wwPDB X-ray Structure Validation Summary Report (i)

Oct 20, 2026 – 02:15 PM JST

PDB ID	:	46GH / pdb_000046gh
Title	:	Crystal structure of a de novo-designed VHH targeting BHRF1
Authors	:	Wang, S.; Yu, Q.L.; Tian, B.H.; Qin, X.Y.; Chen, M.C.
Deposited on	:	2026-09-21
Resolution	:	3.40 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 (i) 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 (1)) were used in the production of this report:

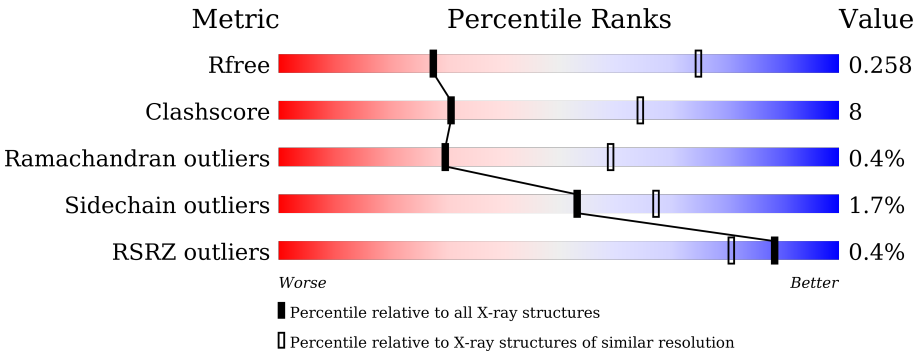
MolProbity	:	4-5-2 with Phenix2.2
Xtriage (Phenix)	:	2.2
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.51

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 3.40 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	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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 <=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	160	% 74% 22% ·
1	C	160	73% 23% · ·
1	E	160	% 77% 20% · ·
1	G	160	74% 22% · · ·
1	I	160	76% 21% · ·
1	K	160	73% 23% ·

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Mol	Chain	Length	Quality of chain
1	M	160	
1	O	160	
1	Q	160	
1	S	160	
2	B	132	
2	D	132	
2	F	132	
2	H	132	
2	J	132	
2	L	132	
2	N	132	
2	P	132	
2	R	132	
2	T	132	

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 22139 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 Apoptosis regulator BHRF1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	160	Total	C	N	O	S	0	0	0
			1285	811	226	239	9			
1	C	160	Total	C	N	O	S	0	0	0
			1285	811	226	239	9			
1	E	160	Total	C	N	O	S	0	0	0
			1285	811	226	239	9			
1	G	158	Total	C	N	O	S	0	0	0
			1273	804	224	237	8			
1	I	160	Total	C	N	O	S	0	0	0
			1285	811	226	239	9			
1	K	160	Total	C	N	O	S	0	0	0
			1285	811	226	239	9			
1	M	159	Total	C	N	O	S	0	0	0
			1281	809	225	238	9			
1	O	160	Total	C	N	O	S	0	0	0
			1285	811	226	239	9			
1	Q	160	Total	C	N	O	S	0	0	0
			1285	811	226	239	9			
1	S	159	Total	C	N	O	S	0	0	0
			1281	809	225	238	9			

- Molecule 2 is a protein called BHRF1_VHH-N13.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	122	Total	C	N	O	S	0	0	0
			936	591	161	179	5			
2	D	122	Total	C	N	O	S	0	0	0
			936	591	161	179	5			
2	F	122	Total	C	N	O	S	0	0	0
			936	591	161	179	5			
2	H	122	Total	C	N	O	S	0	0	0
			936	591	161	179	5			

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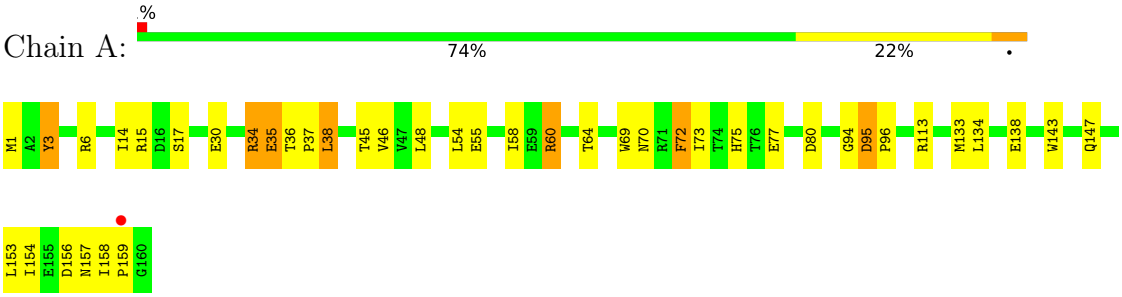
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	J	122	Total	C	N	O	S	0	0	0
			936	591	161	179	5			
2	L	121	Total	C	N	O	S	0	0	0
			927	586	160	176	5			
2	N	122	Total	C	N	O	S	0	0	0
			936	591	161	179	5			
2	P	122	Total	C	N	O	S	0	0	0
			936	591	161	179	5			
2	R	122	Total	C	N	O	S	0	0	0
			936	591	161	179	5			
2	T	117	Total	C	N	O	S	0	0	0
			894	565	153	171	5			

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.

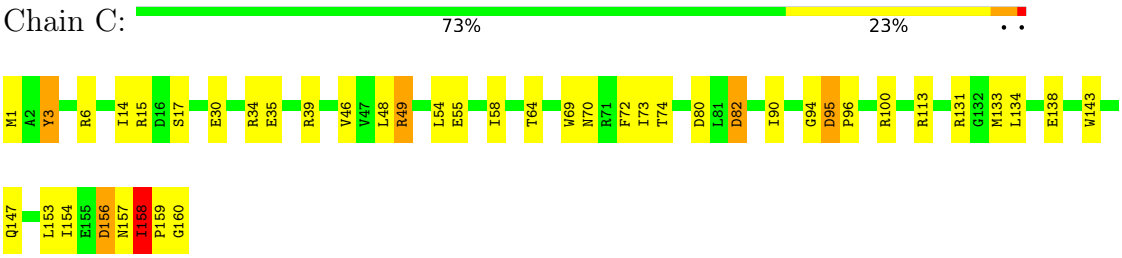
- Molecule 1: Apoptosis regulator BHRF1

Chain A:



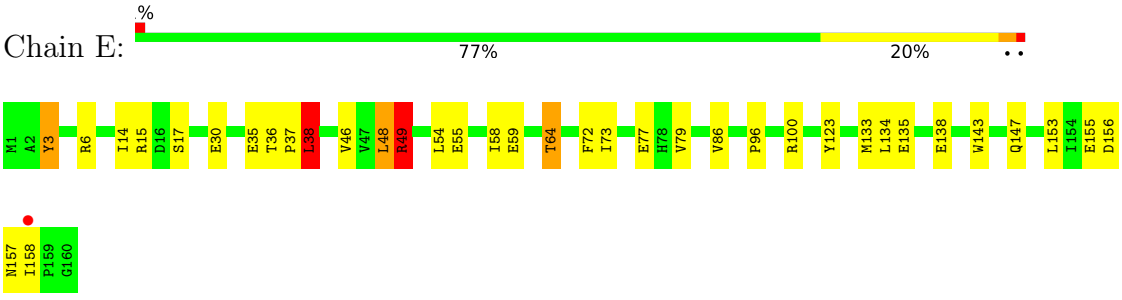
- Molecule 1: Apoptosis regulator BHRF1

Chain C:



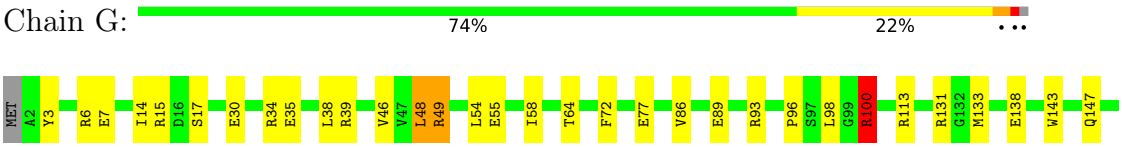
- Molecule 1: Apoptosis regulator BHRF1

Chain E:



- Molecule 1: Apoptosis regulator BHRF1

Chain G:

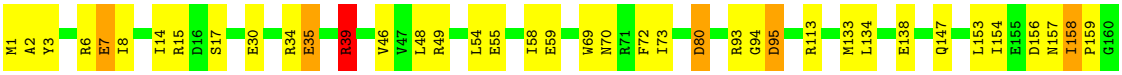




• Molecule 1: Apoptosis regulator BHRF1

Chain I:

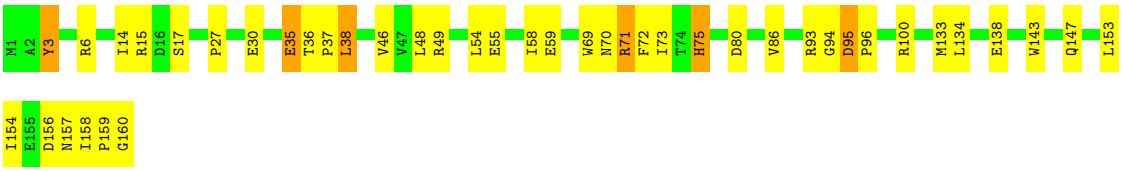




• Molecule 1: Apoptosis regulator BHRF1

Chain K:

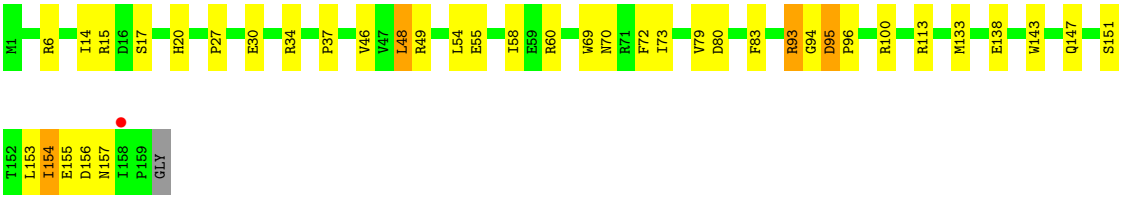




• Molecule 1: Apoptosis regulator BHRF1

Chain M:

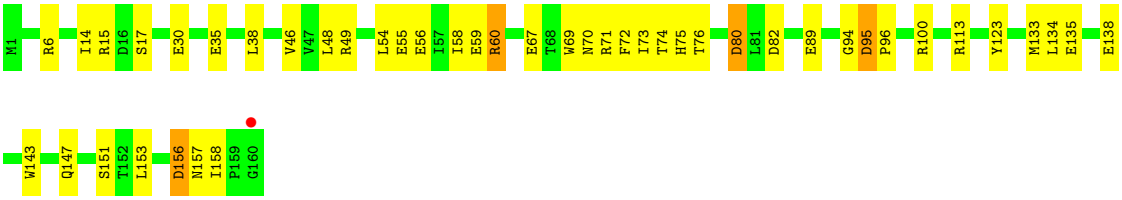




• Molecule 1: Apoptosis regulator BHRF1

Chain O:





• Molecule 1: Apoptosis regulator BHRF1

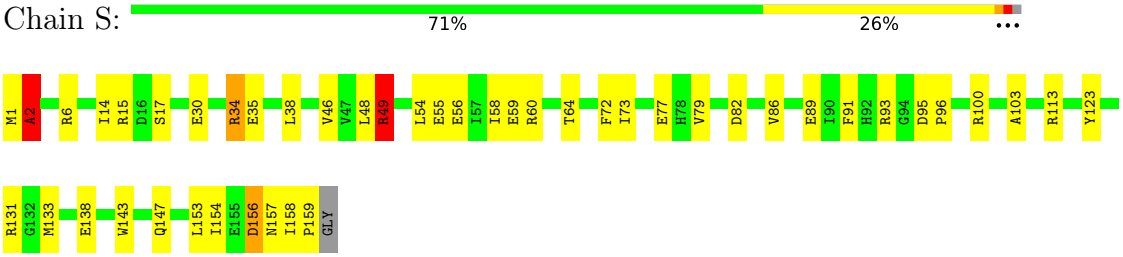
Chain Q:





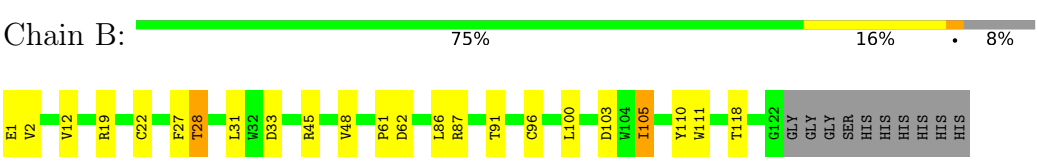
• Molecule 1: Apoptosis regulator BHRF1

Chain S:



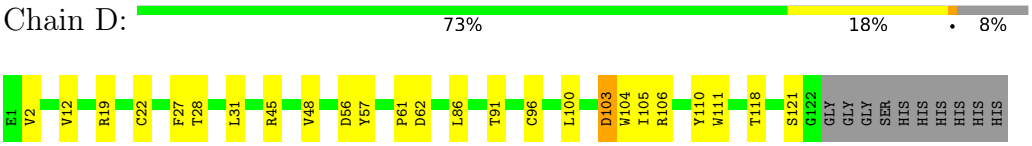
• Molecule 2: BHRF1_VHH-N13

Chain B:



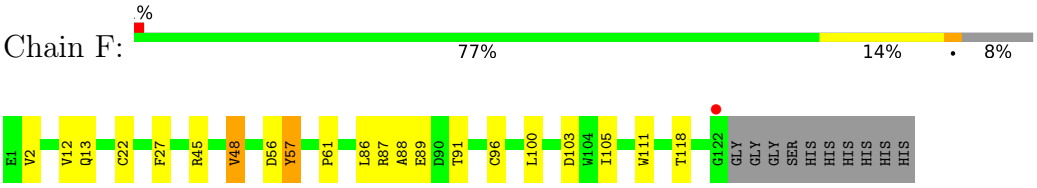
• Molecule 2: BHRF1_VHH-N13

Chain D:



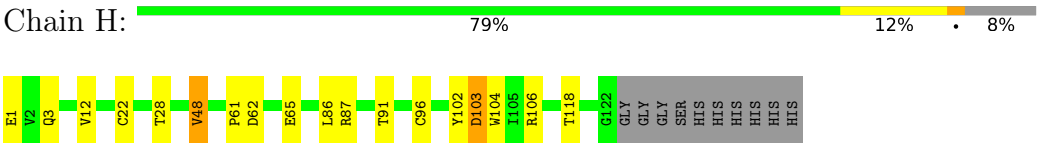
• Molecule 2: BHRF1_VHH-N13

Chain F:



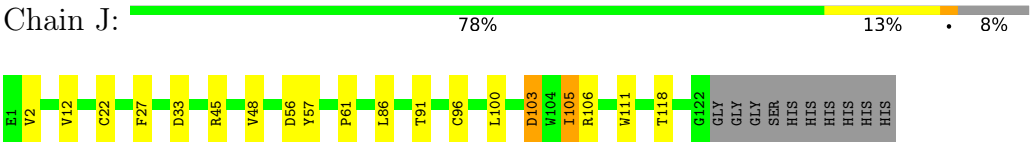
• Molecule 2: BHRF1_VHH-N13

Chain H:



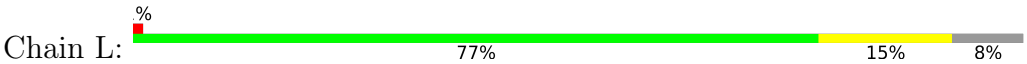
• Molecule 2: BHRF1_VHH-N13

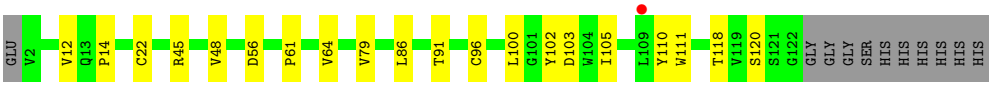
Chain J:



• Molecule 2: BHRF1_VHH-N13

Chain L:

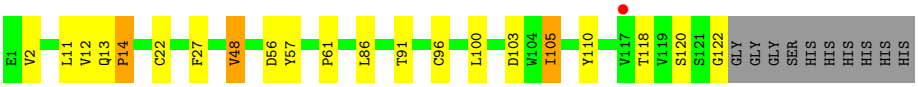




• Molecule 2: BHRF1_VHH-N13

Chain N:

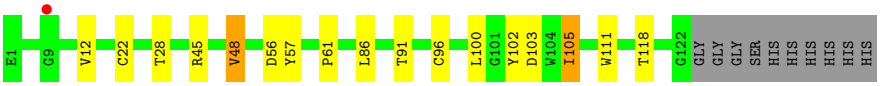




• Molecule 2: BHRF1_VHH-N13

Chain P:

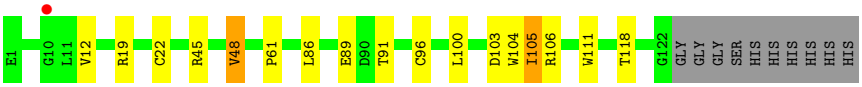




• Molecule 2: BHRF1_VHH-N13

Chain R:

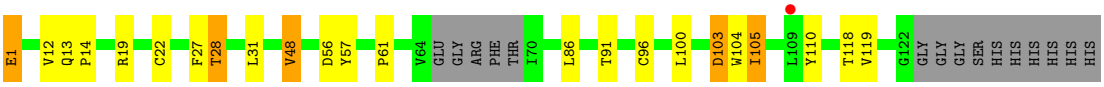




• Molecule 2: BHRF1_VHH-N13

Chain T:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 2 21 21	Depositor
Cell constants a, b, c, α, β, γ	84.64Å 196.38Å 214.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.90 – 3.40 47.90 – 3.40	Depositor EDS
% Data completeness (in resolution range)	99.6 (47.90-3.40) 99.7 (47.90-3.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 3.40Å)	Xtriage
Refinement program	REFMAC 5.8.0431	Depositor
R, R_{free}	0.204 , 0.251 0.210 , 0.258	Depositor DCC
R_{free} test set	2470 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	101.0	Xtriage
Anisotropy	0.568	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 104.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	22139	wwPDB-VP
Average B, all atoms (Å^2)	135.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.91% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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	0.71	0/1317	1.43	17/1794 (0.9%)
1	C	0.68	0/1317	1.38	12/1794 (0.7%)
1	E	0.67	0/1317	1.42	15/1794 (0.8%)
1	G	0.75	1/1305 (0.1%)	1.46	14/1779 (0.8%)
1	I	0.70	0/1317	1.38	10/1794 (0.6%)
1	K	0.67	0/1317	1.39	11/1794 (0.6%)
1	M	0.65	0/1313	1.36	7/1789 (0.4%)
1	O	0.66	0/1317	1.37	10/1794 (0.6%)
1	Q	0.67	0/1317	1.38	11/1794 (0.6%)
1	S	0.65	0/1313	1.35	9/1789 (0.5%)
2	B	0.61	0/958	1.10	5/1298 (0.4%)
2	D	0.64	0/958	1.11	2/1298 (0.2%)
2	F	0.57	0/958	1.02	1/1298 (0.1%)
2	H	0.63	0/958	1.10	3/1298 (0.2%)
2	J	0.60	0/958	1.08	3/1298 (0.2%)
2	L	0.63	0/949	1.12	3/1286 (0.2%)
2	N	0.62	0/958	1.07	3/1298 (0.2%)
2	P	0.59	0/958	1.00	3/1298 (0.2%)
2	R	0.56	0/958	0.98	2/1298 (0.2%)
2	T	0.62	0/914	1.06	3/1238 (0.2%)
All	All	0.65	1/22677 (0.0%)	1.27	144/30823 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	C	0	2
1	E	0	2
1	G	0	3
1	I	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	K	0	3
1	M	0	5
1	Q	0	3
1	S	0	4
2	B	0	1
2	D	0	1
2	F	0	1
2	H	0	1
2	N	0	1
2	R	0	1
2	T	0	1
All	All	0	35

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	100	ARG	NE-CZ	-5.62	1.26	1.33

The worst 5 of 144 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	N	14	PRO	CB-CA-C	10.58	125.11	111.46
2	L	56	ASP	CB-CA-C	9.36	125.57	110.88
1	K	156	ASP	CA-CB-CG	9.24	121.84	112.60
1	Q	156	ASP	CA-CB-CG	8.91	121.52	112.60
1	G	155	GLU	N-CA-CB	7.87	121.48	110.07

There are no chirality outliers.

5 of 35 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	158	ILE	Mainchain
1	A	34	ARG	Sidechain
1	A	60	ARG	Sidechain
2	B	19	ARG	Sidechain
1	C	49	ARG	Sidechain

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	1285	0	1242	17	0
1	C	1285	0	1242	30	0
1	E	1285	0	1242	19	0
1	G	1273	0	1227	27	0
1	I	1285	0	1242	28	0
1	K	1285	0	1242	30	0
1	M	1281	0	1239	20	0
1	O	1285	0	1242	33	0
1	Q	1285	0	1242	20	0
1	S	1281	0	1239	32	0
2	B	936	0	894	13	0
2	D	936	0	894	23	0
2	F	936	0	894	16	0
2	H	936	0	894	14	0
2	J	936	0	894	15	0
2	L	927	0	885	15	0
2	N	936	0	894	15	1
2	P	936	0	894	14	0
2	R	936	0	894	11	0
2	T	894	0	855	15	1
All	All	22139	0	21291	352	1

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 352 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:O:67:GLU:HB3	1:O:71:ARG:HH12	1.06	1.19
1:O:72:PHE:O	1:O:76:THR:HG23	1.56	1.06
1:M:93:ARG:NH1	2:P:102:TYR:OH	2.00	0.94
1:I:157:ASN:O	1:I:158:ILE:HG12	1.71	0.90
2:N:11:LEU:HD21	2:N:122:GLY:HA2	1.54	0.89

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:14:PRO:O	2:T:14:PRO:CB[2_545]	2.06	0.14

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	158/160 (99%)	151 (96%)	5 (3%)	2 (1%)	9 33
1	C	158/160 (99%)	147 (93%)	9 (6%)	2 (1%)	9 33
1	E	158/160 (99%)	152 (96%)	5 (3%)	1 (1%)	21 50
1	G	156/160 (98%)	151 (97%)	4 (3%)	1 (1%)	21 50
1	I	158/160 (99%)	149 (94%)	8 (5%)	1 (1%)	21 50
1	K	158/160 (99%)	146 (92%)	10 (6%)	2 (1%)	9 33
1	M	157/160 (98%)	147 (94%)	9 (6%)	1 (1%)	21 50
1	O	158/160 (99%)	150 (95%)	7 (4%)	1 (1%)	21 50
1	Q	158/160 (99%)	152 (96%)	6 (4%)	0	100 100
1	S	157/160 (98%)	151 (96%)	6 (4%)	0	100 100
2	B	120/132 (91%)	115 (96%)	5 (4%)	0	100 100
2	D	120/132 (91%)	114 (95%)	6 (5%)	0	100 100
2	F	120/132 (91%)	115 (96%)	5 (4%)	0	100 100
2	H	120/132 (91%)	117 (98%)	3 (2%)	0	100 100
2	J	120/132 (91%)	115 (96%)	5 (4%)	0	100 100
2	L	119/132 (90%)	113 (95%)	6 (5%)	0	100 100
2	N	120/132 (91%)	114 (95%)	6 (5%)	0	100 100
2	P	120/132 (91%)	116 (97%)	4 (3%)	0	100 100
2	R	120/132 (91%)	115 (96%)	5 (4%)	0	100 100
2	T	113/132 (86%)	108 (96%)	5 (4%)	0	100 100
All	All	2768/2920 (95%)	2638 (95%)	119 (4%)	11 (0%)	30 59

5 of 11 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	LEU
1	E	38	LEU
1	K	38	LEU
1	C	95	ASP
1	I	95	ASP

5.3.2 Protein sidechains (i)

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	141/141 (100%)	138 (98%)	3 (2%)	47	64
1	C	141/141 (100%)	138 (98%)	3 (2%)	47	64
1	E	141/141 (100%)	138 (98%)	3 (2%)	47	64
1	G	140/141 (99%)	137 (98%)	3 (2%)	47	64
1	I	141/141 (100%)	139 (99%)	2 (1%)	59	70
1	K	141/141 (100%)	138 (98%)	3 (2%)	47	64
1	M	141/141 (100%)	138 (98%)	3 (2%)	47	64
1	O	141/141 (100%)	137 (97%)	4 (3%)	38	60
1	Q	141/141 (100%)	140 (99%)	1 (1%)	76	78
1	S	141/141 (100%)	140 (99%)	1 (1%)	76	78
2	B	95/102 (93%)	94 (99%)	1 (1%)	65	74
2	D	95/102 (93%)	95 (100%)	0	100	100
2	F	95/102 (93%)	93 (98%)	2 (2%)	47	64
2	H	95/102 (93%)	93 (98%)	2 (2%)	47	64
2	J	95/102 (93%)	95 (100%)	0	100	100
2	L	94/102 (92%)	94 (100%)	0	100	100
2	N	95/102 (93%)	93 (98%)	2 (2%)	47	64
2	P	95/102 (93%)	94 (99%)	1 (1%)	65	74
2	R	95/102 (93%)	93 (98%)	2 (2%)	47	64

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	T	91/102 (89%)	88 (97%)	3 (3%)	33 57
All	All	2354/2430 (97%)	2315 (98%)	39 (2%)	53 67

5 of 39 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	O	60	ARG
1	S	46	VAL
1	O	80	ASP
1	Q	46	VAL
2	T	13	GLN

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

Mol	Chain	Res	Type
1	S	157	ASN
1	O	78	HIS
2	H	3	GLN
1	G	157	ASN
2	J	113	GLN

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 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, 95^{th} 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	160/160 (100%)	-0.57	1 (0%) 85 75	66, 93, 167, 231	0
1	C	160/160 (100%)	-0.61	0 100 100	65, 95, 173, 212	0
1	E	160/160 (100%)	-0.45	1 (0%) 85 75	71, 109, 191, 244	0
1	G	158/160 (98%)	-0.62	0 100 100	64, 91, 143, 205	0
1	I	160/160 (100%)	-0.48	0 100 100	78, 108, 178, 244	0
1	K	160/160 (100%)	-0.55	0 100 100	70, 115, 182, 206	0
1	M	159/160 (99%)	-0.31	1 (0%) 85 75	79, 125, 189, 252	0
1	O	160/160 (100%)	-0.45	1 (0%) 85 75	78, 106, 163, 200	0
1	Q	160/160 (100%)	-0.43	0 100 100	72, 113, 171, 206	0
1	S	159/160 (99%)	-0.51	0 100 100	88, 129, 182, 249	0
2	B	122/132 (92%)	-0.57	0 100 100	78, 106, 140, 175	0
2	D	122/132 (92%)	-0.59	0 100 100	74, 97, 144, 186	0
2	F	122/132 (92%)	-0.08	1 (0%) 82 71	115, 182, 234, 263	0
2	H	122/132 (92%)	-0.67	0 100 100	75, 113, 165, 202	0
2	J	122/132 (92%)	-0.61	0 100 100	82, 110, 159, 242	0
2	L	121/132 (91%)	-0.58	1 (0%) 82 71	81, 120, 168, 194	0
2	N	122/132 (92%)	0.17	1 (0%) 82 71	162, 232, 315, 395	0
2	P	122/132 (92%)	0.06	1 (0%) 82 71	180, 245, 301, 333	0
2	R	122/132 (92%)	-0.39	1 (0%) 82 71	137, 197, 264, 275	0
2	T	117/132 (88%)	-0.17	1 (0%) 81 68	140, 192, 289, 358	0
All	All	2810/2920 (96%)	-0.43	10 (0%) 88 81	64, 120, 249, 395	0

The worst 5 of 10 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	P	9	GLY	3.1
1	M	158	ILE	3.0
2	L	109	LEU	2.6
1	O	160	GLY	2.6
2	T	109	LEU	2.5

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)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.