wwPDB EM Validation Summary Report

Jun 10, 2025 – 02:14 PM JST

PDB ID	:	8ZLU / pdb_00008zlu
EMDB ID	:	EMD-60233
Title	:	Cryo-EM strcuture of Cas5-HNH Cascade,Conf1
Authors	:	Liu, Y.N.; Wang, L.; Zhang, H.; Zhu, H.
Deposited on	:	2024-05-21
Resolution	:	2.47 Å(reported)

This is a wwPDB EM Validation Summary 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/EMValidationReportHelp
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:

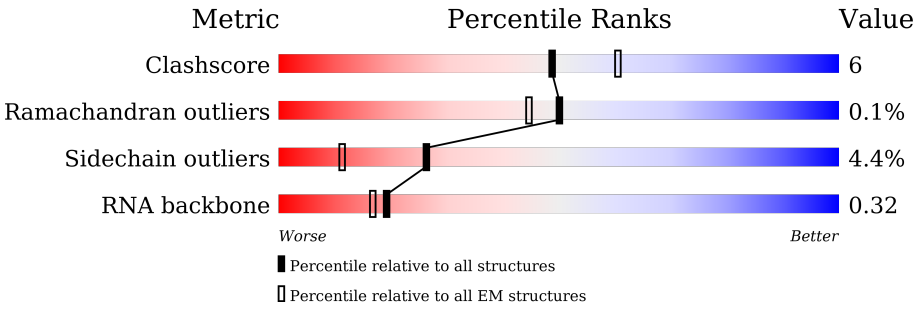
EMDB validation analysis	:	FAILED
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	FAILED
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 2.47 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)	EM structures (#Entries)
Clashscore	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415
RNA backbone	6643	2191

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 <=5%

Mol	Chain	Length	Quality of chain
1	A	61	46% 38% 13% •
2	C	546	69% 11% • 19%
3	E	174	76% 17% • 5%
4	F	378	85% 12% •
4	G	378	58% 8% • 34%
4	H	378	80% 17% • •
4	I	378	79% 17% • •
4	J	378	81% 15% • •

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Mol	Chain	Length	Quality of chain
4	K	378	
5	B	388	
6	D	272	

2 Entry composition (i)

There are 7 unique types of molecules in this entry. The entry contains 27053 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 RNA chain called RNA (61-MER).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	P		
1	A	59	1258	562	225	413	58	0	0

- Molecule 2 is a protein called CRISPR-associated protein Cse1 (CRISPR_cse1).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	C	443	3495	2246	597	633	19	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-10	MET	-	initiating methionine	UNP A0A1V6F8D1
C	-9	HIS	-	expression tag	UNP A0A1V6F8D1
C	-8	HIS	-	expression tag	UNP A0A1V6F8D1
C	-7	HIS	-	expression tag	UNP A0A1V6F8D1
C	-6	HIS	-	expression tag	UNP A0A1V6F8D1
C	-5	HIS	-	expression tag	UNP A0A1V6F8D1
C	-4	HIS	-	expression tag	UNP A0A1V6F8D1
C	-3	HIS	-	expression tag	UNP A0A1V6F8D1
C	-2	HIS	-	expression tag	UNP A0A1V6F8D1
C	-1	HIS	-	expression tag	UNP A0A1V6F8D1
C	0	HIS	-	expression tag	UNP A0A1V6F8D1
C	1	VAL	-	expression tag	UNP A0A1V6F8D1

- Molecule 3 is a protein called CRISPR-associated protein Cse2 (CRISPR_cse2).

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	E	165	1352	875	238	233	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	F	367	Total	C	N	O	S	0	0
			2802	1773	485	532	12		
4	H	367	Total	C	N	O	S	0	0
			2833	1787	495	539	12		
4	I	364	Total	C	N	O	S	0	0
			2787	1762	485	528	12		
4	J	367	Total	C	N	O	S	0	0
			2804	1772	488	532	12		
4	K	352	Total	C	N	O	S	0	0
			2711	1714	476	510	11		
4	G	251	Total	C	N	O	S	0	0
			1919	1222	334	355	8		

- Molecule 5 is a protein called CRISPR system Cascade subunit CasD.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	378	Total	C	N	O	S	0	0
			2955	1866	546	522	21		

- Molecule 6 is a protein called CRISPR-associated endoribonuclease Cse3.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	D	268	Total	C	N	O	S	0	0
			2135	1369	383	379	4		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

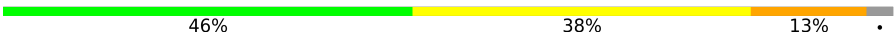
Mol	Chain	Residues	Atoms		AltConf
7	C	1	Total	Mg	0
			1	1	
7	B	1	Total	Mg	0
			1	1	

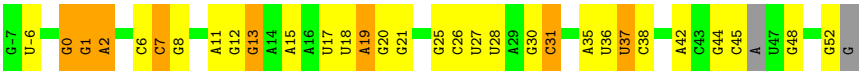
3 Residue-property plots (i)

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. 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. 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: RNA (61-MER)

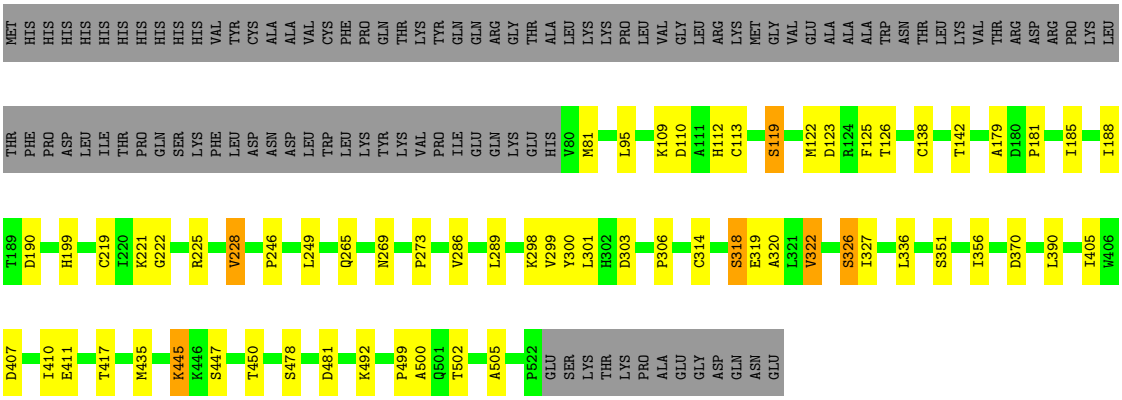
Chain A:





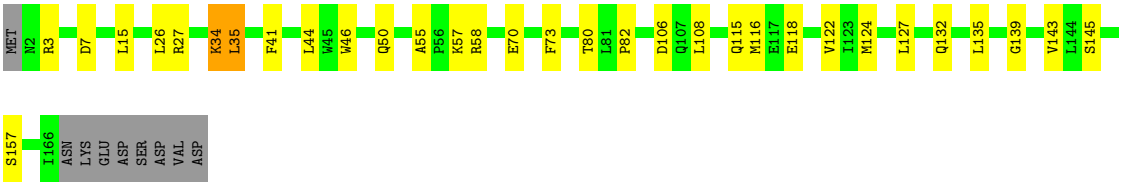
- Molecule 2: CRISPR-associated protein Cse1 (CRISPR_cse1)

Chain C:



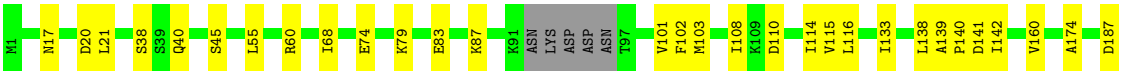
- Molecule 3: CRISPR-associated protein Cse2 (CRISPR_cse2)

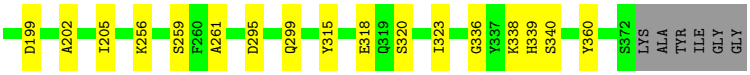
Chain E:



- Molecule 4: CRISPR system Cascade subunit CasC

Chain F:



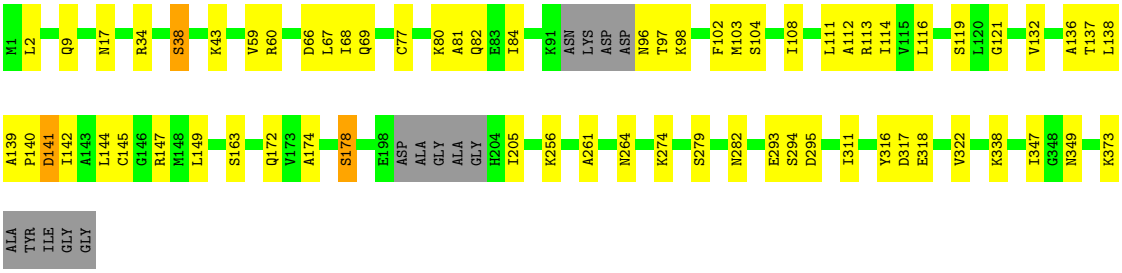


• Molecule 4: CRISPR system Cascade subunit CasC

Chain H:

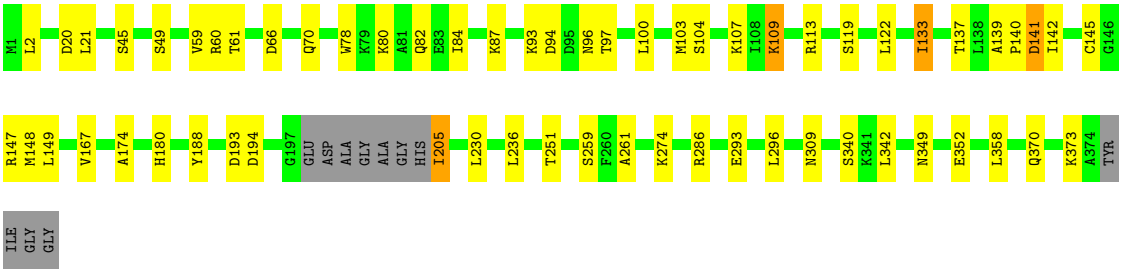
• Molecule 4: CRISPR system Cascade subunit CasC

Chain I:



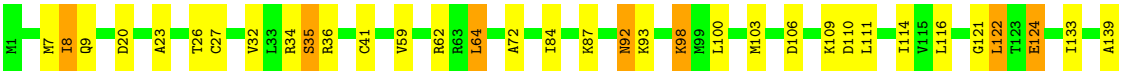
• Molecule 4: CRISPR system Cascade subunit CasC

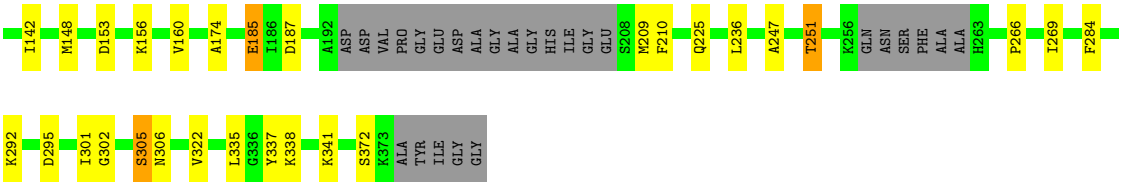
Chain J:



• Molecule 4: CRISPR system Cascade subunit CasC

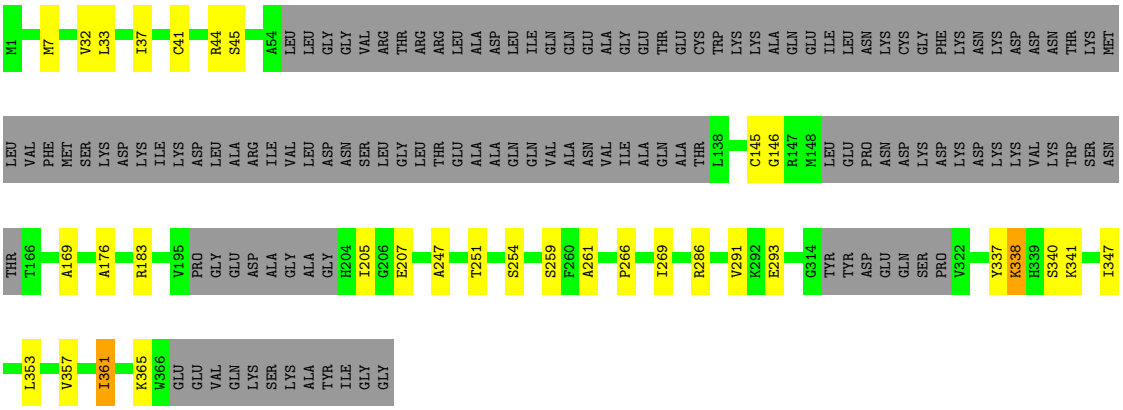
Chain K:





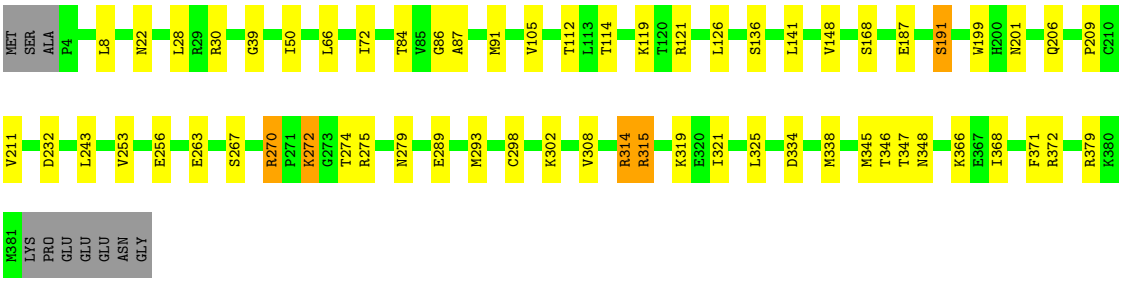
• Molecule 4: CRISPR system Cascade subunit CasC

Chain G:



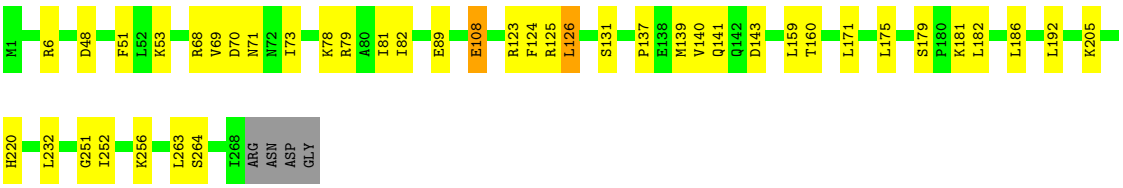
• Molecule 5: CRISPR system Cascade subunit CasD

Chain B:



• Molecule 6: CRISPR-associated endoribonuclease Cse3

Chain D:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	181932	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	12000	Depositor
Maximum defocus (nm)	25000	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG

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	0.11	0/1405	0.31	0/2187
2	C	0.10	0/3596	0.30	0/4901
3	E	0.10	0/1382	0.25	0/1862
4	F	0.09	0/2857	0.25	0/3876
4	G	0.11	0/1960	0.32	0/2658
4	H	0.08	0/2888	0.26	0/3913
4	I	0.11	0/2842	0.32	0/3856
4	J	0.11	0/2858	0.34	0/3876
4	K	0.10	0/2762	0.29	0/3740
5	B	0.10	0/3028	0.28	0/4107
6	D	0.10	0/2193	0.31	0/2976
All	All	0.10	0/27771	0.29	0/37952

There are no bond length outliers.

There are no bond angle outliers.

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	1258	0	638	21	0
2	C	3495	0	3402	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1352	0	1387	19	0
4	F	2802	0	2730	28	0
4	G	1919	0	1852	18	0
4	H	2833	0	2771	36	0
4	I	2787	0	2695	41	0
4	J	2804	0	2723	37	0
4	K	2711	0	2661	41	0
5	B	2955	0	2966	37	0
6	D	2135	0	2096	30	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
All	All	27053	0	25921	297	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 297 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)
4:F:338:LYS:HD2	4:F:339:HIS:H	1.34	0.92
5:B:274:THR:HG22	5:B:275:ARG:H	1.53	0.74
4:I:81:ALA:HB2	4:I:116:LEU:HD21	1.68	0.74
4:I:60:ARG:HH22	4:I:142:ILE:HG12	1.53	0.73
4:J:2:LEU:HB2	4:J:274:LYS:O	1.88	0.73

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 PDB entries followed by that with respect to all EM entries.

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	
2	C	441/546 (81%)	401 (91%)	40 (9%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	163/174 (94%)	158 (97%)	5 (3%)	0	100	100
4	F	363/378 (96%)	344 (95%)	19 (5%)	0	100	100
4	G	241/378 (64%)	224 (93%)	17 (7%)	0	100	100
4	H	363/378 (96%)	340 (94%)	22 (6%)	1 (0%)	37	54
4	I	358/378 (95%)	326 (91%)	30 (8%)	2 (1%)	22	36
4	J	363/378 (96%)	336 (93%)	26 (7%)	1 (0%)	37	54
4	K	346/378 (92%)	318 (92%)	28 (8%)	0	100	100
5	B	376/388 (97%)	355 (94%)	21 (6%)	0	100	100
6	D	266/272 (98%)	256 (96%)	10 (4%)	0	100	100
All	All	3280/3648 (90%)	3058 (93%)	218 (7%)	4 (0%)	50	67

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	I	137	THR
4	I	322	VAL
4	H	76	GLU
4	J	140	PRO

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 PDB entries followed by that with respect to all EM entries.

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	
2	C	370/470 (79%)	354 (96%)	16 (4%)	25	45
3	E	143/153 (94%)	136 (95%)	7 (5%)	21	39
4	F	292/313 (93%)	283 (97%)	9 (3%)	35	59
4	G	199/313 (64%)	189 (95%)	10 (5%)	20	38
4	H	300/313 (96%)	286 (95%)	14 (5%)	22	41
4	I	290/313 (93%)	281 (97%)	9 (3%)	35	59
4	J	291/313 (93%)	277 (95%)	14 (5%)	21	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
4	K	285/313 (91%)	268 (94%)	17 (6%)	16 30
5	B	308/322 (96%)	291 (94%)	17 (6%)	18 34
6	D	223/238 (94%)	218 (98%)	5 (2%)	47 70
All	All	2701/3061 (88%)	2583 (96%)	118 (4%)	26 44

5 of 118 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	J	93	LYS
5	B	314	ARG
4	K	59	VAL
5	B	279	ASN
5	B	114	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 28 such sidechains are listed below:

Mol	Chain	Res	Type
4	I	15	ASN
6	D	120	GLN
4	J	96	ASN
4	G	351	ASN
4	J	69	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	A	57/61 (93%)	19 (33%)	0

5 of 19 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	A	0	G
1	A	1	G
1	A	2	A
1	A	6	C
1	A	7	C

There are no RNA pucker outliers to report.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no oligosaccharides 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.