



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 02:20 AM UTC

PDB ID : 6TQA / pdb_00006tqa
Title : X-ray structure of Roquin ROQ domain in complex with a UCP3 CDE2 SL RNA motif
Authors : Binas, O.; Tants, J.-N.; Peter, S.A.; Janowski, R.; Davydova, E.; Braun, J.; Niessing, D.; Schwalbe, H.; Weigand, J.E.; Schlundt, A.
Deposited on : 2019-12-16
Resolution : 2.40 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
Mogul : 2022.3.0, CSD as543be (2022)
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

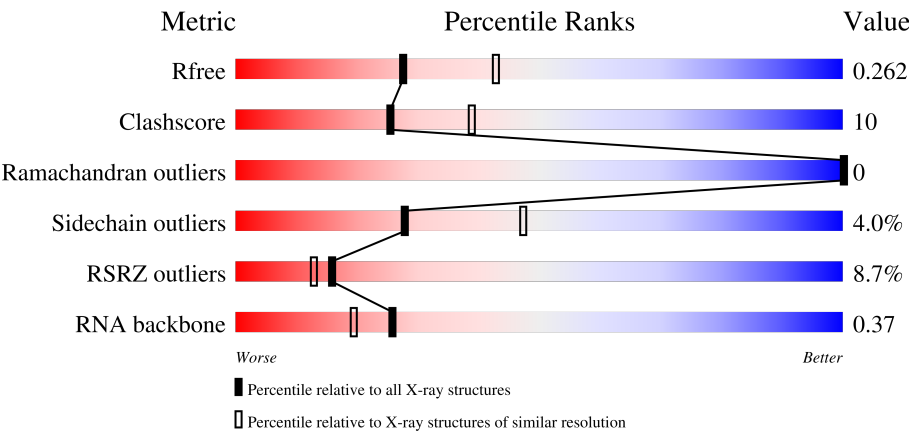
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)
RNA backbone	3983	1155 (2.70-2.10)

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	180	63%19%•16%
1	B	180	6% 62%20%•17%
1	C	180	3% 67%16%•16%
1	D	180	24% 56%24%•17%

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Mol	Chain	Length	Quality of chain
2	E	21	
2	F	21	
2	G	21	
2	H	21	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	CL	F	101	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6938 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 Roquin-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	152	Total	C	N	O	S	0	0	0
			1214	764	220	224	6			
1	B	149	Total	C	N	O	S	0	2	0
			1206	760	221	219	6			
1	C	151	Total	C	N	O	S	0	3	0
			1225	774	223	222	6			
1	D	149	Total	C	N	O	S	0	1	0
			1198	755	218	219	6			

- Molecule 2 is a RNA chain called RNA (5'-R(P*GP*GP*UP*GP*CP*CP*UP*AP*AP*UP*AP*UP*UP*UP*AP*GP*GP*CP*AP*CP*(CCC))-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	21	Total	C	N	O	P	0	0	0
			449	199	77	151	22			
2	F	21	Total	C	N	O	P	0	0	0
			449	199	77	151	22			
2	G	21	Total	C	N	O	P	0	0	0
			449	199	77	151	22			
2	H	21	Total	C	N	O	P	0	0	0
			449	199	77	151	22			

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	F	1	Total	Cl	0	0
			1	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	1	Total 1	Mg 1	0	0

- Molecule 5 is water.

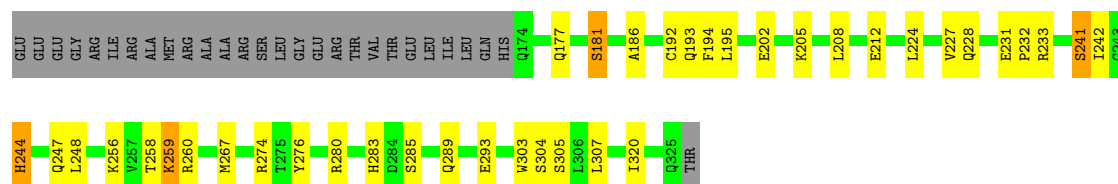
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	58	Total 58	O 58	0	0
5	E	39	Total 39	O 39	0	0
5	B	44	Total 44	O 44	0	0
5	F	31	Total 31	O 31	0	0
5	C	41	Total 41	O 41	0	0
5	G	26	Total 26	O 26	0	0
5	D	37	Total 37	O 37	0	0
5	H	19	Total 19	O 19	0	0

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.

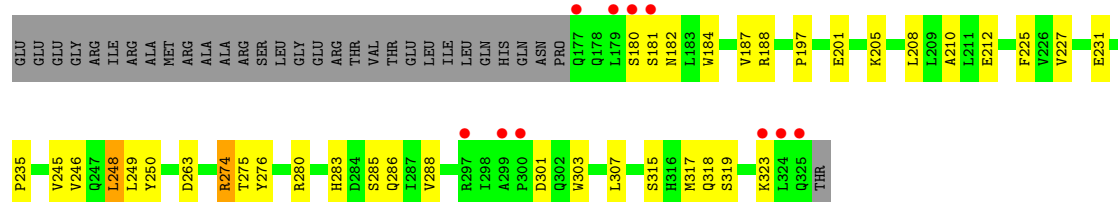
• Molecule 1: Roquin-1

Chain A: 



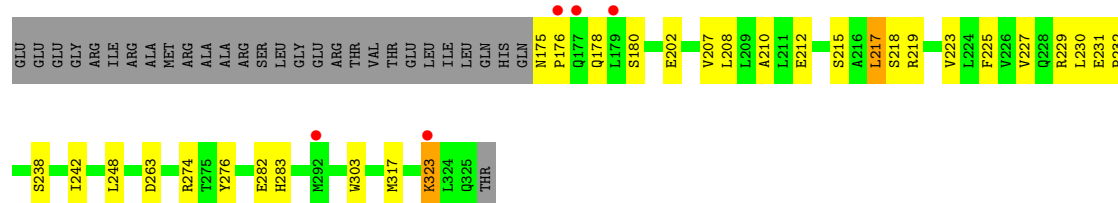
• Molecule 1: Roquin-1

Chain B: 



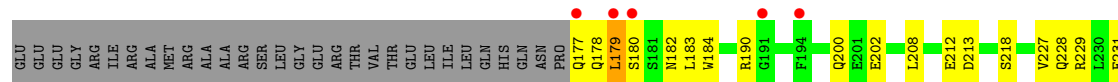
• Molecule 1: Roquin-1

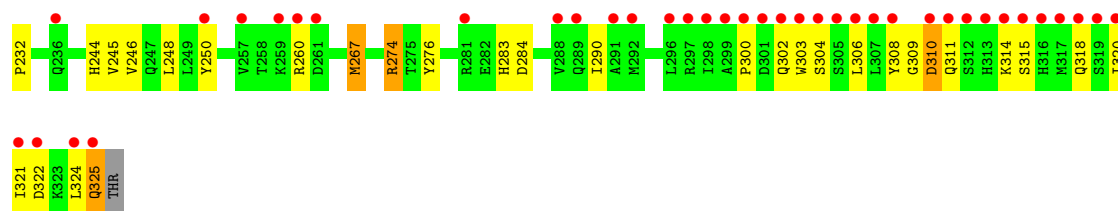
Chain C: 



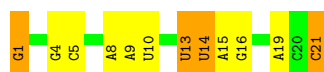
• Molecule 1: Roquin-1

Chain D: 

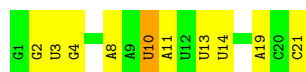




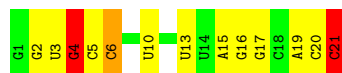
• Molecule 2: RNA (5'-R(P*GP*GP*UP*GP*CP*CP*UP*AP*AP*UP*AP*UP*UP*UP*AP*G P*GP*CP*AP*CP*(CCC))-3')



• Molecule 2: RNA (5'-R(P*GP*GP*UP*GP*CP*CP*UP*AP*AP*UP*AP*UP*UP*UP*AP*G P*GP*CP*AP*CP*(CCC))-3')



• Molecule 2: RNA (5'-R(P*GP*GP*UP*GP*CP*CP*UP*AP*AP*UP*AP*UP*UP*UP*AP*G P*GP*CP*AP*CP*(CCC))-3')



• Molecule 2: RNA (5'-R(P*GP*GP*UP*GP*CP*CP*UP*AP*AP*UP*AP*UP*UP*UP*AP*G P*GP*CP*AP*CP*(CCC))-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.53Å 160.66Å 68.01Å 90.00° 107.96° 90.00°	Depositor
Resolution (Å)	42.40 – 2.40 42.40 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.8 (42.40-2.40) 99.8 (42.40-2.40)	Depositor EDS
R_{merge}	0.01	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.8.0232	Depositor
R, R_{free}	0.197 , 0.259 0.201 , 0.262	Depositor DCC
R_{free} test set	1720 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	36.1	Xtriage
Anisotropy	0.389	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 49.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.049 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6938	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.72% 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: MG, CCC, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	1.23	3/1234 (0.2%)	1.58	5/1662 (0.3%)
1	B	1.22	5/1231 (0.4%)	1.64	1/1655 (0.1%)
1	C	1.17	2/1254 (0.2%)	1.55	6/1686 (0.4%)
1	D	1.11	0/1220	1.61	9/1641 (0.5%)
2	E	0.88	2/475 (0.4%)	1.09	4/736 (0.5%)
2	F	0.62	0/475	1.03	1/736 (0.1%)
2	G	0.63	0/475	1.10	3/736 (0.4%)
2	H	0.60	1/475 (0.2%)	1.10	4/736 (0.5%)
All	All	1.07	13/6839 (0.2%)	1.46	33/9588 (0.3%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	235	PRO	C-O	-7.10	1.14	1.24
1	B	248	LEU	C-O	6.15	1.31	1.24
1	B	283	HIS	CE1-NE2	6.06	1.38	1.32
1	B	318	GLN	C-N	5.92	1.41	1.34
1	A	267	MET	C-O	5.87	1.31	1.24
2	E	5	C	O3'-P	-5.75	1.52	1.61
1	C	283	HIS	CE1-NE2	5.68	1.38	1.32
1	C	217	LEU	C-O	5.64	1.30	1.24
2	E	1	G	OP3-P	5.59	1.59	1.48
1	B	197	PRO	C-O	-5.59	1.16	1.24
2	H	1	G	OP3-P	5.44	1.59	1.48
1	A	186	ALA	C-O	5.27	1.30	1.24
1	A	283	HIS	CE1-NE2	5.08	1.37	1.32

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	13	U	C4'-C3'-O3'	-6.79	102.82	113.00
2	G	2	G	C3'-C2'-O2'	6.30	120.15	110.70
2	H	7	U	C1'-C2'-O2'	6.25	117.77	108.40
1	C	238	SER	CA-C-O	-6.12	114.90	121.45
1	D	310	ASP	CB-CA-C	5.89	122.14	110.42
2	F	10	U	C1'-C2'-O2'	-5.88	102.98	111.80
1	D	218	SER	CA-C-O	-5.66	115.65	121.87
2	H	1	G	C3'-C2'-O2'	5.58	119.07	110.70
1	D	213	ASP	CA-CB-CG	5.52	118.12	112.60
1	D	315	SER	N-CA-C	-5.48	104.95	111.69
2	H	6	C	C4'-C3'-O3'	-5.40	104.89	113.00
2	E	1	G	C1'-C2'-O2'	5.34	116.41	108.40
1	A	305	SER	CA-C-N	5.30	127.65	120.44
1	A	305	SER	C-N-CA	5.30	127.65	120.44
2	G	6	C	C4'-C3'-O3'	-5.29	105.06	113.00
2	H	14	U	C2'-C3'-O3'	5.28	121.62	113.70
2	E	13	U	C3'-C2'-O2'	5.28	118.62	110.70
1	B	187	VAL	N-CA-C	-5.25	105.73	110.82
1	C	227	VAL	CA-C-O	-5.22	115.64	121.17
1	D	245	VAL	N-CA-C	-5.15	105.69	110.53
1	A	244	HIS	CA-CB-CG	5.13	118.93	113.80
1	D	244	HIS	CA-CB-CG	5.11	118.91	113.80
1	A	241	SER	N-CA-C	-5.11	105.89	111.82
2	E	9	A	C1'-C2'-O2'	5.08	116.02	108.40
1	C	207	VAL	N-CA-C	-5.07	105.04	110.36
1	C	263	ASP	CA-CB-CG	5.07	117.67	112.60
1	D	250	TYR	CA-C-N	5.04	127.97	120.31
1	D	250	TYR	C-N-CA	5.04	127.97	120.31
1	C	180	SER	CA-C-N	5.04	127.28	120.38
1	C	180	SER	C-N-CA	5.04	127.28	120.38
1	A	205	LYS	N-CA-C	-5.03	105.87	111.36
2	G	4	G	P-O5'-C5'	-5.03	113.35	120.90
1	D	246	VAL	CA-C-O	-5.01	115.74	120.95

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1214	0	1233	26	0
1	B	1206	0	1238	20	0
1	C	1225	0	1264	24	0
1	D	1198	0	1225	28	0
2	E	449	0	224	6	0
2	F	449	0	224	4	0
2	G	449	0	224	13	0
2	H	449	0	224	2	0
3	A	2	0	0	1	0
3	F	1	0	0	3	0
4	H	1	0	0	0	0
5	A	58	0	0	1	0
5	B	44	0	0	1	0
5	C	41	0	0	2	0
5	D	37	0	0	0	0
5	E	39	0	0	0	0
5	F	31	0	0	1	0
5	G	26	0	0	0	0
5	H	19	0	0	0	0
All	All	6938	0	5856	120	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 10.

All (120) 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:G:21:CCC:H5''	2:G:21:CCC:H6	1.16	1.12
1:C:229[B]:ARG:HH21	1:C:229[B]:ARG:HG2	1.16	1.06
2:G:3:U:H2'	2:G:4:G:H5''	1.52	0.92
2:G:21:CCC:H6	2:G:21:CCC:C5'	2.04	0.86
1:C:229[B]:ARG:HG2	1:C:229[B]:ARG:NH2	1.94	0.81
1:B:184:TRP:O	1:B:188[B]:ARG:HG2	1.83	0.79
2:G:3:U:C2'	2:G:4:G:H5''	2.16	0.74
2:E:14:U:H6	2:E:14:U:H5''	1.55	0.72
2:G:21:CCC:H5''	2:G:21:CCC:C6	2.08	0.72
3:F:101:CL:CL	5:F:217:HOH:O	2.47	0.70
1:C:229[B]:ARG:HH21	1:C:229[B]:ARG:CG	1.97	0.70
1:C:208:LEU:HD11	1:C:276:TYR:HA	1.73	0.69
1:A:259:LYS:NZ	2:E:10:U:O2	2.27	0.67
1:A:227:VAL:HG22	1:A:242:ILE:HG13	1.79	0.65
1:C:229[B]:ARG:NH2	1:C:229[B]:ARG:CG	2.59	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:208:LEU:HD11	1:D:276:TYR:HA	1.78	0.63
1:B:208:LEU:O	1:B:212:GLU:HG2	1.99	0.63
1:D:177:GLN:HG2	1:D:177:GLN:O	1.98	0.63
1:C:248:LEU:HD23	1:C:248:LEU:O	1.99	0.63
1:D:267:MET:HA	1:D:267:MET:HE3	1.83	0.61
1:A:224:LEU:O	1:D:229[A]:ARG:NH2	2.35	0.60
1:A:256:LYS:HD2	3:A:402:CL:CL	2.39	0.59
1:D:200:GLN:NE2	1:D:283:HIS:NE2	2.42	0.59
5:B:417:HOH:O	3:F:101:CL:CL	2.53	0.59
2:F:8:A:N7	3:F:101:CL:CL	2.73	0.59
1:A:285:SER:HA	1:A:320:ILE:HG21	1.85	0.58
1:A:256:LYS:NZ	5:A:501:HOH:O	2.35	0.58
1:A:228:GLN:HB2	1:D:229[A]:ARG:NH2	2.18	0.58
1:C:230:LEU:CD2	1:C:242:ILE:HD11	2.34	0.57
2:H:10:U:O4'	2:H:10:U:O2	2.22	0.57
1:A:202:GLU:OE2	1:A:233:ARG:NH2	2.37	0.57
1:D:303:TRP:O	1:D:304:SER:C	2.47	0.57
1:D:190:ARG:HD3	1:D:290:ILE:HG12	1.87	0.57
2:E:1:G:H5''	2:E:1:G:C8	2.40	0.56
1:D:212:GLU:O	1:D:274:ARG:HD2	2.06	0.56
1:A:231:GLU:N	1:A:232:PRO:CD	2.70	0.55
2:F:3:U:H2'	2:F:4:G:O4'	2.06	0.55
1:C:230:LEU:HD23	1:C:242:ILE:HD11	1.88	0.55
1:D:177:GLN:O	1:D:177:GLN:CG	2.54	0.55
1:C:323[A]:LYS:HA	1:C:323[A]:LYS:CE	2.36	0.54
1:D:284:ASP:OD2	1:D:308:TYR:OH	2.23	0.54
1:C:303:TRP:HB3	1:C:317:MET:HG3	1.90	0.54
1:B:250:TYR:OH	2:F:11:A:OP1	2.25	0.53
1:B:245:VAL:O	1:B:248:LEU:HB3	2.09	0.53
1:C:210:ALA:HB2	1:C:225:PHE:CE1	2.45	0.52
1:D:248:LEU:C	1:D:248:LEU:HD23	2.35	0.52
1:B:319:SER:O	1:B:323:LYS:HB2	2.09	0.52
1:A:289:GLN:O	1:A:293:GLU:HG3	2.10	0.52
1:C:212:GLU:O	1:C:274:ARG:HD3	2.10	0.52
1:B:227:VAL:O	1:B:231:GLU:HB2	2.10	0.51
1:D:179:LEU:O	1:D:183:LEU:N	2.37	0.51
1:A:228:GLN:CB	1:D:229[A]:ARG:NH2	2.74	0.51
1:C:248:LEU:HD23	1:C:248:LEU:C	2.36	0.51
2:G:4:G:H5'	2:G:4:G:H8	1.76	0.50
1:B:201:GLU:O	1:B:205:LYS:HG3	2.11	0.50
1:D:311:GLN:HB3	1:D:314:LYS:HE2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:280:ARG:NH1	1:B:307:LEU:O	2.44	0.49
1:A:208:LEU:HD11	1:A:276:TYR:HA	1.94	0.49
1:D:179:LEU:HD13	1:D:302:GLN:OE1	2.12	0.49
1:A:212:GLU:HA	1:A:274:ARG:HG2	1.94	0.48
1:D:309:GLY:O	1:D:310:ASP:HB2	2.13	0.48
1:B:208:LEU:O	1:B:212:GLU:CG	2.61	0.48
2:G:4:G:H8	2:G:4:G:C5'	2.25	0.48
2:G:19:A:H2'	2:G:20:C:O4'	2.13	0.48
1:A:258:THR:HG22	1:A:260:ARG:HD3	1.97	0.47
1:D:303:TRP:O	1:D:306:LEU:N	2.48	0.47
1:A:247:GLN:HA	1:A:247:GLN:OE1	2.15	0.47
1:D:184:TRP:HA	1:D:184:TRP:CE3	2.50	0.47
1:A:195:LEU:HD21	1:A:241:SER:HB2	1.97	0.47
1:B:201:GLU:HG3	1:B:276:TYR:OH	2.15	0.46
1:B:303:TRP:HB3	1:B:317:MET:HG3	1.97	0.46
1:D:318:GLN:O	1:D:321:ILE:HG22	2.16	0.46
1:C:202:GLU:HG2	5:C:429:HOH:O	2.15	0.46
1:C:303:TRP:HB3	1:C:317:MET:HE2	1.97	0.46
1:C:231:GLU:HB2	1:C:232:PRO:HD3	1.99	0.45
1:A:192:CYS:HB3	1:A:248:LEU:HD13	1.97	0.45
1:C:218:SER:HB2	5:C:426:HOH:O	2.17	0.45
1:D:324:LEU:O	1:D:325:GLN:HG2	2.17	0.45
1:B:208:LEU:HD11	1:B:276:TYR:HA	1.98	0.45
1:B:285:SER:O	1:B:288:VAL:HB	2.17	0.45
1:C:175:ASN:N	1:C:178:GLN:HE21	2.14	0.44
1:C:231:GLU:N	1:C:232:PRO:CD	2.81	0.44
1:B:208:LEU:CD1	1:B:276:TYR:HA	2.47	0.44
1:B:188[B]:ARG:HA	1:B:188[B]:ARG:HD2	1.83	0.44
1:B:286:GLN:NE2	1:B:286:GLN:HA	2.33	0.44
1:D:178:GLN:O	1:D:182:ASN:HB2	2.17	0.44
2:G:20:C:H2'	2:G:21:CCC:H5''	2.00	0.43
1:D:184:TRP:HA	1:D:184:TRP:HE3	1.82	0.43
1:A:177:GLN:O	1:A:181:SER:OG	2.36	0.43
2:E:14:U:H6	2:E:14:U:C5'	2.27	0.43
1:C:175:ASN:O	1:C:178:GLN:HG3	2.19	0.43
1:D:322:ASP:O	1:D:325:GLN:HB3	2.18	0.43
2:G:10:U:OP1	2:G:10:U:H6	2.02	0.43
1:A:303:TRP:O	1:A:304:SER:C	2.61	0.43
1:A:194:PHE:CZ	1:A:307:LEU:HA	2.54	0.43
1:D:227:VAL:O	1:D:231:GLU:HB2	2.19	0.42
1:B:246:VAL:O	1:B:249:LEU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:VAL:HG22	1:A:242:ILE:CG1	2.48	0.42
1:C:215:SER:HB3	1:C:217:LEU:CD1	2.50	0.42
2:G:4:G:H2'	2:G:5:C:O4'	2.20	0.42
2:E:8:A:C2	2:E:15:A:C2	3.08	0.41
1:D:300:PRO:HA	1:D:303:TRP:HD1	1.84	0.41
1:C:208:LEU:HD11	1:C:276:TYR:CA	2.46	0.41
1:A:193:GLN:HB3	1:A:244:HIS:CB	2.51	0.41
1:A:280:ARG:HA	1:A:280:ARG:HD2	1.89	0.41
2:E:4:G:C2	2:E:19:A:C2	3.09	0.41
1:B:212:GLU:HA	1:B:274:ARG:HG2	2.02	0.41
1:C:219:ARG:O	1:C:223:VAL:HG23	2.21	0.41
2:G:4:G:C5'	2:G:4:G:C8	3.03	0.41
1:A:227:VAL:CG2	1:A:242:ILE:HG13	2.50	0.41
2:G:4:G:H5'	2:G:4:G:C8	2.55	0.41
1:D:231:GLU:N	1:D:232:PRO:CD	2.84	0.41
2:H:14:U:H5''	2:H:14:U:C6	2.56	0.41
1:B:210:ALA:HB2	1:B:225:PHE:CD1	2.57	0.40
2:F:2:G:H2'	2:F:3:U:C6	2.56	0.40
1:C:175:ASN:ND2	1:C:176:PRO:HD2	2.36	0.40
1:A:231:GLU:N	1:A:232:PRO:HD3	2.36	0.40
1:D:248:LEU:HD23	1:D:248:LEU:O	2.22	0.40
1:A:285:SER:HA	1:A:320:ILE:CG2	2.51	0.40
1:B:210:ALA:HB2	1:B:225:PHE:CE1	2.57	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	150/180 (83%)	146 (97%)	4 (3%)	0	100	100
1	B	149/180 (83%)	143 (96%)	6 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	152/180 (84%)	148 (97%)	4 (3%)	0	100	100
1	D	148/180 (82%)	135 (91%)	13 (9%)	0	100	100
All	All	599/720 (83%)	572 (96%)	27 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	133/156 (85%)	131 (98%)	2 (2%)	57	77
1	B	132/156 (85%)	124 (94%)	8 (6%)	17	30
1	C	135/156 (86%)	132 (98%)	3 (2%)	45	67
1	D	131/156 (84%)	122 (93%)	9 (7%)	14	24
All	All	531/624 (85%)	509 (96%)	22 (4%)	28	46

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	181	SER
1	A	259	LYS
1	B	180	SER
1	B	181	SER
1	B	182	ASN
1	B	263	ASP
1	B	274	ARG
1	B	275	THR
1	B	301	ASP
1	B	315	SER
1	C	282	GLU
1	C	323[A]	LYS
1	C	323[B]	LYS
1	D	179	LEU

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Mol	Chain	Res	Type
1	D	180	SER
1	D	202	GLU
1	D	228	GLN
1	D	260	ARG
1	D	267	MET
1	D	274	ARG
1	D	320	ILE
1	D	325	GLN

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	236	GLN
1	A	289	GLN
1	B	182	ASN
1	B	193	GLN
1	B	311	GLN
1	B	313	HIS
1	C	289	GLN
1	C	313	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	E	20/21 (95%)	4 (20%)	0
2	F	20/21 (95%)	4 (20%)	0
2	G	20/21 (95%)	7 (35%)	0
2	H	20/21 (95%)	4 (20%)	0
All	All	80/84 (95%)	19 (23%)	0

All (19) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	E	13	U
2	E	14	U
2	E	16	G
2	E	21	CCC
2	F	10	U
2	F	13	U
2	F	14	U

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Mol	Chain	Res	Type
2	F	19	A
2	G	4	G
2	G	6	C
2	G	13	U
2	G	15	A
2	G	16	G
2	G	17	G
2	G	21	CCC
2	H	10	U
2	H	11	A
2	H	13	U
2	H	17	G

There are no RNA pucker outliers to report.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	CCC	F	21	2	20,25,26	1.04	0	27,38,41	1.67	5 (18%)
2	CCC	H	21	2	20,25,26	0.99	0	27,38,41	1.54	3 (11%)
2	CCC	E	21	2	20,25,26	1.03	0	27,38,41	1.63	6 (22%)
2	CCC	G	21	2	20,25,26	1.38	3 (15%)	27,38,41	1.70	7 (25%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CCC	F	21	2	-	0/7/35/36	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	CCC	H	21	2	-	0/7/35/36	0/3/3/3
2	CCC	E	21	2	-	2/7/35/36	0/3/3/3
2	CCC	G	21	2	-	2/7/35/36	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	21	CCC	O4'-C4'	-2.63	1.39	1.45
2	G	21	CCC	C6-N1	-2.63	1.31	1.38
2	G	21	CCC	C5-C4	-2.48	1.37	1.42

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	21	CCC	C2'-C1'-N1	-4.47	105.76	114.24
2	F	21	CCC	C2'-C1'-N1	-4.23	106.22	114.24
2	F	21	CCC	O2C-PC-O1C	4.20	123.46	109.89
2	E	21	CCC	O2C-PC-O1C	4.06	123.01	109.89
2	H	21	CCC	O2C-PC-O1C	3.99	122.78	109.89
2	H	21	CCC	O3'-PC-O1C	-3.95	105.33	115.76
2	G	21	CCC	O2C-PC-O1C	3.88	122.43	109.89
2	G	21	CCC	O3'-PC-O1C	-3.54	106.41	115.76
2	E	21	CCC	O3'-PC-O1C	-3.48	106.58	115.76
2	F	21	CCC	O2'-PC-O1C	-3.37	106.86	115.76
2	E	21	CCC	C2'-C1'-N1	-2.90	108.73	114.24
2	H	21	CCC	O2'-PC-O1C	-2.76	108.48	115.76
2	E	21	CCC	C5'-C4'-C3'	-2.67	105.50	114.38
2	G	21	CCC	O4'-C4'-C5'	-2.57	101.11	109.33
2	F	21	CCC	O4'-C1'-N1	2.46	113.94	108.36
2	E	21	CCC	O4'-C4'-C5'	2.21	116.42	109.33
2	E	21	CCC	O4'-C1'-N1	2.20	113.34	108.36
2	G	21	CCC	O2'-PC-O1C	-2.19	109.97	115.76
2	G	21	CCC	C5'-C4'-C3'	-2.17	107.15	114.38
2	F	21	CCC	O2'-C2'-C1'	-2.08	105.48	111.43
2	G	21	CCC	O2-C2-N3	-2.06	119.09	122.33

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	21	CCC	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	E	21	CCC	C3'-C4'-C5'-O5'
2	G	21	CCC	C3'-C4'-C5'-O5'
2	G	21	CCC	O4'-C4'-C5'-O5'

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	G	21	CCC	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 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](#)

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	152/180 (84%)	-0.09	0 100 100	35, 41, 62, 106	1 (0%)
1	B	149/180 (82%)	0.46	10 (6%) 24 20	31, 51, 89, 124	10 (6%)
1	C	151/180 (83%)	0.18	5 (3%) 49 45	22, 47, 80, 107	9 (5%)
1	D	149/180 (82%)	1.13	44 (29%) 1 1	26, 63, 136, 154	13 (8%)
2	E	20/21 (95%)	-0.48	0 100 100	38, 49, 66, 69	0
2	F	20/21 (95%)	-0.05	0 100 100	50, 73, 89, 100	0
2	G	20/21 (95%)	-0.49	0 100 100	46, 58, 73, 83	0
2	H	20/21 (95%)	0.09	0 100 100	58, 88, 103, 128	0
All	All	681/804 (84%)	0.34	59 (8%) 16 13	22, 50, 107, 154	33 (4%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	324	LEU	5.4
1	C	176	PRO	5.4
1	B	324	LEU	4.4
1	D	321	ILE	4.3
1	D	311	GLN	4.2
1	D	300	PRO	4.0
1	D	320	ILE	3.7
1	D	314	LYS	3.7
1	D	303	TRP	3.6
1	D	261	ASP	3.6
1	D	302	GLN	3.5
1	D	307	LEU	3.4
1	D	319	SER	3.4
1	D	288	VAL	3.4
1	B	177	GLN	3.3
1	D	179	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	296	LEU	3.2
1	B	179	LEU	3.2
1	D	298	ILE	3.2
1	D	301	ASP	3.1
1	C	179	LEU	3.0
1	D	306	LEU	3.0
1	D	299	ALA	2.9
1	D	318	GLN	2.8
1	D	325	GLN	2.8
1	D	281	ARG	2.8
1	D	304	SER	2.7
1	D	312	SER	2.7
1	B	297	ARG	2.7
1	D	297	ARG	2.7
1	D	316	HIS	2.7
1	D	308	TYR	2.6
1	C	177	GLN	2.6
1	D	317	MET	2.5
1	D	292	MET	2.5
1	D	305	SER	2.5
1	D	313	HIS	2.5
1	D	260	ARG	2.5
1	D	177	GLN	2.4
1	B	299	ALA	2.4
1	D	310	ASP	2.3
1	D	250	TYR	2.3
1	D	257	VAL	2.3
1	D	180	SER	2.3
1	D	315	SER	2.2
1	B	325	GLN	2.2
1	B	180	SER	2.2
1	D	291	ALA	2.2
1	C	323[A]	LYS	2.2
1	B	323	LYS	2.2
1	C	292	MET	2.2
1	B	181	SER	2.2
1	D	289	GLN	2.1
1	D	322	ASP	2.1
1	D	191	GLY	2.1
1	D	259	LYS	2.1
1	D	236	GLN	2.0
1	B	300	PRO	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	194	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	CCC	F	21	23/24	0.85	0.10	86,95,103,105	3
2	CCC	G	21	23/24	0.86	0.10	73,86,95,96	3
2	CCC	H	21	23/24	0.91	0.09	77,90,99,101	0
2	CCC	E	21	23/24	0.93	0.08	62,69,77,79	3

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(Å ²)	Q<0.9
3	CL	F	101	1/1	0.89	0.14	49,49,49,49	0
4	MG	H	101	1/1	0.90	0.07	61,61,61,61	0
3	CL	A	401	1/1	0.93	0.15	71,71,71,71	0
3	CL	A	402	1/1	0.98	0.10	45,45,45,45	0

6.5 Other polymers [i](#)

There are no such residues in this entry.