



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 05:57 AM UTC

PDB ID : 3M6N / pdb_00003m6n
Title : Crystal structure of RpffF
Authors : Lim, S.C.; Cheng, Z.; Qamra, R.; Song, H.
Deposited on : 2010-03-16
Resolution : 1.80 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

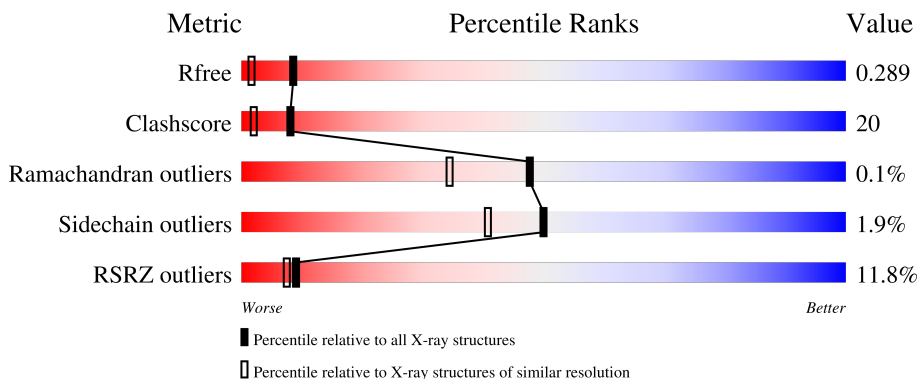
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	305	8% 60% 25% 13%
1	B	305	11% 65% 21% 12%
1	C	305	12% 61% 25% 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 6893 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 RpPf protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	264	Total	C	N	O	S	0	0	0
			2034	1274	371	371	18			
1	B	268	Total	C	N	O	S	0	0	0
			2072	1298	379	377	18			
1	C	264	Total	C	N	O	S	0	0	0
			2036	1277	371	370	18			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-15	MET	-	expression tag	UNP Q7CLS3
A	-14	GLY	-	expression tag	UNP Q7CLS3
A	-13	SER	-	expression tag	UNP Q7CLS3
A	-12	SER	-	expression tag	UNP Q7CLS3
A	-11	HIS	-	expression tag	UNP Q7CLS3
A	-10	HIS	-	expression tag	UNP Q7CLS3
A	-9	HIS	-	expression tag	UNP Q7CLS3
A	-8	HIS	-	expression tag	UNP Q7CLS3
A	-7	HIS	-	expression tag	UNP Q7CLS3
A	-6	HIS	-	expression tag	UNP Q7CLS3
A	-5	SER	-	expression tag	UNP Q7CLS3
A	-4	GLN	-	expression tag	UNP Q7CLS3
A	-3	ASP	-	expression tag	UNP Q7CLS3
A	-2	PRO	-	expression tag	UNP Q7CLS3
A	-1	ASN	-	expression tag	UNP Q7CLS3
A	0	SER	-	expression tag	UNP Q7CLS3
B	-15	MET	-	expression tag	UNP Q7CLS3
B	-14	GLY	-	expression tag	UNP Q7CLS3
B	-13	SER	-	expression tag	UNP Q7CLS3
B	-12	SER	-	expression tag	UNP Q7CLS3
B	-11	HIS	-	expression tag	UNP Q7CLS3
B	-10	HIS	-	expression tag	UNP Q7CLS3
B	-9	HIS	-	expression tag	UNP Q7CLS3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-8	HIS	-	expression tag	UNP Q7CLS3
B	-7	HIS	-	expression tag	UNP Q7CLS3
B	-6	HIS	-	expression tag	UNP Q7CLS3
B	-5	SER	-	expression tag	UNP Q7CLS3
B	-4	GLN	-	expression tag	UNP Q7CLS3
B	-3	ASP	-	expression tag	UNP Q7CLS3
B	-2	PRO	-	expression tag	UNP Q7CLS3
B	-1	ASN	-	expression tag	UNP Q7CLS3
B	0	SER	-	expression tag	UNP Q7CLS3
C	-15	MET	-	expression tag	UNP Q7CLS3
C	-14	GLY	-	expression tag	UNP Q7CLS3
C	-13	SER	-	expression tag	UNP Q7CLS3
C	-12	SER	-	expression tag	UNP Q7CLS3
C	-11	HIS	-	expression tag	UNP Q7CLS3
C	-10	HIS	-	expression tag	UNP Q7CLS3
C	-9	HIS	-	expression tag	UNP Q7CLS3
C	-8	HIS	-	expression tag	UNP Q7CLS3
C	-7	HIS	-	expression tag	UNP Q7CLS3
C	-6	HIS	-	expression tag	UNP Q7CLS3
C	-5	SER	-	expression tag	UNP Q7CLS3
C	-4	GLN	-	expression tag	UNP Q7CLS3
C	-3	ASP	-	expression tag	UNP Q7CLS3
C	-2	PRO	-	expression tag	UNP Q7CLS3
C	-1	ASN	-	expression tag	UNP Q7CLS3
C	0	SER	-	expression tag	UNP Q7CLS3

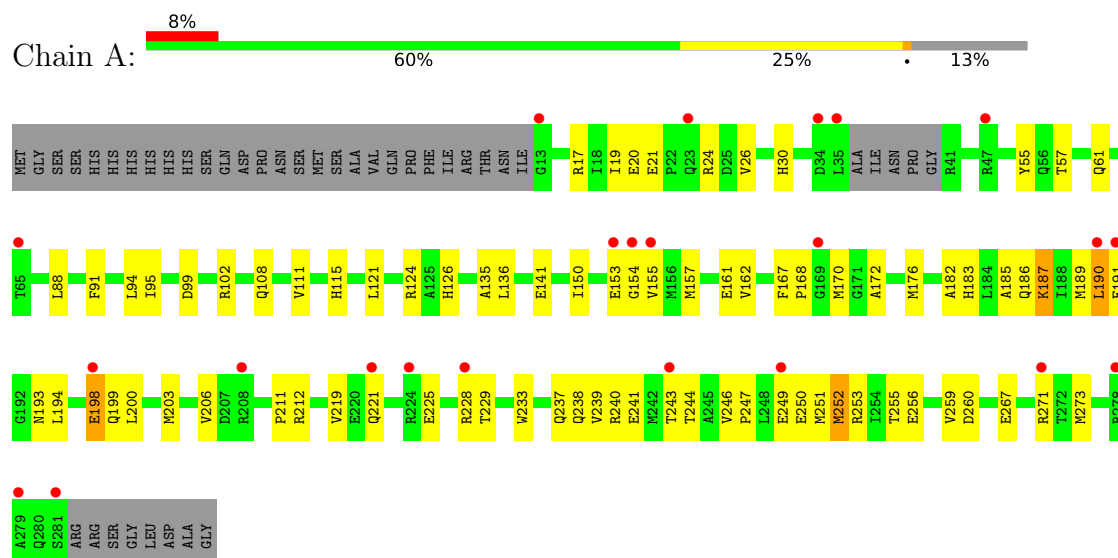
- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	260	Total O 260 260	0	0
2	B	271	Total O 271 271	0	0
2	C	220	Total O 220 220	0	0

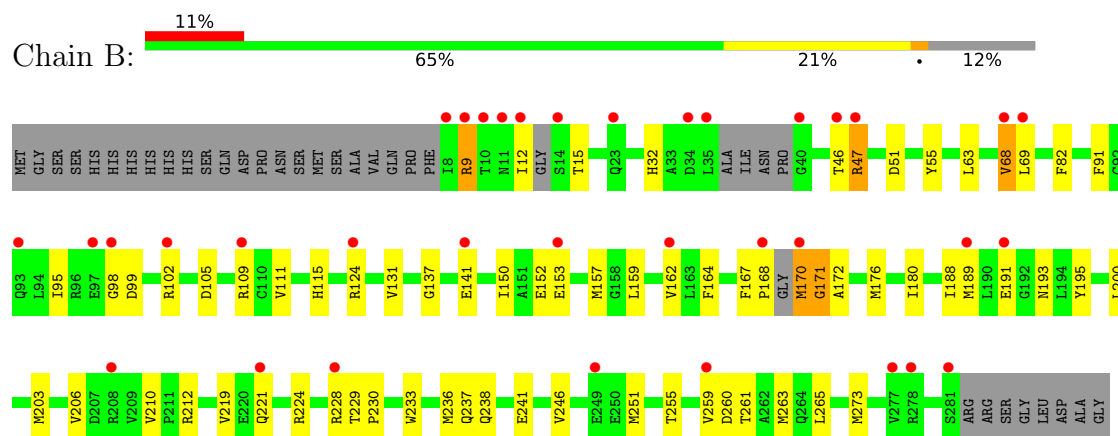
3 Residue-property plots [i](#)

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: RpfF protein

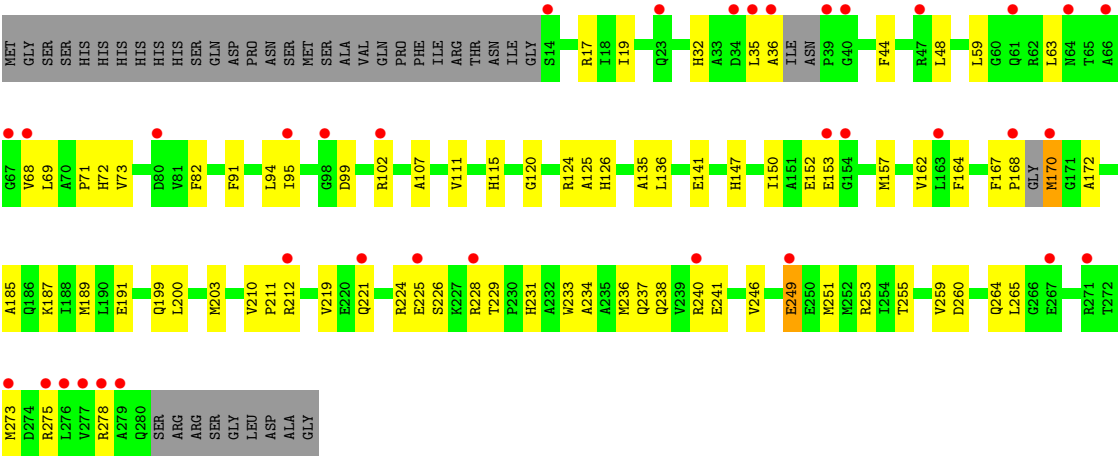


• Molecule 1: RpfF protein



• Molecule 1: RpfF protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.77Å 112.34Å 119.62Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80 30.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.3 (30.00-1.80) 97.3 (30.00-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.37 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.4.0077	Depositor
R, R_{free}	0.225 , 0.243 (Not available) , 0.289	Depositor DCC
R_{free} test set	5925 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	20.4	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 36.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6893	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.40% 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 [i](#)

5.1 Standard geometry [i](#)

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	0.28	0/2067	0.67	0/2792
1	B	0.26	0/2103	0.64	0/2838
1	C	0.27	0/2069	0.64	0/2794
All	All	0.27	0/6239	0.65	0/8424

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	GLY	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	2034	0	2036	86	0
1	B	2072	0	2079	82	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2036	0	2040	78	0
2	A	260	0	0	1	0
2	B	271	0	0	1	1
2	C	220	0	0	1	1
All	All	6893	0	6155	240	1

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 20.

All (240) 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:B:141:GLU:OE1	1:B:170:MET:HB3	1.34	1.26
1:A:249:GLU:OE2	1:A:253:ARG:NH1	1.74	1.19
1:C:225:GLU:O	1:C:228:ARG:HG2	1.42	1.19
1:C:99:ASP:OD2	1:C:102:ARG:NH1	1.76	1.18
1:A:99:ASP:OD2	1:A:102:ARG:NH1	1.80	1.13
1:B:47:ARG:H	1:B:47:ARG:NH1	1.47	1.13
1:B:9:ARG:HH11	1:B:9:ARG:CG	1.64	1.09
1:A:252:MET:HE2	1:A:252:MET:HA	1.37	1.07
1:A:225:GLU:O	1:A:228:ARG:HG2	1.62	1.00
1:B:164:PHE:CE1	1:B:273:MET:HE2	1.96	1.00
1:B:47:ARG:N	1:B:47:ARG:HH11	1.60	0.99
1:A:21:GLU:OE1	1:A:24:ARG:NH1	1.97	0.96
1:B:170:MET:SD	1:B:170:MET:N	2.39	0.96
1:B:47:ARG:H	1:B:47:ARG:HH11	0.98	0.95
1:A:182:ALA:O	1:A:186:GLN:HG3	1.64	0.94
1:B:9:ARG:HH11	1:B:9:ARG:HG3	1.31	0.93
1:B:46:THR:HG22	1:B:47:ARG:NH1	1.84	0.93
1:A:225:GLU:HB3	1:A:228:ARG:HH12	1.31	0.93
1:B:164:PHE:CD1	1:B:273:MET:HE2	2.05	0.92
1:A:191:GLU:HG2	1:A:193:ASN:ND2	1.84	0.91
1:A:249:GLU:CD	1:A:253:ARG:NH1	2.30	0.89
1:B:164:PHE:CD1	1:B:273:MET:CE	2.54	0.89
1:C:164:PHE:CD1	1:C:273:MET:HE3	2.10	0.87
1:A:252:MET:HA	1:A:252:MET:CE	2.04	0.87
1:A:135:ALA:HB3	1:A:157:MET:HG2	1.59	0.84
1:B:153:GLU:HG3	1:B:212:ARG:NH1	1.92	0.84
1:C:225:GLU:O	1:C:228:ARG:CG	2.23	0.84
1:C:164:PHE:CE1	1:C:273:MET:HE2	2.12	0.84
1:C:170:MET:SD	1:C:170:MET:N	2.52	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:THR:O	1:A:61:GLN:HG3	1.78	0.83
1:B:9:ARG:HH11	1:B:9:ARG:HG2	1.42	0.81
1:B:9:ARG:CG	1:B:9:ARG:NH1	2.37	0.81
1:B:46:THR:CG2	1:B:47:ARG:NH1	2.43	0.80
1:B:170:MET:N	1:B:170:MET:HE3	1.95	0.80
1:C:164:PHE:HE1	1:C:273:MET:HE2	1.46	0.79
1:C:200:LEU:HA	1:C:203:MET:HE3	1.63	0.79
1:A:225:GLU:HA	1:A:228:ARG:HH11	1.48	0.78
1:A:176:MET:HE1	1:A:189:MET:CG	2.13	0.78
1:B:170:MET:N	1:B:170:MET:CE	2.46	0.77
1:B:265:LEU:HD13	1:B:273:MET:HE1	1.66	0.77
1:A:225:GLU:HB3	1:A:228:ARG:NH1	2.00	0.77
1:A:176:MET:HE1	1:A:189:MET:HG2	1.65	0.77
1:A:225:GLU:CB	1:A:228:ARG:HH12	1.97	0.76
1:B:164:PHE:CD1	1:B:273:MET:HE3	2.22	0.74
1:C:265:LEU:HD13	1:C:273:MET:HE1	1.69	0.74
1:B:164:PHE:HD1	1:B:273:MET:CE	2.00	0.73
1:C:164:PHE:CE1	1:C:273:MET:CE	2.71	0.73
1:A:191:GLU:CG	1:A:193:ASN:ND2	2.52	0.72
1:A:185:ALA:O	1:A:189:MET:HG3	1.89	0.72
1:A:88:LEU:HD22	1:A:273:MET:HE3	1.71	0.72
1:A:157:MET:HB2	1:A:200:LEU:HD11	1.70	0.72
1:A:183:HIS:O	1:A:187:LYS:HD2	1.89	0.72
1:A:136:LEU:CD2	1:A:194:LEU:HD21	2.19	0.71
1:B:124:ARG:HH21	1:B:238:GLN:HG2	1.55	0.71
1:A:233:TRP:O	1:A:237:GLN:HG2	1.90	0.71
1:C:265:LEU:CD1	1:C:273:MET:HE1	2.20	0.71
1:A:225:GLU:CA	1:A:228:ARG:NH1	2.55	0.70
1:A:225:GLU:HA	1:A:228:ARG:NH1	2.07	0.69
1:A:191:GLU:HG2	1:A:193:ASN:HD21	1.54	0.69
1:B:141:GLU:OE1	1:B:170:MET:CB	2.28	0.69
1:C:153:GLU:HG3	1:C:212:ARG:NH1	2.08	0.69
1:C:164:PHE:HD1	1:C:273:MET:HE3	1.56	0.69
1:B:164:PHE:HD1	1:B:273:MET:HE3	1.57	0.68
1:A:124:ARG:NH2	1:A:238:GLN:HG2	2.08	0.68
1:B:191:GLU:HG2	1:B:193:ASN:OD1	1.94	0.68
1:A:225:GLU:CB	1:A:228:ARG:NH1	2.57	0.67
1:B:265:LEU:CD1	1:B:273:MET:HE1	2.24	0.67
1:A:167:PHE:HE1	1:B:236:MET:HE2	1.58	0.67
1:A:153:GLU:O	1:A:212:ARG:HG2	1.94	0.67
1:B:9:ARG:HG3	1:B:9:ARG:NH1	2.03	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:PHE:CD1	1:C:273:MET:CE	2.79	0.64
1:C:94:LEU:HD21	1:C:102:ARG:HD2	1.78	0.63
1:A:237:GLN:NE2	1:A:240:ARG:HH11	1.97	0.62
1:B:191:GLU:CG	1:B:193:ASN:OD1	2.47	0.62
1:B:12:ILE:HD13	1:B:55:TYR:HD1	1.64	0.62
1:B:164:PHE:HE1	1:B:273:MET:HE2	1.57	0.62
1:B:200:LEU:HA	1:B:203:MET:HE3	1.81	0.62
1:A:249:GLU:OE1	1:A:253:ARG:NH1	2.32	0.62
1:A:228:ARG:HG3	1:A:229:THR:HG23	1.82	0.61
1:A:94:LEU:HD21	1:A:102:ARG:HD2	1.80	0.61
1:B:99:ASP:OD2	1:B:102:ARG:NH1	2.33	0.61
1:A:267:GLU:O	1:A:271:ARG:HG2	2.00	0.61
1:C:168:PRO:O	1:C:170:MET:HB3	2.01	0.61
1:A:251:MET:O	1:A:255:THR:HG23	2.01	0.60
1:B:69:LEU:HD22	1:B:230:PRO:HB2	1.82	0.60
1:A:239:VAL:O	1:A:243:THR:HG23	2.01	0.60
1:A:191:GLU:CG	1:A:193:ASN:HD21	2.15	0.59
1:A:249:GLU:OE2	1:A:253:ARG:HD3	2.02	0.59
1:C:147:HIS:CD2	1:C:240:ARG:HH12	2.20	0.59
1:C:115:HIS:HE1	1:C:246:VAL:O	1.86	0.59
1:B:170:MET:O	1:B:251:MET:CE	2.52	0.58
1:B:170:MET:O	1:B:251:MET:HE2	2.03	0.58
1:A:153:GLU:O	1:A:212:ARG:CG	2.52	0.56
1:A:252:MET:CE	1:A:255:THR:HG21	2.34	0.56
1:C:69:LEU:HD21	1:C:231:HIS:CD2	2.39	0.56
1:C:237:GLN:O	1:C:241:GLU:HG3	2.05	0.56
1:C:91:PHE:O	1:C:95:ILE:HG13	2.06	0.56
1:C:124:ARG:CZ	1:C:238:GLN:HG2	2.35	0.56
1:C:275:ARG:HA	1:C:278:ARG:NH1	2.20	0.56
1:A:221:GLN:NE2	1:A:225:GLU:OE2	2.27	0.55
1:B:15:THR:OG1	1:B:51:ASP:OD2	2.08	0.55
1:A:187:LYS:HD2	1:A:187:LYS:N	2.22	0.55
1:C:200:LEU:HD23	1:C:203:MET:HE3	1.89	0.55
1:B:46:THR:HG23	1:B:47:ARG:HH11	1.72	0.55
1:B:111:VAL:HG21	1:B:255:THR:CG2	2.37	0.55
1:B:162:VAL:HG12	1:B:168:PRO:HD3	1.89	0.55
1:B:9:ARG:HG2	1:B:9:ARG:NH1	2.12	0.55
1:A:150:ILE:HD12	1:A:219:VAL:HG22	1.87	0.54
1:C:185:ALA:O	1:C:189:MET:HG3	2.07	0.54
1:A:111:VAL:HG21	1:A:255:THR:CG2	2.38	0.54
1:A:136:LEU:CD2	1:A:194:LEU:CD2	2.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:63:LEU:HD22	1:B:68:VAL:HG11	1.91	0.53
1:B:141:GLU:HG2	1:B:172:ALA:HB2	1.91	0.53
1:C:150:ILE:HD12	1:C:219:VAL:HG22	1.89	0.53
1:A:198:GLU:CD	1:A:198:GLU:H	2.15	0.53
1:C:71:PRO:HG2	1:C:125:ALA:HB2	1.91	0.53
1:B:189:MET:HB3	1:C:236:MET:HE1	1.91	0.53
1:C:94:LEU:CD2	1:C:102:ARG:HD2	2.39	0.53
1:B:237:GLN:O	1:B:241:GLU:HG3	2.07	0.52
1:B:251:MET:O	1:B:255:THR:HG23	2.09	0.52
1:A:24:ARG:HG3	1:A:26:VAL:HG23	1.90	0.52
1:B:228:ARG:CG	1:B:228:ARG:O	2.58	0.52
1:C:162:VAL:HG11	1:C:189:MET:O	2.09	0.52
1:A:190:LEU:HD22	1:B:236:MET:HE3	1.91	0.52
1:A:136:LEU:HD22	1:A:194:LEU:HD21	1.91	0.52
1:C:187:LYS:O	1:C:191:GLU:HG3	2.09	0.52
1:B:233:TRP:O	1:B:237:GLN:HG2	2.09	0.51
1:A:136:LEU:HD21	1:A:194:LEU:HD21	1.91	0.51
1:C:260:ASP:O	1:C:264:GLN:HG3	2.10	0.51
1:A:191:GLU:HG2	1:A:193:ASN:HD22	1.74	0.51
1:B:162:VAL:HG11	1:B:189:MET:O	2.10	0.51
1:B:69:LEU:HD22	1:B:230:PRO:C	2.35	0.51
1:B:12:ILE:HG22	1:B:12:ILE:O	2.10	0.51
1:A:94:LEU:CD2	1:A:102:ARG:HD2	2.41	0.51
1:A:162:VAL:HG11	1:A:189:MET:O	2.11	0.50
1:A:172:ALA:HB3	1:A:189:MET:HE3	1.92	0.50
1:A:199:GLN:O	1:A:203:MET:HG3	2.10	0.50
1:C:228:ARG:C	1:C:229:THR:HG23	2.37	0.50
1:A:187:LYS:HD2	1:A:187:LYS:H	1.76	0.50
1:A:247:PRO:HD2	1:A:250:GLU:OE1	2.12	0.49
1:B:47:ARG:NH1	1:B:47:ARG:N	2.28	0.49
1:C:107:ALA:HB1	1:C:170:MET:HE1	1.94	0.49
1:C:111:VAL:HG21	1:C:255:THR:HG22	1.94	0.49
1:B:150:ILE:HD12	1:B:219:VAL:HG22	1.95	0.49
1:C:63:LEU:HD13	1:C:71:PRO:HG3	1.94	0.49
1:A:115:HIS:HE1	1:A:246:VAL:O	1.96	0.49
1:A:187:LYS:HA	1:A:187:LYS:HE2	1.95	0.48
1:C:111:VAL:HG21	1:C:255:THR:CG2	2.43	0.48
1:A:161:GLU:OE2	1:A:168:PRO:HA	2.13	0.48
1:C:69:LEU:CD2	1:C:231:HIS:CD2	2.95	0.48
1:A:237:GLN:NE2	1:A:240:ARG:NH1	2.61	0.48
1:C:32:HIS:HE1	1:C:82:PHE:O	1.97	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:105:ASP:O	1:B:109:ARG:HG3	2.13	0.48
1:B:91:PHE:O	1:B:95:ILE:HG13	2.14	0.48
1:B:206:VAL:HB	2:B:651:HOH:O	2.14	0.48
1:C:265:LEU:HD11	1:C:273:MET:HE1	1.95	0.48
1:A:243:THR:OG1	1:A:244:THR:N	2.44	0.47
1:C:228:ARG:C	1:C:229:THR:CG2	2.87	0.47
1:A:206:VAL:HB	2:A:600:HOH:O	2.14	0.47
1:C:233:TRP:O	1:C:237:GLN:HG2	2.14	0.47
1:B:141:GLU:CD	1:B:172:ALA:HB2	2.40	0.47
1:C:200:LEU:HA	1:C:203:MET:CE	2.39	0.47
1:C:210:VAL:HB	1:C:211:PRO:HD2	1.97	0.47
1:A:17:ARG:NH1	1:A:19:ILE:HD11	2.30	0.47
1:C:35:LEU:O	1:C:36:ALA:C	2.58	0.47
1:C:107:ALA:CB	1:C:170:MET:HE1	2.45	0.47
1:C:249:GLU:OE2	1:C:253:ARG:NH2	2.46	0.47
1:A:17:ARG:HH12	1:A:19:ILE:HD11	1.80	0.47
1:C:199:GLN:O	1:C:203:MET:HG3	2.15	0.47
1:A:136:LEU:HD21	1:A:194:LEU:CD2	2.45	0.47
1:A:99:ASP:OD2	1:A:102:ARG:CZ	2.59	0.46
1:C:275:ARG:HG3	1:C:278:ARG:NH2	2.30	0.46
1:B:221:GLN:O	1:B:224:ARG:HG2	2.15	0.46
1:A:91:PHE:O	1:A:95:ILE:HG13	2.15	0.46
1:C:72:HIS:CD2	1:C:126:HIS:HB3	2.50	0.46
1:C:225:GLU:HA	1:C:228:ARG:HE	1.81	0.46
1:A:20:GLU:OE2	1:A:55:TYR:OH	2.29	0.46
1:A:153:GLU:CG	1:A:211:PRO:HA	2.46	0.46
1:B:32:HIS:HE1	1:B:82:PHE:O	1.99	0.46
1:C:167:PHE:CD1	1:C:168:PRO:HD2	2.50	0.46
1:C:221:GLN:O	1:C:225:GLU:HG3	2.16	0.46
1:C:224:ARG:HG2	1:C:228:ARG:HH21	1.81	0.46
1:A:157:MET:HB2	1:A:200:LEU:CD1	2.43	0.46
1:A:237:GLN:HE22	1:A:240:ARG:NH1	2.14	0.46
1:C:199:GLN:C	1:C:203:MET:HE2	2.41	0.45
1:C:251:MET:O	1:C:255:THR:HG23	2.16	0.45
1:A:237:GLN:HE22	1:A:240:ARG:HH11	1.62	0.45
1:B:176:MET:HE1	1:B:188:ILE:HG21	1.99	0.45
1:B:228:ARG:O	1:B:228:ARG:HG2	2.16	0.45
1:A:259:VAL:HG13	1:A:260:ASP:N	2.32	0.45
1:B:137:GLY:HA2	1:B:159:LEU:HD23	2.00	0.44
1:C:275:ARG:HG3	1:C:278:ARG:HH22	1.81	0.44
1:C:157:MET:HB2	1:C:200:LEU:HD11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:131:VAL:HG11	1:B:157:MET:HE2	1.99	0.44
1:C:59:LEU:O	1:C:63:LEU:HG	2.17	0.44
1:B:170:MET:HE3	1:B:170:MET:CA	2.48	0.44
1:C:73:VAL:O	1:C:73:VAL:HG13	2.17	0.44
1:B:115:HIS:HE1	1:B:246:VAL:O	2.01	0.44
1:C:228:ARG:O	1:C:229:THR:CG2	2.65	0.44
1:A:157:MET:HE3	1:A:200:LEU:HD12	1.99	0.43
1:A:126:HIS:HA	1:A:233:TRP:CZ2	2.54	0.43
1:B:46:THR:CG2	1:B:47:ARG:HH11	2.19	0.43
1:C:259:VAL:HG13	1:C:260:ASP:N	2.33	0.43
1:B:46:THR:HG23	1:B:47:ARG:NH1	2.25	0.43
1:B:171:GLY:HA3	1:B:251:MET:HE3	2.00	0.43
1:C:126:HIS:HA	1:C:233:TRP:CZ2	2.54	0.43
1:B:69:LEU:CD2	1:B:230:PRO:C	2.92	0.43
1:B:176:MET:HE2	1:B:180:ILE:HD11	2.01	0.43
1:B:98:GLY:HA2	1:B:263:MET:HE1	2.00	0.42
1:C:120:GLY:HA2	2:C:720:HOH:O	2.19	0.42
1:C:234:ALA:O	1:C:238:GLN:HG3	2.19	0.42
1:C:228:ARG:O	1:C:229:THR:HG22	2.19	0.42
1:A:121:LEU:HD12	1:A:121:LEU:N	2.34	0.42
1:B:12:ILE:HG21	1:B:55:TYR:HB2	2.02	0.42
1:C:17:ARG:NH1	1:C:19:ILE:HD11	2.34	0.42
1:C:141:GLU:HG2	1:C:172:ALA:HB2	2.02	0.42
1:A:237:GLN:O	1:A:241:GLU:HG3	2.20	0.41
1:C:44:PHE:HA	1:C:48:LEU:HD23	2.01	0.41
1:A:167:PHE:CE1	1:B:236:MET:HE2	2.46	0.41
1:C:72:HIS:CE1	1:C:226:SER:HG	2.32	0.41
1:A:17:ARG:HB3	1:A:30:HIS:HB2	2.03	0.41
1:A:256:GLU:O	1:A:259:VAL:HG12	2.20	0.41
1:B:157:MET:HB2	1:B:200:LEU:HD11	2.01	0.41
1:C:17:ARG:HH12	1:C:19:ILE:HD11	1.85	0.41
1:A:108:GLN:HA	1:A:252:MET:HE1	2.02	0.41
1:B:167:PHE:HE1	1:C:236:MET:HE2	1.85	0.41
1:B:229:THR:N	1:B:230:PRO:CD	2.84	0.41
1:B:261:THR:HG23	1:C:231:HIS:HB3	2.03	0.41
1:C:236:MET:O	1:C:240:ARG:HG3	2.21	0.41
1:A:221:GLN:O	1:A:225:GLU:HG3	2.21	0.41
1:B:259:VAL:HG13	1:B:260:ASP:N	2.35	0.41
1:C:135:ALA:C	1:C:136:LEU:HD12	2.46	0.41
1:C:210:VAL:HB	1:C:211:PRO:CD	2.51	0.41
1:B:195:TYR:CD1	1:B:203:MET:HE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:191:GLU:HG3	1:B:193:ASN:OD1	2.18	0.40
1:A:141:GLU:OE2	1:A:170:MET:N	2.40	0.40
1:C:168:PRO:O	1:C:170:MET:CB	2.69	0.40
1:B:46:THR:HG23	1:B:47:ARG:HD3	2.04	0.40
1:B:152:GLU:HA	1:B:210:VAL:O	2.21	0.40
1:C:152:GLU:HA	1:C:210:VAL:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:419:HOH:O	2:C:571:HOH:O[3_744]	2.06	0.14

5.3 Torsion angles

5.3.1 Protein backbone

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	260/305 (85%)	254 (98%)	6 (2%)	0	100	100
1	B	260/305 (85%)	255 (98%)	4 (2%)	1 (0%)	30	19
1	C	258/305 (85%)	253 (98%)	5 (2%)	0	100	100
All	All	778/915 (85%)	762 (98%)	15 (2%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	171	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	212/246 (86%)	207 (98%)	5 (2%)	43	31
1	B	217/246 (88%)	213 (98%)	4 (2%)	51	43
1	C	212/246 (86%)	209 (99%)	3 (1%)	59	52
All	All	641/738 (87%)	629 (98%)	12 (2%)	50	41

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	155	VAL
1	A	187	LYS
1	A	190	LEU
1	A	198	GLU
1	A	252	MET
1	B	9	ARG
1	B	47	ARG
1	B	68	VAL
1	B	170	MET
1	C	68	VAL
1	C	170	MET
1	C	249	GLU

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	32	HIS
1	A	58	ASN
1	A	61	GLN
1	A	186	GLN
1	A	193	ASN
1	A	237	GLN
1	B	23	GLN
1	B	32	HIS
1	B	115	HIS

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Mol	Chain	Res	Type
1	B	132	GLN
1	B	178	GLN
1	B	264	GLN
1	C	32	HIS
1	C	115	HIS
1	C	178	GLN
1	C	193	ASN
1	C	237	GLN

5.3.3 RNA [i](#)

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	264/305 (86%)	0.57	23 (8%) 16 14	11, 17, 24, 28	0
1	B	268/305 (87%)	0.95	35 (13%) 7 6	12, 20, 29, 36	0
1	C	264/305 (86%)	1.05	36 (13%) 7 5	12, 21, 30, 39	0
All	All	796/915 (86%)	0.86	94 (11%) 9 7	11, 19, 28, 39	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	154	GLY	9.0
1	B	170	MET	9.0
1	B	8	ILE	7.9
1	B	12	ILE	6.0
1	A	281	SER	5.4
1	B	11	ASN	5.3
1	B	281	SER	5.2
1	C	36	ALA	4.9
1	A	153	GLU	4.9
1	B	9	ARG	4.6
1	C	228	ARG	4.5
1	B	14	SER	4.5
1	C	170	MET	4.3
1	C	39	PRO	4.2
1	C	102	ARG	4.1
1	A	169	GLY	3.9
1	B	35	LEU	3.9
1	A	155	VAL	3.9
1	C	40	GLY	3.8
1	C	277	VAL	3.8
1	B	191	GLU	3.7
1	B	69	LEU	3.6
1	B	23	GLN	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	47	ARG	3.6
1	A	34	ASP	3.6
1	C	34	ASP	3.4
1	A	228	ARG	3.3
1	A	13	GLY	3.3
1	B	249	GLU	3.2
1	A	35	LEU	3.2
1	A	278	ARG	3.1
1	C	154	GLY	3.0
1	B	162	VAL	3.0
1	B	124	ARG	3.0
1	A	221	GLN	3.0
1	C	35	LEU	2.9
1	B	98	GLY	2.9
1	C	278	ARG	2.8
1	B	34	ASP	2.8
1	C	47	ARG	2.8
1	B	97	GLU	2.8
1	A	190	LEU	2.8
1	B	153	GLU	2.8
1	C	240	ARG	2.7
1	B	10	THR	2.7
1	C	275	ARG	2.7
1	C	279	ALA	2.6
1	C	271	ARG	2.6
1	C	23	GLN	2.6
1	B	228	ARG	2.6
1	C	64	ASN	2.6
1	C	212	ARG	2.6
1	C	225	GLU	2.6
1	C	61	GLN	2.5
1	C	66	ALA	2.5
1	A	191	GLU	2.5
1	B	40	GLY	2.5
1	B	68	VAL	2.5
1	C	80	ASP	2.5
1	C	95	ILE	2.4
1	A	47	ARG	2.4
1	B	278	ARG	2.4
1	B	102	ARG	2.4
1	C	168	PRO	2.4
1	C	153	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	14	SER	2.4
1	C	221	GLN	2.4
1	B	168	PRO	2.3
1	A	271	ARG	2.3
1	C	273	MET	2.2
1	B	46	THR	2.2
1	A	249	GLU	2.2
1	C	249	GLU	2.2
1	B	141	GLU	2.2
1	B	93	GLN	2.2
1	C	67	GLY	2.2
1	A	279	ALA	2.2
1	B	208	ARG	2.2
1	C	267	GLU	2.1
1	C	98	GLY	2.1
1	A	224	ARG	2.1
1	A	198	GLU	2.1
1	B	189	MET	2.1
1	A	65	THR	2.1
1	A	208	ARG	2.1
1	C	276	LEU	2.1
1	B	221	GLN	2.1
1	B	109	ARG	2.1
1	B	259	VAL	2.1
1	C	163	LEU	2.1
1	A	23	GLN	2.0
1	A	243	THR	2.0
1	B	277	VAL	2.0
1	C	68	VAL	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 ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.