Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 10:56 pm BST

PDB ID	:	6I3O
Title	:	Crystal structure of DEAH-box ATPase Prp22
Authors	:	Hamann, F.; Ficner, R.
Deposited on	:	2018-11-07
Resolution	:	3.25 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 ⓘ) were used in the production of this report:

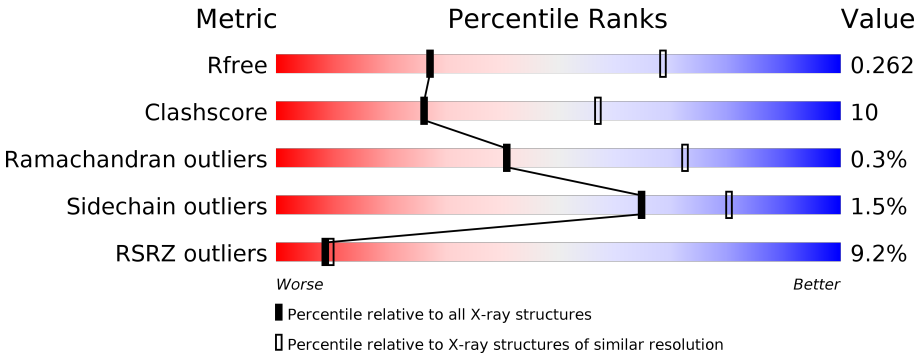
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation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

1 Overall quality at a glance

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

The reported resolution of this entry is 3.25 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	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

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	6% 67% 20% • 13%
1	B	677	10% 69% 16% • 15%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 9208 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.

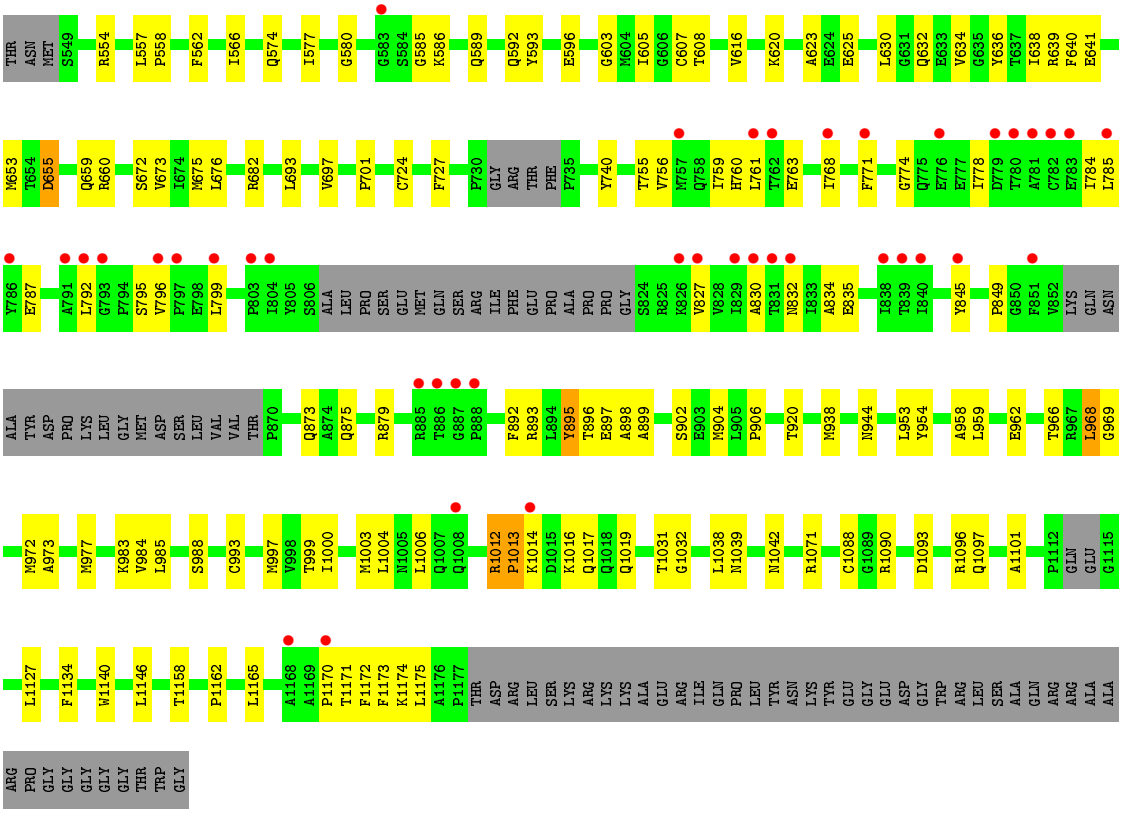
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	589	Total	C	N	O	S	0	0	0
			4652	2970	788	867	27			
1	B	577	Total	C	N	O	S	0	0	0
			4556	2916	772	841	27			

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.

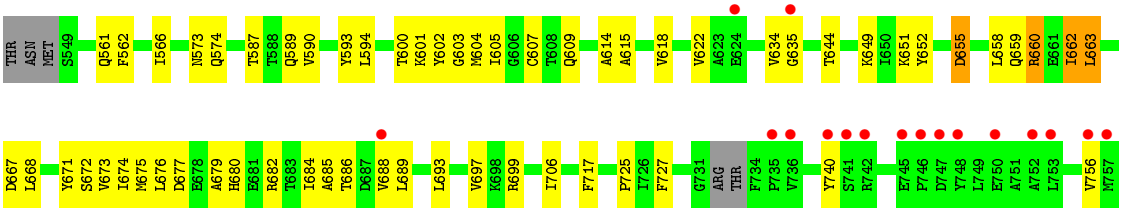
• Molecule 1: Putative pre-mRNA splicing factor

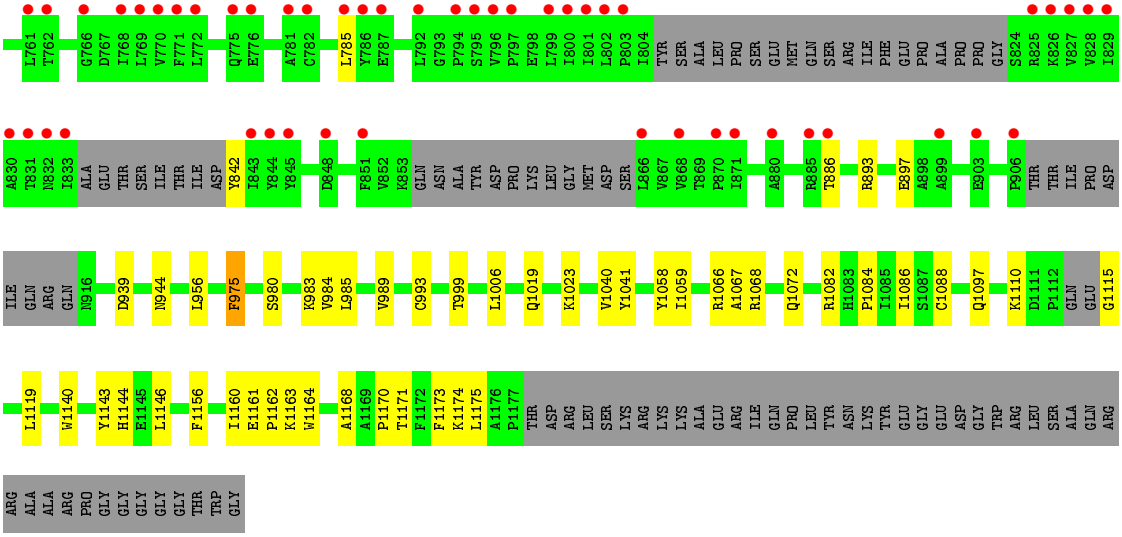
Chain A:



• Molecule 1: Putative pre-mRNA splicing factor

Chain B:




L761 T762 G766 D767 I768 L769 V770 F771 L772 Q775 E776 A781 C782 L785 Y786 E787 L792 G793 P794 S795 V796 P797 E798 L799 I800 I801 L802 P803 I804 TYR SER ALA LEU PRO SER GLU MET GLN SER ARG ILE PHE GLU PRO ALA PRO PRO GLY S824 R825 K826 V827 V828 I829
A830 T831 N832 I833 ALA GLU THR SER ILE THR ILE ASP Y842 I843 Y844 Y845 D848 F851 V852 K853 GLN ASN ALA TYR ASP PRO LYS LEU GLY MET ASP SER L866 V867 V868 T869 P870 I871 A880 R885 T886 R893 E897 A898 A899 E903 P906 THR THR ILE PRO ASP
ILE GLN ARG GLN N916 D939 N944 L956 F975 S980 K983 V984 L985 V989 C993 T999 L1006 Q1019 K1023 Y1040 Y1041 Y1058 I1059 R1066 A1067 R1068 Q1072 R1082 H1083 P1084 I1085 I1086 S1087 C1088 Q1097 K1110 D1111 P1112 GLN GLU G1115
L1119 W1140 Y1143 H1144 E1145 L1146 F1156 I1160 E1161 P1162 K1163 W1164 A1168 A1169 P1170 T1171 F1172 F1173 K1174 L1175 A1176 P1177 THR ASP ARG LEU SER LYS ARG LYS LYS ALA GLU ARG ILE GLN PRO LEU TYR ASN LYS TYR GLU GLY GLU ASP GLY TRP ARG LEU SER ALA GLN ARG
ARG ALA ALA ARG PRO GLY GLY GLY GLY GLY THR TRP GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	67.53Å 93.64Å 218.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	86.06 – 3.25 86.06 – 3.25	Depositor EDS
% Data completeness (in resolution range)	99.6 (86.06-3.25) 99.6 (86.06-3.25)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.63 (at 3.26Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.247 , 0.264 0.248 , 0.262	Depositor DCC
R_{free} test set	1123 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	95.7	Xtriage
Anisotropy	0.269	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 71.4	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	0.92	EDS
Total number of atoms	9208	wwPDB-VP
Average B, all atoms (Å^2)	112.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.60% 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	0.73	0/4745	0.89	0/6429
1	B	0.67	0/4646	0.81	0/6291
All	All	0.70	0/9391	0.85	0/12720

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	4652	0	4686	107	0
1	B	4556	0	4601	86	0
All	All	9208	0	9287	193	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 10.

All (193) 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:761:LEU:HD11	1:A:792:LEU:HD21	1.33	1.06
1:A:1014:LYS:HA	1:A:1017:GLN:HG3	1.50	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:618:VAL:HG12	1:B:652:TYR:HE2	1.42	0.85
1:B:587:THR:HG22	1:B:677:ASP:OD2	1.80	0.82
1:A:608:THR:HA	1:A:653:MET:O	1.80	0.82
1:B:655:ASP:O	1:B:659:GLN:HG3	1.81	0.81
1:A:761:LEU:HD21	1:A:796:VAL:HG13	1.67	0.76
1:B:675:MET:HG3	1:B:706:ILE:HB	1.68	0.76
1:A:1165:LEU:HB3	1:A:1173:PHE:HD2	1.51	0.75
1:B:1082:ARG:HA	1:B:1082:ARG:HE	1.53	0.74
1:B:658:LEU:O	1:B:658:LEU:HD12	1.88	0.73
1:B:1119:LEU:HD23	1:B:1173:PHE:HE2	1.54	0.72
1:A:1038:LEU:HD12	1:A:1090:ARG:NH1	2.06	0.71
1:A:958:ALA:HB2	1:A:972:MET:HE1	1.73	0.70
1:A:1012:ARG:NH1	1:A:1012:ARG:HG2	2.07	0.70
1:A:1012:ARG:HG2	1:A:1012:ARG:HH11	1.55	0.70
1:A:988:SER:HB3	1:A:997:MET:HG3	1.72	0.70
1:A:554:ARG:NH1	1:A:596:GLU:OE2	2.26	0.69
1:B:1006:LEU:HD11	1:B:1067:ALA:HB2	1.74	0.69
1:B:1161:GLU:OE1	1:B:1163:LYS:HE3	1.94	0.68
1:A:592:GLN:NE2	1:A:625:GLU:OE1	2.26	0.68
1:A:659:GLN:HE22	1:A:920:THR:HG23	1.57	0.68
1:A:968:LEU:O	1:A:968:LEU:HD12	1.94	0.67
1:B:1082:ARG:HA	1:B:1082:ARG:NE	2.10	0.67
1:B:660:ARG:CG	1:B:660:ARG:HH11	2.08	0.66
1:B:682:ARG:HD3	1:B:717:PHE:HZ	1.58	0.66
1:B:660:ARG:HH11	1:B:660:ARG:HG3	1.61	0.65
1:A:1038:LEU:C	1:A:1038:LEU:HD13	2.17	0.65
1:B:662:ILE:HG12	1:B:668:LEU:HD11	1.79	0.65
1:A:1175:LEU:O	1:A:1175:LEU:HD12	1.98	0.64
1:B:842:TYR:N	1:B:886:THR:HG1	1.97	0.63
1:A:557:LEU:HD23	1:A:585:GLY:HA3	1.81	0.63
1:B:644:THR:HG21	1:B:651:LYS:HE2	1.81	0.63
1:B:1168:ALA:O	1:B:1170:PRO:HD3	1.99	0.63
1:B:1175:LEU:HD12	1:B:1175:LEU:C	2.19	0.62
1:A:835:GLU:OE2	1:A:875:GLN:NE2	2.33	0.61
1:A:792:LEU:HG	1:A:796:VAL:HG21	1.81	0.61
1:A:1093:ASP:O	1:A:1097:GLN:HB2	2.01	0.61
1:A:1038:LEU:HD11	1:A:1042:ASN:ND2	2.16	0.60
1:A:993:CYS:HB3	1:A:1088:CYS:SG	2.41	0.60
1:A:660:ARG:NH1	1:A:973:ALA:O	2.34	0.60
1:A:1038:LEU:CD1	1:A:1042:ASN:ND2	2.65	0.59
1:A:1003:MET:HA	1:A:1006:LEU:HD23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:655:ASP:O	1:B:659:GLN:CG	2.50	0.59
1:B:684:ILE:HD12	1:B:684:ILE:N	2.17	0.59
1:B:740:TYR:HE1	1:B:893:ARG:HD2	1.67	0.58
1:B:601:LYS:HG3	1:B:602:TYR:HD1	1.70	0.57
1:A:1038:LEU:HD13	1:A:1038:LEU:O	2.05	0.57
1:A:896:THR:O	1:A:899:ALA:HB3	2.04	0.56
1:B:682:ARG:HD3	1:B:717:PHE:CZ	2.37	0.56
1:B:600:THR:HB	1:B:649:LYS:HD3	1.87	0.56
1:B:679:ALA:O	1:B:682:ARG:HG3	2.05	0.56
1:B:671:TYR:HD2	1:B:674:ILE:HD11	1.70	0.56
1:A:1127:LEU:HD13	1:A:1134:PHE:HA	1.87	0.55
1:A:760:HIS:CD2	1:A:799:LEU:HD13	2.42	0.55
1:B:622:VAL:HG12	1:B:634:VAL:HG21	1.87	0.55
1:A:1016:LYS:HD2	1:A:1019:GLN:HG3	1.89	0.55
1:B:993:CYS:HB3	1:B:1088:CYS:HB3	1.89	0.55
1:A:616:VAL:HG22	1:A:636:TYR:CE2	2.42	0.55
1:A:958:ALA:HB2	1:A:972:MET:CE	2.37	0.54
1:A:1165:LEU:HB3	1:A:1173:PHE:CD2	2.39	0.54
1:B:671:TYR:HD2	1:B:674:ILE:CD1	2.20	0.54
1:A:554:ARG:NH2	1:A:592:GLN:OE1	2.40	0.54
1:B:618:VAL:HG12	1:B:652:TYR:CE2	2.32	0.54
1:B:685:ALA:O	1:B:688:VAL:HB	2.07	0.54
1:A:873:GLN:HB2	1:A:906:PRO:HA	1.90	0.54
1:A:895:TYR:CD1	1:A:895:TYR:N	2.77	0.53
1:A:969:GLY:HA2	1:A:972:MET:HE2	1.90	0.53
1:A:759:ILE:HG13	1:A:763:GLU:HG3	1.90	0.53
1:B:589:GLN:HB3	1:B:593:TYR:CZ	2.44	0.53
1:A:562:PHE:O	1:A:566:ILE:HG13	2.09	0.53
1:B:614:ALA:O	1:B:618:VAL:HG23	2.09	0.53
1:A:985:LEU:O	1:A:988:SER:OG	2.26	0.52
1:A:792:LEU:HD23	1:A:796:VAL:HG11	1.92	0.52
1:B:1143:TYR:CE2	1:B:1146:LEU:HG	2.45	0.52
1:B:1097:GLN:HG2	1:B:1164:TRP:CD1	2.45	0.52
1:A:577:ILE:HD12	1:A:724:CYS:SG	2.51	0.51
1:B:609:GLN:HG3	1:B:615:ALA:HA	1.93	0.51
1:A:1038:LEU:CD1	1:A:1090:ARG:NH1	2.72	0.51
1:A:623:ALA:HA	1:A:634:VAL:HG11	1.93	0.51
1:A:999:THR:OG1	1:A:1071:ARG:NH1	2.43	0.51
1:A:607:CYS:HA	1:A:675:MET:O	2.11	0.51
1:A:993:CYS:CB	1:A:1088:CYS:SG	2.99	0.51
1:A:774:GLY:O	1:A:778:ILE:HG12	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:799:LEU:HD11	1:A:827:VAL:HG23	1.93	0.50
1:B:660:ARG:NH2	1:B:975:PHE:O	2.45	0.50
1:B:676:LEU:HD11	1:B:693:LEU:HD12	1.93	0.50
1:B:685:ALA:O	1:B:689:LEU:N	2.43	0.50
1:B:999:THR:HG23	1:B:1041:TYR:CD2	2.47	0.50
1:B:756:VAL:HG11	1:B:785:LEU:HD21	1.93	0.49
1:B:980:SER:O	1:B:984:VAL:HG23	2.12	0.49
1:B:662:ILE:CG1	1:B:668:LEU:HD11	2.42	0.49
1:A:574:GLN:NE2	1:A:697:VAL:HG13	2.28	0.49
1:B:1084:PRO:HG2	1:B:1086:ILE:HD11	1.95	0.49
1:B:680:HIS:ND1	1:B:680:HIS:N	2.59	0.49
1:A:1038:LEU:HD12	1:A:1090:ARG:CZ	2.42	0.49
1:A:1000:ILE:O	1:A:1004:LEU:HG	2.12	0.49
1:B:603:GLY:HA3	1:B:672:SER:HB2	1.94	0.48
1:B:574:GLN:OE1	1:B:697:VAL:HG13	2.13	0.48
1:A:983:LYS:NZ	1:A:1101:ALA:HB1	2.29	0.48
1:A:639:ARG:HG2	1:A:640:PHE:CD2	2.49	0.48
1:A:620:LYS:HG2	1:A:630:LEU:HD22	1.96	0.48
1:B:671:TYR:CD2	1:B:674:ILE:HD11	2.48	0.48
1:A:895:TYR:CE2	1:A:904:MET:CE	2.97	0.47
1:B:660:ARG:NH1	1:B:660:ARG:CG	2.72	0.47
1:A:784:ILE:O	1:A:787:GLU:HG2	2.14	0.47
1:A:1038:LEU:HD11	1:A:1042:ASN:HD21	1.80	0.47
1:B:663:LEU:HD23	1:B:663:LEU:O	2.14	0.47
1:A:1039:ASN:OD1	1:A:1090:ARG:NH1	2.48	0.47
1:B:590:VAL:O	1:B:594:LEU:HG	2.15	0.47
1:A:1039:ASN:OD1	1:A:1090:ARG:NH2	2.48	0.46
1:A:566:ILE:HG12	1:A:727:PHE:CE2	2.50	0.46
1:B:1023:LYS:HG3	1:B:1058:TYR:HD2	1.81	0.46
1:A:1013:PRO:HG2	1:A:1016:LYS:HB2	1.96	0.46
1:B:675:MET:HG3	1:B:706:ILE:CB	2.43	0.46
1:A:574:GLN:HE22	1:A:701:PRO:HA	1.81	0.46
1:A:966:THR:HG23	1:A:968:LEU:N	2.31	0.46
1:A:835:GLU:OE1	1:A:879:ARG:NH1	2.31	0.46
1:A:1175:LEU:O	1:A:1175:LEU:CD1	2.63	0.46
1:A:580:GLY:HA3	1:A:586:LYS:HD3	1.97	0.46
1:B:604:MET:H	1:B:672:SER:H	1.64	0.46
1:B:607:CYS:HA	1:B:675:MET:O	2.16	0.46
1:A:1140:TRP:CD2	1:A:1162:PRO:HG3	2.50	0.45
1:A:755:THR:HG23	1:A:892:PHE:HD2	1.81	0.45
1:A:768:ILE:HB	1:A:827:VAL:HG22	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:605:ILE:HG23	1:A:673:VAL:HG13	1.98	0.45
1:A:832:ASN:O	1:A:835:GLU:HG2	2.16	0.45
1:B:605:ILE:HG12	1:B:673:VAL:HG12	1.98	0.45
1:A:1038:LEU:HD13	1:A:1042:ASN:ND2	2.31	0.45
1:A:953:LEU:HB3	1:A:959:LEU:HD13	1.99	0.45
1:B:655:ASP:OD2	1:B:686:THR:CG2	2.65	0.45
1:B:573:ASN:ND2	1:B:725:PRO:HG2	2.32	0.45
1:B:566:ILE:HG12	1:B:727:PHE:CE2	2.51	0.45
1:A:759:ILE:HD11	1:A:845:TYR:CG	2.52	0.45
1:B:1175:LEU:CD1	1:B:1175:LEU:C	2.84	0.45
1:B:663:LEU:C	1:B:663:LEU:CD2	2.85	0.45
1:A:1031:THR:HB	1:A:1096:ARG:HD3	1.98	0.45
1:A:830:ALA:HB1	1:A:834:ALA:HB3	1.98	0.45
1:A:603:GLY:HA3	1:A:672:SER:HB3	1.99	0.44
1:A:1140:TRP:CE2	1:A:1162:PRO:HG3	2.52	0.44
1:A:966:THR:HG23	1:A:968:LEU:H	1.82	0.44
1:A:589:GLN:HB3	1:A:593:TYR:CZ	2.53	0.44
1:A:574:GLN:NE2	1:A:701:PRO:HA	2.32	0.44
1:A:1170:PRO:O	1:A:1174:LYS:HB2	2.18	0.44
1:A:962:GLU:N	1:A:962:GLU:OE1	2.48	0.44
1:B:740:TYR:CD2	1:B:897:GLU:HA	2.52	0.44
1:B:682:ARG:NH1	1:B:939:ASP:OD2	2.51	0.44
1:B:655:ASP:N	1:B:655:ASP:OD1	2.51	0.43
1:B:956:LEU:O	1:B:983:LYS:HE3	2.19	0.43
1:B:684:ILE:CD1	1:B:684:ILE:N	2.81	0.43
1:B:1140:TRP:CD2	1:B:1162:PRO:HG3	2.54	0.43
1:A:740:TYR:HD2	1:A:897:GLU:HB2	1.82	0.43
1:A:682:ARG:NH1	1:A:938:MET:HE1	2.33	0.43
1:B:1160:ILE:HA	1:B:1164:TRP:HZ3	1.83	0.43
1:B:635:GLY:O	1:B:651:LYS:HA	2.18	0.43
1:B:944:ASN:N	1:B:944:ASN:OD1	2.51	0.43
1:A:1038:LEU:C	1:A:1038:LEU:CD1	2.86	0.42
1:A:1032:GLY:HA3	1:A:1158:THR:HA	2.01	0.42
1:A:893:ARG:HB3	1:A:895:TYR:CE1	2.54	0.42
1:B:1161:GLU:HA	1:B:1162:PRO:HD3	1.80	0.42
1:A:1175:LEU:C	1:A:1175:LEU:HD12	2.40	0.42
1:B:1119:LEU:HD23	1:B:1173:PHE:CE2	2.44	0.42
1:B:562:PHE:CD1	1:B:562:PHE:N	2.87	0.42
1:B:604:MET:SD	1:B:651:LYS:HD2	2.60	0.42
1:B:561:GLN:HB2	1:B:562:PHE:CD1	2.54	0.42
1:B:1068:ARG:O	1:B:1072:GLN:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:954:TYR:CE2	1:A:1171:THR:HG21	2.55	0.42
1:A:676:LEU:HD11	1:A:693:LEU:HD12	2.02	0.41
1:A:944:ASN:N	1:A:944:ASN:OD1	2.53	0.41
1:B:985:LEU:HD23	1:B:985:LEU:HA	1.93	0.41
1:A:660:ARG:HE	1:A:660:ARG:HB3	1.73	0.41
1:A:984:VAL:CG1	1:A:997:MET:SD	3.08	0.41
1:B:989:VAL:HG13	1:B:1084:PRO:HD2	2.03	0.41
1:B:659:GLN:HB3	1:B:659:GLN:HE21	1.69	0.41
1:A:771:PHE:O	1:A:849:PRO:HG2	2.20	0.41
1:A:968:LEU:C	1:A:968:LEU:HD12	2.39	0.41
1:A:1006:LEU:HD13	1:A:1006:LEU:HA	1.84	0.41
1:A:898:ALA:O	1:A:902:SER:N	2.53	0.41
1:B:562:PHE:O	1:B:566:ILE:HG13	2.21	0.41
1:A:638:ILE:HG13	1:A:641:GLU:HB3	2.03	0.41
1:A:655:ASP:N	1:A:655:ASP:OD1	2.53	0.41
1:B:1019:GLN:O	1:B:1023:LYS:HG2	2.20	0.41
1:B:562:PHE:HD1	1:B:562:PHE:N	2.18	0.41
1:B:667:ASP:OD1	1:B:699:ARG:NH1	2.54	0.41
1:A:592:GLN:O	1:A:596:GLU:HG3	2.20	0.41
1:B:1110:LYS:HD2	1:B:1115:GLY:O	2.21	0.41
1:A:756:VAL:O	1:A:759:ILE:HG22	2.21	0.41
1:A:1146:LEU:HD12	1:A:1146:LEU:HA	1.93	0.40
1:A:557:LEU:HA	1:A:558:PRO:HD3	1.94	0.40
1:A:740:TYR:CD2	1:A:897:GLU:HB2	2.56	0.40
1:B:1144:HIS:HB3	1:B:1156:PHE:HB2	2.02	0.40
1:B:1040:VAL:HG13	1:B:1059:ILE:HD13	2.03	0.40
1:A:1013:PRO:CD	1:A:1013:PRO:O	2.69	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	579/677 (86%)	550 (95%)	27 (5%)	2 (0%)	41 72
1	B	563/677 (83%)	536 (95%)	26 (5%)	1 (0%)	47 77
All	All	1142/1354 (84%)	1086 (95%)	53 (5%)	3 (0%)	41 72

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	632	GLN
1	B	1171	THR
1	A	1013	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	507/581 (87%)	499 (98%)	8 (2%)	62 79
1	B	495/581 (85%)	488 (99%)	7 (1%)	67 81
All	All	1002/1162 (86%)	987 (98%)	15 (2%)	65 80

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	655	ASP
1	A	785	LEU
1	A	795	SER
1	A	895	TYR
1	A	968	LEU
1	A	977	MET
1	A	1012	ARG
1	A	1172	PHE
1	B	655	ASP
1	B	660	ARG
1	B	662	ILE
1	B	663	LEU
1	B	975	PHE

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Mol	Chain	Res	Type
1	B	1066	ARG
1	B	1174	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	565	GLN
1	A	574	GLN
1	A	659	GLN
1	A	760	HIS
1	A	1042	ASN
1	A	1046	ASN
1	B	573	ASN
1	B	758	GLN
1	B	1046	ASN
1	B	1081	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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	589/677 (87%)	0.42	41 (6%) 16 15	56, 92, 174, 208	0
1	B	577/677 (85%)	0.67	66 (11%) 5 5	61, 110, 187, 220	0
All	All	1166/1354 (86%)	0.54	107 (9%) 9 10	56, 102, 182, 220	0

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	796	VAL	8.2
1	B	832	ASN	8.1
1	B	801	ILE	8.0
1	B	827	VAL	7.8
1	B	761	LEU	6.2
1	B	747	ASP	6.2
1	A	830	ALA	5.3
1	B	781	ALA	5.1
1	A	826	LYS	4.8
1	B	829	ILE	4.8
1	B	799	LEU	4.8
1	A	827	VAL	4.7
1	B	745	GLU	4.7
1	B	800	ILE	4.6
1	A	792	LEU	4.6
1	B	831	THR	4.6
1	A	803	PRO	4.6
1	A	839	THR	4.4
1	A	781	ALA	4.4
1	B	770	VAL	4.3
1	A	885	ARG	4.3
1	B	762	THR	4.2
1	B	771	PHE	4.1
1	A	829	ILE	4.1

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Mol	Chain	Res	Type	RSRZ
1	B	828	VAL	4.1
1	B	735	PRO	4.0
1	A	851	PHE	4.0
1	B	741	SER	3.8
1	B	785	LEU	3.8
1	A	757	MET	3.8
1	A	831	THR	3.7
1	A	886	THR	3.7
1	A	840	ILE	3.5
1	B	830	ALA	3.5
1	B	786	TYR	3.5
1	B	742	ARG	3.5
1	B	833	ILE	3.4
1	A	762	THR	3.4
1	A	832	ASN	3.4
1	B	880	ALA	3.4
1	B	757	MET	3.3
1	A	780	THR	3.3
1	A	845	TYR	3.2
1	A	779	ASP	3.2
1	B	794	PRO	3.1
1	B	736	VAL	3.1
1	A	793	GLY	3.1
1	B	868	VAL	3.0
1	B	845	TYR	3.0
1	A	785	LEU	3.0
1	A	1170	PRO	3.0
1	B	870	PRO	3.0
1	B	772	LEU	2.9
1	B	826	LYS	2.9
1	B	748	TYR	2.9
1	B	851	PHE	2.9
1	B	871	ILE	2.9
1	A	1014	LYS	2.9
1	A	838	ILE	2.8
1	B	802	LEU	2.8
1	B	782	CYS	2.8
1	B	797	PRO	2.8
1	B	768	ILE	2.8
1	A	761	LEU	2.8
1	B	866	LEU	2.7
1	A	771	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	783	GLU	2.7
1	B	795	SER	2.6
1	B	746	PRO	2.6
1	A	786	TYR	2.5
1	B	740	TYR	2.5
1	A	804	ILE	2.5
1	A	797	PRO	2.5
1	A	888	PRO	2.5
1	B	906	PRO	2.5
1	A	583	GLY	2.5
1	A	887	GLY	2.5
1	B	848	ASP	2.5
1	B	825	ARG	2.5
1	A	768	ILE	2.4
1	B	886	THR	2.4
1	A	791	ALA	2.4
1	B	688	VAL	2.4
1	A	782	CYS	2.4
1	B	776	GLU	2.4
1	B	844	TYR	2.4
1	B	843	ILE	2.3
1	B	769	LEU	2.3
1	B	750	GLU	2.3
1	B	753	LEU	2.3
1	B	624	GLU	2.3
1	B	635	GLY	2.2
1	B	803	PRO	2.2
1	B	787	GLU	2.2
1	A	776	GLU	2.2
1	B	885	ARG	2.2
1	A	1008	GLN	2.1
1	B	775	GLN	2.1
1	A	799	LEU	2.1
1	B	766	GLY	2.1
1	A	1168	ALA	2.1
1	B	899	ALA	2.1
1	A	796	VAL	2.1
1	B	756	VAL	2.0
1	B	792	LEU	2.0
1	B	903	GLU	2.0
1	B	752	ALA	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates

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.