Full wwPDB X-ray Structure Validation Report

Jan 5, 2017 – 03:20 AM EST

PDB ID	:	5GN1
Title	:	Crystal structure of the C-terminal part of Fun30 ATPase domain
Authors	:	Jiang, T.; Liu, L.
Deposited on	:	2016-07-18
Resolution	:	1.95 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 (1)) were used in the production of this report:

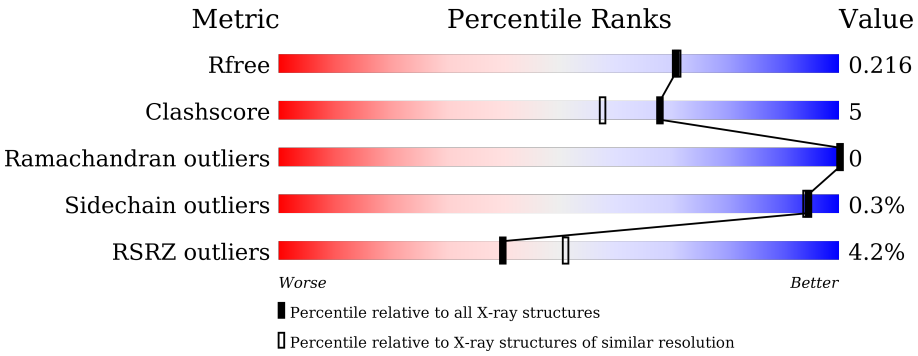
MolProbity	:	4.02b-467
Mogul	:	unknown
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028442
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028442

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 1.95 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	1833 (1.96-1.96)
Clashscore	102246	1953 (1.96-1.96)
Ramachandran outliers	100387	1936 (1.96-1.96)
Sidechain outliers	100360	1936 (1.96-1.96)
RSRZ outliers	91569	1835 (1.96-1.96)

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	366	7% 75% 10% 16%
1	B	366	2% 78% 6% 16%
1	C	366	2% 79% 6% 15%
1	D	366	4% 75% 11% 15%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 11466 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 ATP-dependent helicase FUN30.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	309	Total	C	N	O	S	0	2	0
			2520	1607	418	483	12			
1	B	309	Total	C	N	O	S	0	0	0
			2509	1600	418	479	12			
1	C	310	Total	C	N	O	S	0	2	0
			2533	1615	426	480	12			
1	D	312	Total	C	N	O	S	0	3	0
			2564	1632	431	488	13			

There are 92 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	765	MET	-	expression tag	UNP P31380
A	766	ALA	-	expression tag	UNP P31380
A	767	SER	-	expression tag	UNP P31380
A	768	MET	-	expression tag	UNP P31380
A	769	THR	-	expression tag	UNP P31380
A	770	GLY	-	expression tag	UNP P31380
A	771	GLY	-	expression tag	UNP P31380
A	772	GLN	-	expression tag	UNP P31380
A	773	GLN	-	expression tag	UNP P31380
A	774	MET	-	expression tag	UNP P31380
A	775	GLY	-	expression tag	UNP P31380
A	776	ARG	-	expression tag	UNP P31380
A	777	GLY	-	expression tag	UNP P31380
A	778	SER	-	expression tag	UNP P31380
A	779	MET	-	expression tag	UNP P31380
A	1123	LEU	-	expression tag	UNP P31380
A	1124	GLU	-	expression tag	UNP P31380
A	1125	HIS	-	expression tag	UNP P31380
A	1126	HIS	-	expression tag	UNP P31380
A	1127	HIS	-	expression tag	UNP P31380
A	1128	HIS	-	expression tag	UNP P31380

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Chain	Residue	Modelled	Actual	Comment	Reference
A	1129	HIS	-	expression tag	UNP P31380
A	1130	HIS	-	expression tag	UNP P31380
B	765	MET	-	expression tag	UNP P31380
B	766	ALA	-	expression tag	UNP P31380
B	767	SER	-	expression tag	UNP P31380
B	768	MET	-	expression tag	UNP P31380
B	769	THR	-	expression tag	UNP P31380
B	770	GLY	-	expression tag	UNP P31380
B	771	GLY	-	expression tag	UNP P31380
B	772	GLN	-	expression tag	UNP P31380
B	773	GLN	-	expression tag	UNP P31380
B	774	MET	-	expression tag	UNP P31380
B	775	GLY	-	expression tag	UNP P31380
B	776	ARG	-	expression tag	UNP P31380
B	777	GLY	-	expression tag	UNP P31380
B	778	SER	-	expression tag	UNP P31380
B	779	MET	-	expression tag	UNP P31380
B	1123	LEU	-	expression tag	UNP P31380
B	1124	GLU	-	expression tag	UNP P31380
B	1125	HIS	-	expression tag	UNP P31380
B	1126	HIS	-	expression tag	UNP P31380
B	1127	HIS	-	expression tag	UNP P31380
B	1128	HIS	-	expression tag	UNP P31380
B	1129	HIS	-	expression tag	UNP P31380
B	1130	HIS	-	expression tag	UNP P31380
C	765	MET	-	expression tag	UNP P31380
C	766	ALA	-	expression tag	UNP P31380
C	767	SER	-	expression tag	UNP P31380
C	768	MET	-	expression tag	UNP P31380
C	769	THR	-	expression tag	UNP P31380
C	770	GLY	-	expression tag	UNP P31380
C	771	GLY	-	expression tag	UNP P31380
C	772	GLN	-	expression tag	UNP P31380
C	773	GLN	-	expression tag	UNP P31380
C	774	MET	-	expression tag	UNP P31380
C	775	GLY	-	expression tag	UNP P31380
C	776	ARG	-	expression tag	UNP P31380
C	777	GLY	-	expression tag	UNP P31380
C	778	SER	-	expression tag	UNP P31380
C	779	MET	-	expression tag	UNP P31380
C	1123	LEU	-	expression tag	UNP P31380
C	1124	GLU	-	expression tag	UNP P31380

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Chain	Residue	Modelled	Actual	Comment	Reference
C	1125	HIS	-	expression tag	UNP P31380
C	1126	HIS	-	expression tag	UNP P31380
C	1127	HIS	-	expression tag	UNP P31380
C	1128	HIS	-	expression tag	UNP P31380
C	1129	HIS	-	expression tag	UNP P31380
C	1130	HIS	-	expression tag	UNP P31380
D	765	MET	-	expression tag	UNP P31380
D	766	ALA	-	expression tag	UNP P31380
D	767	SER	-	expression tag	UNP P31380
D	768	MET	-	expression tag	UNP P31380
D	769	THR	-	expression tag	UNP P31380
D	770	GLY	-	expression tag	UNP P31380
D	771	GLY	-	expression tag	UNP P31380
D	772	GLN	-	expression tag	UNP P31380
D	773	GLN	-	expression tag	UNP P31380
D	774	MET	-	expression tag	UNP P31380
D	775	GLY	-	expression tag	UNP P31380
D	776	ARG	-	expression tag	UNP P31380
D	777	GLY	-	expression tag	UNP P31380
D	778	SER	-	expression tag	UNP P31380
D	779	MET	-	expression tag	UNP P31380
D	1123	LEU	-	expression tag	UNP P31380
D	1124	GLU	-	expression tag	UNP P31380
D	1125	HIS	-	expression tag	UNP P31380
D	1126	HIS	-	expression tag	UNP P31380
D	1127	HIS	-	expression tag	UNP P31380
D	1128	HIS	-	expression tag	UNP P31380
D	1129	HIS	-	expression tag	UNP P31380
D	1130	HIS	-	expression tag	UNP P31380

- Molecule 2 is water.

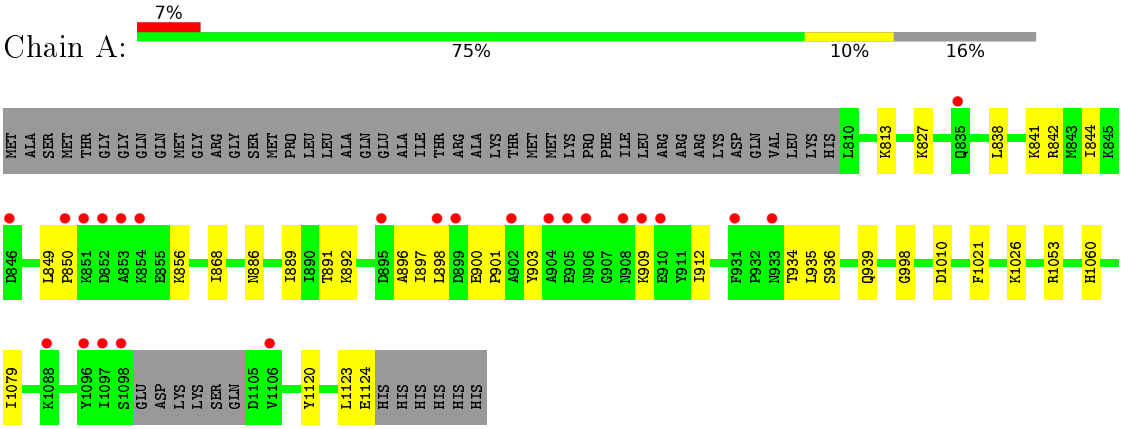
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	268	Total O 268 268	0	0
2	B	396	Total O 396 396	0	0
2	C	347	Total O 347 347	0	0
2	D	329	Total O 329 329	0	0

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 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.

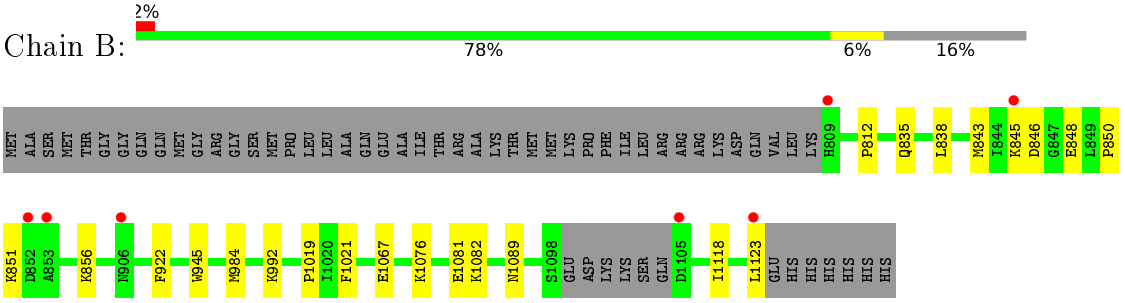
- Molecule 1: ATP-dependent helicase FUN30

Chain A:



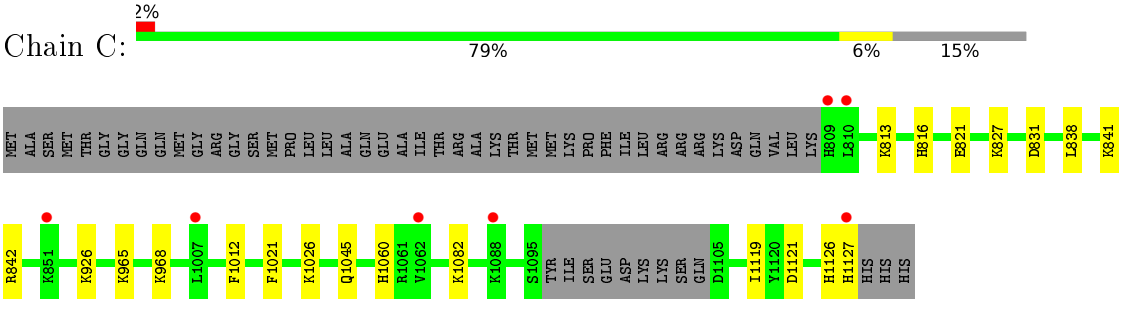
- Molecule 1: ATP-dependent helicase FUN30

Chain B:



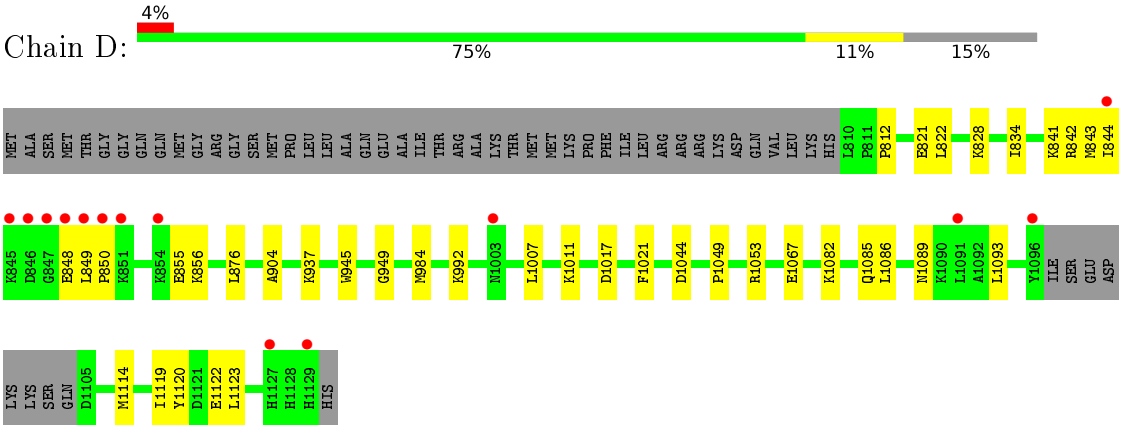
- Molecule 1: ATP-dependent helicase FUN30

Chain C:



- Molecule 1: ATP-dependent helicase FUN30

Chain D:


4%
75%
11%
15%
MET ALA SER MET THR GLY GLY GLN GLN MET GLY ARG GLY SER MET PRO LEU LEU ALA GLN GLU ALA ILE THR ARG ALA LYS THR MET MET LYS PRO PHE ILE LEU ARG ARG ARG LYS ASP GLN VAL LEU LYS HIS L810 P811 P812 E821 L822 K828 I834 K841 R842 M843 I844
K845 D846 G847 E848 L849 P850 K851 K854 E855 K856 L876 A904 K937 W945 G949 M984 K992 H1003 L1007 K1011 D1017 F1021 D1044 P1049 R1053 E1067 K1082 Q1085 L1086 N1089 K1090 L1091 A1092 L1093 Y1096 ILE SER GLU ASP
LYS LYS SER GLN D1105 M1114 I1119 Y1120 D1121 E1122 L1123 H1127 H1128 H1129 HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	114.43Å 118.39Å 111.58Å 90.00° 107.28° 90.00°	Depositor
Resolution (Å)	36.20 – 1.95 36.20 – 1.95	Depositor EDS
% Data completeness (in resolution range)	100.0 (36.20-1.95) 100.0 (36.20-1.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.15 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.10_2155: ???)	Depositor
R, R_{free}	0.187 , 0.216 0.187 , 0.216	Depositor DCC
R_{free} test set	1990 reflections (1.93%)	DCC
Wilson B-factor (Å^2)	25.9	Xtriage
Anisotropy	0.170	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 42.9	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	0.96	EDS
Total number of atoms	11466	wwPDB-VP
Average B, all atoms (Å^2)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 44.68 % of the origin peak, indicating pseudo translational symmetry.The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.4745e-04.The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[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	0.55	0/2562	0.63	0/3446
1	B	0.46	0/2549	0.55	0/3430
1	C	0.50	0/2581	0.58	0/3472
1	D	0.44	0/2611	0.56	0/3514
All	All	0.49	0/10303	0.58	0/13862

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	2520	0	2572	29	1
1	B	2509	0	2556	16	0
1	C	2533	0	2582	18	0
1	D	2564	0	2592	34	1
2	A	268	0	0	2	0
2	B	396	0	0	3	1
2	C	347	0	0	7	0
2	D	329	0	0	4	1
All	All	11466	0	10302	96	2

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 5.

All (96) 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:838:LEU:HD21	1:B:1123:LEU:HD23	1.06	1.02
1:B:838:LEU:CD2	1:B:1123:LEU:HD23	2.00	0.91
1:A:886:ASN:OD1	1:A:889:ILE:HG12	1.70	0.90
1:A:898:LEU:CD1	1:A:909:LYS:HE2	2.04	0.86
1:B:838:LEU:HD21	1:B:1123:LEU:CD2	2.00	0.84
1:D:841:LYS:HD2	1:D:844:ILE:HD11	1.61	0.83
1:C:1026:LYS:HG3	2:C:1359:HOH:O	1.83	0.79
1:D:849:LEU:HD23	1:D:850:PRO:HD2	1.67	0.77
1:A:896:ALA:O	1:A:934:THR:HG21	1.89	0.72
1:A:886:ASN:CG	1:A:889:ILE:HG12	2.11	0.71
1:B:1082:LYS:HE2	2:B:1392:HOH:O	1.94	0.67
1:A:903:TYR:HE2	1:A:912:ILE:HD11	1.62	0.64
1:A:898:LEU:HD11	1:A:909:LYS:HE2	1.79	0.64
1:D:849:LEU:CD2	1:D:850:PRO:HD2	2.27	0.64
1:D:812:PRO:HD2	1:D:1067:GLU:HG2	1.81	0.63
1:A:998:GLY:HA3	1:A:1026:LYS:HE2	1.81	0.61
1:A:842:ARG:NH2	2:A:1201:HOH:O	2.09	0.61
1:A:896:ALA:O	1:A:934:THR:CG2	2.48	0.61
1:B:851:LYS:HE2	2:C:1286:HOH:O	2.01	0.60
1:A:898:LEU:CD1	1:A:909:LYS:CE	2.79	0.60
1:B:1076:LYS:HD3	1:B:1081:GLU:OE2	2.01	0.59
1:A:903:TYR:CE2	1:A:912:ILE:HD11	2.37	0.59
1:B:835:GLN:NE2	2:B:1205:HOH:O	2.32	0.59
1:A:838:LEU:HD21	1:A:1123:LEU:HD13	1.84	0.59
1:D:842:ARG:HB3	1:D:848:GLU:HB2	1.86	0.58
1:D:855:GLU:HA	1:D:855:GLU:OE1	2.03	0.57
1:D:850:PRO:CG	1:D:856:LYS:HA	2.36	0.56
1:C:968:LYS:NZ	1:C:1012:PHE:O	2.38	0.56
1:D:850:PRO:HG2	1:D:856:LYS:HA	1.87	0.56
1:D:1119:ILE:HD12	2:D:1212:HOH:O	2.05	0.55
1:C:827:LYS:HD2	2:C:1203:HOH:O	2.06	0.55
1:A:850:PRO:HD3	2:A:1228:HOH:O	2.07	0.54
1:D:850:PRO:HG2	1:D:856:LYS:HB2	1.89	0.54
1:D:834:ILE:HG23	1:D:1123:LEU:HD11	1.89	0.54
1:D:850:PRO:HG2	1:D:856:LYS:CB	2.37	0.54
1:A:813:LYS:HD3	1:A:1060:HIS:CD2	2.44	0.52
1:B:945:TRP:CE3	1:B:984:MET:HE1	2.44	0.52
1:D:848:GLU:OE2	2:D:1201:HOH:O	2.19	0.51
1:D:1053:ARG:NH2	1:D:1089:ASN:OD1	2.32	0.51
1:B:845:LYS:HG2	1:B:846:ASP:OD1	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:843:MET:HA	1:B:848:GLU:O	2.11	0.50
1:D:1007:LEU:HG	1:D:1011:LYS:HE3	1.93	0.50
1:C:1126:HIS:CE1	2:C:1268:HOH:O	2.65	0.49
1:C:1126:HIS:O	1:C:1127:HIS:HB2	2.13	0.48
1:A:1124:GLU:OE2	1:A:1124:GLU:HA	2.12	0.48
1:A:1053:ARG:NH1	1:D:904:ALA:O	2.46	0.48
1:B:1089:ASN:HB2	2:B:1262:HOH:O	2.14	0.48
1:C:1045:GLN:HG2	2:C:1262:HOH:O	2.13	0.48
1:C:1121:ASP:HB3	1:C:1126:HIS:O	2.15	0.47
1:B:1082:LYS:HE3	1:B:1118:ILE:HG22	1.97	0.47
1:C:821:GLU:HG2	1:C:821:GLU:O	2.15	0.47
1:D:841:LYS:O	1:D:844:ILE:HG13	2.15	0.46
1:C:813:LYS:HD3	1:C:1060:HIS:CG	2.49	0.46
1:C:813:LYS:HD3	1:C:1060:HIS:CD2	2.50	0.46
1:D:850:PRO:HG2	1:D:856:LYS:CA	2.46	0.46
1:D:821:GLU:O	1:D:949:GLY:HA3	2.16	0.45
1:A:868:ILE:HG23	1:A:1079:ILE:HD11	1.99	0.45
1:A:901:PRO:O	1:A:903:TYR:N	2.49	0.45
1:B:812:PRO:HG2	1:B:1067:GLU:HG2	1.98	0.44
1:D:841:LYS:HD2	1:D:844:ILE:CD1	2.42	0.44
1:A:898:LEU:HD11	1:A:909:LYS:CE	2.47	0.44
1:D:876:LEU:HD21	1:D:1044:ASP:HB3	2.00	0.44
1:A:897:ILE:HD12	1:A:935:LEU:HD11	1.99	0.44
1:C:1082:LYS:HD3	1:C:1082:LYS:HA	1.84	0.44
1:D:937:LYS:HE3	1:D:937:LYS:HB2	1.83	0.44
1:D:841:LYS:CD	1:D:844:ILE:HD11	2.40	0.44
1:A:936:SER:HA	1:A:939:GLN:HG3	2.00	0.44
1:C:1119:ILE:HD12	2:C:1213:HOH:O	2.17	0.44
1:D:821:GLU:HG2	1:D:822:LEU:C	2.38	0.44
1:A:827:LYS:HE2	1:A:827:LYS:HB2	1.82	0.43
1:A:841:LYS:HG2	1:A:1120:TYR:CG	2.52	0.43
1:B:992:LYS:O	1:B:1019:PRO:HD2	2.19	0.43
1:B:922:PHE:CE1	1:B:984:MET:HE2	2.53	0.43
1:C:838:LEU:HD22	1:C:842:ARG:CZ	2.49	0.43
1:D:992:LYS:HE2	1:D:1017:ASP:OD2	2.18	0.43
1:B:850:PRO:HD2	1:B:856:LYS:HG2	2.01	0.42
1:A:849:LEU:HD23	1:A:856:LYS:HE3	2.01	0.42
1:C:965:LYS:HB3	1:C:965:LYS:HE3	1.86	0.42
1:D:1049:PRO:HD2	1:D:1089:ASN:HA	2.02	0.42
1:D:828:LYS:HE3	2:D:1433:HOH:O	2.19	0.42
1:C:816:HIS:HB3	2:C:1465:HOH:O	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:844:ILE:HA	1:A:844:ILE:HD13	1.92	0.42
1:A:891:THR:HB	1:A:892:LYS:HE2	2.02	0.42
1:C:926:LYS:HD2	1:C:926:LYS:HA	1.79	0.42
1:D:1114:MET:HG2	2:D:1425:HOH:O	2.20	0.42
1:D:1085:GLN:HG3	1:D:1086:LEU:HG	2.01	0.41
1:A:897:ILE:HA	1:A:934:THR:HG21	2.01	0.41
1:C:827:LYS:HE3	1:C:831:ASP:OD2	2.21	0.41
1:A:898:LEU:HD12	1:A:909:LYS:HE2	1.93	0.41
1:D:843:MET:SD	1:D:849:LEU:HD21	2.61	0.41
1:D:841:LYS:HA	1:D:844:ILE:CG1	2.51	0.41
1:C:841:LYS:HE3	1:C:841:LYS:HB3	1.86	0.41
1:D:1093:LEU:HA	1:D:1093:LEU:HD23	1.97	0.41
1:D:1082:LYS:HE3	1:D:1122:GLU:OE2	2.21	0.40
1:D:945:TRP:CE2	1:D:984:MET:HE2	2.56	0.40
1:A:900:GLU:OE2	1:A:934:THR:OG1	2.35	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1010:ASP:OD2	1:D:1120:TYR:OH[3_555]	2.12	0.08
2:B:1542:HOH:O	2:D:1444:HOH:O[3_555]	2.19	0.01

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	307/366 (84%)	301 (98%)	6 (2%)	0	100	100
1	B	305/366 (83%)	303 (99%)	2 (1%)	0	100	100
1	C	308/366 (84%)	301 (98%)	7 (2%)	0	100	100
1	D	311/366 (85%)	304 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	1231/1464 (84%)	1209 (98%)	22 (2%)	0	100 100

There are no Ramachandran outliers to report.

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	288/335 (86%)	287 (100%)	1 (0%)	94 94
1	B	286/335 (85%)	285 (100%)	1 (0%)	94 94
1	C	289/335 (86%)	288 (100%)	1 (0%)	94 94
1	D	292/335 (87%)	291 (100%)	1 (0%)	94 94
All	All	1155/1340 (86%)	1151 (100%)	4 (0%)	94 94

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1021	PHE
1	B	1021	PHE
1	C	1021	PHE
1	D	1021	PHE

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

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	309/366 (84%)	0.05	24 (7%)	16	25	16, 30, 61, 75	1 (0%)
1	B	309/366 (84%)	-0.25	7 (2%)	64	73	15, 25, 43, 64	2 (0%)
1	C	310/366 (84%)	-0.18	7 (2%)	64	73	14, 28, 50, 83	1 (0%)
1	D	312/366 (85%)	-0.00	14 (4%)	37	48	17, 29, 50, 76	1 (0%)
All	All	1240/1464 (84%)	-0.10	52 (4%)	40	51	14, 28, 53, 83	5 (0%)

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	906	ASN	6.8
1	D	849	LEU	6.7
1	D	1096	TYR	6.3
1	C	809	HIS	5.5
1	D	850	PRO	5.3
1	C	1062	VAL	5.0
1	A	909	LYS	3.8
1	A	898	LEU	3.8
1	D	844	ILE	3.7
1	D	848	GLU	3.7
1	A	931	PHE	3.7
1	C	1127	HIS	3.4
1	B	809	HIS	3.4
1	A	850	PRO	3.4
1	A	906	ASN	3.2
1	A	851	LYS	3.2
1	A	1106	VAL	3.2
1	D	1127	HIS	3.1
1	B	1105	ASP	3.1
1	D	1091	LEU	3.1
1	A	846	ASP	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	845	LYS	2.9
1	B	1123	LEU	2.8
1	A	899	ASP	2.8
1	D	846	ASP	2.8
1	D	854	LYS	2.8
1	C	1088	LYS	2.7
1	D	1003	ASN	2.7
1	D	847	GLY	2.7
1	D	1129	HIS	2.7
1	B	853	ALA	2.6
1	C	810	LEU	2.5
1	B	852	ASP	2.5
1	A	1098	SER	2.4
1	A	902	ALA	2.4
1	A	1096	TYR	2.4
1	A	854	LYS	2.4
1	A	852	ASP	2.4
1	B	845	LYS	2.3
1	D	851	LYS	2.3
1	A	1088	LYS	2.3
1	A	895	ASP	2.3
1	A	910	GLU	2.3
1	A	905	GLU	2.2
1	A	904	ALA	2.2
1	A	1097	ILE	2.1
1	C	1007	LEU	2.1
1	A	853	ALA	2.1
1	A	908	ASN	2.1
1	A	933	ASN	2.1
1	A	835	GLN	2.0
1	C	851	LYS	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

There are no ligands in this entry.

6.5 Other polymers

There are no such residues in this entry.