wwPDB X-ray Structure Validation Summary Report (i)

Feb 1, 2016 – 08:44 PM GMT

PDB ID	:	4TVX
Title	:	Crystal structure of the E. coli CRISPR RNA-guided surveillance complex, Cascade
Authors	:	Jackson, R.N.; Golden, S.M.; Carter, J.; Wiedenheft, B.
Deposited on	:	2014-06-28
Resolution	:	3.24 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:

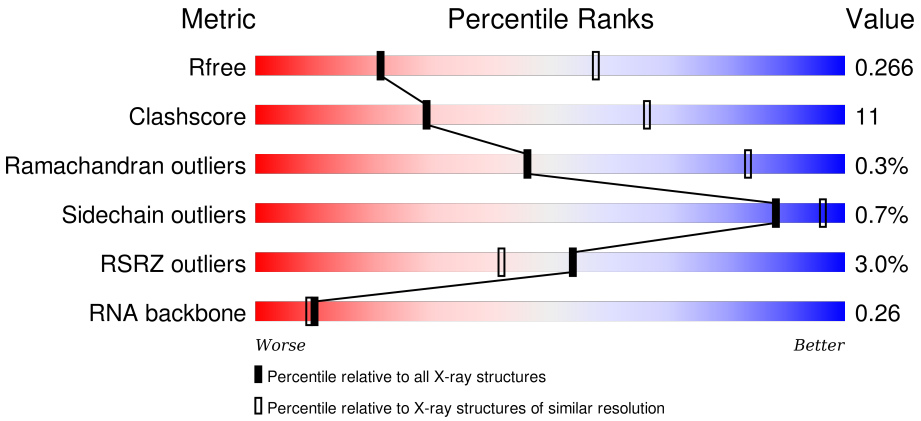
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

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 3.24 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	1092 (3.28-3.20)
Clashscore	102246	1227 (3.28-3.20)
Ramachandran outliers	100387	1204 (3.28-3.20)
Sidechain outliers	100360	1203 (3.28-3.20)
RSRZ outliers	91569	1097 (3.28-3.20)
RNA backbone	2183	1001 (3.74-2.74)

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	J	165	3% 70% 25% • 5%
1	K	165	3% 72% 24% 5%
1	V	165	5% 72% 22% 6%
1	W	165	2% 75% 20% 5%

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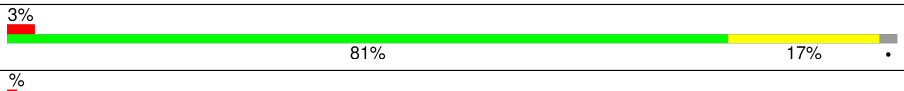
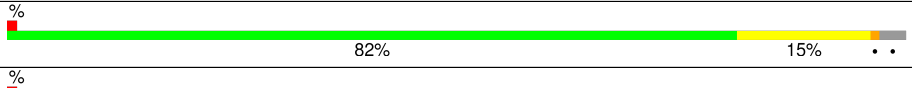
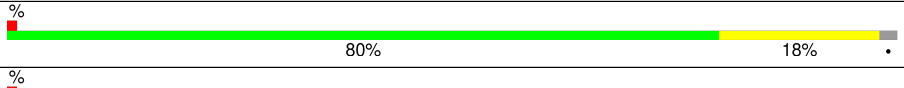
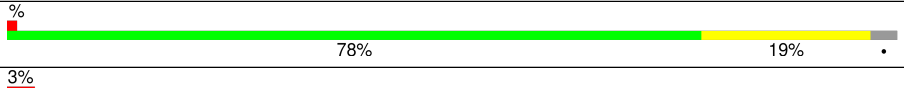
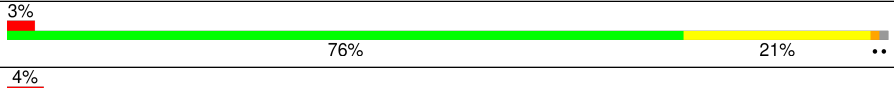
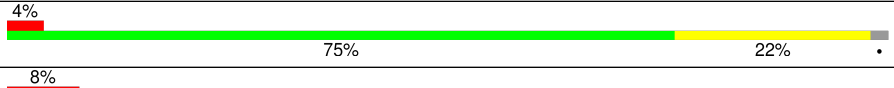
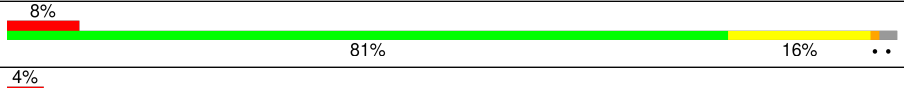
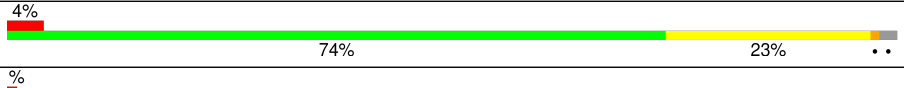
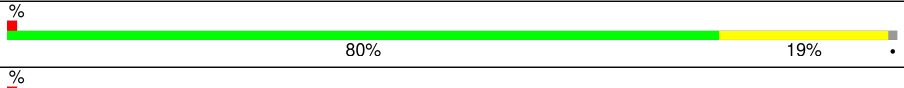
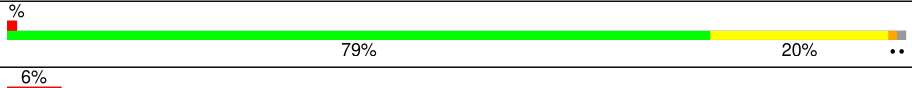
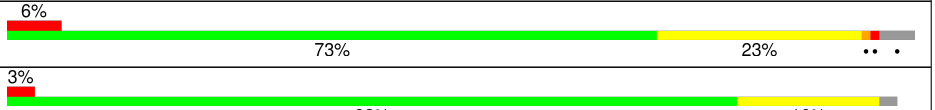
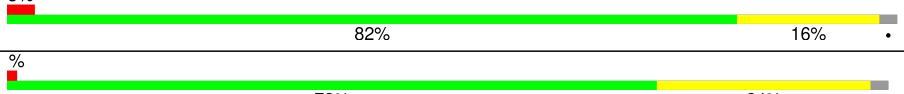
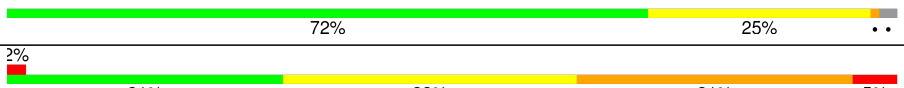
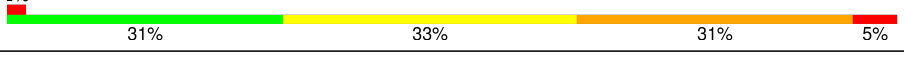
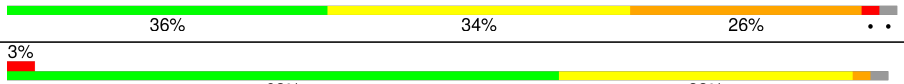
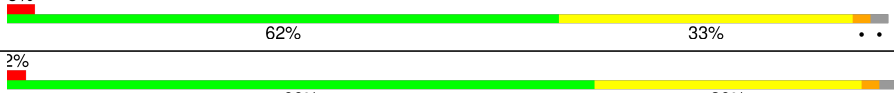
Mol	Chain	Length	Quality of chain
2	B	363	
2	C	363	
2	D	363	
2	E	363	
2	F	363	
2	G	363	
2	N	363	
2	O	363	
2	P	363	
2	Q	363	
2	R	363	
2	S	363	
3	A	199	
3	M	199	
4	H	224	
4	T	224	
5	L	61	
5	X	61	
6	I	502	
6	U	502	

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 103806 atoms, of which 50537 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 CasB.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	W	157	Total	C	H	N	O	S	0	0	0
			2522	795	1255	245	220	7			
1	V	155	Total	C	H	N	O	S	0	0	0
			2322	755	1132	218	210	7			
1	K	157	Total	C	H	N	O	S	0	0	0
			2524	795	1254	245	223	7			
1	J	157	Total	C	H	N	O	S	0	0	0
			2551	800	1280	248	216	7			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
W	-4	GLY	-	expression tag	UNP P76632
W	-3	PRO	-	expression tag	UNP P76632
W	-2	GLY	-	expression tag	UNP P76632
W	-1	TYR	-	expression tag	UNP P76632
W	0	GLN	-	expression tag	UNP P76632
V	-4	GLY	-	expression tag	UNP P76632
V	-3	PRO	-	expression tag	UNP P76632
V	-2	GLY	-	expression tag	UNP P76632
V	-1	TYR	-	expression tag	UNP P76632
V	0	GLN	-	expression tag	UNP P76632
K	-4	GLY	-	expression tag	UNP P76632
K	-3	PRO	-	expression tag	UNP P76632
K	-2	GLY	-	expression tag	UNP P76632
K	-1	TYR	-	expression tag	UNP P76632
K	0	GLN	-	expression tag	UNP P76632
J	-4	GLY	-	expression tag	UNP P76632
J	-3	PRO	-	expression tag	UNP P76632
J	-2	GLY	-	expression tag	UNP P76632
J	-1	TYR	-	expression tag	UNP P76632
J	0	GLN	-	expression tag	UNP P76632

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	F	356	Total	C	H	N	O	S	0	0	0
			5396	1702	2681	487	511	15			
2	D	356	Total	C	H	N	O	S	0	0	0
			5165	1660	2518	476	497	14			
2	E	351	Total	C	H	N	O	S	0	0	0
			5237	1664	2582	476	501	14			
2	C	347	Total	C	H	N	O	S	0	0	0
			5023	1610	2455	469	475	14			
2	B	345	Total	C	H	N	O	S	0	0	0
			4922	1590	2389	458	471	14			
2	G	353	Total	C	H	N	O	S	0	0	0
			5306	1681	2621	482	507	15			
2	R	359	Total	C	H	N	O	S	0	0	0
			5416	1714	2686	485	516	15			
2	P	354	Total	C	H	N	O	S	0	0	0
			5117	1644	2505	471	482	15			
2	Q	354	Total	C	H	N	O	S	0	0	0
			5148	1651	2519	469	494	15			
2	O	355	Total	C	H	N	O	S	0	0	0
			5123	1645	2500	471	493	14			
2	N	358	Total	C	H	N	O	S	0	0	0
			5229	1673	2561	479	502	14			
2	S	361	Total	C	H	N	O	S	0	0	0
			5412	1715	2677	490	515	15			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	A	192	Total	C	H	N	O	S	0	0	0
			2991	954	1506	262	262	7			
3	M	195	Total	C	H	N	O	S	0	1	0
			3057	971	1542	274	263	7			

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

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	H	219	Total	C	H	N	O	S	0	0	0
			3434	1093	1708	307	317	9			
4	T	219	Total	C	H	N	O	S	0	0	0
			3436	1093	1710	307	317	9			

- Molecule 5 is a RNA chain called Escherichia coli strain ECOR44 cluster 1 CRISPR region.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	L	61	Total	C	H	N	O	P	0	0	0
			1957	580	657	233	426	61			
5	X	60	Total	C	H	N	O	P	0	0	0
			1898	562	634	227	415	60			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	42	A	C	conflict	GB 50811866
L	53	C	U	conflict	GB 50811866
X	42	A	C	conflict	GB 50811866
X	53	C	U	conflict	GB 50811866

- Molecule 6 is a protein called CRISPR system Cascade subunit CasA.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
6	U	493	Total	C	H	N	O	S	0	0	0
			7393	2398	3633	668	675	19			
6	I	493	Total	C	H	N	O	S	0	0	0
			7225	2356	3532	658	660	19			

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

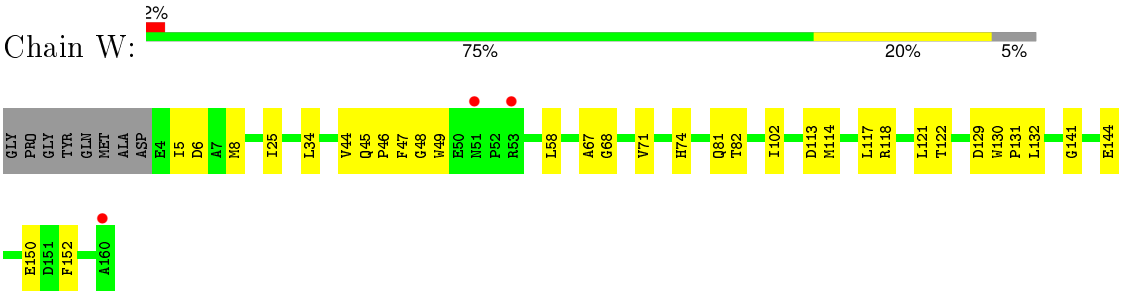
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	I	1	Total	Zn	0	0
			1	1		
7	U	1	Total	Zn	0	0
			1	1		

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.

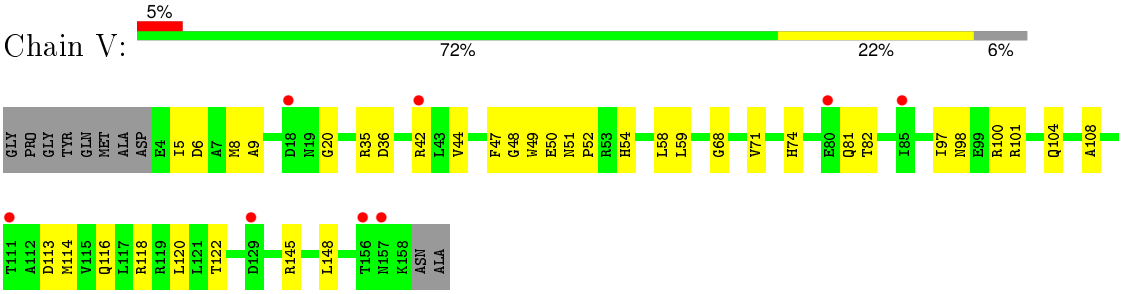
- Molecule 1: CRISPR system Cascade subunit CasB

Chain W:



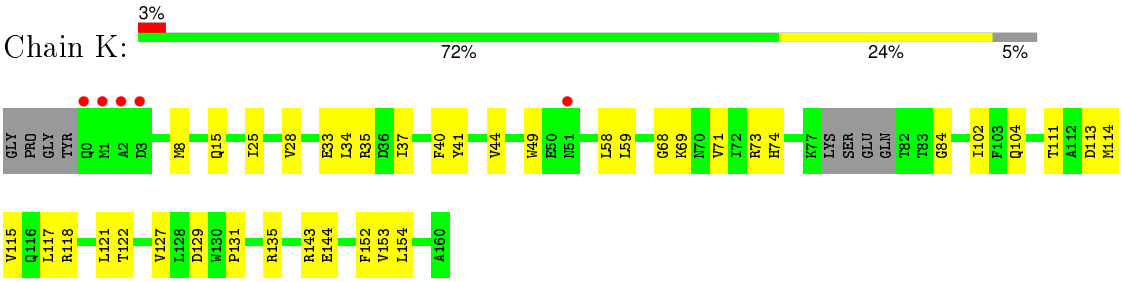
- Molecule 1: CRISPR system Cascade subunit CasB

Chain V:



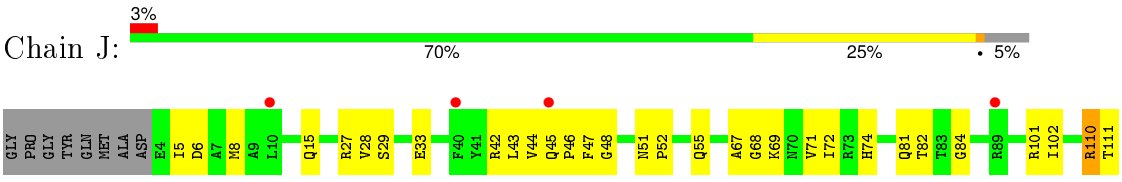
- Molecule 1: CRISPR system Cascade subunit CasB

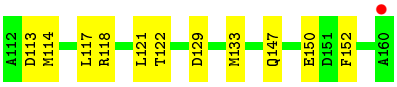
Chain K:



- Molecule 1: CRISPR system Cascade subunit CasB

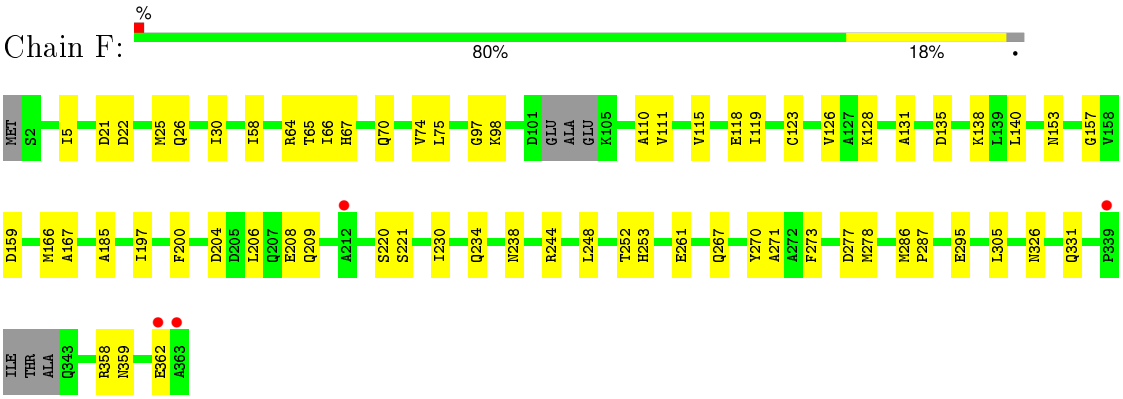
Chain J:





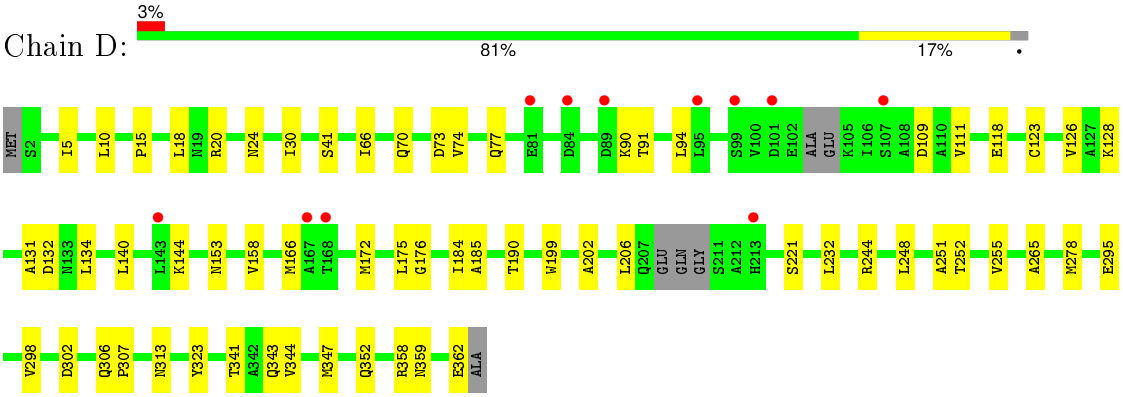
• Molecule 2: CRISPR system Cascade subunit CasC

Chain F:



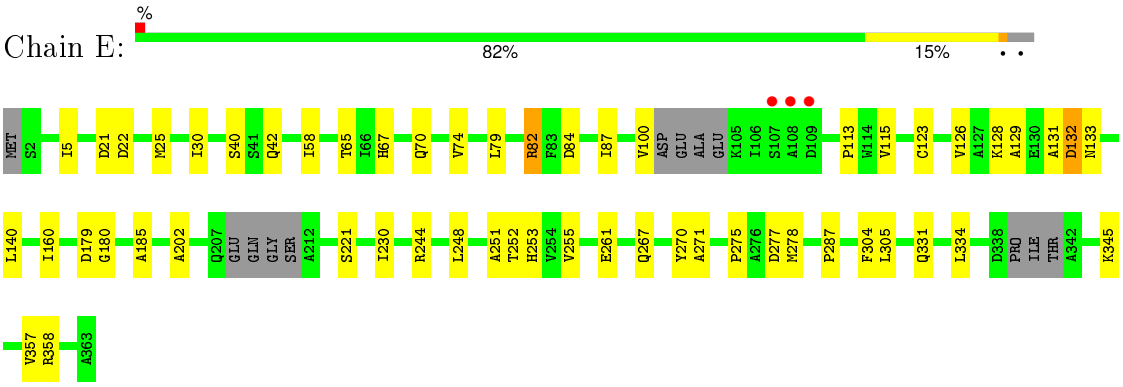
• Molecule 2: CRISPR system Cascade subunit CasC

Chain D:



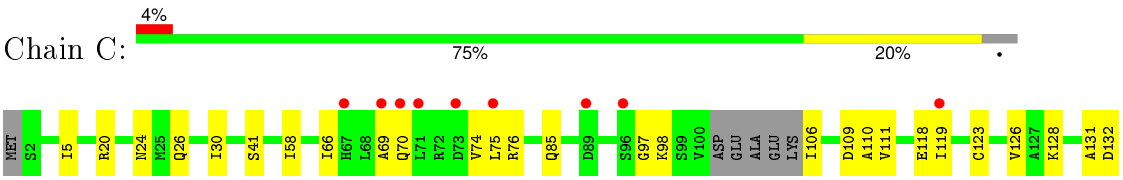
• Molecule 2: CRISPR system Cascade subunit CasC

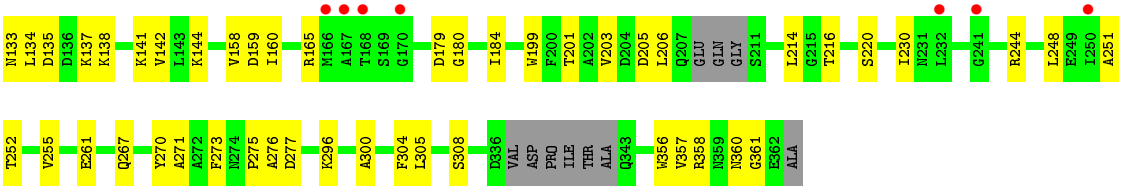
Chain E:



• Molecule 2: CRISPR system Cascade subunit CasC

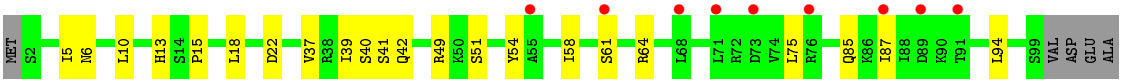
Chain C:

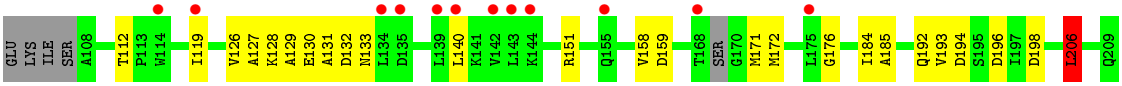


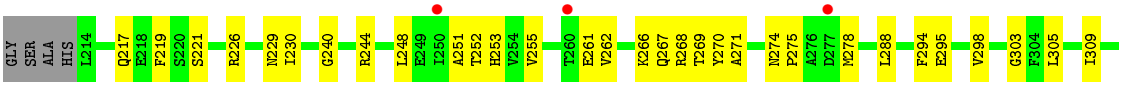


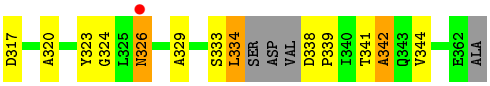
• Molecule 2: CRISPR system Cascade subunit CasC

Chain B:



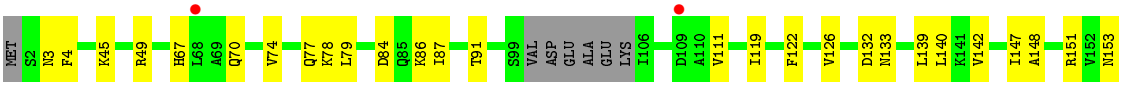


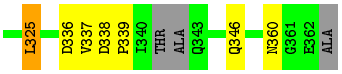




• Molecule 2: CRISPR system Cascade subunit CasC

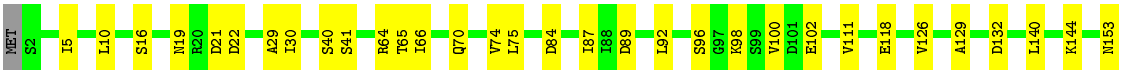
Chain G:

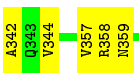




• Molecule 2: CRISPR system Cascade subunit CasC

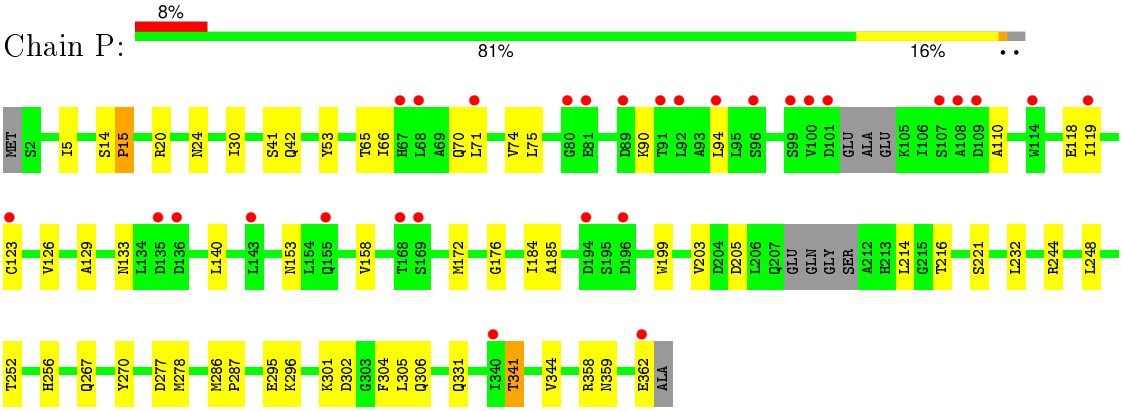
Chain R:





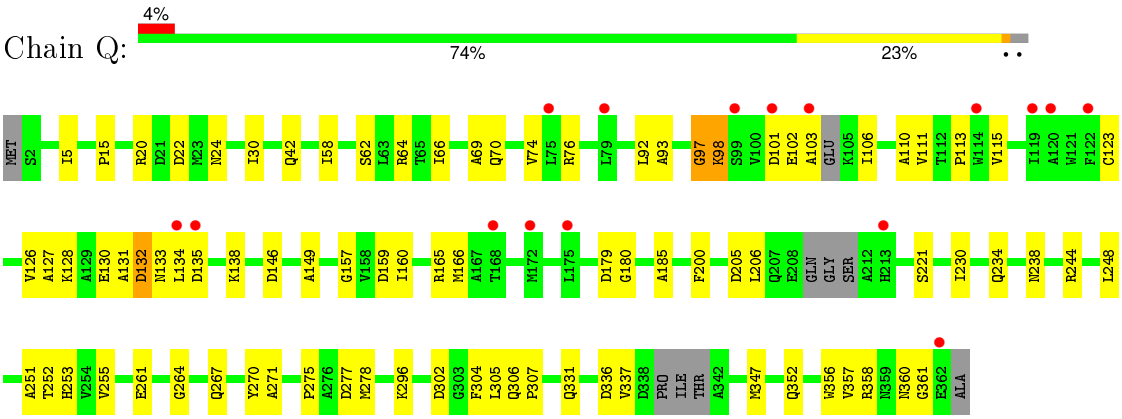
• Molecule 2: CRISPR system Cascade subunit CasC

Chain P:



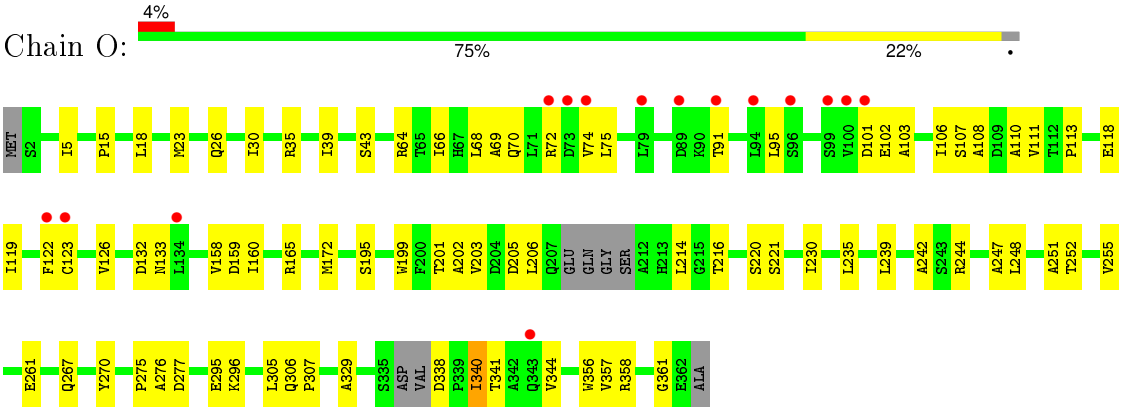
• Molecule 2: CRISPR system Cascade subunit CasC

Chain Q:



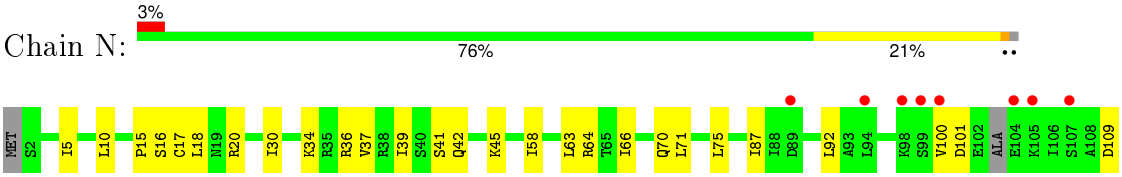
• Molecule 2: CRISPR system Cascade subunit CasC

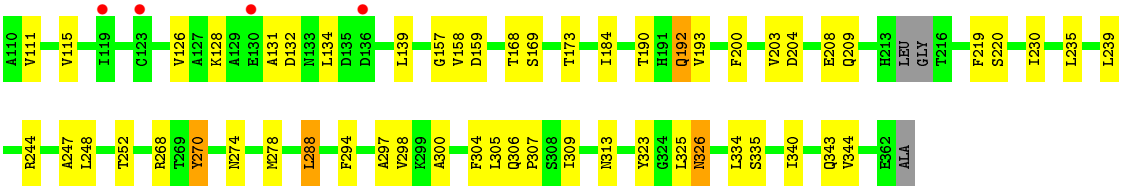
Chain O:



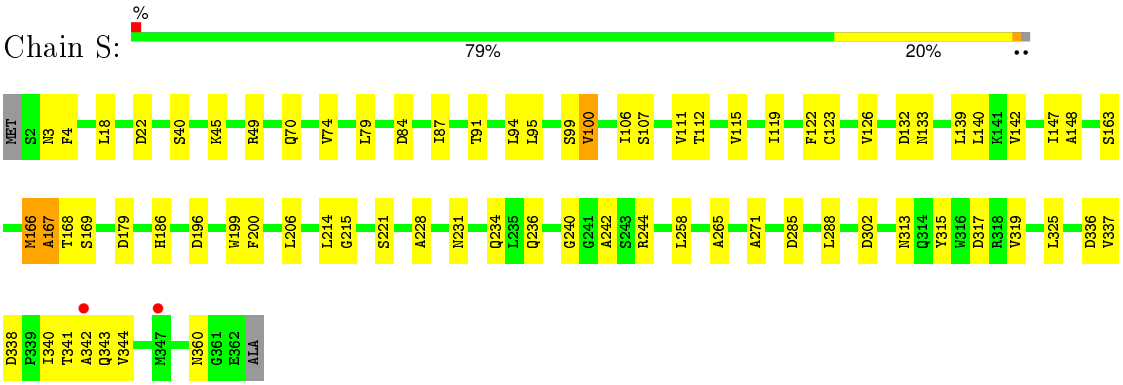
• Molecule 2: CRISPR system Cascade subunit CasC

Chain N:

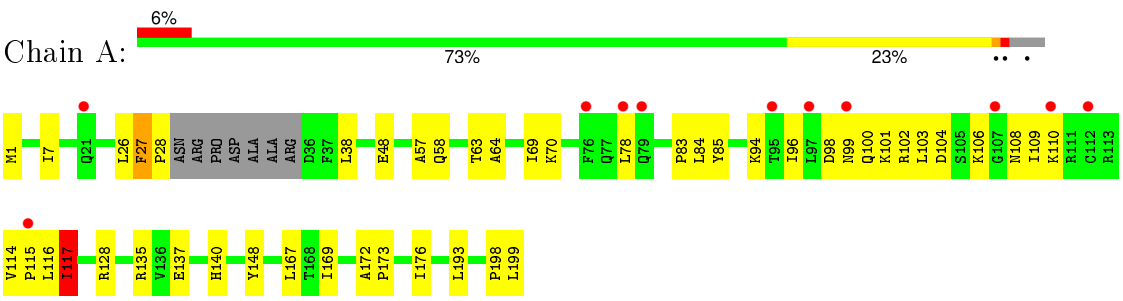




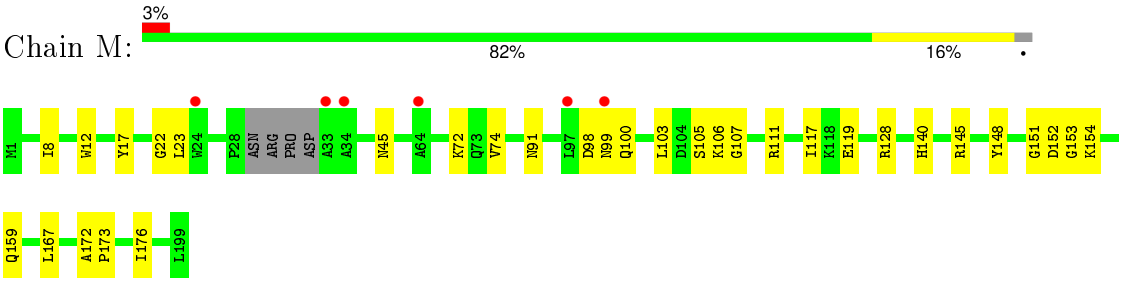
• Molecule 2: CRISPR system Cascade subunit CasC



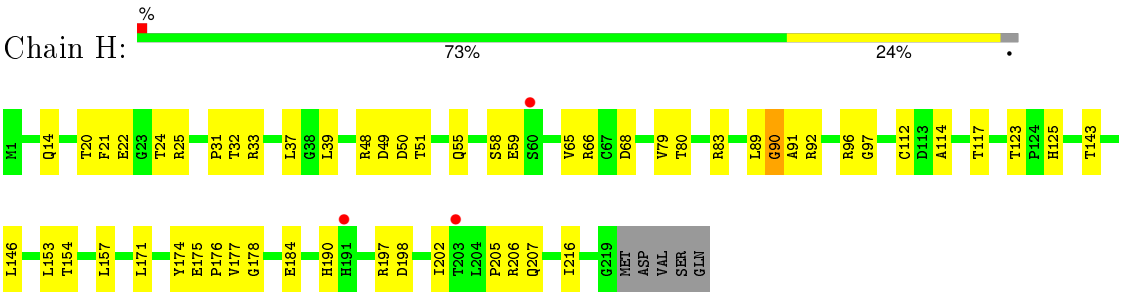
• Molecule 3: CRISPR system Cascade subunit CasE



• Molecule 3: CRISPR system Cascade subunit CasE

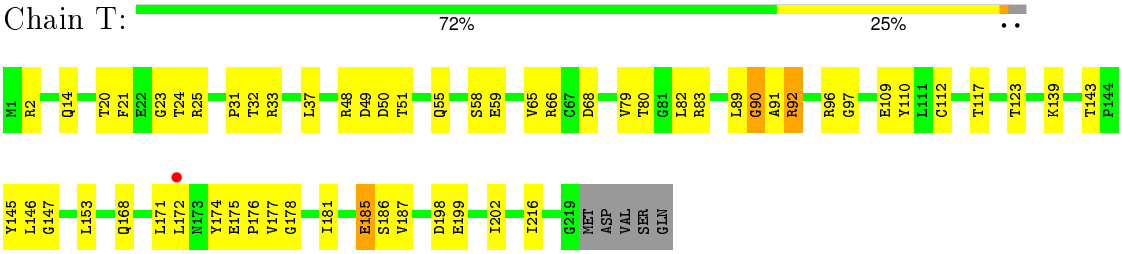


• Molecule 4: CRISPR system Cascade subunit CasD



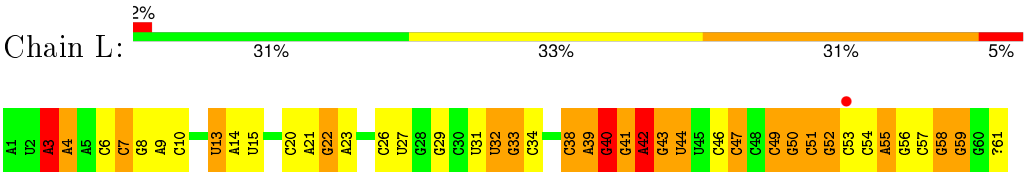
• Molecule 4: CRISPR system Cascade subunit CasD

Chain T:



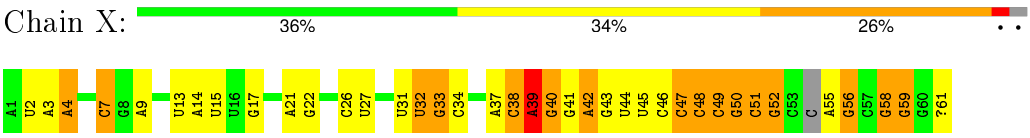
• Molecule 5: Escherichia coli strain ECOR44 cluster 1 CRISPR region

Chain L:



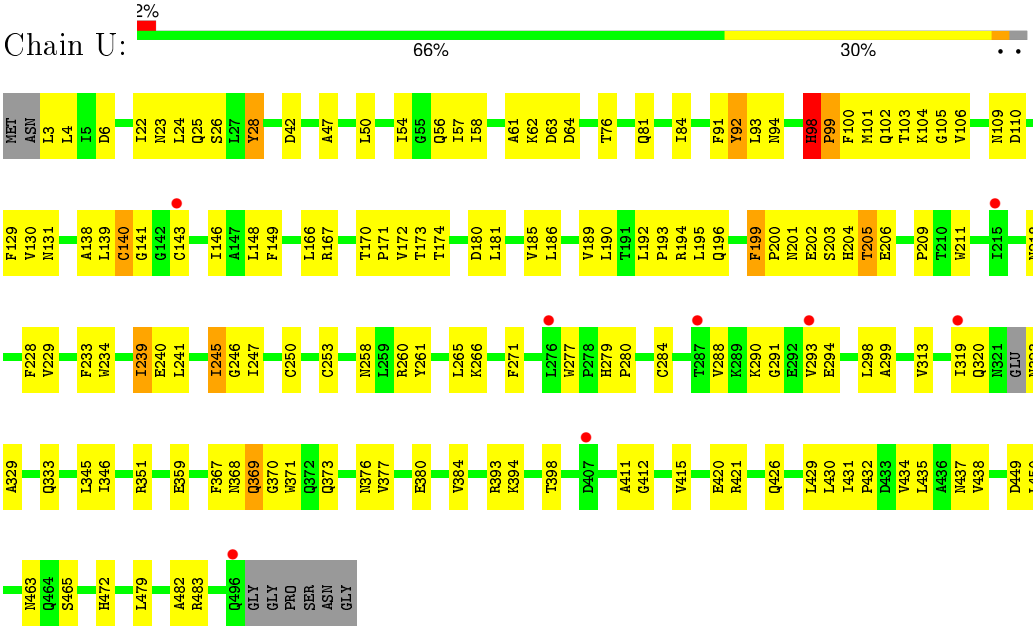
• Molecule 5: Escherichia coli strain ECOR44 cluster 1 CRISPR region

Chain X:



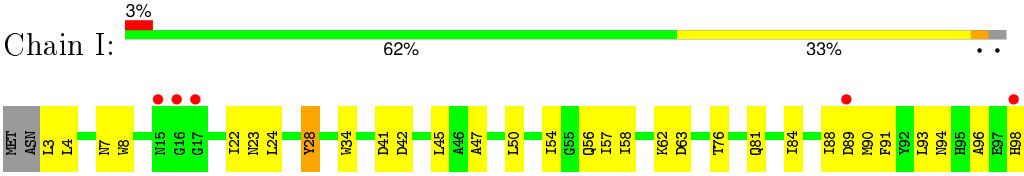
• Molecule 6: CRISPR system Cascade subunit CasA

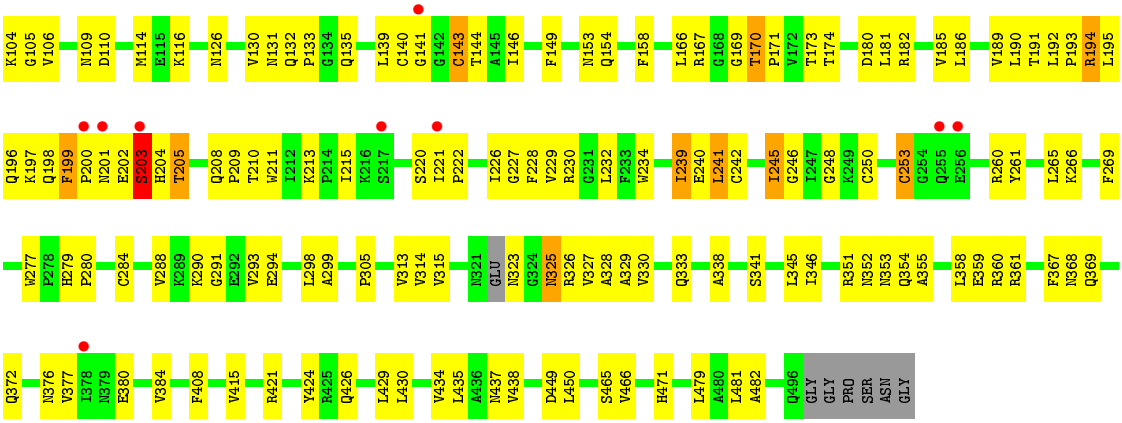
Chain U:



• Molecule 6: CRISPR system Cascade subunit CasA

Chain I:




K104 G105 V106 N109 D110 M114 E115 K116 N126 V130 N131 Q132 P133 G134 Q135 L139 C140 G141 G142 C143 T144 A145 I146 F149 N153 Q154 F158 L166 R167 G168 G169 T170 P171 V172 T173 T174 D180 L181 R182 V185 L186 V189 L190 T191 L192 P193 R194 L195
Q196 K197 Q198 F199 P200 N201 E202 S203 H204 T205 Q208 P209 T210 W211 I212 K213 P214 I215 K216 S217 S220 I221 P222 I226 G227 F228 V229 R230 G231 L232 F233 W234 I239 E240 L241 C242 I245 G246 I247 G248 K249 C250 C253 G254 Q255 E256 R260 Y261 L265 K266 F269
W277 P278 H279 P280 C284 V288 K289 K290 G291 E292 V293 E294 L298 A299 P305 V313 V314 V315 N321 GLU N323 G324 N325 R326 V327 A328 A329 V330 Q333 A338 S341 L345 I346 R351 N352 N353 Q354 A355 L358 E359 R360 R361 F367 N368 Q369
Q372 N376 V377 I378 N379 E380 V384 F408 V415 R421 Y424 R425 Q426 L429 L430 V434 L435 A436 N437 V438 D449 L450 S465 V466 H471 L479 A480 L481 A482 Q496 GLY GLY PRO SER ASN GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	200.85Å 214.54Å 217.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.61 – 3.24 39.61 – 3.24	Depositor EDS
% Data completeness (in resolution range)	99.8 (39.61-3.24) 96.1 (39.61-3.24)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.67 (at 3.25Å)	Xtriage
Refinement program	PHENIX (phenix.refine: dev_1760)	Depositor
R, R_{free}	0.234 , 0.268 0.239 , 0.266	Depositor DCC
R_{free} test set	2034 reflections (1.44%)	DCC
Wilson B-factor (Å^2)	75.0	Xtriage
Anisotropy	0.390	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.2	EDS
Estimated twinning fraction	0.017 for -h,l,k	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 148829 reflections	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	103806	wwPDB-VP
Average B, all atoms (Å^2)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.64% 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	J	0.28	0/1296	0.53	0/1751
1	K	0.29	0/1294	0.55	0/1751
1	V	0.28	0/1215	0.55	0/1656
1	W	0.27	0/1292	0.55	0/1749
2	B	0.31	0/2573	0.65	2/3491 (0.1%)
2	C	0.30	0/2608	0.59	0/3530
2	D	0.29	0/2690	0.58	0/3649
2	E	0.31	0/2696	0.58	2/3648 (0.1%)
2	F	0.31	0/2757	0.59	0/3723
2	G	0.32	0/2728	0.65	2/3687 (0.1%)
2	N	0.30	0/2711	0.63	0/3676
2	O	0.34	1/2665 (0.0%)	0.60	0/3617
2	P	0.29	0/2654	0.58	0/3601
2	Q	0.30	0/2670	0.59	2/3618 (0.1%)
2	R	0.31	0/2773	0.60	0/3747
2	S	0.32	0/2780	0.64	0/3763
3	A	0.28	0/1516	0.55	0/2056
3	M	0.28	0/1549	0.56	0/2100
4	H	0.28	0/1768	0.58	1/2402 (0.0%)
4	T	0.27	0/1768	0.57	1/2402 (0.0%)
5	L	0.38	0/1423	1.02	4/2216 (0.2%)
5	X	0.39	0/1382	1.04	2/2151 (0.1%)
6	I	0.33	0/3782	0.65	2/5159 (0.0%)
6	U	0.37	0/3851	0.66	0/5244
All	All	0.31	1/54441 (0.0%)	0.64	18/74387 (0.0%)

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
2	B	0	3
2	E	0	1
2	F	0	1
2	G	0	1
2	N	0	1
2	P	0	1
2	Q	0	2
2	R	0	2
2	S	0	3
3	A	0	1
4	H	0	2
4	T	0	3
6	I	0	3
6	U	0	7
All	All	0	31

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	102	GLU	CB-CG	6.10	1.63	1.52

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	I	194	ARG	NE-CZ-NH1	8.31	124.46	120.30
2	G	86	LYS	CD-CE-NZ	-7.60	94.22	111.70
2	E	82	ARG	NE-CZ-NH1	7.44	124.02	120.30
6	I	194	ARG	NE-CZ-NH2	-6.94	116.83	120.30
2	Q	97	GLY	N-CA-C	-5.96	98.21	113.10

There are no chirality outliers.

5 of 31 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	206	LEU	Peptide
2	B	221	SER	Peptide
2	B	342	ALA	Peptide
2	E	132	ASP	Peptide
2	F	326	ASN	Peptide

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	J	1271	1280	1280	30	0
1	K	1270	1254	1257	25	0
1	V	1190	1132	1131	29	0
1	W	1267	1255	1255	22	0
2	B	2533	2389	2389	74	0
2	C	2568	2455	2455	59	0
2	D	2647	2518	2518	47	0
2	E	2655	2582	2582	48	0
2	F	2715	2681	2681	56	0
2	G	2685	2621	2621	52	0
2	N	2668	2561	2561	72	0
2	O	2623	2500	2500	65	0
2	P	2612	2505	2505	47	0
2	Q	2629	2519	2519	63	0
2	R	2730	2686	2685	57	0
2	S	2735	2677	2677	69	0
3	A	1485	1506	1505	36	0
3	M	1515	1542	1541	30	0
4	H	1726	1708	1708	40	0
4	T	1726	1710	1710	43	0
5	L	1300	657	656	39	0
5	X	1264	634	633	35	0
6	I	3693	3532	3533	155	0
6	U	3760	3633	3634	136	0
7	I	1	0	0	0	0
7	U	1	0	0	0	0
All	All	53269	50537	50536	1183	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 11.

The worst 5 of 1183 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:73:ASP:OD1	2:D:77:GLN:NE2	1.90	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:52:G:N7	5:L:55:A:N6	2.06	1.03
6:U:202:GLU:O	6:U:205:THR:OG1	1.84	0.94
2:B:58:ILE:HG22	2:B:158:VAL:HG11	1.51	0.92
2:S:244:ARG:NH1	2:S:360:ASN:OD1	2.01	0.92

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	J	155/165 (94%)	154 (99%)	1 (1%)	0	100	100
1	K	153/165 (93%)	151 (99%)	2 (1%)	0	100	100
1	V	153/165 (93%)	152 (99%)	1 (1%)	0	100	100
1	W	155/165 (94%)	153 (99%)	2 (1%)	0	100	100
2	B	335/363 (92%)	315 (94%)	18 (5%)	2 (1%)	30	73
2	C	339/363 (93%)	323 (95%)	16 (5%)	0	100	100
2	D	350/363 (96%)	327 (93%)	20 (6%)	3 (1%)	21	65
2	E	343/363 (94%)	328 (96%)	15 (4%)	0	100	100
2	F	350/363 (96%)	330 (94%)	20 (6%)	0	100	100
2	G	347/363 (96%)	322 (93%)	25 (7%)	0	100	100
2	N	352/363 (97%)	333 (95%)	18 (5%)	1 (0%)	46	83
2	O	349/363 (96%)	325 (93%)	19 (5%)	5 (1%)	14	55
2	P	348/363 (96%)	332 (95%)	14 (4%)	2 (1%)	30	73
2	Q	346/363 (95%)	329 (95%)	15 (4%)	2 (1%)	30	73
2	R	353/363 (97%)	336 (95%)	16 (4%)	1 (0%)	46	83
2	S	359/363 (99%)	336 (94%)	22 (6%)	1 (0%)	46	83

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	A	188/199 (94%)	182 (97%)	4 (2%)	2 (1%)	17 60
3	M	192/199 (96%)	186 (97%)	6 (3%)	0	100 100
4	H	217/224 (97%)	208 (96%)	9 (4%)	0	100 100
4	T	217/224 (97%)	209 (96%)	8 (4%)	0	100 100
6	I	489/502 (97%)	460 (94%)	28 (6%)	1 (0%)	52 87
6	U	489/502 (97%)	458 (94%)	30 (6%)	1 (0%)	52 87
All	All	6579/6866 (96%)	6249 (95%)	309 (5%)	21 (0%)	46 83

5 of 21 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	117	ILE
2	S	100	VAL
6	I	170	THR
2	D	343	GLN
2	N	343	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	J	130/141 (92%)	128 (98%)	2 (2%)	72 90
1	K	130/141 (92%)	130 (100%)	0	100 100
1	V	115/141 (82%)	115 (100%)	0	100 100
1	W	129/141 (92%)	129 (100%)	0	100 100
2	B	243/298 (82%)	240 (99%)	3 (1%)	78 92
2	C	249/298 (84%)	248 (100%)	1 (0%)	93 98
2	D	259/298 (87%)	259 (100%)	0	100 100
2	E	271/298 (91%)	271 (100%)	0	100 100
2	F	282/298 (95%)	282 (100%)	0	100 100
2	G	277/298 (93%)	274 (99%)	3 (1%)	80 93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	N	266/298 (89%)	263 (99%)	3 (1%)	80 93
2	O	257/298 (86%)	257 (100%)	0	100 100
2	P	254/298 (85%)	254 (100%)	0	100 100
2	Q	260/298 (87%)	260 (100%)	0	100 100
2	R	282/298 (95%)	282 (100%)	0	100 100
2	S	280/298 (94%)	280 (100%)	0	100 100
3	A	158/170 (93%)	157 (99%)	1 (1%)	90 96
3	M	159/170 (94%)	159 (100%)	0	100 100
4	H	185/192 (96%)	185 (100%)	0	100 100
4	T	185/192 (96%)	184 (100%)	1 (0%)	92 97
6	I	371/426 (87%)	360 (97%)	11 (3%)	48 81
6	U	386/426 (91%)	376 (97%)	10 (3%)	54 83
All	All	5128/5716 (90%)	5093 (99%)	35 (1%)	88 96

5 of 35 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
6	U	92	TYR
6	U	204	HIS
6	I	241	LEU
6	U	140	CYS
6	U	143	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	292	ASN
2	B	209	GLN
2	G	153	ASN
2	N	331	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	L	59/61 (96%)	33 (55%)	3 (5%)
5	X	56/61 (91%)	28 (50%)	1 (1%)

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Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
All	All	115/122 (94%)	61 (53%)	4 (3%)

5 of 61 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	L	3	A
5	L	4	A
5	L	7	C
5	L	9	A
5	L	13	U

All (4) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	L	9	A
5	L	40	G
5	L	42	A
5	X	9	A

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

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

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	23G	L	61	5	18,29,30	6.73	12 (66%)	19,45,48	2.63	7 (36%)
5	23G	X	61	5	18,29,30	6.84	12 (66%)	19,45,48	2.60	8 (42%)

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
5	23G	X	61	5	-	0/3/35/36	0/4/4/4

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	X	61	23G	C3'-C4'	-7.58	1.30	1.52
5	L	61	23G	C3'-C4'	-7.22	1.32	1.52
5	X	61	23G	O3'-C3'	-6.73	1.30	1.45
5	L	61	23G	O3'-C3'	-6.63	1.30	1.45
5	L	61	23G	O6-C6	-3.08	1.17	1.24

The worst 5 of 15 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	L	61	23G	C1'-N9-C4	-6.20	117.59	126.94
5	X	61	23G	N1-C2-N3	-4.60	115.63	121.79
5	L	61	23G	N1-C2-N3	-4.39	115.91	121.79
5	X	61	23G	C1'-N9-C4	-4.38	120.33	126.94
5	X	61	23G	C5'-C4'-C3'	-2.75	104.39	114.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	L	61	23G	1	0
5	X	61	23G	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 2 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	J	157/165 (95%)	0.24	5 (3%) 51 39	74, 95, 126, 153	0
1	K	157/165 (95%)	0.20	5 (3%) 51 39	51, 75, 108, 152	0
1	V	155/165 (93%)	0.41	8 (5%) 31 20	78, 105, 137, 153	0
1	W	157/165 (95%)	0.06	3 (1%) 70 58	57, 82, 108, 122	0
2	B	345/363 (95%)	0.45	25 (7%) 18 12	74, 115, 160, 168	0
2	C	347/363 (95%)	0.33	16 (4%) 36 25	56, 99, 149, 164	0
2	D	356/363 (98%)	0.34	11 (3%) 52 40	50, 89, 147, 160	0
2	E	351/363 (96%)	0.07	3 (0%) 85 79	36, 67, 98, 121	0
2	F	356/363 (98%)	0.13	4 (1%) 82 73	31, 66, 118, 151	0
2	G	353/363 (97%)	0.01	2 (0%) 90 85	30, 60, 96, 109	0
2	N	358/363 (98%)	0.29	12 (3%) 49 36	49, 87, 140, 160	0
2	O	355/363 (97%)	0.28	15 (4%) 40 28	50, 89, 145, 164	0
2	P	354/363 (97%)	0.42	29 (8%) 14 9	54, 93, 152, 172	0
2	Q	354/363 (97%)	0.24	16 (4%) 37 26	45, 73, 132, 148	0
2	R	359/363 (98%)	0.11	4 (1%) 82 73	31, 61, 99, 122	0
2	S	361/363 (99%)	0.01	2 (0%) 90 85	33, 62, 113, 153	0
3	A	192/199 (96%)	0.48	11 (5%) 27 17	75, 96, 122, 208	0
3	M	195/199 (97%)	0.26	6 (3%) 52 40	67, 93, 122, 139	0
4	H	219/224 (97%)	0.14	3 (1%) 78 67	42, 74, 105, 124	0
4	T	219/224 (97%)	0.15	1 (0%) 91 88	36, 66, 94, 110	0
5	L	60/61 (98%)	0.30	1 (1%) 73 62	43, 83, 167, 186	0
5	X	59/61 (96%)	0.21	0 100 100	40, 79, 141, 174	0
6	I	493/502 (98%)	0.38	14 (2%) 56 44	46, 113, 176, 267	0
6	U	493/502 (98%)	0.18	11 (2%) 65 54	50, 84, 120, 227	0

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Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
All	All	6805/6988 (97%)	0.23	207 (3%)	54	42	30, 84, 142, 267	0

The worst 5 of 207 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	363	ALA	6.8
2	R	363	ALA	6.8
2	B	175	LEU	5.4
1	V	156	THR	4.5
2	D	168	THR	4.5

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, 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	X	61	26/27	0.87	0.22	-	74,105,132,145	0
5	23G	L	61	26/27	0.86	0.23	-	62,102,137,142	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
7	ZN	U	601	1/1	0.88	0.21	-0.24	181,181,181,181	0
7	ZN	I	601	1/1	0.63	0.14	-2.00	181,181,181,181	0

6.5 Other polymers (i)

There are no such residues in this entry.