



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 25, 2024 – 03:41 PM EDT

PDB ID : 6OPM  
Title : Casposase bound to integration product  
Authors : Dyda, F.; Hickman, A.B.; Kailasan, S.  
Deposited on : 2019-04-25  
Resolution : 3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

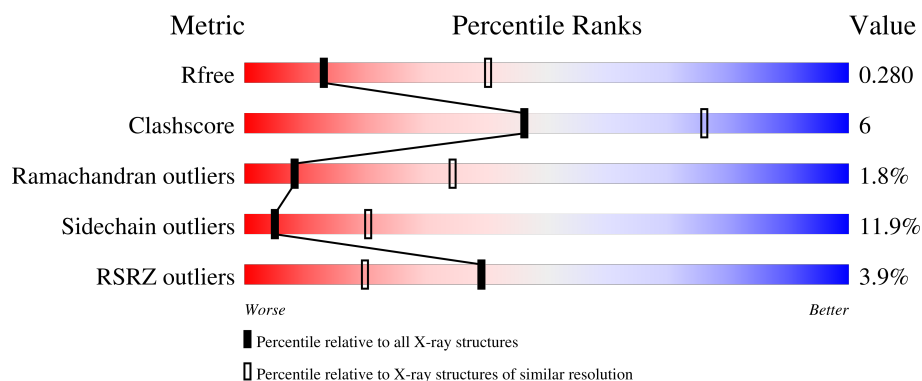
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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.




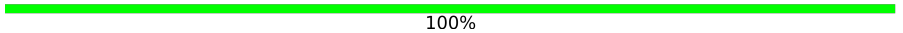
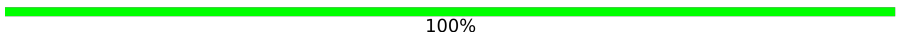
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	431	<div> <div>5%</div> <div>58%19%21%</div> </div>
1	B	431	<div> <div>3%</div> <div>63%17%18%</div> </div>
1	C	431	<div> <div>4%</div> <div>61%19%17%</div> </div>
1	D	431	<div> <div>%</div> <div>59%19%21%</div> </div>
2	E	21	<div> <div>5%</div> <div>76%19%5%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	21	
3	H	13	
3	J	13	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	CA	A	501	-	-	-	X
4	CA	A	502	-	-	-	X
4	CA	C	501	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12315 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-associated endonuclease Cas1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	341	Total	C	N	O	S	Se	0	0	0
			2765	1782	463	511	1	8			
1	B	354	Total	C	N	O	S	Se	0	0	0
			2857	1839	479	530	1	8			
1	C	359	Total	C	N	O	S	Se	0	0	0
			2884	1852	484	539	1	8			
1	D	341	Total	C	N	O	S	Se	0	0	0
			2765	1782	463	511	1	8			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-16	GLY	-	expression tag	UNP A0A0F8IEL4
A	-15	SER	-	expression tag	UNP A0A0F8IEL4
A	-14	ALA	-	expression tag	UNP A0A0F8IEL4
A	-13	MSE	-	expression tag	UNP A0A0F8IEL4
A	-12	ASP	-	expression tag	UNP A0A0F8IEL4
A	-11	PRO	-	expression tag	UNP A0A0F8IEL4
A	-10	GLY	-	expression tag	UNP A0A0F8IEL4
A	-9	SER	-	expression tag	UNP A0A0F8IEL4
A	-8	GLY	-	expression tag	UNP A0A0F8IEL4
A	-7	SER	-	expression tag	UNP A0A0F8IEL4
A	-6	GLY	-	expression tag	UNP A0A0F8IEL4
A	-5	ASN	-	expression tag	UNP A0A0F8IEL4
A	-4	SER	-	expression tag	UNP A0A0F8IEL4
A	-3	HIS	-	expression tag	UNP A0A0F8IEL4
A	-2	ASN	-	expression tag	UNP A0A0F8IEL4
A	-1	SER	-	expression tag	UNP A0A0F8IEL4
A	0	LEU	-	expression tag	UNP A0A0F8IEL4
A	1	MSE	-	expression tag	UNP A0A0F8IEL4
A	184	SER	CYS	engineered mutation	UNP A0A0F8IEL4
A	406	ASP	-	expression tag	UNP A0A0F8IEL4
A	407	GLY	-	expression tag	UNP A0A0F8IEL4

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Chain	Residue	Modelled	Actual	Comment	Reference
A	408	ARG	-	expression tag	UNP A0A0F8IEL4
A	409	GLU	-	expression tag	UNP A0A0F8IEL4
A	410	ASN	-	expression tag	UNP A0A0F8IEL4
A	411	LEU	-	expression tag	UNP A0A0F8IEL4
A	412	TYR	-	expression tag	UNP A0A0F8IEL4
A	413	PHE	-	expression tag	UNP A0A0F8IEL4
A	414	GLN	-	expression tag	UNP A0A0F8IEL4
B	-16	GLY	-	expression tag	UNP A0A0F8IEL4
B	-15	SER	-	expression tag	UNP A0A0F8IEL4
B	-14	ALA	-	expression tag	UNP A0A0F8IEL4
B	-13	MSE	-	expression tag	UNP A0A0F8IEL4
B	-12	ASP	-	expression tag	UNP A0A0F8IEL4
B	-11	PRO	-	expression tag	UNP A0A0F8IEL4
B	-10	GLY	-	expression tag	UNP A0A0F8IEL4
B	-9	SER	-	expression tag	UNP A0A0F8IEL4
B	-8	GLY	-	expression tag	UNP A0A0F8IEL4
B	-7	SER	-	expression tag	UNP A0A0F8IEL4
B	-6	GLY	-	expression tag	UNP A0A0F8IEL4
B	-5	ASN	-	expression tag	UNP A0A0F8IEL4
B	-4	SER	-	expression tag	UNP A0A0F8IEL4
B	-3	HIS	-	expression tag	UNP A0A0F8IEL4
B	-2	ASN	-	expression tag	UNP A0A0F8IEL4
B	-1	SER	-	expression tag	UNP A0A0F8IEL4
B	0	LEU	-	expression tag	UNP A0A0F8IEL4
B	1	MSE	-	expression tag	UNP A0A0F8IEL4
B	184	SER	CYS	engineered mutation	UNP A0A0F8IEL4
B	406	ASP	-	expression tag	UNP A0A0F8IEL4
B	407	GLY	-	expression tag	UNP A0A0F8IEL4
B	408	ARG	-	expression tag	UNP A0A0F8IEL4
B	409	GLU	-	expression tag	UNP A0A0F8IEL4
B	410	ASN	-	expression tag	UNP A0A0F8IEL4
B	411	LEU	-	expression tag	UNP A0A0F8IEL4
B	412	TYR	-	expression tag	UNP A0A0F8IEL4
B	413	PHE	-	expression tag	UNP A0A0F8IEL4
B	414	GLN	-	expression tag	UNP A0A0F8IEL4
C	-16	GLY	-	expression tag	UNP A0A0F8IEL4
C	-15	SER	-	expression tag	UNP A0A0F8IEL4
C	-14	ALA	-	expression tag	UNP A0A0F8IEL4
C	-13	MSE	-	expression tag	UNP A0A0F8IEL4
C	-12	ASP	-	expression tag	UNP A0A0F8IEL4
C	-11	PRO	-	expression tag	UNP A0A0F8IEL4
C	-10	GLY	-	expression tag	UNP A0A0F8IEL4

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-9	SER	-	expression tag	UNP A0A0F8IEL4
C	-8	GLY	-	expression tag	UNP A0A0F8IEL4
C	-7	SER	-	expression tag	UNP A0A0F8IEL4
C	-6	GLY	-	expression tag	UNP A0A0F8IEL4
C	-5	ASN	-	expression tag	UNP A0A0F8IEL4
C	-4	SER	-	expression tag	UNP A0A0F8IEL4
C	-3	HIS	-	expression tag	UNP A0A0F8IEL4
C	-2	ASN	-	expression tag	UNP A0A0F8IEL4
C	-1	SER	-	expression tag	UNP A0A0F8IEL4
C	0	LEU	-	expression tag	UNP A0A0F8IEL4
C	1	MSE	-	expression tag	UNP A0A0F8IEL4
C	184	SER	CYS	engineered mutation	UNP A0A0F8IEL4
C	406	ASP	-	expression tag	UNP A0A0F8IEL4
C	407	GLY	-	expression tag	UNP A0A0F8IEL4
C	408	ARG	-	expression tag	UNP A0A0F8IEL4
C	409	GLU	-	expression tag	UNP A0A0F8IEL4
C	410	ASN	-	expression tag	UNP A0A0F8IEL4
C	411	LEU	-	expression tag	UNP A0A0F8IEL4
C	412	TYR	-	expression tag	UNP A0A0F8IEL4
C	413	PHE	-	expression tag	UNP A0A0F8IEL4
C	414	GLN	-	expression tag	UNP A0A0F8IEL4
D	-16	GLY	-	expression tag	UNP A0A0F8IEL4
D	-15	SER	-	expression tag	UNP A0A0F8IEL4
D	-14	ALA	-	expression tag	UNP A0A0F8IEL4
D	-13	MSE	-	expression tag	UNP A0A0F8IEL4
D	-12	ASP	-	expression tag	UNP A0A0F8IEL4
D	-11	PRO	-	expression tag	UNP A0A0F8IEL4
D	-10	GLY	-	expression tag	UNP A0A0F8IEL4
D	-9	SER	-	expression tag	UNP A0A0F8IEL4
D	-8	GLY	-	expression tag	UNP A0A0F8IEL4
D	-7	SER	-	expression tag	UNP A0A0F8IEL4
D	-6	GLY	-	expression tag	UNP A0A0F8IEL4
D	-5	ASN	-	expression tag	UNP A0A0F8IEL4
D	-4	SER	-	expression tag	UNP A0A0F8IEL4
D	-3	HIS	-	expression tag	UNP A0A0F8IEL4
D	-2	ASN	-	expression tag	UNP A0A0F8IEL4
D	-1	SER	-	expression tag	UNP A0A0F8IEL4
D	0	LEU	-	expression tag	UNP A0A0F8IEL4
D	1	MSE	-	expression tag	UNP A0A0F8IEL4
D	184	SER	CYS	engineered mutation	UNP A0A0F8IEL4
D	406	ASP	-	expression tag	UNP A0A0F8IEL4
D	407	GLY	-	expression tag	UNP A0A0F8IEL4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	408	ARG	-	expression tag	UNP A0A0F8IEL4
D	409	GLU	-	expression tag	UNP A0A0F8IEL4
D	410	ASN	-	expression tag	UNP A0A0F8IEL4
D	411	LEU	-	expression tag	UNP A0A0F8IEL4
D	412	TYR	-	expression tag	UNP A0A0F8IEL4
D	413	PHE	-	expression tag	UNP A0A0F8IEL4
D	414	GLN	-	expression tag	UNP A0A0F8IEL4

- Molecule 2 is a DNA chain called DNA 21-mer.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	E	21	Total	C	N	O	P	0	0	0
			423	203	76	124	20			
2	F	21	Total	C	N	O	P	0	0	0
			423	203	76	124	20			

- Molecule 3 is a protein called unknown.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	H	13	Total	C	N	O	0	0	0
			78	39	13	26			
3	J	13	Total	C	N	O	0	0	0
			78	39	13	26			

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	2	Total	Ca	0	0
			2	2		
4	C	2	Total	Ca	0	0
			2	2		
4	E	1	Total	Ca	0	0
			1	1		
4	F	1	Total	Ca	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	5	Total	O	0	0
			5	5		

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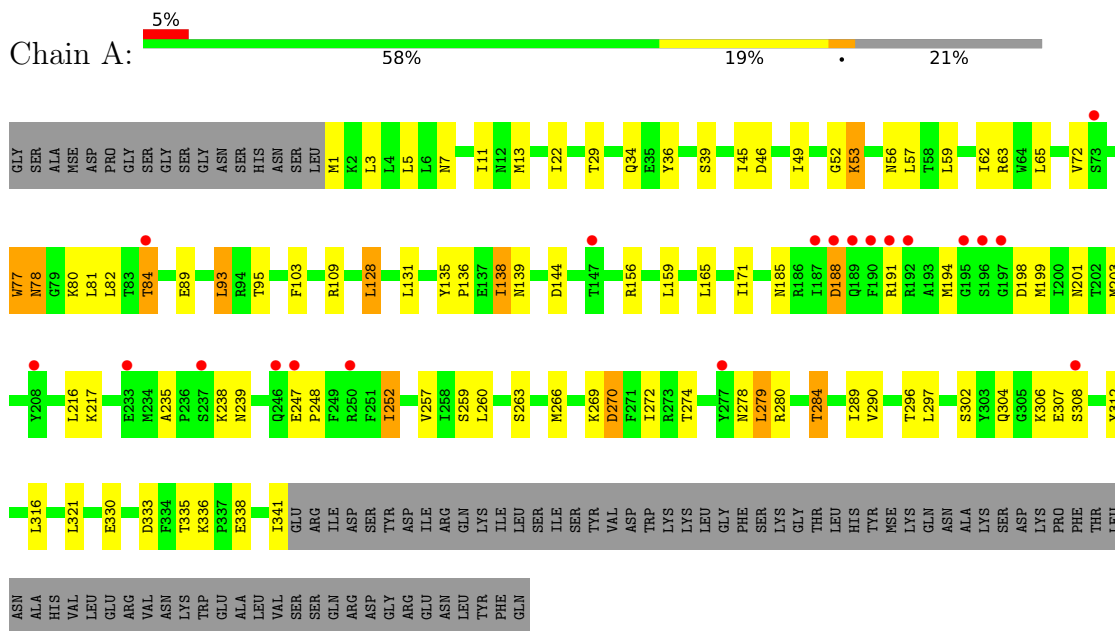
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	11	Total 11	O 11	0	0
5	C	5	Total 5	O 5	0	0
5	D	6	Total 6	O 6	0	0
5	E	3	Total 3	O 3	0	0
5	F	6	Total 6	O 6	0	0



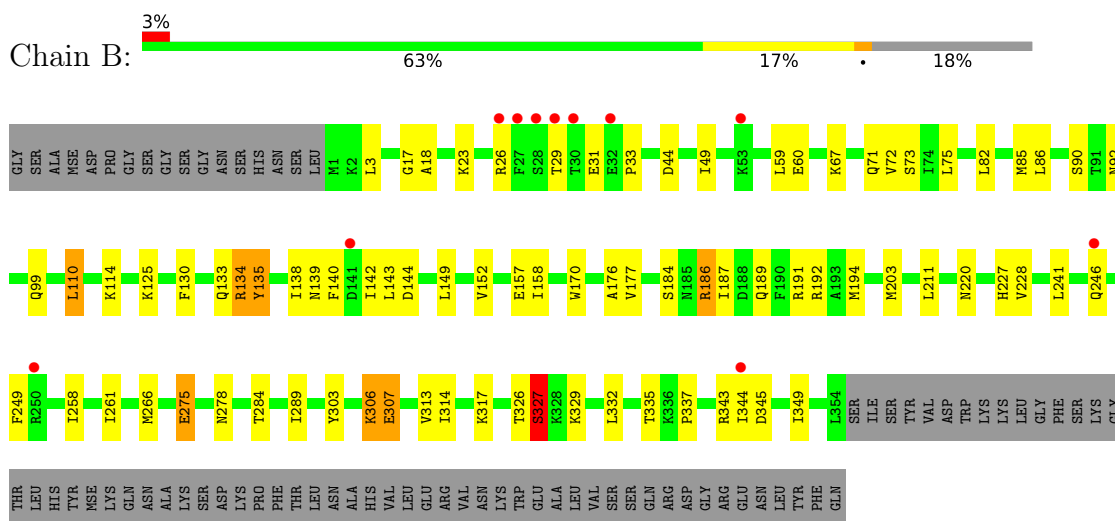
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

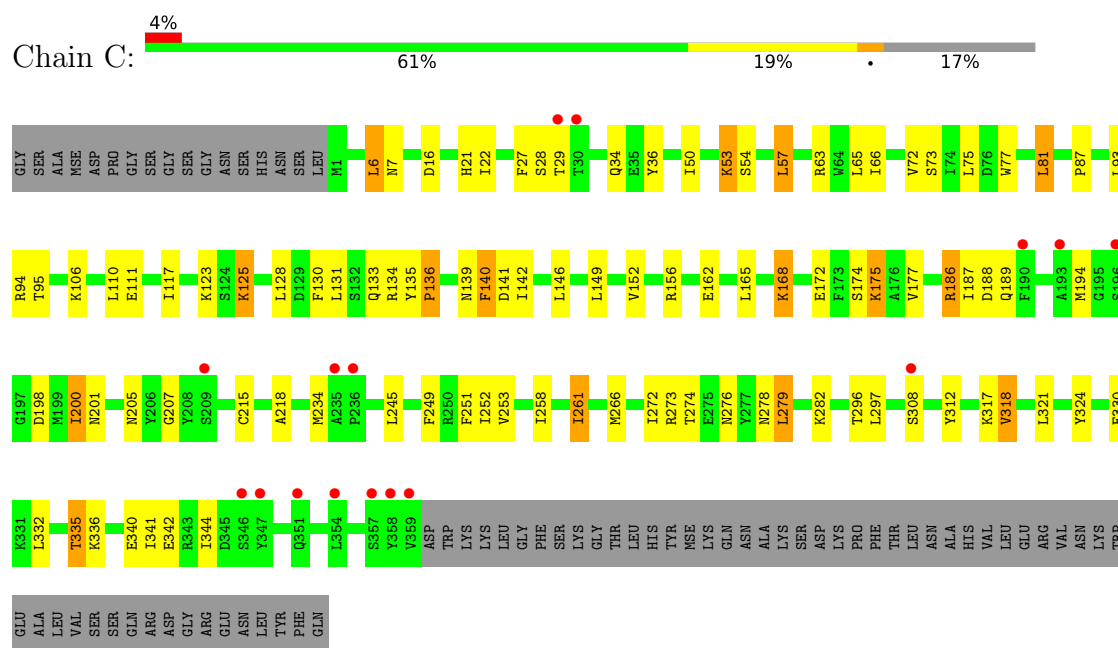
#### • Molecule 1: CRISPR-associated endonuclease Cas1



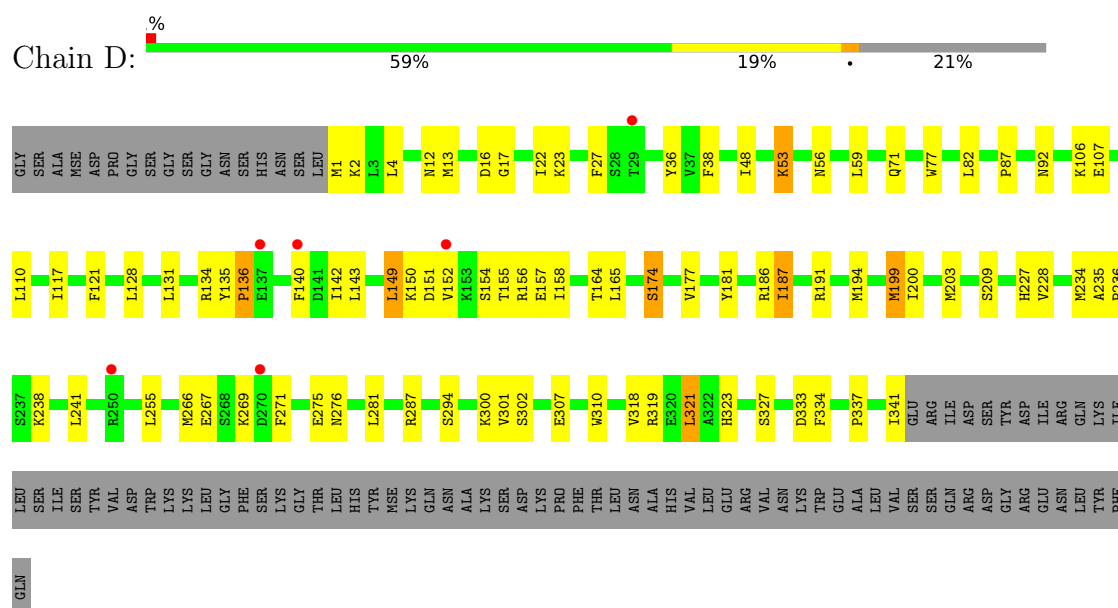
#### • Molecule 1: CRISPR-associated endonuclease Cas1



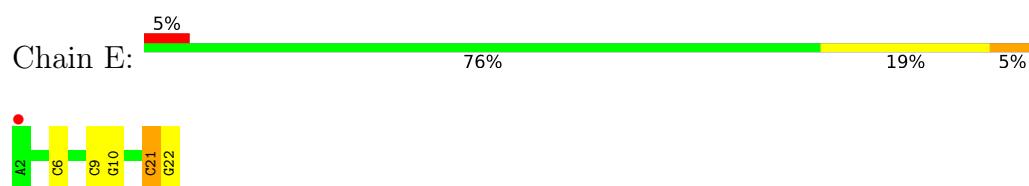
#### • Molecule 1: CRISPR-associated endonuclease Cas1



- Molecule 1: CRISPR-associated endonuclease Cas1



- Molecule 2: DNA 21-mer



- Molecule 2: DNA 21-mer





- Molecule 3: unknown

Chain H:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: unknown

Chain J:  100%

There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	106.39Å 106.39Å 423.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.89 – 3.10 29.89 – 3.10	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.89-3.10) 100.0 (29.89-3.10)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.39 (at 3.11Å)	Xtriage
Refinement program	BUSTER 2.10.3	Depositor
R, $R_{free}$	0.198 , 0.256 0.213 , 0.280	Depositor DCC
$R_{free}$ test set	1135 reflections (2.50%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	107.5	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 108.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12315	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	142.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.48	0/2816	0.70	0/3781
1	B	0.52	0/2909	0.75	0/3908
1	C	0.51	0/2936	0.72	1/3945 (0.0%)
1	D	0.49	0/2816	0.71	0/3781
2	E	1.29	1/473 (0.2%)	1.06	0/727
2	F	1.24	1/473 (0.2%)	1.08	0/727
All	All	0.60	2/12423 (0.0%)	0.76	1/16869 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	21	DC	C3'-O3'	-5.89	1.36	1.44
2	E	21	DC	C3'-O3'	-5.47	1.36	1.44

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	140	PHE	C-N-CA	5.41	135.22	121.70

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	2765	0	2802	33	0
1	B	2857	0	2873	36	0
1	C	2884	0	2882	48	0
1	D	2765	0	2802	42	0
2	E	423	0	238	5	0
2	F	423	0	238	7	0
3	H	78	0	15	0	0
3	J	78	0	15	0	0
4	A	2	0	0	0	0
4	C	2	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	5	0	0	0	0
5	B	11	0	0	0	0
5	C	5	0	0	0	0
5	D	6	0	0	0	0
5	E	3	0	0	0	0
5	F	6	0	0	0	0
All	All	12315	0	11865	152	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.

All (152) 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)
1:D:181:TYR:HB3	1:D:200:ILE:HD11	1.58	0.85
1:D:13:MSE:HE1	1:D:48:ILE:HG21	1.62	0.81
1:A:84:THR:HG21	1:A:216:LEU:HD13	1.68	0.75
1:D:200:ILE:HA	1:D:203:MSE:HE2	1.68	0.74
1:C:186:ARG:HH21	1:C:205:ASN:ND2	1.90	0.69
1:C:125:LYS:HB2	1:C:142:ILE:HG13	1.72	0.69
1:B:125:LYS:HB2	1:B:142:ILE:HG13	1.76	0.68
1:B:90:SER:HB3	1:B:92:ASN:HD22	1.59	0.66
1:A:53:LYS:HE3	1:A:53:LYS:HA	1.79	0.65
1:D:155:THR:HA	1:D:158:ILE:HD12	1.78	0.65
1:D:174:SER:HA	1:D:177:VAL:HG22	1.79	0.65
1:D:199:MSE:HG3	1:D:271:PHE:CZ	2.32	0.65
1:D:22:ILE:HD12	1:D:38:PHE:HE1	1.64	0.63
1:A:198:ASP:HB2	1:A:201:ASN:HB2	1.80	0.61
1:C:130:PHE:HB2	1:C:341:ILE:HD12	1.82	0.61
1:B:152:VAL:HB	1:B:157:GLU:HB3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:135:TYR:N	1:C:136:PRO:HD2	2.17	0.60
1:A:82:LEU:HD21	1:B:67:LYS:HE2	1.82	0.59
1:B:72:VAL:HB	1:B:85:MSE:HE3	1.84	0.59
1:C:172:GLU:HA	1:C:175:LYS:HE2	1.83	0.59
1:C:218:ALA:HB1	1:C:318:VAL:HG21	1.85	0.58
1:C:22:ILE:HB	1:C:36:TYR:HB2	1.86	0.58
1:A:93:LEU:HD13	1:B:227:HIS:HB2	1.86	0.58
1:D:12:ASN:HB3	1:D:23:LYS:HB3	1.86	0.58
1:C:6:LEU:HD12	1:C:50:ILE:HG12	1.84	0.57
1:A:247:GLU:HB2	1:A:248:PRO:HD3	1.88	0.56
1:C:186:ARG:HH21	1:C:205:ASN:HD22	1.53	0.56
1:D:1:MSE:HE1	1:D:319:ARG:HG3	1.88	0.56
1:B:187:ILE:HD12	1:B:191:ARG:HA	1.87	0.55
1:C:335:THR:HG22	1:C:336:LYS:HG3	1.89	0.55
1:B:134:ARG:HG2	1:B:176:ALA:HA	1.89	0.55
1:D:194:MSE:HE1	2:F:18:DG:H2''	1.89	0.55
1:D:117:ILE:HG22	1:D:149:LEU:HD11	1.89	0.55
1:B:26:ARG:HB3	1:B:33:PRO:HG3	1.88	0.55
1:C:198:ASP:HB2	1:C:201:ASN:HB2	1.89	0.54
1:A:93:LEU:HD13	1:B:227:HIS:CB	2.38	0.54
1:A:11:ILE:HD11	1:A:52:GLY:HA3	1.89	0.54
1:C:93:LEU:HD22	1:D:228:VAL:HG23	1.89	0.53
1:A:1:MSE:HE2	1:A:297:LEU:HD23	1.90	0.53
1:D:152:VAL:HB	1:D:157:GLU:HB3	1.91	0.53
1:B:343:ARG:HB3	1:B:349:ILE:HD11	1.91	0.53
1:C:93:LEU:HD13	1:D:227:HIS:HB2	1.91	0.53
1:D:235:ALA:HB3	1:D:238:LYS:HG3	1.90	0.52
1:D:1:MSE:HB3	1:D:323:HIS:HE1	1.74	0.52
1:D:149:LEU:O	1:D:152:VAL:HG22	2.08	0.52
2:E:9:DC:H2'	2:E:10:DG:C8	2.45	0.52
1:D:199:MSE:O	1:D:203:MSE:HG3	2.10	0.52
1:B:306:LYS:HE3	1:B:307:GLU:H	1.75	0.52
1:D:300:LYS:HB3	1:D:307:GLU:HG2	1.91	0.52
1:C:273:ARG:NH1	1:C:279:LEU:HD11	2.25	0.52
1:B:170:TRP:CD2	1:B:186:ARG:HG3	2.45	0.52
1:D:22:ILE:HD12	1:D:38:PHE:CE1	2.45	0.51
1:B:75:LEU:HD21	1:B:220:ASN:HB3	1.92	0.51
1:C:16:ASP:HB2	1:C:21:HIS:CE1	2.45	0.51
1:A:63:ARG:HH22	1:D:275:GLU:HB2	1.76	0.51
1:C:186:ARG:HA	1:C:201:ASN:HD21	1.76	0.51
1:B:170:TRP:CE2	1:B:186:ARG:HG3	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:LEU:HD23	1:C:140:PHE:HB2	1.93	0.50
2:E:21:DC:H2'	2:E:22:DG:C8	2.46	0.50
2:F:9:DC:H2'	2:F:10:DG:C8	2.46	0.50
1:C:274:THR:HB	1:C:278:ASN:H	1.77	0.50
1:D:13:MSE:HG2	1:D:22:ILE:HG12	1.94	0.50
1:C:274:THR:HG22	1:C:276:ASN:H	1.76	0.49
1:B:203:MSE:HG2	1:B:289:ILE:HD11	1.93	0.49
1:C:63:ARG:HA	1:D:82:LEU:HD21	1.95	0.49
1:A:103:PHE:HA	1:A:109:ARG:HG3	1.93	0.49
1:D:13:MSE:HE2	1:D:22:ILE:HD13	1.95	0.49
1:A:78:ASN:HD22	1:A:80:LYS:H	1.61	0.49
1:C:272:ILE:HG13	1:C:282:LYS:CG	2.43	0.49
1:A:93:LEU:HD22	1:B:228:VAL:HG23	1.96	0.48
1:C:177:VAL:HG12	1:C:261:ILE:HG21	1.95	0.48
2:F:4:DA:C8	2:F:4:DA:H5''	2.48	0.48
1:C:140:PHE:CE1	1:C:142:ILE:HD11	2.49	0.48
1:D:22:ILE:HB	1:D:36:TYR:HB2	1.96	0.48
1:D:321:LEU:HG	1:D:334:PHE:HZ	1.79	0.48
1:C:53:LYS:H	1:C:53:LYS:HD2	1.79	0.47
1:C:340:GLU:HB2	1:C:342:GLU:HG3	1.96	0.47
1:A:77:TRP:HB3	1:A:280:ARG:CZ	2.44	0.47
1:C:308:SER:HA	2:E:22:DG:H5''	1.97	0.47
1:A:260:LEU:HA	1:A:263:SER:HB2	1.96	0.47
1:D:199:MSE:HG3	1:D:271:PHE:CE1	2.49	0.47
1:B:135:TYR:CD1	1:B:138:ILE:HD11	2.50	0.47
2:F:4:DA:H8	2:F:5:DT:H72	1.78	0.47
1:A:3:LEU:HD22	1:A:49:ILE:HD11	1.96	0.47
1:A:59:LEU:HA	1:A:62:ILE:HD12	1.96	0.47
1:A:308:SER:HA	2:F:22:DG:H5''	1.96	0.47
1:B:275:GLU:HG3	1:D:77:TRP:HE1	1.78	0.47
1:A:13:MSE:HG2	1:A:22:ILE:HG12	1.96	0.47
1:B:303:TYR:HB2	1:B:337:PRO:HB3	1.96	0.47
2:F:21:DC:H2'	2:F:22:DG:C8	2.50	0.47
1:A:63:ARG:HA	1:B:82:LEU:HD21	1.96	0.47
1:A:312:TYR:O	1:A:316:LEU:HG	2.15	0.47
1:B:99:GLN:HE22	1:B:241:LEU:HD22	1.80	0.47
1:D:134:ARG:C	1:D:136:PRO:HD2	2.35	0.47
1:C:57:LEU:HD21	1:D:59:LEU:HD21	1.97	0.46
1:A:65:LEU:HD13	1:A:72:VAL:HG21	1.97	0.46
1:D:301:VAL:HG21	1:D:310:TRP:CZ2	2.50	0.46
1:A:333:ASP:HB3	1:A:336:LYS:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:302:SER:HA	1:D:307:GLU:HA	1.98	0.46
1:A:203:MSE:HE2	1:A:257:VAL:HG13	1.97	0.46
1:A:306:LYS:HB2	2:F:22:DG:H4'	1.97	0.46
1:B:143:LEU:HD23	1:B:143:LEU:H	1.81	0.46
1:C:149:LEU:O	1:C:152:VAL:HG22	2.16	0.46
1:A:22:ILE:HB	1:A:36:TYR:HB2	1.97	0.45
1:A:199:MSE:HA	1:A:279:LEU:HD12	1.98	0.45
1:A:252:ILE:HG13	1:A:296:THR:HG22	1.97	0.45
1:D:27:PHE:HE2	1:D:53:LYS:HZ1	1.64	0.45
1:A:128:LEU:HA	1:A:131:LEU:HD12	1.97	0.45
1:C:94:ARG:NH2	1:D:236:PRO:HD3	2.32	0.45
1:D:128:LEU:HD12	1:D:140:PHE:CD1	2.52	0.45
1:A:235:ALA:HB3	1:A:238:LYS:HB2	1.99	0.45
1:B:313:VAL:O	1:B:317:LYS:HG2	2.17	0.44
1:C:65:LEU:HD13	1:C:72:VAL:HG21	1.99	0.44
1:C:177:VAL:HG11	1:C:200:ILE:HD13	2.00	0.44
1:B:258:ILE:HA	1:B:261:ILE:HD12	2.00	0.44
1:C:324:TYR:CD1	1:C:332:LEU:HB2	2.53	0.44
1:A:135:TYR:HA	1:A:138:ILE:HG12	1.99	0.43
1:C:249:PHE:HZ	1:C:317:LYS:HG3	1.83	0.43
1:D:187:ILE:HB	1:D:191:ARG:HA	1.99	0.43
1:C:215:CYS:HB3	1:C:245:LEU:HD23	2.00	0.43
1:C:66:ILE:HG23	1:C:87:PRO:HA	2.00	0.43
1:A:270:ASP:HB3	1:A:284:THR:OG1	2.19	0.43
1:C:252:ILE:HG23	1:C:296:THR:HG22	2.00	0.43
1:B:152:VAL:HG21	1:B:158:ILE:HG12	2.00	0.43
1:D:135:TYR:N	1:D:136:PRO:HD2	2.34	0.42
1:B:192:ARG:HB3	1:B:194:MSE:HG2	2.00	0.42
1:D:71:GLN:HA	1:D:87:PRO:HD3	2.02	0.42
1:C:218:ALA:CB	1:C:318:VAL:HG21	2.48	0.42
1:B:90:SER:C	1:B:92:ASN:H	2.23	0.42
1:D:209:SER:HB3	2:E:6:DC:H5''	2.00	0.42
1:A:274:THR:HB	1:A:278:ASN:H	1.85	0.42
1:C:94:ARG:HH21	1:D:236:PRO:HD3	1.85	0.42
1:C:207:GLY:HA3	1:C:253:VAL:HG13	2.01	0.42
1:C:117:ILE:HD12	1:C:162:GLU:HG3	2.00	0.41
1:C:165:LEU:HD23	1:C:165:LEU:HA	1.96	0.41
1:B:149:LEU:O	1:B:152:VAL:HG22	2.21	0.41
1:B:249:PHE:CE2	1:B:314:ILE:HG12	2.55	0.41
1:C:168:LYS:O	1:C:172:GLU:HG2	2.21	0.41
1:B:211:LEU:HG	1:B:246:GLN:HG2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:326:THR:O	1:B:327:SER:HB2	2.20	0.41
1:C:75:LEU:HD23	1:C:81:LEU:HA	2.02	0.41
1:B:114:LYS:HE2	1:B:149:LEU:O	2.21	0.41
1:B:194:MSE:HE3	1:B:194:MSE:HB2	1.99	0.41
1:C:272:ILE:HG13	1:C:282:LYS:HG3	2.02	0.41
1:B:71:GLN:HG3	1:B:86:LEU:HA	2.04	0.40
1:C:312:TYR:CD2	2:E:21:DC:H4'	2.56	0.40
1:D:121:PHE:HB3	1:D:142:ILE:HG23	2.03	0.40
1:B:110:LEU:HD22	1:B:110:LEU:HA	1.86	0.40
1:C:123:LYS:HD2	1:C:251:PHE:CE1	2.56	0.40
1:C:252:ILE:HG21	1:C:297:LEU:HD13	2.04	0.40
1:D:27:PHE:HE2	1:D:53:LYS:NZ	2.19	0.40
1:C:272:ILE:HG13	1:C:282:LYS:HG2	2.04	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	339/431 (79%)	300 (88%)	33 (10%)	6 (2%)	8	34
1	B	352/431 (82%)	320 (91%)	26 (7%)	6 (2%)	9	36
1	C	357/431 (83%)	317 (89%)	33 (9%)	7 (2%)	7	31
1	D	339/431 (79%)	309 (91%)	24 (7%)	6 (2%)	8	34
All	All	1387/1724 (80%)	1246 (90%)	116 (8%)	25 (2%)	8	34

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	191	ARG
1	C	141	ASP

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Mol	Chain	Res	Type
1	C	188	ASP
1	D	92	ASN
1	B	327	SER
1	B	344	ILE
1	D	17	GLY
1	A	77	TRP
1	B	17	GLY
1	B	18	ALA
1	B	345	ASP
1	C	234	MSE
1	D	106	LYS
1	A	188	ASP
1	A	239	ASN
1	B	329	LYS
1	C	27	PHE
1	A	136	PRO
1	A	259	SER
1	D	150	LYS
1	D	327	SER
1	D	136	PRO
1	C	187	ILE
1	C	136	PRO
1	C	344	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	302/371 (81%)	257 (85%)	45 (15%)	3	13
1	B	309/371 (83%)	279 (90%)	30 (10%)	8	30
1	C	311/371 (84%)	274 (88%)	37 (12%)	5	20
1	D	302/371 (81%)	268 (89%)	34 (11%)	6	23
All	All	1224/1484 (82%)	1078 (88%)	146 (12%)	5	20

All (146) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	7	ASN
1	A	29	THR
1	A	34	GLN
1	A	39	SER
1	A	45	ILE
1	A	46	ASP
1	A	53	LYS
1	A	56	ASN
1	A	57	LEU
1	A	78	ASN
1	A	81	LEU
1	A	84	THR
1	A	89	GLU
1	A	93	LEU
1	A	95	THR
1	A	128	LEU
1	A	138	ILE
1	A	139	ASN
1	A	144	ASP
1	A	156	ARG
1	A	159	LEU
1	A	165	LEU
1	A	171	ILE
1	A	185	ASN
1	A	188	ASP
1	A	194	MSE
1	A	217	LYS
1	A	252	ILE
1	A	266	MSE
1	A	269	LYS
1	A	270	ASP
1	A	272	ILE
1	A	279	LEU
1	A	284	THR
1	A	289	ILE
1	A	290	VAL
1	A	302	SER
1	A	304	GLN
1	A	307	GLU
1	A	321	LEU
1	A	330	GLU
1	A	335	THR

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Mol	Chain	Res	Type
1	A	338	GLU
1	A	341	ILE
1	B	3	LEU
1	B	23	LYS
1	B	29	THR
1	B	31	GLU
1	B	44	ASP
1	B	49	ILE
1	B	59	LEU
1	B	60	GLU
1	B	73	SER
1	B	110	LEU
1	B	130	PHE
1	B	133	GLN
1	B	134	ARG
1	B	135	TYR
1	B	139	ASN
1	B	140	PHE
1	B	144	ASP
1	B	177	VAL
1	B	184	SER
1	B	186	ARG
1	B	189	GLN
1	B	266	MSE
1	B	275	GLU
1	B	278	ASN
1	B	284	THR
1	B	306	LYS
1	B	307	GLU
1	B	327	SER
1	B	332	LEU
1	B	335	THR
1	C	6	LEU
1	C	7	ASN
1	C	28	SER
1	C	29	THR
1	C	34	GLN
1	C	53	LYS
1	C	54	SER
1	C	57	LEU
1	C	73	SER
1	C	77	TRP

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Mol	Chain	Res	Type
1	C	81	LEU
1	C	95	THR
1	C	106	LYS
1	C	110	LEU
1	C	111	GLU
1	C	125	LYS
1	C	131	LEU
1	C	133	GLN
1	C	134	ARG
1	C	139	ASN
1	C	146	LEU
1	C	156	ARG
1	C	168	LYS
1	C	174	SER
1	C	175	LYS
1	C	186	ARG
1	C	189	GLN
1	C	194	MSE
1	C	200	ILE
1	C	258	ILE
1	C	261	ILE
1	C	266	MSE
1	C	279	LEU
1	C	318	VAL
1	C	321	LEU
1	C	330	GLU
1	C	335	THR
1	D	2	LYS
1	D	4	LEU
1	D	16	ASP
1	D	53	LYS
1	D	56	ASN
1	D	107	GLU
1	D	110	LEU
1	D	131	LEU
1	D	143	LEU
1	D	149	LEU
1	D	151	ASP
1	D	154	SER
1	D	156	ARG
1	D	164	THR
1	D	165	LEU

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Mol	Chain	Res	Type
1	D	174	SER
1	D	186	ARG
1	D	187	ILE
1	D	199	MSE
1	D	234	MSE
1	D	241	LEU
1	D	255	LEU
1	D	266	MSE
1	D	267	GLU
1	D	269	LYS
1	D	276	ASN
1	D	281	LEU
1	D	287	ARG
1	D	294	SER
1	D	318	VAL
1	D	321	LEU
1	D	333	ASP
1	D	337	PRO
1	D	341	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	34	GLN
1	A	78	ASN
1	A	185	ASN
1	B	92	ASN
1	B	101	HIS
1	C	7	ASN
1	C	21	HIS
1	C	56	ASN
1	C	133	GLN
1	C	201	ASN
1	C	205	ASN
1	C	220	ASN
1	C	298	ASN
1	D	56	ASN
1	D	92	ASN
1	D	276	ASN
1	D	278	ASN
1	D	323	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 6 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	333/431 (77%)	0.27	20 (6%) 21 10	95, 152, 208, 261	0
1	B	346/431 (80%)	-0.02	11 (3%) 47 25	86, 124, 189, 235	0
1	C	351/431 (81%)	0.06	16 (4%) 32 16	89, 134, 211, 242	0
1	D	333/431 (77%)	-0.10	6 (1%) 68 47	92, 139, 190, 212	0
2	E	21/21 (100%)	-0.11	1 (4%) 30 14	99, 114, 141, 237	0
2	F	21/21 (100%)	0.02	1 (4%) 30 14	95, 105, 159, 229	0
3	H	0/13	-	-	-	-
3	J	0/13	-	-	-	-
All	All	1405/1792 (78%)	0.05	55 (3%) 39 20	86, 136, 202, 261	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	SER	12.7
1	A	195	GLY	12.6
1	A	188	ASP	7.0
1	A	197	GLY	6.6
1	A	189	GLN	6.5
1	C	358	TYR	6.2
1	A	190	PHE	5.9
1	A	192	ARG	5.3
1	B	29	THR	4.5
1	B	344	ILE	4.2
1	B	30	THR	4.1
1	B	53	LYS	4.1
1	A	233	GLU	3.9
1	A	187	ILE	3.9
1	A	250	ARG	3.8
1	C	357	SER	3.8
1	C	351	GLN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	237	SER	3.5
1	C	359	VAL	3.4
1	D	29	THR	3.4
1	C	235	ALA	3.3
1	A	191	ARG	3.3
1	A	277	TYR	3.2
1	D	140	PHE	3.2
1	C	196	SER	3.1
1	A	147	THR	3.1
1	B	28	SER	3.1
1	B	250	ARG	3.1
1	C	308	SER	3.0
1	B	26	ARG	3.0
1	C	347	TYR	2.8
1	A	308	SER	2.7
1	A	247	GLU	2.7
1	D	250	ARG	2.7
1	C	30	THR	2.7
1	B	27	PHE	2.6
1	C	29	THR	2.6
1	C	190	PHE	2.5
1	C	193	ALA	2.5
1	D	137	GLU	2.5
1	D	152	VAL	2.5
1	C	209	SER	2.3
1	C	236	PRO	2.3
1	A	73	SER	2.3
2	E	2	DA	2.3
1	B	141	ASP	2.2
2	F	2	DA	2.2
1	B	32	GLU	2.1
1	C	354	LEU	2.1
1	A	208	TYR	2.1
1	C	346	SER	2.1
1	A	246	GLN	2.0
1	A	84	THR	2.0
1	B	246	GLN	2.0
1	D	270	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

### 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	CA	A	502	1/1	0.71	1.13	178,178,178,178	0
4	CA	A	501	1/1	0.72	0.48	157,157,157,157	0
4	CA	C	501	1/1	0.77	0.75	165,165,165,165	0
4	CA	C	502	1/1	0.86	0.10	149,149,149,149	0
4	CA	E	101	1/1	0.95	0.37	112,112,112,112	0
4	CA	F	101	1/1	0.96	0.19	98,98,98,98	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.