



wwPDB X-ray Structure Validation Summary Report ⓘ

May 20, 2025 – 01:05 PM EDT

PDB ID : 9E7E / pdb_00009e7e
Title : Crystal structure of HIV-1 RRE SLII A31CG39C mutant in complex with Fab BL3-6
Authors : Ojha, M.; Koirala, D.
Deposited on : 2024-11-01
Resolution : 2.75 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 Phenix2.0rc1
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.43.1

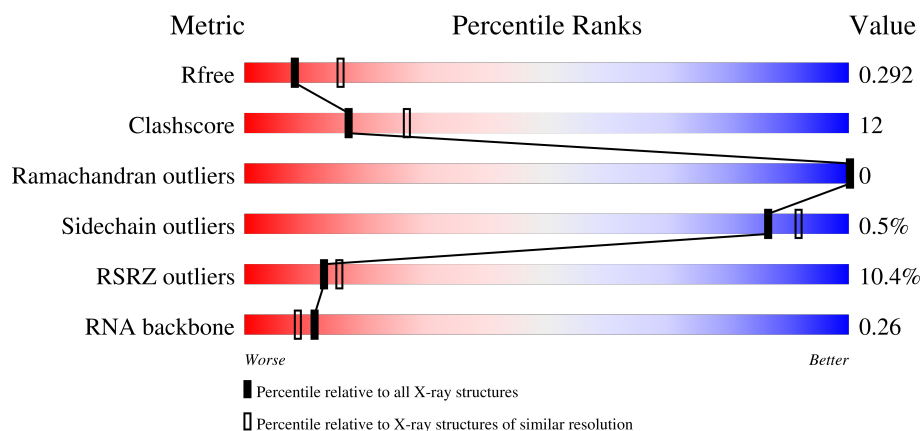
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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}	164625	1606 (2.78-2.74)
Clashscore	180529	1689 (2.78-2.74)
Ramachandran outliers	177936	1665 (2.78-2.74)
Sidechain outliers	177891	1665 (2.78-2.74)
RSRZ outliers	164620	1606 (2.78-2.74)
RNA backbone	3690	1094 (3.00-2.52)

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	233	<div> <div>3%</div> <div>77%</div> <div>20%</div> <div>•</div> </div>
1	D	233	<div> <div>3%</div> <div>81%</div> <div>16%</div> <div>•</div> </div>
1	G	233	<div> <div>28%</div> <div>61%</div> <div>35%</div> <div>••</div> </div>
1	H	233	<div> <div>79%</div> <div>18%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
2	B	215	
2	E	215	
2	I	215	
2	L	215	
3	C	72	
3	F	72	
3	O	72	
3	R	72	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 19620 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 BL3-6 Fab heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	226	Total	C	N	O	S	0	0	0
			1684	1058	288	332	6			
1	A	226	Total	C	N	O	S	0	0	0
			1684	1058	288	332	6			
1	D	226	Total	C	N	O	S	0	0	0
			1684	1058	288	332	6			
1	G	226	Total	C	N	O	S	0	0	0
			1684	1058	288	332	6			

- Molecule 2 is a protein called BL3-6 Fab light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	215	Total	C	N	O	S	0	0	0
			1643	1025	275	337	6			
2	B	215	Total	C	N	O	S	0	0	0
			1643	1025	275	337	6			
2	E	215	Total	C	N	O	S	0	0	0
			1643	1025	275	337	6			
2	I	215	Total	C	N	O	S	0	0	0
			1643	1025	275	337	6			

- Molecule 3 is a RNA chain called Rev Response Element SLII A31C/G39C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	R	72	Total	C	N	O	P	0	0	0
			1538	687	281	498	72			
3	C	72	Total	C	N	O	P	0	0	0
			1538	687	281	498	72			
3	F	72	Total	C	N	O	P	0	0	0
			1538	687	281	498	72			
3	O	72	Total	C	N	O	P	0	0	0
			1538	687	281	498	72			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
R	1	G	A	conflict	GB 902798
R	31	C	A	engineered mutation	GB 902798
R	39	C	G	engineered mutation	GB 902798
R	49	G	U	conflict	GB 902798
R	50	A	U	conflict	GB 902798
R	52	A	-	insertion	GB 902798
R	53	C	-	insertion	GB 902798
R	54	A	-	insertion	GB 902798
R	55	C	-	insertion	GB 902798
R	72	C	A	conflict	GB 902798
C	1	G	A	conflict	GB 902798
C	31	C	A	engineered mutation	GB 902798
C	39	C	G	engineered mutation	GB 902798
C	49	G	U	conflict	GB 902798
C	50	A	U	conflict	GB 902798
C	52	A	-	insertion	GB 902798
C	53	C	-	insertion	GB 902798
C	54	A	-	insertion	GB 902798
C	55	C	-	insertion	GB 902798
C	72	C	A	conflict	GB 902798
F	1	G	A	conflict	GB 902798
F	31	C	A	engineered mutation	GB 902798
F	39	C	G	engineered mutation	GB 902798
F	49	G	U	conflict	GB 902798
F	50	A	U	conflict	GB 902798
F	52	A	-	insertion	GB 902798
F	53	C	-	insertion	GB 902798
F	54	A	-	insertion	GB 902798
F	55	C	-	insertion	GB 902798
F	72	C	A	conflict	GB 902798
O	1	G	A	conflict	GB 902798
O	31	C	A	engineered mutation	GB 902798
O	39	C	G	engineered mutation	GB 902798
O	49	G	U	conflict	GB 902798
O	50	A	U	conflict	GB 902798
O	52	A	-	insertion	GB 902798
O	53	C	-	insertion	GB 902798
O	54	A	-	insertion	GB 902798
O	55	C	-	insertion	GB 902798
O	72	C	A	conflict	GB 902798

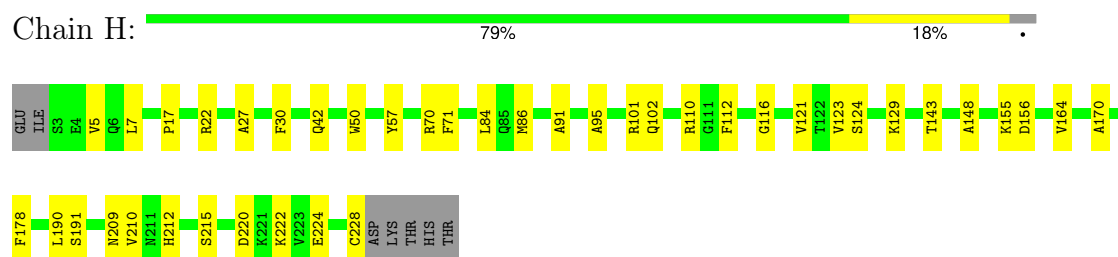
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	H	18	Total 18	O 18	0	0
4	L	14	Total 14	O 14	0	0
4	R	2	Total 2	O 2	0	0
4	A	18	Total 18	O 18	0	0
4	B	13	Total 13	O 13	0	0
4	C	3	Total 3	O 3	0	0
4	F	3	Total 3	O 3	0	0
4	D	21	Total 21	O 21	0	0
4	E	25	Total 25	O 25	0	0
4	O	13	Total 13	O 13	0	0
4	G	26	Total 26	O 26	0	0
4	I	4	Total 4	O 4	0	0

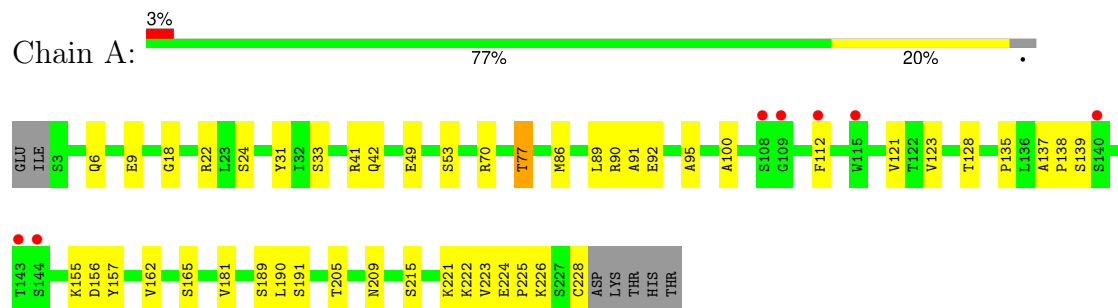
3 Residue-property plots [i](#)

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.

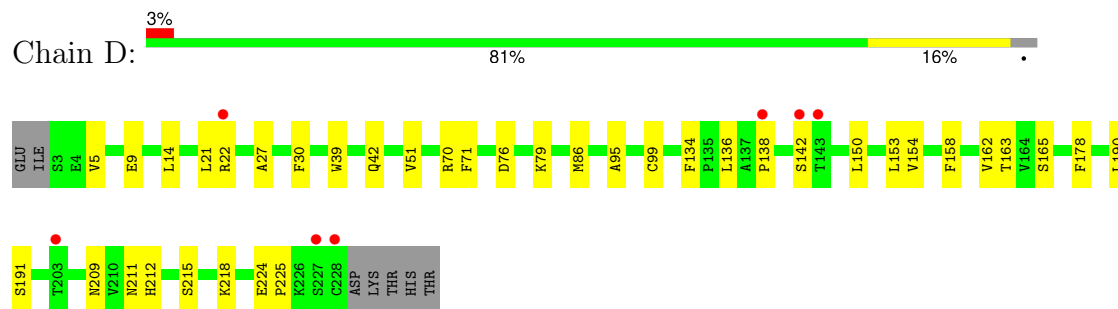
- Molecule 1: BL3-6 Fab heavy chain



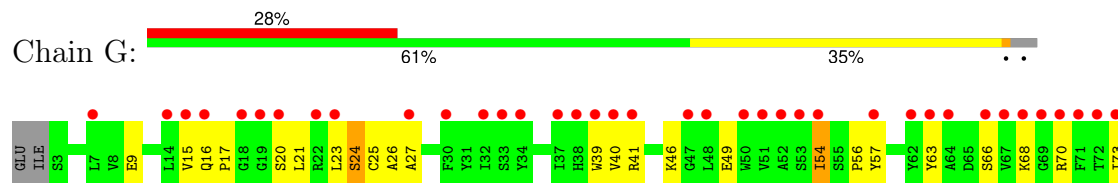
- Molecule 1: BL3-6 Fab heavy chain

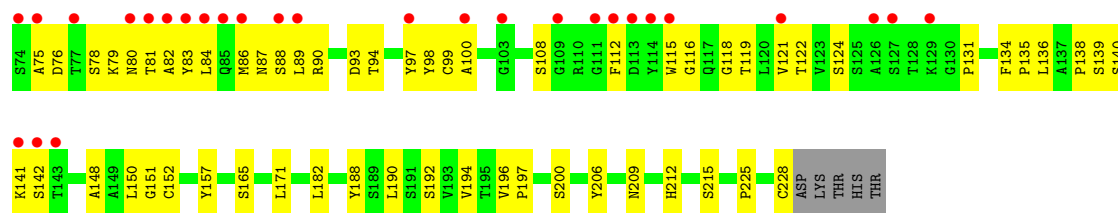


- Molecule 1: BL3-6 Fab heavy chain



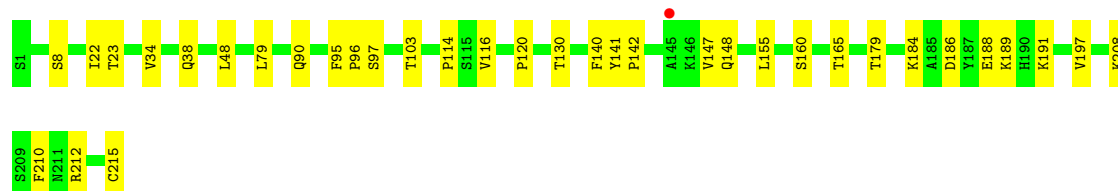
- Molecule 1: BL3-6 Fab heavy chain





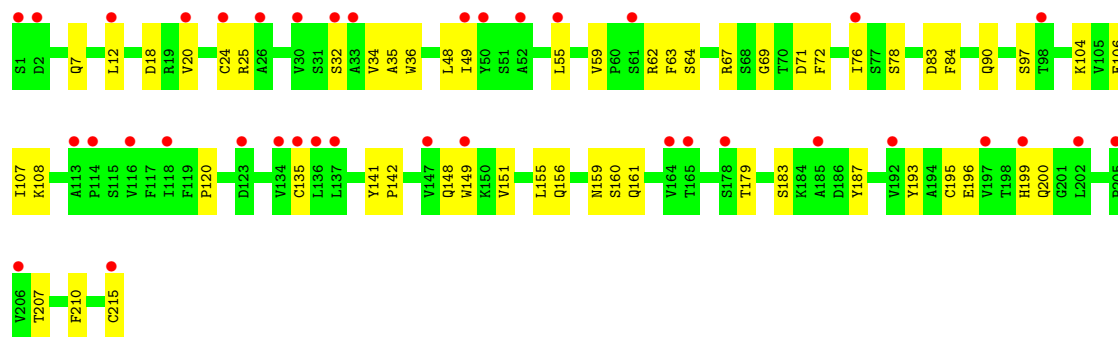
• Molecule 2: BL3-6 Fab light chain

Chain L: 84% 16%



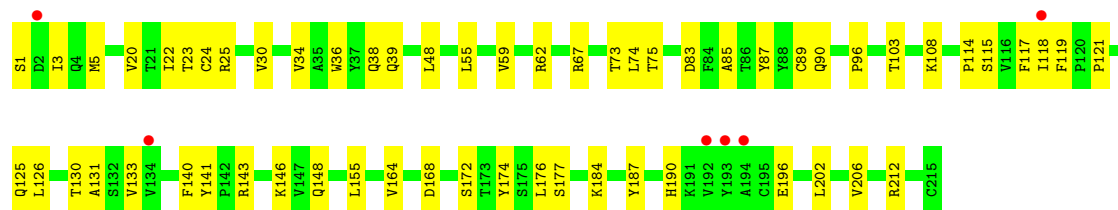
• Molecule 2: BL3-6 Fab light chain

Chain B: 18% 75% 25%



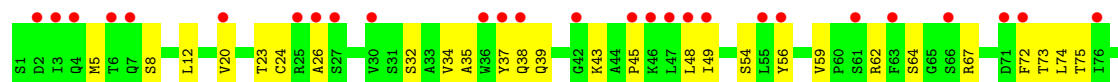
• Molecule 2: BL3-6 Fab light chain

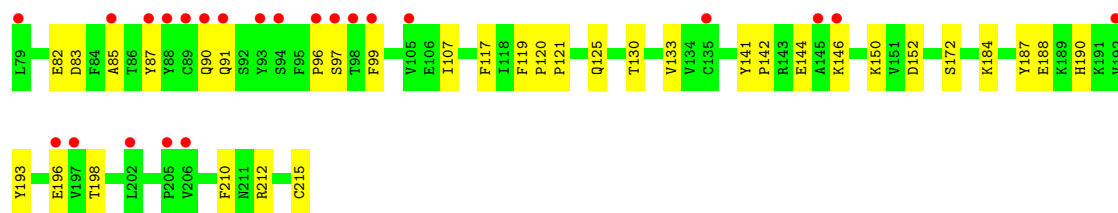
Chain E: 3% 73% 27%



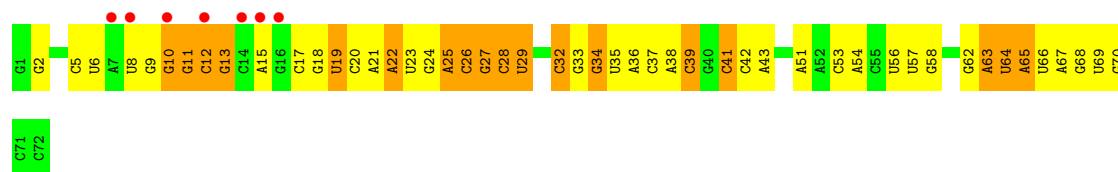
• Molecule 2: BL3-6 Fab light chain

Chain I: 23% 72% 28%

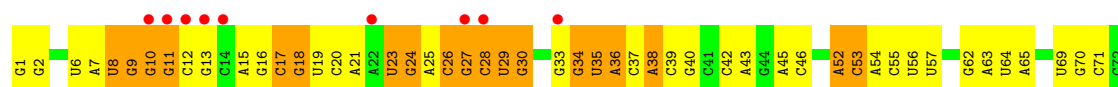




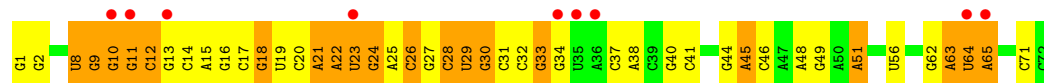
● Molecule 3: Rev Response Element SLII A31C/G39C



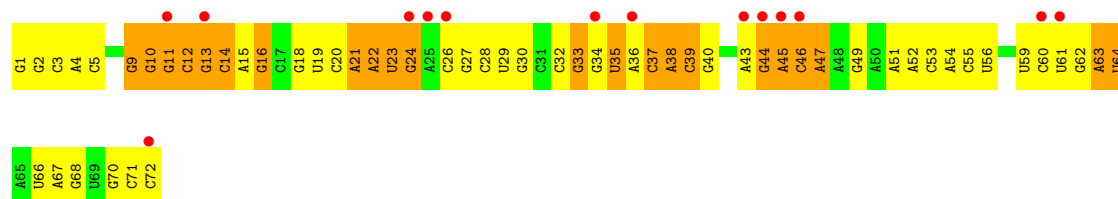
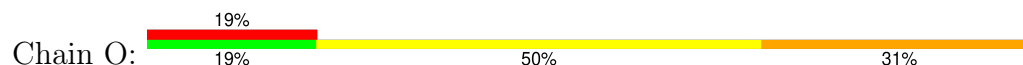
● Molecule 3: Rev Response Element SLII A31C/G39C



● Molecule 3: Rev Response Element SLII A31C/G39C



● Molecule 3: Rev Response Element SLII A31C/G39C



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	84.37Å 95.64Å 111.24Å 77.48° 76.34° 74.25°	Depositor
Resolution (Å)	49.66 – 2.75 49.66 – 2.75	Depositor EDS
% Data completeness (in resolution range)	96.6 (49.66-2.75) 86.8 (49.66-2.75)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.60 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.250 , 0.293 0.251 , 0.292	Depositor DCC
R_{free} test set	80220 reflections (2.45%)	wwPDB-VP
Wilson B-factor (Å ²)	62.3	Xtriage
Anisotropy	0.259	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 83.3	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	0.92	EDS
Total number of atoms	19620	wwPDB-VP
Average B, all atoms (Å ²)	132.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.66% 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	0.52	0/1725	0.80	0/2347
1	D	0.63	0/1725	0.83	0/2347
1	G	0.65	0/1725	0.97	2/2347 (0.1%)
1	H	0.60	0/1725	0.83	0/2347
2	B	0.47	0/1678	0.78	0/2277
2	E	0.63	0/1678	0.85	0/2277
2	I	0.48	0/1678	0.75	0/2277
2	L	0.52	0/1678	0.71	0/2277
3	C	0.32	0/1720	0.56	0/2679
3	F	0.38	0/1720	0.63	0/2679
3	O	0.39	0/1720	0.62	0/2679
3	R	0.29	0/1720	0.50	0/2679
All	All	0.51	0/20492	0.74	2/29212 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	140	SER	CA-C-N	5.88	134.71	122.41
1	G	140	SER	C-N-CA	5.88	134.71	122.41

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	1684	0	1643	34	0
1	D	1684	0	1643	24	0
1	G	1684	0	1643	67	0
1	H	1684	0	1643	29	0
2	B	1643	0	1595	43	0
2	E	1643	0	1595	40	0
2	I	1643	0	1595	45	0
2	L	1643	0	1595	24	0
3	C	1538	0	780	32	0
3	F	1538	0	780	34	0
3	O	1538	0	780	44	0
3	R	1538	0	780	35	0
4	A	18	0	0	2	0
4	B	13	0	0	1	0
4	C	3	0	0	0	0
4	D	21	0	0	0	0
4	E	25	0	0	0	0
4	F	3	0	0	0	0
4	G	26	0	0	0	0
4	H	18	0	0	0	0
4	I	4	0	0	0	0
4	L	14	0	0	2	0
4	O	13	0	0	0	0
4	R	2	0	0	0	0
All	All	19620	0	16072	427	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 12.

The worst 5 of 427 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:G:94:THR:HG23	1:G:122:THR:HA	1.58	0.85
2:E:121:PRO:HD3	2:E:133:VAL:HG22	1.61	0.82
1:G:26:ALA:HA	1:G:81:THR:HG22	1.61	0.81
2:B:62:ARG:NE	2:B:83:ASP:OD2	2.14	0.79
1:G:212:HIS:HD1	1:G:215:SER:HG	1.25	0.77

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	224/233 (96%)	217 (97%)	7 (3%)	0	100	100
1	D	224/233 (96%)	215 (96%)	9 (4%)	0	100	100
1	G	224/233 (96%)	194 (87%)	30 (13%)	0	100	100
1	H	224/233 (96%)	214 (96%)	10 (4%)	0	100	100
2	B	213/215 (99%)	205 (96%)	8 (4%)	0	100	100
2	E	213/215 (99%)	207 (97%)	6 (3%)	0	100	100
2	I	213/215 (99%)	205 (96%)	8 (4%)	0	100	100
2	L	213/215 (99%)	207 (97%)	6 (3%)	0	100	100
All	All	1748/1792 (98%)	1664 (95%)	84 (5%)	0	100	100

There are no Ramachandran outliers to report.

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	187/194 (96%)	185 (99%)	2 (1%)	70	83
1	D	187/194 (96%)	187 (100%)	0	100	100
1	G	187/194 (96%)	183 (98%)	4 (2%)	48	69
1	H	187/194 (96%)	187 (100%)	0	100	100
2	B	190/190 (100%)	190 (100%)	0	100	100
2	E	190/190 (100%)	189 (100%)	1 (0%)	86	92

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	190/190 (100%)	190 (100%)	0	100	100
2	L	190/190 (100%)	190 (100%)	0	100	100
All	All	1508/1536 (98%)	1501 (100%)	7 (0%)	86	92

5 of 7 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	24	SER
1	G	54	ILE
1	G	152	CYS
1	G	150	LEU
2	E	115	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 8 such sidechains are listed below:

Mol	Chain	Res	Type
2	I	138	ASN
1	G	85	GLN
2	E	38	GLN
2	B	211	ASN
2	E	148	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
3	C	72/72 (100%)	30 (41%)	2 (2%)
3	F	71/72 (98%)	31 (43%)	4 (5%)
3	O	71/72 (98%)	34 (47%)	2 (2%)
3	R	71/72 (98%)	28 (39%)	3 (4%)
All	All	285/288 (98%)	123 (43%)	11 (3%)

5 of 123 RNA backbone outliers are listed below:

Mol	Chain	Res	Type
3	R	2	G
3	R	8	U
3	R	9	G
3	R	10	G
3	R	11	G

5 of 11 RNA pucker outliers are listed below:

Mol	Chain	Res	Type
3	F	51	A
3	F	62	G
3	O	63	A
3	O	10	G
3	C	9	G

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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 ⓘ

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, 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	226/233 (96%)	0.37	7 (3%) 51 53	61, 83, 136, 195	0
1	D	226/233 (96%)	0.08	7 (3%) 51 53	46, 72, 135, 238	0
1	G	226/233 (96%)	1.24	66 (29%) 1 2	53, 96, 139, 213	0
1	H	226/233 (96%)	-0.12	0 100 100	51, 66, 112, 174	0
2	B	215/215 (100%)	1.19	38 (17%) 4 5	74, 122, 183, 250	0
2	E	215/215 (100%)	0.29	6 (2%) 55 56	44, 72, 148, 200	0
2	I	215/215 (100%)	1.33	50 (23%) 2 3	71, 120, 170, 213	0
2	L	215/215 (100%)	0.14	1 (0%) 87 89	60, 91, 117, 129	0
3	C	72/72 (100%)	0.55	9 (12%) 9 12	83, 150, 324, 338	0
3	F	72/72 (100%)	0.71	9 (12%) 9 12	66, 166, 333, 376	0
3	O	72/72 (100%)	1.37	14 (19%) 4 4	88, 189, 529, 558	0
3	R	72/72 (100%)	0.74	7 (9%) 15 17	76, 203, 465, 519	0
All	All	2052/2080 (98%)	0.60	214 (10%) 13 16	44, 96, 246, 558	0

The worst 5 of 214 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	71	PHE	6.1
3	O	26	C	6.0
2	I	89	CYS	5.7
1	G	15	VAL	5.3
2	I	91	GLN	5.3

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](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.