



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:09 AM UTC

PDB ID : 5DAR / pdb_00005dar
Title : CRYSTAL STRUCTURE OF THE BASE OF THE RIBOSOMAL P STALK
FROM METHANOCOCCUS JANNASCHII
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Deposited on : 2015-08-20
Resolution : 2.90 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

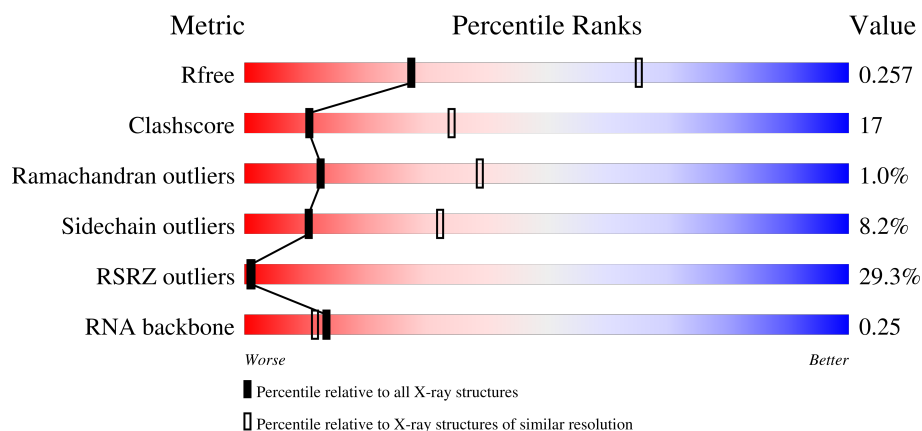
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)
RNA backbone	3983	1120 (3.10-2.70)

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	74	8% 28% 43% 20% 8%
1	D	74	7% 26% 50% 19% 5%
2	B	213	15% 46% 23% 6% 25%
2	E	213	32% 61% 33% . .

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Mol	Chain	Length	Quality of chain
3	C	161	35% 56% 34% 9% .
3	F	161	47% 56% 34% 7% ..

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 8414 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 RNA chain called 74 nt fragment of 23S rRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	74	Total	C	N	O	P	0	0	0
			1588	708	293	513	74			
1	D	74	Total	C	N	O	P	0	0	0
			1588	708	293	513	74			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1224	C	U	conflict	GB 470491724
D	1224	C	U	conflict	GB 470491724

- Molecule 2 is a protein called 50S ribosomal protein L10.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	160	Total	C	N	O	S	0	0	0
			1243	802	213	222	6			
2	E	205	Total	C	N	O	S	0	0	0
			1571	1014	266	284	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	9	MET	VAL	conflict	UNP P54049
E	9	MET	VAL	conflict	UNP P54049

- Molecule 3 is a protein called 50S ribosomal protein L11.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	158	Total	C	N	O	S	0	0	0
			1197	762	197	232	6			
3	F	158	Total	C	N	O	S	0	0	0
			1197	762	197	232	6			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total 5	Mg 5	0	0
4	D	3	Total 3	Mg 3	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Cl 1	0	0
5	B	1	Total 1	Cl 1	0	0
5	F	1	Total 1	Cl 1	0	0

- Molecule 6 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	2	Total 2	K 2	0	0
6	C	1	Total 1	K 1	0	0
6	D	1	Total 1	K 1	0	0
6	F	1	Total 1	K 1	0	0

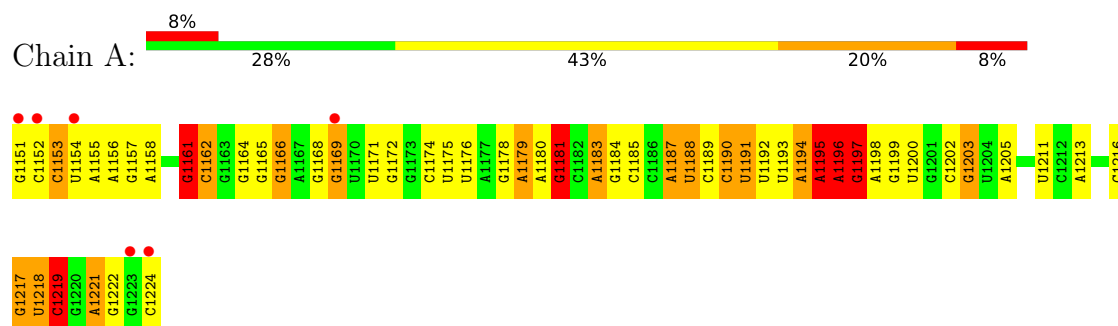
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	5	Total 5	O 5	0	0
7	C	1	Total 1	O 1	0	0
7	D	7	Total 7	O 7	0	0
7	E	1	Total 1	O 1	0	0

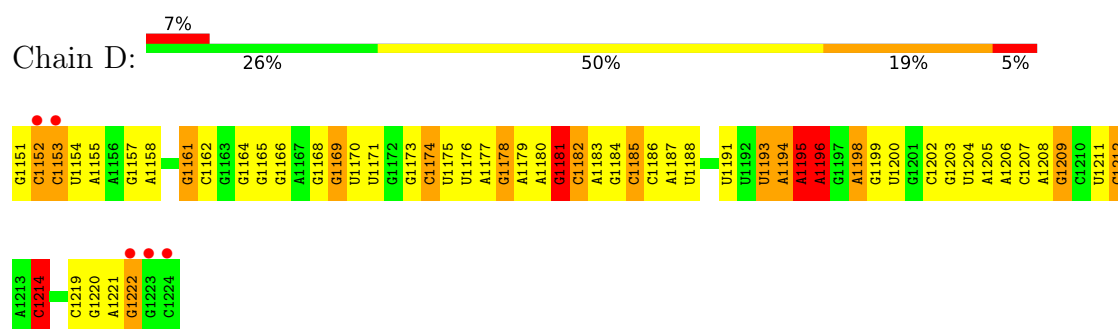
3 Residue-property plots [i](#)

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.

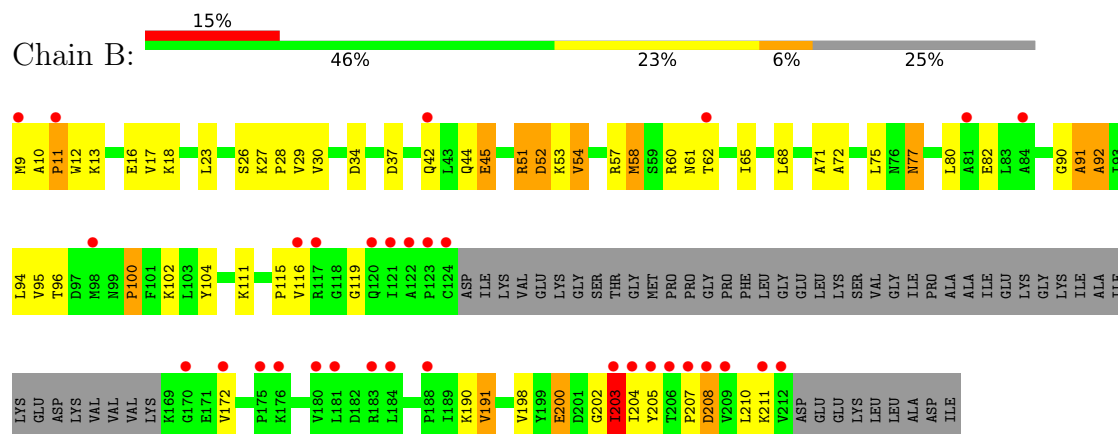
- Molecule 1: 74 nt fragment of 23S rRNA



- Molecule 1: 74 nt fragment of 23S rRNA



- Molecule 2: 50S ribosomal protein L10



- Molecule 2: 50S ribosomal protein L10

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	72.40Å 88.45Å 95.23Å 90.00° 102.19° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 20.00 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.2 (20.00-2.90) 97.2 (20.00-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.14	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 2.90Å)	Xtriage
Refinement program	REFMAC 5.8.0073	Depositor
R, R_{free}	0.264 , 0.297 (Not available) , 0.257	Depositor DCC
R_{free} test set	1295 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.638	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 32.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	8414	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.73% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, MG, K

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	0.61	0/1777	1.15	22/2768 (0.8%)
1	D	0.59	0/1777	1.13	24/2768 (0.9%)
2	B	1.12	4/1259 (0.3%)	1.12	3/1699 (0.2%)
2	E	0.76	0/1593	1.05	5/2149 (0.2%)
3	C	0.91	2/1213 (0.2%)	1.19	10/1639 (0.6%)
3	F	0.85	1/1213 (0.1%)	1.09	2/1639 (0.1%)
All	All	0.80	7/8832 (0.1%)	1.12	66/12662 (0.5%)

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
3	F	0	1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	91	ALA	CA-C	-9.08	1.42	1.52
2	B	91	ALA	C-O	-6.11	1.17	1.24
3	C	72	THR	C-O	-6.09	1.16	1.24
2	B	92	ALA	C-O	-5.87	1.16	1.23
2	B	51	ARG	CA-C	-5.42	1.45	1.52
3	C	72	THR	CA-C	-5.12	1.46	1.52
3	F	109	LYS	N-CA	-5.10	1.40	1.46

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1185	C	C3'-C2'-O2'	10.98	127.17	110.70
1	A	1191	U	C4'-C3'-O3'	-8.76	99.86	113.00
3	C	97	LEU	CB-CA-C	8.43	124.80	109.37
3	C	138	GLY	N-CA-C	-8.36	105.14	115.08
1	A	1196	A	C1'-C2'-O2'	8.33	120.90	108.40
1	D	1195	A	C2'-C3'-O3'	8.11	125.87	113.70
1	A	1181	G	C3'-C2'-O2'	8.00	122.70	110.70
1	A	1203	G	C4'-C3'-O3'	-7.84	101.24	113.00
1	D	1184	G	C3'-C2'-O2'	7.72	122.28	110.70
1	D	1214	C	C3'-C2'-O2'	7.64	122.17	110.70
3	C	73	THR	N-CA-C	-7.28	101.55	112.04
1	D	1196	A	C1'-C2'-O2'	7.22	119.23	108.40
1	A	1195	A	C2'-C3'-O3'	7.10	124.36	113.70
1	A	1213	A	C1'-C2'-O2'	7.10	119.05	108.40
1	A	1162	C	C3'-C2'-O2'	7.01	121.22	110.70
3	C	73	THR	CA-C-N	7.01	129.99	120.38
3	C	73	THR	C-N-CA	7.01	129.99	120.38
3	F	94	VAL	CB-CA-C	6.97	118.48	110.88
1	A	1194	A	C4'-C3'-O3'	-6.89	102.67	113.00
1	D	1181	G	C3'-C2'-O2'	6.64	120.66	110.70
1	D	1205	A	C3'-C2'-O2'	6.63	120.64	110.70
1	D	1219	C	C4'-C3'-O3'	-6.62	103.07	113.00
1	D	1176	U	C2'-C3'-O3'	6.54	123.51	113.70
1	D	1188	U	C2'-C3'-O3'	-6.35	104.18	113.70
2	B	203	ILE	N-CA-C	6.33	116.73	107.75
1	D	1194	A	C4'-C3'-O3'	-6.16	103.75	113.00
1	D	1195	A	C3'-C2'-O2'	6.11	119.86	110.70
3	C	74	ALA	N-CA-C	6.10	118.71	111.33
1	D	1211	U	C1'-C2'-O2'	6.07	117.50	108.40
3	C	88	GLU	CA-C-N	6.05	127.41	119.84
3	C	88	GLU	C-N-CA	6.05	127.41	119.84
1	D	1195	A	C4'-C3'-O3'	6.05	122.08	113.00
1	A	1205	A	C3'-C2'-O2'	6.04	119.75	110.70
1	D	1164	G	C3'-C2'-O2'	6.02	119.73	110.70
1	A	1211	U	C2'-C3'-O3'	5.97	122.66	113.70
1	D	1162	C	C3'-C2'-O2'	5.94	119.61	110.70
2	E	89	ARG	CB-CA-C	-5.92	109.73	116.54
1	A	1184	G	C3'-C2'-O2'	5.79	119.38	110.70
1	D	1161	G	C4'-C3'-O3'	-5.69	104.46	113.00
1	D	1212	C	C3'-C2'-O2'	5.62	119.13	110.70
1	A	1191	U	C2'-C3'-O3'	5.62	122.12	113.70
3	F	108	MET	N-CA-C	-5.61	105.25	111.36
2	E	99	ASN	CA-C-N	5.57	126.80	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	99	ASN	C-N-CA	5.57	126.80	119.84
1	D	1191	U	C4'-C3'-O3'	-5.47	104.80	113.00
1	A	1187	A	C3'-C2'-O2'	5.43	118.85	110.70
1	D	1176	U	C4'-C3'-O3'	-5.42	104.88	113.00
1	D	1185	C	C1'-C2'-O2'	5.38	116.46	108.40
1	A	1219	C	C3'-C2'-O2'	5.35	118.72	110.70
1	D	1161	G	C1'-C2'-O2'	5.30	116.35	108.40
1	A	1211	U	C4'-C3'-O3'	-5.25	105.12	113.00
1	A	1178	G	C1'-C2'-O2'	5.23	116.24	108.40
1	A	1161	G	C1'-C2'-O2'	5.22	116.23	108.40
1	A	1217	G	C2'-C3'-O3'	-5.20	105.90	113.70
1	A	1166	G	C1'-C2'-O2'	5.19	116.19	108.40
1	D	1209	G	C1'-C2'-O2'	5.19	116.19	108.40
2	B	77	ASN	CA-C-N	5.18	124.98	119.28
2	B	77	ASN	C-N-CA	5.18	124.98	119.28
3	C	69	ILE	CA-C-N	-5.14	115.09	120.38
3	C	69	ILE	C-N-CA	-5.14	115.09	120.38
1	A	1188	U	C4'-C3'-O3'	-5.11	105.33	113.00
1	D	1174	C	C4'-C3'-O3'	-5.09	105.36	113.00
1	D	1178	G	C4'-C3'-O3'	-5.07	105.39	113.00
2	E	40	ALA	CA-C-N	-5.03	114.48	119.56
2	E	40	ALA	C-N-CA	-5.03	114.48	119.56
1	A	1197	G	C2'-C3'-O3'	-5.02	106.17	113.70

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	F	138	GLY	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	1588	0	802	35	0
1	D	1588	0	801	38	0
2	B	1243	0	1347	61	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	1571	0	1707	46	0
3	C	1197	0	1256	55	0
3	F	1197	0	1256	49	0
4	A	5	0	0	0	0
4	D	3	0	0	0	0
5	A	1	0	0	1	0
5	B	1	0	0	0	0
5	F	1	0	0	0	0
6	A	2	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	5	0	0	3	0
7	C	1	0	0	0	0
7	D	7	0	0	1	0
7	E	1	0	0	0	0
All	All	8414	0	7169	258	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 17.

All (258) 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)
2:E:207:PRO:HA	2:E:210:LEU:HG	1.32	1.07
2:B:115:PRO:O	2:B:116:VAL:N	1.89	1.06
1:D:1170:U:OP2	3:F:109:LYS:NZ	1.89	1.04
2:B:104:TYR:OH	2:B:211:LYS:NZ	1.91	1.02
1:D:1151:G:H2'	1:D:1152:C:O5'	1.65	0.95
2:B:115:PRO:C	2:B:116:VAL:N	2.26	0.93
2:B:51:ARG:NH2	3:C:116:TYR:CD2	2.38	0.92
2:B:102:LYS:HB3	2:B:102:LYS:HZ2	1.34	0.91
1:A:1172:G:OP1	7:A:1401:HOH:O	1.87	0.90
2:B:51:ARG:HH21	3:C:116:TYR:HD2	1.20	0.89
2:B:29:VAL:HG12	2:B:200:GLU:HG2	1.55	0.88
1:D:1151:G:C2'	1:D:1152:C:O5'	2.22	0.87
1:D:1170:U:H3	1:D:1198:A:H2	1.23	0.86
2:E:46:ILE:HG21	2:E:193:LEU:HD12	1.59	0.84
2:B:54:VAL:HG21	2:B:94:LEU:HD11	1.61	0.83
3:C:98:THR:HG22	3:C:100:GLU:N	1.99	0.78
2:B:52:ASP:O	2:B:53:LYS:HG2	1.85	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:54:VAL:HG21	2:E:94:LEU:HD11	1.66	0.77
2:E:123:PRO:HG3	2:E:189:ILE:CD1	2.14	0.77
1:D:1170:U:N3	1:D:1198:A:H2	1.83	0.76
1:A:1192:U:O4	7:A:1402:HOH:O	2.04	0.74
3:F:104:LYS:O	3:F:108:MET:HG3	1.87	0.74
2:E:123:PRO:HG3	2:E:189:ILE:HD11	1.69	0.74
1:A:1191:U:O2	3:C:114:LEU:HD11	1.90	0.71
3:F:106:ALA:HB2	3:F:122:VAL:HG12	1.71	0.71
1:D:1182:C:H5'	1:D:1182:C:H6	1.55	0.71
1:A:1218:U:H5'	1:A:1219:C:OP2	1.90	0.70
2:E:207:PRO:HA	2:E:210:LEU:CG	2.17	0.70
2:E:34:ASP:OD2	2:E:89:ARG:HD3	1.92	0.70
1:D:1158:A:N1	1:D:1222:G:O2'	2.21	0.70
3:F:128:THR:O	3:F:131:SER:OG	2.09	0.70
1:A:1216:C:H2'	1:A:1217:G:O4'	1.90	0.69
2:B:202:GLY:O	2:B:203:ILE:HG13	1.93	0.67
3:F:5:VAL:HG11	3:F:23:ALA:HB1	1.76	0.67
2:B:23:LEU:O	2:B:26:SER:HB3	1.94	0.67
2:B:102:LYS:HB3	2:B:102:LYS:NZ	2.06	0.67
1:D:1171:U:C5	3:F:8:LEU:HD13	2.30	0.66
1:D:1195:A:O2'	1:D:1214:C:O2'	2.14	0.66
2:B:51:ARG:NH2	3:C:116:TYR:HD2	1.83	0.65
2:B:51:ARG:NH2	3:C:116:TYR:CE2	2.66	0.64
3:F:111:ASP:OD1	3:F:111:ASP:N	2.30	0.64
1:A:1164:G:O2'	2:B:37:ASP:HA	1.98	0.64
1:D:1195:A:HO2'	1:D:1214:C:HO2'	1.45	0.63
3:F:120:ASN:O	3:F:123:LYS:HB2	1.98	0.63
2:B:52:ASP:C	2:B:53:LYS:HG2	2.23	0.63
1:D:1173:G:OP1	3:F:73:THR:HG21	1.98	0.63
2:E:123:PRO:CG	2:E:189:ILE:CD1	2.77	0.63
2:B:42:GLN:HA	2:B:45:GLU:HG2	1.80	0.62
1:A:1187:A:O2'	3:C:90:ARG:NH1	2.32	0.62
2:E:15:GLU:HA	2:E:18:LYS:HG2	1.82	0.61
1:D:1187:A:O2'	3:F:90:ARG:NH1	2.33	0.61
3:C:157:PHE:O	3:C:158:LYS:HB2	2.00	0.60
3:F:128:THR:HG22	3:F:132:MET:HE1	1.82	0.60
2:B:54:VAL:HG21	2:B:94:LEU:CD1	2.30	0.59
3:F:18:PRO:O	3:F:20:LEU:N	2.34	0.59
2:E:10:ALA:HB1	2:E:13:LYS:HG3	1.85	0.59
2:B:10:ALA:HB1	2:B:11:PRO:HD2	1.84	0.58
1:D:1174:C:H2'	1:D:1175:U:O4'	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:78:PRO:O	2:E:81:ALA:HB3	2.04	0.58
3:F:126:LEU:HD23	3:F:136:VAL:HG21	1.86	0.58
2:E:23:LEU:O	2:E:26:SER:HB3	2.04	0.58
3:F:106:ALA:CB	3:F:122:VAL:HG12	2.34	0.58
1:D:1170:U:N3	1:D:1198:A:C2	2.63	0.57
2:E:152:ALA:HB2	2:E:161:LYS:HE3	1.85	0.57
2:B:42:GLN:O	2:B:45:GLU:HG3	2.04	0.57
2:B:34:ASP:HA	2:B:90:GLY:O	2.04	0.57
3:F:128:THR:HG22	3:F:132:MET:CE	2.35	0.57
3:C:72:THR:HG22	3:C:72:THR:O	2.04	0.57
3:C:96:ASN:OD1	3:C:96:ASN:C	2.47	0.57
1:A:1171:U:O4	3:C:8:LEU:HD22	2.05	0.57
3:F:12:GLY:N	3:F:42:THR:O	2.38	0.56
3:F:106:ALA:O	3:F:110:LYS:HB2	2.05	0.56
2:B:100:PRO:HD3	2:B:200:GLU:HG3	1.87	0.56
3:C:93:VAL:HG12	3:C:95:GLY:H	1.70	0.56
1:A:1196:A:H3'	1:A:1196:A:N3	2.20	0.56
2:B:53:LYS:O	2:B:54:VAL:HG12	2.03	0.56
2:B:27:LYS:HG3	2:B:28:PRO:CD	2.36	0.56
1:D:1207:C:H2'	1:D:1208:A:H5'	1.87	0.56
1:D:1204:U:O2'	1:D:1206:A:N7	2.35	0.55
2:E:58:MET:HG3	2:E:59:SER:N	2.21	0.55
3:C:97:LEU:HD13	3:C:101:GLN:HB2	1.88	0.55
3:F:99:LEU:N	3:F:137:GLU:OE2	2.40	0.55
2:E:14:ILE:O	2:E:18:LYS:HG2	2.07	0.54
2:E:128:VAL:O	2:E:163:ASP:HA	2.06	0.54
1:A:1179:A:C4	1:A:1183:A:C2	2.95	0.54
1:A:1168:G:C2'	1:A:1169:G:H5'	2.38	0.54
1:D:1168:G:O2'	1:D:1169:G:H5'	2.08	0.54
1:A:1156:A:C6	2:B:9:MET:SD	3.00	0.53
2:E:35:MET:HE3	2:E:92:ALA:CB	2.38	0.53
3:F:80:LEU:HD11	3:F:134:VAL:HG21	1.90	0.53
2:E:35:MET:HE3	2:E:92:ALA:HB2	1.90	0.53
3:F:103:ILE:HG22	3:F:107:LYS:HD2	1.90	0.53
3:F:140:ASP:OD1	3:F:142:LYS:HB2	2.08	0.53
1:D:1154:U:O2'	1:D:1221:A:N1	2.40	0.53
1:A:1196:A:H5''	1:A:1197:G:OP1	2.08	0.53
1:A:1152:C:O2'	1:A:1153:C:P	2.67	0.53
3:F:96:ASN:ND2	3:F:135:THR:OG1	2.42	0.52
2:E:170:GLY:O	2:E:171:GLU:N	2.43	0.52
3:F:34:VAL:HG13	3:F:65:ILE:HD11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:40:ALA:N	2:E:41:PRO:CD	2.73	0.52
1:D:1193:U:O2	1:D:1195:A:C8	2.62	0.51
2:E:104:TYR:CD1	2:E:210:LEU:HD13	2.45	0.51
2:E:16:GLU:OE2	2:E:16:GLU:HA	2.10	0.51
2:B:203:ILE:HG23	2:B:204:ILE:N	2.25	0.51
3:C:97:LEU:HD12	3:C:102:VAL:HG23	1.93	0.51
2:B:61:ASN:ND2	2:B:91:ALA:CB	2.74	0.50
1:D:1202:C:H5'	1:D:1203:G:OP2	2.10	0.50
3:C:98:THR:HB	3:C:101:GLN:HG3	1.93	0.50
2:E:27:LYS:HG3	2:E:28:PRO:HD2	1.92	0.50
2:B:62:THR:O	2:B:65:ILE:HG13	2.12	0.50
3:C:71:PRO:C	3:C:73:THR:H	2.18	0.50
3:F:69:ILE:HD13	3:F:108:MET:O	2.12	0.50
2:E:35:MET:SD	2:E:58:MET:HE2	2.51	0.49
2:B:16:GLU:OE2	2:B:57:ARG:NH1	2.43	0.49
2:B:29:VAL:HG12	2:B:200:GLU:CG	2.37	0.49
2:B:205:TYR:HB3	2:B:210:LEU:HD21	1.93	0.49
3:C:10:THR:OG1	3:C:49:GLN:NE2	2.45	0.49
2:B:29:VAL:HG22	2:B:96:THR:O	2.11	0.49
3:F:71:PRO:HA	3:F:109:LYS:NZ	2.27	0.49
3:C:18:PRO:O	3:C:20:LEU:N	2.46	0.49
1:D:1157:G:OP1	2:E:60:ARG:NH1	2.44	0.49
1:D:1196:A:OP2	7:D:1401:HOH:O	2.20	0.49
2:E:35:MET:O	2:E:38:VAL:HB	2.13	0.49
2:B:27:LYS:HG3	2:B:28:PRO:HD2	1.95	0.49
2:B:30:VAL:HG13	2:B:95:VAL:HG12	1.95	0.49
2:B:51:ARG:CZ	3:C:116:TYR:CE2	2.96	0.48
2:B:115:PRO:O	2:B:116:VAL:CA	2.61	0.48
2:E:24:ILE:HD12	2:E:68:LEU:HD23	1.96	0.48
2:E:54:VAL:HG21	2:E:94:LEU:CD1	2.41	0.48
1:D:1181:G:O2'	1:D:1199:G:H2'	2.13	0.48
2:B:29:VAL:CG2	2:B:96:THR:HG23	2.44	0.48
1:A:1152:C:O2'	1:A:1153:C:OP2	2.28	0.48
2:E:201:ASP:O	2:E:203:ILE:HG12	2.14	0.48
2:B:58:MET:HG3	2:B:92:ALA:HB2	1.95	0.48
2:B:100:PRO:HG3	2:B:198:VAL:HG11	1.96	0.48
2:B:102:LYS:NZ	2:B:102:LYS:CB	2.73	0.48
1:D:1186:C:H2'	1:D:1187:A:O4'	2.14	0.48
3:F:110:LYS:HG3	3:F:110:LYS:O	2.14	0.47
3:F:75:LEU:O	3:F:76:ILE:C	2.56	0.47
1:A:1175:U:H2'	1:A:1176:U:O4'	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:111:LYS:HD3	2:B:191:VAL:C	2.40	0.47
3:F:39:ASN:O	3:F:43:LYS:HG2	2.14	0.47
3:F:129:CYS:HA	3:F:132:MET:HE3	1.96	0.47
3:F:147:GLU:O	3:F:152:VAL:HB	2.15	0.47
1:A:1164:G:HO2'	2:B:37:ASP:HA	1.79	0.47
2:B:13:LYS:O	2:B:17:VAL:HG23	2.14	0.47
1:D:1195:A:C8	1:D:1195:A:H3'	2.49	0.47
3:C:45:TYR:HA	3:C:48:MET:HE3	1.97	0.47
2:B:12:TRP:O	2:B:16:GLU:HB2	2.15	0.47
1:D:1173:G:H5''	3:F:73:THR:HG21	1.97	0.47
2:B:53:LYS:C	2:B:54:VAL:CG1	2.88	0.46
3:F:70:PRO:O	3:F:109:LYS:NZ	2.47	0.46
3:C:24:ILE:HD13	3:C:34:VAL:HG11	1.98	0.46
1:D:1168:G:C2'	1:D:1169:G:H5'	2.46	0.46
2:E:31:ALA:HB2	2:E:198:VAL:HG13	1.97	0.46
2:B:172:VAL:HG13	2:B:172:VAL:O	2.15	0.46
2:B:203:ILE:HG23	2:B:204:ILE:H	1.79	0.46
2:B:100:PRO:CD	2:B:200:GLU:HG3	2.44	0.46
1:A:1164:G:H2'	1:A:1165:G:O5'	2.16	0.46
1:A:1192:U:O2	2:B:44:GLN:NE2	2.44	0.46
2:B:203:ILE:CG2	2:B:204:ILE:N	2.78	0.46
3:C:98:THR:CG2	3:C:100:GLU:N	2.75	0.46
3:F:18:PRO:O	3:F:19:PRO:C	2.58	0.46
3:C:18:PRO:O	3:C:21:GLY:N	2.46	0.46
1:D:1165:G:H2'	1:D:1166:G:H5'	1.98	0.46
1:A:1168:G:H1'	3:C:114:LEU:HG	1.98	0.45
1:D:1203:G:O2'	1:D:1208:A:N6	2.46	0.45
2:B:207:PRO:O	2:B:208:ASP:C	2.59	0.45
2:B:23:LEU:O	2:B:26:SER:CB	2.62	0.45
1:D:1151:G:O2'	1:D:1152:C:O5'	2.34	0.45
1:D:1173:G:H5''	3:F:73:THR:CG2	2.46	0.45
3:F:139:LYS:NZ	3:F:153:TYR:OH	2.37	0.45
3:F:70:PRO:HG2	3:F:75:LEU:HD21	1.98	0.45
3:C:42:THR:HG22	3:C:67:VAL:HG11	1.99	0.45
2:E:61:ASN:O	2:E:62:THR:C	2.60	0.45
1:A:1174:C:H5''	3:C:84:THR:HG23	1.99	0.45
3:C:126:LEU:O	3:C:129:CYS:HB2	2.17	0.45
2:B:61:ASN:ND2	2:B:91:ALA:HB2	2.33	0.44
3:C:11:GLY:O	3:C:46:GLU:HA	2.16	0.44
1:A:1194:A:N1	5:A:1306:CL:CL	2.88	0.44
3:C:48:MET:SD	3:C:78:LYS:HD2	2.57	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:109:LYS:HB2	3:C:113:MET:HE3	1.99	0.44
3:C:96:ASN:HB2	3:C:135:THR:OG1	2.17	0.44
2:E:17:VAL:HA	2:E:20:LEU:HD12	1.99	0.44
3:F:118:LEU:O	3:F:122:VAL:HG13	2.17	0.44
3:C:126:LEU:HD11	3:C:144:VAL:HG23	1.98	0.44
1:D:1170:U:OP2	3:F:71:PRO:HA	2.17	0.44
3:F:24:ILE:HD13	3:F:34:VAL:HG11	1.99	0.44
2:E:20:LEU:O	2:E:24:ILE:HG12	2.17	0.44
2:B:61:ASN:ND2	2:B:91:ALA:HB3	2.32	0.44
1:D:1152:C:O2'	1:D:1153:C:P	2.75	0.44
1:A:1154:U:O2'	1:A:1221:A:N1	2.50	0.43
1:A:1187:A:H2'	1:A:1188:U:H5'	2.00	0.43
2:B:71:ALA:O	2:B:75:LEU:HG	2.18	0.43
3:C:73:THR:CG2	3:C:74:ALA:N	2.81	0.43
1:D:1196:A:N3	1:D:1196:A:H3'	2.33	0.43
2:E:47:ARG:CZ	2:E:56:LEU:HD23	2.48	0.43
1:D:1200:U:C2	1:D:1212:C:H1'	2.52	0.43
1:A:1181:G:O2'	1:A:1199:G:H2'	2.17	0.43
3:C:98:THR:CG2	3:C:100:GLU:H	2.31	0.43
1:A:1195:A:C8	1:A:1195:A:H3'	2.53	0.43
3:C:14:ALA:O	3:C:35:VAL:HG13	2.18	0.43
1:A:1168:G:O2'	1:A:1169:G:H5'	2.19	0.43
3:C:73:THR:CG2	3:C:74:ALA:H	2.32	0.43
1:A:1165:G:H2'	1:A:1166:G:H5'	2.01	0.43
2:B:65:ILE:HA	2:B:68:LEU:HD12	2.00	0.43
2:E:20:LEU:HD22	2:E:93:ILE:HD12	2.01	0.43
3:C:71:PRO:O	3:C:74:ALA:HB3	2.18	0.43
3:F:75:LEU:O	3:F:78:LYS:N	2.52	0.43
3:C:157:PHE:O	3:C:158:LYS:CB	2.64	0.42
2:E:152:ALA:HB2	2:E:161:LYS:CE	2.49	0.42
1:A:1221:A:OP2	1:A:1221:A:H2'	2.18	0.42
3:C:5:VAL:HG11	3:C:23:ALA:HB1	2.01	0.42
2:E:12:TRP:CE2	2:E:13:LYS:HG2	2.54	0.42
3:C:119:LYS:O	3:C:122:VAL:HB	2.19	0.42
2:E:66:ARG:NH2	2:E:70:GLU:OE2	2.51	0.42
2:E:83:LEU:HD23	2:E:204:ILE:HG12	2.01	0.42
2:E:130:LYS:HG2	2:E:131:GLY:N	2.34	0.42
2:E:123:PRO:CG	2:E:189:ILE:HD13	2.50	0.42
3:C:86:ALA:N	3:C:94:VAL:CG2	2.82	0.42
3:F:39:ASN:O	3:F:43:LYS:CG	2.67	0.42
3:C:87:HIS:N	3:C:92:GLU:OE2	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:72:THR:OG1	3:F:109:LYS:HG2	2.20	0.41
3:C:18:PRO:O	3:C:22:PRO:HD2	2.20	0.41
1:D:1185:C:O2'	1:D:1186:C:H5'	2.20	0.41
1:A:1161:G:C5	1:A:1162:C:C5	3.09	0.41
3:C:120:ASN:HA	3:C:123:LYS:HG3	2.01	0.41
3:F:25:GLY:N	3:F:26:PRO:HD2	2.35	0.41
3:F:137:GLU:HB2	3:F:139:LYS:HZ3	1.85	0.41
2:B:27:LYS:HG3	2:B:28:PRO:HD3	2.01	0.41
2:E:33:VAL:HG21	2:E:193:LEU:HD22	2.02	0.41
3:F:49:GLN:O	3:F:70:PRO:HB3	2.20	0.41
2:B:72:ALA:HB1	2:B:77:ASN:O	2.21	0.41
3:C:99:LEU:HD23	3:C:156:TYR:CE1	2.55	0.41
1:D:1174:C:H4'	3:F:87:HIS:HA	2.03	0.41
1:D:1178:G:H21	1:D:1206:A:H5'	1.85	0.41
3:C:103:ILE:HG23	3:C:118:LEU:HD21	2.03	0.41
3:C:45:TYR:O	3:C:46:GLU:C	2.64	0.41
3:C:73:THR:HG22	3:C:74:ALA:H	1.86	0.41
2:E:65:ILE:HD11	2:E:87:VAL:HB	2.02	0.41
2:E:126:ILE:HB	2:E:167:VAL:CG1	2.51	0.41
3:F:41:LYS:HB2	3:F:67:VAL:HG21	2.02	0.41
1:A:1151:G:N1	1:A:1152:C:N4	2.69	0.40
1:A:1157:G:OP1	2:B:60:ARG:NH1	2.55	0.40
3:C:72:THR:HG23	3:C:105:ILE:CG2	2.50	0.40
3:C:97:LEU:CD1	3:C:102:VAL:HG23	2.51	0.40
1:A:1190:C:O5'	1:A:1190:C:H6	2.04	0.40
7:A:1404:HOH:O	3:C:131:SER:HA	2.21	0.40
2:E:51:ARG:NH1	2:E:52:ASP:OD2	2.54	0.40
3:F:119:LYS:HE2	3:F:157:PHE:CB	2.51	0.40
1:A:1191:U:O2'	3:C:114:LEU:HD12	2.21	0.40
3:C:98:THR:HG21	3:C:100:GLU:HB3	2.03	0.40
2:B:119:GLY:O	2:B:172:VAL:HG23	2.22	0.40
2:E:148:GLY:O	2:E:150:PRO:HD3	2.21	0.40
3:F:14:ALA:O	3:F:35:VAL:HG13	2.21	0.40
1:A:1192:U:O4'	3:C:114:LEU:HD13	2.20	0.40
2:B:80:LEU:C	2:B:82:GLU:N	2.80	0.40
3:C:69:ILE:HG22	3:C:70:PRO:HD2	2.04	0.40

There are no symmetry-related clashes.

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	
2	B	154/213 (72%)	131 (85%)	21 (14%)	2 (1%)	9	32
2	E	201/213 (94%)	179 (89%)	21 (10%)	1 (0%)	24	54
3	C	156/161 (97%)	131 (84%)	23 (15%)	2 (1%)	9	32
3	F	156/161 (97%)	140 (90%)	14 (9%)	2 (1%)	9	32
All	All	667/748 (89%)	581 (87%)	79 (12%)	7 (1%)	12	39

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	18	PRO
3	F	18	PRO
3	F	19	PRO
2	B	11	PRO
3	C	19	PRO
2	B	208	ASP
2	E	100	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	
2	B	137/180 (76%)	127 (93%)	10 (7%)	13	38
2	E	173/180 (96%)	163 (94%)	10 (6%)	18	49
3	C	132/135 (98%)	119 (90%)	13 (10%)	7	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	F	132/135 (98%)	118 (89%)	14 (11%)	6	22
All	All	574/630 (91%)	527 (92%)	47 (8%)	10	32

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	18	LYS
2	B	45	GLU
2	B	52	ASP
2	B	54	VAL
2	B	58	MET
2	B	100	PRO
2	B	190	LYS
2	B	191	VAL
2	B	200	GLU
2	B	203	ILE
3	C	32	MET
3	C	64	GLU
3	C	78	LYS
3	C	84	THR
3	C	98	THR
3	C	101	GLN
3	C	110	LYS
3	C	113	MET
3	C	122	VAL
3	C	132	MET
3	C	142	LYS
3	C	144	VAL
3	C	158	LYS
2	E	14	ILE
2	E	42	GLN
2	E	45	GLU
2	E	53	LYS
2	E	66	ARG
2	E	73	GLU
2	E	109	GLU
2	E	116	VAL
2	E	204	ILE
2	E	206	THR
3	F	8	LEU
3	F	32	MET
3	F	43	LYS

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Mol	Chain	Res	Type
3	F	46	GLU
3	F	64	GLU
3	F	73	THR
3	F	94	VAL
3	F	109	LYS
3	F	110	LYS
3	F	111	ASP
3	F	123	LYS
3	F	139	LYS
3	F	142	LYS
3	F	158	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
3	C	49	GLN
2	E	76	ASN
2	E	99	ASN
3	F	49	GLN
3	F	91	HIS
3	F	96	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	73/74 (98%)	24 (32%)	2 (2%)
1	D	73/74 (98%)	19 (26%)	3 (4%)
All	All	146/148 (98%)	43 (29%)	5 (3%)

All (43) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	1153	C
1	A	1155	A
1	A	1158	A
1	A	1161	G
1	A	1169	G
1	A	1179	A
1	A	1180	A
1	A	1181	G

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Mol	Chain	Res	Type
1	A	1183	A
1	A	1189	C
1	A	1190	C
1	A	1193	U
1	A	1195	A
1	A	1196	A
1	A	1197	G
1	A	1198	A
1	A	1200	U
1	A	1202	C
1	A	1203	G
1	A	1218	U
1	A	1219	C
1	A	1221	A
1	A	1222	G
1	A	1224	C
1	D	1152	C
1	D	1153	C
1	D	1155	A
1	D	1161	G
1	D	1169	G
1	D	1177	A
1	D	1179	A
1	D	1180	A
1	D	1181	G
1	D	1182	C
1	D	1183	A
1	D	1193	U
1	D	1194	A
1	D	1195	A
1	D	1196	A
1	D	1198	A
1	D	1209	G
1	D	1214	C
1	D	1222	G

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	A	1180	A
1	A	1195	A
1	D	1195	A

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Mol	Chain	Res	Type
1	D	1214	C
1	D	1220	G

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](#)

Of 16 ligands modelled in this entry, 16 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	E	1
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	E	170:GLY	C	171:GLU	N	2.81
1	B	115:PRO	C	116:VAL	N	2.26

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	74/74 (100%)	0.79	6 (8%) 18 15	7, 12, 45, 85	0
1	D	74/74 (100%)	0.86	5 (6%) 23 18	10, 15, 66, 102	0
2	B	160/213 (75%)	1.22	32 (20%) 3 2	10, 30, 74, 91	1 (0%)
2	E	205/213 (96%)	1.66	68 (33%) 1 1	12, 41, 102, 132	1 (0%)
3	C	158/161 (98%)	1.85	56 (35%) 1 1	9, 31, 128, 160	0
3	F	158/161 (98%)	2.72	76 (48%) 0 0	18, 42, 178, 209	0
All	All	829/896 (92%)	1.67	243 (29%) 1 1	7, 32, 134, 209	2 (0%)

All (243) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	F	24	ILE	11.7
3	F	38	ILE	9.3
3	F	20	LEU	7.9
3	F	41	LYS	7.7
3	F	40	GLU	7.6
3	F	19	PRO	7.5
3	F	49	GLN	7.4
3	F	18	PRO	7.4
3	F	1	ALA	7.3
3	C	1	ALA	7.3
3	F	27	LEU	7.2
3	F	29	VAL	7.1
3	F	25	GLY	6.7
3	C	24	ILE	6.3
3	F	22	PRO	6.1
3	F	62	LYS	6.1
3	F	35	VAL	6.0
3	F	16	ALA	6.0
3	F	10	THR	6.0

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Mol	Chain	Res	Type	RSRZ
1	D	1223	G	6.0
3	F	26	PRO	5.9
3	F	17	GLY	5.8
3	F	52	VAL	5.7
2	E	213	ASP	5.7
3	F	8	LEU	5.6
3	F	4	VAL	5.5
2	E	9	MET	5.4
3	F	55	ILE	5.4
2	B	211	LYS	5.4
3	F	64	GLU	5.4
3	C	40	GLU	5.3
3	F	9	VAL	5.3
3	F	60	THR	5.3
3	F	31	VAL	5.3
2	B	170	GLY	5.2
3	F	23	ALA	5.2
3	F	34	VAL	5.2
3	F	54	VAL	5.2
3	C	18	PRO	5.1
3	F	56	VAL	5.0
3	F	13	ARG	5.0
2	E	120	GLN	4.9
2	E	118	GLY	4.8
3	F	48	MET	4.8
3	C	20	LEU	4.8
2	B	180	VAL	4.8
3	F	42	THR	4.7
3	F	32	MET	4.7
3	F	37	GLU	4.7
3	C	49	GLN	4.7
3	C	2	LYS	4.7
3	C	26	PRO	4.7
2	B	212	VAL	4.6
3	F	5	VAL	4.6
3	F	11	GLY	4.6
3	C	45	TYR	4.5
3	F	59	GLU	4.5
2	E	126	ILE	4.4
3	F	12	GLY	4.4
3	F	68	GLY	4.3
2	E	161	LYS	4.3

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Mol	Chain	Res	Type	RSRZ
2	E	153	ILE	4.3
3	F	14	ALA	4.3
2	E	165	VAL	4.2
3	C	60	THR	4.2
3	C	65	ILE	4.2
2	E	132	SER	4.2
3	F	15	THR	4.1
2	E	127	LYS	4.1
3	F	28	GLY	4.1
3	F	2	LYS	4.1
3	F	3	GLU	4.1
3	F	36	LYS	4.1
3	F	58	THR	4.1
3	C	34	VAL	4.0
3	F	67	VAL	4.0
3	F	33	GLN	4.0
2	B	172	VAL	4.0
2	B	117	ARG	4.0
3	C	3	GLU	4.0
3	F	43	LYS	4.0
2	E	142	GLY	3.9
2	E	210	LEU	3.9
2	B	184	LEU	3.9
2	E	117	ARG	3.9
3	C	27	LEU	3.8
2	B	120	GLN	3.8
3	C	23	ALA	3.8
3	F	30	ASN	3.8
3	C	58	THR	3.8
2	E	137	PRO	3.8
1	D	1224	C	3.7
3	C	64	GLU	3.7
2	E	156	GLY	3.7
3	F	7	VAL	3.7
1	A	1151	G	3.6
3	C	55	ILE	3.6
2	E	149	ILE	3.6
2	E	136	PRO	3.6
3	C	17	GLY	3.6
3	C	38	ILE	3.6
3	F	51	PRO	3.6
2	E	125	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
2	E	62	THR	3.5
3	C	67	VAL	3.5
1	D	1152	C	3.5
3	C	56	VAL	3.5
3	F	57	ASP	3.5
2	E	152	ALA	3.5
3	C	9	VAL	3.4
3	F	45	TYR	3.4
3	F	63	PHE	3.4
3	F	39	ASN	3.4
3	C	4	VAL	3.4
3	C	8	LEU	3.4
3	F	66	GLU	3.4
3	C	19	PRO	3.4
2	E	141	LEU	3.4
2	E	138	GLY	3.3
3	C	42	THR	3.3
1	A	1224	C	3.3
2	B	11	PRO	3.3
3	F	65	ILE	3.3
3	C	25	GLY	3.3
2	E	154	GLU	3.3
2	E	139	PRO	3.3
3	C	29	VAL	3.3
3	C	16	ALA	3.3
3	C	21	GLY	3.3
3	F	44	ASP	3.2
2	E	188	PRO	3.2
2	E	159	ALA	3.2
3	C	14	ALA	3.2
2	B	116	VAL	3.1
2	B	124	CYS	3.1
3	F	47	GLY	3.1
3	C	46	GLU	3.1
3	F	61	ARG	3.1
2	E	158	ILE	3.1
3	C	32	MET	3.1
2	E	119	GLY	3.1
3	F	133	GLY	3.1
1	D	1222	G	3.1
2	E	167	VAL	3.0
2	B	123	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
3	F	126	LEU	3.0
3	C	54	VAL	3.0
2	E	123	PRO	3.0
3	C	63	PHE	3.0
3	C	44	ASP	2.9
3	C	31	VAL	2.9
3	F	86	ALA	2.9
3	C	13	ARG	2.9
2	B	81	ALA	2.9
2	E	160	ILE	2.9
2	E	197	ALA	2.9
2	E	162	GLU	2.8
2	E	150	PRO	2.8
2	E	10	ALA	2.8
3	C	125	VAL	2.8
2	B	204	ILE	2.8
2	E	181	LEU	2.8
2	B	42	GLN	2.8
2	E	128	VAL	2.8
3	F	50	VAL	2.8
3	F	53	LYS	2.8
2	E	176	LYS	2.8
3	C	48	MET	2.7
2	E	164	LYS	2.7
1	A	1152	C	2.7
1	D	1153	C	2.7
2	B	208	ASP	2.7
2	E	177	LEU	2.7
2	B	98	MET	2.7
3	F	21	GLY	2.7
3	C	7	VAL	2.7
2	E	135	MET	2.6
2	B	205	TYR	2.6
2	E	212	VAL	2.6
3	C	59	GLU	2.6
2	E	104	TYR	2.6
2	E	144	LEU	2.6
3	F	128	THR	2.6
2	B	122	ALA	2.6
3	F	46	GLU	2.5
2	E	145	LYS	2.5
2	B	209	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
2	E	11	PRO	2.5
2	E	175	PRO	2.5
3	C	98	THR	2.5
2	E	78	PRO	2.5
2	E	180	VAL	2.4
2	E	185	GLY	2.4
3	F	117	THR	2.4
2	B	9	MET	2.4
2	E	121	ILE	2.4
3	C	79	GLU	2.4
3	F	157	PHE	2.4
3	C	33	GLN	2.4
3	C	10	THR	2.4
3	F	69	ILE	2.4
2	E	178	ALA	2.4
2	B	188	PRO	2.4
3	C	22	PRO	2.3
3	F	119	LYS	2.3
2	E	186	ILE	2.3
2	E	173	VAL	2.3
3	C	47	GLY	2.3
3	C	15	THR	2.3
3	C	120	ASN	2.2
2	B	121	ILE	2.2
2	B	84	ALA	2.2
2	B	176	LYS	2.2
2	E	143	GLU	2.2
2	E	116	VAL	2.2
3	C	35	VAL	2.2
2	E	155	LYS	2.2
2	B	181	LEU	2.2
2	E	179	ALA	2.2
3	C	61	ARG	2.2
1	A	1223	G	2.2
2	B	62	THR	2.2
2	E	170	GLY	2.2
2	E	41	PRO	2.1
2	E	151	ALA	2.1
3	C	30	ASN	2.1
1	A	1154	U	2.1
2	B	207	PRO	2.1
2	E	166	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	203	ILE	2.1
2	E	172	VAL	2.1
3	C	37	GLU	2.1
1	A	1169	G	2.1
2	E	157	LYS	2.1
3	C	36	LYS	2.1
3	F	114	LEU	2.1
2	B	206	THR	2.1
2	E	97	ASP	2.1
2	B	183	ARG	2.0
2	E	133	THR	2.0
2	B	175	PRO	2.0
2	E	23	LEU	2.0
2	E	169	LYS	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](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CL	B	301	1/1	0.79	0.14	43,43,43,43	0
4	MG	A	1302	1/1	0.82	0.12	7,7,7,7	0
4	MG	A	1303	1/1	0.87	0.12	5,5,5,5	0
6	K	F	202	1/1	0.87	0.08	49,49,49,49	0
6	K	A	1308	1/1	0.88	0.10	30,30,30,30	0
4	MG	A	1305	1/1	0.88	0.11	30,30,30,30	0
4	MG	D	1302	1/1	0.90	0.23	17,17,17,17	0
6	K	C	201	1/1	0.91	0.07	23,23,23,23	0
5	CL	A	1306	1/1	0.91	0.21	9,9,9,9	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	MG	A	1304	1/1	0.92	0.13	4,4,4,4	0
4	MG	D	1301	1/1	0.94	0.08	2,2,2,2	0
4	MG	A	1301	1/1	0.94	0.22	2,2,2,2	0
6	K	D	1304	1/1	0.94	0.05	11,11,11,11	0
5	CL	F	201	1/1	0.94	0.17	38,38,38,38	0
6	K	A	1307	1/1	0.96	0.08	18,18,18,18	0
4	MG	D	1303	1/1	0.98	0.04	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.