Full wwPDB X-ray Structure Validation Report ⓘ

Sep 26, 2023 – 04:35 AM EDT

PDB ID	:	6BB8
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:

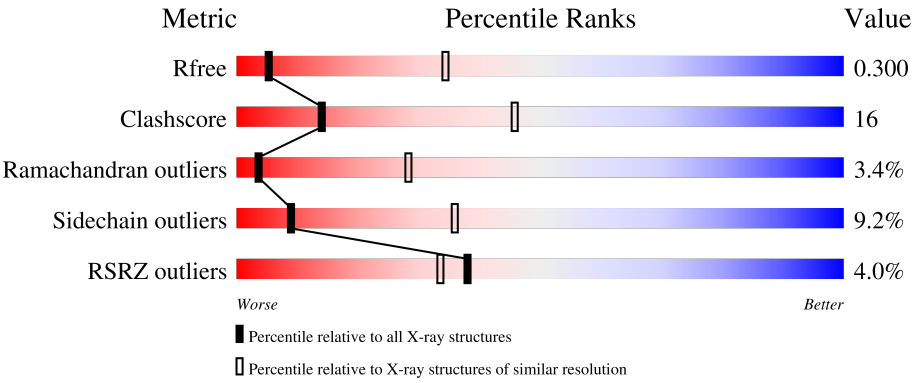
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 3.49 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}	130704	1659 (3.60-3.40)
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 <=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	3% 53% 26% 5% • 16%

2 Entry composition (i)

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.

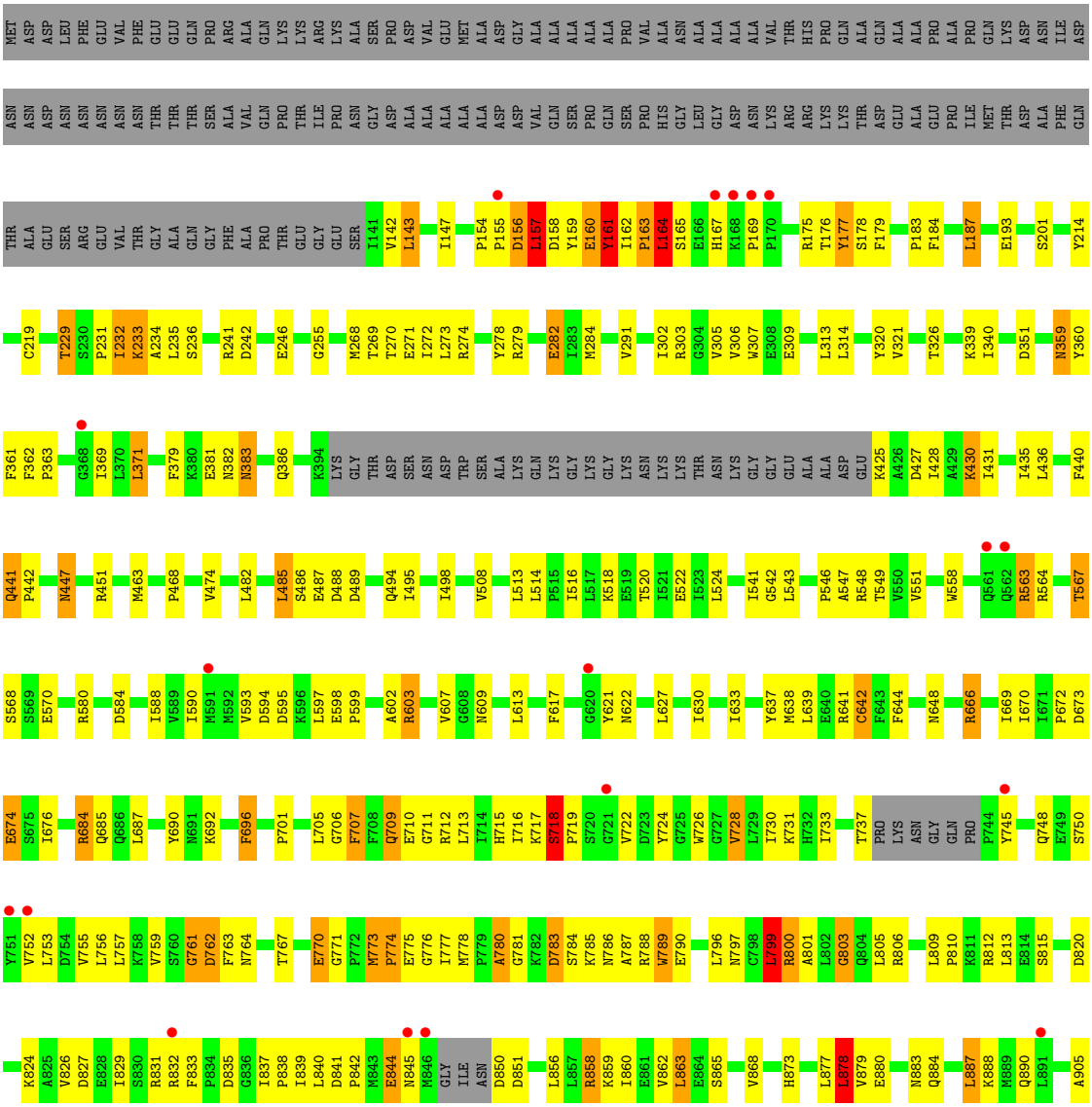
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	927	7226	4623	1241	1322	40	0	0	0

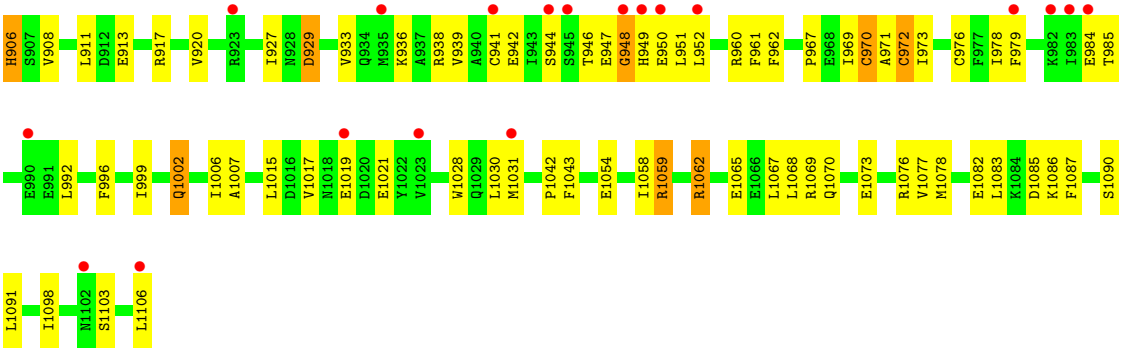
3 Residue-property plots (i)

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

Chain A:




H906 S907 V908 L911 D912 E913 R917 V920 R923 I927 N928 D929 V933 Q934 M935 K936 A937 R938 V939 A940 C941 E942 I943 S944 S945 T946 E947 G948 H949 E950 L951 L952 R960 F961 F962 P967 E968 I969 C970 A971 C972 I973 C976 F977 I978 F979 K982 I983 E984 T985
E990 E991 L992 F996 I999 Q1002 I1006 A1007 L1015 D1016 V1017 N1018 E1019 D1020 E1021 Y1022 V1023 W1028 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 N1102 S1103 L1106

4 Data and refinement statistics (i)

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) 85.8 (30.07-3.49)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.86 (at 3.47Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, R_{free}	0.251 , 0.301 0.251 , 0.300	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)	0.27 , 105.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.31$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.35	0/7361	0.72	10/9959 (0.1%)

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 (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	241	ARG	NE-CZ-NH1	-9.07	115.77	120.30
1	A	707	PHE	CB-CG-CD2	-7.71	115.40	120.80
1	A	241	ARG	NE-CZ-NH2	6.75	123.67	120.30
1	A	878	LEU	CA-CB-CG	-6.61	100.09	115.30
1	A	707	PHE	CB-CG-CD1	6.32	125.22	120.80
1	A	371	LEU	CB-CG-CD2	6.02	121.23	111.00
1	A	232	ILE	C-N-CA	5.91	136.47	121.70
1	A	745	TYR	N-CA-C	5.90	126.92	111.00
1	A	371	LEU	CA-CB-CG	-5.67	102.27	115.30
1	A	229	THR	C-N-CA	-5.14	108.86	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 (i)

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	226	0
All	All	7226	0	7179	226	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 (226) 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: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:156:ASP:HA	1:A:157:LEU:C	2.14	0.67
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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:784:SER:HA	1:A:785:LYS:C	2.25	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
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:486:SER:C	1:A:488:ASP:H	2.15	0.50
1:A:551:VAL:HA	1:A:590:ILE:O	2.12	0.50
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:850:ASP:HB2	1:A:851:ASP:CG	2.36	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: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
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:441:GLN:CD	1:A:441:GLN:H	2.19	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:549:THR:HA	1:A:588:ILE:O	2.16	0.45
1:A:929:ASP:OD1	1:A:929:ASP:N	2.50	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: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: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:548:ARG:HD3	1:A:584:ASP:CG	2.39	0.43
1:A:1091:LEU:HD23	1:A:1091:LEU:HA	1.88	0.43
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:1015:LEU:C	1:A:1017:VAL:H	2.21	0.43
1:A:284:MET:HB2	1:A:284:MET:HE2	1.85	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:627:LEU:HD11	1:A:638:MET:HE3	2.02	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:877:LEU:O	1:A:878:LEU:C	2.57	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:164:LEU:O	1:A:165:SER:OG	2.28	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: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:946:THR:C	1:A:948:GLY:H	2.24	0.41
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:382:ASN:N	1:A:382:ASN:OD1	2.55	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 28

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	9 36

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

Mol	Chain	Res	Type
1	A	143	LEU
1	A	156	ASP
1	A	157	LEU
1	A	160	GLU
1	A	161	TYR
1	A	164	LEU
1	A	167	HIS
1	A	169	PRO
1	A	175	ARG
1	A	184	PHE
1	A	187	LEU
1	A	219	CYS
1	A	242	ASP
1	A	246	GLU
1	A	282	GLU
1	A	302	ILE
1	A	351	ASP
1	A	359	ASN
1	A	383	ASN
1	A	386	GLN
1	A	425	LYS
1	A	430	LYS
1	A	441	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	447	ASN
1	A	451	ARG
1	A	463	MET
1	A	468	PRO
1	A	482	LEU
1	A	563	ARG
1	A	567	THR
1	A	603	ARG
1	A	613	LEU
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	762	ASP
1	A	767	THR
1	A	770	GLU
1	A	778	MET
1	A	783	ASP
1	A	797	ASN
1	A	799	LEU
1	A	812	ARG
1	A	815	SER
1	A	820	ASP
1	A	831	ARG
1	A	833	PHE
1	A	835	ASP
1	A	844	GLU
1	A	856	LEU
1	A	858	ARG
1	A	863	LEU
1	A	873	HIS
1	A	887	LEU
1	A	890	GLN
1	A	906	HIS
1	A	929	ASP
1	A	970	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	972	CYS
1	A	1002	GLN
1	A	1042	PRO
1	A	1059	ARG
1	A	1062	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	386	GLN
1	A	441	GLN
1	A	610	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	927/1106 (83%)	0.12	37 (3%) 38 33	95, 171, 249, 325	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	945	SER	5.0
1	A	751	TYR	4.0
1	A	1106	LEU	3.8
1	A	845	ASN	3.5
1	A	167	HIS	3.4
1	A	984	GLU	3.4
1	A	169	PRO	3.3
1	A	170	PRO	3.3
1	A	944	SER	3.2
1	A	983	ILE	3.1
1	A	1102	ASN	3.0
1	A	368	GLY	2.9
1	A	923	ARG	2.9
1	A	846	MET	2.9
1	A	950	GLU	2.7
1	A	168	LYS	2.7
1	A	949	HIS	2.7
1	A	935	MET	2.7
1	A	752	VAL	2.6
1	A	620	GLY	2.5
1	A	948	GLY	2.4
1	A	561	GLN	2.4
1	A	979	PHE	2.4
1	A	941	CYS	2.4
1	A	1031	MET	2.4
1	A	745	TYR	2.4
1	A	562	GLN	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	721	GLY	2.4
1	A	952	LEU	2.3
1	A	1019	GLU	2.2
1	A	982	LYS	2.2
1	A	832	ARG	2.2
1	A	891	LEU	2.2
1	A	990	GLU	2.2
1	A	1023	VAL	2.1
1	A	155	PRO	2.0
1	A	591	MET	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 monosaccharides 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.