wwPDB X-ray Structure Validation Summary Report (i)

Mar 21, 2016 – 02:07 PM EDT

PDB ID	:	5H9E
Title	:	Crystal structure of E. coli Cascade bound to a PAM-containing dsDNA target (32-nt spacer) at 3.20 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	:	3.21 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

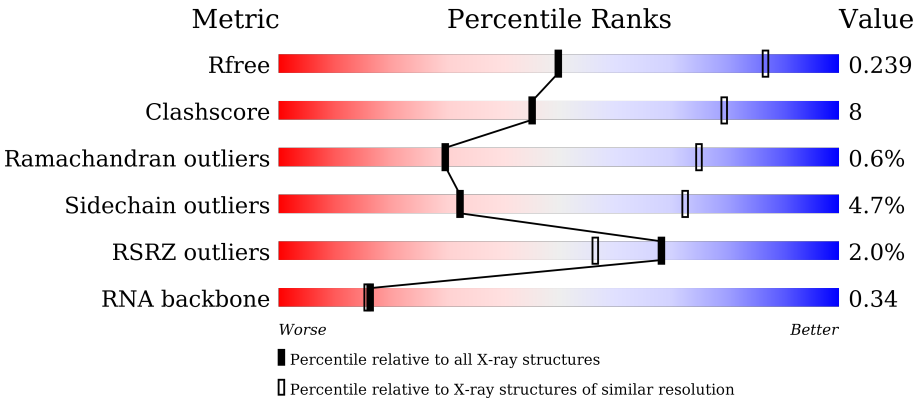
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20027107
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0122
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.21 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}	91344	1095 (3.26-3.18)
Clashscore	102246	1046 (3.24-3.20)
Ramachandran outliers	100387	1026 (3.24-3.20)
Sidechain outliers	100360	1025 (3.24-3.20)
RSRZ outliers	91569	1100 (3.26-3.18)
RNA backbone	2183	1004 (3.72-2.72)

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	76% 19%
2	B	182	2% 70% 12% 17%
2	C	182	70% 12% 18%
3	D	363	3% 67% 18% 12%

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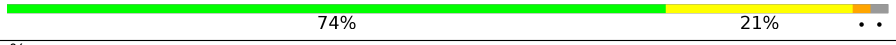
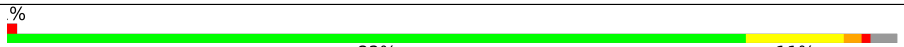
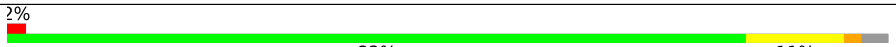
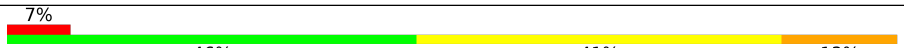
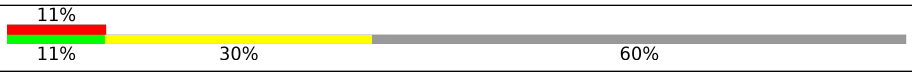
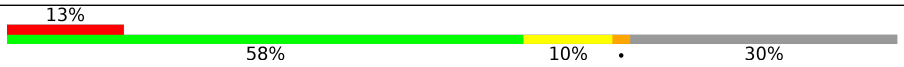
Mol	Chain	Length	Quality of chain
3	E	363	
3	F	363	
3	G	363	
3	H	363	
3	I	363	
4	J	224	
5	L	61	
6	M	47	
7	N	47	
8	K	199	

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 27217 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
			3728	2379	656	674	19			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	151	Total	C	N	O	S	0	0	0
			1216	765	234	210	7			
2	C	150	Total	C	N	O	S	0	0	0
			1219	767	230	215	7			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-21	MET	-	expression tag	UNP P76632
B	-20	ALA	-	expression tag	UNP P76632
B	-19	SER	-	expression tag	UNP P76632
B	-18	HIS	-	expression tag	UNP P76632
B	-17	HIS	-	expression tag	UNP P76632
B	-16	HIS	-	expression tag	UNP P76632
B	-15	HIS	-	expression tag	UNP P76632
B	-14	HIS	-	expression tag	UNP P76632
B	-13	HIS	-	expression tag	UNP P76632
B	-12	GLY	-	expression tag	UNP P76632
B	-11	ALA	-	expression tag	UNP P76632
B	-10	LEU	-	expression tag	UNP P76632
B	-9	GLU	-	expression tag	UNP P76632
B	-8	VAL	-	expression tag	UNP P76632
B	-7	LEU	-	expression tag	UNP P76632
B	-6	PHE	-	expression tag	UNP P76632
B	-5	GLN	-	expression tag	UNP P76632
B	-4	GLY	-	expression tag	UNP P76632

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Chain	Residue	Modelled	Actual	Comment	Reference
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	-21	MET	-	expression tag	UNP P76632
C	-20	ALA	-	expression tag	UNP P76632
C	-19	SER	-	expression tag	UNP P76632
C	-18	HIS	-	expression tag	UNP P76632
C	-17	HIS	-	expression tag	UNP P76632
C	-16	HIS	-	expression tag	UNP P76632
C	-15	HIS	-	expression tag	UNP P76632
C	-14	HIS	-	expression tag	UNP P76632
C	-13	HIS	-	expression tag	UNP P76632
C	-12	GLY	-	expression tag	UNP P76632
C	-11	ALA	-	expression tag	UNP P76632
C	-10	LEU	-	expression tag	UNP P76632
C	-9	GLU	-	expression tag	UNP P76632
C	-8	VAL	-	expression tag	UNP P76632
C	-7	LEU	-	expression tag	UNP P76632
C	-6	PHE	-	expression tag	UNP P76632
C	-5	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
			2356	1476	427	439	14			
3	E	354	Total	C	N	O	S	0	0	0
			2694	1685	479	515	15			
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
			2671	1669	474	513	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 (47-MER) Non-target.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	M	19	Total	C	N	O	P	0	0	0
			387	188	58	122	19			

- Molecule 7 is a DNA chain called DNA (47-MER) Target.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	N	40	Total	C	N	O	P	0	0	0
			820	389	154	237	40			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	K	139	Total	C	N	O	S	0	0	0
			935	597	156	176	6			

- Molecule 9 is ZINC ION (three-letter code: ZN) (formula: Zn).

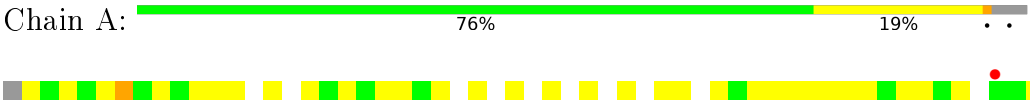
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Zn	0	0
			1	1		

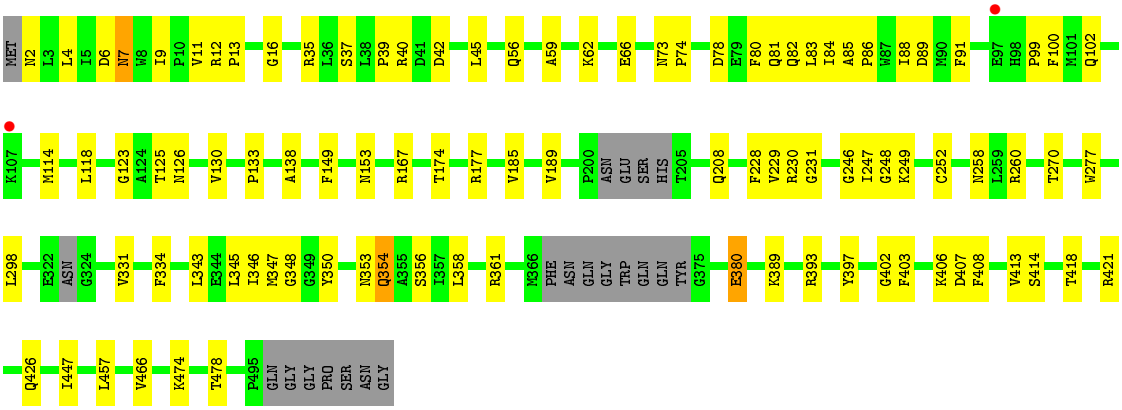
3 Residue-property plots (i)

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

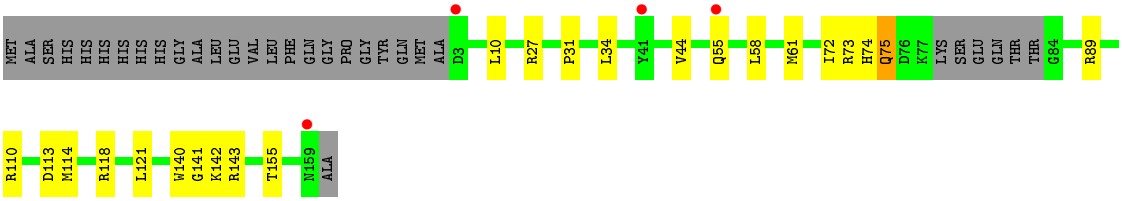
Chain A:





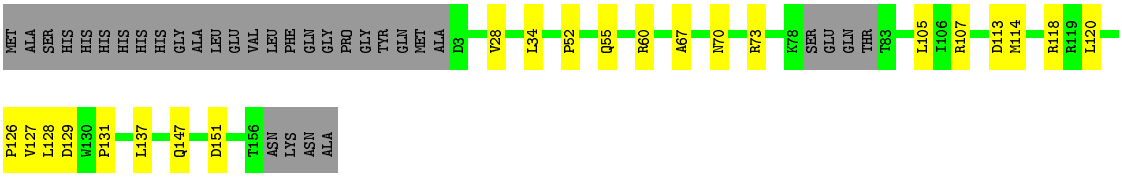
- Molecule 2: CRISPR system Cascade subunit CasB

Chain B:



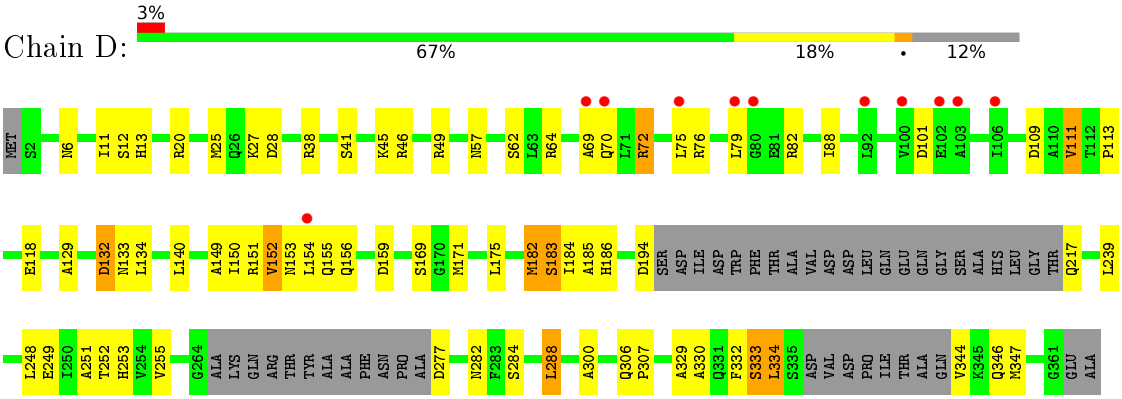
- Molecule 2: CRISPR system Cascade subunit CasB

Chain C:



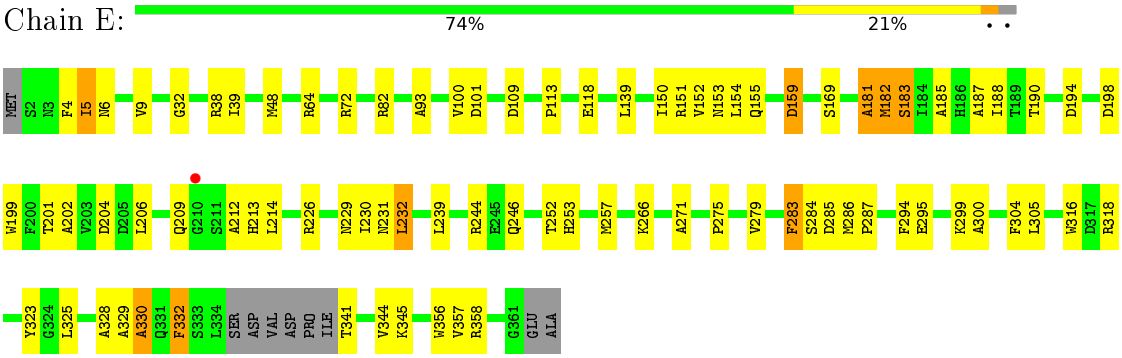
- Molecule 3: CRISPR system Cascade subunit CasC

Chain D:



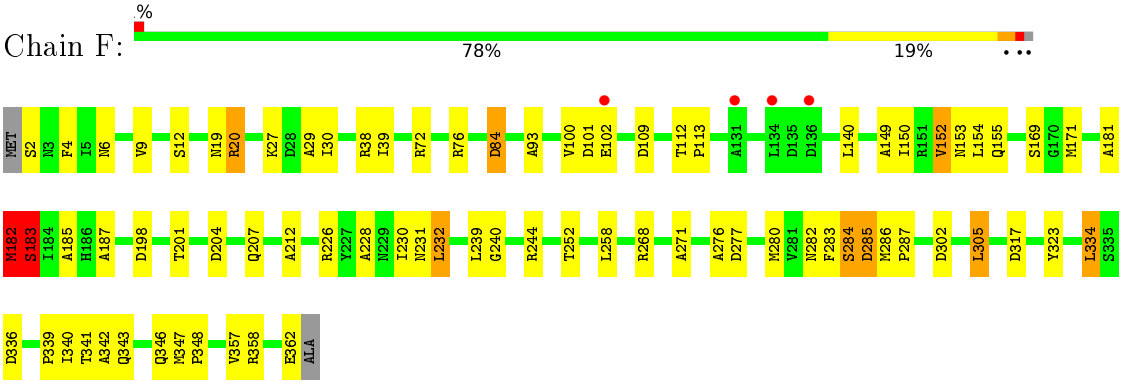
- Molecule 3: CRISPR system Cascade subunit CasC

Chain E:



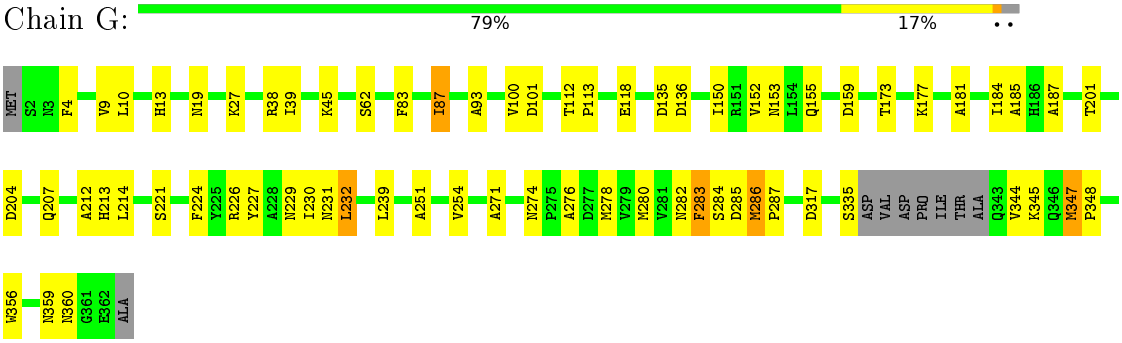
- Molecule 3: CRISPR system Cascade subunit CasC

Chain F:



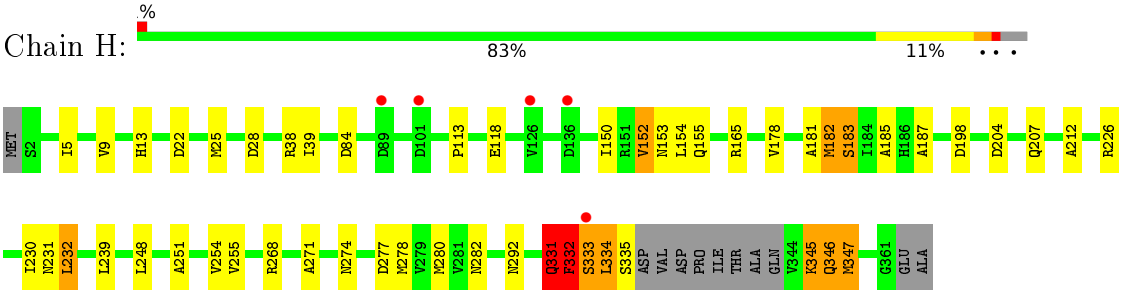
- Molecule 3: CRISPR system Cascade subunit CasC

Chain G:



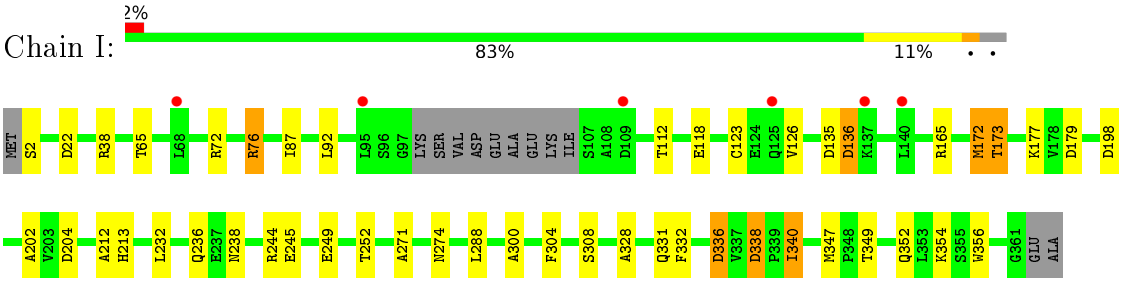
• Molecule 3: CRISPR system Cascade subunit CasC

Chain H:



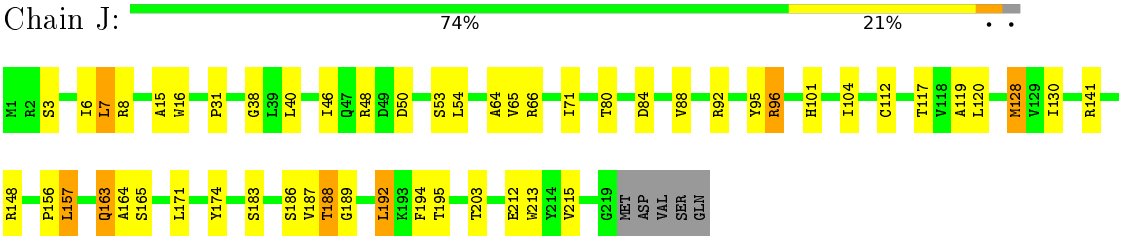
• Molecule 3: CRISPR system Cascade subunit CasC

Chain I:



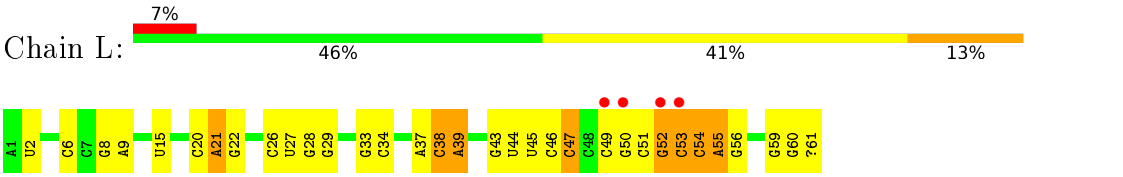
• Molecule 4: CRISPR system Cascade subunit CasD

Chain J:



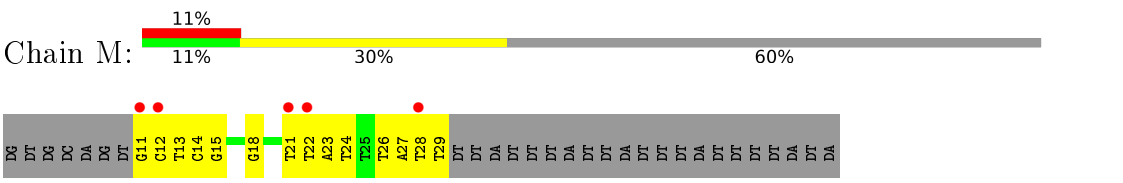
• Molecule 5: crRNA (61-MER)

Chain L:



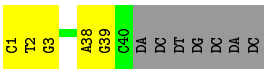
• Molecule 6: DNA (47-MER) Non-target

Chain M:



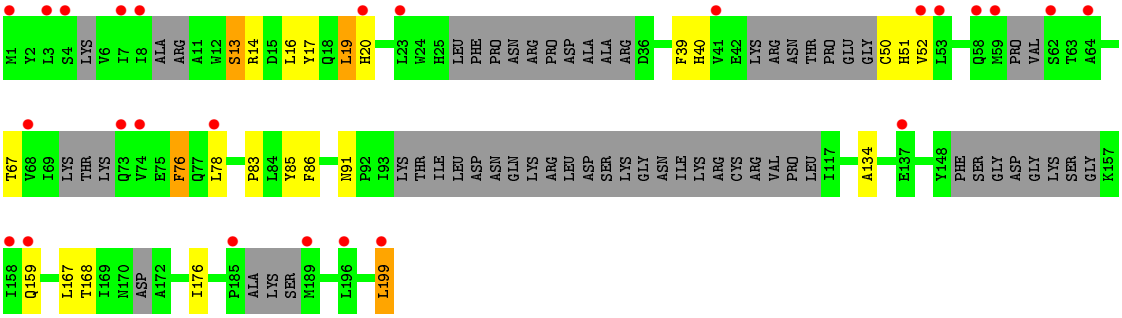
• Molecule 7: DNA (47-MER) Target

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	92.81Å 149.82Å 404.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.09 – 3.21 50.08 – 3.21	Depositor EDS
% Data completeness (in resolution range)	97.2 (50.09-3.21) 91.2 (50.08-3.21)	Depositor EDS
R_{merge}	0.27	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.03 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.209 , 0.247 0.210 , 0.239	Depositor DCC
R_{free} test set	1852 reflections (2.19%)	DCC
Wilson B-factor (Å^2)	49.5	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 17.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.28$	Xtriage
Outliers	1 of 90215 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	27217	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.43% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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	0.27	0/3811	0.46	0/5177
2	B	0.33	0/1240	0.43	0/1679
2	C	0.27	0/1243	0.43	0/1682
3	D	0.26	0/2390	0.42	0/3235
3	E	0.31	0/2737	0.51	1/3702 (0.0%)
3	F	0.31	0/2800	0.53	3/3790 (0.1%)
3	G	0.32	0/2756	0.47	1/3721 (0.0%)
3	H	0.41	2/2734 (0.1%)	0.71	13/3697 (0.4%)
3	I	0.29	0/2715	0.45	1/3676 (0.0%)
4	J	0.33	0/1773	0.52	0/2407
5	L	0.30	0/1423	0.93	6/2216 (0.3%)
6	M	0.74	1/430 (0.2%)	1.07	0/662
7	N	0.59	0/920	0.89	0/1417
8	K	0.22	0/940	0.48	0/1278
All	All	0.33	3/27912 (0.0%)	0.57	25/38339 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	E	0	1
3	H	0	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	M	26	DT	O3'-P	-6.63	1.53	1.61
3	H	345	LYS	C-O	6.48	1.35	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	333	SER	C-O	5.37	1.33	1.23

The worst 5 of 25 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	H	334	LEU	CA-CB-CG	15.85	151.76	115.30
3	F	182	MET	CA-CB-CG	8.32	127.44	113.30
3	E	232	LEU	CA-CB-CG	8.05	133.82	115.30
5	L	38	C	C2-N1-C1'	8.02	127.62	118.80
3	H	333	SER	O-C-N	7.85	135.26	122.70

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	E	181	ALA	Peptide
3	H	331	GLN	Peptide
3	H	332	PHE	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3728	0	3704	56	0
2	B	1216	0	1194	9	0
2	C	1219	0	1203	14	0
3	D	2356	0	2270	45	0
3	E	2694	0	2629	53	0
3	F	2755	0	2692	56	0
3	G	2713	0	2674	41	0
3	H	2691	0	2627	41	0
3	I	2671	0	2595	39	0
4	J	1731	0	1723	41	0
5	L	1300	0	659	26	0
6	M	387	0	221	19	0
7	N	820	0	449	4	0
8	K	935	0	832	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	1	0	0	0	0
All	All	27217	0	25472	407	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 8.

The worst 5 of 407 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)
3:I:172:MET:CE	4:J:96:ARG:HB3	1.60	1.32
8:K:13:SER:HG	8:K:50:CYS:N	1.34	1.25
3:I:172:MET:HE3	4:J:96:ARG:HB3	1.22	1.18
3:H:182:MET:HA	3:H:230:ILE:HA	1.29	1.14
5:L:52:G:N7	5:L:55:A:N6	2.00	1.09

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%)	446 (94%)	26 (6%)	1 (0%)	52 88
2	B	147/182 (81%)	137 (93%)	8 (5%)	2 (1%)	14 57
2	C	146/182 (80%)	141 (97%)	5 (3%)	0	100 100
3	D	310/363 (85%)	286 (92%)	21 (7%)	3 (1%)	19 64
3	E	350/363 (96%)	324 (93%)	21 (6%)	5 (1%)	14 57
3	F	359/363 (99%)	340 (95%)	17 (5%)	2 (1%)	30 75
3	G	350/363 (96%)	334 (95%)	16 (5%)	0	100 100
3	H	348/363 (96%)	332 (95%)	14 (4%)	2 (1%)	30 75

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	I	347/363 (96%)	334 (96%)	13 (4%)	0	100 100
4	J	217/224 (97%)	207 (95%)	9 (4%)	1 (0%)	34 77
8	K	117/199 (59%)	107 (92%)	7 (6%)	3 (3%)	7 40
All	All	3164/3467 (91%)	2988 (94%)	157 (5%)	19 (1%)	30 75

5 of 19 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	354	GLN
2	B	142	LYS
3	D	182	MET
3	D	183	SER
3	D	330	ALA

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	399/426 (94%)	384 (96%)	15 (4%)	40 77
2	B	123/155 (79%)	118 (96%)	5 (4%)	37 76
2	C	126/155 (81%)	126 (100%)	0	100 100
3	D	234/298 (78%)	216 (92%)	18 (8%)	16 54
3	E	278/298 (93%)	264 (95%)	14 (5%)	30 71
3	F	287/298 (96%)	269 (94%)	18 (6%)	22 63
3	G	283/298 (95%)	269 (95%)	14 (5%)	31 72
3	H	280/298 (94%)	272 (97%)	8 (3%)	50 82
3	I	277/298 (93%)	268 (97%)	9 (3%)	46 80
4	J	186/192 (97%)	176 (95%)	10 (5%)	27 69
8	K	82/170 (48%)	74 (90%)	8 (10%)	10 38
All	All	2555/2886 (88%)	2436 (95%)	119 (5%)	32 72

5 of 119 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	F	20	ARG
3	F	305	LEU
4	J	183	SER
3	F	152	VAL
3	F	277	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 7 such sidechains are listed below:

Mol	Chain	Res	Type
3	G	13	HIS
3	H	314	GLN
3	G	282	ASN
3	D	153	ASN
3	H	282	ASN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	L	59/61 (96%)	20 (33%)	1 (1%)

5 of 20 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	L	8	G
5	L	9	A
5	L	15	U
5	L	21	A
5	L	22	G

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	1.46	3 (15%)	21,45,48	2.85	8 (38%)

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 (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	61	23G	C4-N3	-2.35	1.32	1.35
5	L	61	23G	C5-C4	2.50	1.46	1.40
5	L	61	23G	C6-C5	3.64	1.48	1.41

The worst 5 of 8 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	61	23G	C5-C6-N1	-5.70	116.07	123.52
5	L	61	23G	C1'-N9-C4	-5.58	120.58	126.81
5	L	61	23G	C6-C5-C4	-3.31	117.07	120.86
5	L	61	23G	C4'-O4'-C1'	-2.78	106.70	109.64
5	L	61	23G	N3-C2-N1	-2.46	124.21	127.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	61	23G	4	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

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, 95^{th} 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%)	-0.23	2 (0%) 93 90	30, 53, 87, 112	0
2	B	151/182 (82%)	0.34	4 (2%) 59 47	39, 70, 102, 128	0
2	C	150/182 (82%)	-0.09	0 100 100	26, 43, 65, 94	0
3	D	318/363 (87%)	0.22	11 (3%) 48 34	66, 86, 118, 142	0
3	E	354/363 (97%)	-0.12	1 (0%) 94 93	41, 61, 88, 110	0
3	F	361/363 (99%)	-0.12	4 (1%) 82 73	35, 56, 84, 108	0
3	G	354/363 (97%)	-0.17	0 100 100	30, 45, 67, 86	0
3	H	352/363 (96%)	-0.16	5 (1%) 78 67	27, 46, 86, 109	0
3	I	351/363 (96%)	-0.21	6 (1%) 73 62	24, 44, 86, 114	0
4	J	219/224 (97%)	-0.43	0 100 100	27, 44, 72, 103	0
5	L	60/61 (98%)	0.40	4 (6%) 21 13	30, 51, 179, 191	0
6	M	19/47 (40%)	1.05	5 (26%) 1 1	59, 113, 169, 185	0
7	N	40/47 (85%)	-0.38	0 100 100	33, 43, 160, 203	0
8	K	139/199 (69%)	0.91	25 (17%) 2 1	82, 117, 153, 166	0
All	All	3349/3622 (92%)	-0.06	67 (2%) 68 56	24, 55, 110, 203	0

The worst 5 of 67 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
8	K	199	LEU	4.2
8	K	62	SER	3.8
8	K	158	ILE	3.7
6	M	21	DT	3.5
8	K	53	LEU	3.3

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, 95^{th} 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	0.76	0.26	-	86,134,211,233	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, 95^{th} 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	0.99	0.07	-	61,61,61,61	0

6.5 Other polymers (i)

There are no such residues in this entry.