



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 05:24 AM UTC

PDB ID : 5A9V / pdb_00005a9v
Title : Structure of apo BipA
Authors : Kumar, V.; Chen, Y.; Ero, R.; Li, Z.; Gao, Y.
Deposited on : 2015-07-23
Resolution : 3.31 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
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

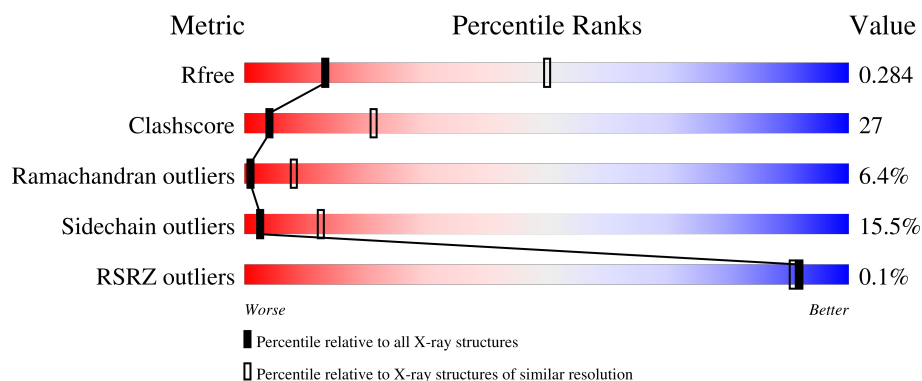
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.31 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	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

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	607	
1	B	607	
1	C	607	
1	D	607	
1	E	607	

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Mol	Chain	Length	Quality of chain
1	F	607	58% 24% 8% • 9%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 25398 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.

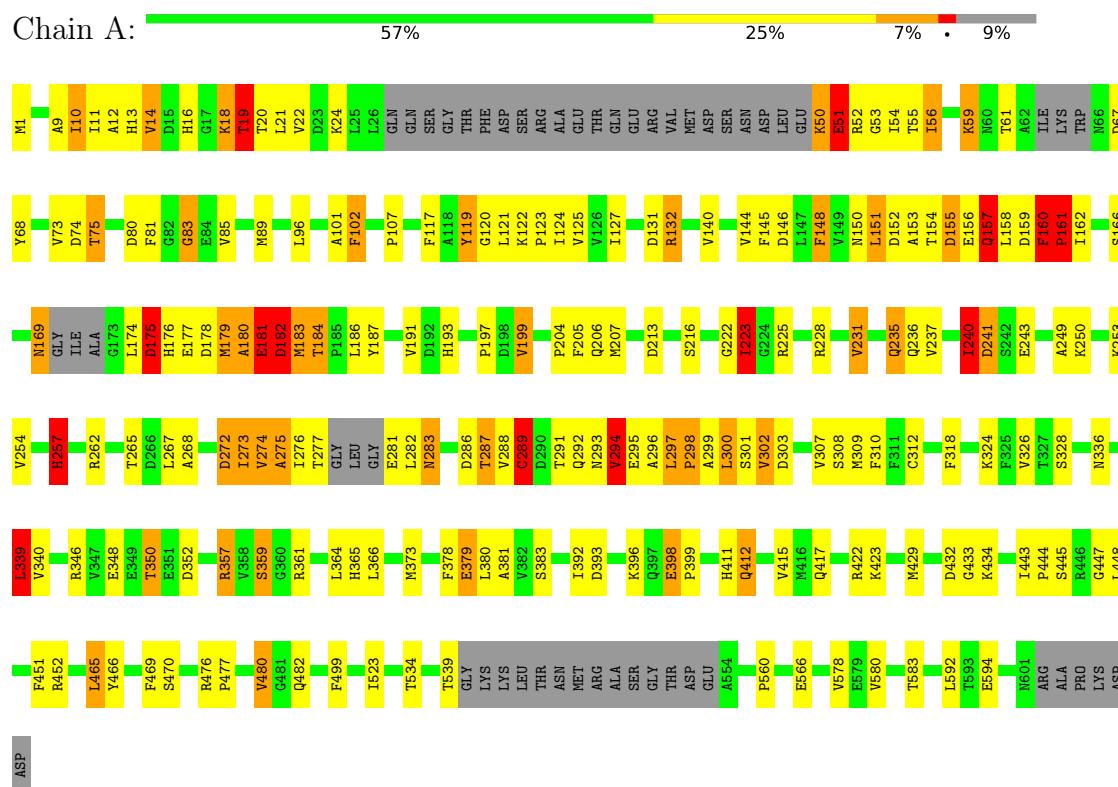
- Molecule 1 is a protein called GTP-BINDING PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	555	Total	C	N	O	S	0	0	0
			4233	2675	736	806	16			
1	B	555	Total	C	N	O	S	0	0	0
			4233	2675	736	806	16			
1	C	555	Total	C	N	O	S	0	0	0
			4233	2675	736	806	16			
1	D	555	Total	C	N	O	S	0	0	0
			4233	2675	736	806	16			
1	E	555	Total	C	N	O	S	0	0	0
			4233	2675	736	806	16			
1	F	555	Total	C	N	O	S	0	0	0
			4233	2675	736	806	16			

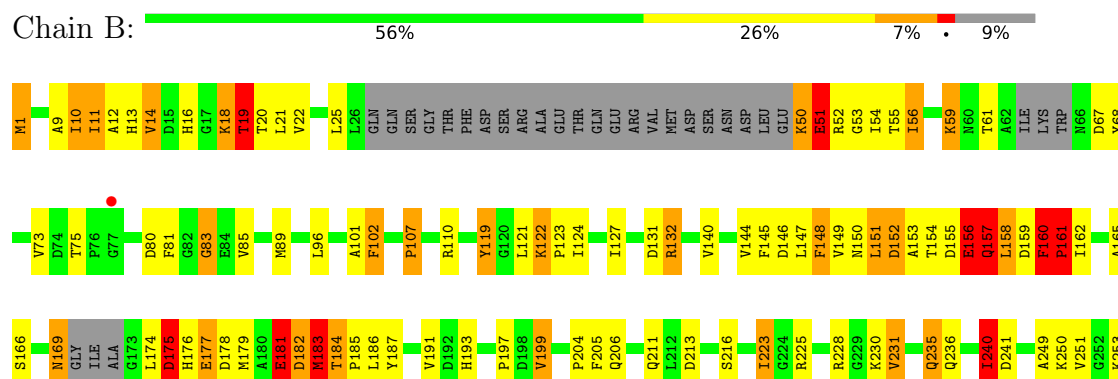
3 Residue-property plots

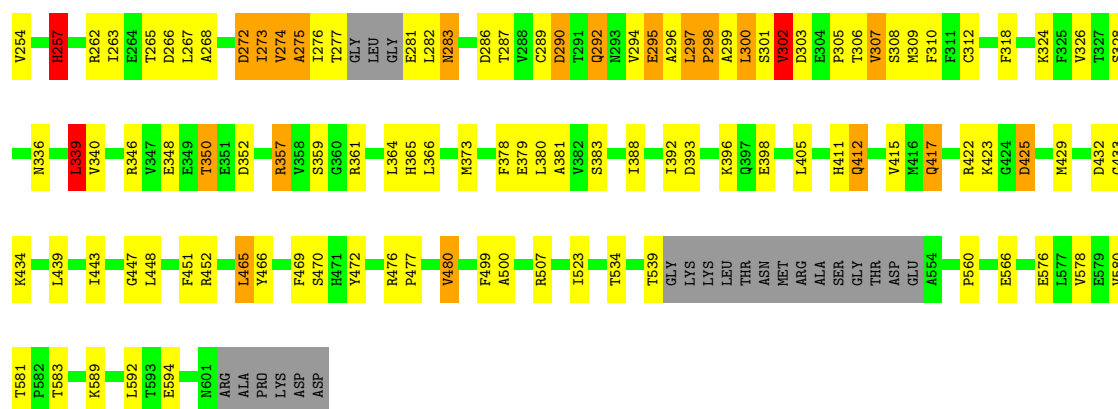
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: GTP-BINDING PROTEIN



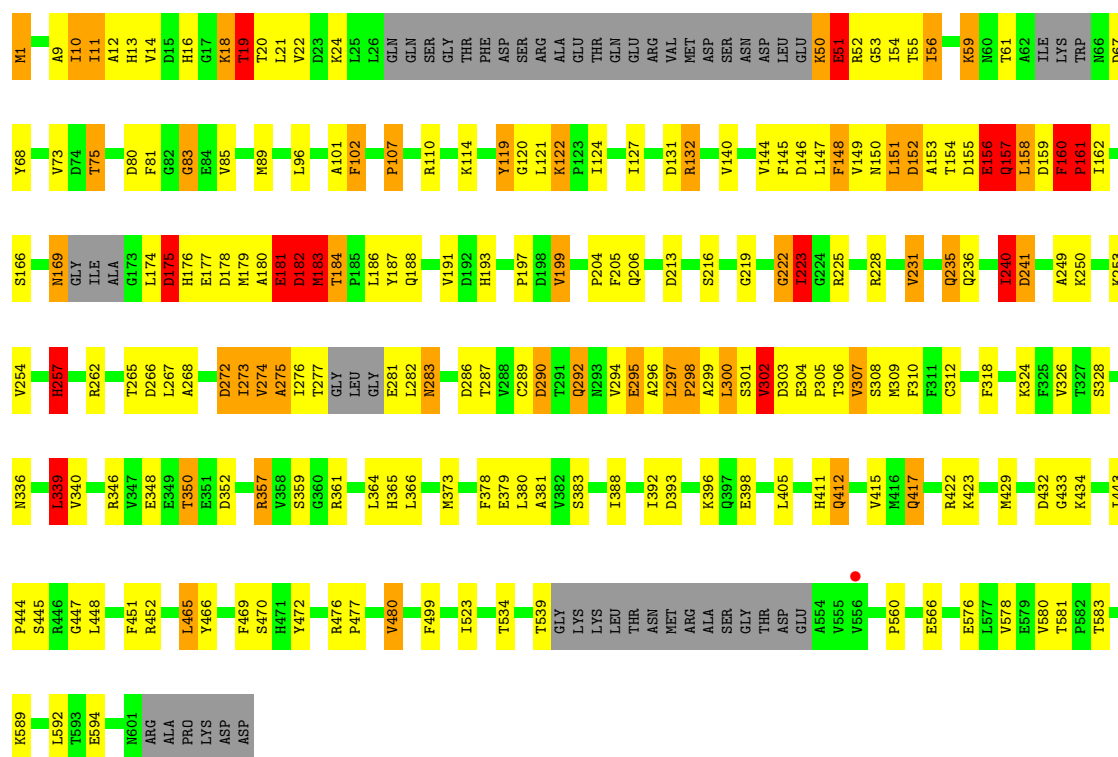
• Molecule 1: GTP-BINDING PROTEIN





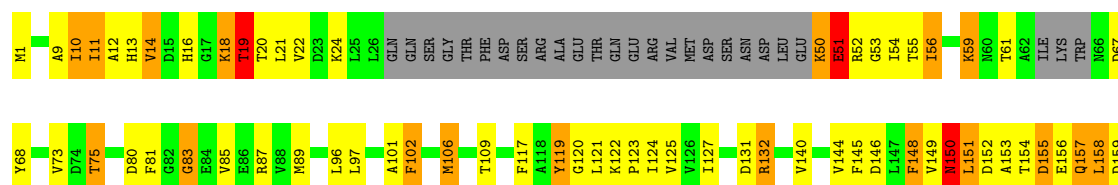
• Molecule 1: GTP-BINDING PROTEIN

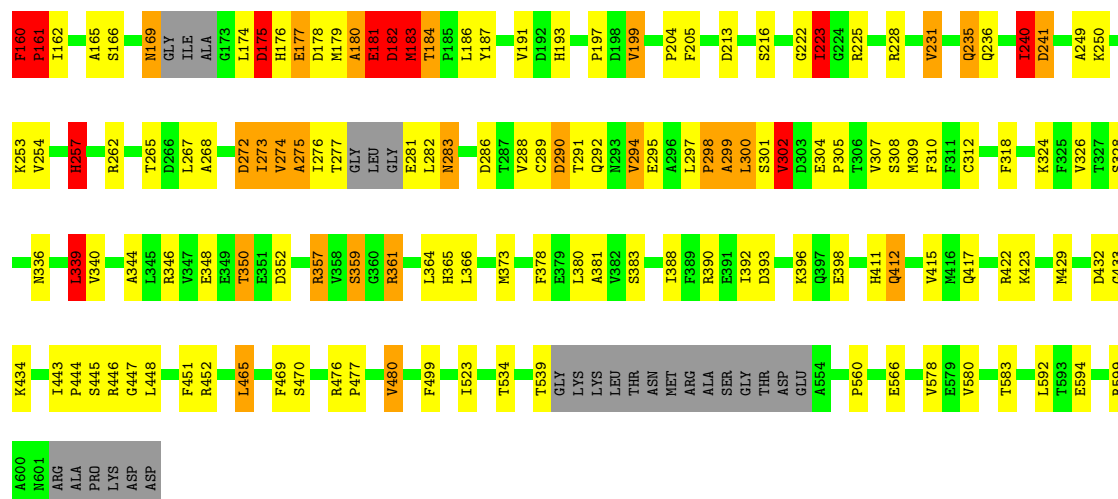
Chain C: 57% 25% 7% 9%



• Molecule 1: GTP-BINDING PROTEIN

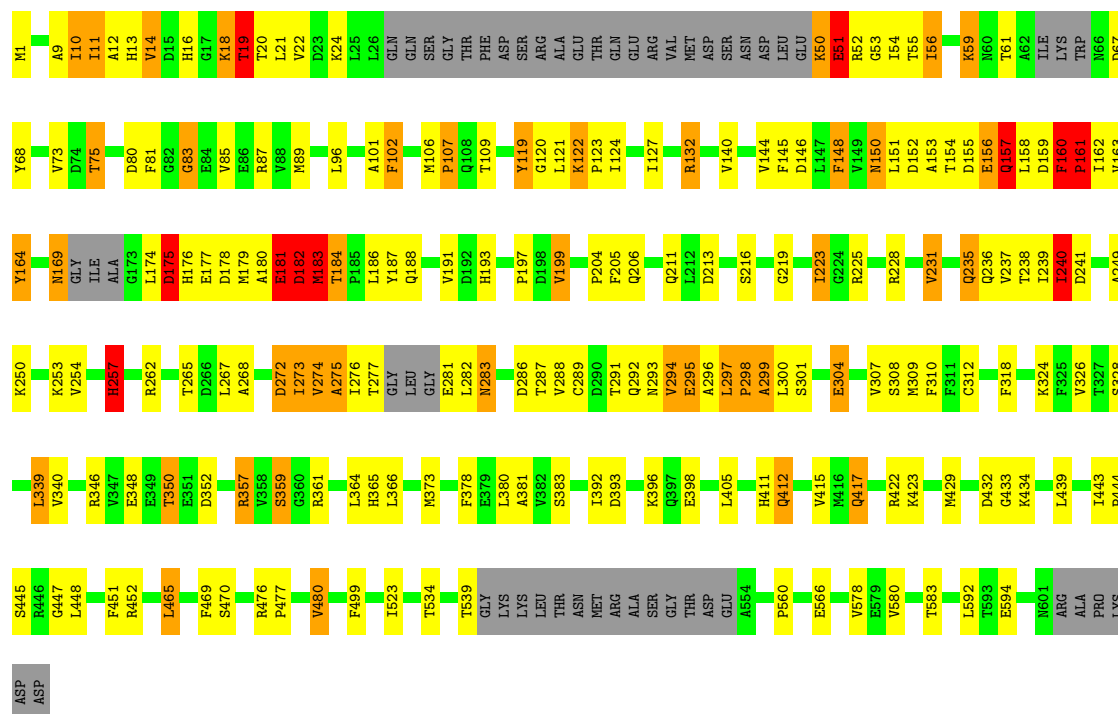
Chain D: 57% 25% 7% 9%





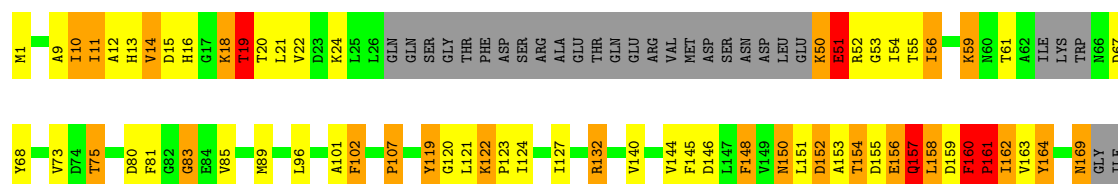
• Molecule 1: GTP-BINDING PROTEIN

Chain E: 58% 25% 7% 9%



• Molecule 1: GTP-BINDING PROTEIN

Chain F: 58% 24% 8% 9%



ALA	G173	L174	D175	H176	E177	D178	M179	A180	E181	D182	M183	T184	F185	L186	Y187	V191	D192	H193	P197	D198	V199	P204	F205	Q206	Q211	I212	D213	S216	G219	I223	G224	R225	R228	V231	Q235	Q236	V237	T238	I239	I240	D241	A249	K250	K253	V254	H257																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
F451	R346	V347	E348	E349	T350	E351	D352	R357	V358	S359	G360	R361	L364	H365	L366	M373	F378	E379	L380	A381	V382	S383	I392	D393	K396	G397	E398	L405	H411	Q412	V415	M416	Q417	R422	K423	M429	D432	G433	K434	L439	I443	P444	S445	R446	G447	L448																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																				
R476	P477	V480	F499	I523	T534	T539	GLY	LYS	LYS	LEU	THR	ASN	MET	ARG	ALA	SER	GLY	THR	ASP	GLU	A554	P560	M563	E566	V578	E579	V580	T583	L592	T593	E594	N601	ARG	ALA	PRO	LYS	ASP	ASP																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
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4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	241.95Å 241.95Å 241.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.39 – 3.31 49.39 – 3.31	Depositor EDS
% Data completeness (in resolution range)	91.8 (49.39-3.31) 91.8 (49.39-3.31)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.02 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.8.0107	Depositor
R, R_{free}	0.263 , 0.288 0.277 , 0.284	Depositor DCC
R_{free} test set	9472 reflections (10.00%)	wwPDB-VP
Wilson B-factor (Å ²)	114.3	Xtriage
Anisotropy	0.029	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 267.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.429 for l,-k,h 0.429 for -l,-k,-h 0.429 for -h,-l,-k 0.429 for -h,l,k 0.439 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	25398	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 1.64% 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

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	0.85	3/4292 (0.1%)	1.14	23/5786 (0.4%)
1	B	0.86	3/4292 (0.1%)	1.15	23/5786 (0.4%)
1	C	0.86	2/4292 (0.0%)	1.14	24/5786 (0.4%)
1	D	0.85	3/4292 (0.1%)	1.14	20/5786 (0.3%)
1	E	0.85	3/4292 (0.1%)	1.13	24/5786 (0.4%)
1	F	0.85	3/4292 (0.1%)	1.13	22/5786 (0.4%)
All	All	0.85	17/25752 (0.1%)	1.14	136/34716 (0.4%)

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	4
1	B	0	4
1	C	0	4
1	D	0	5
1	E	0	4
1	F	0	4
All	All	0	25

The worst 5 of 17 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	240	ILE	CA-C	6.29	1.60	1.52
1	D	240	ILE	CA-C	6.15	1.60	1.52
1	F	240	ILE	CA-C	6.15	1.60	1.52
1	E	240	ILE	CA-C	5.89	1.60	1.52
1	C	240	ILE	CA-C	5.89	1.60	1.52

The worst 5 of 136 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	476	ARG	CA-C-N	-11.37	105.62	119.84
1	A	476	ARG	C-N-CA	-11.37	105.62	119.84
1	C	476	ARG	CA-C-N	-11.28	105.75	119.84
1	C	476	ARG	C-N-CA	-11.28	105.75	119.84
1	B	476	ARG	CA-C-N	-11.25	105.78	119.84

There are no chirality outliers.

5 of 25 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	132	ARG	Peptide
1	A	19	THR	Peptide
1	A	240	ILE	Peptide
1	A	465	LEU	Peptide
1	B	19	THR	Peptide

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	4233	0	4156	224	0
1	B	4233	0	4156	247	0
1	C	4233	0	4156	250	0
1	D	4233	0	4155	223	0
1	E	4233	0	4156	228	0
1	F	4233	0	4156	229	0
All	All	25398	0	24935	1383	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 27.

The worst 5 of 1383 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:A:287:THR:HB	1:A:297:LEU:CD1	1.13	1.55
1:B:169:ASN:HD21	1:B:182:ASP:N	1.09	1.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:287:THR:CB	1:A:297:LEU:CD1	1.94	1.45
1:B:169:ASN:CG	1:B:182:ASP:HB2	1.02	1.41
1:C:287:THR:CB	1:C:297:LEU:HD11	1.53	1.39

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	543/607 (90%)	421 (78%)	85 (16%)	37 (7%)	1	7
1	B	543/607 (90%)	420 (77%)	89 (16%)	34 (6%)	1	8
1	C	543/607 (90%)	418 (77%)	89 (16%)	36 (7%)	1	7
1	D	543/607 (90%)	419 (77%)	87 (16%)	37 (7%)	1	7
1	E	543/607 (90%)	425 (78%)	86 (16%)	32 (6%)	1	9
1	F	543/607 (90%)	424 (78%)	85 (16%)	34 (6%)	1	8
All	All	3258/3642 (90%)	2527 (78%)	521 (16%)	210 (6%)	1	8

5 of 210 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	161	PRO
1	A	181	GLU
1	A	182	ASP
1	A	223	ILE
1	A	393	ASP

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	447/519 (86%)	379 (85%)	68 (15%)	3	13
1	B	448/519 (86%)	376 (84%)	72 (16%)	2	12
1	C	447/519 (86%)	378 (85%)	69 (15%)	2	13
1	D	445/519 (86%)	378 (85%)	67 (15%)	3	13
1	E	449/519 (86%)	383 (85%)	66 (15%)	3	14
1	F	450/519 (87%)	376 (84%)	74 (16%)	2	11
All	All	2686/3114 (86%)	2270 (84%)	416 (16%)	2	12

5 of 416 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	184	THR
1	E	150	ASN
1	F	364	LEU
1	D	235	GLN
1	D	359	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 32 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	157	GLN
1	F	169	ASN
1	C	16	HIS
1	B	428	ASN
1	F	235	GLN

5.3.3 RNA ⓘ

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 [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	555/607 (91%)	-1.13	0 100 100	79, 130, 184, 219	0
1	B	555/607 (91%)	-1.14	1 (0%) 91 86	80, 129, 184, 220	0
1	C	555/607 (91%)	-1.12	1 (0%) 91 86	82, 130, 183, 216	0
1	D	555/607 (91%)	-1.16	0 100 100	85, 131, 183, 218	0
1	E	555/607 (91%)	-1.10	0 100 100	83, 131, 183, 225	0
1	F	555/607 (91%)	-1.16	0 100 100	83, 131, 182, 218	0
All	All	3330/3642 (91%)	-1.13	2 (0%) 92 91	79, 131, 184, 225	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	77	GLY	4.0
1	C	556	VAL	2.7

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.