WORLDWIDE
wwPDB
PROTEIN DATA BANK

wwPDB X-ray Structure Validation Summary Report (i)

Mar 21, 2016 – 03:04 PM EDT

PDB ID : 5H9F
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)

The following versions of software and data (see references (1)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : unknown
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0122
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

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	Percentile Ranks	Value
Rfree		0.233
Clashscore		6
Ramachandran outliers		0.3%
Sidechain outliers		4.2%
RSRZ outliers		3.2%
RNA backbone		0.36

Worse   *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution
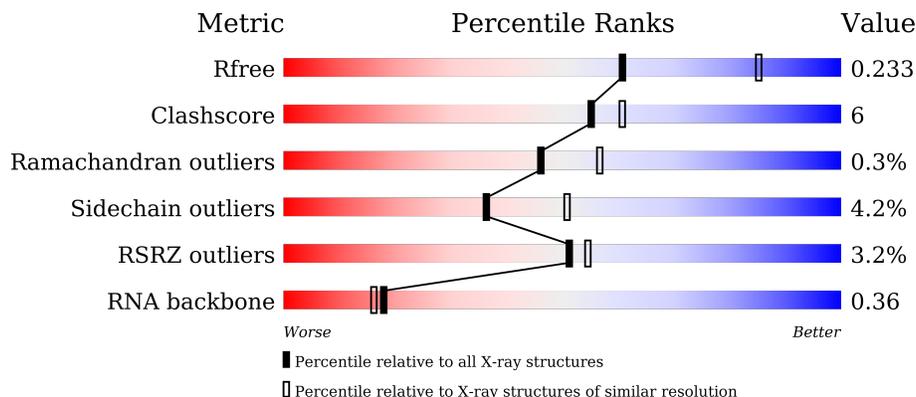
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	91344	4776 (2.50-2.42)
Clashscore	102246	1030 (2.48-2.44)
Ramachandran outliers	100387	1024 (2.48-2.44)
Sidechain outliers	100360	1024 (2.48-2.44)
RSRZ outliers	91569	4787 (2.50-2.42)
RNA backbone	2183	1004 (2.92-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	502	% 82% 13% · ·
2	B	165	5% 73% 19% · 7%
2	C	165	% 84% 6% · 9%
3	D	363	5% 65% 20% · 12%

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Mol	Chain	Length	Quality of chain
3	E	363	82% 14%
3	F	363	2% 85% 13%
3	G	363	88% 9%
3	H	363	% 87% 10%
3	I	363	2% 86% 9%
4	J	224	79% 17%
5	L	61	3% 44% 36% 18%
6	M	28	36% 25% 68% 7%
7	N	50	20% 62% 38%
8	K	199	17% 65% 13% 20%
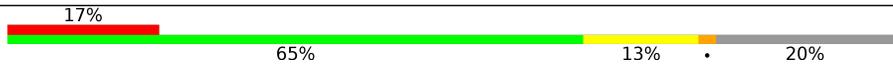
2 Entry composition ⓘ

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 3746	C 2389	N 663	O 675	S 19	0	0	0

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

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

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 2399	C 1503	N 431	O 450	S 15	0	0	0
3	E	354	Total 2694	C 1685	N 479	O 515	S 15	0	0	0

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

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

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

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

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

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

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

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

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

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

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

- Molecule 9 is ZINC ION (three-letter code: 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 ⓘ

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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
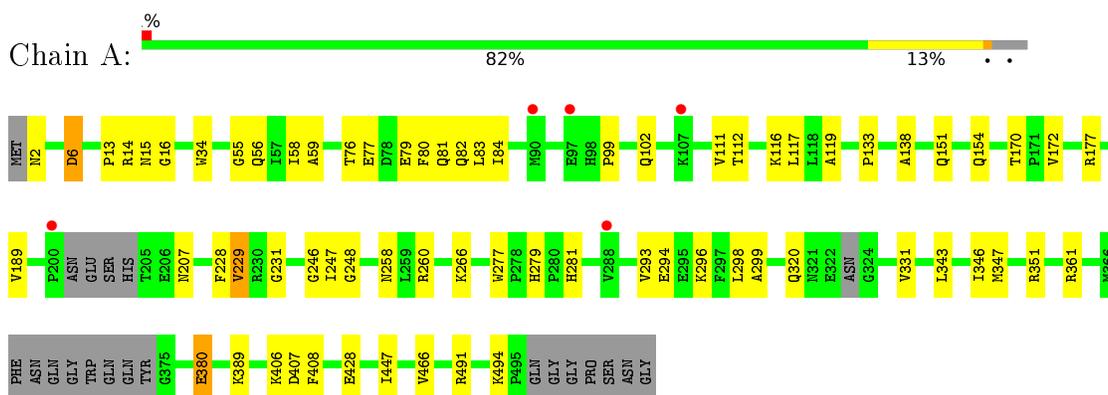
• Molecule 2: CRISPR system Cascade subunit CasB
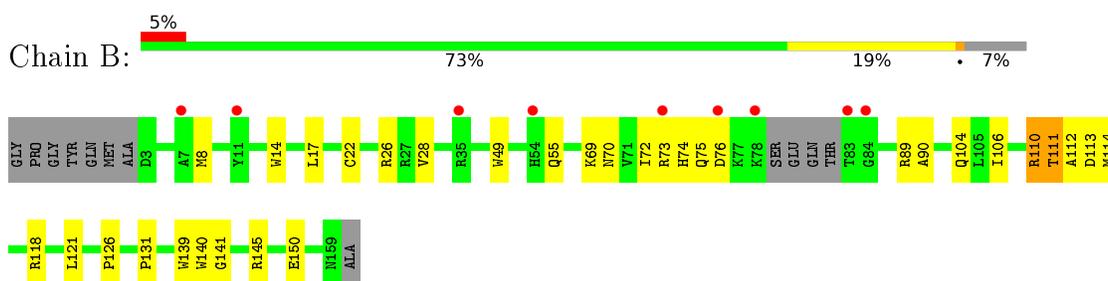
• Molecule 2: CRISPR system Cascade subunit CasB
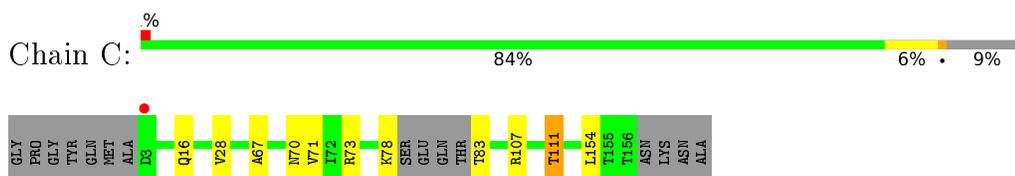

• Molecule 3: CRISPR system Cascade subunit CasC

• Molecule 3: CRISPR system Cascade subunit CasC

Chain E:

• Molecule 3: CRISPR system Cascade subunit CasC

Chain F:

• Molecule 3: CRISPR system Cascade subunit CasC

Chain G:


• Molecule 3: CRISPR system Cascade subunit CasC

Chain H:

• Molecule 3: CRISPR system Cascade subunit CasC

Chain I:
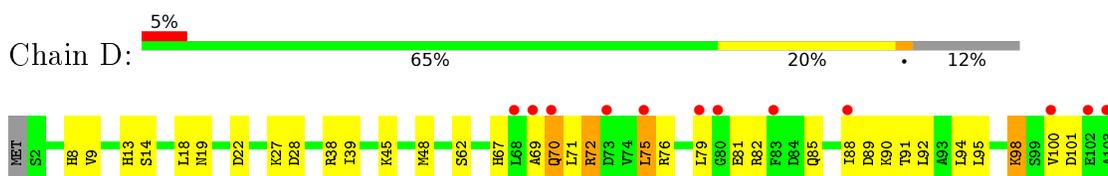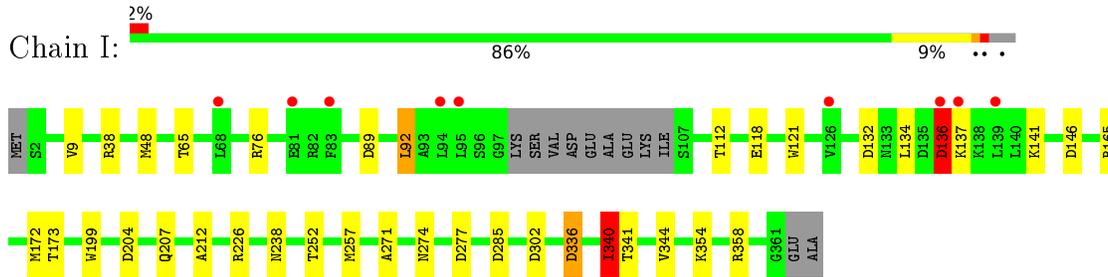
• Molecule 4: CRISPR system Cascade subunit CasD

Chain J:
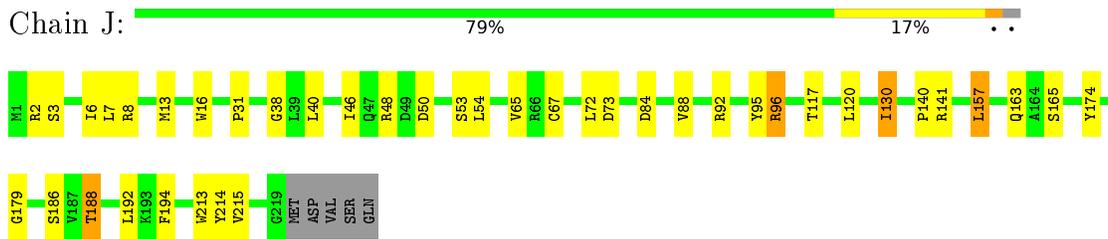
• Molecule 5: crRNA (61-MER)

Chain L:
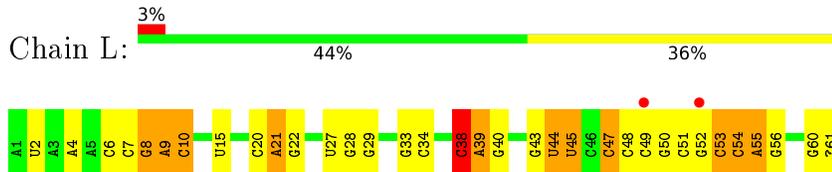
• Molecule 6: DNA (28-MER) Non-target

Chain M:
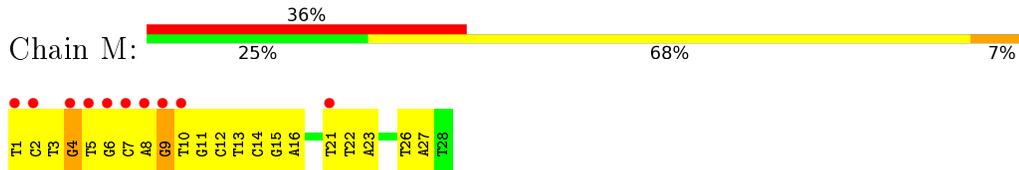
• Molecule 7: DNA (50-MER) Target

Chain N:
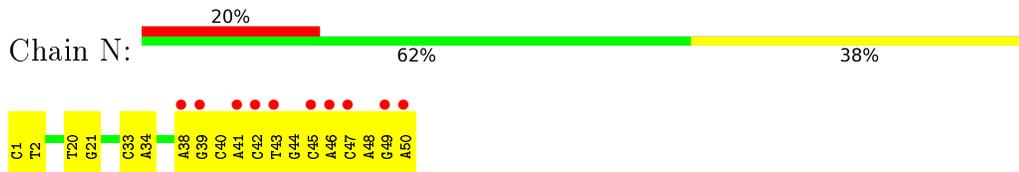
• Molecule 8: CRISPR system Cascade subunit CasE

Chain K:
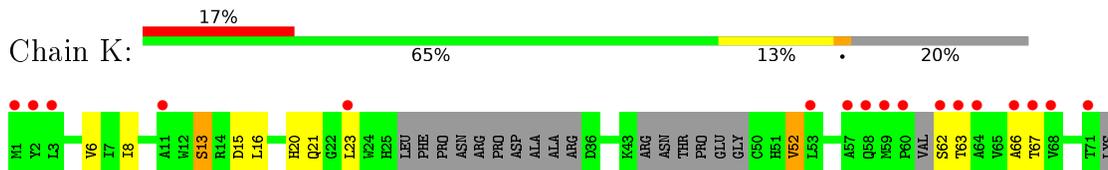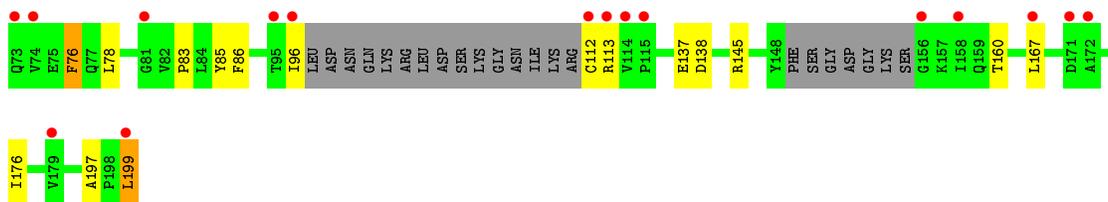
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	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
$< I/\sigma(I) >$ [1]	1.70 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.206 , 0.233 0.200 , 0.233	Depositor DCC
R_{free} test set	1875 reflections (0.98%)	DCC
Wilson B-factor (Å^2)	39.9	Xtriage
Anisotropy	0.225	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 28.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \lvert L \rvert > = 0.48, < L^2 > = 0.31$	Xtriage
Outliers	0 of 205381 reflections	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 2.21% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, 23G

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z|>5	RMSZ	#|Z|>5
1	A	0.28	0/3830	0.42	0/5200
2	B	0.42	0/1270	0.43	0/1717
2	C	0.28	0/1247	0.41	0/1686
3	D	0.26	0/2433	0.41	0/3286
3	E	0.27	0/2737	0.39	0/3702
3	F	0.29	0/2800	0.42	0/3790
3	G	0.29	0/2756	0.41	0/3721
3	H	0.29	0/2734	0.41	0/3697
3	I	0.33	0/2730	0.44	0/3693
4	J	0.37	0/1773	0.50	1/2407 (0.0%)
5	L	0.51	1/1423 (0.1%)	0.95	7/2216 (0.3%)
6	M	0.73	0/637	1.20	3/982 (0.3%)
7	N	0.76	0/1151	0.92	0/1773
8	K	0.23	0/1112	0.42	0/1521
All	All	0.36	1/28633 (0.0%)	0.53	11/39391 (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	-6.49	1.53	1.61

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	38	C	C2-N1-C1'	7.80	127.38	118.80
6	M	4	DG	O4'-C1'-N9	7.80	113.46	108.00
6	M	4	DG	OP1-P-O3'	7.72	122.18	105.20
5	L	38	C	N1-C2-O2	6.75	122.95	118.90
5	L	38	C	N3-C2-O2	-6.02	117.68	121.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3746	0	3735	37	0
2	B	1246	0	1235	17	0
2	C	1223	0	1214	4	0
3	D	2399	0	2350	49	0
3	E	2694	0	2629	32	0
3	F	2755	0	2692	31	0
3	G	2713	0	2674	24	0
3	H	2691	0	2627	25	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	14	0
9	A	1	0	0	0	0
10	A	133	0	0	6	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
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	336	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 6.

The worst 5 of 336 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

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	
1	A	473/502 (94%)	455 (96%)	17 (4%)	1 (0%)	52	64
2	B	149/165 (90%)	144 (97%)	3 (2%)	2 (1%)	15	15
2	C	146/165 (88%)	143 (98%)	2 (1%)	1 (1%)	26	32
3	D	310/363 (85%)	293 (94%)	16 (5%)	1 (0%)	46	57
3	E	350/363 (96%)	338 (97%)	11 (3%)	1 (0%)	46	57
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%)	30	35
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%)	46	57

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	111	THR
2	B	140	TRP
3	I	136	ASP
3	D	133	ASN
3	E	209	GLN

5.3.2 Protein sidechains (i)

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%)	390 (97%)	13 (3%)	46	63
2	B	129/141 (92%)	123 (95%)	6 (5%)	32	45
2	C	127/141 (90%)	122 (96%)	5 (4%)	39	54
3	D	246/298 (83%)	226 (92%)	20 (8%)	15	19
3	E	278/298 (93%)	262 (94%)	16 (6%)	25	34
3	F	287/298 (96%)	274 (96%)	13 (4%)	34	47
3	G	283/298 (95%)	276 (98%)	7 (2%)	55	72
3	H	280/298 (94%)	276 (99%)	4 (1%)	74	85
3	I	281/298 (94%)	272 (97%)	9 (3%)	46	63
4	J	186/192 (97%)	180 (97%)	6 (3%)	46	63
8	K	102/170 (60%)	91 (89%)	11 (11%)	8	8
All	All	2602/2858 (91%)	2492 (96%)	110 (4%)	36	51

5 of 110 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	E	182	MET
3	F	84	ASP
8	K	52	VAL
3	E	194	ASP
3	E	246	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 6 such sidechains are listed below:

Mol	Chain	Res	Type
3	E	207	GLN
3	F	346	GLN
3	F	331	GLN
3	D	234	GLN
3	F	343	GLN

5.3.3　RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	L	59/61 (96%)	21 (35%)	1 (1%)

5 of 21 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

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 (i)

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	19,29,30	1.15	2 (10%)	21,45,48	1.79	5 (23%)

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	-	0/3/35/36	0/4/4/4

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	61	23G	C5-C4	2.64	1.46	1.40
5	L	61	23G	C6-C5	3.08	1.47	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	61	23G	C5-C6-N1	-3.59	118.84	123.52
5	L	61	23G	C6-C5-C4	-2.52	117.98	120.86
5	L	61	23G	N3-C2-N1	-2.32	124.40	127.56
5	L	61	23G	C4'-O4'-C1'	2.49	112.28	109.64
5	L	61	23G	C6-N1-C2	4.18	120.78	115.88

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 carbohydrates 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 (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.08	5 (1%)	84	86	19, 48, 84, 110	0
2	B	153/165 (92%)	0.38	9 (5%)	26	28	33, 59, 87, 100	0
2	C	150/165 (90%)	-0.20	1 (0%)	89	90	19, 32, 56, 84	0
3	D	318/363 (87%)	0.36	19 (5%)	25	27	44, 67, 120, 164	0
3	E	354/363 (97%)	-0.08	0	100	100	33, 49, 75, 101	0
3	F	361/363 (99%)	-0.01	8 (2%)	65	68	22, 44, 74, 147	0
3	G	354/363 (97%)	-0.17	1 (0%)	94	95	19, 32, 55, 73	0
3	H	352/363 (96%)	-0.05	3 (0%)	85	87	16, 33, 79, 112	0
3	I	351/363 (96%)	-0.01	9 (2%)	59	62	18, 39, 89, 131	0
4	J	219/224 (97%)	-0.29	0	100	100	20, 37, 63, 77	0
5	L	60/61 (98%)	0.10	2 (3%)	50	53	20, 36, 130, 134	0
6	M	28/28 (100%)	1.74	10 (35%)	0	0	52, 110, 264, 267	0
7	N	50/50 (100%)	0.32	10 (20%)	1	1	22, 43, 257, 281	0
8	K	159/199 (79%)	1.06	33 (20%)	1	1	67, 93, 108, 125	0
All	All	3390/3572 (94%)	0.05	110 (3%)	51	54	16, 45, 99, 281	0

The worst 5 of 110 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
6	M	9	DG	8.2
8	K	158	ILE	6.9
3	I	137	LYS	5.7
6	M	8	DA	5.6
6	M	10	DT	5.5

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors($Å^2$)	Q<0.9
5	23G	L	61	26/27	0.73	0.17	-	98,123,163,171	0

6.3 Carbohydrates (i)

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors($Å^2$)	Q<0.9
9	ZN	A	601	1/1	0.97	0.10	-0.43	51,51,51,51	0

6.5 Other polymers (i)

There are no such residues in this entry.