



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:33 AM UTC

PDB ID : 5T7F / pdb_00005t7f
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

<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
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

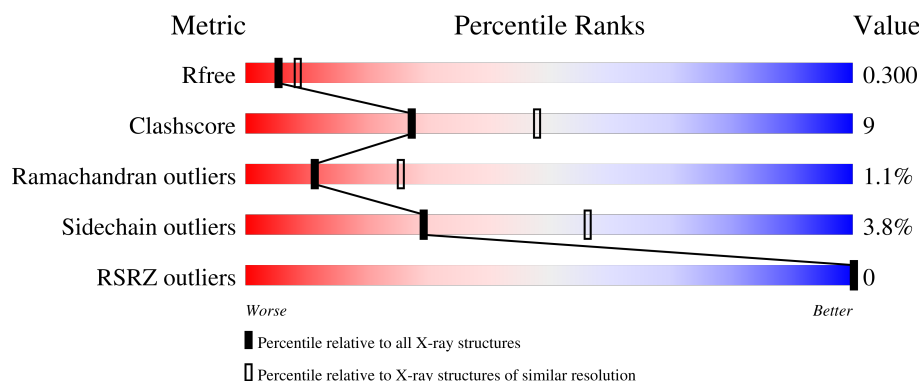
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (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 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	939	 68% 17% • 13%
1	B	939	 67% 17% •• 13%

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.

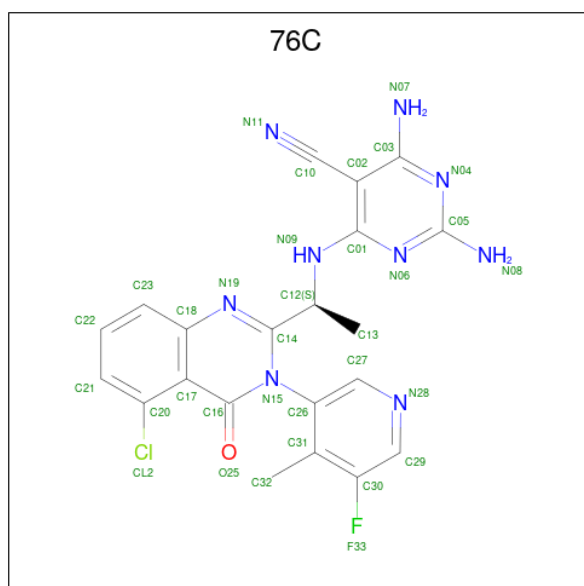
- Molecule 1 is a protein called Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic sub-unit delta isoform.

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 (CCD ID: 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

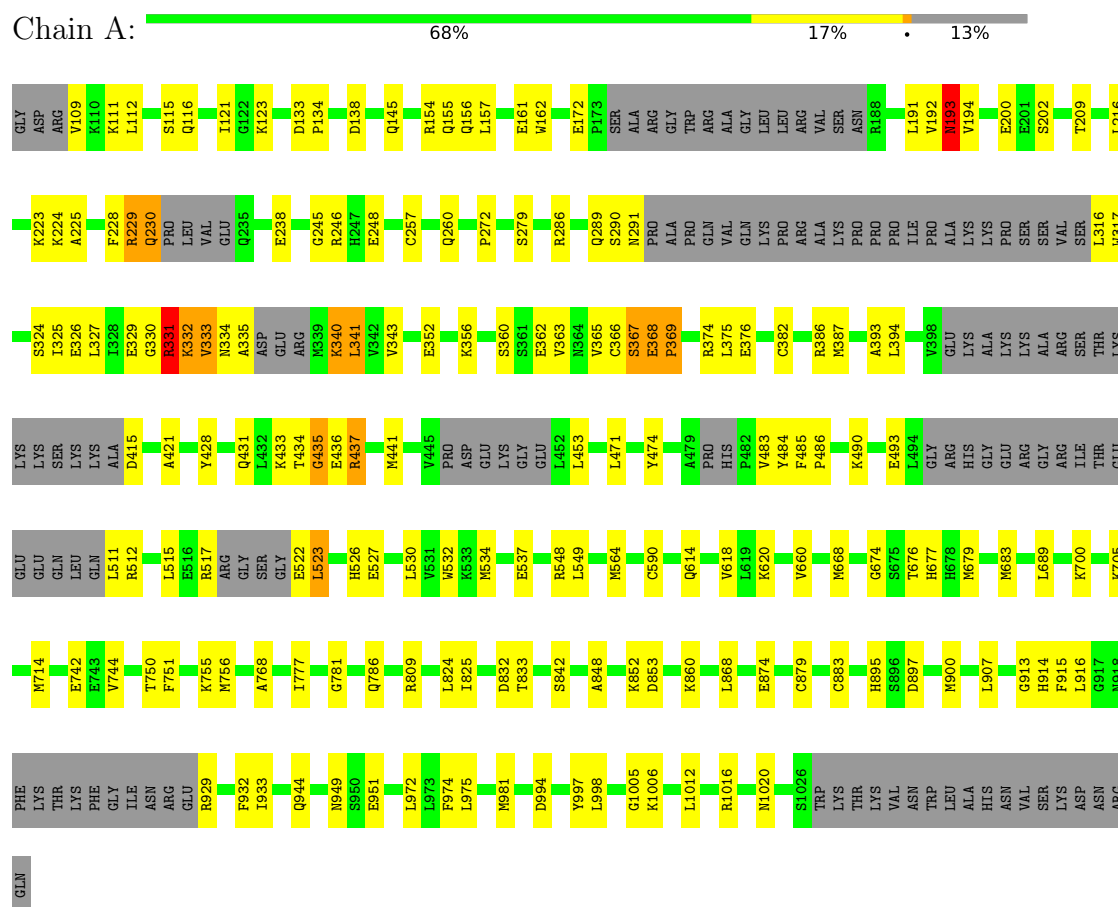
- Molecule 3 is water.

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

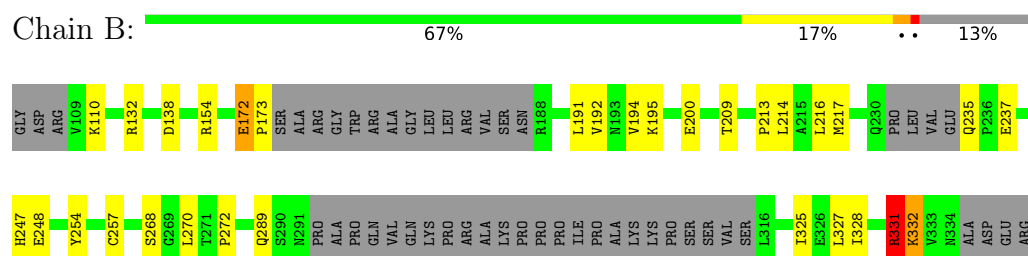
3 Residue-property plots

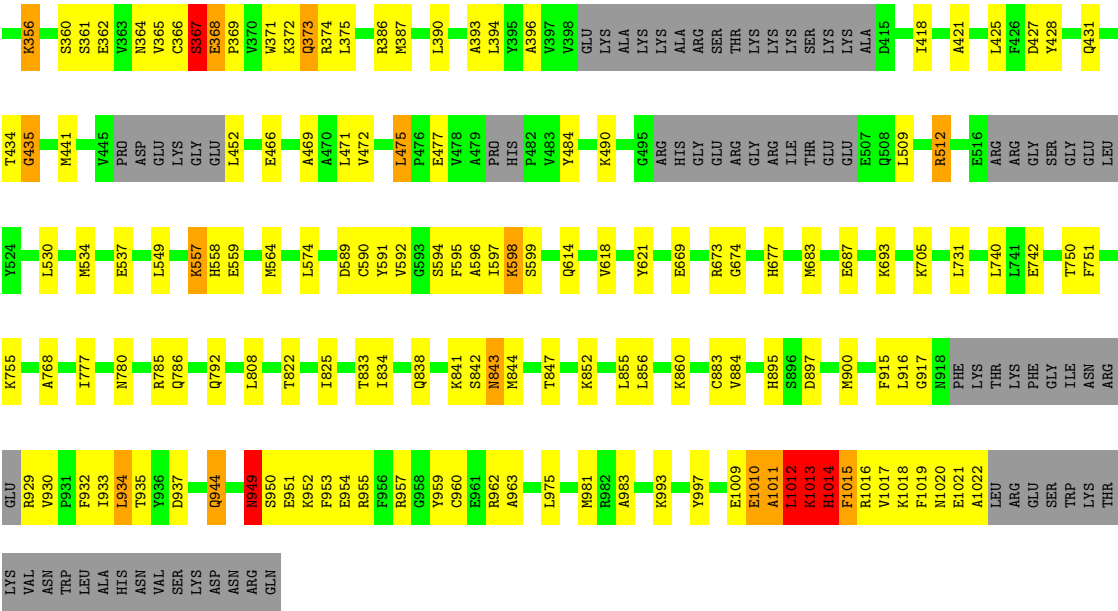
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Phosphatidylinositol 4,5-bisphosphate 3-kinase catalytic subunit delta isoform



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





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	64.23Å 142.79Å 221.07Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	45.90 – 2.60 45.90 – 2.60	Depositor EDS
% Data completeness (in resolution range)	91.4 (45.90-2.60) 86.1 (45.90-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.230 , 0.294 0.239 , 0.300	Depositor DCC
R_{free} test set	1983 reflections (3.23%)	wwPDB-VP
Wilson B-factor (Å ²)	47.4	Xtriage
Anisotropy	0.177	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.467 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	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

5.1 Standard geometry

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	0.28	0/6741	0.73	6/9090 (0.1%)
1	B	0.33	0/6715	0.77	14/9059 (0.2%)
All	All	0.31	0/13456	0.75	20/18149 (0.1%)

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

There are no bond length outliers.

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	331	ARG	N-CA-C	11.38	124.91	108.86
1	B	1010	GLU	N-CA-C	-8.69	102.23	112.92
1	B	332	LYS	N-CA-C	8.27	123.95	108.65
1	B	332	LYS	CB-CG-CD	-7.32	94.46	111.30
1	B	949	ASN	CA-C-N	7.22	129.96	120.28
1	B	949	ASN	C-N-CA	7.22	129.96	120.28
1	B	367	SER	CA-C-N	6.63	133.63	121.70
1	B	367	SER	C-N-CA	6.63	133.63	121.70
1	B	235	GLN	CA-C-N	6.55	126.24	119.82
1	B	235	GLN	C-N-CA	6.55	126.24	119.82
1	A	193	ASN	N-CA-C	6.26	120.03	109.76
1	B	373	GLN	N-CA-C	5.88	117.92	110.33
1	A	331	ARG	N-CA-C	5.71	117.43	107.49
1	A	290	SER	N-CA-C	5.65	118.08	108.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	596	ALA	N-CA-C	-5.51	105.28	112.23
1	A	331	ARG	CG-CD-NE	5.49	124.08	112.00
1	B	475	LEU	CA-C-N	5.48	125.79	119.93
1	B	475	LEU	C-N-CA	5.48	125.79	119.93
1	A	367	SER	CA-C-N	5.05	130.79	121.70
1	A	367	SER	C-N-CA	5.05	130.79	121.70

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 [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	6603	0	6597	106	0
1	B	6575	0	6565	133	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	239	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 9.

All (239) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:387:MET:HE3	1:B:590:CYS:HB3	1.66	0.78
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:B:331:ARG:HD2	1:B:368:GLU:CD	2.12	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:756:MET:HE2	1:A:781:GLY:HA3	1.71	0.72
1:A:331:ARG:HB3	1:A:368:GLU:HB3	1.73	0.70
1:B:834:ILE:HD12	1:B:855:LEU:HD11	1.74	0.69
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:A:332:LYS:HZ2	1:A:369:PRO:HD3	1.59	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:1010:GLU:C	1:B:1012:LEU:H	2.03	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:1005:GLY:C	1:A:1006:LYS:HD3	2.22	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:549:LEU:HG	1:A:564:MET:HE1	1.81	0.63
1:A:387:MET:HE3	1:A:590:CYS:HB3	1.81	0.63
1:B:386:ARG:HG3	1:B:387:MET:HE2	1.79	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1009:GLU:CG	1:B:1014:HIS:HE2	2.14	0.60
1:B:1014:HIS:H	1:B:1014:HIS:CD2	2.17	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:HD3	1:A:1006:LYS:N	2.17	0.59
1:A:386:ARG:HG3	1:A:387:MET:HE2	1.83	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:229:ARG:C	1:A:229:ARG:HD2	2.28	0.58
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
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:B:530:LEU:HG	1:B:534:MET:HE2	1.88	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:785:ARG:N	3:B:1201:HOH:O	2.30	0.54
1:B:884:VAL:HG22	1:B:1015:PHE:CE1	2.42	0.54
1:A:367:SER:HB3	1:A:368:GLU:C	2.32	0.54
1:B:394:LEU:HD13	1:B:441:MET:HE1	1.89	0.54
1:B:944:GLN:HE21	1:B:952:LYS:NZ	2.05	0.54
1:A:879:CYS:HA	1:A:907:LEU:HD23	1.90	0.54
1:A:913:GLY:C	1:A:914:HIS:HD2	2.15	0.54
1:B:614:GLN:HG3	1:B:981:MET:HG2	1.89	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:750:THR:OG1	1:B:751:PHE:N	2.41	0.53
1:B:1012:LEU:HB3	1:B:1014:HIS:HA	1.91	0.53
1:B:246:ARG:NH1	1:B:248:GLU:OE1	2.43	0.52
1:B:138:ASP:OD2	1:B:428:TYR:OH	2.27	0.52
1:A:929:ARG:HA	1:A:997:TYR:HE1	1.75	0.52
1:B:1010:GLU:C	1:B:1012:LEU:N	2.68	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:B:1013:LYS:HE3	1:B:1016:ARG:NE	2.27	0.49
1:B:934:LEU:HD21	1:B:1022:ALA:C	2.38	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: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:394:LEU:HD13	1:A:441:MET:HE1	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:1011:ALA:HB3	1:B:1014:HIS:CE1	2.50	0.46
1:A:913:GLY:C	1:A:914:HIS:CD2	2.94	0.46
1:B:549:LEU:HG	1:B:564:MET:HE1	1.97	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:530:LEU:CG	1:B:534:MET:HE2	2.46	0.45
1:B:1009:GLU:CD	1:B:1014:HIS:HE2	2.24	0.45
1:A:334:ASN:CG	1:A:335:ALA:H	2.23	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:512:ARG:HB2	1:B:534:MET:HE1	1.98	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
1:A:191:LEU:O	1:A:272:PRO:HD2	2.16	0.45
1:A:194:VAL:HG21	1:A:216:LEU:HD21	1.99	0.45
1:A:365:VAL:O	1:A:367:SER:N	2.50	0.45
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:ALA:HB2	1:A:453:LEU:HD13	1.99	0.44
1:A:532:TRP:HZ3	1:A:564:MET:HE2	1.83	0.43
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:225:ALA:HB1	1:A:230:GLN:C	2.44	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:371:TRP:C	1:B:373:GLN:H	2.26	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:842:SER:O	1:B:844:MET:N	2.52	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:A:121:ILE:HB	1:A:668:MET:HE3	2.01	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
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:A:679:MET:HE2	1:A:679:MET:HB3	1.89	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:HE3	1:B:852:LYS:HB2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:1012:LEU:HD23	1:B:1014:HIS:HA	2.01	0.41
1:A:154:ARG:NH2	1:A:674:GLY:O	2.51	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:B:214:LEU:HA	1:B:217:MET:HE3	2.02	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:676:THR:O	1:A:679:MET:HE2	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: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: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
1:A:162:TRP:CE3	1:A:286:ARG:HG3	2.57	0.40
1:B:289:GLN:HG2	1:B:677:HIS:CD2	2.57	0.40
1:B:393:ALA:HB1	1:B:452:LEU:CD2	2.51	0.40
1:B:1010:GLU:O	1:B:1010:GLU:CD	2.65	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

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	794/939 (85%)	752 (95%)	36 (4%)	6 (1%)	16	34
1	B	794/939 (85%)	740 (93%)	43 (5%)	11 (1%)	9	19
All	All	1588/1878 (85%)	1492 (94%)	79 (5%)	17 (1%)	11	25

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
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%)	697 (96%)	29 (4%)	28	55
1	B	723/827 (87%)	697 (96%)	26 (4%)	31	58
All	All	1449/1654 (88%)	1394 (96%)	55 (4%)	29	56

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	VAL
1	A	123	LYS
1	A	145	GLN
1	A	193	ASN
1	A	200	GLU
1	A	223	LYS
1	A	229	ARG
1	A	230	GLN
1	A	291	ASN
1	A	331	ARG
1	A	332	LYS
1	A	333	VAL
1	A	340	LYS
1	A	341	LEU
1	A	352	GLU
1	A	356	LYS
1	A	368	GLU
1	A	437	ARG
1	A	490	LYS
1	A	493	GLU
1	A	522	GLU
1	A	523	LEU
1	A	537	GLU
1	A	714	MET
1	A	744	VAL
1	A	755	LYS
1	A	852	LYS
1	A	933	ILE
1	A	951	GLU
1	B	110	LYS
1	B	132	ARG
1	B	172	GLU
1	B	200	GLU
1	B	237	GLU

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Mol	Chain	Res	Type
1	B	332	LYS
1	B	340	LYS
1	B	352	GLU
1	B	356	LYS
1	B	372	LYS
1	B	374	ARG
1	B	466	GLU
1	B	512	ARG
1	B	557	LYS
1	B	598	LYS
1	B	705	LYS
1	B	731	LEU
1	B	792	GLN
1	B	933	ILE
1	B	934	LEU
1	B	944	GLN
1	B	951	GLU
1	B	993	LYS
1	B	1012	LEU
1	B	1013	LYS
1	B	1014	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	GLN
1	A	193	ASN
1	A	291	ASN
1	A	464	ASN
1	A	536	HIS
1	A	721	GLN
1	A	914	HIS
1	A	976	HIS
1	B	193	ASN
1	B	247	HIS
1	B	351	ASN
1	B	373	GLN
1	B	526	HIS
1	B	536	HIS
1	B	721	GLN
1	B	944	GLN
1	B	976	HIS

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Mol	Chain	Res	Type
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 oligosaccharides 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	B	1101	-	35,36,36	1.10	5 (14%)	41,53,53	1.55	3 (7%)
2	76C	A	1101	-	35,36,36	1.10	5 (14%)	41,53,53	1.54	4 (9%)

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	B	1101	-	-	0/10/14/14	0/4/4/4
2	76C	A	1101	-	-	0/10/14/14	0/4/4/4

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1101	76C	C01-N09	3.30	1.40	1.35
2	A	1101	76C	C01-N09	3.29	1.40	1.35
2	B	1101	76C	C05-N08	2.33	1.38	1.33
2	A	1101	76C	C05-N08	2.32	1.38	1.33
2	A	1101	76C	C03-N07	2.13	1.39	1.34
2	B	1101	76C	C03-N07	2.13	1.39	1.34
2	B	1101	76C	C12-C14	2.13	1.54	1.50
2	A	1101	76C	C12-C14	2.11	1.54	1.50
2	B	1101	76C	C02-C03	-2.03	1.39	1.42
2	A	1101	76C	C02-C03	-2.03	1.39	1.42

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1101	76C	C17-C20-CL2	4.29	125.14	119.62
2	B	1101	76C	C17-C20-CL2	4.28	125.14	119.62
2	A	1101	76C	C31-C26-N15	4.21	122.66	119.05
2	B	1101	76C	C31-C26-N15	4.20	122.64	119.05
2	B	1101	76C	N15-C14-N19	-2.20	122.31	124.21
2	A	1101	76C	N15-C14-N19	-2.18	122.32	124.21
2	A	1101	76C	C26-N15-C14	2.04	122.67	120.49

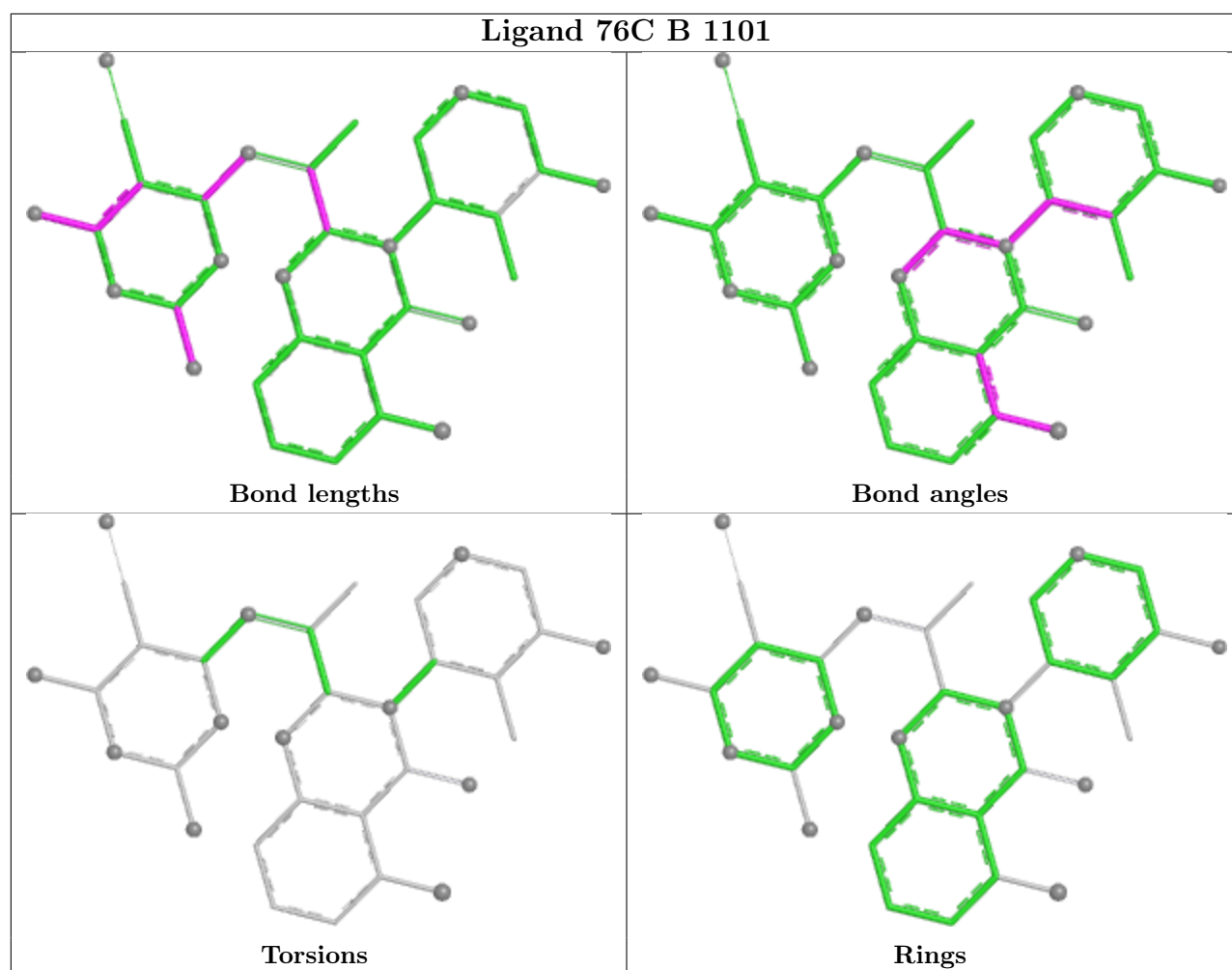
There are no chirality outliers.

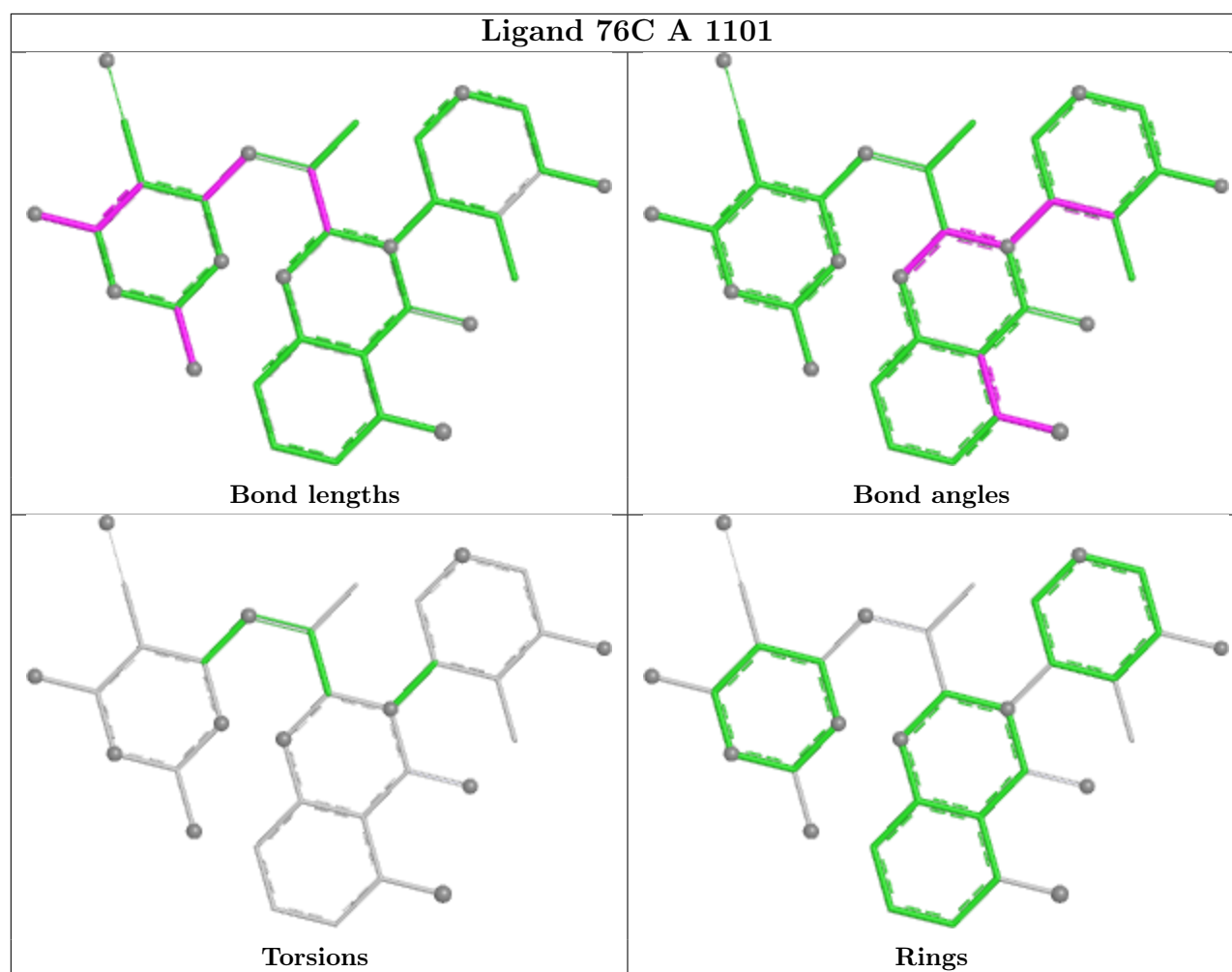
There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





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 [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	819/939 (87%)	-1.09	0 100 100	38, 61, 89, 110	0
1	B	816/939 (86%)	-1.06	0 100 100	37, 61, 92, 118	0
All	All	1635/1878 (87%)	-1.07	0 100 100	37, 61, 90, 118	0

There are no RSRZ outliers to report.

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](#)

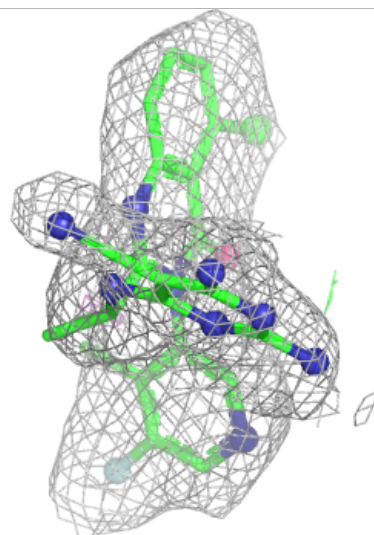
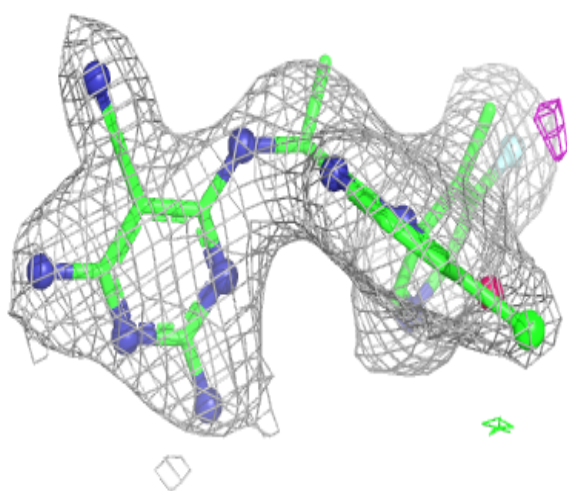
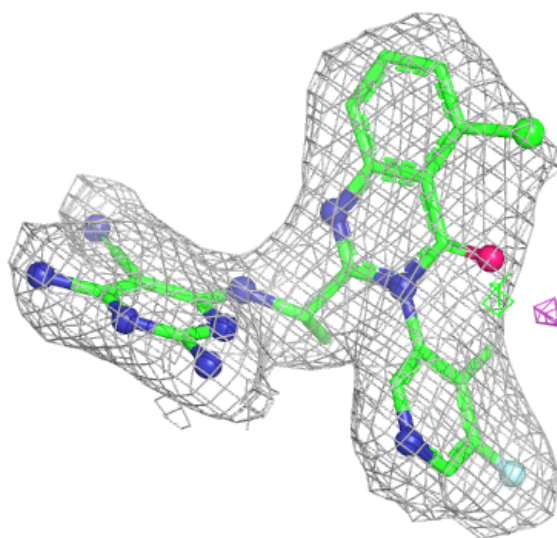
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	76C	A	1101	33/33	0.99	0.04	36,45,56,70	0
2	76C	B	1101	33/33	0.99	0.04	36,46,56,73	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

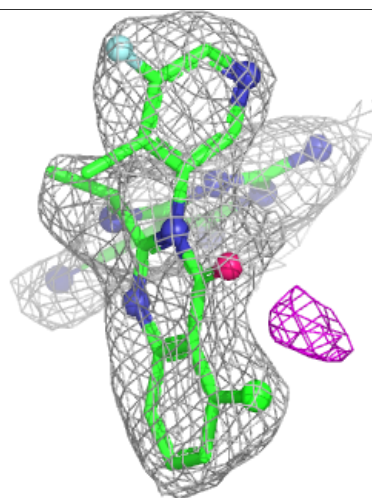
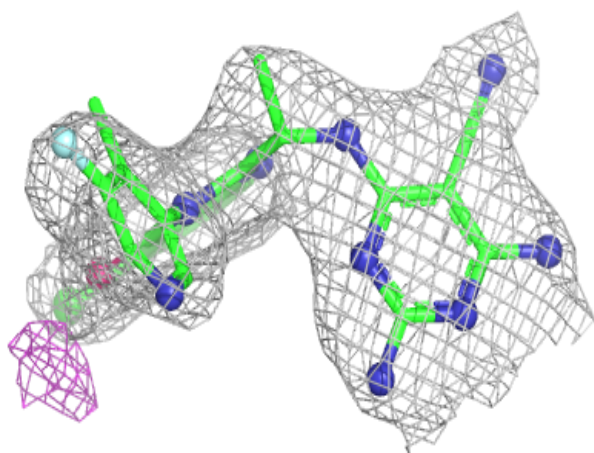
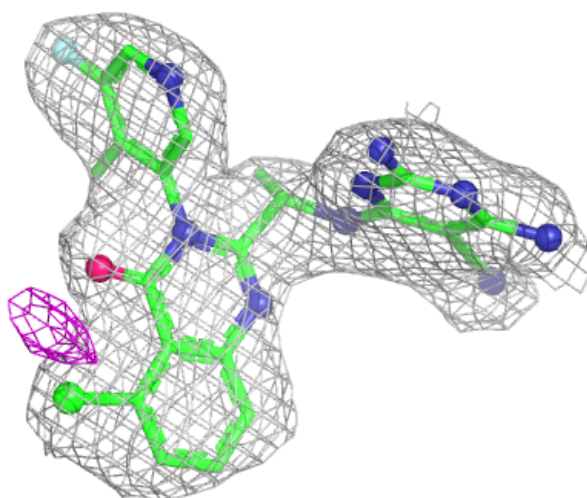
Electron density around 76C A 1101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 76C B 1101:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.