
1:B:1022:LEU:HD12	1:B:1033:VAL:HG22	1.90	0.53
1:C:1068:ILE:HG22	1:C:1069:PRO:HD3	1.91	0.52
1:B:1131:HIS:CG	1:B:1132:PRO:HD2	2.45	0.52
1:B:1098:LEU:O	1:B:1140:ARG:NH2	2.39	0.51
1:C:1106:ILE:HD11	1:C:1143:PRO:HA	1.93	0.51
1:D:1022:LEU:HD12	1:D:1033:VAL:HG22	1.93	0.51
1:C:1144:ASP:OD2	1:C:1191:ARG:NH2	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:972:ARG:HD2	2:A:5:HOH:O	2.12	0.50
1:C:1168:HIS:HB2	1:C:1169:PRO:CD	2.43	0.49
1:B:966:PRO:HD2	1:B:1124:GLN:OE1	2.12	0.49
1:A:1016:ARG:NH1	1:A:1037:SER:OG	2.45	0.49
1:A:1037:SER:OG	1:A:1049:HIS:NE2	2.39	0.48
1:D:1089:SER:O	1:D:1153:GLY:HA2	2.13	0.48
1:D:1168:HIS:HB2	1:D:1169:PRO:CD	2.42	0.48
1:B:1068:ILE:HB	1:B:1069:PRO:HD3	1.96	0.48
1:D:997:ALA:HB3	1:D:1055:SER:HB3	1.97	0.47
1:C:1168:HIS:HB2	1:C:1169:PRO:HD2	1.97	0.47
1:D:1006:PRO:HG3	1:D:1221:PHE:CE1	2.49	0.47
1:A:1168:HIS:HB2	1:A:1169:PRO:HD2	1.97	0.47
1:B:1148:PHE:HZ	1:B:1184:VAL:HG21	1.81	0.46
1:D:1080:THR:HA	1:D:1083:LEU:HD12	1.97	0.46
1:D:1082:THR:O	1:D:1086:ILE:HG12	2.15	0.46
1:C:1065:SER:O	1:C:1066:VAL:HG23	2.16	0.46
1:D:975:ASP:HA	2:D:8:HOH:O	2.15	0.46
1:C:943:GLY:HA3	1:C:958:GLN:HB3	1.96	0.46
1:A:943:GLY:HA3	1:A:958:GLN:HB3	1.98	0.45
1:C:973:VAL:HG12	1:C:974:TYR:CD2	2.52	0.45
1:A:1062:PRO:HB3	1:A:1204:ALA:O	2.17	0.45
1:A:1068:ILE:N	1:A:1069:PRO:HD2	2.31	0.45
1:C:1131:HIS:CG	1:C:1132:PRO:HD2	2.52	0.44
1:A:1164:MSE:HG2	1:A:1208:ILE:HG12	1.99	0.44
1:D:1196:GLN:OE1	1:D:1207:ARG:HG2	2.17	0.44
1:B:1223:LYS:HE3	1:B:1223:LYS:HB2	1.80	0.44
1:D:973:VAL:HG12	1:D:974:TYR:CD2	2.53	0.44
1:B:994:VAL:HG11	1:B:1166:LEU:HD23	2.00	0.43
1:C:1057:ASN:HA	1:C:1058:PRO:HD2	1.80	0.43
1:B:1177:TYR:CE2	1:B:1179:GLU:HG3	2.53	0.43
1:D:948:LEU:HD21	1:D:955:ILE:HD12	2.00	0.43
1:B:1007:LEU:HD12	1:B:1049:HIS:CD2	2.54	0.43
1:B:1148:PHE:HA	1:B:1149:SER:HA	1.83	0.43
1:B:1189:GLN:O	1:B:1214:LYS:HG3	2.19	0.43
1:A:1021:MSE:HE3	1:C:950:SER:HB3	2.00	0.43
1:D:1067:ASP:OD1	1:D:1067:ASP:N	2.49	0.43
1:B:1061:PRO:HA	1:B:1062:PRO:HD3	1.89	0.43
1:A:996:ALA:HA	2:A:17:HOH:O	2.17	0.42
1:A:1011:GLU:OE1	1:A:1011:GLU:HA	2.19	0.42
1:C:983:SER:O	1:C:986:ALA:HB3	2.20	0.41
1:C:1141:LEU:HA	1:C:1145:LEU:HD13	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1005:GLN:HG2	1:C:1005:GLN:H	1.73	0.41
1:C:938:VAL:HG23	1:C:943:GLY:HA2	2.03	0.41
1:A:1086:ILE:HD11	1:A:1146:PHE:HD1	1.85	0.41
1:C:948:LEU:HD11	1:C:955:ILE:HD11	2.02	0.41
1:B:1042:LYS:O	1:B:1043:GLN:HB2	2.20	0.41
1:D:1190:THR:HG22	1:D:1214:LYS:HB2	2.03	0.40
1:A:1066:VAL:O	1:A:1202:GLY:HA3	2.21	0.40
1:D:1164:MSE:HG2	1:D:1208:ILE:HG12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	284/293 (97%)	274 (96%)	9 (3%)	1 (0%)	34	64
1	B	283/293 (97%)	272 (96%)	11 (4%)	0	100	100
1	C	285/293 (97%)	265 (93%)	18 (6%)	2 (1%)	22	50
1	D	283/293 (97%)	274 (97%)	8 (3%)	1 (0%)	34	64
All	All	1135/1172 (97%)	1085 (96%)	46 (4%)	4 (0%)	34	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	1148	PHE
1	A	1149	SER
1	C	1151	ASP
1	D	1041	ALA

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	250/250 (100%)	241 (96%)	9 (4%)	35	66
1	B	249/250 (100%)	240 (96%)	9 (4%)	35	66
1	C	251/250 (100%)	240 (96%)	11 (4%)	28	58
1	D	249/250 (100%)	239 (96%)	10 (4%)	31	62
All	All	999/1000 (100%)	960 (96%)	39 (4%)	32	63

All (39) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	972	ARG
1	A	1091	SER
1	A	1102	ARG
1	A	1119	LYS
1	A	1151	ASP
1	A	1164	MSE
1	A	1180	GLU
1	A	1183	ARG
1	A	1201	THR
1	B	1016	ARG
1	B	1024	THR
1	B	1065	SER
1	B	1081	ASP
1	B	1098	LEU
1	B	1123	PHE
1	B	1147	ASP
1	B	1164	MSE
1	B	1179	GLU
1	C	940	ARG
1	C	950	SER
1	C	1016	ARG
1	C	1021	MSE
1	C	1066	VAL
1	C	1078	LEU

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Mol	Chain	Res	Type
1	C	1082	THR
1	C	1128	GLU
1	C	1142	THR
1	C	1164	MSE
1	C	1223	LYS
1	D	1024	THR
1	D	1066	VAL
1	D	1098	LEU
1	D	1109	GLU
1	D	1128	GLU
1	D	1164	MSE
1	D	1179	GLU
1	D	1183	ARG
1	D	1192	SER
1	D	1219	GLN

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	1043	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

6.1 Protein, DNA and RNA chains

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, 95^{th} 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	281/293 (95%)	0.53	17 (6%) 21 16	68, 83, 98, 114	0
1	B	280/293 (95%)	0.52	13 (4%) 32 26	74, 83, 98, 124	0
1	C	282/293 (96%)	0.98	39 (13%) 2 2	46, 83, 98, 113	0
1	D	280/293 (95%)	0.91	46 (16%) 1 1	74, 84, 104, 113	0
All	All	1123/1172 (95%)	0.74	115 (10%) 6 4	46, 83, 100, 124	0

All (115) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1157	ALA	8.3
1	C	1156	TRP	8.1
1	C	1155	PHE	7.9
1	C	1177	TYR	7.7
1	D	1149	SER	7.6
1	D	1156	TRP	7.0
1	C	1145	LEU	6.7
1	D	1174	PHE	6.0
1	A	938	VAL	6.0
1	D	1189	GLN	5.9
1	C	937	GLN	5.4
1	C	1203	GLN	5.3
1	D	1152	SER	5.2
1	D	1197	LEU	5.2
1	D	1117	VAL	5.2
1	A	1149	SER	4.8
1	D	1198	LEU	4.7
1	C	1077	PRO	4.5
1	C	1106	ILE	4.4
1	B	940	ARG	4.3
1	A	1211	PHE	4.3

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Mol	Chain	Res	Type	RSRZ
1	C	1142	THR	4.3
1	D	1113	LEU	4.2
1	A	1041	ALA	4.2
1	C	1183	ARG	4.1
1	B	1219	GLN	4.0
1	C	1193	TYR	4.0
1	B	1151	ASP	4.0
1	D	1179	GLU	4.0
1	A	1109	GLU	4.0
1	C	1175	TYR	3.9
1	D	1204	ALA	3.8
1	D	1216	ALA	3.8
1	B	1041	ALA	3.7
1	A	1148	PHE	3.7
1	D	1102	ARG	3.6
1	D	1175	TYR	3.6
1	D	1027	ASN	3.6
1	D	1145	LEU	3.6
1	C	1148	PHE	3.6
1	C	1100	ALA	3.5
1	D	1078	LEU	3.4
1	C	1072	CYS	3.4
1	C	1216	ALA	3.4
1	D	1151	ASP	3.3
1	D	1190	THR	3.3
1	D	1115	ILE	3.3
1	D	1153	GLY	3.3
1	A	1223	LYS	3.3
1	A	1155	PHE	3.2
1	C	1221	PHE	3.1
1	C	974	TYR	3.1
1	A	960	ILE	3.1
1	D	1141	LEU	3.1
1	D	1177	TYR	3.1
1	B	1187	GLN	3.1
1	C	1105	TRP	3.0
1	B	1040	GLY	3.0
1	B	1042	LYS	3.0
1	C	1090	ILE	3.0
1	D	1165	THR	3.0
1	B	1211	PHE	3.0
1	D	1186	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	D	1114	GLU	2.9
1	D	1148	PHE	2.9
1	D	1143	PRO	2.9
1	D	1183	ARG	2.9
1	D	991	ALA	2.9
1	C	1153	GLY	2.9
1	D	1205	PHE	2.9
1	D	1077	PRO	2.8
1	D	1215	ARG	2.7
1	B	1153	GLY	2.7
1	B	960	ILE	2.6
1	C	1109	GLU	2.6
1	C	960	ILE	2.6
1	D	1028	VAL	2.6
1	C	1222	LEU	2.5
1	D	1079	ASP	2.5
1	C	1143	PRO	2.5
1	C	1211	PHE	2.5
1	C	1141	LEU	2.5
1	C	1003	PHE	2.5
1	D	960	ILE	2.5
1	D	1119	LYS	2.5
1	C	1167	SER	2.4
1	D	1214	LYS	2.4
1	B	1073	GLU	2.4
1	D	1094	TYR	2.4
1	D	1160	ARG	2.4
1	D	1045	GLU	2.3
1	D	1207	ARG	2.3
1	C	1123	PHE	2.3
1	A	1213	VAL	2.2
1	A	940	ARG	2.2
1	C	1113	LEU	2.2
1	A	1123	PHE	2.2
1	A	1042	LYS	2.2
1	B	1190	THR	2.2
1	D	1188	LEU	2.2
1	A	1086	ILE	2.1
1	D	1223	LYS	2.1
1	C	1102	ARG	2.1
1	D	1112	LEU	2.1
1	C	1176	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	1112	LEU	2.1
1	A	1003	PHE	2.1
1	C	969	GLY	2.1
1	C	1200	GLU	2.1
1	A	1221	PHE	2.1
1	B	974	TYR	2.0
1	D	1150	SER	2.0
1	A	1168	HIS	2.0
1	C	1104	ALA	2.0
1	C	938	VAL	2.0

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.