Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 05:35 am BST

PDB ID	:	6HYU
Title	:	Crystal structure of DHX8 helicase bound to single stranded poly-adenine RNA
Authors	:	Felisberto-Rodrigues, C.; Thomas, J.C.; McAndrew, P.C.; Le Bihan, Y.V.; Burke, R.; Workman, P.; van Montfort, R.L.M.
Deposited on	:	2018-10-22
Resolution	:	3.22 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:

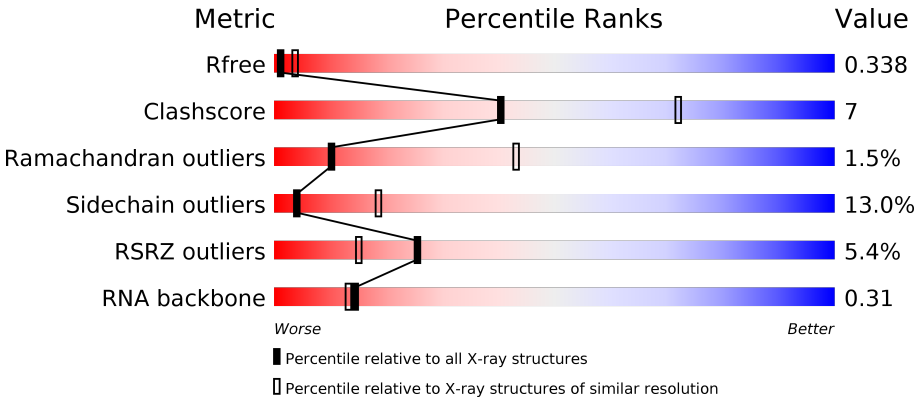
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, 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 3.22 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	1335 (3.24-3.20)
Clashscore	141614	1460 (3.24-3.20)
Ramachandran outliers	138981	1437 (3.24-3.20)
Sidechain outliers	138945	1436 (3.24-3.20)
RSRZ outliers	127900	1291 (3.24-3.20)
RNA backbone	3102	1023 (3.54-2.90)

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	673	67% 22% • 9%
1	C	673	10% 68% 16% • 13%
2	B	6	67% 33%
3	D	3	33% 100%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8921 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 RNA helicase DHX8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	614	Total	C	N	O	S	0	0	1
			4547	2907	745	861	34			
1	C	587	Total	C	N	O	S	0	0	4
			4182	2660	691	801	30			

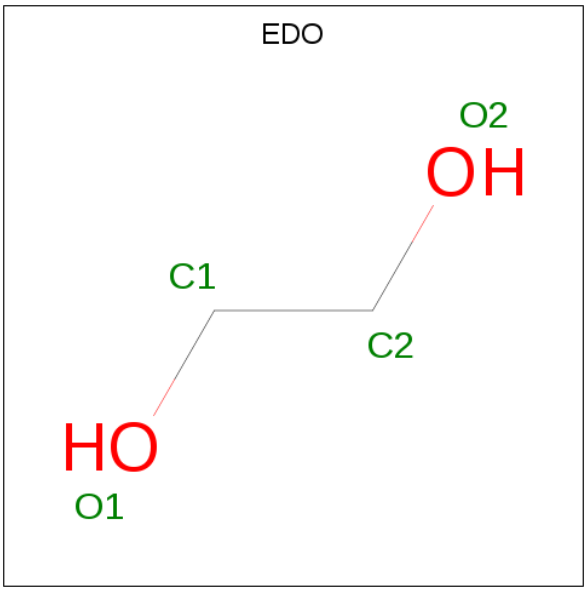
- Molecule 2 is a RNA chain called RNA (5'-R(*AP*AP*AP*AP*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	6	Total	C	N	O	P	0	0	0
			129	60	30	34	5			

- Molecule 3 is a RNA chain called RNA (5'-R(*A*AP*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	3	Total	C	N	O	P	0	0	0
			32	18	6	7	1			

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

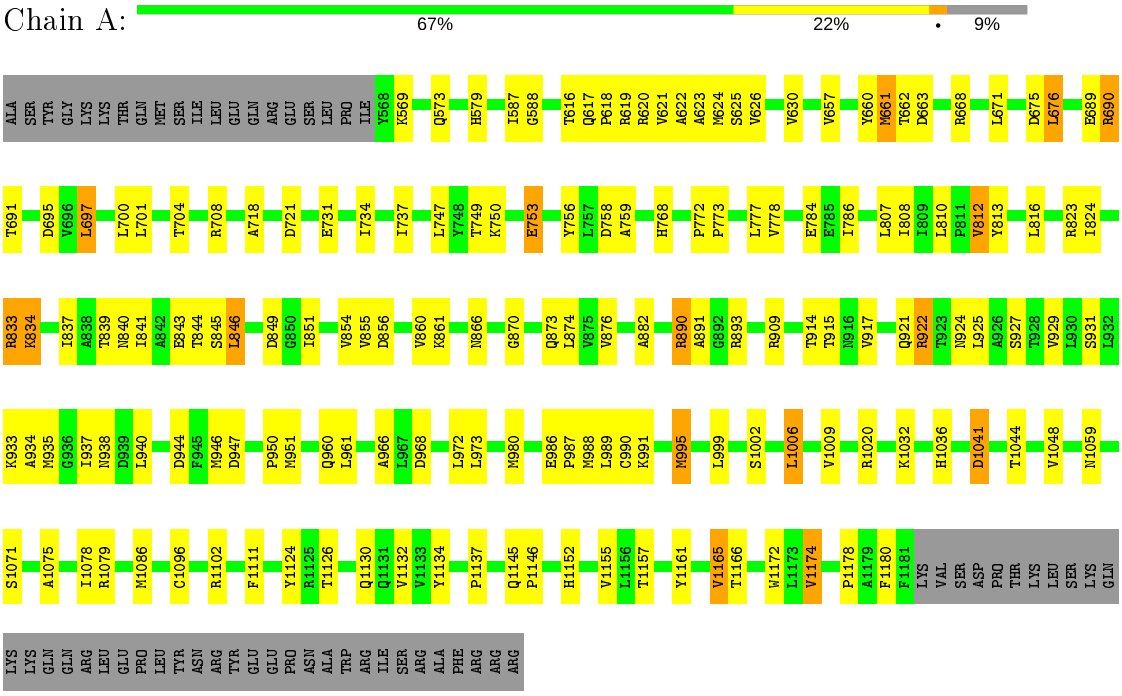
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	22	Total O 22 22	0	0
5	B	1	Total O 1 1	0	0
5	C	4	Total O 4 4	0	0

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.

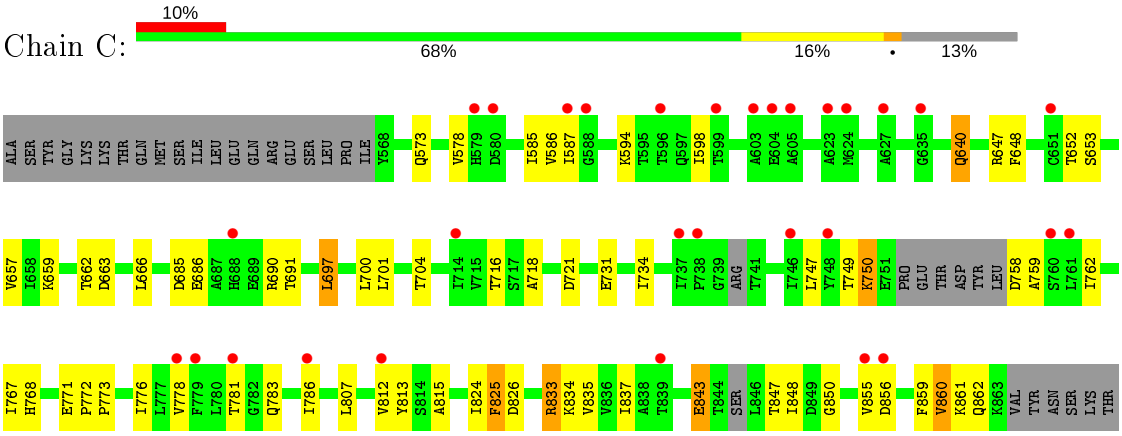
- Molecule 1: ATP-dependent RNA helicase DHX8

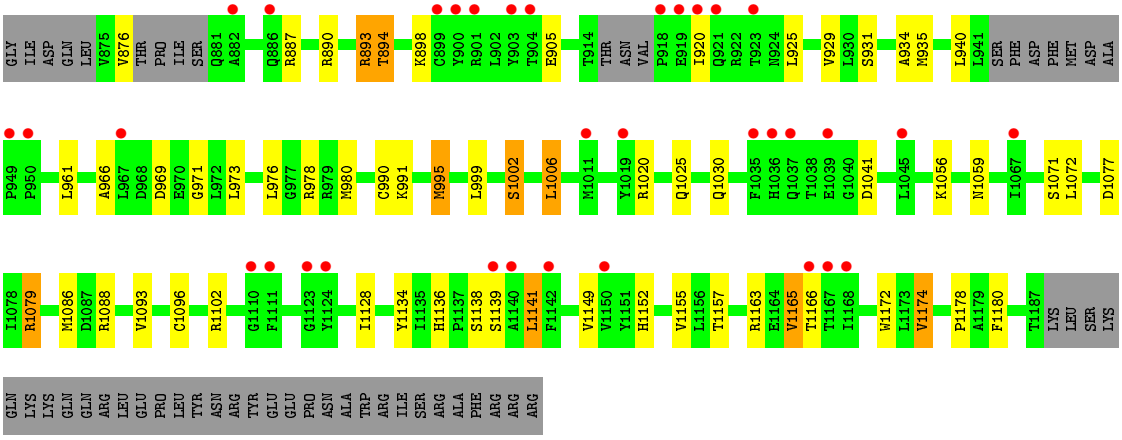
Chain A:



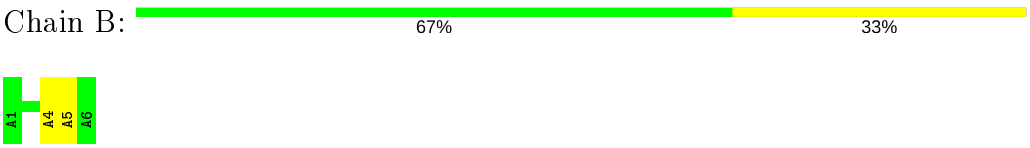
- Molecule 1: ATP-dependent RNA helicase DHX8

Chain C:

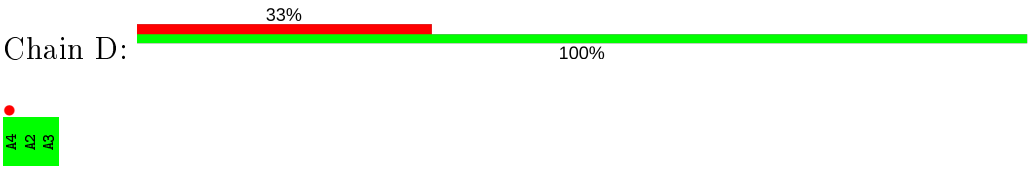




• Molecule 2: RNA (5'-R(*AP*AP*AP*AP*AP*A)-3')



• Molecule 3: RNA (5'-R(*A*AP*A)-3')



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 2 21	Depositor
Cell constants a, b, c, α, β, γ	66.10Å 138.60Å 169.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.75 – 3.22 48.75 – 3.22	Depositor EDS
% Data completeness (in resolution range)	99.8 (48.75-3.22) 99.8 (48.75-3.22)	Depositor EDS
R_{merge}	0.38	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.13 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.226 , 0.289 0.264 , 0.338	Depositor DCC
R_{free} test set	1292 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	87.0	Xtriage
Anisotropy	0.299	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 146.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.44$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	8921	wwPDB-VP
Average B, all atoms (Å^2)	117.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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

Bond lengths and bond angles in the following residue types are not validated in this section: EDO

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	0.53	0/4639	0.75	0/6322
1	C	0.50	0/4256	0.74	2/5808 (0.0%)
2	B	1.26	0/146	0.92	0/226
3	D	1.41	0/34	0.84	0/49
All	All	0.54	0/9075	0.75	2/12405 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	749	THR	C-N-CA	6.31	137.47	121.70
1	C	825	PHE	C-N-CA	5.05	134.33	121.70

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	4547	0	4180	75	0
1	C	4182	0	3666	45	0
2	B	129	0	68	2	0
3	D	32	0	17	0	0
4	A	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	A	22	0	0	0	0
5	B	1	0	0	0	0
5	C	4	0	0	0	0
All	All	8921	0	7937	121	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 7.

All (121) 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:C:861:LYS:HG2	1:C:876:VAL:HG22	1.44	0.99
1:A:844:THR:C	1:A:846:LEU:H	1.81	0.81
1:A:701:LEU:HA	1:A:704:THR:HG22	1.68	0.75
1:A:861:LYS:HD3	1:A:874:LEU:HD23	1.71	0.72
1:C:701:LEU:HA	1:C:704:THR:HG22	1.69	0.72
1:C:759:ALA:HA	1:C:762:ILE:HD12	1.74	0.70
1:A:777:LEU:HB2	1:A:851:ILE:HD13	1.74	0.69
1:C:781:THR:HB	1:C:861:LYS:HG3	1.75	0.68
1:A:843:GLU:O	1:A:890:ARG:NH2	2.30	0.65
1:A:882:ALA:HB2	1:A:915:THR:HG22	1.79	0.64
1:A:1032:LYS:HD3	1:A:1036:HIS:CE1	2.32	0.64
1:A:1032:LYS:HD3	1:A:1036:HIS:HE1	1.63	0.62
1:A:924:ASN:HD21	1:A:960:GLN:HE22	1.48	0.62
1:C:594:LYS:HA	1:C:598:ILE:HD12	1.80	0.62
1:A:844:THR:C	1:A:846:LEU:N	2.52	0.62
1:A:1111:PHE:CE2	1:A:1152:HIS:HD2	2.18	0.61
1:C:768:HIS:ND1	1:C:833:ARG:HD2	2.19	0.57
1:A:844:THR:O	1:A:846:LEU:N	2.36	0.57
1:A:668:ARG:HA	1:A:671:LEU:HD12	1.86	0.57
1:C:686:GLU:HB3	1:C:716:THR:O	2.05	0.56
1:C:1006:LEU:HB3	1:C:1079:ARG:HD3	1.87	0.56
1:A:810:LEU:HD13	1:A:824:ILE:HA	1.88	0.55
1:A:938:ASN:O	1:A:940:LEU:HD22	2.06	0.55
1:C:980:MET:HG2	1:C:990:CYS:HB3	1.88	0.55
1:A:750:LYS:HD2	1:A:750:LYS:H	1.71	0.54
1:C:772:PRO:HB2	1:C:773:PRO:HD2	1.89	0.54
1:C:587:ILE:HD11	1:C:734:ILE:HB	1.90	0.54
1:A:812:VAL:CG2	1:A:824:ILE:HG21	2.38	0.54
1:A:690:ARG:HB2	1:A:690:ARG:HH11	1.72	0.54
1:A:917:VAL:HG12	1:A:922:ARG:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:934:ALA:HA	1:A:973:LEU:HD11	1.90	0.54
1:A:980:MET:HG2	1:A:990:CYS:HB3	1.90	0.54
1:C:860:VAL:HB	1:C:887:ARG:HH22	1.73	0.54
1:C:833:ARG:HG2	1:C:834:LYS:N	2.23	0.53
1:C:778:VAL:HG22	1:C:855:VAL:HB	1.91	0.53
1:A:989:LEU:HD22	1:A:1009:VAL:HG13	1.89	0.53
1:C:666:LEU:HB3	1:C:697:LEU:HD11	1.91	0.53
1:A:587:ILE:HD11	1:A:734:ILE:HB	1.90	0.53
1:A:778:VAL:HG22	1:A:855:VAL:HB	1.92	0.52
1:C:594:LYS:O	1:C:598:ILE:HB	2.09	0.52
1:A:753:GLU:HG3	1:A:759:ALA:HB2	1.91	0.51
1:C:934:ALA:HA	1:C:973:LEU:HD11	1.92	0.51
1:C:1096:CYS:HB2	1:C:1102:ARG:HD2	1.92	0.51
1:A:616:THR:HA	1:A:661:MET:O	2.10	0.51
1:A:938:ASN:O	1:A:940:LEU:CD2	2.59	0.50
1:C:652:THR:HG21	1:C:659:LYS:HE2	1.94	0.50
1:C:767:ILE:HG23	1:C:771:GLU:HB2	1.93	0.50
1:C:697:LEU:HA	1:C:700:LEU:HD12	1.92	0.50
1:A:921:GLN:HG2	1:A:950:PRO:HD3	1.93	0.50
1:A:938:ASN:C	1:A:940:LEU:HD22	2.31	0.50
1:A:933:LYS:CE	1:A:940:LEU:HD21	2.42	0.49
1:C:850:GLY:H	1:C:894:THR:HG21	1.77	0.49
1:A:1132:VAL:HG23	1:A:1132:VAL:O	2.13	0.49
1:A:808:ILE:HB	1:A:834:LYS:HB3	1.94	0.49
1:A:1096:CYS:HB2	1:A:1102:ARG:HD2	1.94	0.48
1:A:991:LYS:O	1:A:995:MET:HB2	2.13	0.48
1:A:772:PRO:HB2	1:A:773:PRO:HD2	1.94	0.48
1:C:1136:HIS:O	1:C:1141:LEU:HB2	2.13	0.48
1:C:585:ILE:O	1:C:734:ILE:HA	2.14	0.48
1:C:825:PHE:HA	1:C:848:ILE:HG23	1.96	0.48
1:A:768:HIS:ND1	1:A:833:ARG:HD2	2.30	0.47
1:A:925:LEU:O	1:A:929:VAL:HG23	2.15	0.47
1:C:847:THR:HA	1:C:890:ARG:HH22	1.79	0.47
1:A:927:SER:HB2	1:A:987:PRO:HD3	1.95	0.47
1:C:991:LYS:O	1:C:995:MET:HB2	2.14	0.47
1:A:1075:ALA:HA	1:A:1078:ILE:HD12	1.96	0.47
1:C:786:ILE:HG12	1:C:837:ILE:HG22	1.97	0.47
1:A:1155:VAL:HG22	1:A:1157:THR:HG23	1.97	0.46
1:A:621:VAL:HA	1:A:624:MET:HE2	1.98	0.46
1:A:931:SER:O	1:A:935:MET:HG2	2.16	0.46
1:A:812:VAL:HG22	1:A:824:ILE:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:PRO:HG2	1:A:844:THR:CB	2.46	0.45
1:A:1172:TRP:C	1:A:1174:VAL:H	2.20	0.45
1:C:890:ARG:O	1:C:893:ARG:HB3	2.16	0.45
1:A:695:ASP:OD1	1:A:947:ASP:HB2	2.17	0.45
1:C:843:GLU:HG3	1:C:887:ARG:HG3	1.98	0.45
1:C:861:LYS:CG	1:C:876:VAL:HG22	2.31	0.45
1:A:1006:LEU:HD11	1:A:1086:MET:HG3	1.99	0.45
1:A:630:VAL:HG21	1:A:660:TYR:OH	2.17	0.45
1:A:622:ALA:O	1:A:626:VAL:HG23	2.17	0.44
1:A:986:GLU:HG2	1:A:988:MET:H	1.82	0.44
1:A:588:GLY:HA3	1:A:737:ILE:HB	1.99	0.44
1:A:617:GLN:HG3	1:A:623:ALA:HA	1.98	0.44
1:A:1124:TYR:O	1:A:1132:VAL:HA	2.18	0.44
1:A:1041:ASP:HB2	1:A:1165:VAL:O	2.17	0.44
1:A:675:ASP:O	1:A:708:ARG:HD3	2.17	0.44
1:A:697:LEU:HA	1:A:700:LEU:HD12	1.98	0.44
1:C:925:LEU:O	1:C:929:VAL:HG23	2.18	0.44
1:A:1134:TYR:O	1:A:1161:TYR:HA	2.18	0.44
1:A:813:TYR:O	1:A:816:LEU:HB2	2.18	0.44
1:C:1172:TRP:C	1:C:1174:VAL:H	2.21	0.44
1:C:718:ALA:HB3	1:C:721:ASP:HB2	2.00	0.44
1:C:1149:VAL:HB	1:C:1165:VAL:HG12	2.00	0.43
1:A:676:LEU:HD12	1:A:704:THR:HG21	2.01	0.43
1:C:1155:VAL:HG22	1:C:1157:THR:HG23	1.99	0.43
1:C:776:ILE:O	1:C:835:VAL:HA	2.18	0.43
1:A:961:LEU:HB3	1:A:966:ALA:HB3	2.01	0.43
1:A:1137:PRO:HD3	1:A:1161:TYR:CE1	2.53	0.43
1:C:747:LEU:HD11	1:C:898:LYS:HB3	2.01	0.43
1:A:924:ASN:HD21	1:A:960:GLN:NE2	2.14	0.42
1:C:1178:PRO:C	1:C:1180:PHE:H	2.22	0.42
1:A:986:GLU:HB3	1:A:989:LEU:HD12	2.01	0.42
1:C:1002:SER:HB2	1:C:1093:VAL:HA	2.01	0.42
1:C:640:GLN:HA	1:C:653:SER:OG	2.19	0.42
1:C:813:TYR:HD2	1:C:815:ALA:HB3	1.84	0.42
1:C:961:LEU:HB3	1:C:966:ALA:HB3	2.01	0.42
1:C:1152:HIS:HB3	1:C:1163:ARG:O	2.20	0.42
1:A:854:VAL:HG23	1:A:891:ALA:HB2	2.02	0.42
1:A:937:ILE:HG22	1:A:937:ILE:O	2.20	0.42
1:A:861:LYS:HD3	1:A:874:LEU:CD2	2.46	0.42
1:C:973:LEU:HD13	1:C:978:ARG:HG3	2.02	0.42
1:A:718:ALA:HB3	1:A:721:ASP:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:756:TYR:HD1	1:A:756:TYR:H	1.67	0.41
1:A:620:ARG:HG3	2:B:5:A:H5"	2.03	0.41
1:A:786:ILE:HG12	1:A:837:ILE:HG22	2.01	0.41
1:A:1178:PRO:C	1:A:1180:PHE:H	2.24	0.41
1:A:968:ASP:HB3	1:A:972:LEU:H	1.85	0.41
2:B:4:A:H2'	2:B:5:A:O4'	2.20	0.41
1:A:619:ARG:HD2	1:A:841:ILE:HA	2.02	0.41
1:A:1044:THR:O	1:A:1048:VAL:HG23	2.21	0.40
1:A:1145:GLN:HA	1:A:1146:PRO:HD3	1.87	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	612/673 (91%)	550 (90%)	59 (10%)	3 (0%)	29 66
1	C	569/673 (84%)	497 (87%)	57 (10%)	15 (3%)	5 30
All	All	1181/1346 (88%)	1047 (89%)	116 (10%)	18 (2%)	10 43

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	870	GLY
1	C	750	LYS
1	C	826	ASP
1	C	1056	LYS
1	C	1128	ILE
1	C	1134	TYR
1	A	845	SER
1	C	640	GLN
1	C	647	ARG

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Mol	Chain	Res	Type
1	C	824	ILE
1	C	1139	SER
1	A	846	LEU
1	C	648	PHE
1	C	935	MET
1	C	969	ASP
1	C	1138	SER
1	C	843	GLU
1	C	971	GLY

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	416/596 (70%)	362 (87%)	54 (13%)	4	18
1	C	359/596 (60%)	312 (87%)	47 (13%)	4	18
All	All	775/1192 (65%)	674 (87%)	101 (13%)	4	18

All (101) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	569	LYS
1	A	573	GLN
1	A	579	HIS
1	A	625	SER
1	A	657	VAL
1	A	661	MET
1	A	662	THR
1	A	663	ASP
1	A	676	LEU
1	A	689	GLU
1	A	690	ARG
1	A	691	THR
1	A	697	LEU
1	A	731	GLU

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Mol	Chain	Res	Type
1	A	747	LEU
1	A	749	THR
1	A	753	GLU
1	A	758	ASP
1	A	784	GLU
1	A	807	LEU
1	A	812	VAL
1	A	823	ARG
1	A	833	ARG
1	A	834	LYS
1	A	839	THR
1	A	840	ASN
1	A	849	ASP
1	A	856	ASP
1	A	860	VAL
1	A	866	ASN
1	A	873	GLN
1	A	876	VAL
1	A	890	ARG
1	A	893	ARG
1	A	909	ARG
1	A	914	THR
1	A	922	ARG
1	A	944	ASP
1	A	946	MET
1	A	951	MET
1	A	995	MET
1	A	999	LEU
1	A	1002	SER
1	A	1006	LEU
1	A	1020	ARG
1	A	1041	ASP
1	A	1059	ASN
1	A	1071	SER
1	A	1079	ARG
1	A	1126	THR
1	A	1130	GLN
1	A	1165	VAL
1	A	1166	THR
1	A	1174	VAL
1	C	573	GLN
1	C	578	VAL

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Mol	Chain	Res	Type
1	C	586	VAL
1	C	657	VAL
1	C	662	THR
1	C	663	ASP
1	C	685	ASP
1	C	690	ARG
1	C	691	THR
1	C	697	LEU
1	C	731	GLU
1	C	750	LYS
1	C	758	ASP
1	C	783	GLN
1	C	807	LEU
1	C	812	VAL
1	C	833	ARG
1	C	856	ASP
1	C	859	PHE
1	C	860	VAL
1	C	862	GLN
1	C	893	ARG
1	C	894	THR
1	C	905	GLU
1	C	920	ILE
1	C	931	SER
1	C	940	LEU
1	C	976	LEU
1	C	995	MET
1	C	999	LEU
1	C	1002	SER
1	C	1006	LEU
1	C	1020	ARG
1	C	1025	GLN
1	C	1030	GLN
1	C	1041	ASP
1	C	1059	ASN
1	C	1071	SER
1	C	1072	LEU
1	C	1077	ASP
1	C	1079	ARG
1	C	1086	MET
1	C	1088	ARG
1	C	1141	LEU

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Mol	Chain	Res	Type
1	C	1165	VAL
1	C	1166	THR
1	C	1174	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	866	ASN
1	A	924	ASN
1	A	960	GLN
1	A	1025	GLN
1	A	1036	HIS
1	A	1130	GLN
1	A	1145	GLN
1	A	1152	HIS
1	C	1152	HIS

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	5/6 (83%)	0	0
3	D	0/3	-	-
All	All	5/9 (55%)	0	0

There are no RNA backbone outliers to report.

There are no RNA pucker outliers to report.

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

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	EDO	A	1301	-	3,3,3	1.05	0	2,2,2	0.30	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	1301	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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

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	614/673 (91%)	-0.22	0 100 100	49, 88, 116, 139	0
1	C	587/673 (87%)	0.66	64 (10%) 5 4	87, 147, 186, 215	0
2	B	6/6 (100%)	0.39	0 100 100	82, 92, 101, 106	0
3	D	3/3 (100%)	1.42	1 (33%) 0 0	153, 153, 160, 160	0
All	All	1210/1355 (89%)	0.21	65 (5%) 25 15	49, 115, 175, 215	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	588	GLY	9.4
1	C	1123	GLY	7.1
1	C	899	CYS	6.6
1	C	737	ILE	6.5
1	C	949	PRO	6.0
1	C	839	THR	5.3
1	C	918	PRO	5.3
1	C	1036	HIS	4.4
1	C	904	THR	4.4
1	C	856	ASP	4.3
1	C	919	GLU	4.0
1	C	812	VAL	4.0
1	C	901	ARG	3.9
1	C	738	PRO	3.9
1	C	1167	THR	3.8
1	C	1035	PHE	3.8
1	C	920	ILE	3.8
1	C	746	ILE	3.7
1	C	604	GLU	3.5
1	C	1110	GLY	3.5
1	C	855	VAL	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	635	GLY	3.3
1	C	903	TYR	3.3
1	C	580	ASP	3.3
1	C	605	ALA	3.3
1	C	1139	SER	3.3
1	C	1140	ALA	3.2
1	C	624	MET	3.2
1	C	1019	TYR	3.1
1	C	1011	MET	3.0
1	C	900	TYR	3.0
1	C	760	SER	3.0
1	C	761	LEU	2.9
1	C	921	GLN	2.9
1	C	1150	VAL	2.8
1	C	923	THR	2.8
1	C	1111	PHE	2.8
1	C	714	ILE	2.7
1	C	748	TYR	2.7
1	C	627	ALA	2.6
1	C	1124	TYR	2.6
1	C	603	ALA	2.5
1	C	1037	GLN	2.5
1	C	688	HIS	2.5
1	C	1168	ILE	2.5
1	C	1166	THR	2.5
1	C	587	ILE	2.5
1	C	1067	ILE	2.5
1	C	950	PRO	2.4
1	C	778	VAL	2.4
3	D	4	A	2.3
1	C	779	PHE	2.3
1	C	599	THR	2.2
1	C	651	CYS	2.2
1	C	596	THR	2.2
1	C	579	HIS	2.1
1	C	786	ILE	2.1
1	C	967	LEU	2.1
1	C	1045	LEU	2.1
1	C	1039	GLU	2.1
1	C	1142	PHE	2.0
1	C	623	ALA	2.0
1	C	882	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	886	GLN	2.0
1	C	781	THR	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)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	EDO	A	1301	4/4	0.68	0.30	63,69,74,75	0

6.5 Other polymers (i)

There are no such residues in this entry.