



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 12:19 AM UTC

PDB ID : 7VYX / pdb_00007vyx
Title : Crystal structure of the selenomethionine(SeMet)-derived Cas12c1 (D969A) ternary complex
Authors : Zhang, B.; Lin, J.Y.; Perculija, V.; OuYang, S.Y.
Deposited on : 2021-11-15
Resolution : 3.20 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

<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

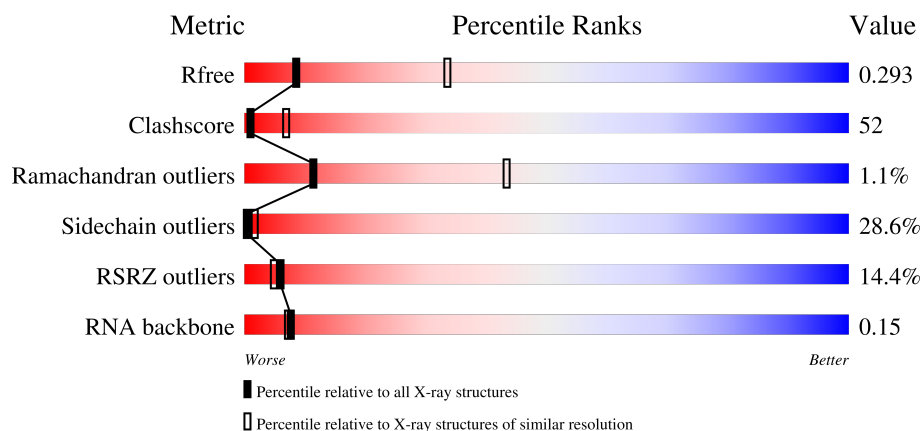
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 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	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)
RNA backbone	3983	1222 (3.50-2.90)

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	1310	
1	B	1310	
2	C	136	
2	D	136	

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Mol	Chain	Length	Quality of chain
3	E	31	13%45%16%10%29%
3	F	31	10%52%23%10%16%
4	G	23	9%9%30%9%52%
4	H	23	4%13%35%52%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 24465 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 Selenomethionine (SeMet)-labeled Cas12c1 D969A mutant.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	1211	Total	C	N	O	S	Se	0	0	0
			9533	6075	1639	1788	20	11			
1	B	1193	Total	C	N	O	S	Se	0	0	0
			9369	5977	1607	1754	20	11			

- Molecule 2 is a RNA chain called sgRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	103	Total	C	N	O	P	0	0	0
			2188	978	387	720	103			
2	D	91	Total	C	N	O	P	0	0	0
			1934	865	344	634	91			

- Molecule 3 is a DNA chain called Target DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	22	Total	C	N	O	P	0	0	0
			451	216	78	135	22			
3	F	26	Total	C	N	O	P	0	0	0
			534	256	92	160	26			

- Molecule 4 is a DNA chain called Non-target DNA strand.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	G	11	Total	C	N	O	P	0	0	0
			227	108	42	66	11			
4	H	11	Total	C	N	O	P	0	0	0
			227	108	42	66	11			

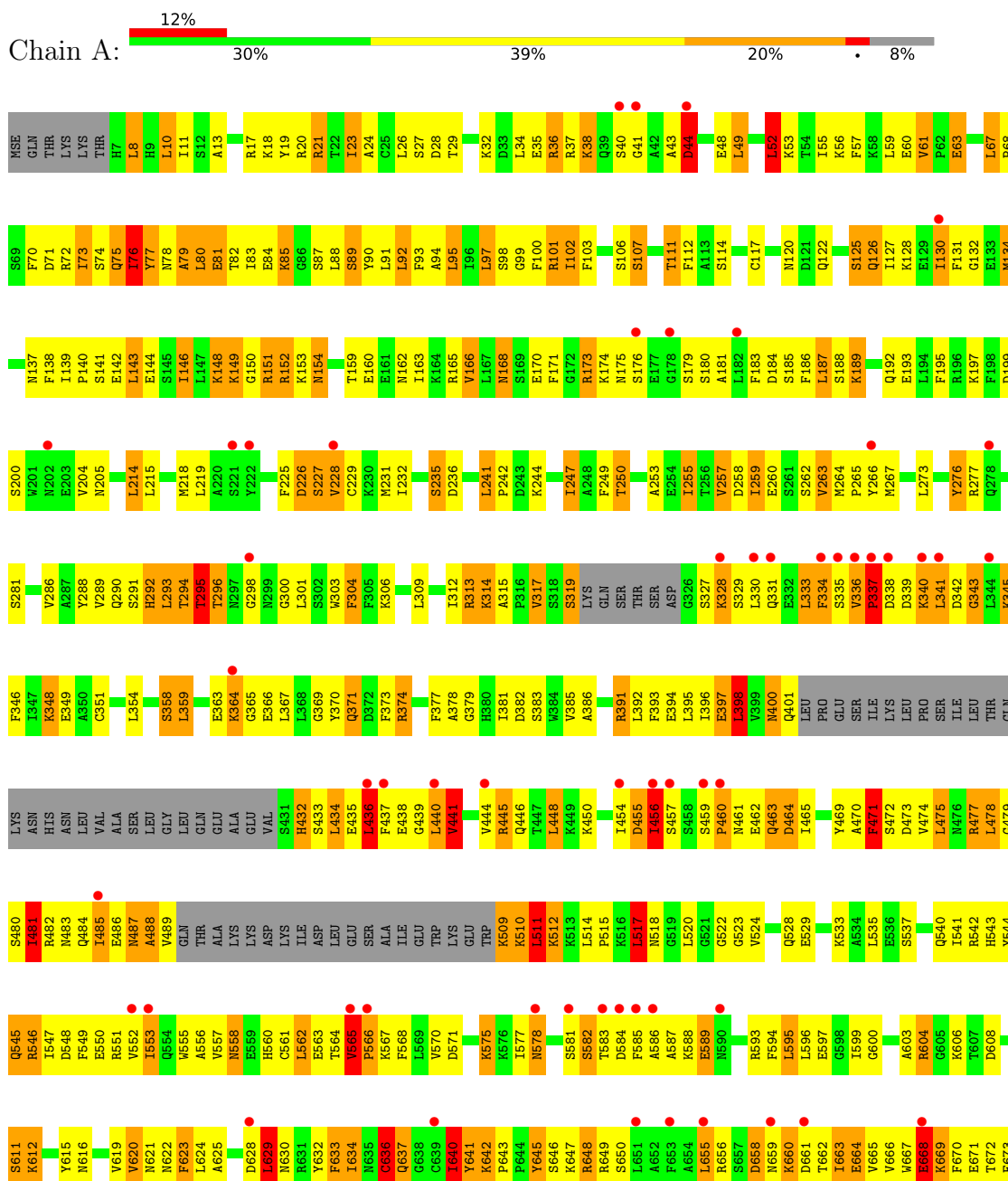
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total 1	Zn 1	0	0
5	B	1	Total 1	Zn 1	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.

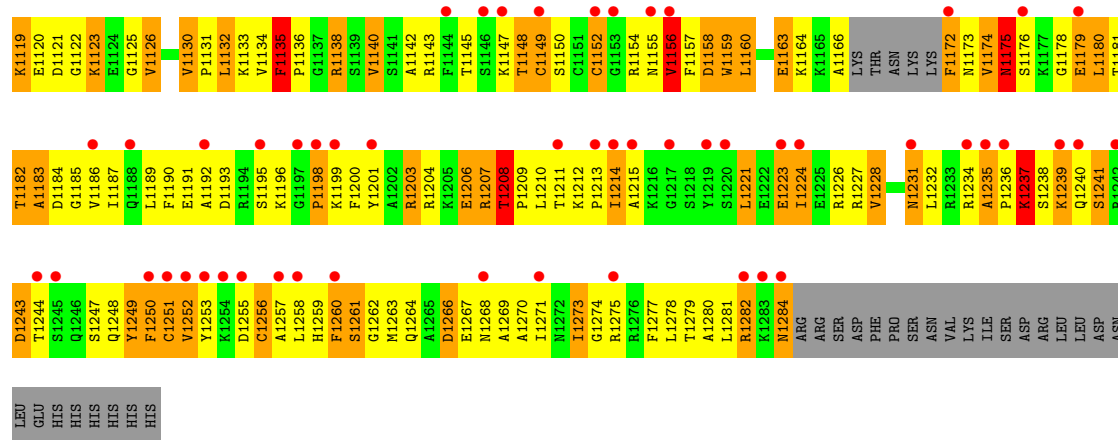
- Molecule 1: Selenomethionine (SeMet)-labeled Cas12c1 D969A mutant



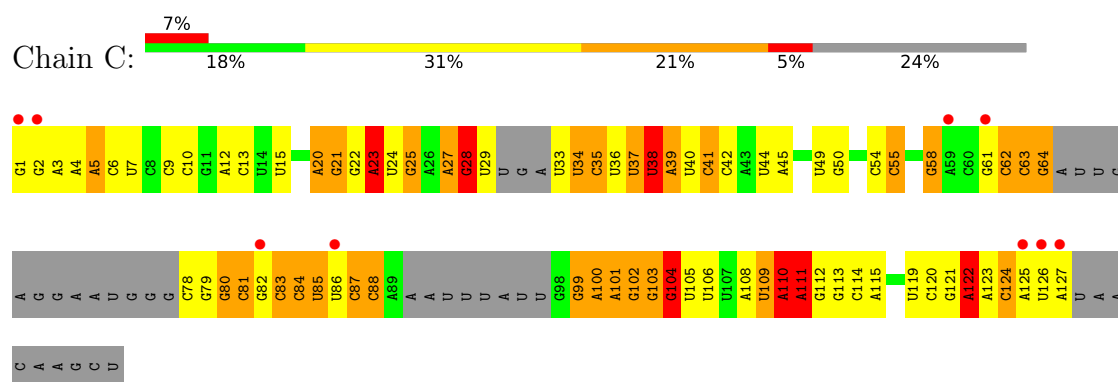


E142	I73	R5E
L143	S74	GLN
E144	Q75	THR
S145	I76	LVS
I146	Y77	LVS
L147	N78	THR
K148	A79	HIS
K149	L80	L8
G150	E81	H9
R151	T82	L10
R152	I83	
K153	E84	A13
M154		K14
M155	L88	A15
S156	S89	S16
D157	Y90	R17
W158	L91	
T159	L92	R20
E160		R21
E161	L95	T22
M162	I96	I23
I163	L97	A24
	S98	C25
V166	G99	L26
L167	F100	S27
M168	R101	D28
S169	I102	T29
E170	F103	A30
F171		K31
G172	S107	
R173		L34
K174	K110	E35
M175	T111	R36
S176	F112	A37
	A113	K38
	S114	
S180		D44
A181	C117	P45
F183	Y118	A46
D184	K119	Q47
S185	N120	F48
F186	D121	L49
L187	Q122	
S188	F123	L52
K189	A124	K53
F190	S125	T54
S191	Q126	I55
Q192	I127	
E193	K128	K58
	E129	L59
R196	I130	E60
F197		V61
F198	M134	P62
D199	V135	E63
	K136	
S200	N137	L67
W201	F138	P68
M202	I139	
E203	A140	
V204	S141	D71
S205		S72

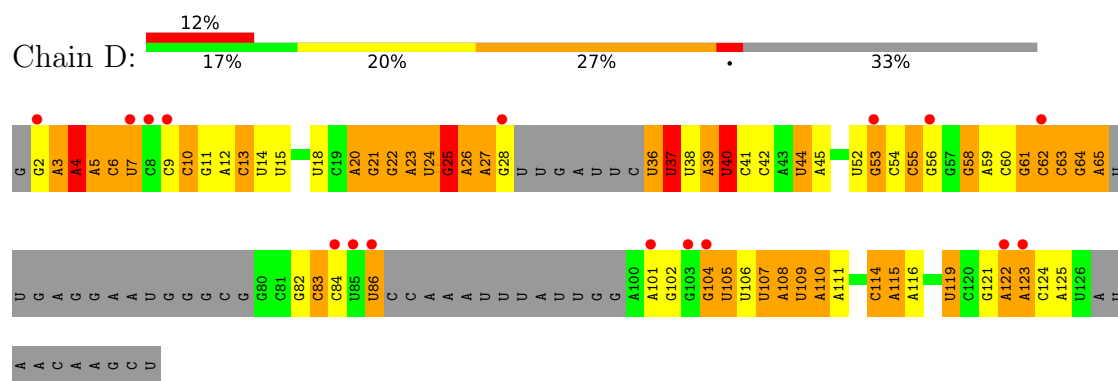




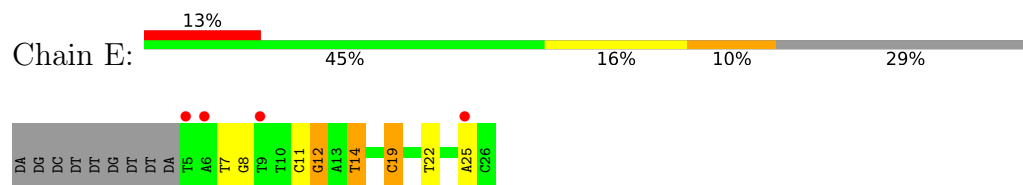
• Molecule 2: sgRNA



• Molecule 2: sgRNA

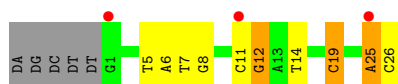


• Molecule 3: Target DNA strand

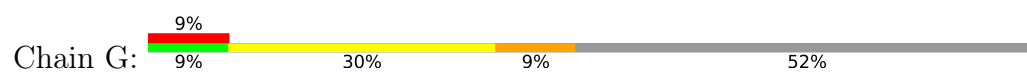


• Molecule 3: Target DNA strand

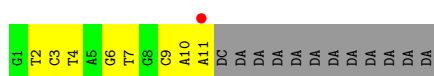




- Molecule 4: Non-target DNA strand



- Molecule 4: Non-target DNA strand



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	93.13Å 149.85Å 173.25Å 90.00° 91.59° 90.00°	Depositor
Resolution (Å)	49.73 – 3.20 49.73 – 3.20	Depositor EDS
% Data completeness (in resolution range)	79.4 (49.73-3.20) 79.4 (49.73-3.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 3.19Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.256 , 0.292 0.256 , 0.293	Depositor DCC
R_{free} test set	2973 reflections (3.79%)	wwPDB-VP
Wilson B-factor (Å ²)	53.0	Xtriage
Anisotropy	0.063	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 73.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.045 for h,-k,-l	Xtriage
F_o, F_c correlation	0.83	EDS
Total number of atoms	24465	wwPDB-VP
Average B, all atoms (Å ²)	73.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.86% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	1.70	70/9713 (0.7%)	1.50	185/13105 (1.4%)
1	B	1.56	52/9549 (0.5%)	1.51	197/12891 (1.5%)
2	C	0.73	5/2441 (0.2%)	0.99	9/3793 (0.2%)
2	D	0.65	2/2158 (0.1%)	1.00	7/3352 (0.2%)
3	E	0.56	0/504	1.05	6/776 (0.8%)
3	F	0.55	0/597	1.00	6/920 (0.7%)
4	G	0.96	1/254 (0.4%)	0.99	1/390 (0.3%)
4	H	0.49	0/254	0.87	0/390
All	All	1.46	130/25470 (0.5%)	1.39	411/35617 (1.2%)

The worst 5 of 130 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1190	PHE	C-N	15.43	1.55	1.33
1	A	337	PRO	N-CD	14.04	1.67	1.47
1	A	290	GLN	C-N	10.83	1.47	1.33
1	B	956	PRO	N-CD	10.11	1.61	1.47
1	A	515	PRO	N-CD	9.99	1.61	1.47

The worst 5 of 411 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	731	PRO	CA-C-N	17.75	138.00	119.19
1	B	731	PRO	C-N-CA	17.75	138.00	119.19
1	A	731	PRO	CA-C-N	17.61	137.53	119.56
1	A	731	PRO	C-N-CA	17.61	137.53	119.56
1	A	1235	ALA	CA-C-N	17.42	137.45	119.85

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	9533	0	9379	1025	0
1	B	9369	0	9165	1103	0
2	C	2188	0	1113	139	0
2	D	1934	0	984	123	0
3	E	451	0	251	10	0
3	F	534	0	297	7	0
4	G	227	0	125	15	0
4	H	227	0	125	6	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
All	All	24465	0	21439	2367	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 52.

The worst 5 of 2367 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:B:1159:TRP:CH2	1:B:1183:ALA:HB2	1.29	1.67
1:B:565:VAL:HB	1:B:708:ARG:CD	1.31	1.60
1:B:565:VAL:CB	1:B:708:ARG:HD3	1.34	1.52
1:A:444:VAL:HG21	1:A:471:PHE:CD2	1.43	1.49
1:A:1201:TYR:CE2	1:A:1209:PRO:HD2	1.48	1.47

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	1197/1310 (91%)	1130 (94%)	59 (5%)	8 (1%)	18	52
1	B	1177/1310 (90%)	1092 (93%)	68 (6%)	17 (1%)	9	39
All	All	2374/2620 (91%)	2222 (94%)	127 (5%)	25 (1%)	11	43

5 of 25 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	656	ARG
1	B	841	ARG
1	A	175	ASN
1	A	328	LYS
1	A	881	VAL

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	1018/1144 (89%)	729 (72%)	289 (28%)	0	2
1	B	993/1144 (87%)	707 (71%)	286 (29%)	0	1
All	All	2011/2288 (88%)	1436 (71%)	575 (29%)	0	2

5 of 575 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	811	LEU
1	B	1282	ARG
1	B	861	VAL
1	B	806	GLU
1	B	1037	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 59 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	9	HIS
1	B	1259	HIS
1	B	205	ASN
1	B	1240	GLN
1	B	961	GLN

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	99/136 (72%)	51 (51%)	9 (9%)
2	D	87/136 (63%)	49 (56%)	5 (5%)
All	All	186/272 (68%)	100 (53%)	14 (7%)

5 of 100 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	2	G
2	C	5	A
2	C	7	U
2	C	13	C
2	C	15	U

5 of 14 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	C	110	A
2	C	114	C
2	D	114	C
2	D	82	G
2	D	110	A

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

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

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	1200/1310 (91%)	0.82	159 (13%) 7 6	12, 61, 132, 179	0
1	B	1182/1310 (90%)	0.99	186 (15%) 5 4	16, 72, 129, 161	0
2	C	103/136 (75%)	0.79	9 (8%) 16 11	10, 81, 167, 198	0
2	D	91/136 (66%)	1.10	16 (17%) 4 3	13, 97, 168, 199	0
3	E	22/31 (70%)	0.64	4 (18%) 3 3	9, 44, 145, 166	0
3	F	26/31 (83%)	0.86	3 (11%) 9 7	14, 63, 139, 152	0
4	G	11/23 (47%)	0.75	2 (18%) 3 3	23, 41, 91, 122	0
4	H	11/23 (47%)	0.58	1 (9%) 15 9	26, 38, 78, 132	0
All	All	2646/3000 (88%)	0.90	380 (14%) 6 5	9, 67, 139, 199	0

The worst 5 of 380 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	733	ASN	12.5
1	A	1187	ILE	8.3
1	A	1178	GLY	7.6
1	A	1189	LEU	6.0
1	B	1224	ILE	5.8

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($\text{\AA}^2$)	Q<0.9
5	ZN	B	1401	1/1	0.91	0.08	79,79,79,79	0
5	ZN	A	1401	1/1	0.96	0.04	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.