



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 20, 2016 – 06:56 AM EST

PDB ID : 5T7F
Title : PI3Kdelta in complex with the inhibitor GS-643624
Authors : Somoza, J.R.; Villasenor, A.
Deposited on : 2016-09-04
Resolution : 2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/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
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028442
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20028442

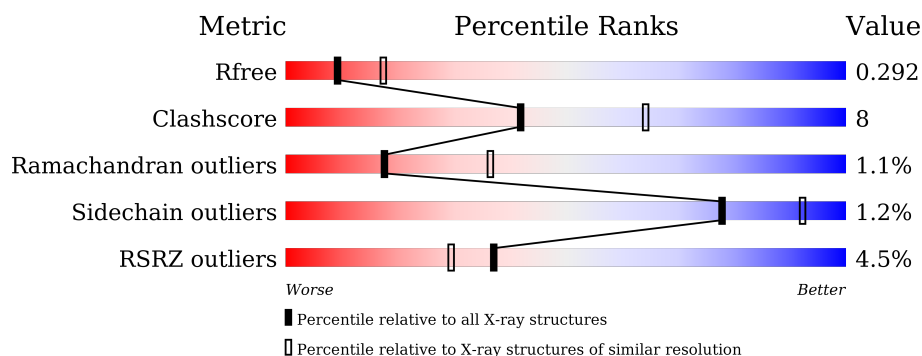
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	939	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>15%</div> <div>•</div> <div>13%</div> </div> </div>
1	B	939	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>16%</div> <div>••</div> <div>13%</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 13339 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.

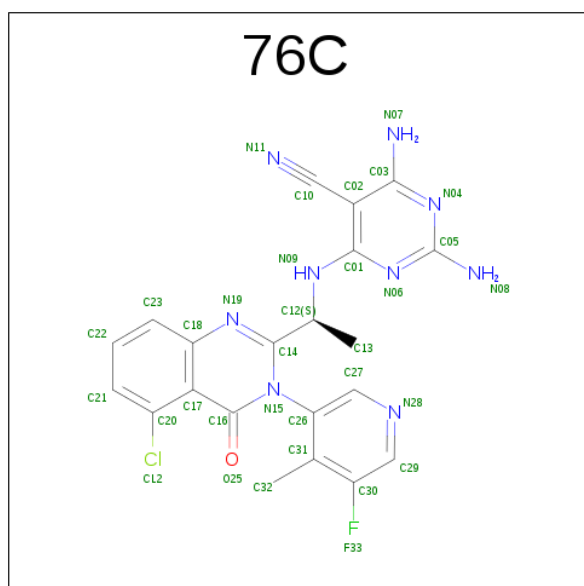
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	819	Total	C	N	O	S	0	0	0
			6603	4233	1121	1195	54			
1	B	816	Total	C	N	O	S	0	0	0
			6575	4216	1114	1191	54			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	508	GLN	-	insertion	UNP O35904
B	508	GLN	-	insertion	UNP O35904

- Molecule 2 is 2,4-bis(azanyl)-6-[[[(1 {S})-1-[5-chloranyl-3-(5-fluoranyl-4-methyl-pyridin-3-yl)-4-oxidanylidene-quinazolin-2-yl]ethyl]amino]pyrimidine-5-carbonitrile (three-letter code: 76C) (formula: C₂₁H₁₇ClFN₉O).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total 33	C 21	Cl 1	F 1	N 9	O 1	0	0
2	B	1	Total 33	C 21	Cl 1	F 1	N 9	O 1	0	0

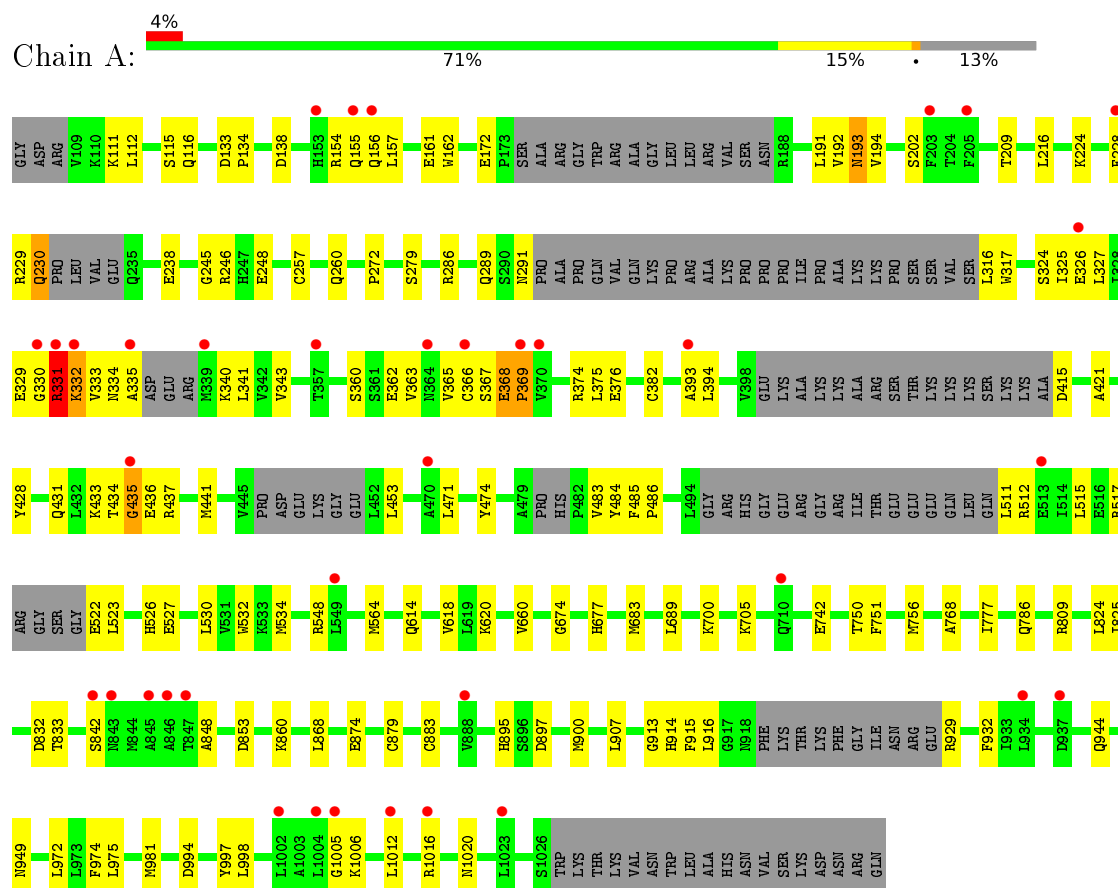
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	48	Total 48	O 48	0	0
3	B	47	Total 47	O 47	0	0

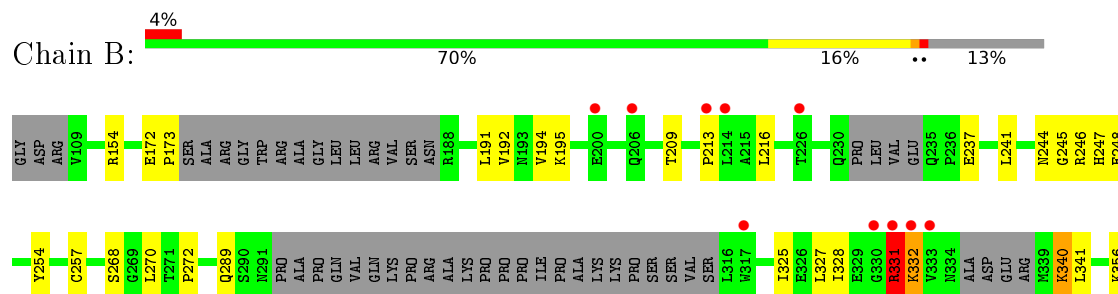
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit delta isoform



- Molecule 1: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit delta isoform



HIS	ASN	VAL	SER	LYS	ASP	ASN	ARG	GLN	L934	T935	T936	D937	F938	Q944	M949	E950	E951	K952	F953	E954	R955	F956	R957	G958	Y959	C960	R961	R962	A963	L975	M981	R982	A983	Y997	E1008	E1009	E1010	A1011	L1012	K1013	H1014	F1015	R1016	V1017	K1018	F1019	N1020	E1021	A1022	LEU	ARG	GLU	SER	TRP	LYS	THR	LYS	VAL	ASN	TRP	LEU	ALA																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
ASP	GLU	LYS	GLY	L452	E466	M564	T833	I834	Q838	K841	S842	M843	M844	T847	K852	L855	L856	K860	C883	V884	Y887	H895	S896	D897	M900	G913	H914	F915	L916	G917	R918	PHE	LYS	THR	LYS	PHE	PHE	GLY	ILE	ASN	ARG	GLU	R929	V930	P931	F932	I933																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
S360	S361	E362	V363	N364	V365	C366	S367	S368	P369	V370	H371	K372	Q373	R374	L375	L390	A393	A396	V397	V398	GLU	LYS	ALA	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS	LYS

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	64.23 Å 142.79 Å 221.07 Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	45.90 – 2.60 45.87 – 2.60	Depositor EDS
% Data completeness (in resolution range)	91.4 (45.90-2.60) 85.9 (45.87-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.70 (at 2.61 Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.230 , 0.294 0.233 , 0.292	Depositor DCC
R_{free} test set	1878 reflections (3.56%)	DCC
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.154	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.467 for h,-k,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	13339	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.96% 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: 76C

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	0.24	0/6741	0.42	1/9090 (0.0%)
1	B	0.27	1/6715 (0.0%)	0.47	3/9059 (0.0%)
All	All	0.26	1/13456 (0.0%)	0.44	4/18149 (0.0%)

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	B	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	332	LYS	CB-CG	-5.12	1.38	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	331	ARG	NE-CZ-NH1	-7.28	116.66	120.30
1	B	332	LYS	CB-CG-CD	-6.59	94.46	111.60
1	A	331	ARG	CG-CD-NE	5.85	124.08	111.80
1	B	331	ARG	N-CA-C	5.15	124.91	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	1012	LEU	Peptide
1	B	1013	LYS	Peptide
1	B	1014	HIS	Peptide
1	B	331	ARG	Peptide
1	B	366	CYS	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	6603	0	6597	97	0
1	B	6575	0	6565	124	1
2	A	33	0	0	0	0
2	B	33	0	0	0	0
3	A	48	0	0	3	0
3	B	47	0	0	2	0
All	All	13339	0	13162	221	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.

All (221) 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:331:ARG:HD3	1:A:368:GLU:HB3	1.56	0.85
1:A:193:ASN:ND2	1:A:202:SER:OG	2.10	0.84
1:A:883:CYS:HB3	1:A:932:PHE:HZ	1.44	0.81
1:B:557:LYS:HE3	1:B:559:GLU:HG2	1.65	0.77
1:A:324:SER:OG	1:A:374:ARG:NH1	2.18	0.76
1:B:856:LEU:HG	1:B:860:LYS:HE3	1.68	0.76
1:A:511:LEU:HB2	1:A:530:LEU:HD21	1.69	0.75
1:B:955:ARG:NH2	1:B:959:TYR:OH	2.19	0.74
1:A:944:GLN:OE1	1:A:949:ASN:ND2	2.21	0.74
1:A:1016:ARG:O	1:A:1020:ASN:ND2	2.22	0.72
1:A:331:ARG:HB3	1:A:368:GLU:HB3	1.73	0.70
1:B:331:ARG:HD2	1:B:368:GLU:CD	2.12	0.70
1:B:834:ILE:HD12	1:B:855:LEU:HD11	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:245:GLY:HA3	1:B:768:ALA:HB2	1.75	0.69
1:A:156:GLN:OE1	1:A:157:LEU:N	2.25	0.68
1:B:365:VAL:O	1:B:367:SER:HB3	1.92	0.68
1:B:331:ARG:HG2	1:B:368:GLU:H	1.57	0.68
1:B:341:LEU:HD11	1:B:365:VAL:HA	1.75	0.68
1:A:326:GLU:HB3	1:A:474:TYR:HB3	1.75	0.68
1:A:209:THR:HB	1:A:257:CYS:HB3	1.76	0.67
1:B:1010:GLU:O	1:B:1012:LEU:N	2.27	0.66
1:A:245:GLY:HA3	1:A:768:ALA:HB2	1.77	0.66
1:B:838:GLN:NE2	1:B:937:ASP:OD2	2.28	0.66
1:B:786:GLN:OE1	3:B:1201:HOH:O	2.13	0.66
1:B:1015:PHE:O	1:B:1019:PHE:N	2.28	0.66
1:A:512:ARG:HH22	1:A:534:MET:HB3	1.62	0.65
1:B:361:SER:OG	1:B:373:GLN:NE2	2.30	0.65
1:B:154:ARG:NH2	1:B:674:GLY:O	2.30	0.65
1:B:1016:ARG:O	1:B:1020:ASN:ND2	2.30	0.64
1:A:192:VAL:HG11	1:A:216:LEU:HD11	1.79	0.64
1:A:343:VAL:H	1:A:360:SER:HB3	1.62	0.63
1:A:246:ARG:NH1	1:A:248:GLU:OE1	2.32	0.62
1:B:361:SER:H	1:B:373:GLN:HE22	1.48	0.61
1:A:229:ARG:NH1	1:A:230:GLN:HG3	2.15	0.61
1:B:1010:GLU:C	1:B:1012:LEU:H	2.03	0.61
1:B:1013:LYS:HE3	1:B:1016:ARG:CD	2.32	0.60
1:A:340:LYS:HG2	1:A:362:GLU:HB3	1.84	0.60
1:B:1014:HIS:CD2	1:B:1014:HIS:H	2.17	0.60
1:B:1009:GLU:CG	1:B:1014:HIS:HE2	2.14	0.60
1:B:929:ARG:HA	1:B:997:TYR:HE1	1.67	0.60
1:B:1013:LYS:HE3	1:B:1016:ARG:HD2	1.84	0.60
1:A:1006:LYS:N	1:A:1006:LYS:HD3	2.17	0.59
1:A:1005:GLY:C	1:A:1006:LYS:HD3	2.22	0.59
1:A:332:LYS:NZ	1:A:369:PRO:HD3	2.16	0.59
1:A:883:CYS:HB3	1:A:932:PHE:CZ	2.32	0.59
1:A:325:ILE:HD11	1:A:375:LEU:HD12	1.84	0.58
1:A:517:ARG:H	1:A:548:ARG:NH2	2.01	0.58
1:A:224:LYS:HZ2	1:A:228:PHE:HD2	1.51	0.58
1:B:331:ARG:CG	1:B:368:GLU:H	2.17	0.57
1:B:780:ASN:ND2	1:B:822:THR:OG1	2.36	0.57
1:B:1011:ALA:O	1:B:1012:LEU:HB2	2.04	0.57
1:A:155:GLN:HA	1:A:156:GLN:NE2	2.18	0.57
1:A:809:ARG:NE	1:A:874:GLU:OE1	2.32	0.57
1:B:369:PRO:HG2	1:B:371:TRP:CZ3	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:614:GLN:HG3	1:A:981:MET:HG2	1.86	0.57
1:B:683:MET:O	1:B:687:GLU:HG3	2.05	0.57
1:B:512:ARG:NH2	1:B:534:MET:SD	2.78	0.57
1:A:331:ARG:HB3	1:A:368:GLU:CB	2.35	0.56
1:A:860:LYS:HG2	1:A:868:LEU:HD13	1.88	0.55
1:B:192:VAL:HG11	1:B:216:LEU:HD11	1.87	0.55
1:B:598:LYS:HD3	1:B:598:LYS:N	2.22	0.55
1:B:917:GLY:HA2	1:B:930:VAL:HG23	1.89	0.55
1:A:172:GLU:HB3	1:A:260:GLN:HG3	1.87	0.55
1:A:786:GLN:HG2	1:A:915:PHE:CE2	2.42	0.54
1:B:884:VAL:HG22	1:B:1015:PHE:CE1	2.42	0.54
1:B:785:ARG:N	3:B:1201:HOH:O	2.30	0.54
1:B:944:GLN:HE21	1:B:952:LYS:NZ	2.05	0.54
1:A:229:ARG:HD2	1:A:229:ARG:C	2.28	0.54
1:A:879:CYS:HA	1:A:907:LEU:HD23	1.90	0.54
1:B:614:GLN:HG3	1:B:981:MET:HG2	1.89	0.54
1:A:332:LYS:HZ2	1:A:369:PRO:HD3	1.71	0.53
1:A:532:TRP:HZ3	1:A:564:MET:HE2	1.74	0.53
1:B:512:ARG:HH12	1:B:537:GLU:HB2	1.73	0.53
1:B:883:CYS:HB3	1:B:932:PHE:CZ	2.44	0.53
1:A:833:THR:HG22	1:A:900:MET:HG2	1.91	0.53
1:B:341:LEU:O	1:B:362:GLU:HA	2.07	0.53
1:A:750:THR:OG1	1:A:751:PHE:N	2.41	0.53
1:B:591:TYR:O	1:B:595:PHE:HD2	1.92	0.53
1:B:1012:LEU:HB3	1:B:1014:HIS:HA	1.91	0.53
1:B:750:THR:OG1	1:B:751:PHE:N	2.41	0.53
1:B:246:ARG:NH1	1:B:248:GLU:OE1	2.43	0.52
1:B:530:LEU:HG	1:B:534:MET:HE2	1.90	0.52
1:A:929:ARG:HA	1:A:997:TYR:HE1	1.75	0.52
1:B:1018:LYS:HA	1:B:1021:GLU:HB2	1.91	0.52
1:A:324:SER:HB3	1:A:376:GLU:HA	1.91	0.51
1:A:415:ASP:N	3:A:1207:HOH:O	2.44	0.51
1:B:960:CYS:HB3	1:B:1015:PHE:CZ	2.46	0.51
1:A:162:TRP:HH2	1:A:289:GLN:HE21	1.58	0.51
1:A:289:GLN:OE1	1:A:677:HIS:CE1	2.64	0.51
1:A:786:GLN:NE2	3:A:1208:HOH:O	2.44	0.50
1:B:247:HIS:HD2	1:B:740:LEU:HD11	1.77	0.50
1:B:856:LEU:O	1:B:860:LYS:HG3	2.12	0.50
1:A:289:GLN:OE1	1:A:677:HIS:ND1	2.45	0.50
1:A:316:LEU:HD12	1:A:483:VAL:HG12	1.93	0.50
1:A:913:GLY:C	1:A:914:HIS:HD2	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1013:LYS:HE3	1:B:1016:ARG:NE	2.27	0.49
1:A:367:SER:HB3	1:A:368:GLU:C	2.32	0.49
1:B:532:TRP:HZ3	1:B:564:MET:HE2	1.78	0.49
1:A:229:ARG:O	1:A:230:GLN:HB3	2.12	0.49
1:B:833:THR:HG22	1:B:900:MET:HG2	1.94	0.48
1:B:512:ARG:NE	1:B:534:MET:HE3	2.29	0.48
1:B:421:ALA:HB2	1:B:441:MET:HG2	1.94	0.48
1:A:421:ALA:HB2	1:A:441:MET:HG2	1.95	0.48
1:B:331:ARG:HG2	1:B:368:GLU:N	2.26	0.48
1:A:895:HIS:CE1	1:A:897:ASP:HB2	2.48	0.48
1:B:883:CYS:HB3	1:B:932:PHE:HZ	1.79	0.48
1:B:557:LYS:HD2	1:B:558:HIS:N	2.29	0.48
1:A:777:ILE:HB	1:A:825:ILE:HB	1.96	0.48
1:B:777:ILE:HB	1:B:825:ILE:HB	1.96	0.48
1:B:390:LEU:HB2	1:B:425:LEU:HD21	1.96	0.47
1:B:341:LEU:HA	1:B:341:LEU:HD23	1.62	0.47
1:B:209:THR:HB	1:B:257:CYS:HB3	1.96	0.47
1:B:1016:ARG:HA	1:B:1019:PHE:HB3	1.96	0.47
1:A:526:HIS:CE1	1:A:527:GLU:HG3	2.50	0.47
1:B:952:LYS:HA	1:B:955:ARG:HG2	1.96	0.47
1:A:434:THR:HA	1:A:435:GLY:HA2	1.68	0.47
1:B:194:VAL:HG21	1:B:216:LEU:HD21	1.97	0.47
1:A:436:GLU:HA	1:A:474:TYR:HA	1.96	0.46
1:A:112:LEU:O	1:A:116:GLN:HG2	2.14	0.46
1:B:435:GLY:HA2	1:B:475:LEU:HB2	1.98	0.46
1:B:393:ALA:HB1	1:B:452:LEU:HD23	1.96	0.46
1:B:434:THR:HG21	1:B:477:GLU:HA	1.97	0.46
1:B:1011:ALA:HB3	1:B:1014:HIS:CE1	2.50	0.46
1:B:396:ALA:HB2	1:B:418:ILE:HD11	1.97	0.46
1:B:509:LEU:HB2	1:B:512:ARG:HH21	1.79	0.46
1:B:895:HIS:CE1	1:B:897:ASP:HB2	2.51	0.46
1:A:332:LYS:HD3	1:A:394:LEU:HD21	1.98	0.46
1:B:435:GLY:O	1:B:475:LEU:N	2.47	0.46
1:A:436:GLU:HB2	1:A:474:TYR:HD1	1.81	0.45
1:B:915:PHE:HD1	1:B:916:LEU:HG	1.82	0.45
1:B:1014:HIS:HB2	1:B:1015:PHE:H	1.45	0.45
1:B:331:ARG:NE	1:B:367:SER:O	2.49	0.45
1:B:954:GLU:OE2	1:B:957:ARG:NH2	2.49	0.45
1:B:195:LYS:HE3	1:B:244:ASN:HD21	1.82	0.45
1:A:116:GLN:HB2	1:A:683:MET:SD	2.57	0.45
1:A:154:ARG:HG3	1:A:157:LEU:HD12	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:VAL:HG21	1:A:216:LEU:HD21	1.99	0.45
1:A:191:LEU:O	1:A:272:PRO:HD2	2.16	0.45
1:A:365:VAL:O	1:A:367:SER:N	2.50	0.45
1:B:934:LEU:HD21	1:B:1022:ALA:C	2.38	0.44
1:B:595:PHE:HA	1:B:598:LYS:HG2	2.00	0.44
1:A:848:ALA:HB1	1:A:853:ASP:HB2	2.00	0.44
1:B:574:LEU:O	1:B:599:SER:HB3	2.17	0.44
1:B:693:LYS:NZ	1:B:780:ASN:OD1	2.47	0.44
1:A:1012:LEU:O	1:A:1016:ARG:HG3	2.18	0.44
1:A:515:LEU:HD13	1:A:523:LEU:HD21	1.99	0.44
1:B:895:HIS:ND1	1:B:897:ASP:HB2	2.33	0.44
1:B:950:SER:HA	1:B:953:PHE:HB3	2.00	0.44
1:A:620:LYS:HE2	1:A:660:VAL:HG11	1.99	0.44
1:B:431:GLN:HB2	1:B:484:TYR:CE1	2.53	0.44
1:B:331:ARG:CD	1:B:368:GLU:H	2.29	0.44
1:A:367:SER:HB3	1:A:369:PRO:N	2.33	0.44
1:A:393:ALA:HB2	1:A:453:LEU:HD13	1.99	0.44
1:B:591:TYR:O	1:B:595:PHE:CD2	2.70	0.43
1:B:944:GLN:HE21	1:B:952:LYS:HZ3	1.66	0.43
1:B:884:VAL:HG22	1:B:1015:PHE:HE1	1.83	0.43
1:A:327:LEU:HD11	1:A:471:LEU:HD11	1.99	0.43
1:B:341:LEU:CD1	1:B:365:VAL:HA	2.47	0.43
1:B:213:PRO:HD3	1:B:254:TYR:O	2.18	0.43
1:B:327:LEU:HD11	1:B:471:LEU:HD11	1.99	0.43
1:B:621:TYR:CZ	1:B:983:ALA:HB2	2.53	0.43
1:A:341:LEU:HB2	1:A:363:VAL:O	2.18	0.43
1:B:808:LEU:HD11	1:B:963:ALA:HB2	2.01	0.43
1:A:157:LEU:HD22	1:A:161:GLU:HB3	2.00	0.43
1:B:950:SER:O	1:B:954:GLU:N	2.47	0.43
1:B:191:LEU:O	1:B:272:PRO:HD2	2.19	0.42
1:B:490:LYS:HD2	1:B:490:LYS:HA	1.84	0.42
1:B:1009:GLU:CG	1:B:1014:HIS:NE2	2.81	0.42
1:B:1012:LEU:CD2	1:B:1014:HIS:HA	2.49	0.42
1:B:1017:VAL:O	1:B:1021:GLU:HG2	2.19	0.42
1:B:842:SER:O	1:B:844:MET:N	2.52	0.42
1:B:213:PRO:HB3	1:B:241:LEU:HD12	2.02	0.42
1:B:957:ARG:HG3	1:B:1019:PHE:CE2	2.54	0.42
1:A:329:GLU:HB2	1:A:330:GLY:H	1.61	0.42
1:A:317:TRP:HA	1:A:382:CYS:HB2	2.02	0.42
1:A:512:ARG:O	1:A:515:LEU:HG	2.20	0.42
1:A:689:LEU:HD21	1:A:824:LEU:HD11	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:ILE:HD11	1:B:375:LEU:HD12	2.01	0.42
1:B:841:LYS:O	1:B:847:THR:HG22	2.20	0.42
1:B:268:SER:HB2	1:B:270:LEU:HG	2.01	0.42
1:A:154:ARG:NE	3:A:1205:HOH:O	2.40	0.42
1:A:431:GLN:HB2	1:A:484:TYR:CE1	2.55	0.42
1:A:972:LEU:HD23	1:A:975:LEU:HD12	2.01	0.42
1:B:328:ILE:HD12	1:B:472:VAL:HG12	2.02	0.42
1:A:111:LYS:O	1:A:115:SER:N	2.50	0.42
1:B:852:LYS:HB2	1:B:852:LYS:HE3	1.78	0.41
1:A:138:ASP:OD2	1:A:428:TYR:OH	2.28	0.41
1:A:974:PHE:HB3	1:A:998:LEU:HD21	2.02	0.41
1:B:975:LEU:HD23	1:B:975:LEU:HA	1.93	0.41
1:A:433:LYS:HD3	1:A:437:ARG:HH11	1.85	0.41
1:B:1012:LEU:HD23	1:B:1014:HIS:HA	2.01	0.41
1:B:356:LYS:HB3	1:B:356:LYS:HE2	1.55	0.41
1:B:594:SER:O	1:B:597:ILE:HB	2.21	0.41
1:A:162:TRP:CZ2	1:A:289:GLN:NE2	2.88	0.41
1:A:433:LYS:HD3	1:A:437:ARG:NH1	2.35	0.41
1:A:154:ARG:NH2	1:A:674:GLY:O	2.51	0.41
1:B:589:ASP:HB3	1:B:592:VAL:HB	2.02	0.41
1:A:614:GLN:O	1:A:618:VAL:HG23	2.20	0.41
1:A:705:LYS:HE2	1:A:705:LYS:HB3	1.85	0.41
1:A:832:ASP:OD1	1:A:833:THR:N	2.53	0.41
1:A:913:GLY:C	1:A:914:HIS:CD2	2.94	0.41
1:A:916:LEU:HD13	1:A:994:ASP:HB3	2.02	0.41
1:B:949:ASN:OD1	1:B:952:LYS:HB2	2.21	0.41
1:B:669:GLU:O	1:B:673:ARG:HG2	2.20	0.41
1:B:962:ARG:HE	1:B:962:ARG:HB2	1.48	0.41
1:B:614:GLN:O	1:B:618:VAL:HG23	2.20	0.41
1:B:427:ASP:OD1	1:B:431:GLN:N	2.47	0.41
1:B:1009:GLU:CD	1:B:1014:HIS:HE2	2.24	0.41
1:A:334:ASN:CG	1:A:335:ALA:H	2.23	0.41
1:A:485:PHE:HA	1:A:486:PRO:HD3	1.98	0.41
1:B:340:LYS:HE2	1:B:364:ASN:N	2.36	0.41
1:A:700:LYS:HE3	1:A:756:MET:O	2.21	0.40
1:B:331:ARG:O	1:B:469:ALA:HA	2.21	0.40
1:B:512:ARG:HH12	1:B:537:GLU:CB	2.33	0.40
1:B:172:GLU:HG3	1:B:173:PRO:HD2	2.02	0.40
1:A:133:ASP:HA	1:A:134:PRO:HD2	1.95	0.40
1:A:238:GLU:OE1	1:A:279:SER:OG	2.23	0.40
1:B:360:SER:OG	1:B:361:SER:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:162:TRP:CE3	1:A:286:ARG:HG3	2.57	0.40
1:B:393:ALA:HB1	1:B:452:LEU:CD2	2.51	0.40
1:B:289:GLN:HG2	1:B:677:HIS:CD2	2.57	0.40

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)
1:B:356:LYS:NZ	1:B:843:ASN:O[3_555]	2.02	0.18

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	794/939 (85%)	752 (95%)	36 (4%)	6 (1%)	24	46
1	B	794/939 (85%)	740 (93%)	43 (5%)	11 (1%)	14	28
All	All	1588/1878 (85%)	1492 (94%)	79 (5%)	17 (1%)	17	36

All (17) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	367	SER
1	B	1012	LEU
1	A	333	VAL
1	A	366	CYS
1	B	755	LYS
1	B	843	ASN
1	B	935	THR
1	B	1011	ALA
1	B	1015	PHE
1	B	742	GLU

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Mol	Chain	Res	Type
1	B	949	ASN
1	A	742	GLU
1	A	842	SER
1	B	435	GLY
1	A	435	GLY
1	A	369	PRO
1	B	368	GLU

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	726/827 (88%)	719 (99%)	7 (1%)	82	94
1	B	723/827 (87%)	712 (98%)	11 (2%)	72	90
All	All	1449/1654 (88%)	1431 (99%)	18 (1%)	78	92

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193	ASN
1	A	230	GLN
1	A	291	ASN
1	A	331	ARG
1	A	332	LYS
1	A	368	GLU
1	A	522	GLU
1	B	237	GLU
1	B	332	LYS
1	B	340	LYS
1	B	374	ARG
1	B	466	GLU
1	B	512	ARG
1	B	933	ILE
1	B	1012	LEU
1	B	1013	LYS

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Mol	Chain	Res	Type
1	B	1014	HIS
1	B	1015	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	193	ASN
1	A	291	ASN
1	A	914	HIS
1	B	247	HIS
1	B	373	GLN
1	B	526	HIS
1	B	944	GLN
1	B	1020	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	76C	A	1101	-	36,36,36	1.51	8 (22%)	32,53,53	1.37	4 (12%)
2	76C	B	1101	-	36,36,36	1.51	8 (22%)	32,53,53	1.37	4 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	76C	A	1101	-	-	0/10/14/14	0/4/4/4
2	76C	B	1101	-	-	0/10/14/14	0/4/4/4

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1101	76C	C26-N15	-2.18	1.43	1.45
2	B	1101	76C	C26-N15	-2.16	1.43	1.45
2	B	1101	76C	C02-C03	-2.09	1.39	1.42
2	A	1101	76C	C02-C03	-2.08	1.39	1.42
2	A	1101	76C	C16-N15	2.07	1.41	1.37
2	B	1101	76C	C03-N07	2.08	1.39	1.34
2	A	1101	76C	C03-N07	2.08	1.39	1.34
2	B	1101	76C	C16-N15	2.11	1.41	1.37
2	A	1101	76C	C05-N08	2.12	1.38	1.34
2	B	1101	76C	C05-N08	2.13	1.38	1.34
2	A	1101	76C	C14-C12	2.58	1.54	1.50
2	B	1101	76C	C14-C12	2.61	1.54	1.50
2	A	1101	76C	C01-N09	3.23	1.40	1.35
2	B	1101	76C	C01-N09	3.23	1.40	1.35
2	A	1101	76C	C16-C17	4.88	1.49	1.41
2	B	1101	76C	C16-C17	4.90	1.49	1.41

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	76C	C26-C27-N28	2.15	124.58	122.20
2	B	1101	76C	C26-C27-N28	2.16	124.59	122.20
2	B	1101	76C	C31-C26-N15	2.65	122.65	119.45
2	A	1101	76C	C31-C26-N15	2.65	122.66	119.45
2	B	1101	76C	C13-C12-N09	3.02	113.70	109.08
2	A	1101	76C	C13-C12-N09	3.03	113.71	109.08
2	B	1101	76C	F33-C30-C31	3.05	120.73	117.69

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	1101	76C	F33-C30-C31	3.06	120.73	117.69

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	A	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	A	155:GLN	C	156:GLN	N	6.51
1	A	156:GLN	C	157:LEU	N	6.22

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	819/939 (87%)	0.29	37 (4%) 37 29	38, 61, 89, 110	0
1	B	816/939 (86%)	0.24	37 (4%) 37 29	37, 61, 92, 118	0
All	All	1635/1878 (87%)	0.26	74 (4%) 37 29	37, 61, 90, 118	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	366	CYS	8.8
1	A	330	GLY	8.3
1	B	1015	PHE	7.7
1	B	932	PHE	5.1
1	B	366	CYS	4.9
1	B	332	LYS	4.4
1	B	934	LEU	4.4
1	B	370	VAL	4.3
1	A	846	ALA	4.2
1	B	1011	ALA	4.0
1	A	470	ALA	4.0
1	B	843	ASN	3.9
1	B	915	PHE	3.6
1	A	435	GLY	3.6
1	B	936	TYR	3.4
1	B	333	VAL	3.4
1	B	510	GLN	3.3
1	A	843	ASN	3.2
1	A	228	PHE	3.2
1	B	963	ALA	3.1
1	A	153	HIS	3.1
1	A	155	GLN	3.0
1	B	938	PHE	3.0
1	A	331	ARG	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	842	SER	2.8
1	A	845	ALA	2.8
1	A	156	GLN	2.8
1	A	1004	LEU	2.8
1	A	370	VAL	2.7
1	A	205	PHE	2.7
1	B	317	TRP	2.7
1	B	913	GLY	2.7
1	A	937	ASP	2.7
1	B	567	LEU	2.7
1	B	950	SER	2.7
1	A	364	ASN	2.7
1	B	596	ALA	2.7
1	B	214	LEU	2.7
1	A	1023	LEU	2.7
1	A	339	MET	2.6
1	B	914	HIS	2.6
1	A	1016	ARG	2.6
1	B	1008	GLU	2.6
1	B	1010	GLU	2.6
1	B	844	MET	2.5
1	A	888	VAL	2.5
1	A	332	LYS	2.5
1	A	393	ALA	2.5
1	A	1005	GLY	2.5
1	B	512	ARG	2.4
1	A	847	THR	2.4
1	A	934	LEU	2.4
1	B	213	PRO	2.4
1	A	710	GLN	2.3
1	B	200	GLU	2.3
1	A	335	ALA	2.3
1	B	887	TYR	2.3
1	B	931	PRO	2.2
1	B	1012	LEU	2.2
1	B	226	THR	2.2
1	A	369	PRO	2.2
1	B	330	GLY	2.2
1	A	1002	LEU	2.2
1	B	599	SER	2.1
1	A	357	THR	2.1
1	B	838	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	477	GLU	2.1
1	B	206	GLN	2.1
1	A	513	GLU	2.1
1	A	203	PHE	2.0
1	B	331	ARG	2.0
1	A	326	GLU	2.0
1	A	549	LEU	2.0
1	A	1012	LEU	2.0

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	76C	B	1101	33/33	0.94	0.20	0.50	36,46,56,73	0
2	76C	A	1101	33/33	0.95	0.18	0.11	36,45,56,70	0

6.5 Other polymers [i](#)

There are no such residues in this entry.