



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 07:24 PM UTC

PDB ID : 6I3O / pdb_00006i3o
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 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
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

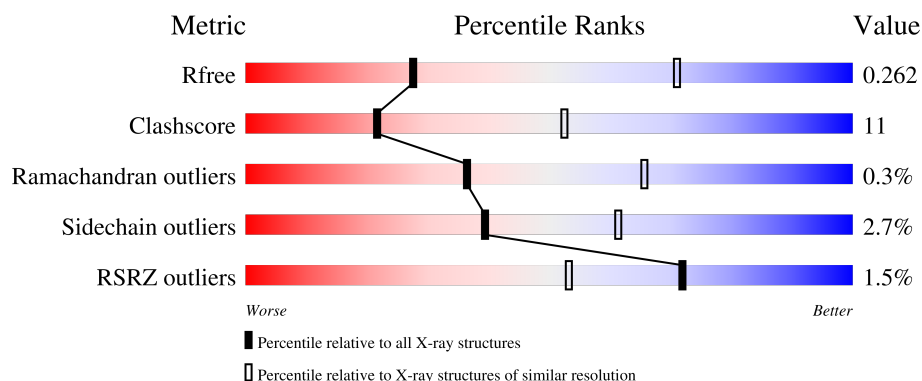
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 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}	180053	1605 (3.30-3.22)
Clashscore	190562	1660 (3.30-3.22)
Ramachandran outliers	187476	1630 (3.30-3.22)
Sidechain outliers	187428	1629 (3.30-3.22)
RSRZ outliers	180081	1605 (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 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	677	64% 21% 13%
1	B	677	66% 18% 15%

2 Entry composition

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			



4 Data and refinement statistics

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
$\langle I/\sigma(I) \rangle$ 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 , 80.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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.*

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

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	1.08	10/4745 (0.2%)	1.34	12/6429 (0.2%)
1	B	1.00	5/4646 (0.1%)	1.24	4/6291 (0.1%)
All	All	1.04	15/9391 (0.2%)	1.29	16/12720 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	929	ILE	C-O	-8.97	1.14	1.24
1	A	780	THR	C-O	6.72	1.31	1.24
1	A	787	GLU	C-O	6.65	1.31	1.24
1	A	578	VAL	C-O	-6.09	1.17	1.24
1	B	1019	GLN	C-O	6.04	1.31	1.24
1	A	674	ILE	C-O	-6.01	1.17	1.24
1	A	1152	GLU	C-O	5.84	1.30	1.23
1	A	709	SER	C-O	5.61	1.30	1.23
1	B	1037	LEU	C-O	5.49	1.30	1.24
1	A	909	ILE	N-CA	5.45	1.50	1.46
1	A	1157	THR	C-O	-5.44	1.17	1.23
1	B	1092	THR	C-O	5.26	1.30	1.24
1	B	645	SER	N-CA	5.17	1.49	1.46
1	A	554	ARG	C-O	-5.08	1.18	1.24
1	A	1002	SER	CA-CB	-5.01	1.45	1.53

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1171	THR	CA-C-N	6.13	128.42	120.44
1	A	1171	THR	C-N-CA	6.13	128.42	120.44
1	A	1097	GLN	CB-CG-CD	-6.05	102.32	112.60
1	A	1080	ARG	CB-CG-CD	5.69	124.39	111.30
1	A	1017	GLN	CB-CA-C	-5.69	101.95	110.88
1	B	1175	LEU	N-CA-C	-5.67	104.94	112.94
1	A	943	VAL	CA-C-O	-5.66	115.06	120.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	662	ILE	N-CA-C	-5.64	104.87	110.62
1	A	679	ALA	N-CA-C	-5.50	105.37	111.36
1	A	681	GLU	CB-CA-C	5.46	119.49	111.73
1	B	592	GLN	CB-CA-C	5.42	119.47	110.90
1	B	941	PRO	O-C-N	5.40	123.69	121.15
1	A	944	ASN	CB-CA-C	-5.38	101.86	110.79
1	A	687	ASP	N-CA-C	5.20	117.69	111.71
1	A	685	ALA	N-CA-C	-5.09	105.91	111.82
1	A	944	ASN	N-CA-CB	5.01	117.48	110.12

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	109	0
1	B	4556	0	4601	91	0
All	All	9208	0	9287	200	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 11.

All (200) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1082:ARG:HA	1:B:1082:ARG:HE	1.53	0.74
1:B:658:LEU:HD12	1:B:658:LEU:O	1.88	0.73
1:B:1119:LEU:HD23	1:B:1173:PHE:HE2	1.54	0.72
1:A:958:ALA:HB2	1:A:972:MET:HE1	1.71	0.72
1:A:1038:LEU:HD12	1:A:1090:ARG:NH1	2.06	0.71
1:A:1012:ARG:HG2	1:A:1012:ARG:NH1	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:A:1038:LEU:C	1:A:1038:LEU:HD13	2.17	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:HD12	1:A:968:LEU:O	1.94	0.67
1:B:1175:LEU:HD12	1:B:1175:LEU:C	2.19	0.67
1:B:1082:ARG:HA	1:B:1082:ARG:NE	2.10	0.67
1:A:1078:MET:HE2	1:A:1083:HIS:HB3	1.76	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:B:1078:MET:HE2	1:B:1083:HIS:HB3	1.78	0.65
1:B:662:ILE:HG12	1:B:668:LEU:HD11	1.79	0.65
1:A:895:TYR:CE2	1:A:904:MET:HE1	2.32	0.64
1:A:1175:LEU:O	1:A:1175:LEU:HD12	1.98	0.64
1:B:975:PHE:HB3	1:B:977:MET:HE3	1.79	0.64
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:842:TYR:N	1:B:886:THR:HG1	1.97	0.63
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:760:HIS:CD2	1:A:799:LEU:HD13	2.42	0.55
1:A:1127:LEU:HD13	1:A:1134:PHE:HA	1.87	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: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:969:GLY:HA2	1:A:972:MET:HE2	1.90	0.54
1:A:895:TYR:CD1	1:A:895:TYR:N	2.77	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:A:958:ALA:HB2	1:A:972:MET:CE	2.37	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:663:LEU:C	1:B:663:LEU:CD2	2.85	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:B:1175:LEU:C	1:B:1175:LEU:CD1	2.84	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:CG	1:B:660:ARG:NH1	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:A:1175:LEU:HD12	1:A:1175:LEU:C	2.40	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:A:968:LEU:HD12	1:A:968:LEU:C	2.39	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:580:GLY:HA3	1:A:586:LYS:HD3	1.97	0.46
1:A:1175:LEU:O	1:A:1175:LEU:CD1	2.63	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:755:THR:HG23	1:A:892:PHE:HD2	1.81	0.45
1:A:1140:TRP:CD2	1:A:1162:PRO:HG3	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:768:ILE:HB	1:A:827:VAL:HG22	1.97	0.45
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:566:ILE:HG12	1:B:727:PHE:CE2	2.51	0.45
1:B:573:ASN:ND2	1:B:725:PRO:HG2	2.32	0.45
1:B:655:ASP:OD2	1:B:686:THR:CG2	2.65	0.45
1:A:759:ILE:HD11	1:A:845:TYR:CG	2.52	0.45
1:A:830:ALA:HB1	1:A:834:ALA:HB3	1.98	0.45
1:A:1031:THR:HB	1:A:1096:ARG:HD3	1.98	0.45
1:A:603:GLY:HA3	1:A:672:SER:HB3	1.99	0.44
1:A:966:THR:HG23	1:A:968:LEU:H	1.82	0.44
1:A:1140:TRP:CE2	1:A:1162:PRO:HG3	2.52	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:962:GLU:OE1	1:A:962:GLU:N	2.48	0.44
1:A:1170:PRO:O	1:A:1174:LYS:HB2	2.18	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:OD1	1:B:655:ASP:N	2.51	0.43
1:B:956:LEU:O	1:B:983:LYS:HE3	2.19	0.43
1:B:684:ILE:N	1:B:684:ILE:CD1	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:B:1160:ILE:HA	1:B:1164:TRP:HZ3	1.83	0.43
1:A:1038:LEU:C	1:A:1038:LEU:CD1	2.86	0.43
1:B:843:ILE:C	1:B:844:TYR:HD1	2.26	0.43
1:B:635:GLY:O	1:B:651:LYS:HA	2.18	0.43
1:B:944:ASN:OD1	1:B:944:ASN:N	2.51	0.43
1:A:677:ASP:C	1:A:677:ASP:OD1	2.61	0.42
1:A:893:ARG:HB3	1:A:895:TYR:CE1	2.54	0.42
1:A:1032:GLY:HA3	1:A:1158:THR:HA	2.01	0.42
1:B:1161:GLU:HA	1:B:1162:PRO:HD3	1.80	0.42
1:B:1119:LEU:HD23	1:B:1173:PHE:CE2	2.44	0.42
1:B:562:PHE:N	1:B:562:PHE:CD1	2.87	0.42
1:B:658:LEU:HD12	1:B:658:LEU:C	2.41	0.42
1:B:604:MET:SD	1:B:651:LYS:HD2	2.60	0.42
1:B:662:ILE:O	1:B:665:ASP:C	2.63	0.42
1:B:561:GLN:HB2	1:B:562:PHE:CD1	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1068:ARG:O	1:B:1072:GLN:HG3	2.20	0.42
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:659:GLN:HE21	1:B:659:GLN:HB3	1.69	0.41
1:B:989:VAL:HG13	1:B:1084:PRO:HD2	2.03	0.41
1:A:771:PHE:O	1:A:849:PRO:HG2	2.20	0.41
1:A:898:ALA:O	1:A:902:SER:N	2.53	0.41
1:A:1006:LEU:HA	1:A:1006:LEU:HD13	1.84	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:OD1	1:A:655:ASP:N	2.53	0.41
1:B:1019:GLN:O	1:B:1023:LYS:HG2	2.20	0.41
1:A:718:SER:OG	1:A:724:CYS:O	2.34	0.41
1:B:562:PHE:N	1:B:562:PHE:HD1	2.18	0.41
1:A:592:GLN:O	1:A:596:GLU:HG3	2.20	0.41
1:B:667:ASP:OD1	1:B:699:ARG:NH1	2.54	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:557:LEU:HA	1:A:558:PRO:HD3	1.94	0.40
1:A:1146:LEU:HD12	1:A:1146:LEU:HA	1.93	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

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%)	36	66
1	B	563/677 (83%)	536 (95%)	26 (5%)	1 (0%)	43	70
All	All	1142/1354 (84%)	1086 (95%)	53 (5%)	3 (0%)	36	66

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 ⓘ

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%)	493 (97%)	14 (3%)	38	60
1	B	495/581 (85%)	482 (97%)	13 (3%)	40	62
All	All	1002/1162 (86%)	975 (97%)	27 (3%)	39	61

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	577	ILE
1	A	655	ASP
1	A	663	LEU
1	A	676	LEU
1	A	697	VAL
1	A	754	THR
1	A	785	LEU
1	A	795	SER
1	A	895	TYR
1	A	968	LEU
1	A	977	MET
1	A	1006	LEU
1	A	1012	ARG

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Mol	Chain	Res	Type
1	A	1017	GLN
1	B	550	ILE
1	B	576	LEU
1	B	655	ASP
1	B	660	ARG
1	B	662	ILE
1	B	663	LEU
1	B	684	ILE
1	B	694	LYS
1	B	697	VAL
1	B	754	THR
1	B	1026	LYS
1	B	1166	VAL
1	B	1174	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) 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	878	GLN
1	A	915	GLN
1	A	1042	ASN
1	A	1046	ASN
1	B	573	ASN
1	B	589	GLN
1	B	758	GLN
1	B	1046	ASN
1	B	1057	ASN
1	B	1081	HIS
1	B	1083	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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	589/677 (87%)	0.05	8 (1%)	73 54	56, 92, 174, 208	0
1	B	577/677 (85%)	0.20	10 (1%)	69 50	61, 110, 187, 220	0
All	All	1166/1354 (86%)	0.13	18 (1%)	72 53	56, 102, 182, 220	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	678	GLU	3.9
1	B	684	ILE	3.2
1	B	1168	ALA	3.0
1	A	980	SER	2.8
1	A	852	VAL	2.7
1	B	761	LEU	2.7
1	B	1172	PHE	2.7
1	A	1168	ALA	2.6
1	B	688	VAL	2.6
1	B	1170	PRO	2.6
1	A	1170	PRO	2.4
1	B	833	ILE	2.3
1	B	796	VAL	2.3
1	A	1172	PHE	2.2
1	A	679	ALA	2.2
1	B	831	THR	2.2
1	B	828	VAL	2.0
1	A	888	PRO	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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.