



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2021 – 12:33 PM EDT

PDB ID : 7JXI
Title : EGFR kinase (T790M/V948R) in complex with PF-06747775
Authors : Beyett, T.S.; Eck, M.J.
Deposited on : 2020-08-27
Resolution : 3.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

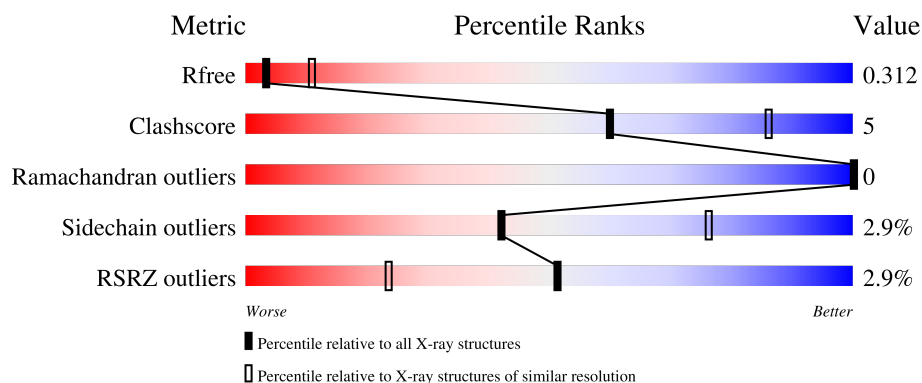
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

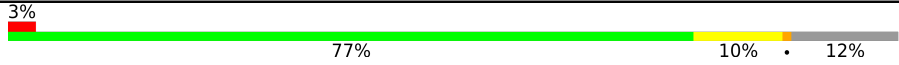



The reported resolution of this entry is 3.00 Å.

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}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	331	 3% 77% 10% • 12%
1	B	331	 3% 72% 10% • 17%
1	C	331	 2% 74% 11% • 15%
1	D	331	 2% 73% 14% • 13%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 9311 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.

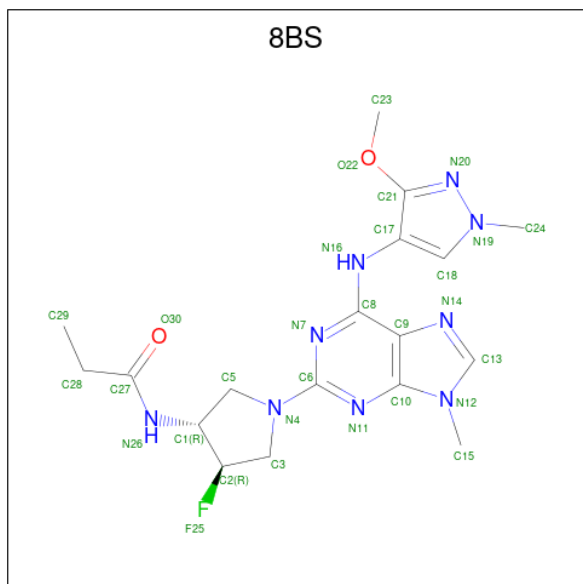
- Molecule 1 is a protein called Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	289	Total	C	N	O	S	0	1	0
			2338	1506	396	417	19			
1	A	290	Total	C	N	O	S	0	1	0
			2347	1508	399	421	19			
1	C	283	Total	C	N	O	S	0	0	0
			2286	1471	387	410	18			
1	B	274	Total	C	N	O	S	0	1	0
			2220	1434	374	394	18			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	692	GLY	-	expression tag	UNP P00533
D	693	SER	-	expression tag	UNP P00533
D	694	THR	-	expression tag	UNP P00533
D	790	MET	THR	engineered mutation	UNP P00533
D	948	ARG	VAL	engineered mutation	UNP P00533
A	692	GLY	-	expression tag	UNP P00533
A	693	SER	-	expression tag	UNP P00533
A	694	THR	-	expression tag	UNP P00533
A	790	MET	THR	engineered mutation	UNP P00533
A	948	ARG	VAL	engineered mutation	UNP P00533
C	692	GLY	-	expression tag	UNP P00533
C	693	SER	-	expression tag	UNP P00533
C	694	THR	-	expression tag	UNP P00533
C	790	MET	THR	engineered mutation	UNP P00533
C	948	ARG	VAL	engineered mutation	UNP P00533
B	692	GLY	-	expression tag	UNP P00533
B	693	SER	-	expression tag	UNP P00533
B	694	THR	-	expression tag	UNP P00533
B	790	MET	THR	engineered mutation	UNP P00533
B	948	ARG	VAL	engineered mutation	UNP P00533

- Molecule 2 is N-[(3R,4R)-4-fluoro-1-{6-[(3-methoxy-1-methyl-1H-pyrazol-4-yl)amino]-9-methyl-9H-purin-2-yl}pyrrolidin-3-yl]propanamide (three-letter code: 8BS) (formula: C₁₈H₂₄FN₉O₂) (labeled as "Ligand of Interest" by depositor).

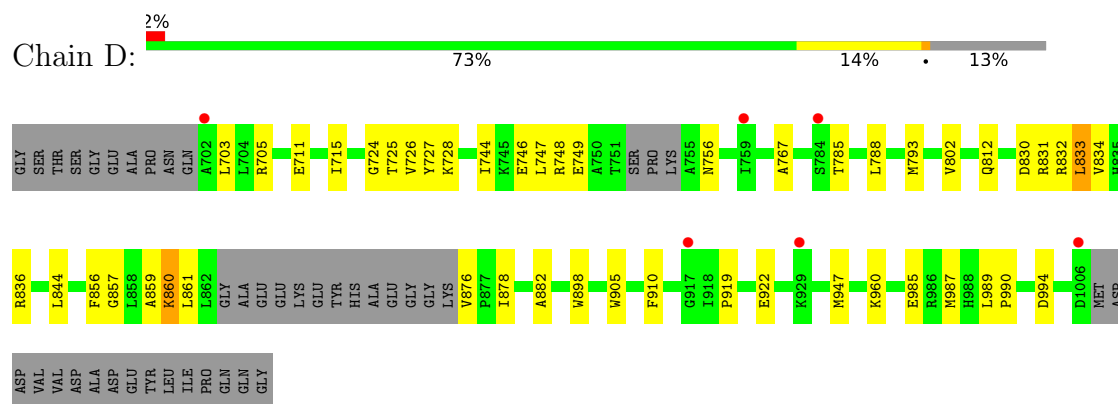


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	D	1	Total	C	F	N	O	0	0
			30	18	1	9	2		
2	A	1	Total	C	F	N	O	0	0
			30	18	1	9	2		
2	C	1	Total	C	F	N	O	0	0
			30	18	1	9	2		
2	B	1	Total	C	F	N	O	0	0
			30	18	1	9	2		

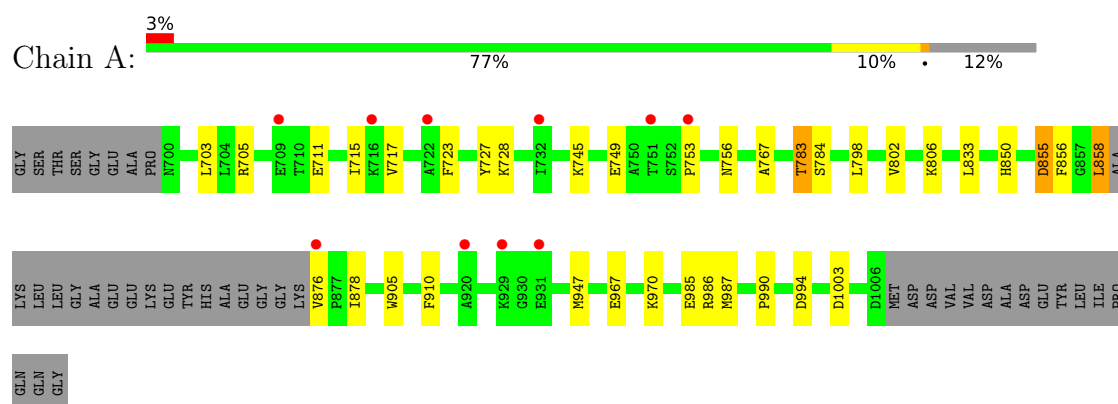
3 Residue-property plots

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.

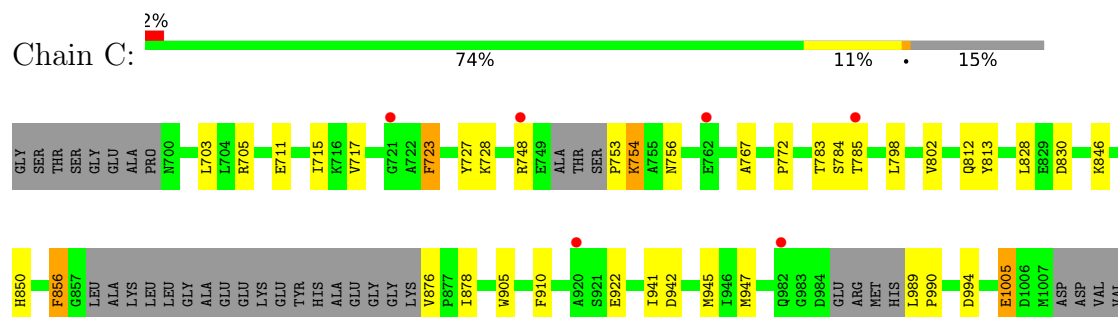
- Molecule 1: Epidermal growth factor receptor



- Molecule 1: Epidermal growth factor receptor

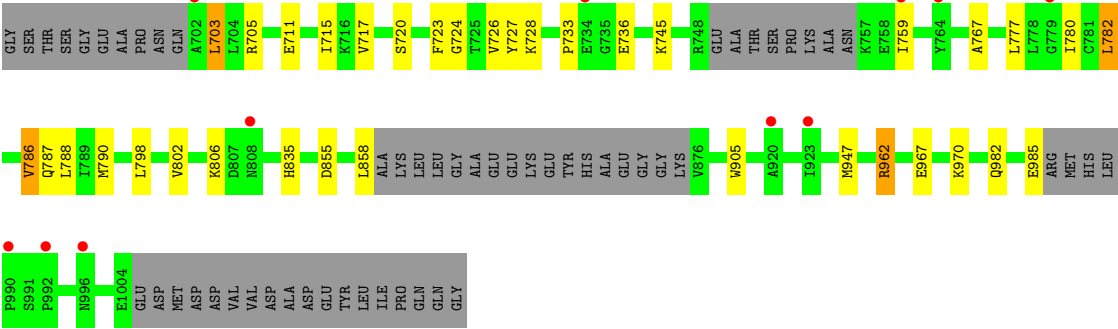


- Molecule 1: Epidermal growth factor receptor



ASP
ALA
ASP
GLU
TYR
LEU
ILE
PRO
GLN
GLY

● Molecule 1: Epidermal growth factor receptor



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	70.63Å 100.78Å 87.16Å 90.00° 101.17° 90.00°	Depositor
Resolution (Å)	85.50 – 3.00 85.50 – 3.00	Depositor EDS
% Data completeness (in resolution range)	98.0 (85.50-3.00) 98.0 (85.50-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 3.01Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.276 , 0.312 0.277 , 0.312	Depositor DCC
R_{free} test set	1175 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	59.7	Xtriage
Anisotropy	0.642	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	9311	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 17.47% 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: 8BS

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	0.27	0/2402	0.49	0/3248
1	B	0.27	0/2271	0.51	0/3067
1	C	0.26	0/2335	0.46	0/3154
1	D	0.29	0/2391	0.51	0/3231
All	All	0.27	0/9399	0.49	0/12700

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	2347	0	2391	20	0
1	B	2220	0	2272	19	0
1	C	2286	0	2327	24	0
1	D	2338	0	2391	26	0
2	A	30	0	0	0	0
2	B	30	0	0	0	0
2	C	30	0	0	0	0
2	D	30	0	0	0	0
All	All	9311	0	9381	85	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 5.

All (85) 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:B:726:VAL:HG22	1:B:745:LYS:HG2	1.59	0.83
1:A:703:LEU:O	1:A:767:ALA:HB1	2.00	0.60
1:D:703:LEU:O	1:D:767:ALA:HB1	2.03	0.58
1:D:833:LEU:HG	1:D:856:PHE:CZ	2.38	0.58
1:D:747:LEU:HD11	1:D:788:LEU:HD11	1.87	0.57
1:A:990:PRO:HB2	1:A:994:ASP:HB2	1.87	0.56
1:A:745:LYS:NZ	1:A:855:ASP:OD1	2.38	0.56
1:A:798:LEU:O	1:A:802:VAL:HG23	2.07	0.55
1:B:703:LEU:O	1:B:767:ALA:HB1	2.07	0.54
1:C:703:LEU:O	1:C:767:ALA:HB1	2.08	0.54
1:A:705:ARG:NH2	1:A:711:GLU:OE2	2.41	0.53
1:D:749:GLU:HB3	1:D:861:LEU:HD22	1.90	0.53
1:D:830:ASP:HA	1:B:720:SER:HB3	1.90	0.53
1:A:783:THR:OG1	1:A:784:SER:N	2.38	0.53
1:A:905:TRP:HD1	1:A:947:MET:HE1	1.75	0.52
1:C:905:TRP:HD1	1:C:947:MET:HE1	1.75	0.51
1:B:835:HIS:CE1	1:B:855:ASP:O	2.64	0.51
1:A:715:ILE:HG12	1:A:728:LYS:O	2.11	0.51
1:C:723:PHE:O	1:C:748:ARG:HG2	2.11	0.50
1:D:919:PRO:HD2	1:D:922:GLU:OE1	2.11	0.50
1:B:759:ILE:HG21	1:B:786:VAL:HG11	1.94	0.50
1:D:832:ARG:HH22	1:B:724:GLY:HA2	1.77	0.50
1:D:812:GLN:HG2	1:D:989:LEU:HG	1.93	0.50
1:B:780:ILE:HA	1:B:787:GLN:O	2.12	0.50
1:D:746:GLU:OE2	1:D:785:THR:OG1	2.23	0.49
1:A:717:VAL:HG22	1:A:727:TYR:CE2	2.47	0.49
1:D:705:ARG:NH2	1:D:711:GLU:OE2	2.45	0.49
1:D:724:GLY:HA2	1:D:748:ARG:CZ	2.42	0.49
1:B:985:GLU:H	1:B:985:GLU:CD	2.15	0.49
1:D:831:ARG:O	1:D:833:LEU:HD13	2.13	0.48
1:D:793:MET:HG3	1:D:844:LEU:HD13	1.95	0.48
1:C:783:THR:HG22	1:C:784:SER:H	1.78	0.48
1:B:715:ILE:HG12	1:B:728:LYS:O	2.14	0.48
1:B:777:LEU:HD11	1:B:788:LEU:HB3	1.96	0.48
1:B:733:PRO:HG2	1:B:736:GLU:HB2	1.96	0.48
1:D:727:TYR:HE1	1:D:746:GLU:HG3	1.79	0.47
1:C:941:ILE:O	1:C:945:MET:HG3	2.13	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:942:ASP:HA	1:C:945:MET:HE2	1.96	0.47
1:D:715:ILE:HG12	1:D:728:LYS:O	2.15	0.47
1:C:812:GLN:HG2	1:C:989:LEU:HG	1.97	0.47
1:B:723:PHE:CD1	1:B:723:PHE:N	2.83	0.47
1:C:784:SER:OG	1:C:785:THR:N	2.48	0.47
1:D:905:TRP:HD1	1:D:947:MET:HE1	1.80	0.46
1:A:833:LEU:HB3	1:A:856:PHE:CZ	2.51	0.46
1:D:990:PRO:HB2	1:D:994:ASP:HB2	1.98	0.46
1:C:717:VAL:HG22	1:C:727:TYR:CE2	2.51	0.46
1:B:717:VAL:HG22	1:B:727:TYR:CE2	2.51	0.46
1:C:715:ILE:HG12	1:C:728:LYS:O	2.16	0.46
1:C:813:TYR:OH	1:C:990:PRO:HD3	2.16	0.45
1:A:802:VAL:CG1	1:A:910:PHE:HA	2.47	0.45
1:A:850:HIS:ND1	1:A:1003:ASP:OD2	2.49	0.45
1:A:802:VAL:HG12	1:A:910:PHE:HA	1.98	0.44
1:B:782:LEU:HD23	1:B:786:VAL:HG22	1.99	0.44
1:A:753:PRO:HA	1:A:756:ASN:HB2	1.99	0.44
1:C:990:PRO:HB2	1:C:994:ASP:HB2	1.98	0.44
1:C:753:PRO:O	1:C:756:ASN:HB2	2.18	0.44
1:A:967:GLU:O	1:A:970:LYS:HB3	2.18	0.44
1:B:745:LYS:NZ	1:B:855:ASP:OD1	2.51	0.44
1:C:705:ARG:NH2	1:C:711:GLU:OE2	2.46	0.44
1:D:834:VAL:HG12	1:D:836:ARG:HG3	1.99	0.44
1:D:876:VAL:HG23	1:D:878:ILE:HG12	1.98	0.44
1:B:705:ARG:NH2	1:B:711:GLU:OE2	2.46	0.44
1:C:772:PRO:O	1:C:850:HIS:NE2	2.51	0.43
1:C:783:THR:HG22	1:C:784:SER:N	2.33	0.43
1:D:724:GLY:HA2	1:D:748:ARG:NH2	2.33	0.43
1:B:962:ARG:H	1:B:962:ARG:HG2	1.45	0.43
1:D:726:VAL:HA	1:D:744:ILE:O	2.19	0.43
1:C:798:LEU:O	1:C:802:VAL:HG23	2.19	0.43
1:A:876:VAL:HG23	1:A:878:ILE:HG12	2.01	0.43
1:C:876:VAL:HG23	1:C:878:ILE:HG12	2.00	0.43
1:D:724:GLY:HA3	1:D:746:GLU:O	2.19	0.42
1:A:717:VAL:HG11	1:C:830:ASP:HB3	2.01	0.42
1:A:858:LEU:HD13	1:A:858:LEU:HA	1.87	0.42
1:C:846:LYS:NZ	1:C:1005:GLU:OE2	2.42	0.42
1:B:798:LEU:O	1:B:802:VAL:HG23	2.20	0.42
1:A:802:VAL:O	1:A:806:LYS:HB3	2.19	0.42
1:D:882:ALA:HA	1:D:898:TRP:CD2	2.55	0.42
1:D:802:VAL:HG12	1:D:910:PHE:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:857:GLY:C	1:D:859:ALA:H	2.23	0.41
1:B:905:TRP:HD1	1:B:947:MET:HE1	1.85	0.41
1:C:802:VAL:HG12	1:C:910:PHE:HA	2.03	0.41
1:D:860:LYS:HD3	1:D:860:LYS:HA	1.42	0.41
1:C:754:LYS:O	1:C:754:LYS:HG2	2.19	0.41
1:C:828:LEU:HD11	1:C:856:PHE:CE2	2.55	0.40
1:A:717:VAL:CG1	1:C:830:ASP:HB3	2.52	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	287/331 (87%)	278 (97%)	9 (3%)	0	100	100
1	B	267/331 (81%)	261 (98%)	6 (2%)	0	100	100
1	C	275/331 (83%)	266 (97%)	9 (3%)	0	100	100
1	D	284/331 (86%)	272 (96%)	12 (4%)	0	100	100
All	All	1113/1324 (84%)	1077 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	261/290 (90%)	253 (97%)	8 (3%)	40	75
1	B	247/290 (85%)	237 (96%)	10 (4%)	31	68
1	C	254/290 (88%)	249 (98%)	5 (2%)	55	83
1	D	259/290 (89%)	252 (97%)	7 (3%)	44	77
All	All	1021/1160 (88%)	991 (97%)	30 (3%)	42	76

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	725	THR
1	D	756	ASN
1	D	833	LEU
1	D	860	LYS
1	D	960	LYS
1	D	985	GLU
1	D	987	MET
1	A	723	PHE
1	A	749	GLU
1	A	783	THR
1	A	855	ASP
1	A	858	LEU
1	A	985	GLU
1	A	986	ARG
1	A	987	MET
1	C	723	PHE
1	C	754	LYS
1	C	856	PHE
1	C	922	GLU
1	C	1005	GLU
1	B	703	LEU
1	B	782	LEU
1	B	786	VAL
1	B	790	MET
1	B	806	LYS
1	B	858	LEU
1	B	962	ARG
1	B	967	GLU
1	B	970	LYS
1	B	982	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	8BS	D	1101	1	26,33,33	2.90	12 (46%)	21,48,48	3.38	11 (52%)
2	8BS	B	1101	1	26,33,33	2.38	9 (34%)	21,48,48	2.48	8 (38%)
2	8BS	A	1101	1	26,33,33	2.41	9 (34%)	21,48,48	2.69	10 (47%)
2	8BS	C	1101	1	26,33,33	2.68	12 (46%)	21,48,48	2.94	9 (42%)

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	8BS	D	1101	1	-	7/12/28/28	0/4/4/4
2	8BS	B	1101	1	-	7/12/28/28	0/4/4/4
2	8BS	A	1101	1	-	2/12/28/28	0/4/4/4
2	8BS	C	1101	1	-	4/12/28/28	0/4/4/4

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1101	8BS	C6-N4	7.62	1.49	1.35
2	C	1101	8BS	C6-N4	6.57	1.47	1.35
2	D	1101	8BS	C8-N7	5.93	1.40	1.32
2	B	1101	8BS	C6-N4	5.57	1.46	1.35
2	A	1101	8BS	C6-N4	5.36	1.45	1.35
2	C	1101	8BS	C18-C17	5.24	1.43	1.38
2	C	1101	8BS	C18-N19	5.19	1.40	1.35
2	B	1101	8BS	C18-C17	4.82	1.43	1.38
2	D	1101	8BS	C6-N7	4.82	1.43	1.34
2	A	1101	8BS	C18-C17	4.36	1.43	1.38
2	C	1101	8BS	C8-N7	4.25	1.38	1.32
2	B	1101	8BS	C18-N19	4.24	1.40	1.35
2	C	1101	8BS	C8-N16	4.10	1.42	1.36
2	A	1101	8BS	C18-N19	3.96	1.39	1.35
2	D	1101	8BS	C18-N19	3.91	1.39	1.35
2	A	1101	8BS	C8-N7	3.87	1.38	1.32
2	B	1101	8BS	C5-N4	3.77	1.51	1.46
2	D	1101	8BS	C18-C17	3.57	1.42	1.38
2	D	1101	8BS	C1-N26	3.54	1.52	1.46
2	D	1101	8BS	C3-C2	3.51	1.59	1.51
2	B	1101	8BS	C21-N20	3.47	1.39	1.34
2	A	1101	8BS	C21-N20	3.45	1.39	1.34
2	B	1101	8BS	C27-N26	3.37	1.41	1.34
2	D	1101	8BS	C27-N26	3.35	1.41	1.34
2	A	1101	8BS	C5-N4	3.24	1.50	1.46
2	A	1101	8BS	C8-N16	3.23	1.41	1.36
2	D	1101	8BS	C21-N20	3.09	1.38	1.34
2	A	1101	8BS	C27-N26	2.78	1.39	1.34
2	C	1101	8BS	C3-C2	2.68	1.57	1.51
2	D	1101	8BS	C8-N16	2.67	1.40	1.36
2	C	1101	8BS	C17-N16	2.66	1.47	1.39
2	C	1101	8BS	C21-N20	2.53	1.37	1.34
2	A	1101	8BS	C6-N7	2.50	1.38	1.34
2	B	1101	8BS	C8-N7	2.44	1.36	1.32
2	B	1101	8BS	C8-N16	2.42	1.39	1.36
2	C	1101	8BS	C5-N4	2.35	1.49	1.46
2	C	1101	8BS	O22-C21	2.15	1.38	1.35
2	D	1101	8BS	C5-C1	2.12	1.56	1.52
2	C	1101	8BS	O22-C23	2.11	1.49	1.42
2	C	1101	8BS	C27-N26	2.08	1.38	1.34
2	D	1101	8BS	C3-N4	2.07	1.49	1.46
2	B	1101	8BS	C3-C2	2.00	1.55	1.51

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1101	8BS	C28-C27-N26	8.41	126.59	115.77
2	D	1101	8BS	N7-C6-N4	8.16	127.17	117.11
2	C	1101	8BS	C3-N4-C5	-6.33	103.33	111.67
2	D	1101	8BS	C3-N4-C5	-6.16	103.55	111.67
2	D	1101	8BS	C28-C27-N26	6.09	123.61	115.77
2	B	1101	8BS	C3-N4-C5	-5.98	103.79	111.67
2	A	1101	8BS	N7-C6-N4	5.71	124.16	117.11
2	B	1101	8BS	C28-C27-N26	5.58	122.95	115.77
2	A	1101	8BS	C28-C27-N26	5.17	122.42	115.77
2	D	1101	8BS	C1-N26-C27	4.64	131.31	123.48
2	A	1101	8BS	C3-N4-C5	-4.44	105.81	111.67
2	D	1101	8BS	N16-C8-N7	4.33	122.72	118.66
2	C	1101	8BS	N7-C6-N4	3.77	121.77	117.11
2	A	1101	8BS	C1-N26-C27	3.60	129.55	123.48
2	D	1101	8BS	C5-N4-C6	3.41	129.08	123.40
2	A	1101	8BS	C5-N4-C6	3.31	128.92	123.40
2	A	1101	8BS	C9-C8-N7	-3.25	118.11	120.81
2	D	1101	8BS	C23-O22-C21	3.18	120.37	117.21
2	B	1101	8BS	C15-N12-C10	3.15	130.99	124.18
2	C	1101	8BS	C9-C8-N7	-3.14	118.20	120.81
2	B	1101	8BS	C9-C8-N7	-3.11	118.23	120.81
2	A	1101	8BS	C15-N12-C10	2.99	130.63	124.18
2	B	1101	8BS	C17-N16-C8	-2.95	121.14	129.29
2	B	1101	8BS	N7-C6-N4	2.85	120.62	117.11
2	C	1101	8BS	O30-C27-N26	-2.83	118.18	122.95
2	C	1101	8BS	C17-N16-C8	-2.74	121.72	129.29
2	D	1101	8BS	C9-C8-N7	-2.73	118.54	120.81
2	C	1101	8BS	C23-O22-C21	2.69	119.88	117.21
2	A	1101	8BS	C17-N16-C8	-2.68	121.87	129.29
2	B	1101	8BS	C1-N26-C27	2.63	127.91	123.48
2	D	1101	8BS	C15-N12-C10	2.56	129.70	124.18
2	C	1101	8BS	O30-C27-C28	-2.46	115.22	122.08
2	A	1101	8BS	C23-O22-C21	2.37	119.56	117.21
2	A	1101	8BS	F25-C2-C3	-2.36	104.97	109.06
2	C	1101	8BS	C15-N12-C10	2.35	129.26	124.18
2	B	1101	8BS	O30-C27-N26	-2.14	119.34	122.95
2	D	1101	8BS	O30-C27-C28	-2.04	116.39	122.08
2	D	1101	8BS	C17-N16-C8	-2.02	123.71	129.29

There are no chirality outliers.

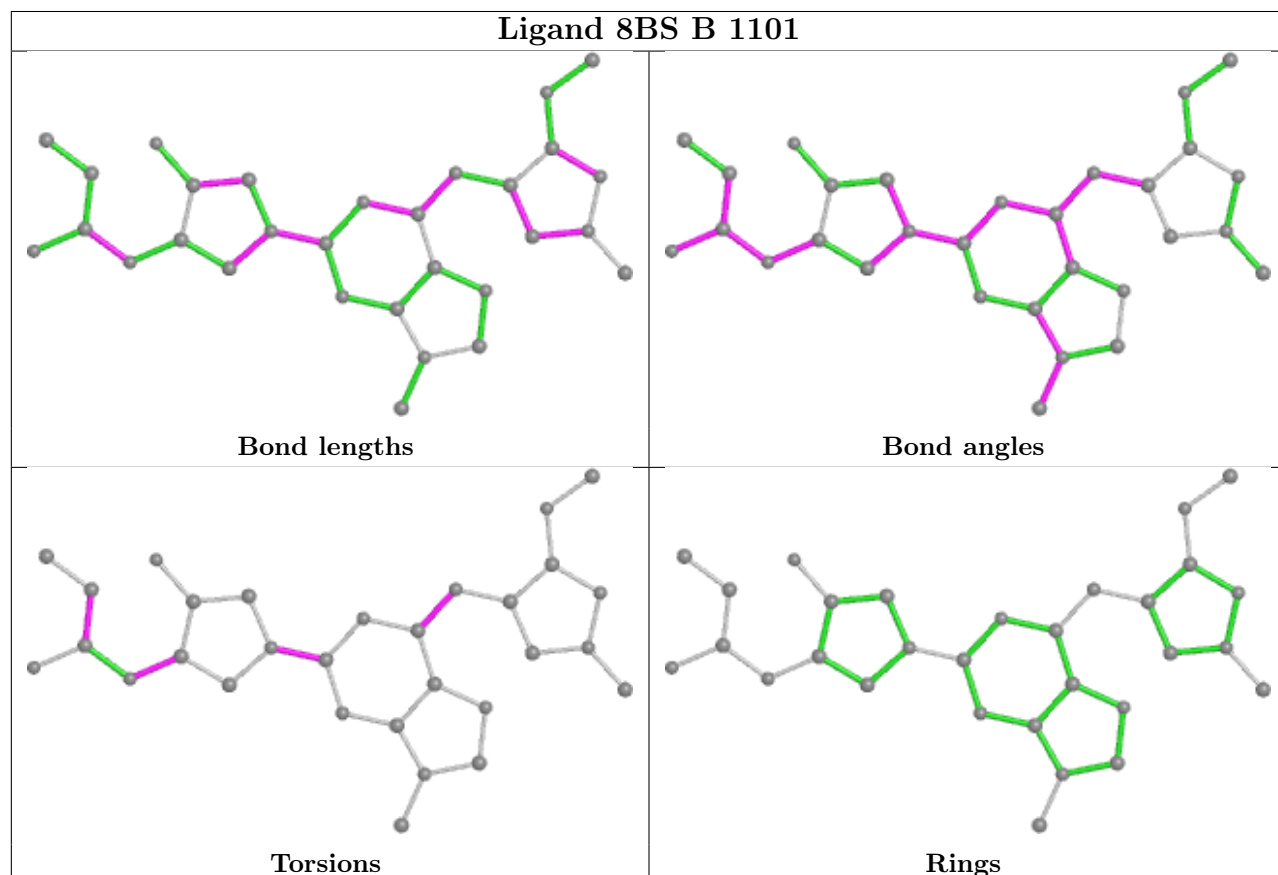
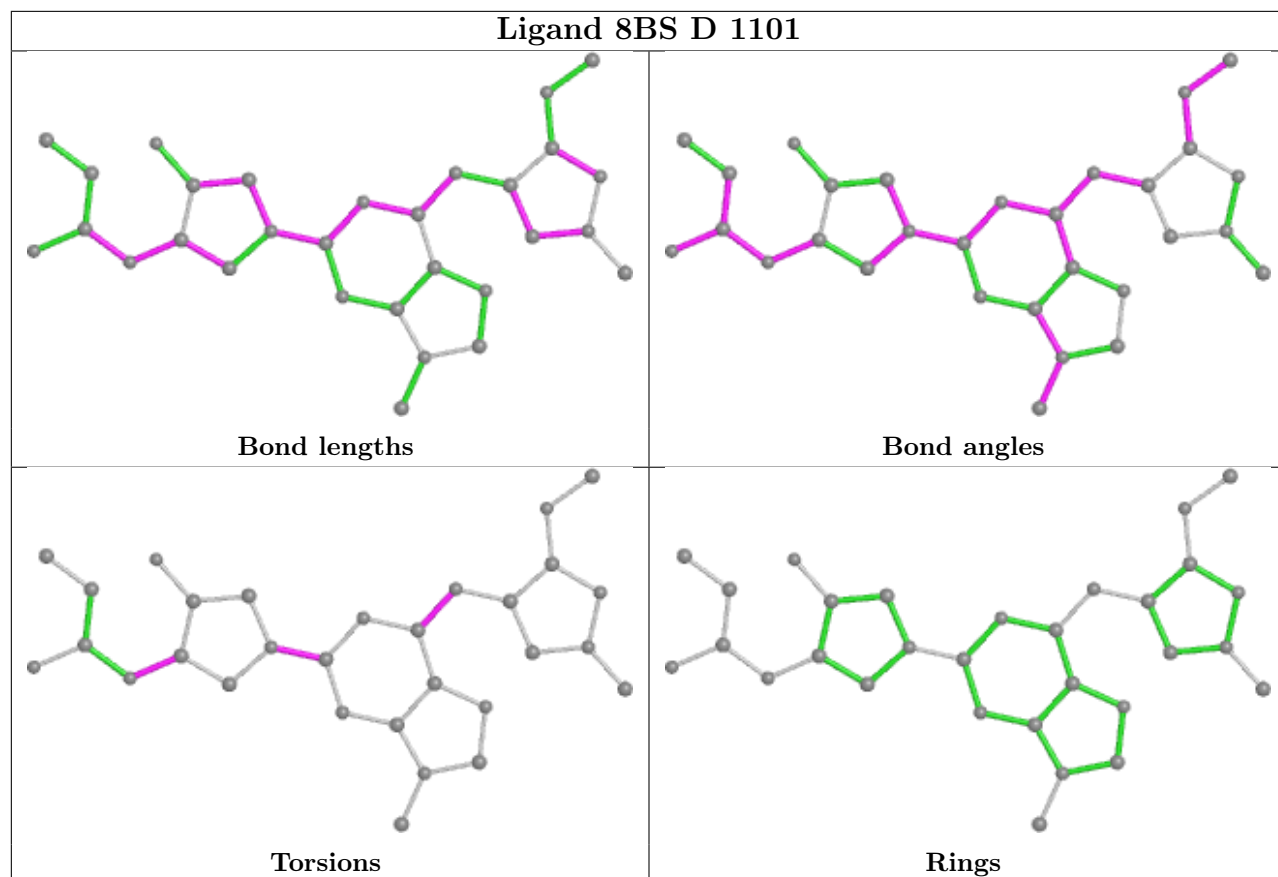
All (20) torsion outliers are listed below:

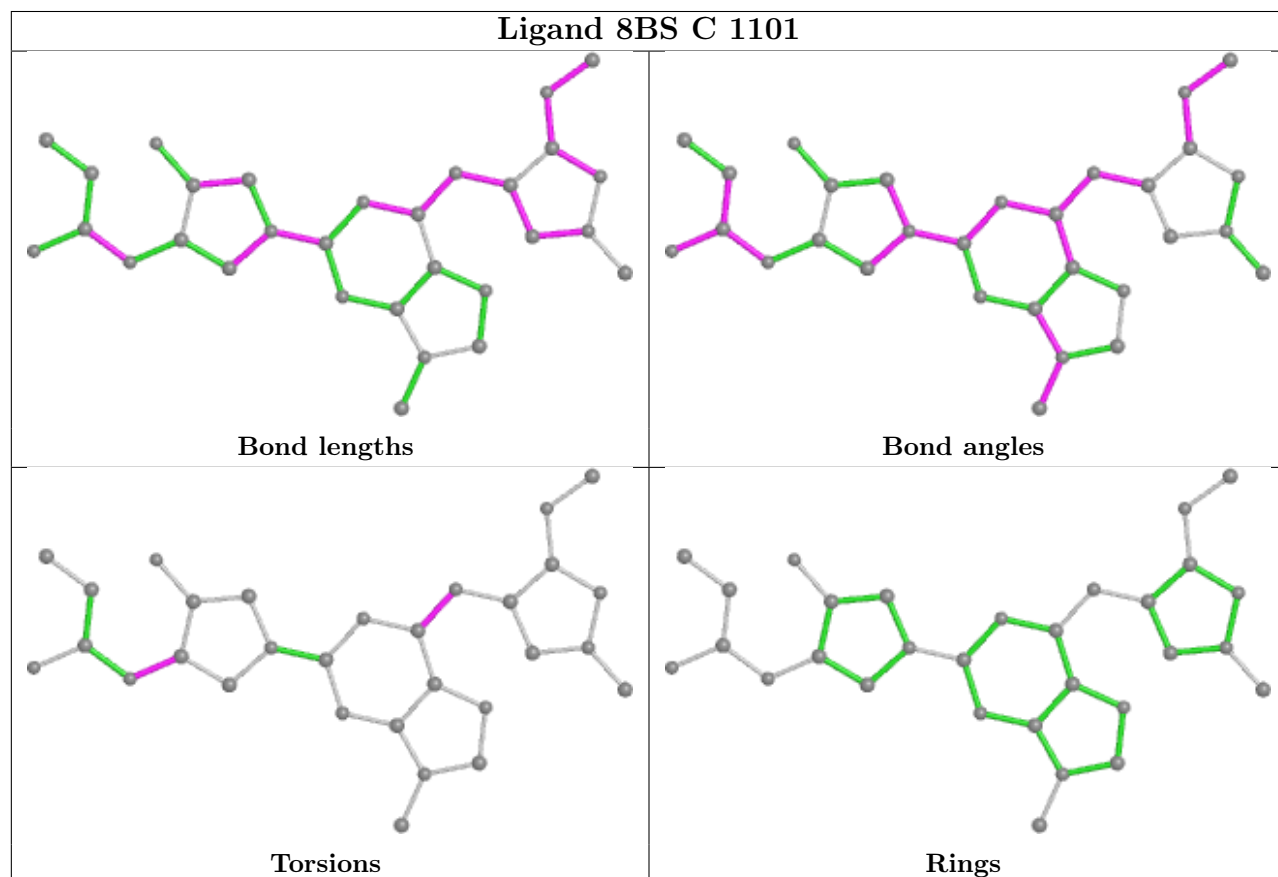
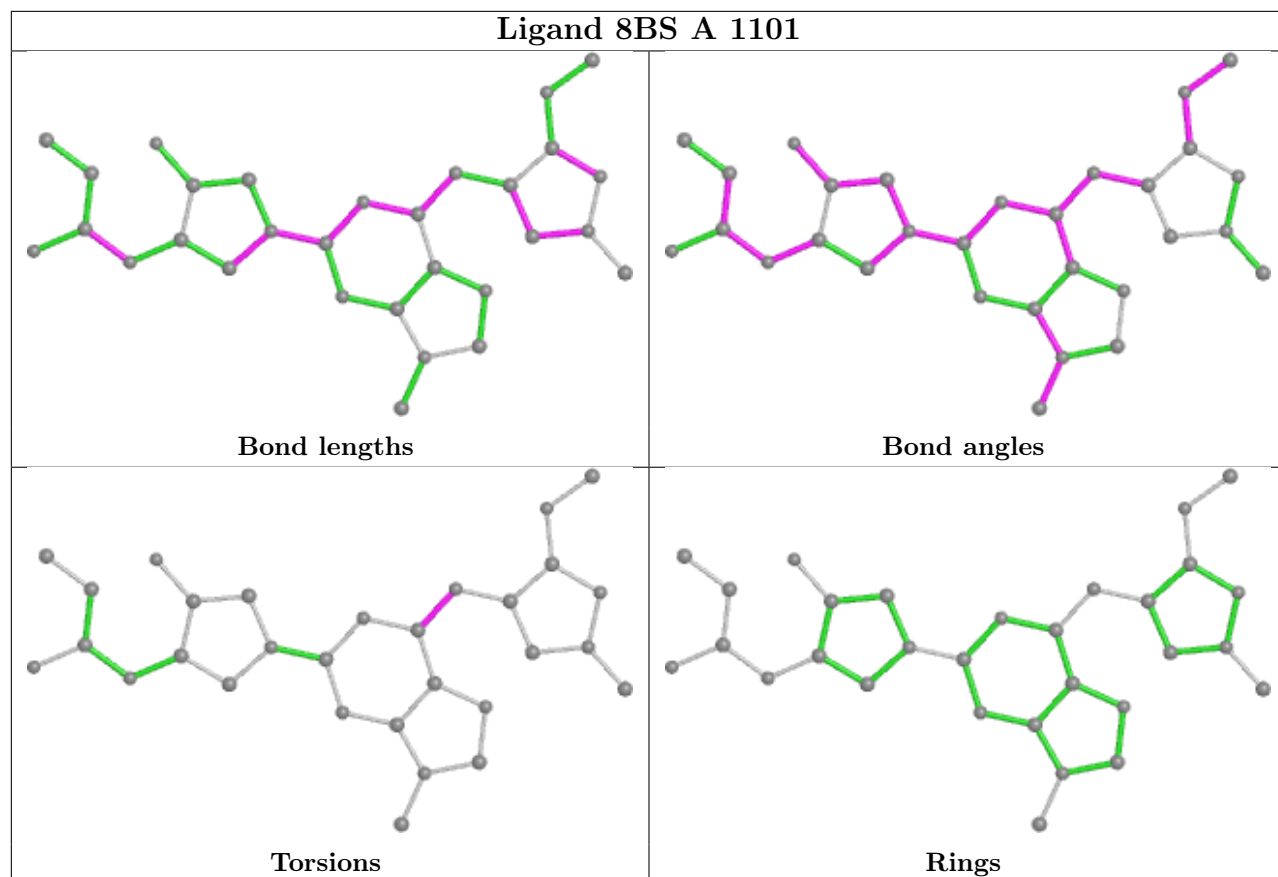
Mol	Chain	Res	Type	Atoms
2	D	1101	8BS	N7-C6-N4-C5
2	D	1101	8BS	N11-C6-N4-C5
2	D	1101	8BS	N7-C8-N16-C17
2	D	1101	8BS	C9-C8-N16-C17
2	D	1101	8BS	C2-C1-N26-C27
2	C	1101	8BS	N7-C8-N16-C17
2	C	1101	8BS	C9-C8-N16-C17
2	B	1101	8BS	N7-C6-N4-C3
2	B	1101	8BS	N11-C6-N4-C3
2	B	1101	8BS	N7-C8-N16-C17
2	B	1101	8BS	C9-C8-N16-C17
2	A	1101	8BS	N7-C8-N16-C17
2	A	1101	8BS	C9-C8-N16-C17
2	B	1101	8BS	N26-C27-C28-C29
2	B	1101	8BS	O30-C27-C28-C29
2	C	1101	8BS	C2-C1-N26-C27
2	D	1101	8BS	N7-C6-N4-C3
2	D	1101	8BS	N11-C6-N4-C3
2	C	1101	8BS	C5-C1-N26-C27
2	B	1101	8BS	C5-C1-N26-C27

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

There are no such residues in this entry.

5.8 Polymer linkage issues

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	290/331 (87%)	0.19	10 (3%)	45 19	36, 60, 85, 106	0
1	B	274/331 (82%)	0.18	11 (4%)	38 15	31, 57, 85, 101	0
1	C	283/331 (85%)	0.19	6 (2%)	63 34	46, 67, 90, 102	0
1	D	289/331 (87%)	0.01	6 (2%)	63 34	29, 49, 73, 90	0
All	All	1136/1324 (85%)	0.14	33 (2%)	51 23	29, 58, 86, 106	0

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	753	PRO	5.1
1	C	920	ALA	4.2
1	C	785	THR	4.1
1	B	920	ALA	3.8
1	A	722	ALA	3.7
1	A	920	ALA	3.6
1	A	751	THR	3.6
1	A	709	GLU	3.1
1	B	923	ILE	3.1
1	A	931	GLU	3.0
1	B	990	PRO	2.9
1	D	1006	ASP	2.7
1	B	779	GLY	2.7
1	B	996	ASN	2.6
1	C	762	GLU	2.6
1	C	748	ARG	2.5
1	D	759	ILE	2.4
1	B	734	GLU	2.4
1	B	702	ALA	2.4
1	A	876	VAL	2.4
1	A	716	LYS	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	929	LYS	2.3
1	B	808	ASN	2.2
1	A	929	LYS	2.2
1	C	721	GLY	2.2
1	B	759	ILE	2.2
1	C	982	GLN	2.2
1	A	732	ILE	2.2
1	D	784	SER	2.1
1	D	917	GLY	2.1
1	B	764	TYR	2.1
1	B	992	PRO	2.1
1	D	702	ALA	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 monosaccharides in this entry.

6.4 Ligands [i](#)

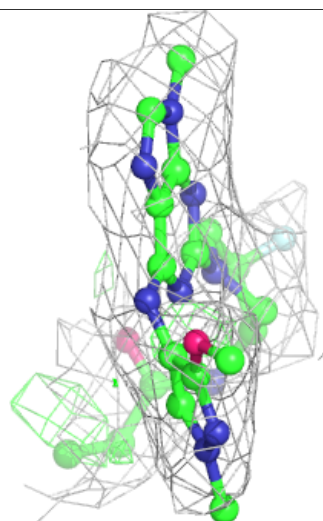
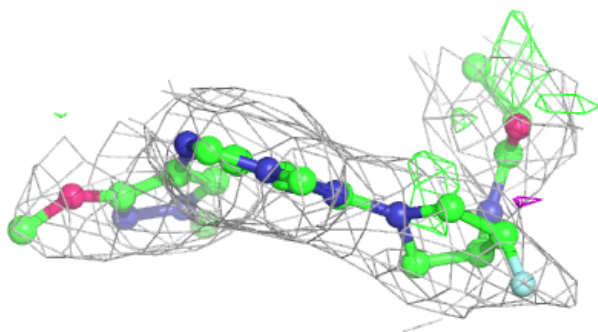
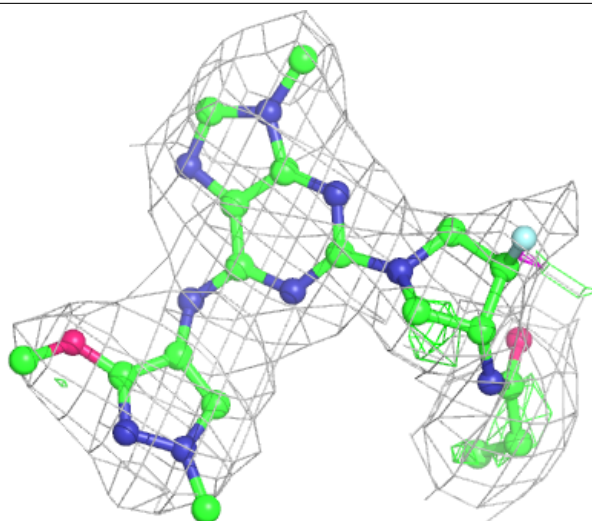
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	8BS	D	1101	30/30	0.88	0.20	39,44,52,59	0
2	8BS	B	1101	30/30	0.89	0.23	37,46,56,60	0
2	8BS	C	1101	30/30	0.91	0.19	44,51,63,77	0
2	8BS	A	1101	30/30	0.92	0.18	42,51,58,60	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.

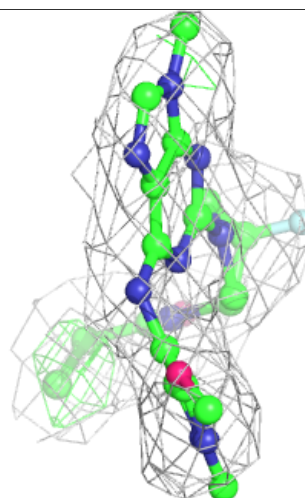
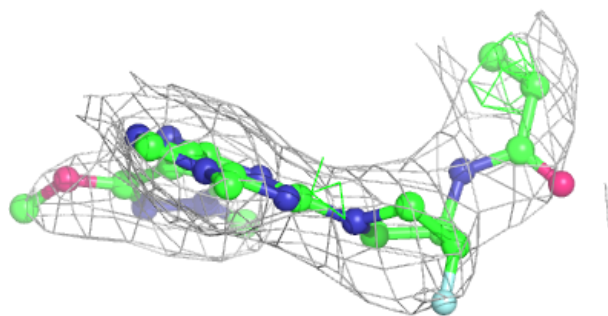
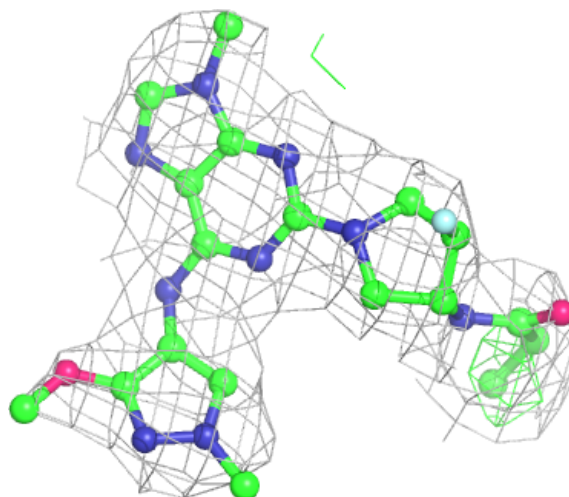
Electron density around 8BS D 1101:

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



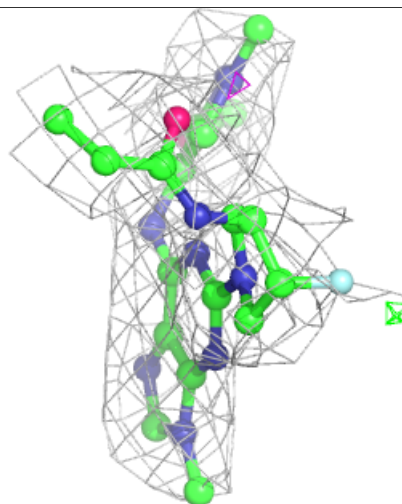
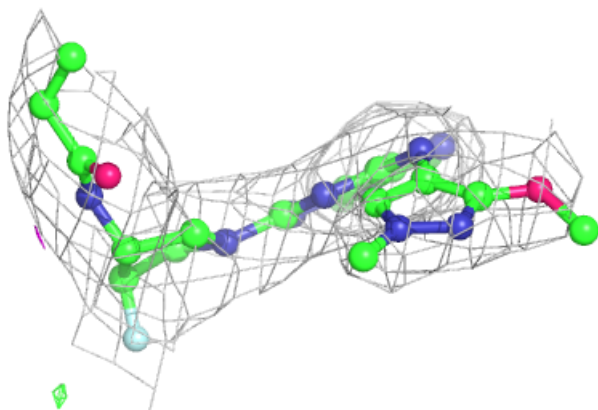
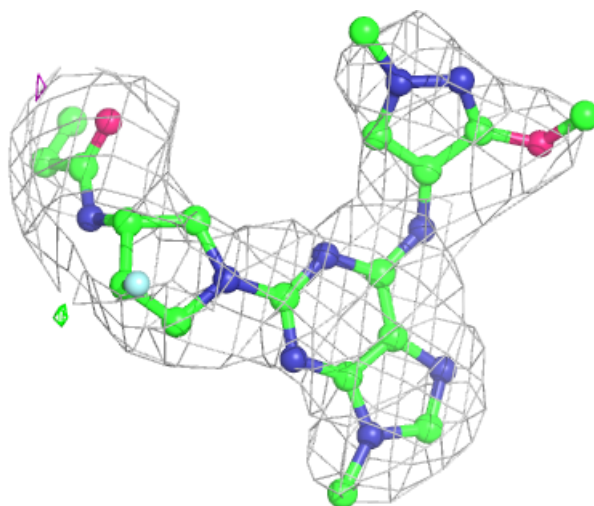
Electron density around 8BS B 1101:

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



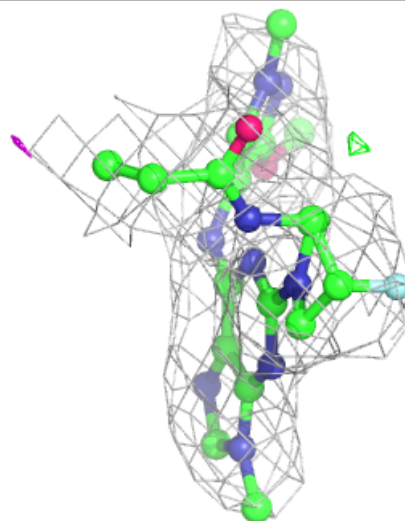
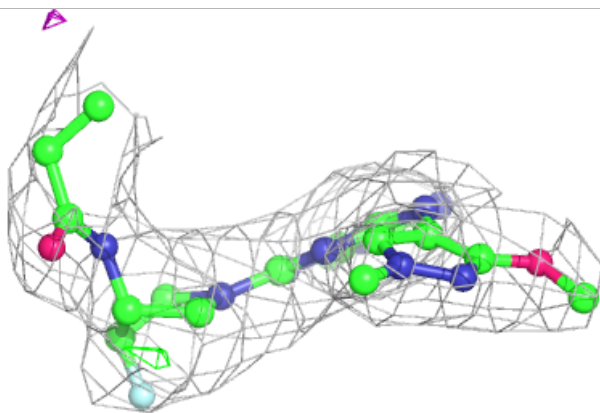
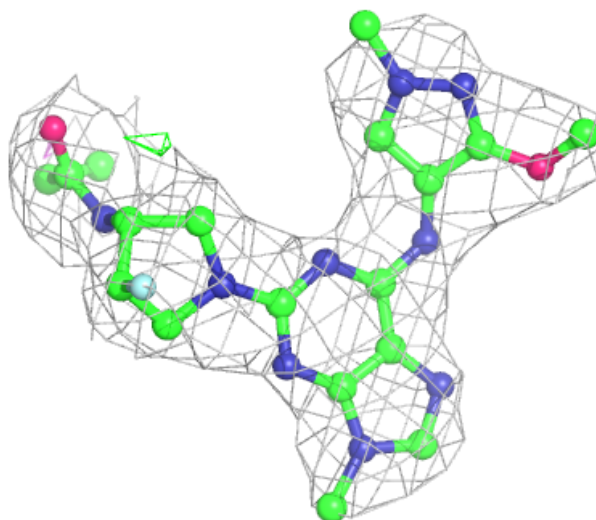
Electron density around 8BS C 1101:

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



Electron density around 8BS 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 ⓘ

There are no such residues in this entry.