



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 8, 2026 – 08:57 PM JST

PDB ID : 9WR8 / pdb_00009wr8
Title : EGFR 20ins complexed with Furmonertinib
Authors : Liu, Q.F.; Jia, Q.Q.
Deposited on : 2025-09-11
Resolution : 2.33 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 : 1.8.5 (274361), CSD as541be (2020)
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 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

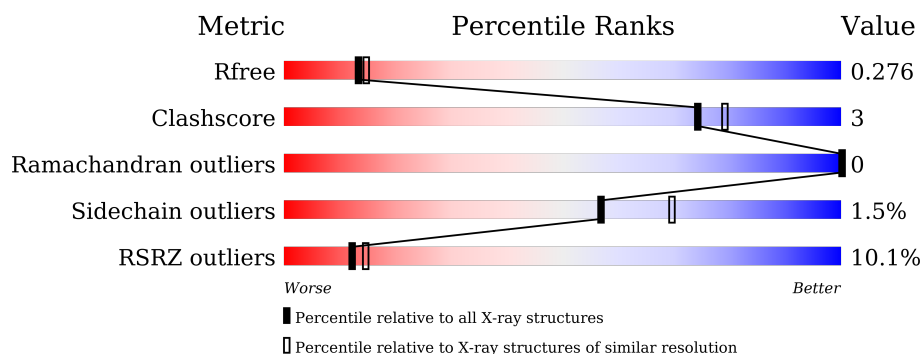
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	330	
1	B	330	
1	C	330	
1	D	330	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9242 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.

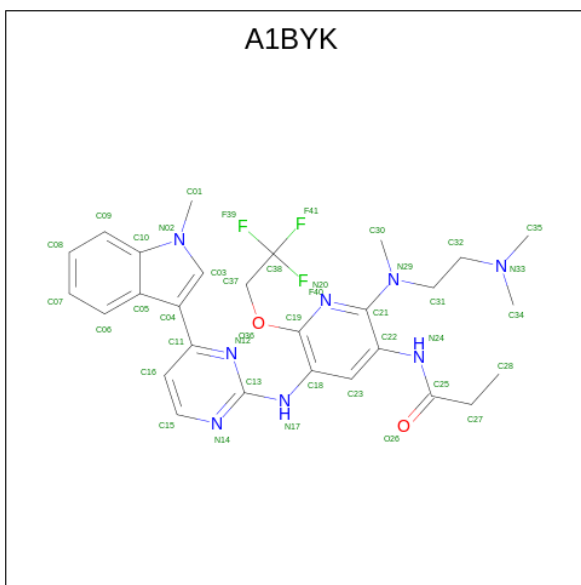
- Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	277	Total	C	N	O	S	0	0	0
			2221	1433	379	394	15			
1	B	278	Total	C	N	O	S	0	0	0
			2217	1430	379	393	15			
1	C	287	Total	C	N	O	S	0	0	0
			2296	1478	393	410	15			
1	D	280	Total	C	N	O	S	0	0	0
			2248	1448	384	401	15			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	773	GLY	-	insertion	UNP P00533
A	774	ASN	-	insertion	UNP P00533
A	775	PRO	-	insertion	UNP P00533
A	951	ARG	VAL	conflict	UNP P00533
B	773	GLY	-	insertion	UNP P00533
B	774	ASN	-	insertion	UNP P00533
B	775	PRO	-	insertion	UNP P00533
B	951	ARG	VAL	conflict	UNP P00533
C	773	GLY	-	insertion	UNP P00533
C	774	ASN	-	insertion	UNP P00533
C	775	PRO	-	insertion	UNP P00533
C	951	ARG	VAL	conflict	UNP P00533
D	773	GLY	-	insertion	UNP P00533
D	774	ASN	-	insertion	UNP P00533
D	775	PRO	-	insertion	UNP P00533
D	951	ARG	VAL	conflict	UNP P00533

- Molecule 2 is Alflutinib, bound form (CCD ID: A1BYK) (formula: C₂₈H₃₃F₃N₈O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			41	28	3	8	2		
2	B	1	Total	C	F	N	O	0	0
			41	28	3	8	2		
2	C	1	Total	C	F	N	O	0	0
			41	28	3	8	2		
2	D	1	Total	C	F	N	O	0	0
			41	28	3	8	2		

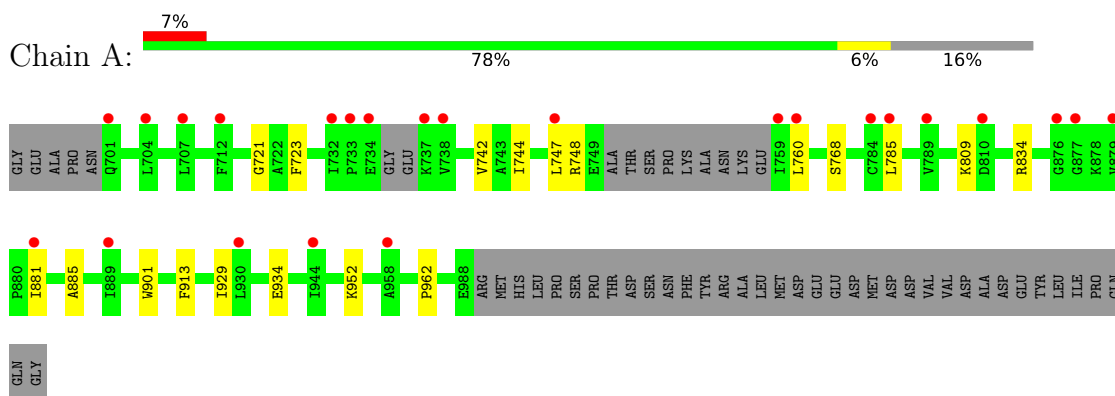
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total	O	0	0
			30	30		
3	B	29	Total	O	0	0
			29	29		
3	C	26	Total	O	0	0
			26	26		
3	D	11	Total	O	0	0
			11	11		

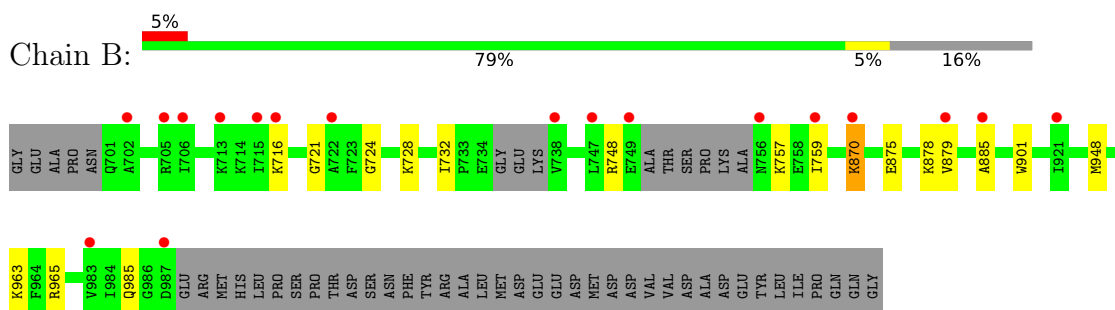
3 Residue-property plots [i](#)

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.

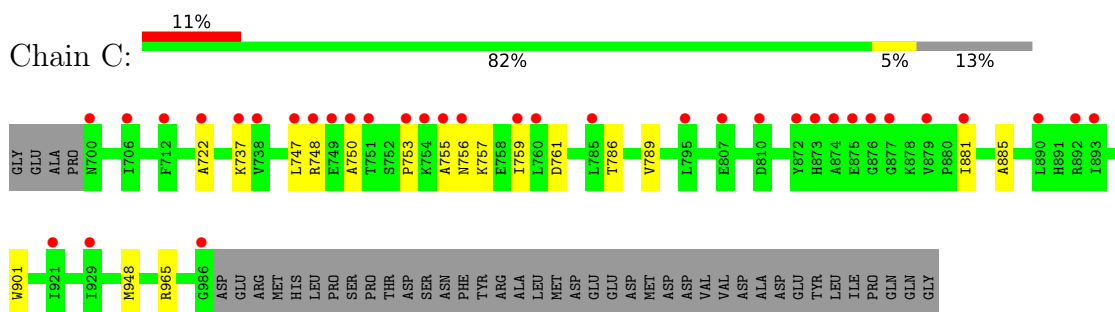
- Molecule 1: Epidermal growth factor receptor



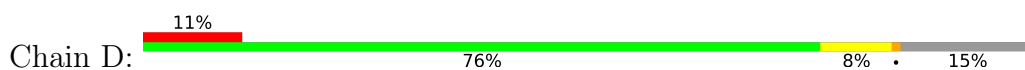
- Molecule 1: Epidermal growth factor receptor

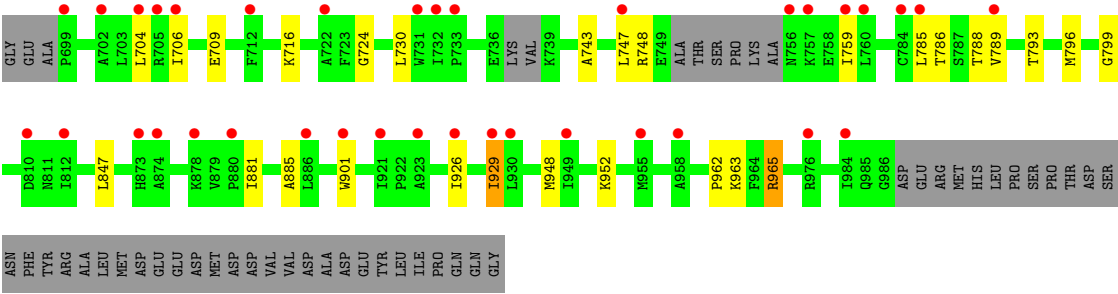


- Molecule 1: Epidermal growth factor receptor



- Molecule 1: Epidermal growth factor receptor





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.30Å 70.66Å 73.47Å 73.40° 85.04° 72.45°	Depositor
Resolution (Å)	70.41 – 2.33 70.41 – 2.33	Depositor EDS
% Data completeness (in resolution range)	98.5 (70.41-2.33) 98.5 (70.41-2.33)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.41 (at 2.34Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.241 , 0.280 0.242 , 0.276	Depositor DCC
R_{free} test set	2461 reflections (4.66%)	wwPDB-VP
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	9242	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.70% 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: A1BYK

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	0.98	0/2269	1.39	0/3066
1	B	1.00	0/2265	1.39	0/3063
1	C	0.99	0/2347	1.40	0/3174
1	D	1.00	0/2297	1.41	0/3103
All	All	0.99	0/9178	1.40	0/12406

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2221	0	2270	8	0
1	B	2217	0	2255	11	0
1	C	2296	0	2355	16	0
1	D	2248	0	2297	22	0
2	A	41	0	0	0	0
2	B	41	0	0	1	0
2	C	41	0	0	0	0
2	D	41	0	0	1	0
3	A	30	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	29	0	0	0	0
3	C	26	0	0	0	0
3	D	11	0	0	1	0
All	All	9242	0	9177	56	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 3.

All (56) 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:D:747:LEU:HD12	1:D:759:ILE:HB	1.42	0.99
1:C:759:ILE:HG21	1:C:789:VAL:HB	1.65	0.79
1:D:747:LEU:HG	1:D:759:ILE:HD12	1.67	0.77
1:A:723:PHE:O	1:A:747:LEU:HD12	1.87	0.74
1:C:747:LEU:HD13	1:C:759:ILE:HG23	1.70	0.73
1:D:747:LEU:HD12	1:D:759:ILE:CB	2.19	0.73
1:B:948:MET:HA	1:B:948:MET:HE2	1.74	0.69
1:C:747:LEU:HD22	1:C:759:ILE:HG12	1.76	0.66
1:B:724:GLY:HA2	1:B:748:ARG:HG2	1.84	0.60
1:A:742:VAL:HG23	1:A:744:ILE:HD11	1.84	0.59
1:B:728:LYS:HD3	2:B:1101:A1BYK:F39	1.93	0.59
1:A:721:GLY:O	1:A:748:ARG:NH2	2.36	0.59
1:C:756:ASN:HA	1:C:759:ILE:HD12	1.85	0.58
1:D:786:THR:OG1	1:D:788:THR:O	2.21	0.58
1:C:948:MET:HA	1:C:948:MET:HE2	1.84	0.58
1:D:724:GLY:HA2	1:D:748:ARG:HG2	1.85	0.57
1:C:750:ALA:HA	1:C:755:ALA:CB	2.35	0.57
1:D:926:ILE:O	1:D:929:ILE:HG22	2.05	0.56
1:C:753:PRO:O	1:C:757:LYS:HB3	2.06	0.55
1:D:709:GLU:OE2	1:D:786:THR:HG21	2.07	0.54
1:C:750:ALA:HA	1:C:755:ALA:HB3	1.90	0.54
1:C:753:PRO:HA	1:C:757:LYS:H	1.75	0.52
1:D:759:ILE:HG21	1:D:789:VAL:HB	1.92	0.51
1:C:756:ASN:OD1	1:C:789:VAL:HG21	2.12	0.49
1:D:709:GLU:HB2	1:D:786:THR:HG22	1.93	0.49
1:B:985:GLN:HG2	1:D:730:LEU:HD11	1.94	0.49
1:D:706:ILE:HG23	1:D:785:LEU:HG	1.95	0.48
1:A:885:ALA:HA	1:A:901:TRP:CD2	2.50	0.47
1:B:878:LYS:HD3	1:B:878:LYS:C	2.40	0.46
1:C:885:ALA:HA	1:C:901:TRP:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:LYS:O	1:A:913:PHE:CG	2.69	0.46
1:C:750:ALA:HB1	1:C:756:ASN:HB2	1.98	0.46
1:C:753:PRO:O	1:C:757:LYS:CB	2.64	0.45
1:A:952:LYS:HB3	1:A:962:PRO:HD3	1.97	0.45
1:B:885:ALA:HA	1:B:901:TRP:CD2	2.51	0.45
1:D:743:ALA:HB3	1:D:793:THR:HG23	1.98	0.44
1:D:963:LYS:HB3	1:D:965:ARG:HD3	2.00	0.44
1:D:952:LYS:HB3	1:D:962:PRO:HD3	2.00	0.44
1:B:870:LYS:HE2	1:B:870:LYS:HA	2.00	0.44
1:D:759:ILE:HD13	1:D:789:VAL:O	2.16	0.44
1:A:929:ILE:HG23	1:A:934:GLU:HB2	1.99	0.44
1:C:786:THR:O	1:C:786:THR:OG1	2.30	0.43
1:C:757:LYS:O	1:C:761:ASP:N	2.48	0.43
1:D:885:ALA:HA	1:D:901:TRP:CD2	2.54	0.43
1:D:706:ILE:CG2	1:D:785:LEU:HG	2.50	0.42
1:B:963:LYS:HG3	1:B:965:ARG:CZ	2.50	0.42
1:C:722:ALA:O	1:C:748:ARG:HD3	2.20	0.41
1:B:721:GLY:O	1:B:748:ARG:NH2	2.54	0.41
1:D:799:GLY:HA3	2:D:1101:A1BYK:C34	2.50	0.41
1:D:796:MET:HG3	1:D:847:LEU:HB3	2.02	0.41
1:A:768:SER:O	1:A:834:ARG:NH2	2.55	0.40
1:D:747:LEU:HD12	1:D:759:ILE:CA	2.51	0.40
1:B:878:LYS:HD3	1:B:879:VAL:N	2.36	0.40
1:D:948:MET:HA	1:D:948:MET:HE2	2.03	0.40
1:B:757:LYS:C	1:B:759:ILE:N	2.79	0.40
1:D:793:THR:HG21	3:D:1205:HOH:O	2.20	0.40

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	271/330 (82%)	263 (97%)	8 (3%)	0	100	100
1	B	272/330 (82%)	266 (98%)	6 (2%)	0	100	100
1	C	285/330 (86%)	275 (96%)	10 (4%)	0	100	100
1	D	274/330 (83%)	271 (99%)	3 (1%)	0	100	100
All	All	1102/1320 (84%)	1075 (98%)	27 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	242/289 (84%)	239 (99%)	3 (1%)	63	75
1	B	240/289 (83%)	236 (98%)	4 (2%)	53	66
1	C	251/289 (87%)	248 (99%)	3 (1%)	63	75
1	D	246/289 (85%)	241 (98%)	5 (2%)	48	61
All	All	979/1156 (85%)	964 (98%)	15 (2%)	57	69

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	760	LEU
1	A	785	LEU
1	A	881	ILE
1	B	716	LYS
1	B	732	ILE
1	B	870	LYS
1	B	875	GLU
1	C	737	LYS
1	C	881	ILE
1	C	965	ARG
1	D	704	LEU
1	D	716	LYS
1	D	881	ILE

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Mol	Chain	Res	Type
1	D	929	ILE
1	D	965	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	790	GLN
1	A	829	ASN
1	B	790	GLN
1	B	811	ASN
1	B	815	GLN
1	B	819	ASN
1	B	979	GLN
1	C	701	GLN
1	C	790	GLN
1	C	819	ASN
1	C	829	ASN
1	D	790	GLN
1	D	811	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](#)

4 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	A1BYK	D	1101	1	41,44,44	0.44	0	54,63,63	0.89	2 (3%)
2	A1BYK	B	1101	1	41,44,44	0.48	0	54,63,63	0.85	3 (5%)
2	A1BYK	A	1101	1	41,44,44	0.42	0	54,63,63	0.88	4 (7%)
2	A1BYK	C	1101	1	41,44,44	0.44	0	54,63,63	0.87	1 (1%)

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	A1BYK	D	1101	1	-	6/29/29/29	0/4/4/4
2	A1BYK	B	1101	1	-	10/29/29/29	0/4/4/4
2	A1BYK	A	1101	1	-	12/29/29/29	0/4/4/4
2	A1BYK	C	1101	1	-	11/29/29/29	0/4/4/4

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1101	A1BYK	N14-C13-N12	-2.37	124.30	126.55
2	A	1101	A1BYK	C23-C18-C19	2.31	119.24	117.01
2	B	1101	A1BYK	C04-C03-N02	-2.17	110.38	111.05
2	A	1101	A1BYK	N14-C13-N12	-2.14	124.52	126.55
2	B	1101	A1BYK	C16-C11-N12	-2.13	120.43	122.92
2	C	1101	A1BYK	N14-C13-N12	-2.12	124.54	126.55
2	D	1101	A1BYK	C16-C11-N12	-2.11	120.45	122.92
2	B	1101	A1BYK	C23-C18-C19	2.09	119.02	117.01
2	A	1101	A1BYK	C16-C11-N12	-2.06	120.50	122.92
2	A	1101	A1BYK	C04-C03-N02	-2.03	110.42	111.05

There are no chirality outliers.

All (39) torsion outliers are listed below:

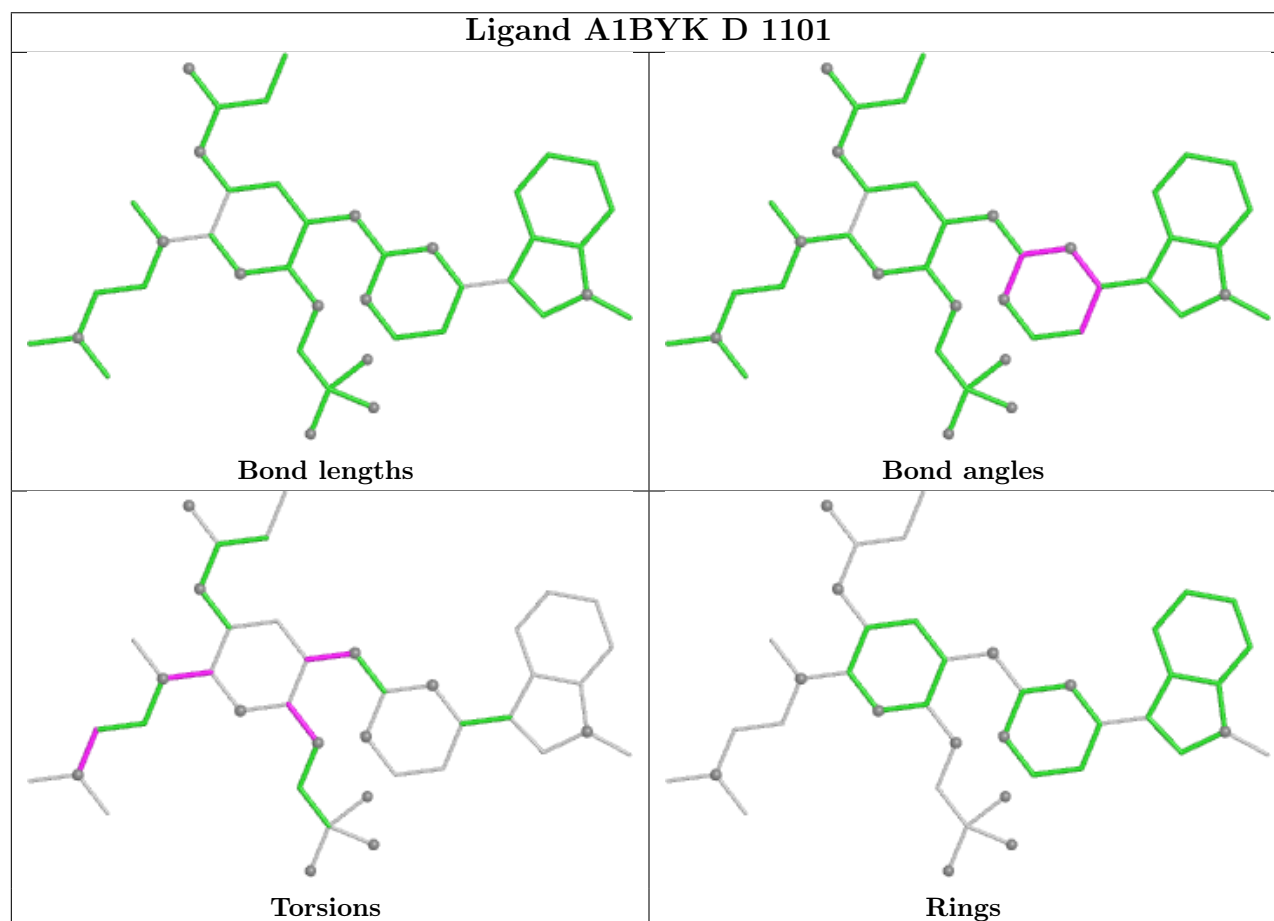
Mol	Chain	Res	Type	Atoms
2	A	1101	A1BYK	C22-C21-N29-C30
2	A	1101	A1BYK	C22-C21-N29-C31
2	A	1101	A1BYK	N20-C21-N29-C31
2	B	1101	A1BYK	C18-C19-O36-C37
2	B	1101	A1BYK	C22-C21-N29-C31
2	B	1101	A1BYK	N20-C21-N29-C31
2	C	1101	A1BYK	C22-C21-N29-C30
2	C	1101	A1BYK	C22-C21-N29-C31
2	C	1101	A1BYK	N20-C21-N29-C31
2	D	1101	A1BYK	C22-C21-N29-C31
2	D	1101	A1BYK	N20-C21-N29-C31
2	B	1101	A1BYK	O36-C37-C38-F39
2	B	1101	A1BYK	O36-C37-C38-F41
2	B	1101	A1BYK	O36-C37-C38-F40
2	B	1101	A1BYK	N20-C19-O36-C37
2	C	1101	A1BYK	O36-C37-C38-F41
2	A	1101	A1BYK	N20-C21-N29-C30
2	C	1101	A1BYK	N20-C21-N29-C30
2	C	1101	A1BYK	O36-C37-C38-F40
2	A	1101	A1BYK	N29-C31-C32-N33
2	C	1101	A1BYK	N29-C31-C32-N33
2	D	1101	A1BYK	C31-C32-N33-C35
2	C	1101	A1BYK	N20-C19-O36-C37
2	C	1101	A1BYK	O36-C37-C38-F39
2	C	1101	A1BYK	C18-C19-O36-C37
2	B	1101	A1BYK	C22-C21-N29-C30
2	A	1101	A1BYK	O36-C37-C38-F41
2	C	1101	A1BYK	C31-C32-N33-C34
2	A	1101	A1BYK	N20-C19-O36-C37
2	A	1101	A1BYK	O36-C37-C38-F40
2	A	1101	A1BYK	C19-C18-N17-C13
2	B	1101	A1BYK	C19-C18-N17-C13
2	D	1101	A1BYK	C19-C18-N17-C13
2	A	1101	A1BYK	O36-C37-C38-F39
2	D	1101	A1BYK	C22-C21-N29-C30
2	B	1101	A1BYK	N20-C21-N29-C30
2	A	1101	A1BYK	C31-C32-N33-C34
2	A	1101	A1BYK	C18-C19-O36-C37
2	D	1101	A1BYK	C18-C19-O36-C37

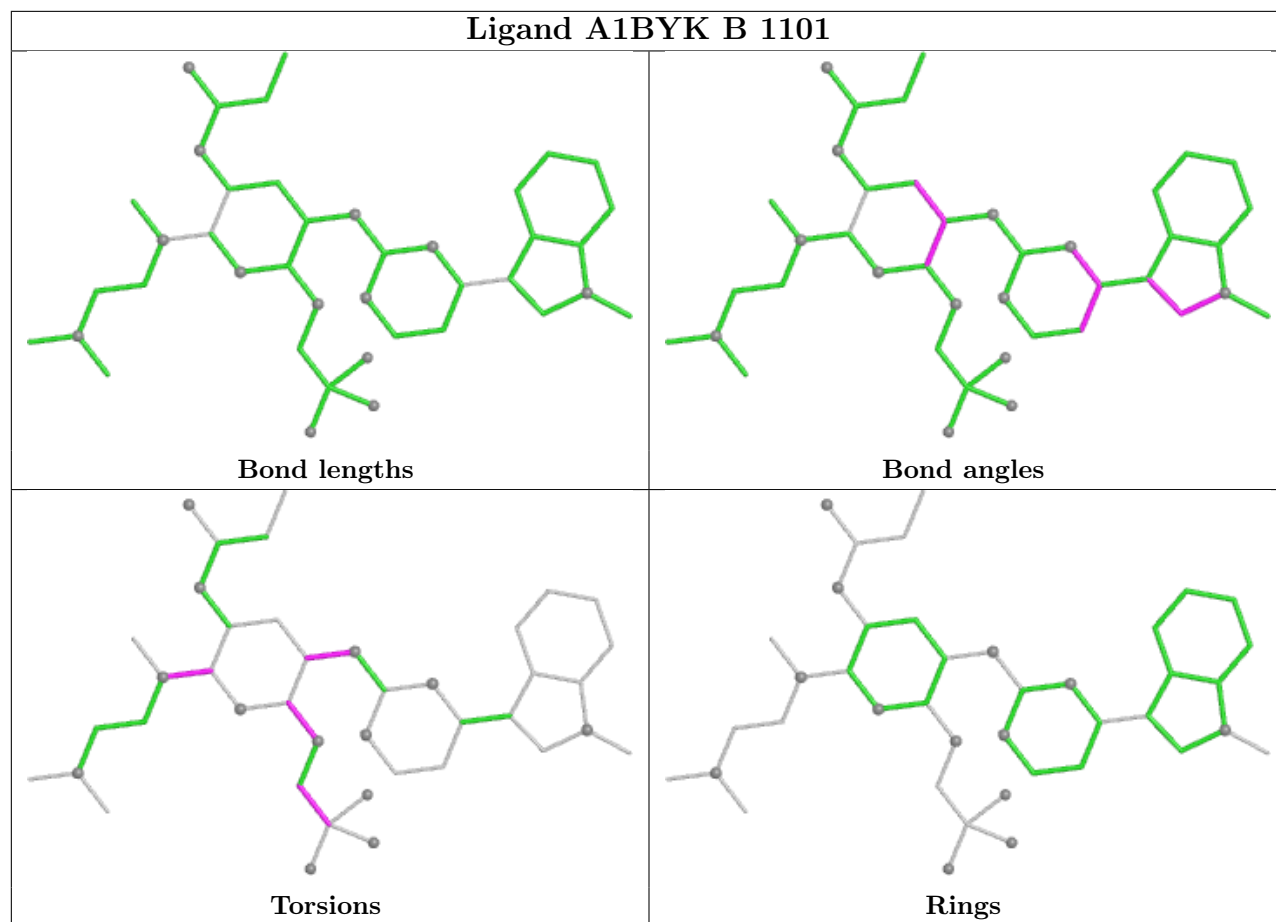
There are no ring outliers.

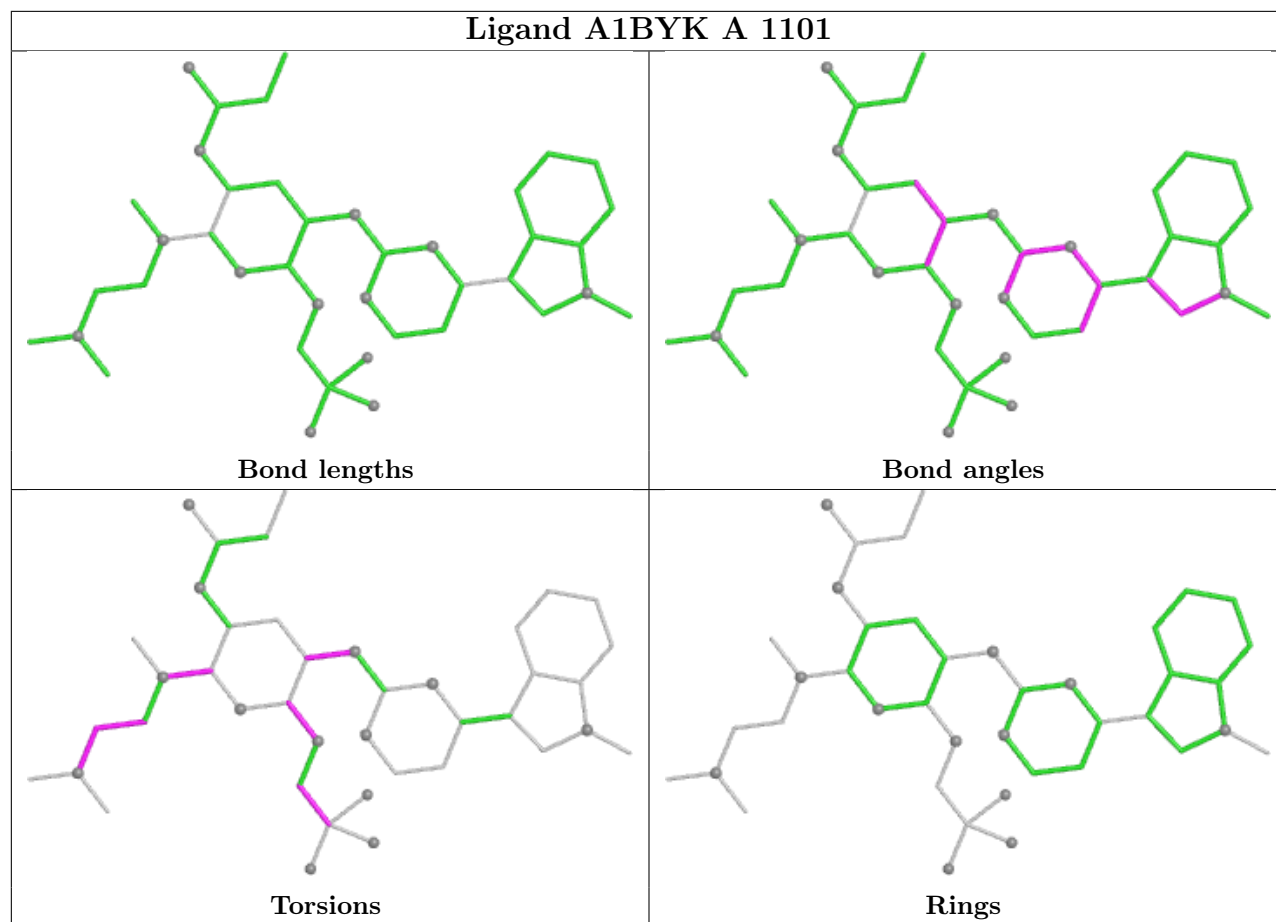
2 monomers are involved in 2 short contacts:

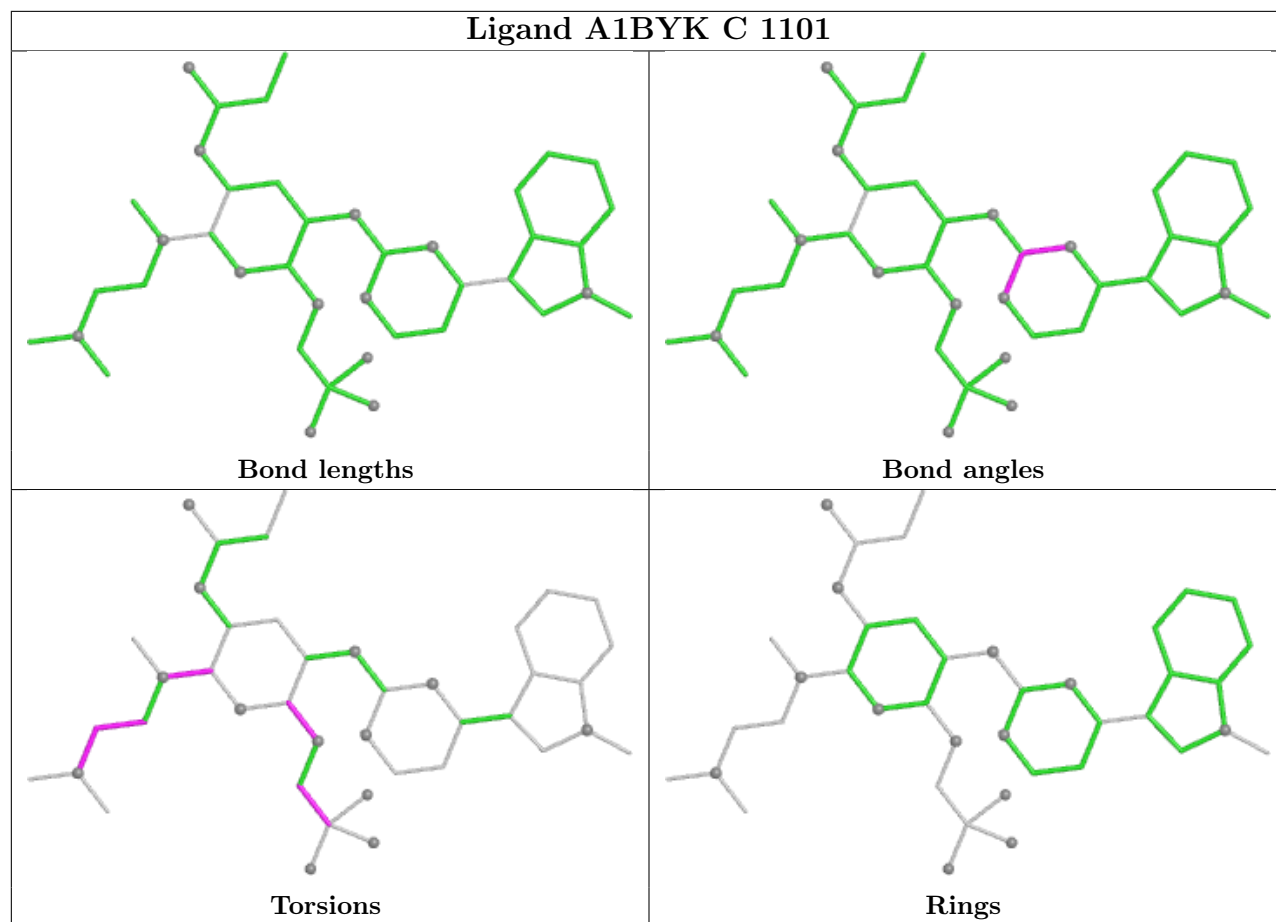
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1101	A1BYK	1	0
2	B	1101	A1BYK	1	0

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](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	277/330 (83%)	0.79	24 (8%)	16 19	29, 51, 94, 108	0
1	B	278/330 (84%)	0.85	18 (6%)	25 29	35, 56, 89, 101	0
1	C	287/330 (86%)	0.94	35 (12%)	8 10	33, 57, 100, 142	0
1	D	280/330 (84%)	1.08	36 (12%)	7 8	39, 65, 101, 131	0
All	All	1122/1320 (85%)	0.92	113 (10%)	12 15	29, 57, 96, 142	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	751	THR	4.4
1	B	756	ASN	4.2
1	B	747	LEU	4.1
1	C	747	LEU	4.1
1	C	873	HIS	4.1
1	D	930	LEU	4.0
1	A	732	ILE	4.0
1	A	738	VAL	4.0
1	D	789	VAL	4.0
1	A	785	LEU	3.9
1	D	923	ALA	3.9
1	A	759	ILE	3.7
1	C	760	LEU	3.7
1	A	747	LEU	3.6
1	D	705	ARG	3.6
1	B	738	VAL	3.5
1	C	890	LEU	3.5
1	A	789	VAL	3.4
1	B	759	ILE	3.4
1	D	955	MET	3.4
1	C	756	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	D	785	LEU	3.3
1	D	759	ILE	3.3
1	D	760	LEU	3.3
1	B	716	LYS	3.2
1	C	738	VAL	3.2
1	C	750	ALA	3.2
1	D	784	CYS	3.2
1	B	722	ALA	3.1
1	B	749	GLU	3.0
1	A	704	LEU	2.9
1	D	732	ILE	2.9
1	A	737	LYS	2.9
1	D	704	LEU	2.8
1	D	699	PRO	2.8
1	C	876	GLY	2.7
1	A	733	PRO	2.7
1	D	926	ILE	2.7
1	D	880	PRO	2.7
1	A	958	ALA	2.7
1	C	700	ASN	2.7
1	C	881	ILE	2.6
1	D	706	ILE	2.6
1	A	930	LEU	2.6
1	C	874	ALA	2.6
1	C	759	ILE	2.6
1	D	747	LEU	2.6
1	D	702	ALA	2.6
1	D	874	ALA	2.6
1	B	870	LYS	2.6
1	D	722	ALA	2.5
1	C	877	GLY	2.5
1	C	748	ARG	2.5
1	C	754	LYS	2.5
1	A	877	GLY	2.5
1	B	715	ILE	2.5
1	D	929	ILE	2.5
1	D	949	ILE	2.5
1	C	753	PRO	2.5
1	A	784	CYS	2.4
1	C	875	GLU	2.4
1	C	785	LEU	2.4
1	C	810	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	873	HIS	2.4
1	B	885	ALA	2.4
1	C	722	ALA	2.4
1	C	892	ARG	2.4
1	D	733	PRO	2.4
1	D	712	PHE	2.4
1	D	878	LYS	2.4
1	B	702	ALA	2.4
1	A	879	VAL	2.4
1	D	757	LYS	2.3
1	C	706	ILE	2.3
1	C	986	GLY	2.3
1	A	712	PHE	2.3
1	C	755	ALA	2.3
1	D	812	ILE	2.3
1	D	886	LEU	2.2
1	A	734	GLU	2.2
1	C	872	TYR	2.2
1	D	921	ILE	2.2
1	A	707	LEU	2.2
1	B	921	ILE	2.2
1	C	921	ILE	2.2
1	A	810	ASP	2.2
1	C	712	PHE	2.2
1	B	713	LYS	2.1
1	C	737	LYS	2.1
1	C	807	GLU	2.1
1	A	876	GLY	2.1
1	A	889	ILE	2.1
1	B	706	ILE	2.1
1	B	987	ASP	2.1
1	D	756	ASN	2.1
1	D	810	ASP	2.1
1	A	701	GLN	2.1
1	A	760	LEU	2.1
1	A	944	ILE	2.1
1	C	893	ILE	2.1
1	C	879	VAL	2.1
1	D	731	TRP	2.1
1	D	901	TRP	2.1
1	C	749	GLU	2.1
1	C	795	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	881	ILE	2.1
1	B	879	VAL	2.1
1	D	976	ARG	2.1
1	D	958	ALA	2.0
1	B	983	VAL	2.0
1	B	705	ARG	2.0
1	C	929	ILE	2.0
1	D	984	ILE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

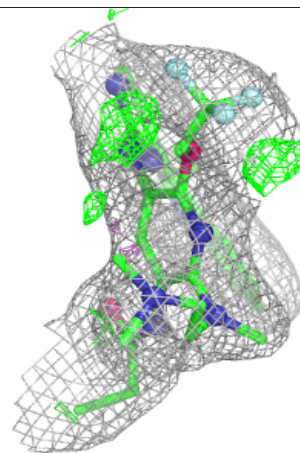
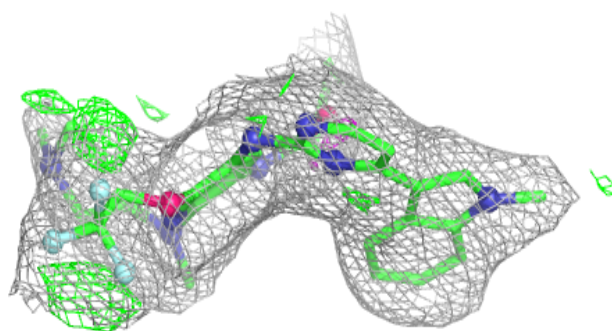
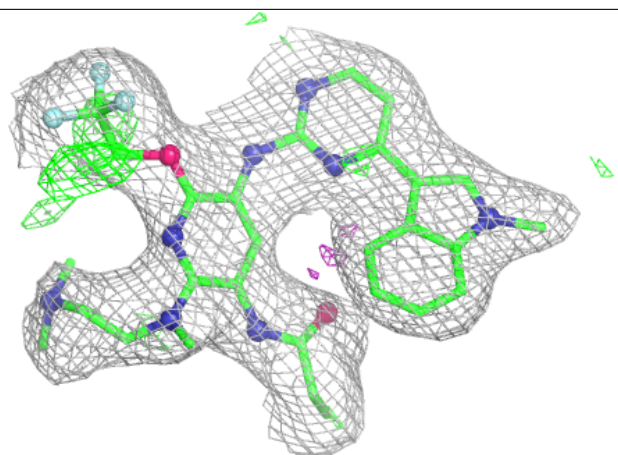
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	A1BYK	C	1101	41/41	0.87	0.13	49,57,77,82	0
2	A1BYK	D	1101	41/41	0.87	0.11	46,49,61,64	0
2	A1BYK	B	1101	41/41	0.89	0.12	50,54,74,81	0
2	A1BYK	A	1101	41/41	0.92	0.09	38,45,61,67	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.

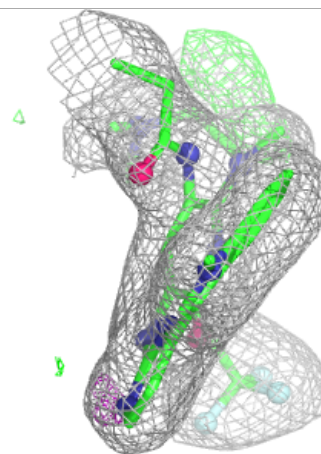
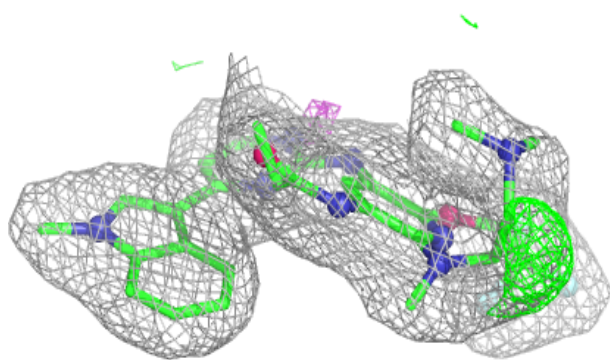
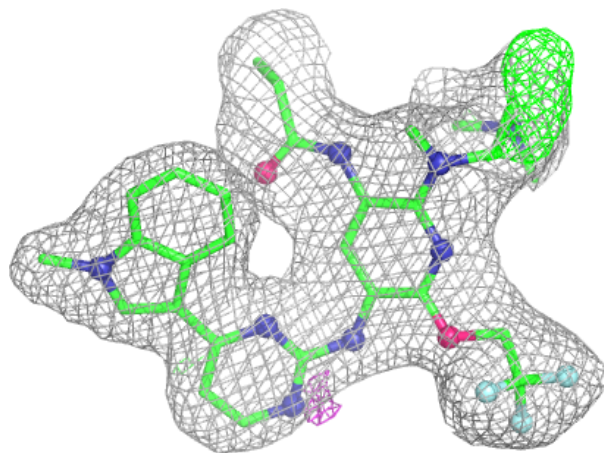
Electron density around A1BYK C 1101:

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



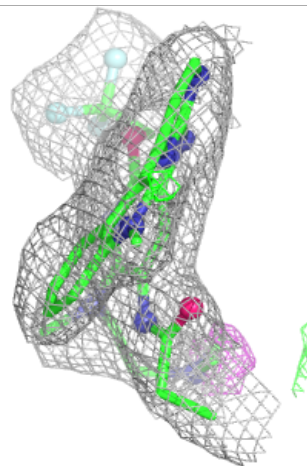
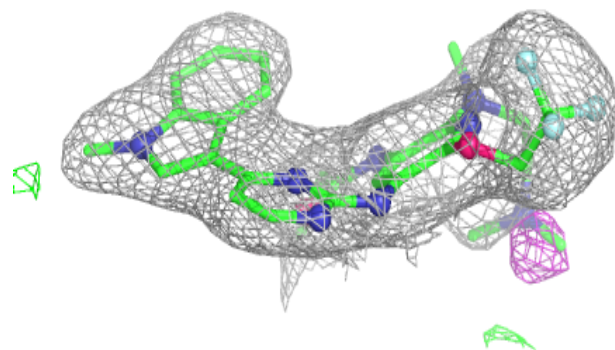
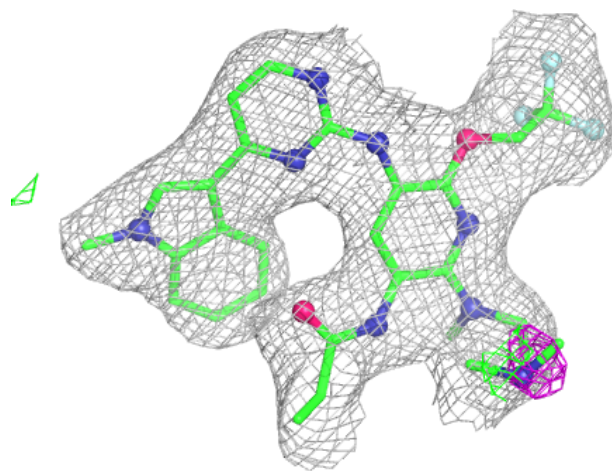
Electron density around A1BYK D 1101:

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



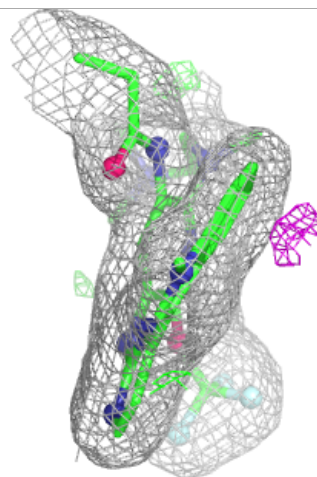
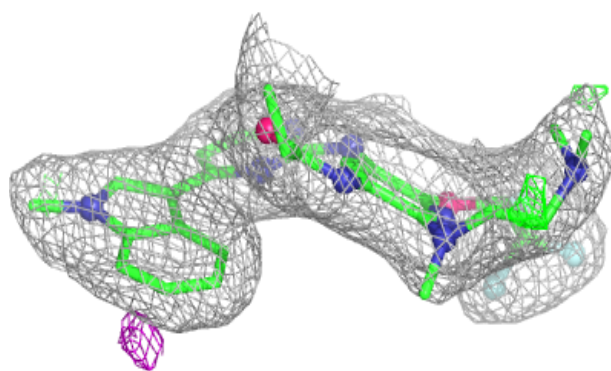
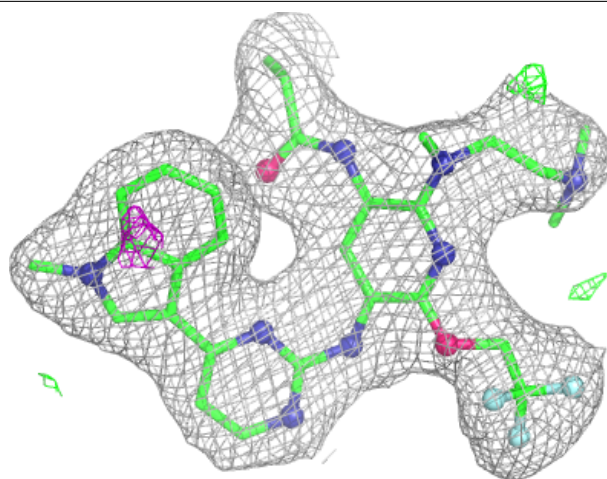
Electron density around A1BYK B 1101:

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



Electron density around A1BYK 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.