Full wwPDB X-ray Structure Validation Report (i)

May 13, 2020 – 05:09 am BST

PDB ID	:	5CQS
Title	:	Dimerization of Elp1 is essential for Elongator complex assembly
Authors	:	Lin, Z.; Xu, H.; Li, F.; Diao, W.; Long, J.; Shen, Y.
Deposited on	:	2015-07-22
Resolution	:	2.70 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 (i)) were used in the production of this report:

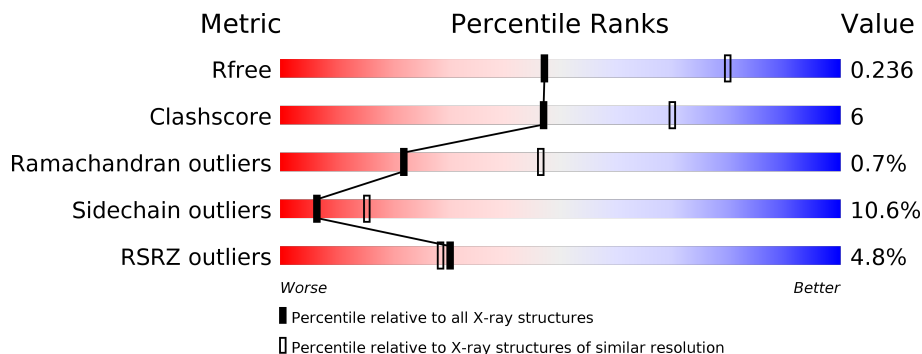|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.70 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	Percentile Ranks	Value
Rfree		0.236
Clashscore		6
Ramachandran outliers		0.7%
Sidechain outliers		10.6%
RSRZ outliers		4.8%

Worse   Better

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	435	4% 55% 18% • 25%
1	B	435	3% 58% 14% • 26%
1	C	435	4% 58% 12% • 28%
1	D	435	3% 62% 11% • 26%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9999 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.

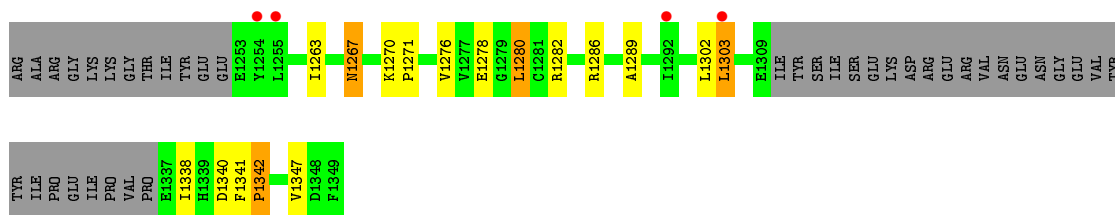- Molecule 1 is a protein called Elongator complex protein 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	325	Total	C	N	O	S	Se	0	0	0
			2515	1594	421	491	3	6			
1	B	323	Total	C	N	O	S	Se	0	0	0
			2492	1580	414	489	3	6			
1	C	313	Total	C	N	O	S	Se	0	0	0
			2450	1556	405	480	3	6			
1	D	324	Total	C	N	O	S	Se	0	0	0
			2521	1601	417	494	3	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	915	GLY	-	expression tag	UNP Q06706
A	916	PRO	-	expression tag	UNP Q06706
A	917	GLY	-	expression tag	UNP Q06706
A	918	SER	-	expression tag	UNP Q06706
B	915	GLY	-	expression tag	UNP Q06706
B	916	PRO	-	expression tag	UNP Q06706
B	917	GLY	-	expression tag	UNP Q06706
B	918	SER	-	expression tag	UNP Q06706
C	915	GLY	-	expression tag	UNP Q06706
C	916	PRO	-	expression tag	UNP Q06706
C	917	GLY	-	expression tag	UNP Q06706
C	918	SER	-	expression tag	UNP Q06706
D	915	GLY	-	expression tag	UNP Q06706
D	916	PRO	-	expression tag	UNP Q06706
D	917	GLY	-	expression tag	UNP Q06706
D	918	SER	-	expression tag	UNP Q06706

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	5	Total 5	O 5	0	0
2	B	1	Total 1	O 1	0	0
2	C	7	Total 7	O 7	0	0
2	D	8	Total 8	O 8	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: Elongator complex protein 1

- Molecule 1: Elongator complex protein 1

• Molecule 1: Elongator complex protein 1

Chain C:

• Molecule 1: Elongator complex protein 1

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	127.75Å 157.74Å 139.26Å 90.00° 93.09° 90.00°	Depositor
Resolution (Å)	45.79 – 2.70 48.61 – 2.70	Depositor EDS
% Data completeness (in resolution range)	98.3 (45.79-2.70) 98.6 (48.61-2.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.69Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.234 , 0.256 0.236 , 0.236	Depositor DCC
R_{free} test set	7553 reflections (10.09%)	wwPDB-VP
Wilson B-factor (Å^2)	60.5	Xtriage
Anisotropy	0.808	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 43.3	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9999	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.01% 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, 0.333 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	0.38	0/2550	0.54	0/3446
1	B	0.39	0/2526	0.56	0/3413
1	C	0.39	0/2484	0.58	0/3353
1	D	0.45	0/2555	0.59	0/3449
All	All	0.40	0/10115	0.57	0/13661

There are no bond length outliers.

There are no bond angle outliers.

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	2515	0	2379	45	0
1	B	2492	0	2349	34	0
1	C	2450	0	2342	32	0
1	D	2521	0	2406	28	0
2	A	5	0	0	0	0
2	B	1	0	0	0	0
2	C	7	0	0	0	0
2	D	8	0	0	0	0
All	All	9999	0	9476	120	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 6.

All (120) 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:1073:GLN:NE2	1:D:1136:ASP:OD2	2.19	0.72
1:B:988:ASP:N	1:B:988:ASP:OD1	2.24	0.69
1:C:941:ALA:HA	1:C:946:MSE:HE3	1.73	0.68
1:B:1128:LEU:HD21	1:C:1065:ARG:HB3	1.76	0.67
1:B:998:ILE:HG23	1:B:1027:ILE:HD12	1.75	0.67
1:A:922:ASN:ND2	1:A:946:MSE:HE2	2.09	0.67
1:B:981:LEU:HD12	1:B:1006:LEU:HD13	1.76	0.67
1:A:925:TYR:HB2	1:A:946:MSE:HE1	1.76	0.67
1:A:1052:LYS:NZ	1:A:1078:GLU:OE2	2.29	0.66
1:A:1348:ASP:OD2	1:D:1008:LYS:NZ	2.26	0.66
1:B:1303:LEU:HB3	1:B:1338:ILE:HD13	1.78	0.66
1:B:1065:ARG:HB3	1:C:1128:LEU:HD13	1.78	0.64
1:A:1278:GLU:OE1	1:D:1063:ARG:NH2	2.33	0.62
1:C:961:ASN:O	1:C:966:ARG:NH2	2.33	0.61
1:D:998:ILE:HG23	1:D:1027:ILE:HD13	1.83	0.61
1:C:1124:ASP:O	1:C:1128:LEU:HB2	2.01	0.60
1:A:1063:ARG:NH2	1:D:1278:GLU:OE1	2.33	0.60
1:C:988:ASP:HB3	1:C:990:ASP:HB2	1.83	0.59
1:A:941:ALA:HA	1:A:946:MSE:HE3	1.85	0.58
1:A:1051:LEU:HD12	1:A:1074:LYS:HG3	1.86	0.58
1:C:1288:GLN:OE1	1:C:1288:GLN:N	2.34	0.57
1:B:1286:ARG:HE	1:C:1047:MSE:HE2	1.69	0.57
1:B:1055:MSE:HE1	1:B:1075:PHE:HB2	1.85	0.57
1:B:1043:VAL:O	1:B:1047:MSE:HG3	2.05	0.57
1:C:955:LEU:HD23	1:C:958:LEU:HD12	1.87	0.56
1:A:984:LEU:HD11	1:A:996:GLU:HG2	1.88	0.56
1:A:922:ASN:HD21	1:A:946:MSE:HE2	1.71	0.56
1:D:1068:MSE:HE1	1:D:1079:VAL:HG13	1.87	0.55
1:A:1136:ASP:OD2	1:D:1073:GLN:NE2	2.41	0.54
1:D:1147:LEU:HD22	1:D:1280:LEU:HD13	1.89	0.54
1:B:1047:MSE:HE3	1:C:1281:CYS:O	2.08	0.53
1:A:1106:TYR:OH	1:D:1128:LEU:HD11	2.09	0.53
1:B:1270:LYS:HB3	1:B:1271:PRO:HD3	1.89	0.53
1:C:1075:PHE:HB3	1:C:1078:GLU:HG3	1.91	0.51
1:A:1109:ASN:HB3	1:A:1112:GLU:CG	2.41	0.50
1:A:1109:ASN:HB3	1:A:1112:GLU:HG3	1.93	0.50
1:B:1076:PRO:O	1:B:1078:GLU:N	2.44	0.50
1:C:968:PHE:CD1	1:C:984:LEU:HB2	2.47	0.50
1:B:1276:VAL:HG12	1:B:1280:LEU:HD22	1.94	0.49
1:B:989:LYS:N	1:B:990:ASP:HA	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1047:MSE:HE1	1:D:1286:ARG:HB3	1.95	0.49
1:A:1285:MSE:HE2	1:A:1285:MSE:HB3	1.75	0.48
1:B:932:TYR:HD1	1:B:970:ILE:HD12	1.77	0.48
1:B:936:LEU:O	1:B:940:VAL:HG23	2.13	0.48
1:B:1064:TRP:HB2	1:B:1086:LEU:HD13	1.96	0.48
1:B:1286:ARG:NE	1:C:1047:MSE:HE2	2.27	0.48
1:B:1065:ARG:HB3	1:C:1128:LEU:CD1	2.44	0.47
1:A:947:ASP:OD2	1:A:949:ARG:NH1	2.48	0.47
1:A:984:LEU:HD12	1:A:987:ILE:HD12	1.96	0.47
1:B:981:LEU:HD11	1:B:1001:VAL:HG22	1.95	0.47
1:C:1032:LEU:HD12	1:C:1037:MSE:HG3	1.96	0.47
1:B:1052:LYS:HD3	1:B:1075:PHE:CE2	2.49	0.47
1:A:1064:TRP:HB2	1:A:1086:LEU:HD13	1.97	0.47
1:C:1096:TYR:HB2	1:C:1120:ALA:HB2	1.96	0.47
1:B:1069:SER:HB2	1:C:1128:LEU:HD21	1.96	0.46
1:B:1263:ILE:O	1:B:1267:ASN:HB2	2.15	0.46
1:D:919:GLN:HB2	1:D:945:GLN:O	2.15	0.46
1:D:965:ARG:NH1	1:D:987:ILE:HD13	2.31	0.46
1:A:1047:MSE:HE2	1:D:1286:ARG:HE	1.81	0.46
1:A:1064:TRP:O	1:A:1068:MSE:HG2	2.17	0.45
1:C:931:LEU:HD23	1:C:931:LEU:HA	1.76	0.45
1:A:968:PHE:CD1	1:A:984:LEU:HB2	2.52	0.45
1:A:951:TYR:CE1	1:A:952:LEU:HD13	2.52	0.45
1:C:982:GLU:HA	1:C:1013:LEU:HD11	1.98	0.45
1:B:1128:LEU:CD2	1:C:1065:ARG:HB3	2.46	0.45
1:D:1280:LEU:HB3	1:D:1289:ALA:HB2	1.98	0.45
1:A:1165:ILE:HG21	1:A:1302:LEU:HD21	1.99	0.45
1:C:1086:LEU:O	1:C:1090:LEU:HB2	2.17	0.45
1:B:968:PHE:CD1	1:B:984:LEU:HB2	2.51	0.44
1:A:948:PRO:O	1:A:952:LEU:HB2	2.18	0.44
1:A:999:ASP:O	1:A:1003:SER:OG	2.27	0.44
1:C:1270:LYS:HE2	1:C:1342:PRO:HG3	2.00	0.44
1:A:1038:TYR:CG	1:A:1060:SER:HB2	2.53	0.43
1:A:952:LEU:HD12	1:A:952:LEU:HA	1.91	0.43
1:B:1278:GLU:O	1:B:1282:ARG:HG3	2.18	0.43
1:D:1171:ARG:O	1:D:1173:ARG:N	2.50	0.43
1:A:1346:ILE:HD11	1:D:1044:ALA:HB2	2.01	0.43
1:D:1293:GLN:HG3	1:D:1341:PHE:HE2	1.83	0.43
1:B:1341:PHE:HA	1:B:1342:PRO:HD3	1.85	0.43
1:A:932:TYR:CD1	1:A:967:LYS:HG2	2.54	0.43
1:B:1037:MSE:HE2	1:B:1037:MSE:HB3	1.73	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:990:ASP:OD2	1:D:992:ASN:ND2	2.40	0.43
1:D:982:GLU:HG2	1:D:1013:LEU:HD21	2.01	0.42
1:B:951:TYR:HD1	1:B:955:LEU:HD12	1.85	0.42
1:C:988:ASP:HB3	1:C:990:ASP:H	1.84	0.42
1:A:934:VAL:HG13	1:A:955:LEU:HD22	2.01	0.42
1:B:1052:LYS:HB2	1:B:1075:PHE:CZ	2.55	0.42
1:A:941:ALA:HA	1:A:946:MSE:CE	2.49	0.42
1:B:1280:LEU:HB3	1:B:1289:ALA:HB2	2.02	0.42
1:D:939:LEU:HA	1:D:939:LEU:HD23	1.85	0.42
1:A:1078:GLU:O	1:A:1082:VAL:HG23	2.18	0.42
1:A:997:VAL:O	1:A:1001:VAL:HG23	2.20	0.42
1:A:962:GLU:HG2	1:A:963:PRO:N	2.33	0.42
1:C:1136:ASP:OD1	1:C:1136:ASP:N	2.53	0.42
1:B:963:PRO:O	1:B:967:LYS:HG3	2.20	0.42
1:C:1030:LYS:HA	1:C:1030:LYS:HD2	1.78	0.42
1:D:1074:LYS:HD3	1:D:1074:LYS:HA	1.93	0.42
1:D:1294:LYS:HE2	1:D:1294:LYS:HB3	1.78	0.42
1:C:1114:VAL:HG13	1:C:1126:ALA:HB1	2.02	0.42
1:D:1064:TRP:HB2	1:D:1086:LEU:HD13	2.01	0.41
1:A:1280:LEU:HA	1:A:1280:LEU:HD12	1.91	0.41
1:A:1290:HIS:HB2	1:A:1347:VAL:HG22	2.01	0.41
1:A:964:LEU:HA	1:A:964:LEU:HD12	1.78	0.41
1:A:1015:ARG:HH11	1:D:1349:PHE:HE1	1.67	0.41
1:B:971:ASP:OD2	1:B:983:HIS:HD2	2.02	0.41
1:C:1028:TYR:O	1:C:1032:LEU:HB2	2.20	0.41
1:A:1154:ILE:HD13	1:A:1273:ALA:HA	2.02	0.41
1:A:989:LYS:HA	1:A:990:ASP:HA	1.72	0.41
1:B:1109:ASN:HB3	1:B:1112:GLU:OE1	2.20	0.41
1:A:1100:ALA:HB2	1:A:1116:LEU:HB2	2.03	0.41
1:A:1349:PHE:HB2	1:D:1012:ALA:HB2	2.03	0.41
1:D:1283:ARG:HA	1:D:1283:ARG:HD2	1.85	0.41
1:A:1308:LYS:C	1:A:1310:ILE:H	2.24	0.40
1:C:1024:ILE:HA	1:C:1027:ILE:HG12	2.03	0.40
1:C:932:TYR:HD1	1:C:970:ILE:HD12	1.86	0.40
1:C:1037:MSE:HE2	1:C:1037:MSE:HB3	1.48	0.40
1:C:1066:GLU:OE1	1:C:1066:GLU:N	2.49	0.40
1:C:1280:LEU:HB3	1:C:1289:ALA:HB2	2.03	0.40
1:D:1090:LEU:HD12	1:D:1090:LEU:HA	1.86	0.40
1:D:1030:LYS:HA	1:D:1030:LYS:HD3	1.81	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	319/435 (73%)	304 (95%)	13 (4%)	2 (1%)	25	50
1	B	317/435 (73%)	292 (92%)	22 (7%)	3 (1%)	17	40
1	C	307/435 (71%)	287 (94%)	17 (6%)	3 (1%)	15	37
1	D	318/435 (73%)	301 (95%)	16 (5%)	1 (0%)	41	66
All	All	1261/1740 (72%)	1184 (94%)	68 (5%)	9 (1%)	22	46

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1077	GLU
1	C	965	ARG
1	D	1172	LEU
1	A	1309	GLU
1	C	963	PRO
1	C	987	ILE
1	A	1089	SER
1	B	1342	PRO
1	B	963	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	255/371 (69%)	224 (88%)	31 (12%)	5	11
1	B	251/371 (68%)	223 (89%)	28 (11%)	6	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	252/371 (68%)	227 (90%)	25 (10%)	8	18
1	D	258/371 (70%)	234 (91%)	24 (9%)	9	21
All	All	1016/1484 (68%)	908 (89%)	108 (11%)	6	15

All (108) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	920	ASP
1	A	927	SER
1	A	929	LEU
1	A	930	SER
1	A	952	LEU
1	A	960	ASP
1	A	965	ARG
1	A	979	LYS
1	A	1003	SER
1	A	1005	ASP
1	A	1011	LEU
1	A	1028	TYR
1	A	1032	LEU
1	A	1036	GLN
1	A	1037	MSE
1	A	1060	SER
1	A	1062	LYS
1	A	1081	SER
1	A	1090	LEU
1	A	1094	HIS
1	A	1104	LEU
1	A	1111	LYS
1	A	1127	SER
1	A	1167	SER
1	A	1280	LEU
1	A	1284	ASN
1	A	1285	MSE
1	A	1286	ARG
1	A	1340	ASP
1	A	1346	ILE
1	A	1347	VAL
1	B	929	LEU
1	B	930	SER
1	B	939	LEU

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Mol	Chain	Res	Type
1	B	960	ASP
1	B	964	LEU
1	B	988	ASP
1	B	1013	LEU
1	B	1021	GLN
1	B	1027	ILE
1	B	1028	TYR
1	B	1032	LEU
1	B	1037	MSE
1	B	1045	TYR
1	B	1062	LYS
1	B	1080	GLU
1	B	1084	GLU
1	B	1090	LEU
1	B	1093	GLU
1	B	1104	LEU
1	B	1128	LEU
1	B	1138	LEU
1	B	1140	GLU
1	B	1267	ASN
1	B	1280	LEU
1	B	1302	LEU
1	B	1303	LEU
1	B	1340	ASP
1	B	1347	VAL
1	C	924	VAL
1	C	929	LEU
1	C	957	GLU
1	C	986	GLU
1	C	990	ASP
1	C	1011	LEU
1	C	1013	LEU
1	C	1028	TYR
1	C	1032	LEU
1	C	1037	MSE
1	C	1084	GLU
1	C	1090	LEU
1	C	1104	LEU
1	C	1105	GLU
1	C	1109	ASN
1	C	1128	LEU
1	C	1132	LYS

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Mol	Chain	Res	Type
1	C	1136	ASP
1	C	1164	GLN
1	C	1165	ILE
1	C	1266	LEU
1	C	1269	THR
1	C	1280	LEU
1	C	1302	LEU
1	C	1347	VAL
1	D	919	GLN
1	D	923	VAL
1	D	929	LEU
1	D	939	LEU
1	D	959	GLN
1	D	964	LEU
1	D	965	ARG
1	D	979	LYS
1	D	1005	ASP
1	D	1011	LEU
1	D	1028	TYR
1	D	1032	LEU
1	D	1037	MSE
1	D	1090	LEU
1	D	1093	GLU
1	D	1094	HIS
1	D	1104	LEU
1	D	1160	ASP
1	D	1268	GLN
1	D	1280	LEU
1	D	1286	ARG
1	D	1294	LYS
1	D	1303	LEU
1	D	1347	VAL

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

Mol	Chain	Res	Type
1	C	1109	ASN

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(Å²)	Q<0.9
1	A	319/435 (73%)	0.43	16 (5%)	28	27	40, 74, 124, 147	0
1	B	317/435 (72%)	0.35	15 (4%)	31	30	40, 73, 130, 147	0
1	C	307/435 (70%)	0.47	19 (6%)	20	19	42, 68, 115, 137	0
1	D	318/435 (73%)	0.42	11 (3%)	44	44	38, 53, 116, 152	0
All	All	1261/1740 (72%)	0.42	61 (4%)	30	28	38, 68, 123, 152	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1166	ASN	4.9
1	C	1296	PHE	4.5
1	B	1166	ASN	4.2
1	C	1153	ILE	4.0
1	C	1266	LEU	3.9
1	A	981	LEU	3.8
1	A	1168	GLN	3.7
1	B	1254	TYR	3.6
1	C	1259	VAL	3.5
1	B	964	LEU	3.5
1	B	1024	ILE	3.4
1	C	1292	ILE	3.2
1	C	1277	VAL	3.1
1	D	1299	VAL	3.0
1	B	1013	LEU	2.9
1	B	1167	SER	2.9
1	C	1300	LEU	2.9
1	A	1252	GLU	2.8
1	C	981	LEU	2.8
1	D	1349	PHE	2.8
1	C	952	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1266	LEU	2.6
1	C	1151	PHE	2.6
1	C	1289	ALA	2.6
1	A	1062	LYS	2.5
1	B	998	ILE	2.5
1	D	1157	LEU	2.4
1	D	1159	ALA	2.4
1	A	1092	PHE	2.4
1	B	1255	LEU	2.4
1	B	1292	ILE	2.4
1	D	1266	LEU	2.4
1	C	954	PHE	2.4
1	A	1255	LEU	2.3
1	C	1303	LEU	2.3
1	C	1349	PHE	2.3
1	B	1303	LEU	2.3
1	A	1035	ASN	2.3
1	D	1166	ASN	2.3
1	B	1153	ILE	2.3
1	A	1292	ILE	2.2
1	B	1027	ILE	2.2
1	A	1013	LEU	2.2
1	D	1277	VAL	2.1
1	D	1161	CYS	2.1
1	C	928	ALA	2.1
1	A	1024	ILE	2.1
1	A	1262	LEU	2.1
1	B	981	LEU	2.1
1	C	1155	ALA	2.1
1	B	1032	LEU	2.1
1	D	1153	ILE	2.1
1	C	925	TYR	2.1
1	C	1024	ILE	2.1
1	A	952	LEU	2.1
1	B	1169	LEU	2.0
1	A	1277	VAL	2.0
1	D	1164	GLN	2.0
1	A	1253	GLU	2.0
1	C	1163	GLY	2.0
1	D	1259	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.