



wwPDB X-ray Structure Validation Summary Report ⓘ

Jun 13, 2022 – 12:03 PM EDT

PDB ID : 7N9V
Title : CA-targeting nanobody is a tool for studying HIV-1 capsid lattice interactions
Authors : Tripler, T.N.
Deposited on : 2021-06-18
Resolution : 3.45 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.13
EDS	:	2.28.1
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)	:	2.28.1

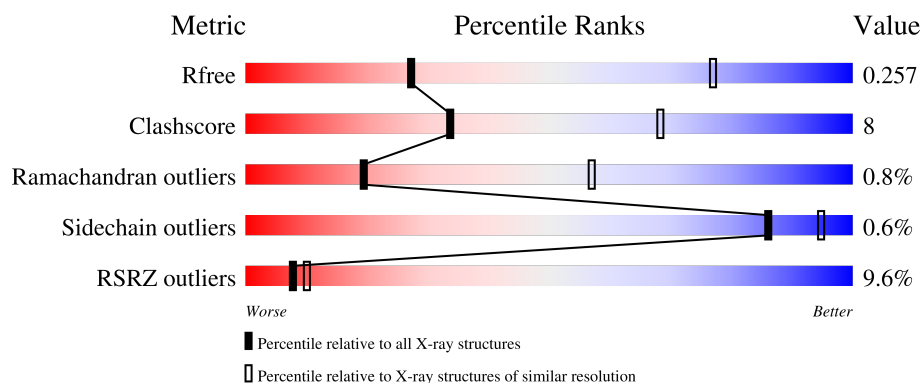
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION






The reported resolution of this entry is 3.45 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	1291 (3.52-3.40)
Clashscore	141614	1372 (3.52-3.40)
Ramachandran outliers	138981	1337 (3.52-3.40)
Sidechain outliers	138945	1338 (3.52-3.40)
RSRZ outliers	127900	1205 (3.52-3.40)

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	223	
1	C	223	
1	D	223	
1	G	223	
1	I	223	

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Mol	Chain	Length	Quality of chain
1	K	223	<p>2% 84% 13%</p>
2	B	113	<p>54% 76% 22%</p>
2	E	113	<p>22% 73% 26%</p>
2	F	113	<p>9% 79% 19%</p>
2	H	113	<p>45% 82% 16%</p>
2	J	113	<p>8% 81% 19%</p>
2	L	113	<p>21% 74% 25%</p>

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 15089 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 Capsid protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	216	Total	C	N	O	S	0	0	0
			1643	1034	285	310	14			
1	A	217	Total	C	N	O	S	0	0	0
			1652	1039	287	312	14			
1	D	220	Total	C	N	O	S	0	0	0
			1668	1049	290	315	14			
1	G	223	Total	C	N	O	S	0	0	0
			1678	1058	292	314	14			
1	I	223	Total	C	N	O	S	0	0	0
			1687	1062	293	318	14			
1	K	218	Total	C	N	O	S	0	0	0
			1649	1040	286	309	14			

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	14	CYS	ALA	conflict	UNP B6DRA0
C	45	CYS	GLU	conflict	UNP B6DRA0
C	184	ALA	TRP	conflict	UNP B6DRA0
C	185	ALA	MET	conflict	UNP B6DRA0
C	223	PRO	-	expression tag	UNP B6DRA0
A	14	CYS	ALA	conflict	UNP B6DRA0
A	45	CYS	GLU	conflict	UNP B6DRA0
A	184	ALA	TRP	conflict	UNP B6DRA0
A	185	ALA	MET	conflict	UNP B6DRA0
A	223	PRO	-	expression tag	UNP B6DRA0
D	14	CYS	ALA	conflict	UNP B6DRA0
D	45	CYS	GLU	conflict	UNP B6DRA0
D	184	ALA	TRP	conflict	UNP B6DRA0
D	185	ALA	MET	conflict	UNP B6DRA0
D	223	PRO	-	expression tag	UNP B6DRA0
G	14	CYS	ALA	conflict	UNP B6DRA0
G	45	CYS	GLU	conflict	UNP B6DRA0

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Chain	Residue	Modelled	Actual	Comment	Reference
G	184	ALA	TRP	conflict	UNP B6DRA0
G	185	ALA	MET	conflict	UNP B6DRA0
G	223	PRO	-	expression tag	UNP B6DRA0
I	14	CYS	ALA	conflict	UNP B6DRA0
I	45	CYS	GLU	conflict	UNP B6DRA0
I	184	ALA	TRP	conflict	UNP B6DRA0
I	185	ALA	MET	conflict	UNP B6DRA0
I	223	PRO	-	expression tag	UNP B6DRA0
K	14	CYS	ALA	conflict	UNP B6DRA0
K	45	CYS	GLU	conflict	UNP B6DRA0
K	184	ALA	TRP	conflict	UNP B6DRA0
K	185	ALA	MET	conflict	UNP B6DRA0
K	223	PRO	-	expression tag	UNP B6DRA0

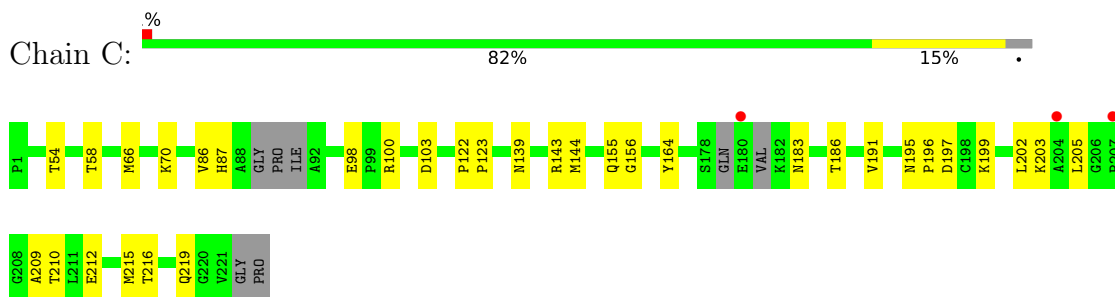
- Molecule 2 is a protein called Nanobody-GYAR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	113	Total	C	N	O	S	0	0	0
			852	534	151	163	4			
2	B	113	Total	C	N	O	S	0	0	0
			852	534	151	163	4			
2	E	113	Total	C	N	O	S	0	0	0
			852	534	151	163	4			
2	F	113	Total	C	N	O	S	0	0	0
			852	534	151	163	4			
2	H	113	Total	C	N	O	S	0	0	0
			852	534	151	163	4			
2	L	113	Total	C	N	O	S	0	0	0
			852	534	151	163	4			

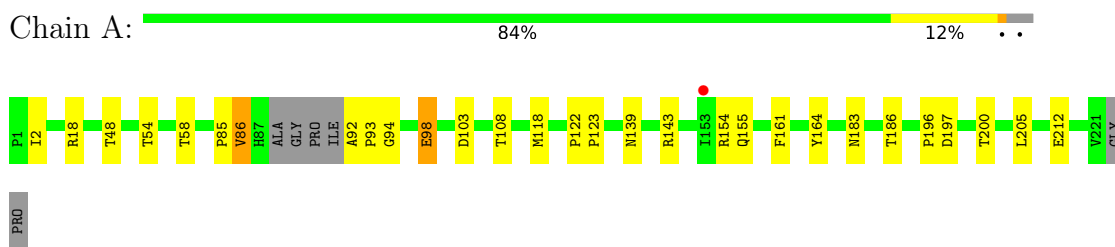
3 Residue-property plots [i](#)

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.

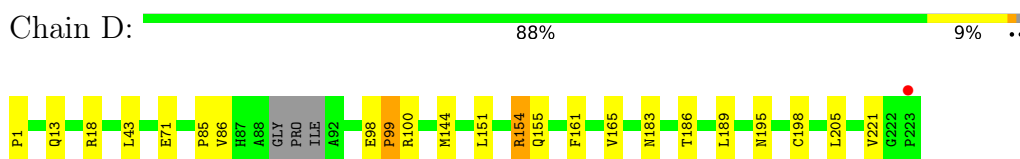
- Molecule 1: Capsid protein



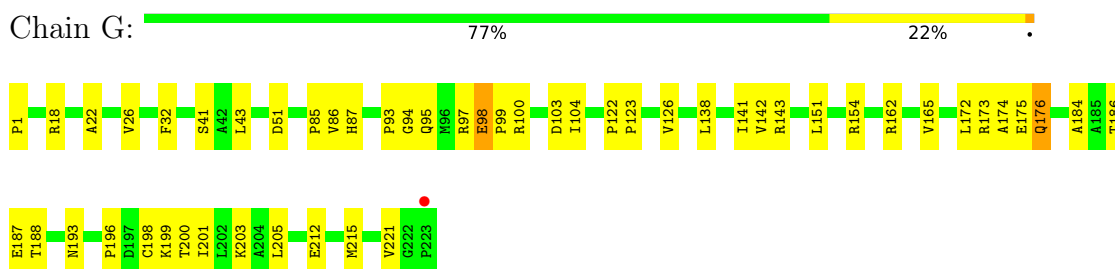
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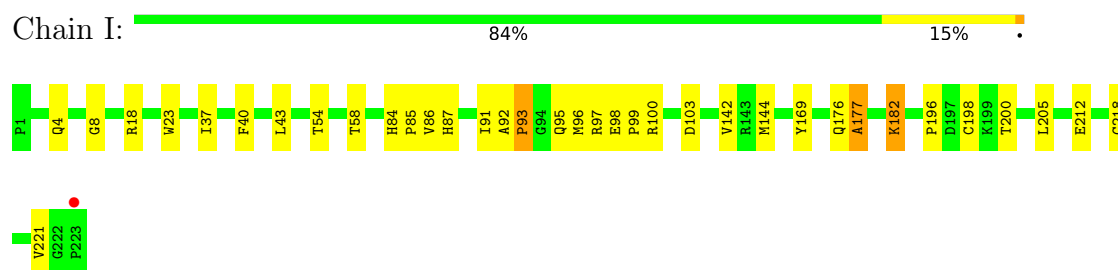
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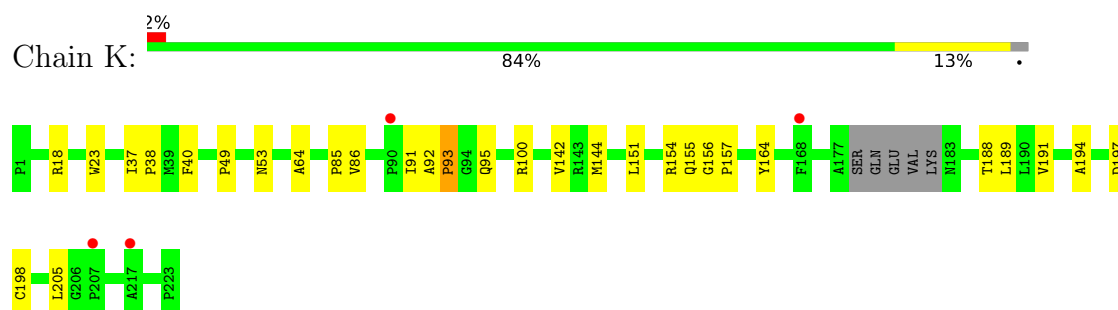
- Molecule 1: Capsid protein



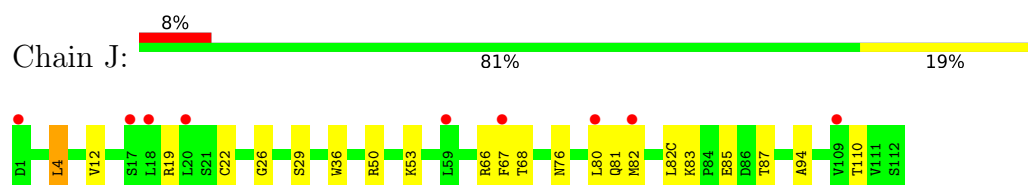
- Molecule 1: Capsid protein



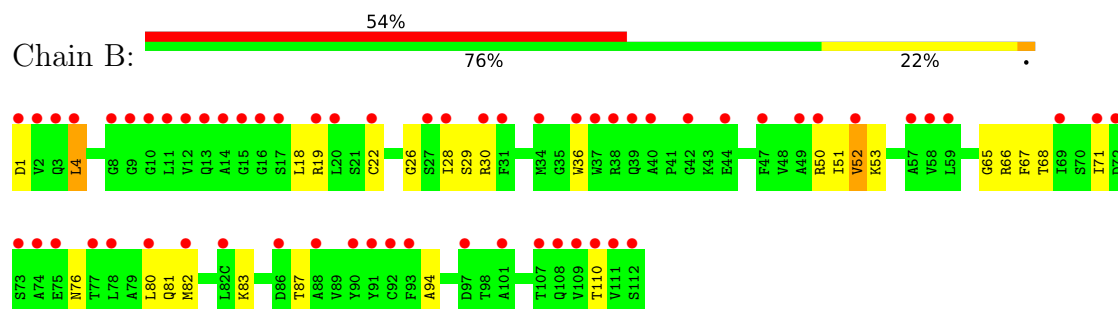
- Molecule 1: Capsid protein



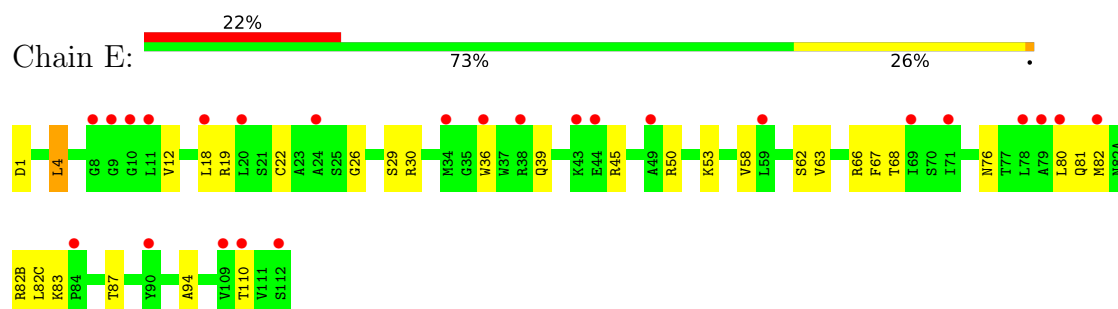
- Molecule 2: Nanobody-GYAR



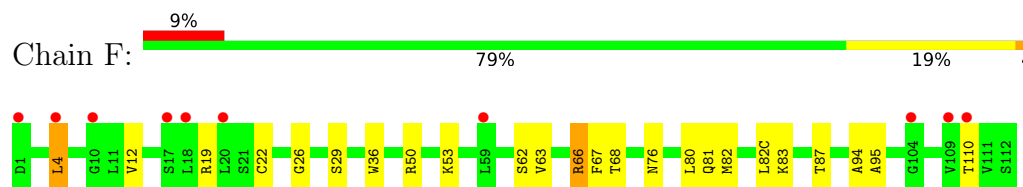
- Molecule 2: Nanobody-GYAR



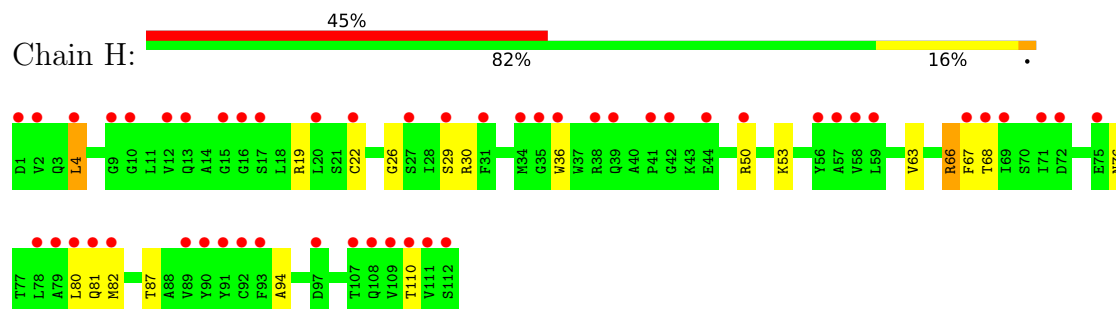
- Molecule 2: Nanobody-GYAR



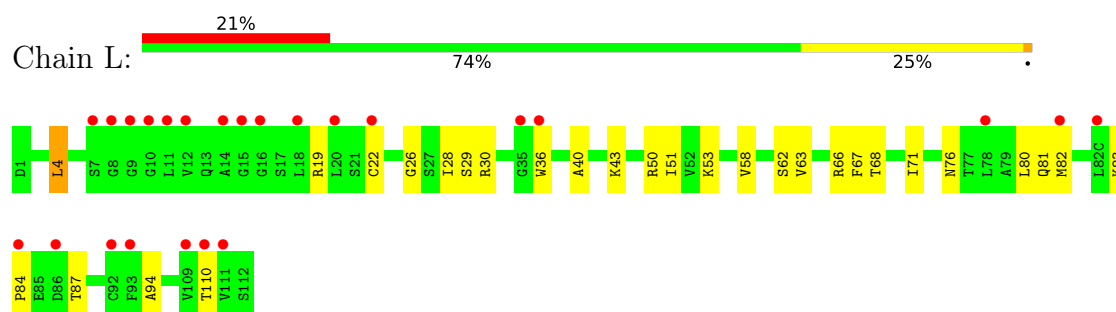
● Molecule 2: Nanobody-GYAR



● Molecule 2: Nanobody-GYAR



● Molecule 2: Nanobody-GYAR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.55Å 140.38Å 125.19Å 90.00° 113.90° 90.00°	Depositor
Resolution (Å)	46.88 – 3.45 46.88 – 3.45	Depositor EDS
% Data completeness (in resolution range)	91.9 (46.88-3.45) 92.0 (46.88-3.45)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.59 (at 3.48Å)	Xtriage
Refinement program	PHENIX 1.19.1_4122	Depositor
R, R_{free}	0.212 , 0.258 0.211 , 0.257	Depositor DCC
R_{free} test set	1998 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	116.1	Xtriage
Anisotropy	0.381	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 82.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	15089	wwPDB-VP
Average B, all atoms (Å ²)	168.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.79% 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](#)

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	0.33	0/1686	0.65	1/2292 (0.0%)
1	C	0.34	0/1675	0.67	1/2274 (0.0%)
1	D	0.33	0/1703	0.62	0/2316
1	G	0.35	0/1715	0.69	0/2336
1	I	0.35	0/1724	0.70	3/2347 (0.1%)
1	K	0.36	0/1685	0.68	1/2294 (0.0%)
2	B	0.45	1/867 (0.1%)	0.96	3/1172 (0.3%)
2	E	0.41	0/867	0.95	3/1172 (0.3%)
2	F	0.41	0/867	0.94	3/1172 (0.3%)
2	H	0.41	0/867	0.94	3/1172 (0.3%)
2	J	0.44	0/867	0.97	3/1172 (0.3%)
2	L	0.44	0/867	0.97	3/1172 (0.3%)
All	All	0.37	1/15390 (0.0%)	0.78	24/20891 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	52	VAL	CB-CG1	-5.60	1.41	1.52

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	4	LEU	CA-CB-CG	13.28	145.84	115.30
2	H	4	LEU	CA-CB-CG	13.10	145.44	115.30
2	F	4	LEU	CA-CB-CG	13.01	145.21	115.30
2	J	4	LEU	CA-CB-CG	12.82	144.78	115.30
2	E	4	LEU	CA-CB-CG	12.79	144.73	115.30

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	1652	0	1616	22	0
1	C	1643	0	1609	23	0
1	D	1668	0	1631	17	0
1	G	1678	0	1640	42	0
1	I	1687	0	1653	26	0
1	K	1649	0	1618	23	0
2	B	852	0	836	22	0
2	E	852	0	836	22	0
2	F	852	0	836	20	0
2	H	852	0	836	16	0
2	J	852	0	836	23	0
2	L	852	0	836	24	0
All	All	15089	0	14783	253	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 8.

The worst 5 of 253 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:66:ARG:HH12	2:J:83:LYS:HE2	1.27	0.99
2:J:29:SER:O	2:J:53:LYS:NZ	2.09	0.85
2:B:29:SER:O	2:B:53:LYS:NZ	2.11	0.84
2:L:29:SER:O	2:L:53:LYS:NZ	2.11	0.84
1:K:92:ALA:HB1	1:K:95:GLN:O	1.77	0.83

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	213/223 (96%)	208 (98%)	2 (1%)	3 (1%)	11	44
1	C	209/223 (94%)	205 (98%)	3 (1%)	1 (0%)	29	66
1	D	216/223 (97%)	211 (98%)	3 (1%)	2 (1%)	17	54
1	G	221/223 (99%)	212 (96%)	5 (2%)	4 (2%)	8	39
1	I	221/223 (99%)	213 (96%)	5 (2%)	3 (1%)	11	44
1	K	214/223 (96%)	209 (98%)	3 (1%)	2 (1%)	17	54
2	B	111/113 (98%)	108 (97%)	3 (3%)	0	100	100
2	E	111/113 (98%)	108 (97%)	3 (3%)	0	100	100
2	F	111/113 (98%)	108 (97%)	3 (3%)	0	100	100
2	H	111/113 (98%)	108 (97%)	3 (3%)	0	100	100
2	J	111/113 (98%)	108 (97%)	3 (3%)	0	100	100
2	L	111/113 (98%)	108 (97%)	3 (3%)	0	100	100
All	All	1960/2016 (97%)	1906 (97%)	39 (2%)	15 (1%)	19	57

5 of 15 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	86	VAL
1	G	94	GLY
1	G	98	GLU
1	I	86	VAL
1	A	94	GLY

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	174/188 (93%)	172 (99%)	2 (1%)	73	88
1	C	173/188 (92%)	173 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	175/188 (93%)	174 (99%)	1 (1%)	86	95
1	G	174/188 (93%)	173 (99%)	1 (1%)	86	95
1	I	177/188 (94%)	176 (99%)	1 (1%)	86	95
1	K	173/188 (92%)	173 (100%)	0	100	100
2	B	86/86 (100%)	85 (99%)	1 (1%)	71	87
2	E	86/86 (100%)	85 (99%)	1 (1%)	71	87
2	F	86/86 (100%)	85 (99%)	1 (1%)	71	87
2	H	86/86 (100%)	85 (99%)	1 (1%)	71	87
2	J	86/86 (100%)	86 (100%)	0	100	100
2	L	86/86 (100%)	86 (100%)	0	100	100
All	All	1562/1644 (95%)	1553 (99%)	9 (1%)	86	95

5 of 9 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	F	66	ARG
2	H	66	ARG
1	G	41	SER
1	I	182	LYS
2	B	1	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	139	ASN
1	D	195	ASN
1	G	193	ASN

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 [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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 [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	217/223 (97%)	-0.05	1 (0%) 91 89	76, 127, 203, 275	0
1	C	216/223 (96%)	-0.03	3 (1%) 75 72	62, 102, 237, 283	0
1	D	220/223 (98%)	-0.08	1 (0%) 91 89	67, 125, 192, 281	0
1	G	223/223 (100%)	-0.09	1 (0%) 92 90	70, 112, 208, 296	0
1	I	223/223 (100%)	-0.15	1 (0%) 92 90	71, 112, 203, 274	0
1	K	218/223 (97%)	-0.08	4 (1%) 68 65	70, 127, 245, 312	0
2	B	113/113 (100%)	2.77	61 (53%) 0 0	227, 324, 432, 657	0
2	E	113/113 (100%)	1.12	25 (22%) 0 1	151, 245, 316, 354	0
2	F	113/113 (100%)	0.54	10 (8%) 10 12	118, 196, 245, 321	0
2	H	113/113 (100%)	2.00	51 (45%) 0 0	210, 307, 399, 484	0
2	J	113/113 (100%)	0.48	9 (7%) 12 14	117, 180, 248, 277	0
2	L	113/113 (100%)	1.09	24 (21%) 0 1	152, 235, 397, 446	0
All	All	1995/2016 (98%)	0.40	191 (9%) 8 10	62, 147, 336, 657	0

The worst 5 of 191 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	2	VAL	17.7
2	L	8	GLY	11.6
2	B	10	GLY	11.2
2	H	69	ILE	9.1
2	B	1	ASP	8.6

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 monosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.