Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 12:06 pm BST

PDB ID	:	6I3P
Title	:	Crystal structure of DEAH-box ATPase Prp22 with bound ssRNA
Authors	:	Hamann, F.; Ficner, R.
Deposited on	:	2018-11-07
Resolution	:	2.75 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 ⓘ symbol.

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

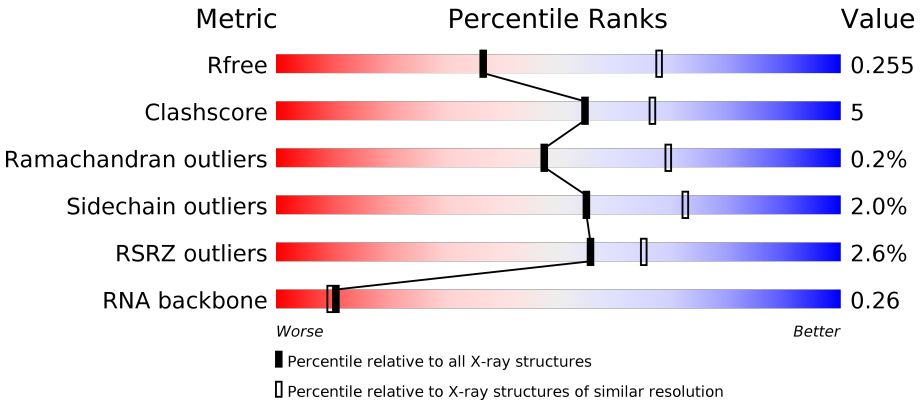
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation 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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)
RNA backbone	3102	1060 (3.02-2.50)

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 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	677	3% 78% 14% • 8%
1	B	677	3% 81% 10% • 8%
1	C	677	2% 82% 10% 7%
1	D	677	2% 83% 10% • 7%

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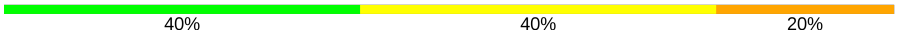
Mol	Chain	Length	Quality of chain
2	E	10	
2	F	10	
2	G	10	
2	H	10	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 20540 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 Putative pre-mRNA splicing factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	626	Total	C	N	O	S	0	0	0
			4934	3147	836	922	29			
1	B	623	Total	C	N	O	S	0	0	0
			4917	3135	833	920	29			
1	C	630	Total	C	N	O	S	0	0	0
			4976	3171	844	931	30			
1	D	630	Total	C	N	O	S	0	0	0
			4977	3172	844	931	30			

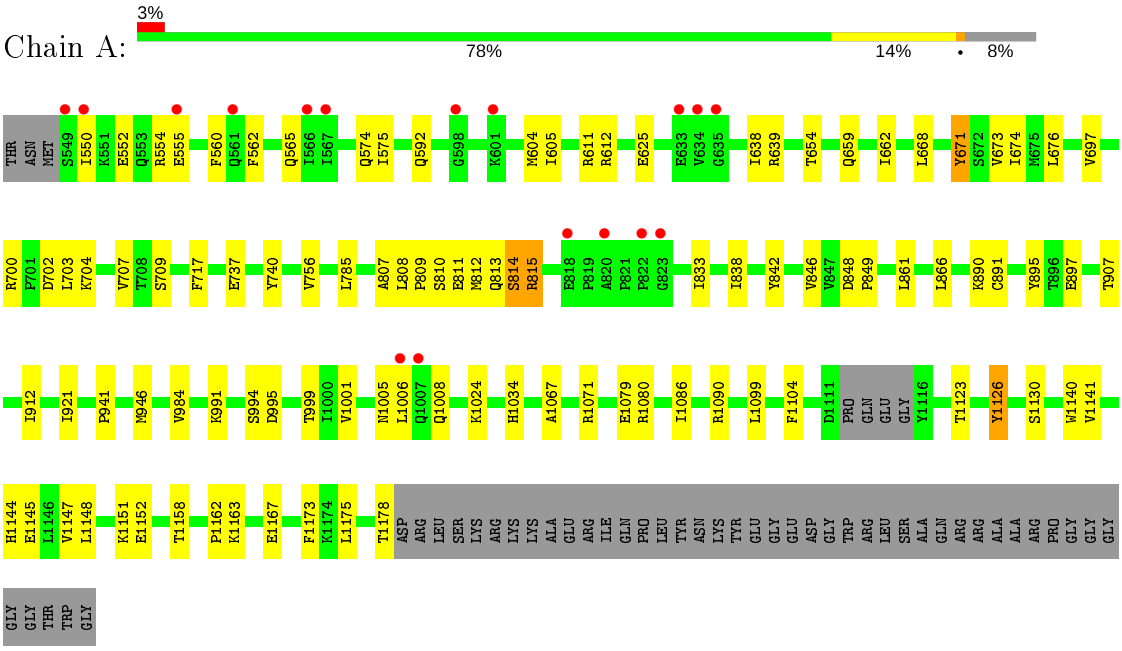
- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	10	Total	C	N	O	P	0	0	0
			184	81	18	75	10			
2	F	10	Total	C	N	O	P	0	0	0
			184	81	18	75	10			
2	G	10	Total	C	N	O	P	0	0	0
			184	81	18	75	10			
2	H	10	Total	C	N	O	P	0	0	0
			184	81	18	75	10			

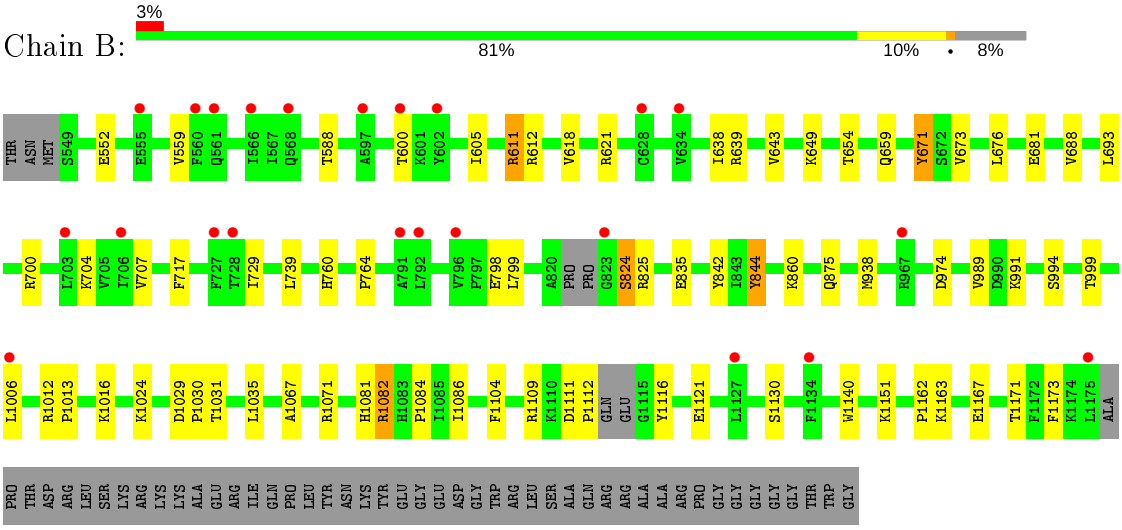
3 Residue-property plots (i)

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: Putative pre-mRNA splicing factor

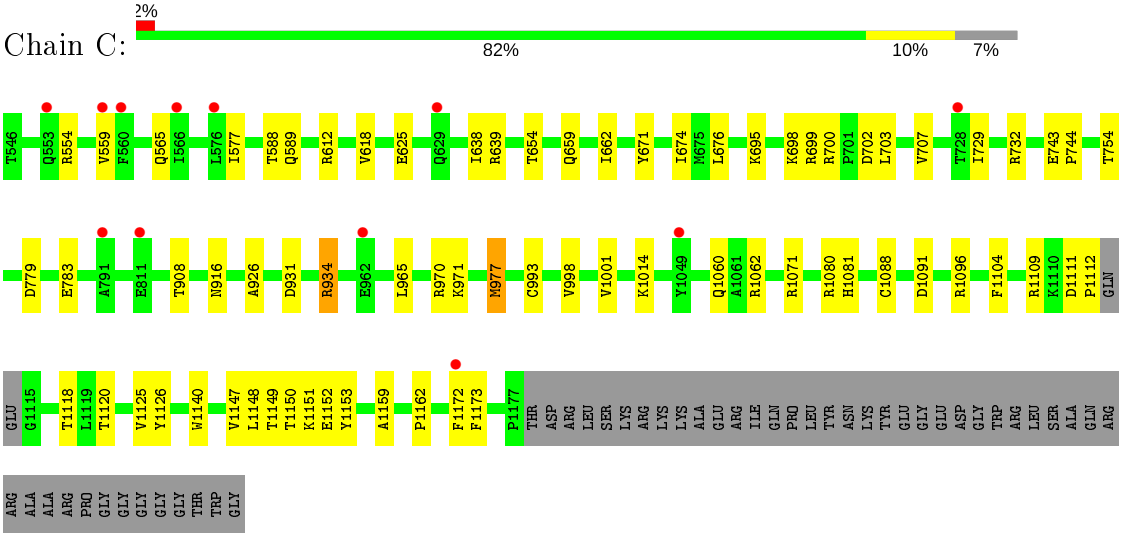


- Molecule 1: Putative pre-mRNA splicing factor



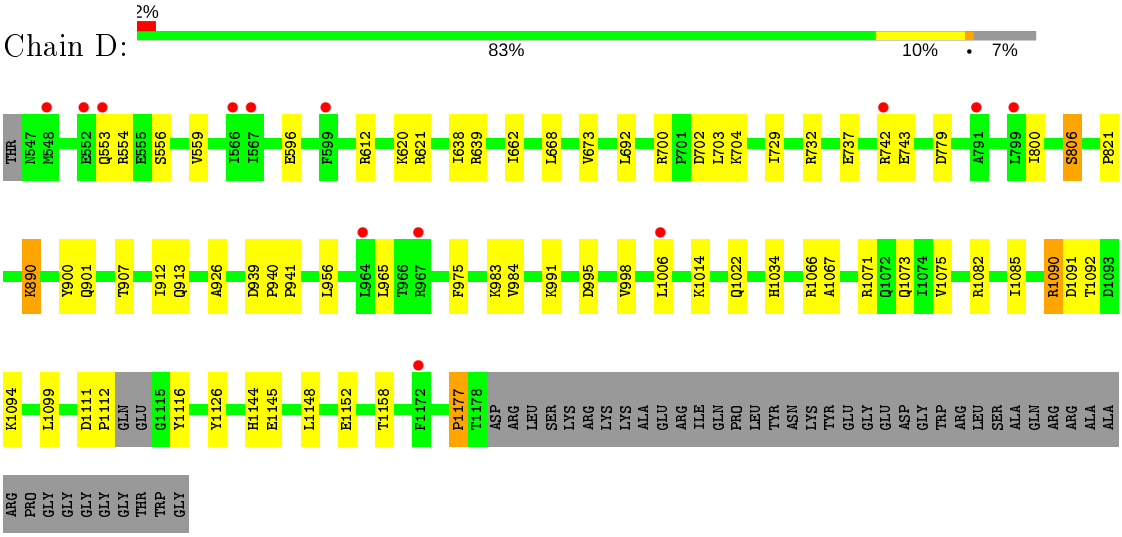
- Molecule 1: Putative pre-mRNA splicing factor

Chain C:



• Molecule 1: Putative pre-mRNA splicing factor

Chain D:



• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

Chain E:

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

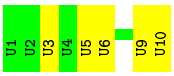
Chain F:

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

Chain G:

• Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3')

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	139.79Å 140.50Å 159.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.24 – 2.75 49.24 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.24-2.75) 100.0 (49.24-2.75)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.66 (at 2.77Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.222 , 0.253 0.224 , 0.255	Depositor DCC
R_{free} test set	4107 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	72.2	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20540	wwPDB-VP
Average B, all atoms (Å^2)	78.0	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 38.45 % 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 3.6788e-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	0.52	0/5036	0.71	0/6828
1	B	0.52	0/5017	0.73	0/6798
1	C	0.52	0/5080	0.71	0/6887
1	D	0.50	0/5081	0.70	0/6889
2	E	0.62	1/201 (0.5%)	1.19	0/309
2	F	0.85	2/201 (1.0%)	1.09	0/309
2	G	0.62	0/201	1.20	0/309
2	H	0.76	1/201 (0.5%)	1.17	0/309
All	All	0.53	4/21018 (0.0%)	0.74	0/28638

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	8	U	O3'-P	-5.92	1.54	1.61
2	F	1	U	O3'-P	-5.65	1.54	1.61
2	H	3	U	O3'-P	-5.58	1.54	1.61
2	E	1	U	O3'-P	-5.11	1.55	1.61

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	4934	0	4957	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	4917	0	4941	53	0
1	C	4976	0	5005	50	0
1	D	4977	0	5009	59	0
2	E	184	0	90	1	0
2	F	184	0	90	1	0
2	G	184	0	90	3	0
2	H	184	0	90	3	0
All	All	20540	0	20272	214	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 5.

All (214) 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:D:662:ILE:CD1	1:D:668:LEU:HG	1.72	1.19
1:C:700:ARG:NH1	1:C:703:LEU:HB2	1.58	1.18
1:A:921:ILE:HD11	1:A:946:MET:CE	1.83	1.09
1:C:977:MET:CE	1:C:1001:VAL:HG11	1.91	1.00
1:D:662:ILE:HD11	1:D:668:LEU:HG	1.40	1.00
1:D:662:ILE:CD1	1:D:668:LEU:CG	2.42	0.96
1:C:700:ARG:HH11	1:C:703:LEU:HB2	1.25	0.95
1:C:977:MET:CE	1:C:1001:VAL:CG1	2.45	0.95
1:A:921:ILE:HD11	1:A:946:MET:HE2	1.50	0.91
1:C:1126:TYR:O	1:C:1153:TYR:HA	1.72	0.89
1:A:811:GLU:N	1:A:811:GLU:OE1	2.07	0.85
1:D:1111:ASP:OD1	1:D:1112:PRO:HD2	1.81	0.80
1:C:977:MET:HE2	1:C:1001:VAL:HG11	1.63	0.80
1:C:977:MET:HE1	1:C:1001:VAL:HG11	1.67	0.77
1:B:760:HIS:HA	1:B:825:ARG:HH21	1.51	0.75
1:C:977:MET:HE1	1:C:1001:VAL:CG1	2.16	0.75
1:B:612:ARG:NH2	1:B:639:ARG:O	2.20	0.74
1:A:1006:LEU:HD11	1:A:1067:ALA:HB2	1.70	0.74
1:B:611:ARG:NH1	1:B:681:GLU:OE1	2.22	0.72
1:A:921:ILE:CD1	1:A:946:MET:CE	2.66	0.71
1:D:662:ILE:HD12	1:D:668:LEU:HG	1.71	0.70
1:D:700:ARG:HH11	1:D:703:LEU:HB2	1.57	0.70
1:A:740:TYR:CE2	1:A:897:GLU:HA	2.27	0.69
1:D:800:ILE:HD11	1:D:821:PRO:HD2	1.75	0.68
1:D:662:ILE:HD13	1:D:668:LEU:HD11	1.76	0.67
1:B:671:TYR:O	1:B:700:ARG:NH2	2.27	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:779:ASP:HB3	1:C:1014:LYS:HD2	1.76	0.66
1:D:662:ILE:HD13	1:D:668:LEU:CG	2.24	0.66
1:D:737:GLU:OE1	1:D:890:LYS:HE2	1.96	0.66
1:B:999:THR:OG1	1:B:1071:ARG:NH1	2.29	0.66
1:B:760:HIS:HA	1:B:825:ARG:NH2	2.11	0.65
1:A:575:ILE:HD11	1:A:697:VAL:HG21	1.78	0.64
1:A:991:LYS:NZ	1:A:1167:GLU:OE2	2.28	0.64
1:A:994:SER:HB2	1:A:1086:ILE:H	1.63	0.64
1:C:700:ARG:HH12	1:C:703:LEU:HB2	1.58	0.64
1:B:760:HIS:ND1	1:B:825:ARG:HD2	2.14	0.63
1:C:1109:ARG:NE	1:C:1140:TRP:CZ2	2.68	0.62
1:B:991:LYS:NZ	1:B:1167:GLU:OE2	2.34	0.61
1:D:737:GLU:OE1	1:D:890:LYS:CE	2.48	0.61
1:D:1111:ASP:OD1	1:D:1112:PRO:CD	2.49	0.60
1:A:995:ASP:OD1	1:A:1071:ARG:NH2	2.33	0.60
1:C:1104:PHE:HB2	1:C:1173:PHE:HE2	1.66	0.60
1:A:740:TYR:CD2	1:A:897:GLU:HA	2.37	0.60
1:A:812:MET:HA	1:A:815:ARG:HD3	1.84	0.59
1:C:700:ARG:NH1	1:C:703:LEU:CB	2.50	0.59
1:D:662:ILE:CD1	1:D:668:LEU:CD2	2.80	0.59
1:D:662:ILE:HD13	1:D:668:LEU:CD1	2.32	0.59
1:B:798:GLU:HB3	1:B:824:SER:HB3	1.85	0.59
1:D:673:VAL:HG22	1:D:704:LYS:HB2	1.84	0.58
1:A:1104:PHE:HB2	1:A:1173:PHE:HE2	1.69	0.58
1:A:921:ILE:CD1	1:A:946:MET:HE2	2.29	0.58
1:B:860:LYS:NZ	1:B:1121:GLU:OE1	2.37	0.58
1:B:717:PHE:CE1	1:B:938:MET:HE1	2.40	0.57
1:B:1006:LEU:HD11	1:B:1067:ALA:HB2	1.86	0.57
1:B:612:ARG:HG3	2:F:8:U:OP1	2.04	0.57
1:B:717:PHE:CD1	1:B:938:MET:CE	2.88	0.57
1:A:1178:THR:HG21	1:B:1171:THR:O	2.05	0.57
1:A:1163:LYS:HB2	1:B:1163:LYS:HB2	1.88	0.56
1:C:1111:ASP:HB2	1:C:1112:PRO:HD2	1.88	0.56
1:B:605:ILE:HG12	1:B:673:VAL:HG22	1.88	0.55
1:B:673:VAL:HG12	1:B:704:LYS:HB2	1.87	0.55
1:A:810:SER:O	1:A:814:SER:OG	2.24	0.55
1:D:1034:HIS:ND1	1:D:1158:THR:OG1	2.33	0.54
1:C:1096:ARG:NH1	1:C:1159:ALA:O	2.39	0.54
1:D:1006:LEU:HD11	1:D:1067:ALA:HB2	1.90	0.54
1:B:676:LEU:HD12	1:B:707:VAL:HG22	1.90	0.53
1:B:994:SER:HB2	1:B:1086:ILE:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:612:ARG:NH2	1:D:639:ARG:O	2.41	0.53
1:A:605:ILE:HG12	1:A:673:VAL:HG22	1.89	0.53
1:D:662:ILE:HD13	1:D:668:LEU:HD21	1.91	0.53
1:D:662:ILE:CD1	1:D:668:LEU:CD1	2.86	0.52
1:D:553:GLN:OE1	1:D:621:ARG:NH1	2.42	0.52
1:B:717:PHE:CD1	1:B:938:MET:HE3	2.44	0.52
1:A:912:ILE:HG12	1:A:941:PRO:HG3	1.92	0.52
1:B:974:ASP:OD2	1:B:1081:HIS:NE2	2.42	0.52
1:C:1118:THR:HG23	1:C:1125:VAL:HG13	1.92	0.52
1:A:1080:ARG:HH12	1:D:1075:VAL:HG11	1.75	0.52
1:D:662:ILE:HD11	1:D:668:LEU:CG	2.24	0.52
1:B:1031:THR:OG1	1:B:1035:LEU:HD12	2.11	0.51
1:C:1148:LEU:HD13	1:C:1152:GLU:HG3	1.91	0.51
1:D:1090:ARG:O	1:D:1092:THR:N	2.43	0.51
1:D:702:ASP:OD1	1:D:702:ASP:N	2.42	0.51
1:C:1149:THR:OG1	1:C:1150:THR:N	2.44	0.50
1:D:1144:HIS:CD2	1:D:1145:GLU:HG3	2.46	0.50
1:A:668:LEU:O	1:A:700:ARG:NH1	2.43	0.50
1:D:559:VAL:HG23	1:D:729:ILE:HD13	1.94	0.50
1:C:1111:ASP:HB2	1:C:1112:PRO:CD	2.41	0.50
1:D:995:ASP:OD1	1:D:1071:ARG:NH2	2.43	0.50
1:C:559:VAL:HG23	1:C:729:ILE:HD13	1.93	0.50
1:A:1144:HIS:CD2	1:A:1145:GLU:HG3	2.46	0.50
1:C:783:GLU:OE1	1:C:1014:LYS:NZ	2.37	0.50
1:A:1178:THR:CG2	1:B:1171:THR:O	2.60	0.49
1:A:833:ILE:HG12	1:A:838:ILE:HG12	1.93	0.49
1:B:600:THR:HB	1:B:649:LYS:HD3	1.94	0.49
1:C:1060:GLN:NE2	1:C:1062:ARG:HH21	2.11	0.49
1:C:700:ARG:HG2	1:C:700:ARG:NH1	2.28	0.49
1:C:700:ARG:HH11	1:C:703:LEU:CB	2.11	0.49
1:A:562:PHE:CD1	1:A:562:PHE:N	2.81	0.48
1:B:611:ARG:HH12	1:B:681:GLU:CD	2.15	0.48
1:B:717:PHE:HD1	1:B:938:MET:HE3	1.77	0.48
1:A:848:ASP:OD2	1:A:895:TYR:OH	2.30	0.48
1:C:998:VAL:HG12	1:C:1071:ARG:HG3	1.95	0.48
1:C:702:ASP:N	1:C:702:ASP:OD1	2.44	0.48
1:C:971:LYS:HG3	1:C:1081:HIS:CD2	2.48	0.48
1:C:1147:VAL:HG21	2:G:4:U:C4	2.49	0.48
1:C:588:THR:HG22	1:C:618:VAL:HG13	1.95	0.48
1:D:612:ARG:HE	1:D:638:ILE:HD12	1.79	0.48
1:A:861:LEU:HD22	1:A:1123:THR:HG21	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:806:SER:HG	2:H:6:U:P	2.36	0.48
1:A:846:VAL:HG12	1:A:891:CYS:SG	2.54	0.48
1:C:674:ILE:HG12	1:C:703:LEU:HD11	1.96	0.48
1:B:559:VAL:HG23	1:B:729:ILE:HD13	1.96	0.47
1:D:662:ILE:HD12	1:D:668:LEU:CD2	2.44	0.47
1:A:984:VAL:HG11	1:A:1099:LEU:HD23	1.96	0.47
1:D:662:ILE:CD1	1:D:668:LEU:HD21	2.44	0.47
1:B:799:LEU:HA	1:B:825:ARG:O	2.15	0.47
1:D:1148:LEU:HD13	1:D:1152:GLU:HG3	1.97	0.47
1:A:737:GLU:OE1	1:A:890:LYS:NZ	2.48	0.47
1:D:912:ILE:HG12	1:D:941:PRO:HG3	1.96	0.47
1:A:1148:LEU:HD13	1:A:1152:GLU:HG3	1.98	0.47
1:D:926:ALA:HA	1:D:965:LEU:HD22	1.95	0.47
1:C:700:ARG:HG2	1:C:700:ARG:HH11	1.79	0.46
1:B:764:PRO:O	1:B:825:ARG:NH1	2.48	0.46
1:C:926:ALA:HA	1:C:965:LEU:HD22	1.97	0.46
1:B:739:LEU:HD12	1:B:739:LEU:N	2.30	0.46
1:C:1118:THR:HG23	1:C:1125:VAL:CG1	2.46	0.46
1:D:991:LYS:O	1:D:1094:LYS:HE2	2.14	0.46
1:A:1001:VAL:O	1:A:1005:ASN:ND2	2.48	0.46
1:C:612:ARG:NH2	1:C:639:ARG:O	2.48	0.46
1:B:588:THR:HG22	1:B:618:VAL:HG13	1.97	0.45
1:B:1082:ARG:CZ	1:C:1080:ARG:HH21	2.30	0.45
1:C:589:GLN:NE2	1:C:625:GLU:OE1	2.47	0.45
1:A:676:LEU:HD12	1:A:707:VAL:HG22	1.97	0.45
1:B:1024:LYS:NZ	1:B:1130:SER:O	2.47	0.45
1:D:662:ILE:HD12	1:D:668:LEU:CG	2.39	0.45
1:C:977:MET:HE3	1:C:1001:VAL:CG1	2.42	0.45
1:C:659:GLN:O	1:C:662:ILE:HG22	2.17	0.45
1:A:1090:ARG:HD3	1:C:1091:ASP:HB2	1.99	0.44
1:D:662:ILE:HD13	1:D:668:LEU:CD2	2.44	0.44
1:D:662:ILE:HG21	1:D:692:LEU:HD13	1.98	0.44
1:A:554:ARG:NH2	1:A:592:GLN:OE1	2.51	0.44
1:A:612:ARG:NH2	1:A:639:ARG:O	2.50	0.44
1:C:1120:THR:HA	1:D:1177:PRO:HG2	1.99	0.44
1:A:756:VAL:HG11	1:A:785:LEU:HD21	1.98	0.44
1:A:555:GLU:HG2	1:A:560:PHE:CZ	2.53	0.44
1:A:574:GLN:HA	1:A:704:LYS:HE3	2.00	0.44
1:D:662:ILE:HD12	1:D:662:ILE:HA	1.89	0.44
1:A:604:MET:H	1:A:671:TYR:HA	1.82	0.44
1:A:1024:LYS:NZ	1:A:1130:SER:O	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:550:ILE:HD11	1:A:625:GLU:HA	2.00	0.44
1:B:1029:ASP:OD1	1:B:1030:PRO:HD2	2.18	0.44
1:B:638:ILE:HG22	1:B:654:THR:HG23	1.99	0.44
1:B:659:GLN:HE21	1:B:688:VAL:HG11	1.83	0.44
1:A:702:ASP:N	1:A:702:ASP:OD1	2.51	0.43
1:A:921:ILE:CD1	1:A:946:MET:HE1	2.44	0.43
1:A:709:SER:HB2	1:A:717:PHE:CD2	2.53	0.43
1:D:1073:GLN:NE2	2:H:10:U:OP2	2.51	0.43
1:B:1111:ASP:HA	1:B:1112:PRO:HD3	1.88	0.43
1:B:717:PHE:CD1	1:B:938:MET:HE1	2.52	0.43
1:A:1126:TYR:CE2	1:A:1151:LYS:HE2	2.53	0.43
1:D:554:ARG:NH2	1:D:596:GLU:OE2	2.45	0.43
1:D:984:VAL:HG11	1:D:1099:LEU:HD23	2.01	0.43
1:D:998:VAL:HG12	1:D:1071:ARG:HG3	2.01	0.43
1:A:1175:LEU:HD21	1:B:1173:PHE:CD1	2.53	0.43
1:A:659:GLN:O	1:A:662:ILE:HG22	2.18	0.43
1:A:1034:HIS:ND1	1:A:1158:THR:OG1	2.40	0.43
1:C:1111:ASP:CB	1:C:1112:PRO:CD	2.97	0.43
1:D:940:PRO:HA	1:D:941:PRO:HD3	1.94	0.43
1:C:1140:TRP:CE2	1:C:1162:PRO:HG3	2.54	0.42
1:D:900:TYR:CD2	1:D:901:GLN:HG3	2.54	0.42
1:D:900:TYR:HD2	1:D:901:GLN:HG3	1.85	0.42
1:C:699:ARG:HG3	1:C:699:ARG:HH11	1.83	0.42
1:C:676:LEU:HD12	1:C:707:VAL:HG12	2.01	0.42
1:A:1079:GLU:OE2	1:D:1071:ARG:NH1	2.53	0.42
1:D:956:LEU:HD22	1:D:983:LYS:HG2	2.01	0.42
1:C:695:LYS:O	1:C:698:LYS:HG2	2.20	0.42
1:D:779:ASP:HB3	1:D:1014:LYS:HD2	2.01	0.42
1:B:1035:LEU:HD23	1:B:1035:LEU:HA	1.90	0.42
1:A:1140:TRP:CD2	1:A:1162:PRO:HG3	2.55	0.42
1:B:989:VAL:HG13	1:B:1084:PRO:HG2	2.02	0.42
1:C:638:ILE:HG22	1:C:654:THR:HG23	2.02	0.42
1:B:676:LEU:HD11	1:B:693:LEU:HD12	2.02	0.41
2:G:2:U:O2'	2:G:3:U:H5	2.03	0.41
1:B:835:GLU:OE2	1:B:875:GLN:HG3	2.20	0.41
1:D:913:GLN:NE2	1:D:939:ASP:HB3	2.35	0.41
1:A:674:ILE:HG12	1:A:703:LEU:HD11	2.02	0.41
1:C:577:ILE:HG13	1:C:707:VAL:HG23	2.03	0.41
1:C:993:CYS:HB3	1:C:1088:CYS:HB3	2.02	0.41
2:G:1:U:C2'	2:G:1:U:O2	2.69	0.41
1:D:612:ARG:NH1	1:D:1066:ARG:HH22	2.18	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:806:SER:OG	2:H:6:U:P	2.78	0.41
1:A:1175:LEU:HD21	1:B:1173:PHE:CG	2.55	0.41
1:A:807:ALA:HA	1:A:1008:GLN:HG2	2.02	0.41
1:A:1175:LEU:CD2	1:B:1173:PHE:CD1	3.04	0.41
1:B:799:LEU:HD12	1:B:825:ARG:O	2.21	0.41
1:A:813:GLN:HB3	1:A:813:GLN:HE21	1.62	0.41
1:D:737:GLU:OE1	1:D:890:LYS:HE3	2.20	0.41
1:A:1147:VAL:HG11	2:E:4:U:C4	2.55	0.41
1:A:740:TYR:CD2	1:A:897:GLU:CA	3.04	0.41
1:B:1013:PRO:HG2	1:B:1016:LYS:HB2	2.02	0.41
1:C:743:GLU:HG2	1:C:744:PRO:HD2	2.03	0.41
1:C:931:ASP:OD1	1:C:934:ARG:HD3	2.21	0.41
1:D:742:ARG:NH2	1:D:743:GLU:OE1	2.50	0.41
1:B:842:TYR:HA	1:B:844:TYR:HE1	1.86	0.41
1:B:1104:PHE:HB2	1:B:1173:PHE:HE2	1.86	0.40
1:B:760:HIS:CE1	1:B:825:ARG:HB3	2.56	0.40
1:D:1085:ILE:H	1:D:1085:ILE:HG13	1.55	0.40
1:A:638:ILE:HG22	1:A:654:THR:HG23	2.01	0.40
1:B:1140:TRP:CD2	1:B:1162:PRO:HG3	2.56	0.40
1:D:700:ARG:NH1	1:D:703:LEU:HB2	2.30	0.40
1:B:621:ARG:HD2	1:B:621:ARG:HA	1.87	0.40
1:A:808:LEU:HA	1:A:809:PRO:HD3	1.97	0.40
1:A:866:LEU:HA	1:A:866:LEU:HD23	1.96	0.40
1:D:556:SER:O	1:D:732:ARG:NH1	2.33	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	622/677 (92%)	605 (97%)	16 (3%)	1 (0%)	47 69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	617/677 (91%)	598 (97%)	18 (3%)	1 (0%)	47 69
1	C	626/677 (92%)	608 (97%)	18 (3%)	0	100 100
1	D	626/677 (92%)	607 (97%)	17 (3%)	2 (0%)	41 60
All	All	2491/2708 (92%)	2418 (97%)	69 (3%)	4 (0%)	47 69

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	1091	ASP
1	D	1177	PRO
1	A	842	TYR
1	B	643	VAL

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	539/581 (93%)	528 (98%)	11 (2%)	55 72
1	B	537/581 (92%)	527 (98%)	10 (2%)	57 73
1	C	545/581 (94%)	533 (98%)	12 (2%)	52 70
1	D	545/581 (94%)	535 (98%)	10 (2%)	59 75
All	All	2166/2324 (93%)	2123 (98%)	43 (2%)	55 72

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	552	GLU
1	A	565	GLN
1	A	611	ARG
1	A	671	TYR
1	A	814	SER
1	A	815	ARG
1	A	849	PRO

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Mol	Chain	Res	Type
1	A	907	THR
1	A	999	THR
1	A	1126	TYR
1	A	1141	VAL
1	B	552	GLU
1	B	611	ARG
1	B	671	TYR
1	B	824	SER
1	B	844	TYR
1	B	1012	ARG
1	B	1082	ARG
1	B	1109	ARG
1	B	1116	TYR
1	B	1151	LYS
1	C	554	ARG
1	C	565	GLN
1	C	671	TYR
1	C	732	ARG
1	C	754	THR
1	C	908	THR
1	C	916	ASN
1	C	934	ARG
1	C	970	ARG
1	C	977	MET
1	C	1151	LYS
1	C	1172	PHE
1	D	620	LYS
1	D	806	SER
1	D	890	LYS
1	D	907	THR
1	D	975	PHE
1	D	1022	GLN
1	D	1082	ARG
1	D	1090	ARG
1	D	1116	TYR
1	D	1126	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	680	HIS
1	A	813	GLN

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Mol	Chain	Res	Type
1	A	1005	ASN
1	A	1144	HIS
1	B	573	ASN
1	B	574	GLN
1	B	609	GLN
1	B	659	GLN
1	B	680	HIS
1	C	573	ASN
1	C	680	HIS
1	C	916	ASN
1	C	1083	HIS
1	D	1007	GLN
1	D	1072	GLN
1	D	1081	HIS
1	D	1106	ASN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	8/10 (80%)	2 (25%)	0
2	F	8/10 (80%)	2 (25%)	1 (12%)
2	G	8/10 (80%)	4 (50%)	1 (12%)
2	H	8/10 (80%)	2 (25%)	0
All	All	32/40 (80%)	10 (31%)	2 (6%)

All (10) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	5	U
2	E	9	U
2	F	5	U
2	F	9	U
2	G	2	U
2	G	3	U
2	G	5	U
2	G	9	U
2	H	5	U
2	H	9	U

All (2) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	F	9	U
2	G	2	U

5.4 Non-standard residues in protein, DNA, RNA chains

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	626/677 (92%)	0.40	17 (2%) 54 63	53, 77, 109, 152	0
1	B	623/677 (92%)	0.36	23 (3%) 41 49	54, 74, 102, 128	0
1	C	630/677 (93%)	0.28	12 (1%) 66 75	53, 73, 102, 123	0
1	D	630/677 (93%)	0.25	13 (2%) 63 72	53, 75, 107, 133	0
2	E	10/10 (100%)	0.59	0 100 100	64, 84, 110, 116	0
2	F	10/10 (100%)	0.44	0 100 100	63, 73, 86, 101	0
2	G	10/10 (100%)	0.28	0 100 100	63, 79, 96, 107	0
2	H	10/10 (100%)	0.20	0 100 100	67, 84, 104, 107	0
All	All	2549/2748 (92%)	0.32	65 (2%) 56 65	53, 75, 106, 152	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	822	PRO	4.7
1	A	550	ILE	3.8
1	C	728	THR	3.6
1	B	602	TYR	3.6
1	A	566	ILE	3.5
1	A	633	GLU	3.3
1	B	561	GLN	3.2
1	A	820	ALA	3.2
1	A	818	GLU	3.1
1	C	811	GLU	3.0
1	D	599	PHE	3.0
1	B	706	ILE	2.8
1	B	555	GLU	2.8
1	C	553	GLN	2.8
1	D	742	ARG	2.7
1	B	1175	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	567	ILE	2.7
1	A	634	VAL	2.7
1	D	567	ILE	2.7
1	D	553	GLN	2.6
1	B	792	LEU	2.6
1	B	967	ARG	2.6
1	C	560	PHE	2.6
1	B	703	LEU	2.6
1	D	566	ILE	2.5
1	D	1006	LEU	2.5
1	D	799	LEU	2.5
1	C	962	GLU	2.4
1	B	566	ILE	2.4
1	A	549	SER	2.4
1	B	560	PHE	2.4
1	B	600	THR	2.4
1	A	561	GLN	2.3
1	A	635	GLY	2.3
1	A	823	GLY	2.3
1	B	597	ALA	2.3
1	D	552	GLU	2.3
1	B	728	THR	2.3
1	D	548	MET	2.3
1	B	727	PHE	2.3
1	B	796	VAL	2.2
1	A	1006	LEU	2.2
1	B	1127	LEU	2.2
1	B	568	GLN	2.2
1	B	634	VAL	2.2
1	B	628	CYS	2.1
1	C	1172	PHE	2.1
1	A	1007	GLN	2.1
1	A	598	GLY	2.1
1	C	1049	TYR	2.1
1	D	791	ALA	2.1
1	D	1172	PHE	2.1
1	D	964	LEU	2.1
1	A	555	GLU	2.1
1	B	1006	LEU	2.1
1	A	601	LYS	2.1
1	C	791	ALA	2.1
1	D	967	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	576	LEU	2.0
1	B	823	GLY	2.0
1	B	791	ALA	2.0
1	B	1134	PHE	2.0
1	C	559	VAL	2.0
1	C	566	ILE	2.0
1	C	629	GLN	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.