



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 11:25 AM UTC

PDB ID : 6BB8 / pdb_00006bb8
Title : Crystal Structure of Frequency-Interacting RNA helicase (FRH)
Authors : Morales, Y.; Johnson, S.J.; Olsen, K.J.
Deposited on : 2017-10-17
Resolution : 3.49 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

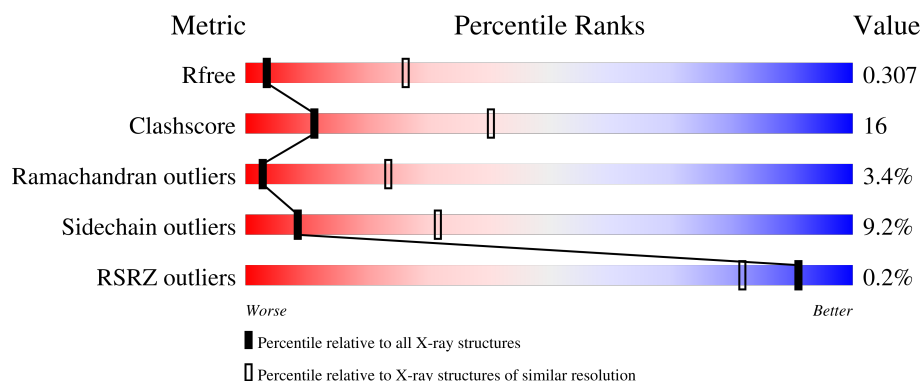
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.49 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	1106	52% 26% 5% 16%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7226 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.

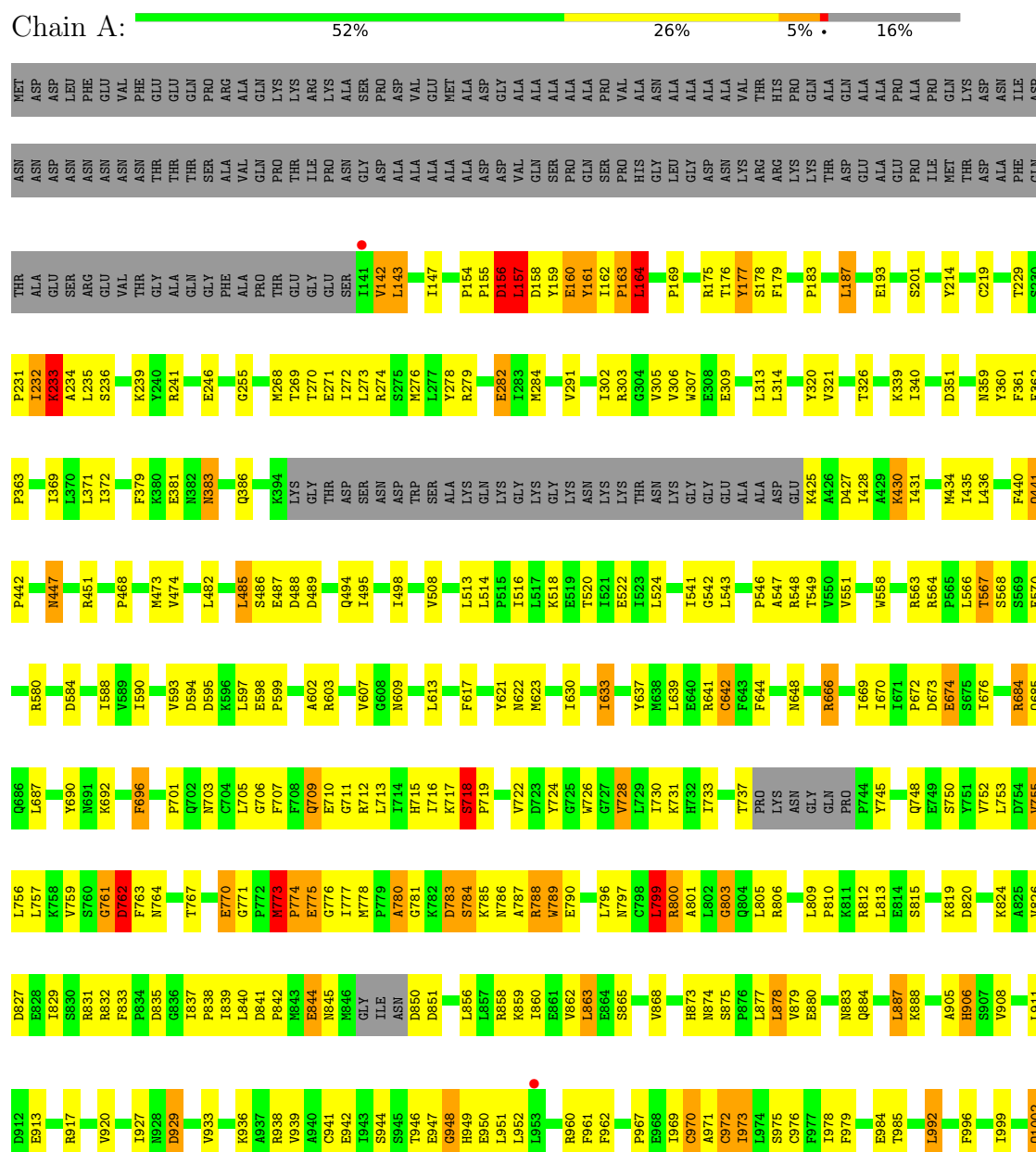
- Molecule 1 is a protein called FRQ-interacting RNA helicase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	927	7226	4623	1241	1322	40	0	0	0

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: FRQ-interacting RNA helicase



I1006	A1007	L1015	D1016	V1017	M1018	E1019	D1020	E1021	H1028	Q1029	L1030	M1031	P1042	F1043	E1054	I1058	R1059	R1062	E1065	E1066	L1067	L1068	R1069	Q1070	E1073	R1076	V1077	M1078	E1082	L1083	K1084	D1085	K1086	F1087	S1090	L1091	I1098	S1103	L1106
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4 Data and refinement statistics

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	117.77Å 117.77Å 180.41Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.07 – 3.49 30.07 – 3.49	Depositor EDS
% Data completeness (in resolution range)	98.8 (30.07-3.49) 85.7 (30.07-3.49)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.86 (at 3.47Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.251 , 0.301 0.253 , 0.307	Depositor DCC
R_{free} test set	937 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	139.8	Xtriage
Anisotropy	0.031	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 167.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.048 for -h,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7226	wwPDB-VP
Average B, all atoms (Å ²)	174.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.37% 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	0.30	0/7361	0.90	18/9959 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	232	ILE	CA-C-N	7.81	136.47	121.54
1	A	232	ILE	C-N-CA	7.81	136.47	121.54
1	A	745	TYR	N-CA-C	7.74	126.92	109.81
1	A	833	PHE	N-CA-C	6.65	119.21	109.30
1	A	775	GLU	CA-C-N	6.17	127.85	120.14
1	A	775	GLU	C-N-CA	6.17	127.85	120.14
1	A	233	LYS	N-CA-C	6.14	123.89	110.80
1	A	788	ARG	N-CA-C	6.03	121.20	113.18
1	A	241	ARG	NE-CZ-NH1	-5.74	115.77	121.50
1	A	156	ASP	CA-C-N	5.63	131.84	121.70
1	A	156	ASP	C-N-CA	5.63	131.84	121.70
1	A	703	ASN	CA-C-N	5.62	131.86	121.52
1	A	703	ASN	C-N-CA	5.62	131.86	121.52
1	A	819	LYS	N-CA-C	-5.56	105.12	111.07
1	A	784	SER	CA-C-N	5.39	131.41	121.70
1	A	784	SER	C-N-CA	5.39	131.41	121.70
1	A	762	ASP	CA-C-N	5.13	130.94	121.70
1	A	762	ASP	C-N-CA	5.13	130.94	121.70

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	177	TYR	Peptide
1	A	984	GLU	Peptide

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	7226	0	7179	233	0
All	All	7226	0	7179	233	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 16.

All (233) 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:274:ARG:HD2	1:A:306:VAL:HG13	1.62	0.80
1:A:949:HIS:O	1:A:951:LEU:N	2.13	0.79
1:A:939:VAL:HG11	1:A:1078:MET:HB3	1.67	0.76
1:A:435:ILE:HG23	1:A:440:PHE:HB2	1.69	0.74
1:A:235:LEU:HD11	1:A:541:ILE:O	1.87	0.73
1:A:717:LYS:N	1:A:799:LEU:O	2.22	0.73
1:A:546:PRO:HG2	1:A:580:ARG:HG2	1.71	0.72
1:A:156:ASP:HA	1:A:157:LEU:C	2.14	0.71
1:A:564:ARG:NH1	1:A:570:GLU:OE2	2.25	0.70
1:A:803:GLY:HA2	1:A:839:ILE:HA	1.74	0.70
1:A:728:VAL:HG23	1:A:756:LEU:HB3	1.73	0.70
1:A:715:HIS:HB3	1:A:801:ALA:HB3	1.73	0.70
1:A:278:TYR:CE2	1:A:313:LEU:HD11	2.27	0.70
1:A:603:ARG:O	1:A:607:VAL:HG22	1.93	0.68
1:A:622:ASN:ND2	1:A:941:CYS:O	2.26	0.68
1:A:944:SER:OG	1:A:1070:GLN:OE1	2.13	0.67
1:A:709:GLN:N	1:A:709:GLN:OE1	2.27	0.66
1:A:927:ILE:HG22	1:A:933:VAL:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:ASN:OD1	1:A:447:ASN:N	2.30	0.65
1:A:597:LEU:HD11	1:A:602:ALA:HB2	1.78	0.65
1:A:908:VAL:HA	1:A:911:LEU:HB2	1.79	0.65
1:A:800:ARG:HG2	1:A:801:ALA:H	1.62	0.65
1:A:474:VAL:HG23	1:A:524:LEU:HD22	1.77	0.64
1:A:947:GLU:O	1:A:949:HIS:N	2.26	0.64
1:A:362:PHE:HB2	1:A:369:ILE:HG22	1.80	0.63
1:A:436:LEU:HD12	1:A:441:GLN:HE21	1.64	0.62
1:A:759:VAL:HG11	1:A:777:ILE:HD12	1.81	0.62
1:A:639:LEU:HD22	1:A:911:LEU:HD22	1.81	0.62
1:A:642:CYS:SG	1:A:644:PHE:HB3	2.39	0.62
1:A:684:ARG:HH12	1:A:685:GLN:HG2	1.64	0.62
1:A:701:PRO:O	1:A:705:LEU:HB2	2.00	0.61
1:A:784:SER:HA	1:A:785:LYS:C	2.25	0.61
1:A:159:TYR:CD2	1:A:160:GLU:HG3	2.36	0.60
1:A:340:ILE:HG13	1:A:641:ARG:HD3	1.84	0.60
1:A:687:LEU:HD21	1:A:863:LEU:HB2	1.83	0.60
1:A:231:PRO:O	1:A:303:ARG:NH1	2.35	0.60
1:A:1069:ARG:HG3	1:A:1091:LEU:HD11	1.82	0.60
1:A:177:TYR:HB3	1:A:178:SER:HA	1.83	0.59
1:A:810:PRO:HD2	1:A:813:LEU:HD13	1.84	0.59
1:A:162:ILE:N	1:A:163:PRO:HD3	2.17	0.59
1:A:690:TYR:HB3	1:A:860:ILE:HG12	1.84	0.59
1:A:773:MET:HE3	1:A:773:MET:HA	1.84	0.59
1:A:648:ASN:HB3	1:A:905:ALA:O	2.03	0.59
1:A:155:PRO:O	1:A:157:LEU:HB2	2.04	0.58
1:A:255:GLY:O	1:A:1069:ARG:NH1	2.37	0.58
1:A:428:ILE:O	1:A:431:ILE:HG22	2.03	0.58
1:A:279:ARG:HH22	1:A:1073:GLU:CG	2.17	0.57
1:A:630:ILE:HG23	1:A:633:ILE:HG22	1.86	0.57
1:A:278:TYR:HE2	1:A:313:LEU:HD11	1.66	0.57
1:A:229:THR:HA	1:A:268:MET:O	2.04	0.57
1:A:759:VAL:O	1:A:788:ARG:N	2.38	0.57
1:A:359:ASN:O	1:A:371:LEU:HD12	2.05	0.57
1:A:674:GLU:HB3	1:A:676:ILE:HG22	1.87	0.56
1:A:711:GLY:O	1:A:728:VAL:HG12	2.05	0.56
1:A:235:LEU:HD22	1:A:543:LEU:HB2	1.86	0.56
1:A:495:ILE:HA	1:A:498:ILE:HG22	1.88	0.56
1:A:962:PHE:O	1:A:1086:LYS:NZ	2.38	0.56
1:A:436:LEU:HA	1:A:441:GLN:HE21	1.70	0.56
1:A:598:GLU:HG3	1:A:599:PRO:HD2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:748:GLN:O	1:A:796:LEU:HB3	2.06	0.56
1:A:594:ASP:OD1	1:A:595:ASP:N	2.38	0.55
1:A:1073:GLU:OE1	1:A:1076:ARG:NH2	2.39	0.55
1:A:967:PRO:HG3	1:A:1086:LYS:HG3	1.87	0.55
1:A:178:SER:OG	1:A:179:PHE:N	2.38	0.55
1:A:305:VAL:HG23	1:A:617:PHE:HD2	1.71	0.55
1:A:274:ARG:NE	1:A:309:GLU:OE1	2.37	0.55
1:A:859:LYS:O	1:A:863:LEU:HD13	2.06	0.55
1:A:160:GLU:HA	1:A:161:TYR:HB2	1.89	0.55
1:A:762:ASP:OD1	1:A:762:ASP:N	2.39	0.55
1:A:952:LEU:HD11	1:A:1002:GLN:HB3	1.88	0.55
1:A:486:SER:C	1:A:488:ASP:H	2.15	0.54
1:A:840:LEU:O	1:A:842:PRO:HD3	2.08	0.54
1:A:232:ILE:HD11	1:A:541:ILE:HD11	1.89	0.54
1:A:233:LYS:HD2	1:A:1059:ARG:NH2	2.22	0.54
1:A:1073:GLU:O	1:A:1077:VAL:HG23	2.08	0.53
1:A:1062:ARG:O	1:A:1065:GLU:HG2	2.07	0.53
1:A:621:TYR:CE1	1:A:951:LEU:HD11	2.44	0.53
1:A:705:LEU:O	1:A:707:PHE:N	2.42	0.53
1:A:757:LEU:O	1:A:789:TRP:HA	2.08	0.52
1:A:824:LYS:HA	1:A:827:ASP:OD1	2.09	0.52
1:A:147:ILE:HD12	1:A:183:PRO:HB2	1.91	0.52
1:A:865:SER:HA	1:A:868:VAL:HG22	1.90	0.52
1:A:1021:GLU:OE2	1:A:1021:GLU:N	2.42	0.52
1:A:764:ASN:OD1	1:A:776:GLY:HA3	2.09	0.52
1:A:229:THR:HG21	1:A:273:LEU:HD22	1.92	0.51
1:A:1082:GLU:HA	1:A:1085:ASP:OD1	2.10	0.51
1:A:568:SER:OG	1:A:609:ASN:O	2.15	0.51
1:A:233:LYS:O	1:A:236:SER:OG	2.29	0.51
1:A:880:GLU:O	1:A:884:GLN:HG3	2.11	0.51
1:A:233:LYS:H	1:A:233:LYS:HD3	1.75	0.51
1:A:755:VAL:HG23	1:A:757:LEU:HG	1.92	0.51
1:A:850:ASP:HB2	1:A:851:ASP:CG	2.36	0.51
1:A:271:GLU:HG2	1:A:306:VAL:HG11	1.92	0.50
1:A:826:VAL:HA	1:A:829:ILE:HG22	1.92	0.50
1:A:642:CYS:SG	1:A:644:PHE:N	2.84	0.50
1:A:340:ILE:CD1	1:A:641:ARG:HB3	2.42	0.50
1:A:759:VAL:HG13	1:A:777:ILE:HG23	1.93	0.50
1:A:279:ARG:NH2	1:A:1073:GLU:OE1	2.44	0.50
1:A:551:VAL:HA	1:A:590:ILE:O	2.12	0.50
1:A:441:GLN:CD	1:A:441:GLN:H	2.19	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1058:ILE:HD11	1:A:1098:ILE:HD12	1.93	0.49
1:A:803:GLY:H	1:A:839:ILE:HG23	1.77	0.49
1:A:862:VAL:O	1:A:865:SER:OG	2.21	0.49
1:A:270:THR:HG21	1:A:307:TRP:CE2	2.46	0.49
1:A:379:PHE:CE2	1:A:381:GLU:HG2	2.47	0.49
1:A:1043:PHE:CD1	1:A:1098:ILE:HD11	2.46	0.49
1:A:232:ILE:HD11	1:A:541:ILE:CD1	2.43	0.49
1:A:724:TYR:HB3	1:A:757:LEU:HD13	1.94	0.49
1:A:920:VAL:HG21	1:A:1015:LEU:HD11	1.93	0.49
1:A:976:CYS:SG	1:A:1031:MET:HG2	2.52	0.49
1:A:716:ILE:HG22	1:A:718:SER:H	1.78	0.49
1:A:305:VAL:HG23	1:A:617:PHE:CD2	2.47	0.49
1:A:508:VAL:HG13	1:A:513:LEU:HD11	1.94	0.49
1:A:841:ASP:HB3	1:A:844:GLU:HB3	1.94	0.49
1:A:969:ILE:O	1:A:973:ILE:HG12	2.12	0.49
1:A:730:ILE:HG22	1:A:731:LYS:HG3	1.95	0.49
1:A:883:ASN:O	1:A:887:LEU:HD13	2.13	0.49
1:A:800:ARG:CG	1:A:801:ALA:H	2.25	0.48
1:A:713:LEU:HD12	1:A:728:VAL:HG13	1.95	0.48
1:A:548:ARG:HD3	1:A:584:ASP:CG	2.39	0.48
1:A:363:PRO:HA	1:A:593:VAL:HG22	1.95	0.48
1:A:1028:TRP:O	1:A:1031:MET:HG3	2.14	0.48
1:A:1015:LEU:C	1:A:1017:VAL:H	2.21	0.48
1:A:282:GLU:O	1:A:282:GLU:HG3	2.12	0.47
1:A:157:LEU:O	1:A:159:TYR:N	2.47	0.47
1:A:785:LYS:HA	1:A:786:ASN:HA	1.38	0.47
1:A:783:ASP:OD2	1:A:783:ASP:N	2.48	0.47
1:A:858:ARG:HE	1:A:858:ARG:HA	1.80	0.47
1:A:235:LEU:HD21	1:A:542:GLY:HA2	1.97	0.47
1:A:617:PHE:HE2	1:A:623:MET:HE1	1.80	0.47
1:A:761:GLY:O	1:A:763:PHE:HB2	2.15	0.47
1:A:427:ASP:HA	1:A:430:LYS:HG3	1.97	0.47
1:A:558:TRP:CD1	1:A:563:ARG:HG3	2.50	0.46
1:A:143:LEU:HD22	1:A:183:PRO:HD3	1.96	0.46
1:A:518:LYS:O	1:A:522:GLU:HG3	2.15	0.46
1:A:314:LEU:HD13	1:A:320:TYR:HE2	1.79	0.46
1:A:567:THR:HG23	1:A:570:GLU:OE2	2.15	0.46
1:A:718:SER:HB3	1:A:722:VAL:HG23	1.98	0.46
1:A:877:LEU:O	1:A:878:LEU:C	2.57	0.46
1:A:996:PHE:O	1:A:999:ILE:HG12	2.16	0.46
1:A:799:LEU:O	1:A:800:ARG:HB3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:829:ILE:HD13	1:A:832:ARG:NH1	2.30	0.46
1:A:271:GLU:HG3	1:A:303:ARG:NH2	2.30	0.46
1:A:276:MET:HE2	1:A:276:MET:HB3	1.78	0.46
1:A:621:TYR:CD1	1:A:951:LEU:HD11	2.50	0.46
1:A:799:LEU:HB3	1:A:800:ARG:H	1.55	0.46
1:A:972:CYS:SG	1:A:973:ILE:N	2.89	0.46
1:A:666:ARG:O	1:A:669:ILE:HG13	2.16	0.46
1:A:161:TYR:CE2	1:A:163:PRO:HG3	2.50	0.46
1:A:973:ILE:O	1:A:976:CYS:HB2	2.16	0.46
1:A:759:VAL:CG1	1:A:777:ILE:HD12	2.46	0.46
1:A:946:THR:C	1:A:948:GLY:H	2.24	0.45
1:A:160:GLU:HA	1:A:161:TYR:CB	2.45	0.45
1:A:773:MET:SD	1:A:773:MET:N	2.89	0.45
1:A:992:LEU:HD11	1:A:1031:MET:CB	2.46	0.45
1:A:1054:GLU:OE1	1:A:1054:GLU:N	2.43	0.45
1:A:291:VAL:HG22	1:A:321:VAL:HB	1.98	0.45
1:A:1103:SER:HB3	1:A:1106:LEU:HG	1.99	0.45
1:A:143:LEU:HD12	1:A:143:LEU:H	1.81	0.45
1:A:949:HIS:C	1:A:951:LEU:H	2.16	0.45
1:A:549:THR:HA	1:A:588:ILE:O	2.16	0.45
1:A:155:PRO:CD	1:A:339:LYS:HA	2.46	0.45
1:A:633:ILE:HD12	1:A:633:ILE:HA	1.84	0.45
1:A:877:LEU:O	1:A:879:VAL:N	2.50	0.45
1:A:726:TRP:HH2	1:A:839:ILE:HG12	1.82	0.45
1:A:929:ASP:OD1	1:A:929:ASP:N	2.50	0.44
1:A:978:ILE:HD11	1:A:1067:LEU:HD22	1.99	0.44
1:A:160:GLU:CA	1:A:161:TYR:HB2	2.47	0.44
1:A:516:ILE:O	1:A:520:THR:HG23	2.17	0.44
1:A:157:LEU:C	1:A:159:TYR:N	2.75	0.44
1:A:824:LYS:O	1:A:827:ASP:OD1	2.35	0.44
1:A:270:THR:HG21	1:A:307:TRP:NE1	2.32	0.44
1:A:485:LEU:HD13	1:A:489:ASP:HB3	1.99	0.44
1:A:598:GLU:HG3	1:A:599:PRO:CD	2.48	0.44
1:A:756:LEU:HA	1:A:790:GLU:O	2.18	0.44
1:A:774:PRO:O	1:A:775:GLU:HB2	2.18	0.44
1:A:784:SER:HB3	1:A:787:ALA:N	2.32	0.44
1:A:913:GLU:O	1:A:917:ARG:HG3	2.18	0.44
1:A:383:ASN:N	1:A:383:ASN:OD1	2.51	0.43
1:A:785:LYS:H	1:A:785:LYS:HG3	1.54	0.43
1:A:201:SER:OG	1:A:326:THR:HA	2.18	0.43
1:A:1091:LEU:HD23	1:A:1091:LEU:HA	1.88	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:ILE:HD12	1:A:431:ILE:HA	1.93	0.43
1:A:780:ALA:HB1	1:A:781:GLY:O	2.17	0.43
1:A:163:PRO:HB2	1:A:164:LEU:H	1.37	0.43
1:A:269:THR:OG1	1:A:272:ILE:HD12	2.18	0.43
1:A:340:ILE:HD12	1:A:641:ARG:HB3	2.01	0.43
1:A:803:GLY:O	1:A:840:LEU:HG	2.19	0.43
1:A:979:PHE:CG	1:A:1030:LEU:HD12	2.54	0.43
1:A:486:SER:O	1:A:488:ASP:N	2.49	0.43
1:A:666:ARG:CD	1:A:888:LYS:HG3	2.49	0.43
1:A:193:GLU:OE1	1:A:214:TYR:OH	2.36	0.43
1:A:369:ILE:HD13	1:A:434:MET:HE1	2.00	0.43
1:A:1007:ALA:HB1	1:A:1019:GLU:HA	2.01	0.43
1:A:233:LYS:HB2	1:A:234:ALA:H	1.29	0.43
1:A:161:TYR:HB3	1:A:162:ILE:H	1.57	0.42
1:A:692:LYS:O	1:A:696:PHE:HB2	2.19	0.42
1:A:874:ASN:O	1:A:875:SER:C	2.60	0.42
1:A:952:LEU:HD13	1:A:1006:ILE:HD12	2.02	0.42
1:A:1043:PHE:CE1	1:A:1098:ILE:HD11	2.55	0.42
1:A:154:PRO:HA	1:A:155:PRO:HD3	1.92	0.42
1:A:440:PHE:HB3	1:A:549:THR:OG1	2.20	0.42
1:A:279:ARG:NH2	1:A:942:GLU:OE2	2.52	0.42
1:A:494:GLN:O	1:A:498:ILE:HB	2.20	0.42
1:A:710:GLU:O	1:A:806:ARG:HD2	2.19	0.42
1:A:906:HIS:HB3	1:A:908:VAL:HG12	2.02	0.42
1:A:949:HIS:C	1:A:951:LEU:N	2.77	0.42
1:A:276:MET:SD	1:A:284:MET:HE1	2.60	0.41
1:A:690:TYR:HB3	1:A:860:ILE:CG1	2.48	0.41
1:A:770:GLU:HA	1:A:771:GLY:HA3	1.82	0.41
1:A:878:LEU:HA	1:A:878:LEU:HD12	1.48	0.41
1:A:938:ARG:O	1:A:941:CYS:HB2	2.21	0.41
1:A:187:LEU:HD13	1:A:187:LEU:HA	1.84	0.41
1:A:710:GLU:HB3	1:A:809:LEU:HD22	2.02	0.41
1:A:837:ILE:HA	1:A:838:PRO:HD3	1.97	0.41
1:A:844:GLU:O	1:A:845:ASN:HB2	2.20	0.41
1:A:360:TYR:HB2	1:A:590:ILE:HG12	2.03	0.41
1:A:514:LEU:HD21	1:A:1054:GLU:HB3	2.02	0.41
1:A:712:ARG:HA	1:A:805:LEU:O	2.21	0.41
1:A:279:ARG:HH22	1:A:1073:GLU:CD	2.29	0.41
1:A:361:PHE:N	1:A:361:PHE:CD2	2.89	0.41
1:A:733:ILE:O	1:A:752:VAL:HG22	2.21	0.41
1:A:972:CYS:O	1:A:975:SER:OG	2.25	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1068:LEU:HD21	1:A:1090:SER:OG	2.21	0.41
1:A:970:CYS:SG	1:A:971:ALA:N	2.94	0.41
1:A:1083:LEU:HD11	1:A:1087:PHE:CZ	2.55	0.41
1:A:436:LEU:HA	1:A:441:GLN:NE2	2.36	0.40
1:A:637:TYR:OH	1:A:641:ARG:NH1	2.54	0.40
1:A:936:LYS:HA	1:A:939:VAL:HG22	2.03	0.40
1:A:780:ALA:HA	1:A:781:GLY:HA3	1.80	0.40
1:A:442:PRO:O	1:A:547:ALA:HB1	2.21	0.40
1:A:764:ASN:OD1	1:A:764:ASN:N	2.54	0.40
1:A:973:ILE:HG12	1:A:973:ILE:H	1.70	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	919/1106 (83%)	816 (89%)	72 (8%)	31 (3%)	3 23

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	ASP
1	A	163	PRO
1	A	233	LYS
1	A	487	GLU
1	A	780	ALA
1	A	800	ARG
1	A	950	GLU
1	A	960	ARG
1	A	161	TYR
1	A	164	LEU
1	A	485	LEU

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Mol	Chain	Res	Type
1	A	706	GLY
1	A	789	TRP
1	A	803	GLY
1	A	948	GLY
1	A	961	PHE
1	A	157	LEU
1	A	878	LEU
1	A	176	THR
1	A	761	GLY
1	A	774	PRO
1	A	799	LEU
1	A	985	THR
1	A	142	VAL
1	A	673	ASP
1	A	674	GLU
1	A	750	SER
1	A	670	ILE
1	A	773	MET
1	A	718	SER
1	A	719	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	759/952 (80%)	689 (91%)	70 (9%)	8	32

All (70) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	VAL
1	A	143	LEU
1	A	156	ASP
1	A	157	LEU
1	A	160	GLU
1	A	164	LEU

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Mol	Chain	Res	Type
1	A	169	PRO
1	A	175	ARG
1	A	187	LEU
1	A	219	CYS
1	A	239	LYS
1	A	246	GLU
1	A	282	GLU
1	A	302	ILE
1	A	351	ASP
1	A	372	ILE
1	A	383	ASN
1	A	386	GLN
1	A	425	LYS
1	A	430	LYS
1	A	441	GLN
1	A	447	ASN
1	A	451	ARG
1	A	468	PRO
1	A	473	MET
1	A	482	LEU
1	A	566	LEU
1	A	567	THR
1	A	613	LEU
1	A	633	ILE
1	A	642	CYS
1	A	666	ARG
1	A	672	PRO
1	A	684	ARG
1	A	696	PHE
1	A	709	GLN
1	A	718	SER
1	A	728	VAL
1	A	737	THR
1	A	753	LEU
1	A	755	VAL
1	A	762	ASP
1	A	767	THR
1	A	770	GLU
1	A	773	MET
1	A	778	MET
1	A	783	ASP
1	A	797	ASN

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Mol	Chain	Res	Type
1	A	799	LEU
1	A	812	ARG
1	A	815	SER
1	A	820	ASP
1	A	831	ARG
1	A	835	ASP
1	A	844	GLU
1	A	856	LEU
1	A	863	LEU
1	A	873	HIS
1	A	887	LEU
1	A	906	HIS
1	A	929	ASP
1	A	970	CYS
1	A	972	CYS
1	A	973	ILE
1	A	992	LEU
1	A	1002	GLN
1	A	1042	PRO
1	A	1059	ARG
1	A	1062	ARG
1	A	1068	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	343	GLN
1	A	386	GLN
1	A	441	GLN
1	A	610	GLN
1	A	685	GLN
1	A	748	GLN
1	A	883	ASN
1	A	884	GLN

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 [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	927/1106 (83%)	-0.56	2 (0%) 91 82	95, 171, 249, 325	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	141	ILE	2.8
1	A	953	LEU	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 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.