



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 03:15 AM UTC

PDB ID : 5H9F / pdb_00005h9f
Title : Crystal structure of E. coli Cascade bound to a PAM-containing dsDNA target at 2.45 angstrom resolution.
Authors : Hayes, R.P.; Xiao, Y.; Ding, F.; van Erp, P.B.G.; Rajashankar, K.; Bailey, S.; Wiedenheft, B.; Ke, A.
Deposited on : 2015-12-28
Resolution : 2.45 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:

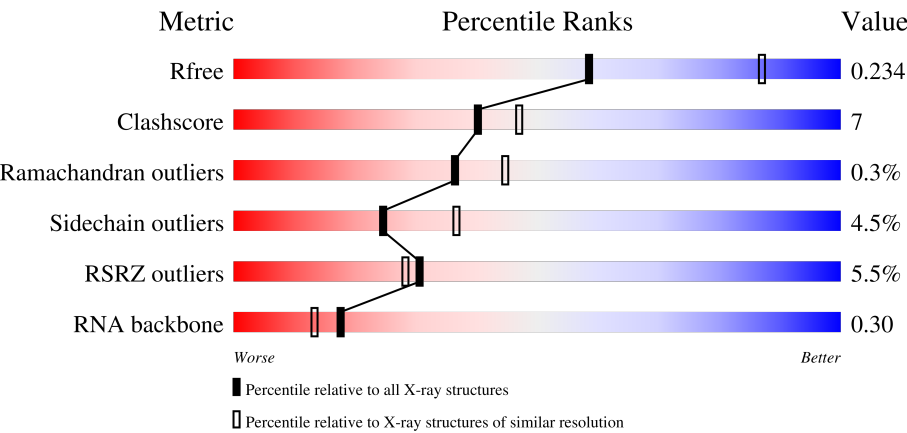
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (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 2.45 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)
RNA backbone	3983	1023 (2.72-2.20)

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	502	4% 81%14%.
2	B	165	4% 72%19%.7%
2	C	165	% 82%8%.9%
3	D	363	8% 65%20%.12%

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Mol	Chain	Length	Quality of chain
3	E	363	3% 81% 16% ..
3	F	363	2% 85% 14% ..
3	G	363	% 87% 10% .
3	H	363	% 85% 12% .
3	I	363	4% 86% 9% ..
4	J	224	% 79% 17% ..
5	L	61	2% 46% 34% 18% .
6	M	28	14% 25% 75%
7	N	50	16% 62% 38%
8	K	199	36% 62% 15% . 20%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 28930 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 CRISPR system Cascade subunit CasA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	481	Total	C	N	O	S	0	0	0
			3746	2389	663	675	19			

- Molecule 2 is a protein called CRISPR system Cascade subunit CasB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	153	Total	C	N	O	S	0	0	0
			1246	782	239	218	7			
2	C	150	Total	C	N	O	S	0	0	0
			1223	770	231	215	7			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-4	GLY	-	expression tag	UNP P76632
B	-3	PRO	-	expression tag	UNP P76632
B	-2	GLY	-	expression tag	UNP P76632
B	-1	TYR	-	expression tag	UNP P76632
B	0	GLN	-	expression tag	UNP P76632
C	-4	GLY	-	expression tag	UNP P76632
C	-3	PRO	-	expression tag	UNP P76632
C	-2	GLY	-	expression tag	UNP P76632
C	-1	TYR	-	expression tag	UNP P76632
C	0	GLN	-	expression tag	UNP P76632

- Molecule 3 is a protein called CRISPR system Cascade subunit CasC.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	318	Total	C	N	O	S	0	0	0
			2399	1503	431	450	15			
3	E	354	Total	C	N	O	S	0	0	0
			2694	1685	479	515	15			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	F	361	Total	C	N	O	S	0	0	0
			2755	1721	490	529	15			
3	G	354	Total	C	N	O	S	0	0	0
			2713	1698	484	516	15			
3	H	352	Total	C	N	O	S	0	0	0
			2691	1681	479	516	15			
3	I	351	Total	C	N	O	S	0	0	0
			2686	1680	476	515	15			

- Molecule 4 is a protein called CRISPR system Cascade subunit CasD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	219	Total	C	N	O	S	0	0	0
			1731	1097	308	317	9			

- Molecule 5 is a RNA chain called crRNA (61-MER).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	L	61	Total	C	N	O	P	0	0	0
			1300	580	233	426	61			

- Molecule 6 is a DNA chain called DNA (28-MER) Non-target.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	28	Total	C	N	O	P	0	0	0
			572	276	90	178	28			

- Molecule 7 is a DNA chain called DNA (50-MER) Target.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	N	50	Total	C	N	O	P	0	0	0
			1025	486	195	294	50			

- Molecule 8 is a protein called CRISPR system Cascade subunit CasE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	K	159	Total	C	N	O	S	0	0	0
			1098	704	182	205	7			

- Molecule 9 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total 1	Zn 1	0	0

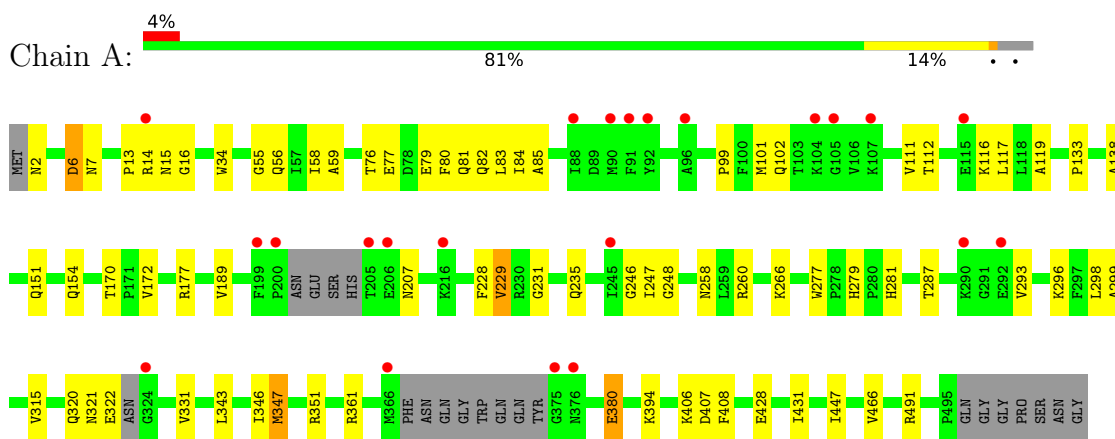
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	133	Total 133	O 133	0	0
10	B	22	Total 22	O 22	0	0
10	C	63	Total 63	O 63	0	0
10	D	32	Total 32	O 32	0	0
10	E	95	Total 95	O 95	0	0
10	F	99	Total 99	O 99	0	0
10	G	144	Total 144	O 144	0	0
10	H	130	Total 130	O 130	0	0
10	I	128	Total 128	O 128	0	0
10	J	69	Total 69	O 69	0	0
10	L	67	Total 67	O 67	0	0
10	M	13	Total 13	O 13	0	0
10	N	49	Total 49	O 49	0	0
10	K	6	Total 6	O 6	0	0

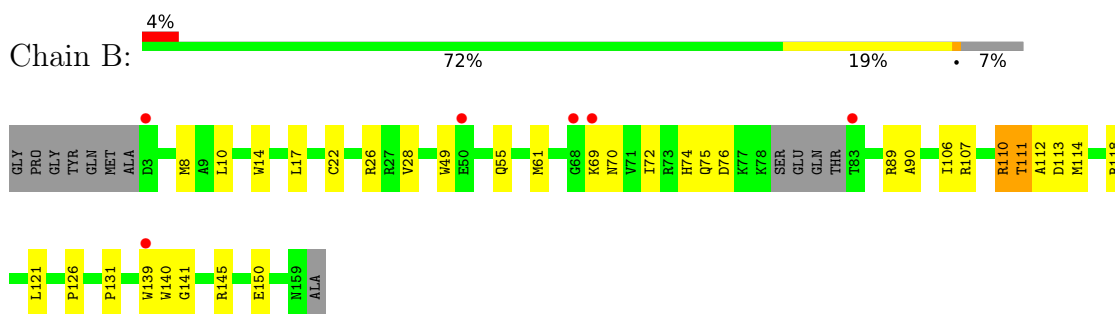
3 Residue-property plots [i](#)

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.

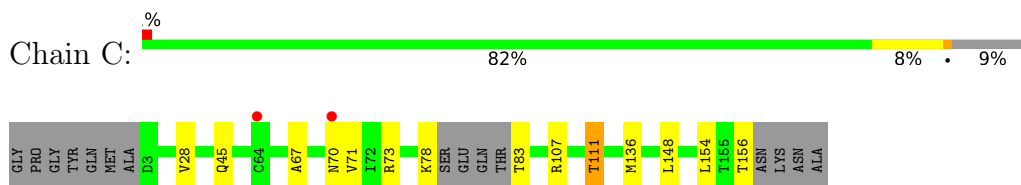
- Molecule 1: CRISPR system Cascade subunit CasA



- Molecule 2: CRISPR system Cascade subunit CasB

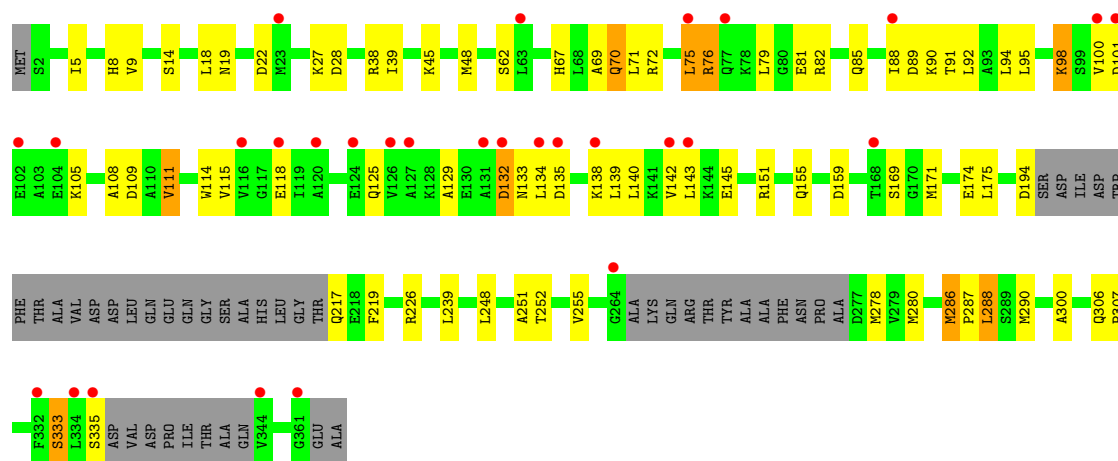


- Molecule 2: CRISPR system Cascade subunit CasB

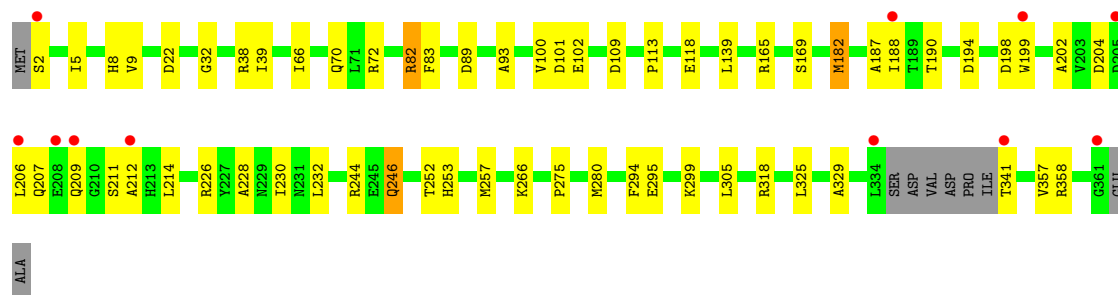
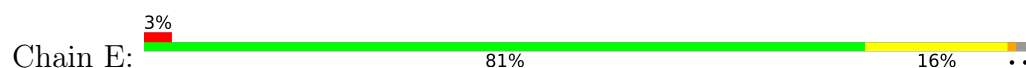


- Molecule 3: CRISPR system Cascade subunit CasC

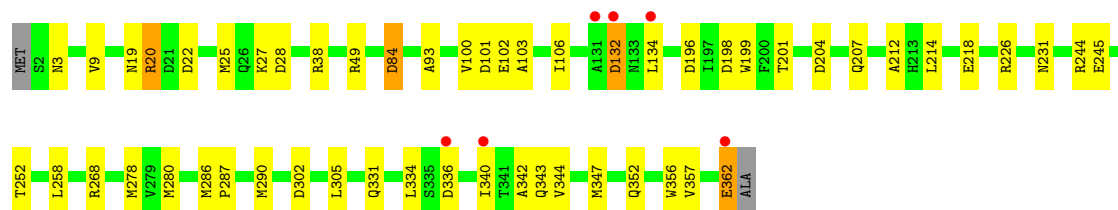
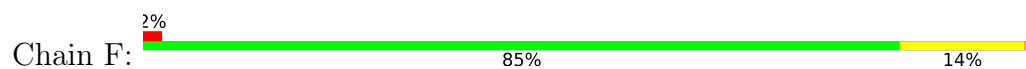




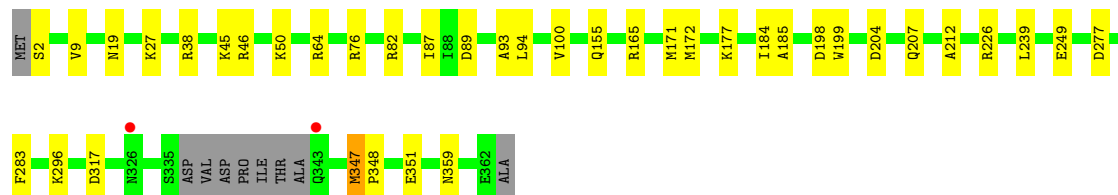
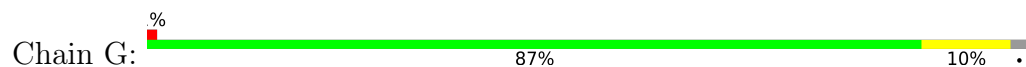
• Molecule 3: CRISPR system Cascade subunit CasC



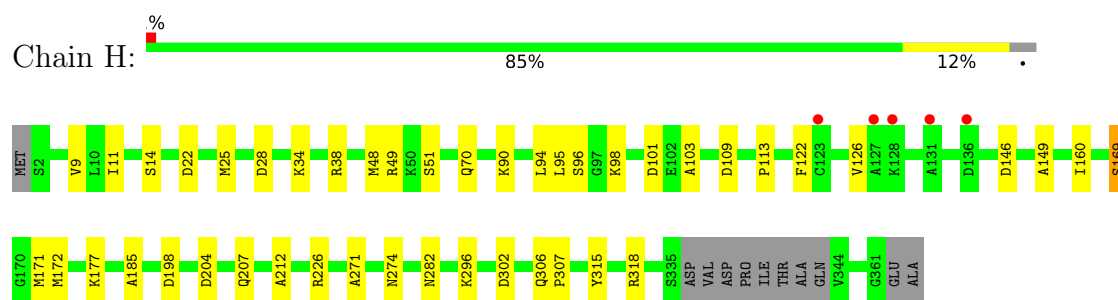
• Molecule 3: CRISPR system Cascade subunit CasC



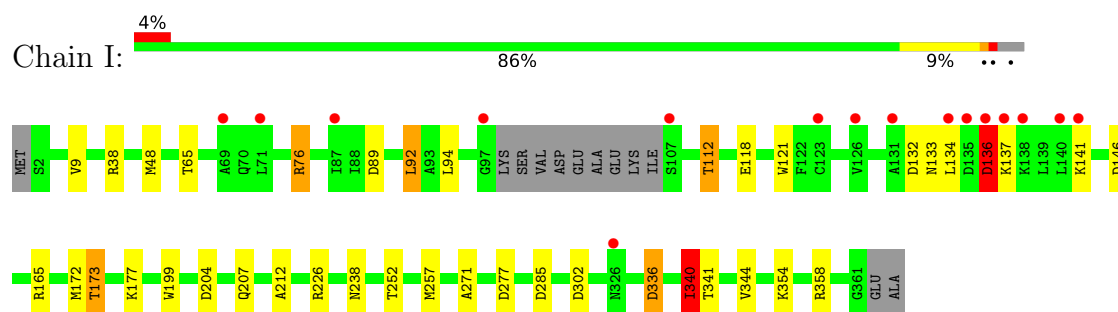
• Molecule 3: CRISPR system Cascade subunit CasC



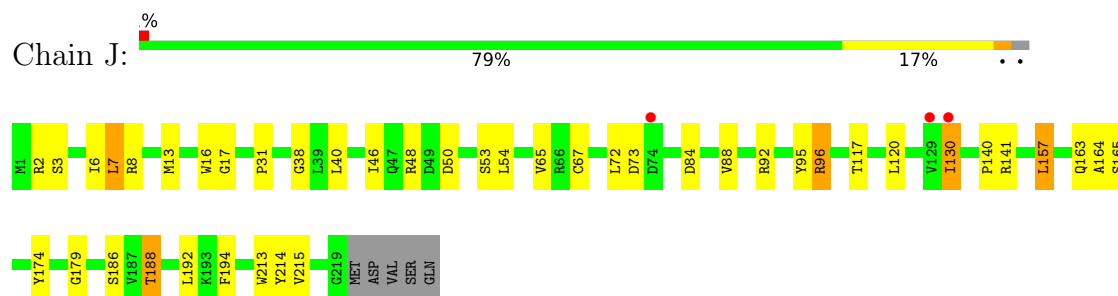
• Molecule 3: CRISPR system Cascade subunit CasC



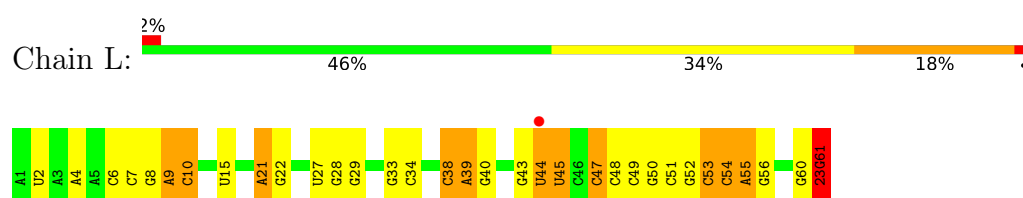
- Molecule 3: CRISPR system Cascade subunit CasC



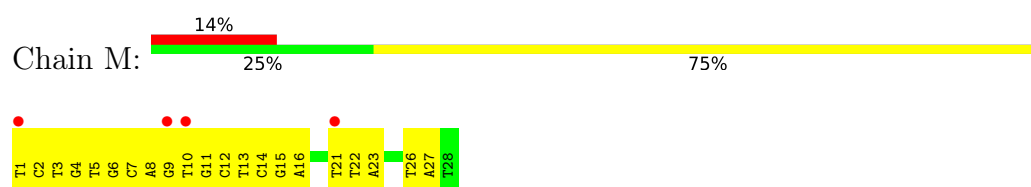
- Molecule 4: CRISPR system Cascade subunit CasD



- Molecule 5: crRNA (61-MER)

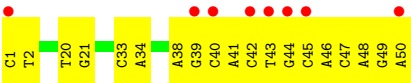


- Molecule 6: DNA (28-MER) Non-target

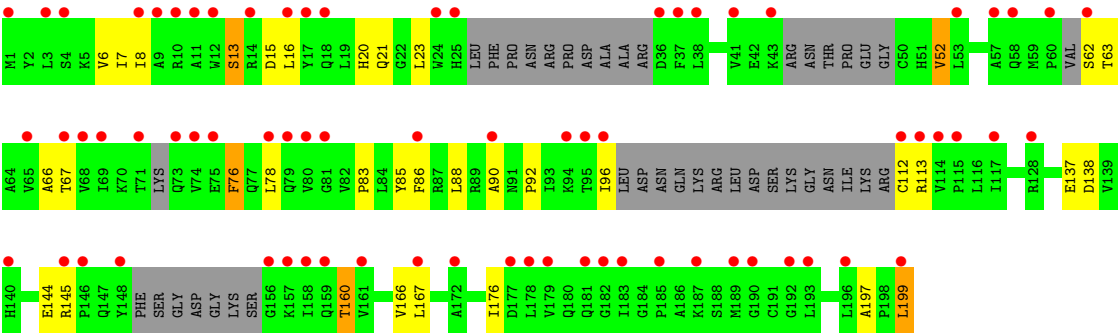


- Molecule 7: DNA (50-MER) Target





• Molecule 8: CRISPR system Cascade subunit CasE



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	92.98Å 150.06Å 400.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.87 – 2.45 49.87 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.87-2.45) 92.9 (49.87-2.45)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.99 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.206 , 0.233 0.210 , 0.234	Depositor DCC
R_{free} test set	2000 reflections (0.97%)	wwPDB-VP
Wilson B-factor (Å ²)	40.7	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 50.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	28930	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.19% 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: 23G, ZN

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	0.40	0/3830	0.73	4/5200 (0.1%)
2	B	0.52	0/1270	0.75	0/1717
2	C	0.42	0/1247	0.73	2/1686 (0.1%)
3	D	0.37	0/2433	0.72	0/3286
3	E	0.38	0/2737	0.69	1/3702 (0.0%)
3	F	0.40	0/2800	0.72	1/3790 (0.0%)
3	G	0.41	0/2756	0.67	0/3721
3	H	0.42	0/2734	0.68	0/3697
3	I	0.45	0/2730	0.72	4/3693 (0.1%)
4	J	0.51	0/1773	0.78	3/2407 (0.1%)
5	L	0.33	1/1423 (0.1%)	0.54	0/2216
6	M	0.36	0/637	0.62	0/982
7	N	0.34	0/1151	0.50	0/1773
8	K	0.31	0/1112	0.78	0/1521
All	All	0.41	1/28633 (0.0%)	0.70	15/39391 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	44	U	O3'-P	-5.20	1.53	1.61

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	188	THR	N-CA-C	8.55	125.48	111.37
1	A	321	ASN	N-CA-C	6.71	121.86	112.93
4	J	17	GLY	N-CA-C	5.98	118.91	112.33
3	F	342	ALA	N-CA-C	5.82	119.91	112.34
1	A	85	ALA	CA-C-N	-5.42	115.30	120.83
1	A	85	ALA	C-N-CA	-5.42	115.30	120.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	112	THR	CA-C-N	5.33	124.78	119.24
3	I	112	THR	C-N-CA	5.33	124.78	119.24
2	C	45	GLN	CA-C-N	-5.31	114.56	120.45
2	C	45	GLN	C-N-CA	-5.31	114.56	120.45
3	I	177	LYS	N-CA-C	-5.31	98.65	107.99
3	I	173	THR	N-CA-C	5.25	118.10	110.17
4	J	164	ALA	N-CA-C	5.24	116.25	108.60
3	E	66	ILE	N-CA-C	-5.13	108.28	113.47
1	A	431	ILE	CB-CA-C	-5.05	109.00	114.35

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	3746	0	3735	39	0
2	B	1246	0	1235	19	0
2	C	1223	0	1214	5	0
3	D	2399	0	2350	50	0
3	E	2694	0	2629	34	0
3	F	2755	0	2692	34	0
3	G	2713	0	2674	26	0
3	H	2691	0	2627	29	0
3	I	2686	0	2630	28	0
4	J	1731	0	1723	29	0
5	L	1300	0	659	39	0
6	M	572	0	323	30	0
7	N	1025	0	560	23	0
8	K	1098	0	1010	16	0
9	A	1	0	0	0	0
10	A	133	0	0	7	0
10	B	22	0	0	2	0
10	C	63	0	0	0	0
10	D	32	0	0	0	0
10	E	95	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
10	F	99	0	0	3	0
10	G	144	0	0	4	0
10	H	130	0	0	4	0
10	I	128	0	0	3	0
10	J	69	0	0	1	0
10	K	6	0	0	1	0
10	L	67	0	0	1	0
10	M	13	0	0	0	0
10	N	49	0	0	0	0
All	All	28930	0	26061	355	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 7.

All (355) 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)
5:L:52:G:N7	5:L:55:A:N6	1.88	1.20
5:L:50:G:C6	5:L:51:C:N4	2.13	1.17
3:H:28:ASP:O	3:H:38:ARG:NH1	1.92	1.03
5:L:52:G:C8	5:L:55:A:N6	2.29	0.98
3:D:72:ARG:NH1	3:D:101:ASP:O	1.98	0.95
3:F:20:ARG:NH1	5:L:29:G:OP2	2.01	0.93
3:D:28:ASP:O	3:D:38:ARG:NH1	2.02	0.93
5:L:44:U:O2'	5:L:45:U:OP2	1.86	0.92
6:M:14:DC:H2''	6:M:15:DG:H5'	1.48	0.92
1:A:296:LYS:NZ	6:M:21:DT:OP2	2.04	0.89
1:A:116:LYS:NZ	10:A:701:HOH:O	2.06	0.86
5:L:60:G:C3'	5:L:61:23G:H5'	2.05	0.86
1:A:101:MET:HE2	1:A:235:GLN:HG2	1.62	0.82
7:N:38:DA:H2'	7:N:39:DG:C8	2.15	0.82
3:I:137:LYS:NZ	7:N:46:DA:OP2	2.12	0.82
1:A:246:GLY:O	1:A:260:ARG:NH1	2.12	0.81
6:M:7:DC:H42	7:N:44:DG:H1	1.26	0.80
5:L:60:G:H3'	5:L:61:23G:H5'	1.63	0.80
3:G:93:ALA:HB2	3:G:100:VAL:HG22	1.64	0.80
3:G:82:ARG:NH1	10:G:402:HOH:O	2.14	0.79
3:D:27:LYS:NZ	5:L:39:A:OP1	2.15	0.79
2:B:26:ARG:HH21	2:B:69:LYS:HB2	1.48	0.79
6:M:9:DG:H4'	6:M:10:DT:OP1	1.83	0.77
3:E:93:ALA:HB2	3:E:100:VAL:HG22	1.67	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:M:9:DG:OP2	6:M:9:DG:H3'	1.84	0.76
2:C:70:ASN:O	2:C:73:ARG:NH1	2.19	0.75
5:L:50:G:C5	5:L:51:C:N4	2.55	0.75
4:J:92:ARG:NH1	5:L:6:C:O2	2.21	0.73
2:B:139:TRP:O	2:B:141:GLY:N	2.22	0.73
6:M:10:DT:H3	7:N:41:DA:H61	1.36	0.72
10:I:523:HOH:O	4:J:13:MET:SD	2.47	0.71
6:M:6:DG:O6	7:N:45:DC:N4	2.16	0.70
3:F:84:ASP:OD1	3:F:84:ASP:N	2.24	0.70
1:A:320:GLN:NE2	10:A:704:HOH:O	2.23	0.69
3:D:109:ASP:OD2	3:D:169:SER:OG	2.07	0.69
3:E:318:ARG:NH2	3:F:336:ASP:OD1	2.26	0.69
3:F:28:ASP:O	3:F:38:ARG:NH1	2.26	0.68
1:A:428:GLU:OE2	10:A:702:HOH:O	2.10	0.68
4:J:50:ASP:OD2	4:J:53:SER:OG	2.12	0.68
6:M:10:DT:H2''	6:M:11:DG:C8	2.28	0.68
3:G:351:GLU:OE2	10:G:401:HOH:O	2.12	0.68
6:M:3:DT:H2''	6:M:4:DG:C8	2.29	0.67
6:M:14:DC:C2'	6:M:15:DG:H5'	2.22	0.66
3:F:93:ALA:HB2	3:F:100:VAL:HG22	1.78	0.66
3:F:196:ASP:OD2	10:F:401:HOH:O	2.14	0.65
10:A:707:HOH:O	6:M:23:DA:N1	2.30	0.65
1:A:99:PRO:HB2	1:A:102:GLN:HB2	1.80	0.64
2:C:67:ALA:HB3	2:C:71:VAL:HG21	1.79	0.63
3:E:72:ARG:NH1	3:E:101:ASP:O	2.31	0.63
5:L:61:23G:OP1	10:L:102:HOH:O	2.15	0.63
6:M:9:DG:O6	7:N:42:DC:N4	2.28	0.63
1:A:2:ASN:N	1:A:6:ASP:OD2	2.31	0.63
3:I:76:ARG:HH11	3:I:89:ASP:CG	2.07	0.63
5:L:50:G:H2'	5:L:51:C:C6	2.33	0.63
3:D:278:MET:HG2	3:D:333:SER:HB2	1.79	0.62
3:I:38:ARG:NH2	4:J:84:ASP:OD1	2.31	0.62
3:F:204:ASP:HB2	3:F:212:ALA:HB2	1.82	0.62
7:N:49:DG:H2''	7:N:50:DA:OP2	1.98	0.62
3:F:38:ARG:NH2	3:G:198:ASP:OD1	2.34	0.61
2:B:89:ARG:NH2	10:B:203:HOH:O	2.33	0.61
4:J:72:LEU:O	4:J:73:ASP:HB2	1.99	0.61
3:F:347:MET:HE3	3:F:352:GLN:HB3	1.82	0.61
3:G:204:ASP:HB2	3:G:212:ALA:HB2	1.81	0.61
7:N:45:DC:H2''	7:N:46:DA:C8	2.35	0.61
6:M:11:DG:H2''	6:M:12:DC:H5''	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:51:C:H2'	5:L:52:G:O4'	2.00	0.60
3:I:252:THR:HG23	3:I:354:LYS:HB3	1.82	0.60
3:E:9:VAL:HB	3:E:226:ARG:HB2	1.82	0.60
6:M:4:DG:H2''	6:M:5:DT:OP1	2.01	0.60
3:E:8:HIS:HB2	3:E:280:MET:HB3	1.84	0.60
4:J:3:SER:HB3	4:J:130:ILE:HD13	1.84	0.59
1:A:380:GLU:HG2	1:A:447:ILE:HD13	1.84	0.59
3:G:155:GLN:HG2	3:G:239:LEU:HD22	1.83	0.59
4:J:8:ARG:NH2	4:J:117:THR:OG1	2.36	0.59
5:L:52:G:HO2'	5:L:53:C:H5	1.47	0.59
4:J:7:LEU:HG	4:J:157:LEU:HD22	1.84	0.59
3:H:204:ASP:HB3	3:H:207:GLN:HB3	1.85	0.59
4:J:3:SER:OG	4:J:163:GLN:OE1	2.21	0.59
3:E:39:ILE:HB	3:E:187:ALA:HB3	1.85	0.58
3:D:62:SER:OG	3:D:159:ASP:OD2	2.14	0.58
3:I:76:ARG:NH1	3:I:89:ASP:OD2	2.36	0.58
3:I:118:GLU:OE2	3:I:173:THR:OG1	2.15	0.57
2:C:136:MET:HE1	2:C:148:LEU:HD23	1.86	0.57
1:A:361:ARG:NH2	10:A:713:HOH:O	2.35	0.57
2:B:110:ARG:O	2:B:112:ALA:N	2.27	0.57
5:L:50:G:C6	5:L:51:C:C4	2.91	0.57
1:A:331:VAL:HG13	1:A:343:LEU:HD21	1.87	0.57
6:M:6:DG:H2'	6:M:7:DC:O4'	2.04	0.57
3:G:204:ASP:HB3	3:G:207:GLN:HB3	1.86	0.57
6:M:10:DT:H3	7:N:41:DA:N6	2.02	0.57
3:H:98:LYS:NZ	3:H:109:ASP:OD1	2.36	0.57
2:B:74:HIS:NE2	2:B:75:GLN:O	2.37	0.57
3:H:90:LYS:NZ	10:H:401:HOH:O	2.13	0.57
3:D:18:LEU:HD13	3:D:39:ILE:HD11	1.87	0.56
3:F:204:ASP:HB3	3:F:207:GLN:HG2	1.87	0.56
3:I:112:THR:HG23	3:I:238:ASN:HA	1.87	0.56
3:D:79:LEU:HD12	3:D:88:ILE:HD11	1.87	0.56
3:I:136:ASP:OD1	3:I:136:ASP:N	2.38	0.56
3:G:38:ARG:NH2	3:H:198:ASP:OD1	2.33	0.56
6:M:10:DT:H2''	6:M:11:DG:H8	1.71	0.56
3:G:9:VAL:HB	3:G:226:ARG:HB2	1.88	0.55
3:F:22:ASP:HB3	3:G:199:TRP:CE2	2.42	0.55
3:D:288:LEU:HD12	3:D:290:MET:HE2	1.86	0.55
1:A:112:THR:OG1	1:A:266:LYS:NZ	2.38	0.54
3:H:315:TYR:OH	10:H:402:HOH:O	2.17	0.54
3:E:182:MET:HB2	3:E:230:ILE:HD13	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:48:ARG:NH1	5:L:2:U:OP2	2.34	0.54
3:F:226:ARG:NH1	3:F:258:LEU:O	2.39	0.54
5:L:47:C:H42	5:L:60:G:H1	1.55	0.54
3:D:129:ALA:HB2	3:D:139:LEU:HD13	1.90	0.54
5:L:53:C:H5''	5:L:54:C:C5	2.42	0.54
3:H:95:LEU:HD22	3:H:172:MET:HE3	1.89	0.53
3:F:9:VAL:HB	3:F:226:ARG:HB2	1.90	0.53
3:D:140:LEU:HD13	3:D:171:MET:HG3	1.90	0.53
3:F:286:MET:HG3	3:F:287:PRO:HD2	1.90	0.53
3:H:296:LYS:HG3	3:I:302:ASP:HB3	1.90	0.53
3:D:69:ALA:O	3:D:72:ARG:HG3	2.08	0.52
7:N:46:DA:H2''	7:N:47:DC:O4'	2.10	0.52
6:M:7:DC:H3'	6:M:8:DA:C8	2.45	0.52
6:M:8:DA:H1'	6:M:9:DG:H5'	1.90	0.52
3:G:94:LEU:HB3	3:G:171:MET:HE2	1.91	0.52
1:A:13:PRO:HG2	1:A:16:GLY:HA3	1.89	0.52
3:D:38:ARG:NH2	3:E:198:ASP:OD1	2.39	0.52
1:A:247:ILE:HG13	1:A:258:ASN:HA	1.92	0.52
3:G:27:LYS:NZ	5:L:21:A:OP1	2.30	0.52
3:H:9:VAL:HB	3:H:226:ARG:HB2	1.91	0.52
4:J:6:ILE:HG13	4:J:174:TYR:CE1	2.44	0.52
3:E:252:THR:HG21	3:E:358:ARG:HG3	1.90	0.51
1:A:177:ARG:HB2	1:A:346:ILE:HG13	1.92	0.51
3:I:204:ASP:HB2	3:I:212:ALA:HB2	1.92	0.51
5:L:52:G:O2'	5:L:53:C:H5	1.94	0.51
5:L:38:C:N4	5:L:40:G:O2'	2.43	0.51
5:L:50:G:C4	5:L:51:C:C5	2.98	0.51
8:K:8:ILE:O	8:K:13:SER:OG	2.28	0.51
3:D:95:LEU:HD23	3:D:114:TRP:HZ3	1.76	0.51
3:D:76:ARG:NH2	3:D:89:ASP:OD2	2.44	0.51
3:H:34:LYS:NZ	10:H:405:HOH:O	2.33	0.51
2:B:106:ILE:HA	2:B:145:ARG:HH11	1.75	0.50
3:D:76:ARG:HG2	3:D:88:ILE:HG21	1.94	0.50
3:D:155:GLN:HG3	3:D:239:LEU:HD22	1.92	0.50
3:G:46:ARG:NH1	3:G:50:LYS:HE3	2.26	0.50
1:A:315:VAL:HG21	1:A:347:MET:HE3	1.94	0.50
3:E:204:ASP:HB2	3:E:212:ALA:HB2	1.93	0.50
5:L:54:C:H4'	5:L:55:A:O5'	2.12	0.50
3:D:45:LYS:HA	3:D:48:MET:HE2	1.93	0.50
3:I:9:VAL:HB	3:I:226:ARG:HB2	1.92	0.50
1:A:491:ARG:NH2	6:M:27:DA:OP1	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:N:48:DA:H2''	7:N:49:DG:OP2	2.12	0.50
5:L:38:C:N4	5:L:40:G:HO2'	2.09	0.49
6:M:12:DC:H2''	6:M:13:DT:OP1	2.12	0.49
3:F:344:VAL:O	10:F:402:HOH:O	2.20	0.49
4:J:194:PHE:HB3	4:J:213:TRP:HB2	1.94	0.49
5:L:9:A:O2'	5:L:10:C:H5''	2.11	0.49
3:F:49:ARG:HD3	10:F:406:HOH:O	2.13	0.49
5:L:50:G:N1	5:L:51:C:N4	2.59	0.49
3:H:94:LEU:HB3	3:H:171:MET:HE2	1.93	0.49
3:E:252:THR:HG22	3:E:357:VAL:HB	1.95	0.49
6:M:1:DT:H2''	6:M:2:DC:O4'	2.13	0.49
6:M:21:DT:H2''	6:M:22:DT:OP2	2.13	0.49
2:B:75:GLN:CG	2:B:76:ASP:N	2.76	0.48
2:C:107:ARG:HB3	3:H:25:MET:HE1	1.95	0.48
3:D:151:ARG:NH2	3:D:175:LEU:O	2.46	0.48
8:K:83:PRO:HG2	8:K:199:LEU:HD11	1.95	0.48
2:B:14:TRP:HE1	2:B:69:LYS:HA	1.79	0.48
1:A:117:LEU:HD23	1:A:151:GLN:HG3	1.95	0.48
3:E:199:TRP:CZ2	3:E:214:LEU:HD23	2.49	0.48
5:L:50:G:C2	5:L:51:C:C4	3.01	0.48
3:D:67:HIS:CE1	3:E:207:GLN:HE21	2.31	0.48
3:F:19:ASN:OD1	3:F:27:LYS:HD2	2.14	0.48
3:I:340:ILE:HD12	3:I:344:VAL:HG21	1.96	0.48
3:E:246:GLN:O	3:E:246:GLN:NE2	2.47	0.48
8:K:76:PHE:HB2	8:K:78:LEU:HD13	1.94	0.48
1:A:77:GLU:O	1:A:81:GLN:HG2	2.14	0.48
2:B:10:LEU:HD23	2:B:61:MET:HE2	1.95	0.48
3:E:182:MET:HE2	3:E:228:ALA:HB1	1.94	0.48
3:H:101:ASP:OD1	3:H:103:ALA:N	2.42	0.47
5:L:50:G:O6	5:L:51:C:N4	2.44	0.47
1:A:247:ILE:HD12	1:A:247:ILE:H	1.78	0.47
3:G:2:SER:HB2	3:G:283:PHE:HB3	1.96	0.47
3:H:122:PHE:O	3:H:126:VAL:HG23	2.15	0.47
1:A:138:ALA:HB1	1:A:260:ARG:HE	1.79	0.47
3:I:358:ARG:NH2	10:I:410:HOH:O	2.42	0.47
5:L:38:C:O2	5:L:39:A:H4'	2.15	0.47
1:A:228:PHE:HA	1:A:277:TRP:HZ2	1.79	0.47
1:A:248:GLY:N	1:A:260:ARG:NH1	2.63	0.47
3:D:89:ASP:HB3	3:D:100:VAL:HG11	1.97	0.47
3:D:288:LEU:HD21	3:E:275:PRO:HG3	1.95	0.47
8:K:86:PHE:CD1	8:K:167:LEU:HG	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:K:85:TYR:CE2	8:K:199:LEU:HB3	2.50	0.47
5:L:50:G:C5	5:L:51:C:C4	3.02	0.47
6:M:4:DG:O5'	6:M:4:DG:H8	1.97	0.47
7:N:44:DG:H2''	7:N:45:DC:H5'	1.97	0.47
3:E:82:ARG:HD2	3:E:83:PHE:CZ	2.50	0.47
1:A:133:PRO:HB3	4:J:95:TYR:CD1	2.50	0.47
4:J:40:LEU:HD11	4:J:120:LEU:HD11	1.97	0.47
3:D:132:ASP:OD1	3:D:132:ASP:N	2.47	0.47
8:K:144:GLU:OE2	8:K:160:THR:OG1	2.19	0.47
3:D:71:LEU:O	3:D:75:LEU:HG	2.15	0.46
3:H:70:GLN:N	3:H:70:GLN:OE1	2.48	0.46
3:H:185:ALA:HB2	3:I:271:ALA:HB3	1.97	0.46
1:A:13:PRO:HD3	1:A:34:TRP:HZ3	1.81	0.46
3:E:253:HIS:O	3:E:257:MET:HG3	2.16	0.46
7:N:1:DC:H2'	7:N:2:DT:C6	2.50	0.46
3:G:89:ASP:O	3:G:100:VAL:HG21	2.15	0.46
3:D:67:HIS:CE1	3:E:204:ASP:OD2	2.69	0.46
7:N:42:DC:H2''	7:N:43:DT:H5'	1.98	0.46
3:D:125:GLN:HG2	3:D:143:LEU:HD21	1.98	0.46
3:I:137:LYS:O	3:I:141:LYS:N	2.48	0.46
3:F:252:THR:HG22	3:F:357:VAL:HB	1.98	0.46
3:I:136:ASP:HB2	3:I:137:LYS:H	1.46	0.46
5:L:44:U:HO2'	5:L:45:U:P	2.27	0.46
8:K:78:LEU:HD22	8:K:176:ILE:HD11	1.97	0.46
3:D:85:GLN:O	3:D:88:ILE:HG22	2.16	0.46
8:K:85:TYR:N	8:K:197:ALA:O	2.49	0.46
3:H:204:ASP:HB2	3:H:212:ALA:HB2	1.98	0.45
3:I:165:ARG:HH11	4:J:92:ARG:NH1	2.14	0.45
4:J:192:LEU:HB3	4:J:215:VAL:HB	1.98	0.45
8:K:15:ASP:OD1	8:K:16:LEU:N	2.46	0.45
3:D:91:THR:O	3:D:95:LEU:HB2	2.17	0.45
3:F:356:TRP:CD1	3:F:362:GLU:HB2	2.51	0.45
3:E:89:ASP:O	3:E:100:VAL:HG21	2.16	0.45
3:E:280:MET:HE1	3:E:329:ALA:HB1	1.98	0.45
3:H:96:SER:O	3:H:169:SER:OG	2.34	0.45
7:N:39:DG:H2''	7:N:40:DC:H5''	1.97	0.45
7:N:46:DA:H2''	7:N:47:DC:C6	2.52	0.45
2:C:154:LEU:HD22	6:M:26:DT:C2	2.51	0.45
3:G:45:LYS:HD2	3:G:184:ILE:HG21	1.98	0.45
3:D:115:VAL:HG12	3:D:118:GLU:H	1.80	0.45
3:E:32:GLY:HA2	3:E:295:GLU:OE2	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:2:ARG:NH1	10:J:304:HOH:O	2.49	0.45
4:J:38:GLY:HA3	5:L:2:U:O4'	2.16	0.45
5:L:50:G:N1	5:L:51:C:C4	2.85	0.45
1:A:231:GLY:HA3	1:A:277:TRP:CZ2	2.51	0.45
2:B:113:ASP:OD1	2:B:114:MET:N	2.49	0.45
3:I:76:ARG:HD2	3:I:89:ASP:OD1	2.17	0.45
1:A:59:ALA:HB2	1:A:83:LEU:HD13	1.99	0.45
3:D:300:ALA:HB2	3:D:307:PRO:HG2	1.98	0.45
3:G:19:ASN:OD1	3:G:27:LYS:HD2	2.16	0.45
3:H:113:PRO:HB2	3:H:160:ILE:HD11	1.99	0.45
5:L:53:C:H5''	5:L:54:C:H5	1.81	0.45
2:B:75:GLN:CG	2:B:76:ASP:H	2.30	0.45
3:D:8:HIS:HB2	3:D:280:MET:HB3	1.99	0.45
3:D:98:LYS:HD3	3:D:108:ALA:HA	1.99	0.45
7:N:20:DT:H72	7:N:21:DG:N1	2.31	0.45
3:I:204:ASP:HB3	3:I:207:GLN:HB3	1.98	0.45
3:E:22:ASP:HB3	3:F:199:TRP:CE2	2.52	0.44
3:H:22:ASP:OD1	3:H:22:ASP:N	2.50	0.44
3:H:318:ARG:NH1	10:H:411:HOH:O	2.49	0.44
3:D:138:LYS:O	3:D:142:VAL:HG23	2.17	0.44
1:A:56:GLN:HA	1:A:189:VAL:HG13	2.00	0.44
3:D:88:ILE:HD12	3:D:88:ILE:HA	1.90	0.44
4:J:186:SER:HB3	4:J:214:TYR:CE1	2.53	0.44
3:E:109:ASP:OD2	3:E:169:SER:OG	2.18	0.44
4:J:50:ASP:O	4:J:54:LEU:HB2	2.18	0.44
3:E:118:GLU:OE1	10:E:401:HOH:O	2.21	0.44
3:D:135:ASP:O	3:D:138:LYS:N	2.48	0.44
3:E:38:ARG:NH2	3:F:198:ASP:OD1	2.51	0.44
7:N:42:DC:H1'	7:N:43:DT:H5'	2.00	0.44
8:K:145:ARG:O	10:K:201:HOH:O	2.21	0.44
3:D:70:GLN:H	3:D:70:GLN:HG2	1.39	0.43
3:D:251:ALA:O	3:D:255:VAL:HG23	2.18	0.43
4:J:48:ARG:NH1	5:L:2:U:P	2.91	0.43
6:M:3:DT:C4	7:N:47:DC:N4	2.86	0.43
1:A:154:GLN:O	1:A:170:THR:HA	2.19	0.43
3:D:174:GLU:OE2	3:D:174:GLU:N	2.51	0.43
8:K:63:THR:OG1	8:K:66:ALA:N	2.50	0.43
2:B:110:ARG:C	2:B:112:ALA:H	2.21	0.43
3:F:278:MET:CE	3:F:331:GLN:HE21	2.31	0.43
3:D:14:SER:OG	8:K:138:ASP:OD1	2.35	0.43
3:F:278:MET:HE2	3:F:331:GLN:HE21	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:306:GLN:HB2	3:D:307:PRO:HD3	2.00	0.43
3:H:48:MET:O	3:H:51:SER:OG	2.34	0.43
3:H:172:MET:HA	3:H:172:MET:HE2	2.00	0.43
3:I:336:ASP:OD1	3:I:336:ASP:N	2.50	0.43
8:K:6:VAL:HB	8:K:52:VAL:HG12	1.99	0.43
3:E:82:ARG:HD2	3:E:83:PHE:CE2	2.53	0.43
2:B:8:MET:HG2	2:B:131:PRO:HG3	2.01	0.42
3:H:146:ASP:OD2	3:H:149:ALA:HB2	2.19	0.42
1:A:80:PHE:CE2	1:A:84:ILE:HD13	2.53	0.42
3:F:132:ASP:OD1	3:F:132:ASP:N	2.52	0.42
3:F:199:TRP:CZ2	3:F:214:LEU:HD23	2.54	0.42
7:N:41:DA:H2''	7:N:42:DC:OP1	2.19	0.42
3:I:121:TRP:CE2	3:I:172:MET:HG2	2.54	0.42
4:J:31:PRO:HD2	4:J:65:VAL:HG11	2.02	0.42
5:L:52:G:O2'	5:L:53:C:C5	2.70	0.42
3:F:3:ASN:ND2	3:F:231:ASN:OD1	2.52	0.42
6:M:4:DG:C2'	6:M:5:DT:OP1	2.67	0.42
3:D:9:VAL:HB	3:D:226:ARG:HB2	2.01	0.42
4:J:186:SER:HB3	4:J:214:TYR:CD1	2.55	0.42
6:M:22:DT:H2''	6:M:23:DA:O5'	2.19	0.42
3:I:92:LEU:HD12	3:I:92:LEU:HA	1.80	0.42
3:F:134:LEU:HD12	3:F:134:LEU:H	1.85	0.42
3:G:64:ARG:HD3	10:G:459:HOH:O	2.19	0.42
5:L:49:C:H2'	5:L:50:G:C8	2.55	0.42
2:B:49:TRP:CZ3	2:B:55:GLN:HB2	2.55	0.41
3:I:146:ASP:OD2	4:J:96:ARG:NH2	2.53	0.41
7:N:48:DA:H1'	7:N:49:DG:O4'	2.21	0.41
8:K:20:HIS:ND1	8:K:21:GLN:HG3	2.35	0.41
1:A:207:ASN:OD1	1:A:229:VAL:HG13	2.20	0.41
3:G:177:LYS:HB2	3:G:177:LYS:NZ	2.35	0.41
3:H:306:GLN:HB2	3:H:307:PRO:HD3	2.02	0.41
3:I:48:MET:HG2	3:I:257:MET:HB3	2.02	0.41
1:A:76:THR:OG1	1:A:79:GLU:HG3	2.19	0.41
1:A:172:VAL:HG23	1:A:299:ALA:HA	2.02	0.41
1:A:279:HIS:CE1	1:A:281:HIS:HB2	2.56	0.41
3:D:286:MET:HA	3:D:287:PRO:HD3	1.96	0.41
4:J:46:ILE:HG21	4:J:54:LEU:HD13	2.01	0.41
7:N:33:DC:H2'	7:N:34:DA:O4'	2.20	0.41
3:D:22:ASP:HB3	3:E:199:TRP:CD2	2.56	0.41
3:D:72:ARG:O	3:D:76:ARG:HG3	2.20	0.41
3:F:245:GLU:CD	3:F:245:GLU:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394:LYS:NZ	10:A:718:HOH:O	2.43	0.41
3:E:101:ASP:OD1	3:E:101:ASP:N	2.52	0.41
3:E:113:PRO:HG2	3:E:165:ARG:HD3	2.02	0.41
3:E:232:LEU:HD13	3:E:244:ARG:HE	1.85	0.41
3:G:82:ARG:NH2	10:G:413:HOH:O	2.43	0.41
7:N:46:DA:H2''	7:N:47:DC:H6	1.85	0.41
1:A:55:GLY:HA2	1:A:58:ILE:HG12	2.01	0.41
3:D:219:PHE:CE2	8:K:137:GLU:HB3	2.55	0.41
3:F:22:ASP:HB3	3:G:199:TRP:CD2	2.55	0.41
1:A:406:LYS:HB3	1:A:408:PHE:HD1	1.86	0.41
2:B:17:LEU:HD23	2:B:22:CYS:HB3	2.02	0.41
1:A:14:ARG:NH1	1:A:15:ASN:OD1	2.52	0.41
3:D:90:LYS:HG3	3:D:94:LEU:HD23	2.02	0.41
3:D:248:LEU:O	3:D:252:THR:HG23	2.21	0.41
3:G:100:VAL:O	3:G:100:VAL:HG23	2.21	0.41
3:I:118:GLU:OE1	3:I:172:MET:N	2.50	0.41
8:K:90:ALA:C	8:K:92:PRO:HD3	2.45	0.41
2:B:150:GLU:OE2	10:B:201:HOH:O	2.22	0.41
3:D:111:VAL:HG21	3:E:202:ALA:HB1	2.03	0.41
3:F:290:MET:HE2	3:F:290:MET:HA	2.03	0.41
3:G:165:ARG:NH1	3:G:172:MET:HE1	2.36	0.41
3:G:185:ALA:HB2	3:H:271:ALA:HB3	2.02	0.41
3:I:277:ASP:OD1	10:I:401:HOH:O	2.22	0.41
4:J:67:CYS:O	4:J:179:GLY:HA3	2.21	0.41
4:J:88:VAL:HG22	5:L:7:C:H1'	2.02	0.41
6:M:15:DG:H2''	6:M:16:DA:C8	2.56	0.41
2:B:90:ALA:HB1	2:B:126:PRO:HB2	2.03	0.41
6:M:22:DT:H4'	6:M:23:DA:OP1	2.20	0.41
3:F:103:ALA:HB3	3:F:106:ILE:HD11	2.02	0.40
3:G:347:MET:HA	3:G:348:PRO:HD3	1.89	0.40
1:A:151:GLN:NE2	10:A:703:HOH:O	2.20	0.40
3:D:171:MET:HG2	3:D:175:LEU:HD12	2.02	0.40
3:E:299:LYS:NZ	3:F:302:ASP:OD1	2.54	0.40
3:H:11:ILE:HD11	3:H:274:ASN:O	2.21	0.40
2:B:72:ILE:HD11	2:B:121:LEU:HD13	2.03	0.40
3:F:101:ASP:HB2	3:F:102:GLU:H	1.68	0.40
2:B:107:ARG:HB2	3:F:25:MET:HE1	2.03	0.40
3:D:75:LEU:HD11	3:D:92:LEU:HD22	2.04	0.40
3:E:190:THR:HG23	3:E:294:PHE:CD1	2.57	0.40
3:G:296:LYS:HG3	3:H:302:ASP:HB3	2.03	0.40
3:H:22:ASP:HB3	3:I:199:TRP:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:285:ASP:O	4:J:140:PRO:HD2	2.21	0.40
4:J:16:TRP:CG	4:J:31:PRO:HA	2.56	0.40
5:L:53:C:O5'	5:L:53:C:H6	2.04	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	473/502 (94%)	455 (96%)	17 (4%)	1 (0%)	43	54
2	B	149/165 (90%)	144 (97%)	3 (2%)	2 (1%)	9	9
2	C	146/165 (88%)	143 (98%)	2 (1%)	1 (1%)	18	24
3	D	310/363 (85%)	293 (94%)	16 (5%)	1 (0%)	36	45
3	E	350/363 (96%)	338 (97%)	11 (3%)	1 (0%)	36	45
3	F	359/363 (99%)	345 (96%)	14 (4%)	0	100	100
3	G	350/363 (96%)	343 (98%)	7 (2%)	0	100	100
3	H	348/363 (96%)	339 (97%)	9 (3%)	0	100	100
3	I	347/363 (96%)	338 (97%)	7 (2%)	2 (1%)	21	27
4	J	217/224 (97%)	215 (99%)	2 (1%)	0	100	100
8	K	145/199 (73%)	137 (94%)	8 (6%)	0	100	100
All	All	3194/3433 (93%)	3090 (97%)	96 (3%)	8 (0%)	36	45

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	111	THR
2	B	140	TRP
3	I	136	ASP

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Mol	Chain	Res	Type
3	D	133	ASN
3	E	209	GLN
1	A	119	ALA
2	C	111	THR
3	I	340	ILE

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	403/426 (95%)	389 (96%)	14 (4%)	32	46
2	B	129/141 (92%)	124 (96%)	5 (4%)	28	42
2	C	127/141 (90%)	122 (96%)	5 (4%)	28	42
3	D	246/298 (83%)	227 (92%)	19 (8%)	12	15
3	E	278/298 (93%)	262 (94%)	16 (6%)	18	27
3	F	287/298 (96%)	274 (96%)	13 (4%)	24	37
3	G	283/298 (95%)	276 (98%)	7 (2%)	42	56
3	H	280/298 (94%)	275 (98%)	5 (2%)	51	65
3	I	281/298 (94%)	270 (96%)	11 (4%)	28	42
4	J	186/192 (97%)	179 (96%)	7 (4%)	29	43
8	K	102/170 (60%)	88 (86%)	14 (14%)	3	3
All	All	2602/2858 (91%)	2486 (96%)	116 (4%)	24	37

All (116) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ASP
1	A	7	ASN
1	A	82	GLN
1	A	111	VAL
1	A	229	VAL
1	A	287	THR

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Mol	Chain	Res	Type
1	A	293	VAL
1	A	298	LEU
1	A	322	GLU
1	A	347	MET
1	A	351	ARG
1	A	380	GLU
1	A	407	ASP
1	A	466	VAL
2	B	28	VAL
2	B	70	ASN
2	B	110	ARG
2	B	111	THR
2	B	118	ARG
2	C	28	VAL
2	C	78	LYS
2	C	83	THR
2	C	111	THR
2	C	156	THR
3	D	5	ILE
3	D	19	ASN
3	D	70	GLN
3	D	75	LEU
3	D	76	ARG
3	D	81	GLU
3	D	82	ARG
3	D	98	LYS
3	D	105	LYS
3	D	111	VAL
3	D	132	ASP
3	D	134	LEU
3	D	145	GLU
3	D	194	ASP
3	D	217	GLN
3	D	286	MET
3	D	288	LEU
3	D	333	SER
3	D	335	SER
3	E	2	SER
3	E	5	ILE
3	E	70	GLN
3	E	82	ARG
3	E	102	GLU

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Mol	Chain	Res	Type
3	E	139	LEU
3	E	182	MET
3	E	188	ILE
3	E	194	ASP
3	E	206	LEU
3	E	211	SER
3	E	246	GLN
3	E	266	LYS
3	E	305	LEU
3	E	325	LEU
3	E	341	THR
3	F	20	ARG
3	F	84	ASP
3	F	132	ASP
3	F	201	THR
3	F	218	GLU
3	F	244	ARG
3	F	268	ARG
3	F	280	MET
3	F	305	LEU
3	F	334	LEU
3	F	340	ILE
3	F	343	GLN
3	F	362	GLU
3	G	76	ARG
3	G	87	ILE
3	G	249	GLU
3	G	277	ASP
3	G	317	ASP
3	G	347	MET
3	G	359	ASN
3	H	14	SER
3	H	49	ARG
3	H	169	SER
3	H	177	LYS
3	H	282	ASN
3	I	65	THR
3	I	76	ARG
3	I	92	LEU
3	I	94	LEU
3	I	132	ASP
3	I	133	ASN

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Mol	Chain	Res	Type
3	I	134	LEU
3	I	136	ASP
3	I	336	ASP
3	I	340	ILE
3	I	341	THR
4	J	7	LEU
4	J	96	ARG
4	J	130	ILE
4	J	141	ARG
4	J	157	LEU
4	J	165	SER
4	J	188	THR
8	K	7	ILE
8	K	13	SER
8	K	23	LEU
8	K	52	VAL
8	K	62	SER
8	K	67	THR
8	K	76	PHE
8	K	88	LEU
8	K	96	ILE
8	K	112	CYS
8	K	113	ARG
8	K	160	THR
8	K	166	VAL
8	K	199	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	281	HIS
2	B	56	GLN
2	B	159	ASN
2	C	147	GLN
3	D	19	ASN
3	D	57	ASN
3	D	125	GLN
3	D	217	GLN
3	D	234	GLN
3	E	77	GLN
3	E	207	GLN
3	E	274	ASN

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Mol	Chain	Res	Type
3	F	26	GLN
3	F	57	ASN
3	F	274	ASN
3	F	331	GLN
3	F	343	GLN
3	F	346	GLN
3	G	234	GLN
3	H	234	GLN
3	H	352	GLN
3	I	192	GLN
3	I	274	ASN
3	I	306	GLN
3	I	331	GLN
3	I	346	GLN
4	J	47	GLN
8	K	170	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	L	60/61 (98%)	22 (36%)	1 (1%)

All (22) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	L	4	A
5	L	8	G
5	L	9	A
5	L	10	C
5	L	15	U
5	L	21	A
5	L	22	G
5	L	27	U
5	L	28	G
5	L	33	G
5	L	34	C
5	L	38	C
5	L	39	A
5	L	43	G
5	L	45	U
5	L	47	C

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Mol	Chain	Res	Type
5	L	48	C
5	L	53	C
5	L	54	C
5	L	55	A
5	L	56	G
5	L	61	23G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	L	54	C

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

1 non-standard protein/DNA/RNA residue is 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
5	23G	L	61	5	24,29,30	1.37	3 (12%)	34,45,48	2.20	9 (26%)

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
5	23G	L	61	5	-	0/7/35/36	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	61	23G	C6-N1	-3.52	1.32	1.38
5	L	61	23G	C5-C4	2.82	1.46	1.38
5	L	61	23G	C5-N7	-2.78	1.33	1.39

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	61	23G	C5-C4-N3	-7.15	117.02	128.39
5	L	61	23G	N9-C4-N3	5.46	136.88	125.95
5	L	61	23G	C2-N3-C4	5.04	120.98	112.30
5	L	61	23G	C6-C5-N7	2.84	135.47	130.29
5	L	61	23G	C4-C5-N7	-2.60	106.56	110.67
5	L	61	23G	C2-N1-C6	-2.39	120.78	125.11
5	L	61	23G	OC1-PC-OC2	2.24	117.13	109.89
5	L	61	23G	C8-N7-C5	2.20	108.18	104.26
5	L	61	23G	C5-C6-N1	2.19	118.84	113.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	61	23G	3	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 1 ligands modelled in this entry, 1 is 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

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	481/502 (95%)	0.32	22 (4%) 37 36	19, 48, 84, 110	0
2	B	153/165 (92%)	0.45	6 (3%) 43 43	33, 59, 87, 100	0
2	C	150/165 (90%)	-0.27	2 (1%) 75 77	19, 32, 56, 84	0
3	D	318/363 (87%)	0.91	29 (9%) 15 12	44, 67, 120, 164	0
3	E	354/363 (97%)	0.25	11 (3%) 51 52	33, 49, 75, 101	0
3	F	361/363 (99%)	0.10	6 (1%) 69 71	22, 44, 74, 147	0
3	G	354/363 (97%)	-0.28	2 (0%) 85 87	19, 32, 55, 73	0
3	H	352/363 (96%)	-0.17	5 (1%) 73 75	16, 33, 79, 112	0
3	I	351/363 (96%)	0.09	16 (4%) 37 36	18, 39, 89, 131	0
4	J	219/224 (97%)	-0.11	3 (1%) 73 75	20, 37, 63, 77	0
5	L	60/61 (98%)	-0.18	1 (1%) 69 71	20, 36, 130, 134	0
6	M	28/28 (100%)	1.28	4 (14%) 6 4	52, 110, 264, 267	0
7	N	50/50 (100%)	0.18	8 (16%) 5 3	22, 43, 257, 281	0
8	K	159/199 (79%)	2.12	72 (45%) 0 0	67, 93, 108, 125	0
All	All	3390/3572 (94%)	0.24	187 (5%) 30 28	16, 45, 99, 281	0

All (187) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	K	156	GLY	6.1
8	K	96	ILE	5.8
3	D	264	GLY	5.7
8	K	158	ILE	5.7
8	K	12	TRP	5.2
3	D	344	VAL	5.2
8	K	148	TYR	5.1
8	K	24	TRP	5.0

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Mol	Chain	Res	Type	RSRZ
8	K	17	TYR	4.8
8	K	43	LYS	4.7
8	K	60	PRO	4.7
8	K	4	SER	4.4
3	D	335	SER	4.3
6	M	21	DT	4.1
3	E	206	LEU	4.1
8	K	73	GLN	4.0
3	D	101	ASP	3.8
1	A	107	LYS	3.7
8	K	41	VAL	3.7
8	K	65	VAL	3.7
3	E	209	GLN	3.7
1	A	104	LYS	3.7
8	K	68	VAL	3.6
3	I	134	LEU	3.5
1	A	90	MET	3.5
8	K	57	ALA	3.5
3	D	138	LYS	3.5
3	D	102	GLU	3.5
8	K	16	LEU	3.5
3	D	142	VAL	3.5
3	D	134	LEU	3.5
8	K	62	SER	3.5
8	K	187	LYS	3.5
3	E	341	THR	3.4
8	K	95	THR	3.4
3	D	135	ASP	3.3
2	B	50	GLU	3.2
8	K	117	ILE	3.2
8	K	181	GLN	3.2
8	K	128	ARG	3.2
8	K	193	LEU	3.2
3	I	97	GLY	3.1
8	K	145	ARG	3.1
8	K	178	LEU	3.1
8	K	74	VAL	3.1
8	K	36	ASP	3.1
8	K	114	VAL	3.1
3	H	131	ALA	3.1
1	A	115	GLU	3.1
8	K	112	CYS	3.1

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Mol	Chain	Res	Type	RSRZ
8	K	25	HIS	3.1
3	D	126	VAL	3.1
8	K	157	LYS	3.0
8	K	167	LEU	3.0
8	K	190	GLY	3.0
8	K	172	ALA	2.9
8	K	8	ILE	2.9
3	D	143	LEU	2.9
8	K	86	PHE	2.9
8	K	75	GLU	2.9
8	K	14	ARG	2.9
6	M	10	DT	2.9
8	K	37	PHE	2.9
1	A	14	ARG	2.8
3	I	137	LYS	2.8
8	K	11	ALA	2.8
3	D	361	GLY	2.8
3	I	138	LYS	2.8
8	K	10	ARG	2.8
3	D	75	LEU	2.8
8	K	18	GLN	2.8
8	K	182	GLY	2.8
3	I	326	ASN	2.8
3	H	123	CYS	2.8
8	K	94	LYS	2.8
3	F	132	ASP	2.8
3	I	140	LEU	2.7
3	D	104	GLU	2.7
3	F	340	ILE	2.7
6	M	9	DG	2.7
1	A	96	ALA	2.7
1	A	324	GLY	2.7
2	B	68	GLY	2.7
7	N	50	DA	2.7
8	K	179	VAL	2.7
3	E	188	ILE	2.7
2	B	83	THR	2.7
3	D	124	GLU	2.7
3	D	131	ALA	2.7
8	K	183	ILE	2.6
3	E	334	LEU	2.6
7	N	42	DC	2.6

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Mol	Chain	Res	Type	RSRZ
3	I	131	ALA	2.6
1	A	375	GLY	2.6
7	N	43	DT	2.6
4	J	74	ASP	2.5
3	I	123	CYS	2.5
8	K	67	THR	2.5
8	K	113	ARG	2.5
7	N	40	DC	2.5
7	N	39	DG	2.5
3	D	88	ILE	2.5
8	K	115	PRO	2.5
8	K	81	GLY	2.5
2	B	3	ASP	2.5
3	E	205	ASP	2.5
3	D	63	LEU	2.5
8	K	58	GLN	2.5
8	K	161	VAL	2.5
8	K	189	MET	2.5
8	K	146	PRO	2.4
7	N	1	DC	2.4
3	E	212	ALA	2.4
1	A	105	GLY	2.4
3	H	128	LYS	2.4
6	M	1	DT	2.4
8	K	53	LEU	2.4
3	D	116	VAL	2.4
3	D	127	ALA	2.4
3	G	326	ASN	2.4
8	K	1	MET	2.4
4	J	129	VAL	2.4
3	E	199	TRP	2.4
3	D	334	LEU	2.3
3	I	135	ASP	2.3
8	K	199	LEU	2.3
3	D	100	VAL	2.3
3	F	362	GLU	2.3
3	I	69	ALA	2.3
1	A	200	PRO	2.3
8	K	71	THR	2.3
8	K	38	LEU	2.3
3	H	136	ASP	2.3
1	A	206	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
7	N	44	DG	2.3
3	D	23	MET	2.3
2	B	69	LYS	2.3
3	F	336	ASP	2.3
3	I	141	LYS	2.3
3	E	208	GLU	2.3
1	A	290	LYS	2.2
3	I	107	SER	2.2
1	A	376	ASN	2.2
3	D	120	ALA	2.2
3	F	131	ALA	2.2
3	G	343	GLN	2.2
1	A	245	ILE	2.2
1	A	292	GLU	2.2
3	H	127	ALA	2.2
8	K	140	HIS	2.2
1	A	366	MET	2.2
3	E	361	GLY	2.2
8	K	192	GLY	2.2
1	A	88	ILE	2.2
8	K	79	GLN	2.2
1	A	92	TYR	2.2
3	F	134	LEU	2.2
3	I	71	LEU	2.2
3	D	132	ASP	2.2
3	I	126	VAL	2.1
8	K	80	VAL	2.1
1	A	205	THR	2.1
3	D	168	THR	2.1
3	I	87	ILE	2.1
1	A	216	LYS	2.1
8	K	185	PRO	2.1
1	A	91	PHE	2.1
1	A	199	PHE	2.1
5	L	44	U	2.1
8	K	9	ALA	2.1
4	J	130	ILE	2.1
2	C	64	CYS	2.1
8	K	196	LEU	2.1
3	E	2	SER	2.1
3	D	77	GLN	2.1
2	B	139	TRP	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	70	ASN	2.1
8	K	78	LEU	2.1
7	N	45	DC	2.1
3	I	136	ASP	2.1
8	K	177	ASP	2.1
8	K	90	ALA	2.0
8	K	69	ILE	2.0
8	K	159	GLN	2.0
3	D	332	PHE	2.0
3	D	118	GLU	2.0
8	K	3	LEU	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
5	23G	L	61	26/27	0.66	0.22	98,123,163,171	0

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
9	ZN	A	601	1/1	0.99	0.03	51,51,51,51	0

6.5 Other polymers [i](#)

There are no such residues in this entry.