



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:42 PM UTC

PDB ID : 6OPM / pdb_00006opm
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

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>.

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

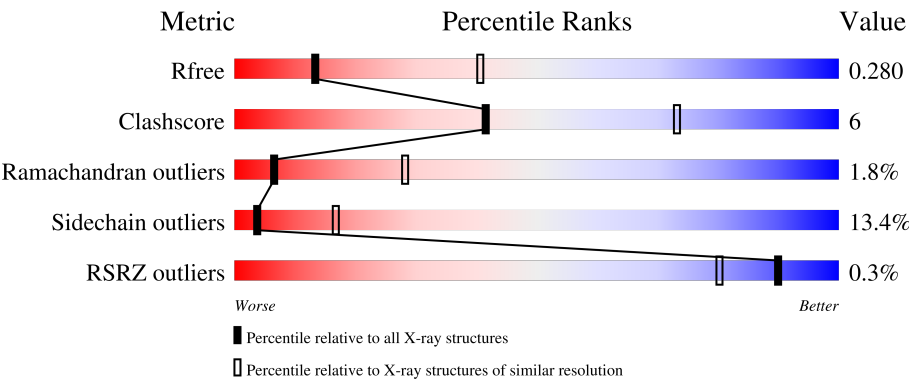
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.10 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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (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 ≥ 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	
1	B	431	
1	C	431	
1	D	431	
2	E	21	

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Mol	Chain	Length	Quality of chain
2	F	21	 67%33%
3	H	13	 100%
3	J	13	 100%

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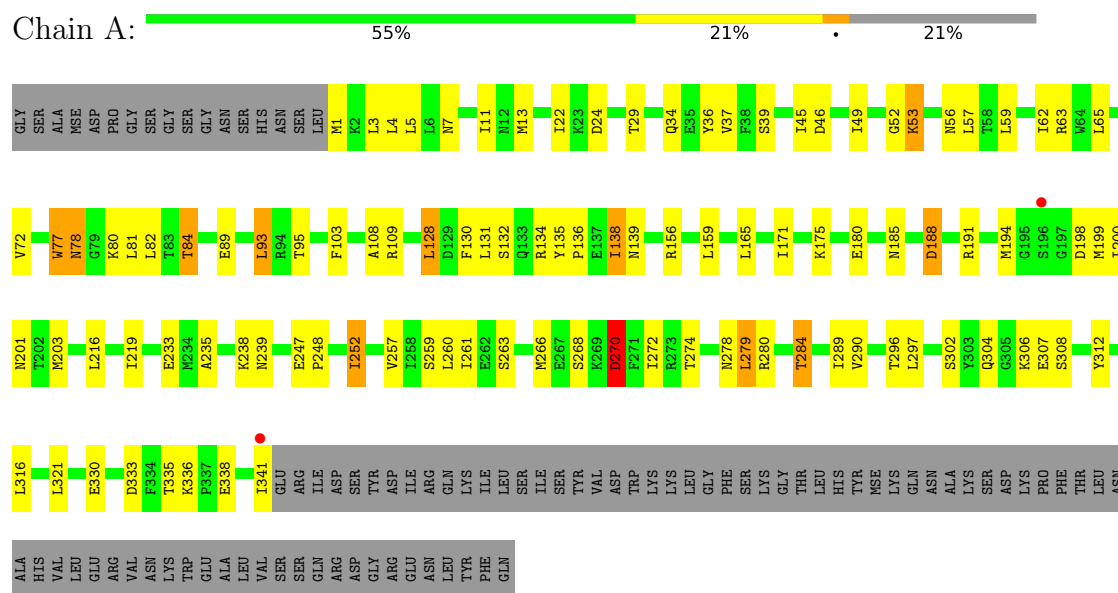
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	11	Total 11	O 11	0	0
5	C	5	Total 5	O 5	0	0
5	D	6	Total 6	O 6	0	0
5	E	3	Total 3	O 3	0	0
5	F	6	Total 6	O 6	0	0

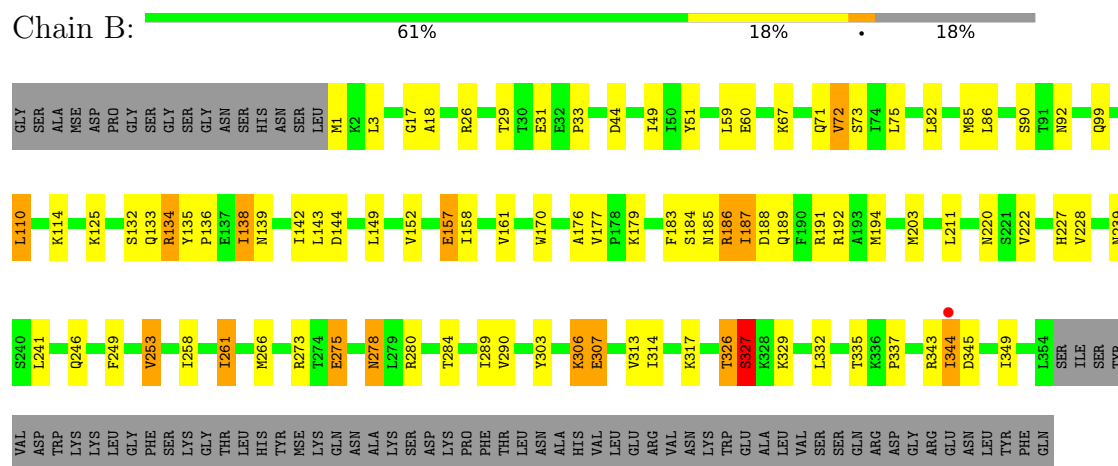
3 Residue-property plots

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

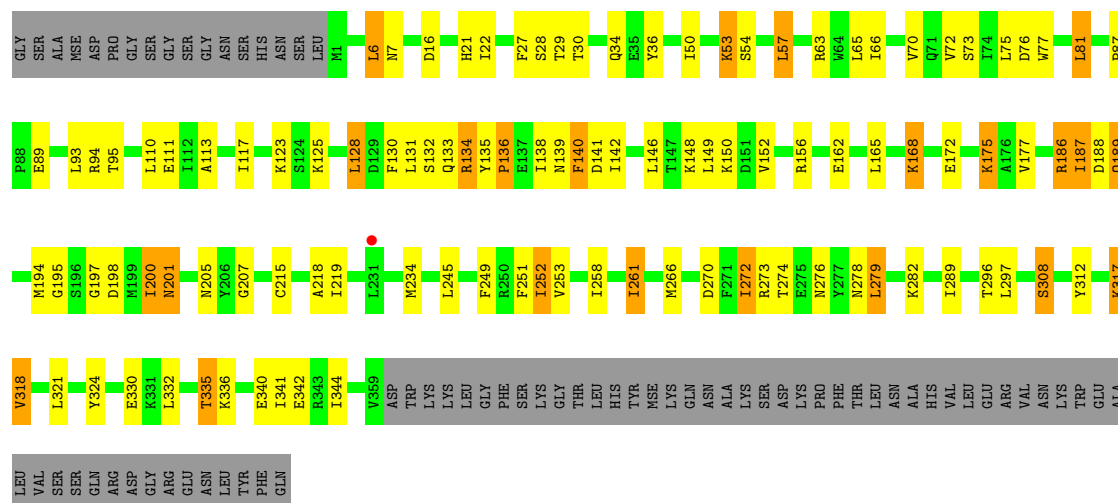


• Molecule 1: CRISPR-associated endonuclease Cas1



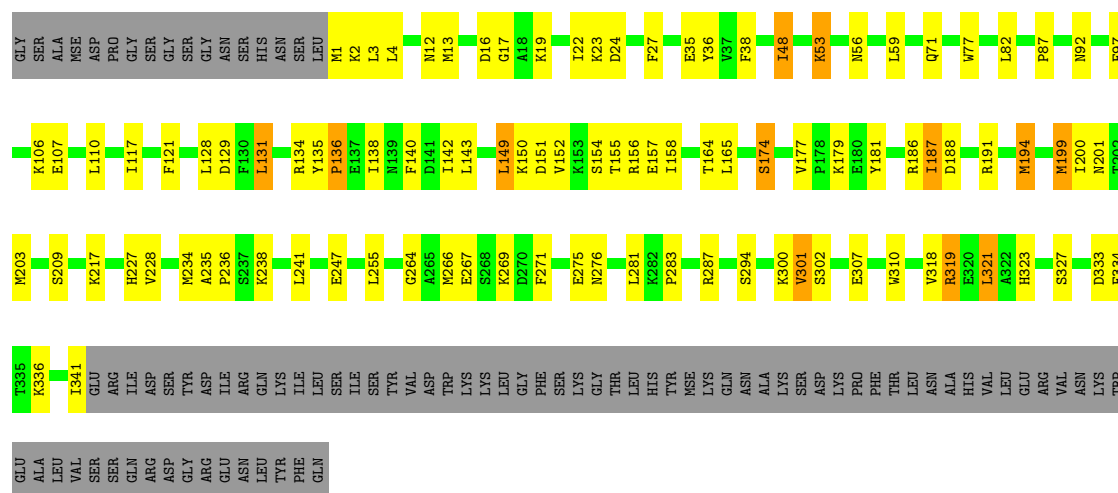
• Molecule 1: CRISPR-associated endonuclease Cas1





- Molecule 1: CRISPR-associated endonuclease Cas1

Chain D: 56% 21% 21%



- Molecule 2: DNA 21-mer

Chain E: 76% 24%



- Molecule 2: DNA 21-mer

Chain F: 67% 33%



- 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, α , β , γ	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) 99.8 (29.89-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	107.5	Xtriage
Anisotropy	0.531	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 105.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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

5.1 Standard geometry

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	0.83	0/2816	1.41	11/3781 (0.3%)
1	B	0.87	1/2909 (0.0%)	1.47	23/3908 (0.6%)
1	C	0.86	0/2936	1.47	22/3945 (0.6%)
1	D	0.83	0/2816	1.42	14/3781 (0.4%)
2	E	0.63	0/473	0.69	0/727
2	F	0.60	0/473	0.70	0/727
All	All	0.83	1/12423 (0.0%)	1.40	70/16869 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	187	ILE	CG1-CD1	-6.38	1.26	1.51

All (70) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	270	ASP	CA-CB-CG	8.24	120.84	112.60
1	B	132	SER	N-CA-C	-7.30	104.90	113.88
1	C	140	PHE	CA-C-N	7.16	135.22	121.54
1	C	140	PHE	C-N-CA	7.16	135.22	121.54
1	B	290	VAL	N-CA-CB	6.63	118.31	110.55
1	B	179	LYS	CA-C-N	6.61	129.43	120.38
1	B	179	LYS	C-N-CA	6.61	129.43	120.38
1	C	138	ILE	N-CA-CB	6.54	118.08	110.82
1	B	278	ASN	CA-CB-CG	6.51	119.11	112.60
1	B	185	ASN	CA-CB-CG	6.51	119.11	112.60
1	D	24	ASP	CA-CB-CG	6.44	119.04	112.60
1	C	201	ASN	N-CA-C	-6.40	104.31	111.28
1	C	270	ASP	CA-CB-CG	6.17	118.77	112.60
1	A	268	SER	CA-C-N	6.04	130.35	120.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	SER	C-N-CA	6.04	130.35	120.63
1	B	51	TYR	N-CA-C	-6.02	100.56	109.11
1	D	179	LYS	CA-C-N	6.02	130.23	120.60
1	D	179	LYS	C-N-CA	6.02	130.23	120.60
1	B	188	ASP	CA-CB-CG	5.87	118.47	112.60
1	C	219	ILE	CA-C-N	5.86	128.41	120.38
1	C	219	ILE	C-N-CA	5.86	128.41	120.38
1	B	136	PRO	CA-C-N	5.84	130.66	122.36
1	B	136	PRO	C-N-CA	5.84	130.66	122.36
1	C	201	ASN	CA-C-N	5.82	128.87	120.79
1	C	201	ASN	C-N-CA	5.82	128.87	120.79
1	B	144	ASP	CA-CB-CG	5.79	118.39	112.60
1	B	183	PHE	CA-C-N	5.72	127.88	120.44
1	B	183	PHE	C-N-CA	5.72	127.88	120.44
1	A	37	VAL	CB-CA-C	5.66	116.86	110.41
1	D	97	PHE	CA-CB-CG	-5.64	108.16	113.80
1	B	326	THR	CA-C-N	5.64	132.32	121.54
1	B	326	THR	C-N-CA	5.64	132.32	121.54
1	C	134	ARG	N-CA-C	-5.62	103.56	110.65
1	B	261	ILE	CA-C-N	5.58	128.07	120.54
1	B	261	ILE	C-N-CA	5.58	128.07	120.54
1	D	264	GLY	CA-C-N	5.56	128.29	120.28
1	D	264	GLY	C-N-CA	5.56	128.29	120.28
1	C	150	LYS	CA-C-N	5.54	128.16	120.29
1	C	150	LYS	C-N-CA	5.54	128.16	120.29
1	B	273	ARG	CA-C-N	5.50	129.06	120.75
1	B	273	ARG	C-N-CA	5.50	129.06	120.75
1	B	239	ASN	CA-C-N	5.43	128.96	120.82
1	B	239	ASN	C-N-CA	5.43	128.96	120.82
1	C	189	GLN	N-CA-C	-5.35	107.77	114.56
1	C	113	ALA	CA-C-N	5.33	127.68	120.38
1	C	113	ALA	C-N-CA	5.33	127.68	120.38
1	A	134	ARG	CA-C-N	5.31	127.59	120.58
1	A	134	ARG	C-N-CA	5.31	127.59	120.58
1	D	247	GLU	CB-CG-CD	5.28	121.58	112.60
1	C	30	THR	N-CA-C	-5.28	108.61	114.62
1	C	70	VAL	N-CA-CB	5.21	118.02	111.46
1	D	188	ASP	CA-CB-CG	5.20	117.80	112.60
1	B	253	VAL	N-CA-CB	5.15	118.31	110.58
1	C	148	LYS	CA-C-N	5.15	127.19	120.28
1	C	148	LYS	C-N-CA	5.15	127.19	120.28
1	B	161	VAL	N-CA-CB	5.13	116.55	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	76	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	24	ASP	CA-CB-CG	5.11	117.71	112.60
1	D	283	PRO	CA-C-N	5.11	127.44	120.54
1	D	283	PRO	C-N-CA	5.11	127.44	120.54
1	D	319	ARG	N-CA-C	-5.11	105.60	111.07
1	D	129	ASP	N-CA-C	-5.07	105.41	111.03
1	A	219	ILE	CA-C-N	5.05	127.01	120.44
1	A	219	ILE	C-N-CA	5.05	127.01	120.44
1	C	187	ILE	CA-C-N	5.05	131.19	121.54
1	C	187	ILE	C-N-CA	5.05	131.19	121.54
1	A	108	ALA	CA-C-N	5.04	127.03	120.28
1	A	108	ALA	C-N-CA	5.04	127.03	120.28
1	D	131	LEU	CA-C-N	5.03	129.95	121.14
1	D	131	LEU	C-N-CA	5.03	129.95	121.14

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	35	0
1	B	2857	0	2873	36	0
1	C	2884	0	2882	50	0
1	D	2765	0	2802	41	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	155	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 (155) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:134:ARG:C	1:D:136:PRO:HD2	2.35	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:90:SER:C	1:B:92:ASN:H	2.23	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: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
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:C:195:GLY:C	1:C:197:GLY:H	2.24	0.45
1:A:252:ILE:HG13	1:A:296:THR:HG22	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:109:ARG:HH22	1:A:233:GLU:CD	2.27	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:C:130:PHE:C	1:C:132:SER:H	2.27	0.42
1:A:130:PHE:C	1:A:132:SER:H	2.27	0.42
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: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
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:D:27:PHE:HE2	1:D:53:LYS:NZ	2.19	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:ILE:HG21	1:C:297:LEU:HD13	2.04	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%)	6	28
1	B	352/431 (82%)	320 (91%)	26 (7%)	6 (2%)	7	30
1	C	357/431 (83%)	317 (89%)	33 (9%)	7 (2%)	6	25
1	D	339/431 (79%)	309 (91%)	24 (7%)	6 (2%)	6	28
All	All	1387/1724 (80%)	1246 (90%)	116 (8%)	25 (2%)	6	28

All (25) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
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%)	255 (84%)	47 (16%)	2	12
1	B	309/371 (83%)	276 (89%)	33 (11%)	6	25
1	C	311/371 (84%)	270 (87%)	41 (13%)	4	17
1	D	302/371 (81%)	259 (86%)	43 (14%)	3	14
All	All	1224/1484 (82%)	1060 (87%)	164 (13%)	4	17

All (164) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	LEU
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

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Mol	Chain	Res	Type
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	156	ARG
1	A	159	LEU
1	A	165	LEU
1	A	171	ILE
1	A	175	LYS
1	A	180	GLU
1	A	185	ASN
1	A	188	ASP
1	A	194	MSE
1	A	200	ILE
1	A	252	ILE
1	A	261	ILE
1	A	266	MSE
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
1	A	338	GLU
1	A	341	ILE
1	B	1	MSE
1	B	3	LEU
1	B	29	THR
1	B	31	GLU

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Mol	Chain	Res	Type
1	B	44	ASP
1	B	49	ILE
1	B	59	LEU
1	B	60	GLU
1	B	72	VAL
1	B	73	SER
1	B	110	LEU
1	B	133	GLN
1	B	134	ARG
1	B	138	ILE
1	B	139	ASN
1	B	157	GLU
1	B	177	VAL
1	B	184	SER
1	B	186	ARG
1	B	189	GLN
1	B	222	VAL
1	B	253	VAL
1	B	266	MSE
1	B	275	GLU
1	B	278	ASN
1	B	280	ARG
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	B	344	ILE
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
1	C	81	LEU
1	C	89	GLU
1	C	95	THR

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Mol	Chain	Res	Type
1	C	110	LEU
1	C	111	GLU
1	C	128	LEU
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	175	LYS
1	C	186	ARG
1	C	189	GLN
1	C	194	MSE
1	C	200	ILE
1	C	252	ILE
1	C	258	ILE
1	C	261	ILE
1	C	266	MSE
1	C	272	ILE
1	C	279	LEU
1	C	289	ILE
1	C	308	SER
1	C	317	LYS
1	C	318	VAL
1	C	321	LEU
1	C	330	GLU
1	C	335	THR
1	D	2	LYS
1	D	3	LEU
1	D	4	LEU
1	D	16	ASP
1	D	19	LYS
1	D	35	GLU
1	D	48	ILE
1	D	53	LYS
1	D	56	ASN
1	D	107	GLU
1	D	110	LEU
1	D	131	LEU
1	D	138	ILE
1	D	143	LEU

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Mol	Chain	Res	Type
1	D	149	LEU
1	D	151	ASP
1	D	154	SER
1	D	156	ARG
1	D	164	THR
1	D	165	LEU
1	D	174	SER
1	D	186	ARG
1	D	187	ILE
1	D	194	MSE
1	D	199	MSE
1	D	201	ASN
1	D	217	LYS
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	301	VAL
1	D	318	VAL
1	D	321	LEU
1	D	333	ASP
1	D	336	LYS
1	D	341	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	ASN
1	A	34	GLN
1	A	56	ASN
1	A	78	ASN
1	A	139	ASN
1	A	227	HIS
1	A	246	GLN
1	A	278	ASN
1	A	291	ASN

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Mol	Chain	Res	Type
1	B	12	ASN
1	B	92	ASN
1	B	227	HIS
1	C	9	HIS
1	C	21	HIS
1	C	133	GLN
1	C	189	GLN
1	C	201	ASN
1	C	205	ASN
1	C	239	ASN
1	C	278	ASN
1	C	298	ASN
1	D	7	ASN
1	D	12	ASN
1	D	71	GLN
1	D	278	ASN
1	D	291	ASN
1	D	304	GLN
1	D	323	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	333/431 (77%)	-0.28	2 (0%) 85 70	95, 152, 208, 261	0
1	B	346/431 (80%)	-0.41	1 (0%) 90 80	86, 124, 189, 235	0
1	C	351/431 (81%)	-0.39	1 (0%) 90 80	89, 134, 211, 242	0
1	D	333/431 (77%)	-0.44	0 100 100	92, 139, 190, 212	0
2	E	21/21 (100%)	-0.59	0 100 100	99, 114, 141, 237	0
2	F	21/21 (100%)	-0.53	0 100 100	95, 105, 159, 229	0
3	H	0/13	-	-	-	-
3	J	0/13	-	-	-	-
All	All	1405/1792 (78%)	-0.39	4 (0%) 90 80	86, 136, 202, 261	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	SER	5.2
1	B	344	ILE	2.9
1	A	341	ILE	2.4
1	C	231	LEU	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	CA	C	501	1/1	0.66	0.26	165,165,165,165	0
4	CA	A	502	1/1	0.83	0.13	178,178,178,178	0
4	CA	A	501	1/1	0.89	0.12	157,157,157,157	0
4	CA	C	502	1/1	0.91	0.07	149,149,149,149	0
4	CA	E	101	1/1	0.94	0.10	112,112,112,112	0
4	CA	F	101	1/1	0.99	0.07	98,98,98,98	0

6.5 Other polymers [i](#)

There are no such residues in this entry.