



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 06:24 PM UTC

PDB ID : 6HYU / pdb_00006hyu
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

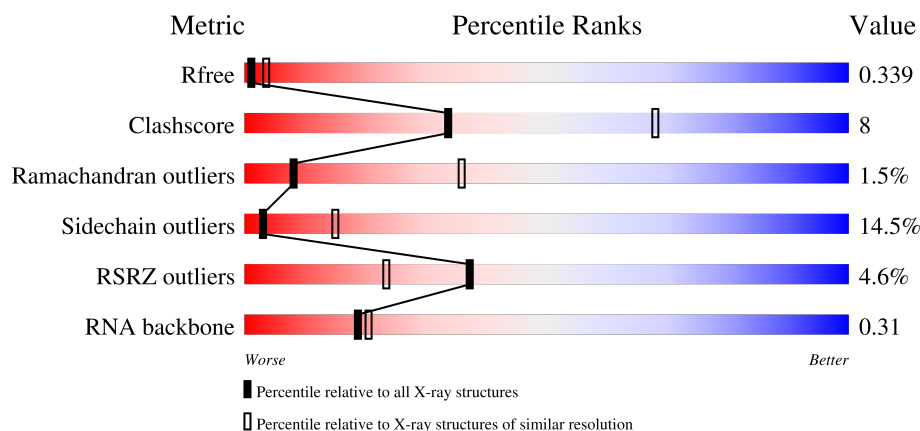
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.22 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}	180053	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)
RNA backbone	3983	1055 (3.50-2.94)

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 of 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 $\leq 5\%$. 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	7% 64% 22% 9%
1	C	673	7% 64% 19% 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*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			

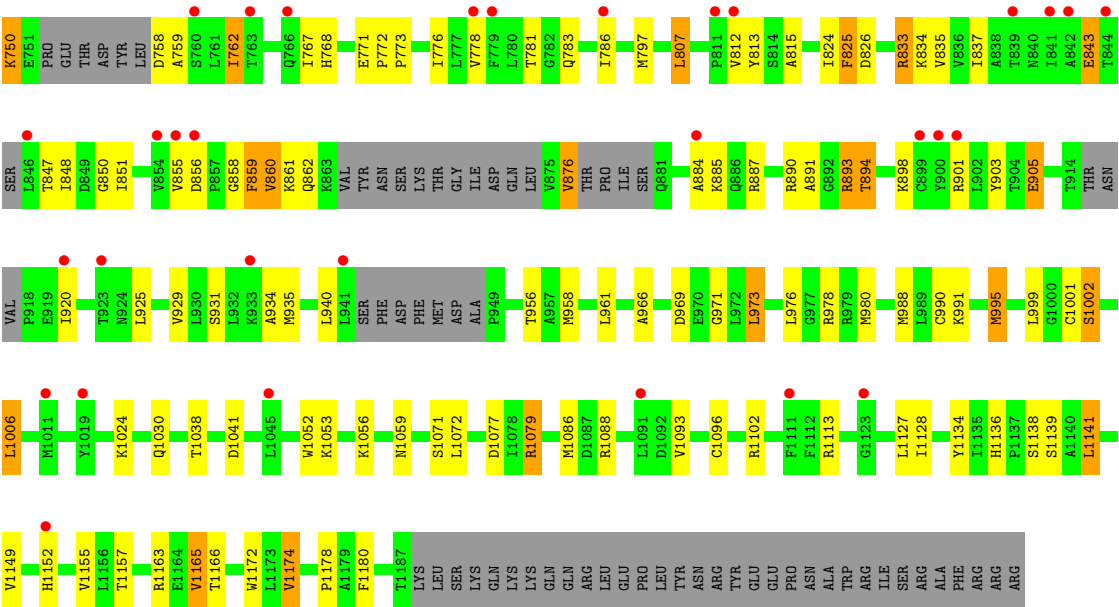
- Molecule 4 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 5 is water.

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



• 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

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
$\langle I/\sigma(I) \rangle$ ¹	1.13 (at 3.19Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, R_{free}	0.226 , 0.289 0.265 , 0.339	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)	0.32 , 167.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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	0.91	1/4639 (0.0%)	1.51	49/6322 (0.8%)
1	C	0.90	0/4256	1.52	40/5808 (0.7%)
2	B	0.72	0/146	0.76	0/226
3	D	0.61	0/34	0.45	0/49
All	All	0.90	1/9075 (0.0%)	1.50	89/12405 (0.7%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	589	GLU	CA-C	5.13	1.59	1.52

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	856	ASP	CA-CB-CG	9.37	121.97	112.60
1	C	749	THR	CA-C-N	8.76	137.47	121.70
1	C	749	THR	C-N-CA	8.76	137.47	121.70
1	C	891	ALA	N-CA-C	-8.66	101.79	111.14
1	C	858	GLY	CA-C-N	7.23	131.08	120.95
1	C	858	GLY	C-N-CA	7.23	131.08	120.95
1	C	685	ASP	CA-CB-CG	6.71	119.31	112.60
1	C	884	ALA	N-CA-C	-6.46	105.33	113.72
1	C	657	VAL	CB-CA-C	6.45	116.70	110.63
1	A	657	VAL	CB-CA-C	6.12	116.38	110.63
1	A	571	LYS	CA-C-N	6.08	128.71	120.38
1	A	571	LYS	C-N-CA	6.08	128.71	120.38
1	A	762	ILE	N-CA-C	-6.06	104.83	110.53
1	A	919	GLU	CA-C-N	5.99	130.45	120.62
1	A	919	GLU	C-N-CA	5.99	130.45	120.62
1	C	1024	LYS	CA-C-N	5.98	128.21	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1024	LYS	C-N-CA	5.98	128.21	120.44
1	A	753	GLU	CA-C-N	5.91	128.68	120.29
1	A	753	GLU	C-N-CA	5.91	128.68	120.29
1	A	626	VAL	N-CA-C	-5.86	105.02	110.53
1	C	721	ASP	CA-C-N	5.77	129.47	120.82
1	C	721	ASP	C-N-CA	5.77	129.47	120.82
1	A	958	MET	CA-C-N	5.73	127.96	120.28
1	A	958	MET	C-N-CA	5.73	127.96	120.28
1	A	868	LYS	CA-C-N	5.66	130.00	121.40
1	A	868	LYS	C-N-CA	5.66	130.00	121.40
1	C	905	GLU	CA-C-N	5.63	128.14	120.54
1	C	905	GLU	C-N-CA	5.63	128.14	120.54
1	C	669	GLU	N-CA-C	-5.58	104.83	111.69
1	A	782	GLY	CA-C-N	5.56	127.67	120.44
1	A	782	GLY	C-N-CA	5.56	127.67	120.44
1	A	676	LEU	CA-C-N	5.56	129.50	120.60
1	A	676	LEU	C-N-CA	5.56	129.50	120.60
1	A	766	GLN	CA-C-N	5.54	127.75	120.60
1	A	766	GLN	C-N-CA	5.54	127.75	120.60
1	A	915	THR	CA-C-N	5.52	128.69	120.90
1	A	915	THR	C-N-CA	5.52	128.69	120.90
1	C	1001	CYS	CA-C-N	5.50	127.65	120.28
1	C	1001	CYS	C-N-CA	5.50	127.65	120.28
1	C	885	LYS	N-CA-C	-5.49	106.71	113.41
1	C	958	MET	CA-C-N	5.45	127.59	120.28
1	C	958	MET	C-N-CA	5.45	127.59	120.28
1	C	736	THR	CA-C-N	5.45	128.69	123.02
1	C	736	THR	C-N-CA	5.45	128.69	123.02
1	C	1053	LYS	CA-C-N	5.43	127.50	120.44
1	C	1053	LYS	C-N-CA	5.43	127.50	120.44
1	A	867	SER	CA-C-N	5.39	128.04	120.28
1	A	867	SER	C-N-CA	5.39	128.04	120.28
1	A	736	THR	CA-C-N	5.35	128.59	123.02
1	A	736	THR	C-N-CA	5.35	128.59	123.02
1	C	1038	THR	CA-C-N	5.35	127.71	120.44
1	C	1038	THR	C-N-CA	5.35	127.71	120.44
1	C	859	PHE	N-CA-C	5.34	117.97	109.96
1	A	572	GLU	CA-C-N	5.29	127.63	120.44
1	A	572	GLU	C-N-CA	5.29	127.63	120.44
1	C	1127	LEU	CA-C-N	5.28	131.47	121.97
1	C	1127	LEU	C-N-CA	5.28	131.47	121.97
1	C	721	ASP	CA-CB-CG	5.26	117.86	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	709	GLN	CA-C-N	5.26	128.30	120.31
1	A	709	GLN	C-N-CA	5.26	128.30	120.31
1	A	620	ARG	CA-C-N	5.24	127.35	120.60
1	A	620	ARG	C-N-CA	5.24	127.35	120.60
1	A	626	VAL	N-CA-CB	5.20	117.22	110.57
1	C	762	ILE	N-CA-C	-5.17	105.67	110.53
1	A	726	SER	CA-C-N	5.16	127.50	120.54
1	A	726	SER	C-N-CA	5.16	127.50	120.54
1	C	746	ILE	CB-CA-C	5.14	117.10	111.08
1	A	1054	ASN	CA-CB-CG	5.14	117.74	112.60
1	C	825	PHE	CA-C-N	5.14	134.33	121.80
1	C	825	PHE	C-N-CA	5.14	134.33	121.80
1	C	1052	TRP	CA-C-N	5.13	127.16	120.28
1	C	1052	TRP	C-N-CA	5.13	127.16	120.28
1	A	845	SER	CA-C-N	5.12	131.33	121.54
1	A	845	SER	C-N-CA	5.12	131.33	121.54
1	A	851	ILE	N-CA-CB	5.10	116.28	110.72
1	C	725	PHE	CA-CB-CG	5.09	118.89	113.80
1	A	985	LEU	CA-C-N	5.08	127.46	120.39
1	A	985	LEU	C-N-CA	5.08	127.46	120.39
1	C	956	THR	N-CA-C	-5.08	105.63	111.07
1	A	1140	ALA	CA-C-N	5.08	130.34	122.26
1	A	1140	ALA	C-N-CA	5.08	130.34	122.26
1	A	755	ASP	CA-C-N	5.07	127.08	120.28
1	A	755	ASP	C-N-CA	5.07	127.08	120.28
1	A	734	ILE	CA-C-N	5.07	128.52	121.02
1	A	734	ILE	C-N-CA	5.07	128.52	121.02
1	A	708	ARG	CA-C-N	5.07	127.58	120.28
1	A	708	ARG	C-N-CA	5.07	127.58	120.28
1	C	695	ASP	CA-C-N	5.06	126.94	120.56
1	C	695	ASP	C-N-CA	5.06	126.94	120.56

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	79	0
1	C	4182	0	3666	49	0
2	B	129	0	68	2	0
3	D	32	0	17	0	0
4	A	4	0	6	0	0
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	129	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 8.

All (129) 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	0.84
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:844:THR:C	1:A:846:LEU:N	2.52	0.65
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:1111:PHE:CE2	1:A:1152:HIS:HD2	2.18	0.61
1:A:951:MET:HE2	1:A:954:LEU:HD23	1.84	0.58
1:C:768:HIS:ND1	1:C:833:ARG:HD2	2.19	0.57
1:A:668:ARG:HA	1:A:671:LEU:HD12	1.86	0.57
1:A:797:MET:HE2	1:A:807:LEU:HB2	1.85	0.57
1:A:844:THR:O	1:A:846:LEU:N	2.36	0.56
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:938:ASN:C	1:A:940:LEU:HD22	2.31	0.55
1:A:750:LYS:H	1:A:750:LYS:HD2	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
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:778:VAL:HG22	1:C:855:VAL:HB	1.91	0.53
1:C:833:ARG:HG2	1:C:834:LYS:N	2.23	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:797:MET:HE2	1:C:807:LEU: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:933:LYS:CE	1:A:940:LEU:HD21	2.42	0.49
1:A:1172:TRP:C	1:A:1174:VAL:H	2.20	0.49
1:C:850:GLY:H	1:C:894:THR:HG21	1.77	0.49
1:A:808:ILE:HB	1:A:834:LYS:HB3	1.94	0.49
1:A:991:LYS:O	1:A:995:MET:HB2	2.13	0.48
1:A:1096:CYS:HB2	1:A:1102:ARG:HD2	1.94	0.48
1:C:1172:TRP:C	1:C:1174:VAL:H	2.21	0.48
1:A:1132:VAL:HG23	1:A:1132:VAL:O	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:988:MET:HE1	1:C:1113:ARG:HB3	1.96	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:708:ARG:NH2	1:A:711:MET:HE2	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:C:1178:PRO:C	1:C:1180:PHE:H	2.22	0.47
1:A:1155:VAL:HG22	1:A:1157:THR:HG23	1.97	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
1:A:1178:PRO:C	1:A:1180:PHE:H	2.24	0.46
1:A:618:PRO:HG2	1:A:844:THR:CB	2.46	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:630:VAL:HG21	1:A:660:TYR:OH	2.17	0.45
1:A:1006:LEU:HD11	1:A:1086:MET:HG3	1.99	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:1041:ASP:HB2	1:A:1165:VAL:O	2.17	0.44
1:A:1124:TYR:O	1:A:1132:VAL:HA	2.18	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:813:TYR:O	1:A:816:LEU:HB2	2.18	0.44
1:A:1134:TYR:O	1:A:1161:TYR:HA	2.18	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:775:ASP:CG	1:A:834:LYS:HG3	2.44	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:989:LEU:HD23	1:A:992:MET:HE2	2.01	0.42
1:A:861:LYS:HD3	1:A:874:LEU:CD2	2.46	0.42
1:C:901:ARG:C	1:C:903:TYR:H	2.28	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
1:A:756:TYR:H	1:A:756:TYR:HD1	1.67	0.41
1:A:937:ILE:O	1:A:937:ILE:HG22	2.20	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: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
1:C:645:THR:HG22	1:C:665:MET:HE2	2.04	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%)	24	58
1	C	569/673 (84%)	497 (87%)	57 (10%)	15 (3%)	4	25
All	All	1181/1346 (88%)	1047 (89%)	116 (10%)	18 (2%)	8	36

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
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 ⓘ

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%)	356 (86%)	60 (14%)	3	15
1	C	359/596 (60%)	307 (86%)	52 (14%)	3	15
All	All	775/1192 (65%)	663 (86%)	112 (14%)	3	15

All (112) 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	621	VAL
1	A	625	SER

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Mol	Chain	Res	Type
1	A	626	VAL
1	A	657	VAL
1	A	661	MET
1	A	662	THR
1	A	689	GLU
1	A	690	ARG
1	A	691	THR
1	A	697	LEU
1	A	711	MET
1	A	723	VAL
1	A	731	GLU
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	847	THR
1	A	849	ASP
1	A	856	ASP
1	A	860	VAL
1	A	861	LYS
1	A	863	LYS
1	A	866	ASN
1	A	873	GLN
1	A	874	LEU
1	A	876	VAL
1	A	890	ARG
1	A	893	ARG
1	A	909	ARG
1	A	914	THR
1	A	917	VAL
1	A	944	ASP
1	A	946	MET
1	A	951	MET
1	A	973	LEU

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Mol	Chain	Res	Type
1	A	991	LYS
1	A	995	MET
1	A	999	LEU
1	A	1002	SER
1	A	1006	LEU
1	A	1041	ASP
1	A	1059	ASN
1	A	1071	SER
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
1	C	586	VAL
1	C	621	VAL
1	C	657	VAL
1	C	661	MET
1	C	662	THR
1	C	685	ASP
1	C	690	ARG
1	C	691	THR
1	C	697	LEU
1	C	705	VAL
1	C	711	MET
1	C	723	VAL
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	851	ILE
1	C	856	ASP
1	C	859	PHE
1	C	860	VAL
1	C	862	GLN
1	C	876	VAL
1	C	893	ARG
1	C	894	THR

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Mol	Chain	Res	Type
1	C	905	GLU
1	C	920	ILE
1	C	931	SER
1	C	940	LEU
1	C	973	LEU
1	C	976	LEU
1	C	995	MET
1	C	999	LEU
1	C	1002	SER
1	C	1006	LEU
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
1	C	1165	VAL
1	C	1166	THR
1	C	1174	VAL

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

Mol	Chain	Res	Type
1	A	821	GLN
1	A	840	ASN
1	A	883	GLN
1	A	924	ASN
1	A	1025	GLN
1	A	1036	HIS
1	A	1059	ASN
1	A	1130	GLN
1	A	1145	GLN
1	A	1152	HIS
1	C	597	GLN
1	C	783	GLN
1	C	862	GLN
1	C	938	ASN
1	C	1030	GLN

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Mol	Chain	Res	Type
1	C	1076	GLN
1	C	1081	GLN

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 oligosaccharides 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	0.96	0	2,2,2	0.23	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	614/673 (91%)	0.10	7 (1%) 78 60	49, 88, 116, 139	0
1	C	587/673 (87%)	0.79	48 (8%) 17 11	87, 147, 186, 215	0
2	B	6/6 (100%)	-0.38	0 100 100	82, 92, 101, 106	0
3	D	3/3 (100%)	2.68	1 (33%) 1 1	153, 153, 160, 160	0
All	All	1210/1355 (89%)	0.44	56 (4%) 37 23	49, 115, 175, 215	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	737	ILE	4.7
3	D	2	A	4.5
1	C	899	CYS	4.2
1	C	839	THR	4.0
1	C	588	GLY	3.9
1	C	812	VAL	3.8
1	C	779	PHE	3.8
1	C	856	ASP	3.7
1	C	599	THR	3.7
1	C	842	ALA	3.4
1	C	746	ILE	3.3
1	C	841	ILE	3.2
1	C	901	ARG	3.0
1	C	705	VAL	3.0
1	C	605	ALA	3.0
1	C	778	VAL	2.9
1	C	658	ILE	2.7
1	C	714	ILE	2.7
1	C	855	VAL	2.6
1	C	687	ALA	2.6
1	C	1019	TYR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	745	GLU	2.5
1	C	763	THR	2.5
1	C	844	THR	2.5
1	C	618	PRO	2.5
1	A	1066	PHE	2.5
1	C	654	PRO	2.5
1	C	1123	GLY	2.5
1	C	1111	PHE	2.4
1	C	900	TYR	2.3
1	C	603	ALA	2.3
1	C	923	THR	2.3
1	C	786	ILE	2.3
1	C	920	ILE	2.3
1	A	687	ALA	2.3
1	C	1152	HIS	2.3
1	C	619	ARG	2.2
1	C	884	ALA	2.2
1	C	941	LEU	2.2
1	A	689	GLU	2.2
1	C	688	HIS	2.2
1	C	760	SER	2.2
1	C	811	PRO	2.2
1	C	595	THR	2.1
1	C	846	LEU	2.1
1	A	589	GLU	2.1
1	C	677	THR	2.1
1	C	623	ALA	2.1
1	A	609	SER	2.1
1	A	1141	LEU	2.1
1	C	1045	LEU	2.1
1	C	933	LYS	2.1
1	C	854	VAL	2.0
1	C	1091	LEU	2.0
1	C	766	GLN	2.0
1	C	1011	MET	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 [i](#)

There are no oligosaccharides 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, 95th 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($\text{\AA}^2$)	Q<0.9
4	EDO	A	1301	4/4	0.83	0.13	63,69,74,75	0

6.5 Other polymers [i](#)

There are no such residues in this entry.