



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2020 – 05:49 pm BST

PDB ID : 5PZP
Title : CRYSTAL STRUCTURE OF THE HEPATITIS C VIRUS NS5B RNA-DEPENDENT RNA POLYMERASE IN COMPLEX WITH 4-FLUORO-2-(4-FLUOROPHENYL)-N-METHYL-5-(2-METHYL-5-{{1-(PYRIMIDIN-2-YL)CYCLOPROPYL}CARBAMOYL}PHENYL)-1-BENZOFURAN-3-CARBOXAMIDE (BMS-929075)
Authors : Sheriff, S.
Deposited on : 2017-02-27
Resolution : 2.95 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 : 2.11
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) : 2.11

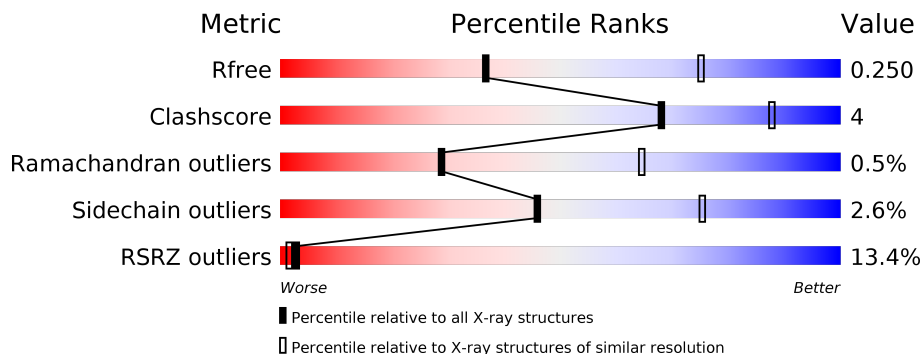
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 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	574	 10% 84% 10% • 5%
1	B	574	 15% 83% 10% • 7%

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 8657 atoms, of which 124 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.

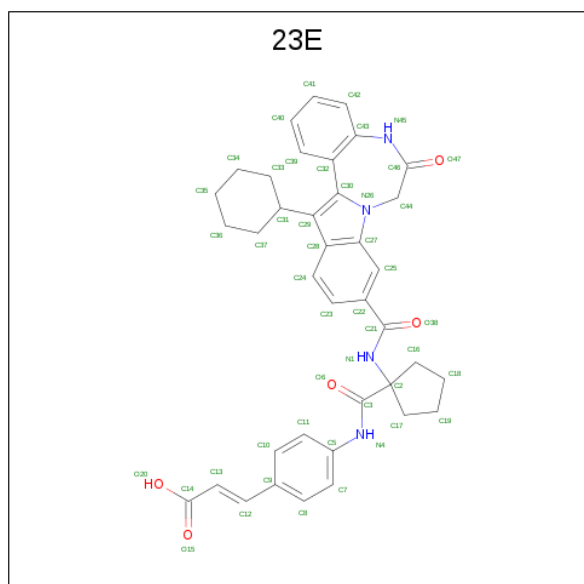
- Molecule 1 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	545	Total 4205	C 2653	N 740	O 779	S 33	0	0	0
1	B	535	Total 4080	C 2567	N 717	O 764	S 32	0	0	0

There are 2 discrepancies between the modelled and reference sequences:

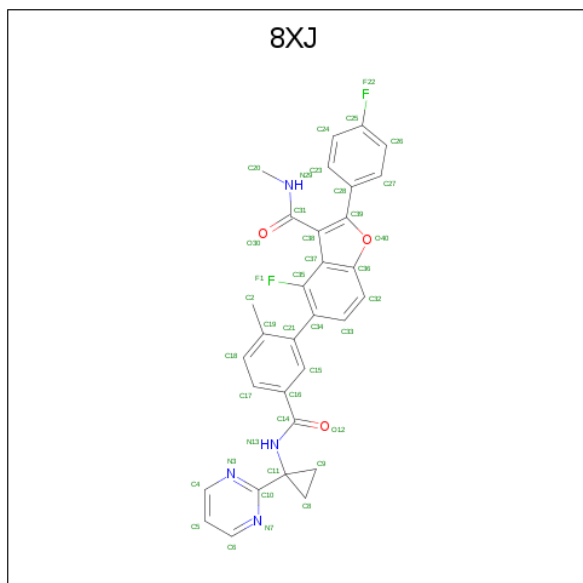
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP Q9WMX2
B	0	MET	-	expression tag	UNP Q9WMX2

- Molecule 2 is (2E)-3-(4-{{(1-{{(13-cyclohexyl-6-oxo-6,7-dihydro-5H-indolo[1,2-d][1,4]benzodiazepin-10-yl)carbonyl}amino}cyclopentyl)carbonyl}amino}phenyl)prop-2-enoic acid (three-letter code: 23E) (formula: C₃₈H₃₈N₄O₅).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
2	A	1	Total	C	H	N	O	38	0
			85	38	38	4	5		
2	B	1	Total	C	H	N	O	38	0
			85	38	38	4	5		

- Molecule 3 is 4-fluoro-2-(4-fluorophenyl)-N-methyl-5-(2-methyl-5-{[1-(pyrimidin-2-yl)cyclopropyl]carbamoyl}phenyl)-1-benzofuran-3-carboxamide (three-letter code: 8XJ) (formula: C₃₁H₂₄F₂N₄O₃).



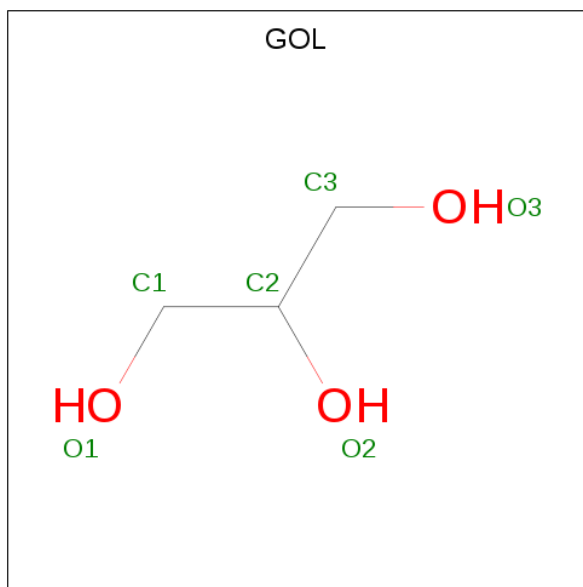
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
			Total	C	F	H	N			O
3	A	1	Total	C	F	H	N	O	24	0
			64	31	2	24	4	3		
3	B	1	Total	C	F	H	N	O	24	0
			64	31	2	24	4	3		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

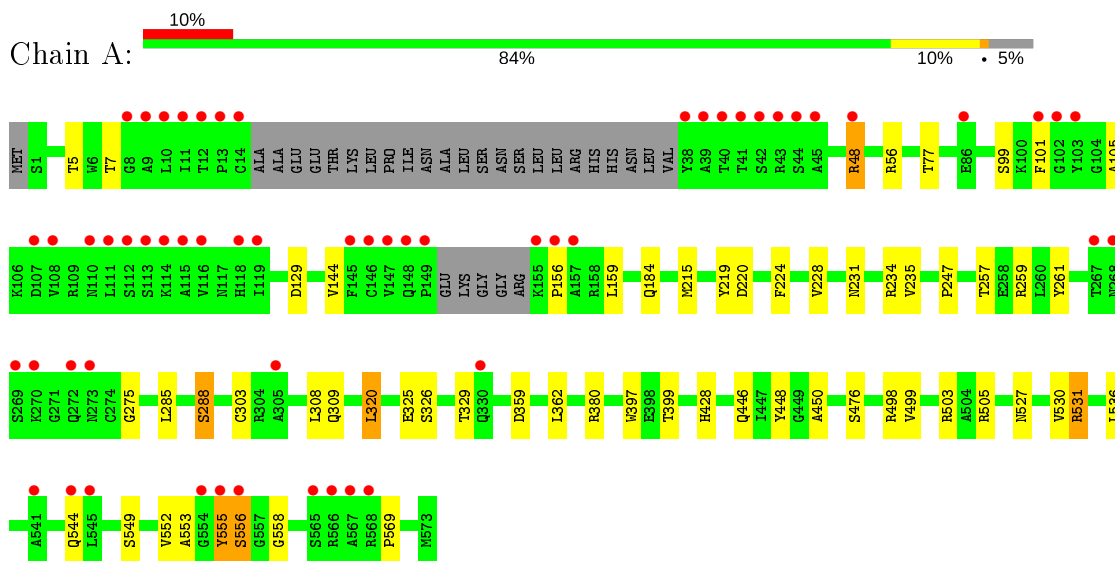
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	9	Total	O	0	0
			9	9		
6	B	1	Total	O	0	0
			1	1		

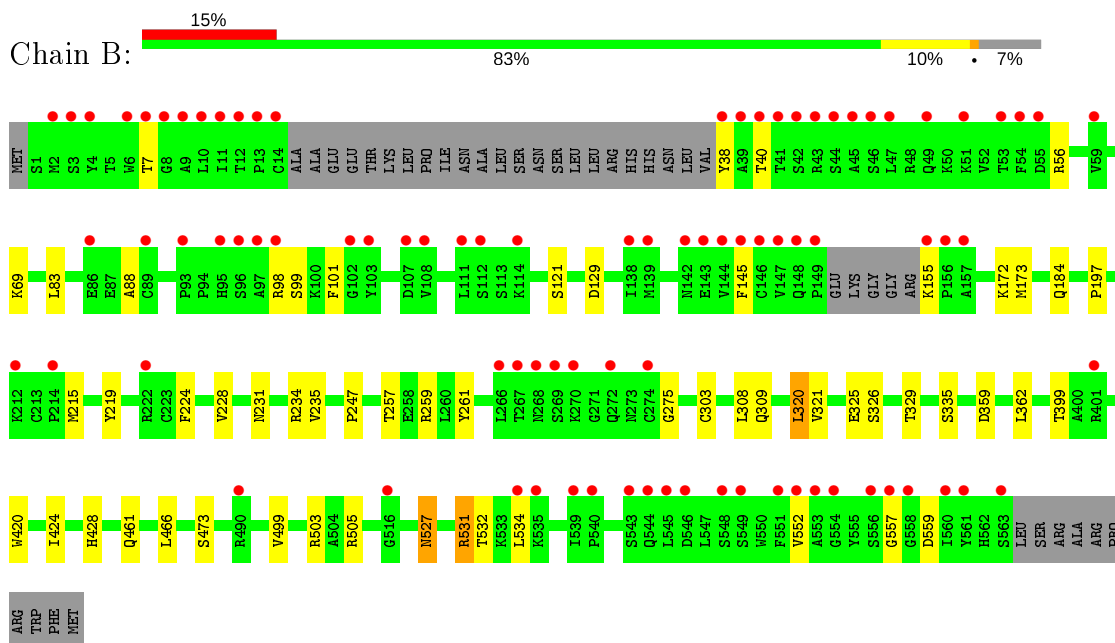
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: RNA-directed RNA polymerase



- Molecule 1: RNA-directed RNA polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	65.20Å 90.70Å 234.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.86 – 2.95 43.86 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.7 (43.86-2.95) 99.7 (43.86-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.76 (at 2.96Å)	Xtrriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.199 , 0.244 0.203 , 0.250	Depositor DCC
R_{free} test set	1057 reflections (3.51%)	wwPDB-VP
Wilson B-factor (Å ²)	59.1	Xtrriage
Anisotropy	0.584	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 73.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8657	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.24% 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: 8XJ, GOL, SO4, 23E

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	0.54	0/4298	0.70	0/5839
1	B	0.52	0/4164	0.70	0/5660
All	All	0.53	0/8462	0.70	0/11499

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

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	4205	0	4155	35	0
1	B	4080	0	4027	31	0
2	A	47	38	37	0	0
2	B	47	38	37	0	0
3	A	40	24	0	0	0
3	B	40	24	0	0	0
4	A	20	0	0	0	0
4	B	20	0	0	0	0
5	A	18	0	24	1	0
5	B	6	0	8	0	0
6	A	9	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	1	0	0	1	0
All	All	8533	124	8288	63	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 4.

All (63) 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:309:GLN:HG3	1:A:325:GLU:HB3	1.61	0.81
1:B:309:GLN:HG3	1:B:325:GLU:HB3	1.61	0.80
1:A:359:ASP:HB2	1:A:362:LEU:HD12	1.73	0.69
1:A:505:ARG:HH21	1:A:531:ARG:HG3	1.57	0.68
1:A:288:SER:CB	1:A:555:TYR:HB3	2.23	0.67
1:B:359:ASP:HB2	1:B:362:LEU:HD12	1.78	0.65
1:A:247:PRO:HG3	1:B:234:ARG:HD3	1.79	0.65
1:B:531:ARG:HD3	1:B:532:THR:HG22	1.79	0.64
1:A:448:TYR:O	1:A:556:SER:HA	2.00	0.62
1:A:505:ARG:NH2	1:A:531:ARG:HG3	2.17	0.60
1:B:303:CYS:HA	1:B:308:LEU:HD12	1.89	0.55
1:A:505:ARG:HD3	5:A:609:GOL:H32	1.88	0.55
1:A:288:SER:HB2	1:A:555:TYR:HB3	1.86	0.55
1:A:285:LEU:HA	1:A:558:GLY:HA2	1.88	0.54
1:A:303:CYS:HA	1:A:308:LEU:HD12	1.90	0.54
1:B:531:ARG:HG3	1:B:531:ARG:HH11	1.73	0.53
1:A:219:TYR:HB3	1:A:320:LEU:HD23	1.90	0.53
1:A:399:THR:HG21	1:A:428:HIS:NE2	2.23	0.53
1:A:446:GLN:HA	1:A:450:ALA:O	2.08	0.52
1:B:399:THR:HG21	1:B:428:HIS:NE2	2.24	0.52
1:B:505:ARG:HE	1:B:531:ARG:HH12	1.59	0.49
1:A:184:GLN:HB2	6:A:703:HOH:O	2.12	0.49
1:A:288:SER:HB3	1:A:555:TYR:HB3	1.92	0.49
1:A:231:ASN:O	1:A:235:VAL:HG23	2.12	0.49
1:B:527:ASN:HD21	1:B:534:LEU:HB2	1.77	0.49
1:B:231:ASN:O	1:B:235:VAL:HG23	2.13	0.48
1:A:215:MET:HB2	1:A:326:SER:HB2	1.95	0.48
1:A:499:VAL:O	1:A:503:ARG:HG3	2.13	0.48
1:B:99:SER:C	1:B:101:PHE:H	2.17	0.48
1:A:549:SER:HA	1:A:552:VAL:HG22	1.95	0.47
1:A:553:ALA:HA	1:A:555:TYR:CZ	2.49	0.47
1:B:219:TYR:HB3	1:B:320:LEU:HD23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:LYS:HE2	1:B:559:ASP:O	2.13	0.47
1:A:48:ARG:HG2	1:A:159:LEU:HD13	1.97	0.47
1:B:88:ALA:HB2	1:B:173:MET:HG2	1.97	0.47
1:B:499:VAL:O	1:B:503:ARG:HG3	2.14	0.47
1:B:184:GLN:HB2	6:B:701:HOH:O	2.15	0.46
1:B:38:TYR:HH	1:B:155:LYS:N	2.13	0.46
1:B:531:ARG:NH1	1:B:531:ARG:HG3	2.31	0.45
1:B:215:MET:HB2	1:B:326:SER:HB2	1.98	0.45
1:A:144:VAL:HG21	1:A:397:TRP:CG	2.52	0.45
1:A:129:ASP:HB3	1:A:259:ARG:NH1	2.32	0.45
1:B:7:THR:HG23	1:B:275:GLY:HA2	1.99	0.44
1:A:234:ARG:HD3	1:B:247:PRO:HG3	2.00	0.44
1:B:505:ARG:HE	1:B:531:ARG:NH1	2.15	0.44
1:B:129:ASP:HB3	1:B:259:ARG:NH1	2.33	0.44
1:A:7:THR:HG23	1:A:275:GLY:HA2	1.99	0.43
1:A:224:PHE:O	1:A:228:VAL:HG23	2.18	0.43
1:B:197:PRO:HD2	1:B:466:LEU:HB3	2.01	0.43
1:A:288:SER:HB2	1:A:555:TYR:CB	2.48	0.43
1:A:48:ARG:HB2	1:A:156:PRO:HB2	1.99	0.43
1:B:224:PHE:O	1:B:228:VAL:HG23	2.19	0.42
1:B:531:ARG:HD2	1:B:532:THR:H	1.84	0.42
1:A:527:ASN:O	1:A:530:VAL:HG22	2.19	0.42
1:A:77:THR:HA	1:B:69:LYS:HD3	2.02	0.42
1:A:99:SER:C	1:A:101:PHE:H	2.23	0.41
1:B:257:THR:HA	1:B:261:TYR:HB2	2.02	0.41
1:B:420:TRP:HA	1:B:424:ILE:HD12	2.01	0.41
1:A:257:THR:HA	1:A:261:TYR:HB2	2.02	0.41
1:B:83:LEU:HB2	1:B:173:MET:HA	2.02	0.41
1:A:5:THR:O	1:A:275:GLY:HA3	2.20	0.41
1:A:544:GLN:OE1	1:A:569:PRO:HA	2.21	0.40
1:B:38:TYR:CE1	1:B:145:PHE:HB2	2.56	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	539/574 (94%)	511 (95%)	25 (5%)	3 (1%)	25	60
1	B	529/574 (92%)	495 (94%)	32 (6%)	2 (0%)	34	69
All	All	1068/1148 (93%)	1006 (94%)	57 (5%)	5 (0%)	29	64

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	552	VAL
1	A	105	ALA
1	B	557	GLY
1	A	531	ARG
1	A	556	SER

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	448/486 (92%)	437 (98%)	11 (2%)	47	76
1	B	434/486 (89%)	422 (97%)	12 (3%)	43	74
All	All	882/972 (91%)	859 (97%)	23 (3%)	46	75

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	ARG
1	A	56	ARG
1	A	220	ASP
1	A	288	SER
1	A	320	LEU
1	A	329	THR
1	A	380	ARG
1	A	476	SER

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Mol	Chain	Res	Type
1	A	498	ARG
1	A	536	LEU
1	A	555	TYR
1	B	40	THR
1	B	56	ARG
1	B	98	ARG
1	B	121	SER
1	B	320	LEU
1	B	321	VAL
1	B	329	THR
1	B	335	SER
1	B	461	GLN
1	B	473	SER
1	B	527	ASN
1	B	531	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	142	ASN
1	B	117	ASN
1	B	142	ASN
1	B	527	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

16 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
4	SO4	A	606	-	4,4,4	0.25	0	6,6,6	0.36	0
4	SO4	B	605	-	4,4,4	0.42	0	6,6,6	0.32	0
4	SO4	A	603	-	4,4,4	0.20	0	6,6,6	0.22	0
4	SO4	B	603	-	4,4,4	0.26	0	6,6,6	0.19	0
2	23E	A	601	-	44,53,53	0.89	2 (4%)	57,77,77	0.62	0
4	SO4	B	604	-	4,4,4	0.33	0	6,6,6	0.38	0
3	8XJ	B	602	-	38,45,45	0.90	2 (5%)	49,67,67	1.33	4 (8%)
5	GOL	A	608	-	5,5,5	0.19	0	5,5,5	0.30	0
3	8XJ	A	602	-	38,45,45	0.74	3 (7%)	49,67,67	1.23	5 (10%)
5	GOL	A	607	-	5,5,5	0.10	0	5,5,5	0.19	0
4	SO4	A	605	-	4,4,4	0.32	0	6,6,6	0.30	0
4	SO4	B	606	-	4,4,4	0.32	0	6,6,6	0.37	0
5	GOL	A	609	-	5,5,5	0.13	0	5,5,5	0.22	0
4	SO4	A	604	-	4,4,4	0.29	0	6,6,6	0.30	0
2	23E	B	601	-	44,53,53	0.80	2 (4%)	57,77,77	0.68	0
5	GOL	B	607	-	5,5,5	0.09	0	5,5,5	0.25	0

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
5	GOL	A	609	-	-	1/4/4/4	-
2	23E	A	601	-	-	4/22/57/57	0/6/7/7
3	8XJ	B	602	-	-	2/17/33/33	0/6/6/6
5	GOL	A	608	-	-	0/4/4/4	-
3	8XJ	A	602	-	-	0/17/33/33	0/6/6/6
5	GOL	A	607	-	-	3/4/4/4	-
5	GOL	B	607	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	23E	B	601	-	-	4/22/57/57	0/6/7/7

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	602	8XJ	C38-C31	-4.23	1.45	1.51
2	A	601	23E	C29-C28	4.16	1.45	1.40
2	B	601	23E	C29-C28	3.42	1.44	1.40
2	A	601	23E	C44-N26	-2.31	1.46	1.48
3	A	602	8XJ	C38-C37	2.25	1.45	1.41
3	A	602	8XJ	C38-C31	-2.19	1.48	1.51
2	B	601	23E	C44-N26	-2.06	1.46	1.48
3	B	602	8XJ	C37-C36	-2.04	1.39	1.43
3	A	602	8XJ	C37-C36	-2.00	1.39	1.43

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	8XJ	C38-C39-C28	5.22	134.60	127.13
3	A	602	8XJ	C38-C39-C28	5.18	134.53	127.13
3	B	602	8XJ	C10-C11-N13	-4.62	112.41	117.12
3	A	602	8XJ	C32-C36-C37	3.13	123.04	117.84
3	B	602	8XJ	C32-C36-C37	3.09	122.98	117.84
3	A	602	8XJ	C10-C11-N13	-3.02	114.04	117.12
3	A	602	8XJ	C38-C37-C36	-2.93	106.42	110.52
3	B	602	8XJ	C38-C37-C36	-2.84	106.55	110.52
3	A	602	8XJ	C39-C38-C37	-2.20	105.76	109.16

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	23E	C3-C2-N1-C21
2	A	601	23E	C16-C2-N1-C21
2	B	601	23E	C3-C2-N1-C21
2	B	601	23E	C16-C2-N1-C21
5	A	607	GOL	C1-C2-C3-O3
2	A	601	23E	C17-C2-N1-C21
5	A	607	GOL	O2-C2-C3-O3
2	B	601	23E	C17-C2-N1-C21
5	A	609	GOL	O2-C2-C3-O3

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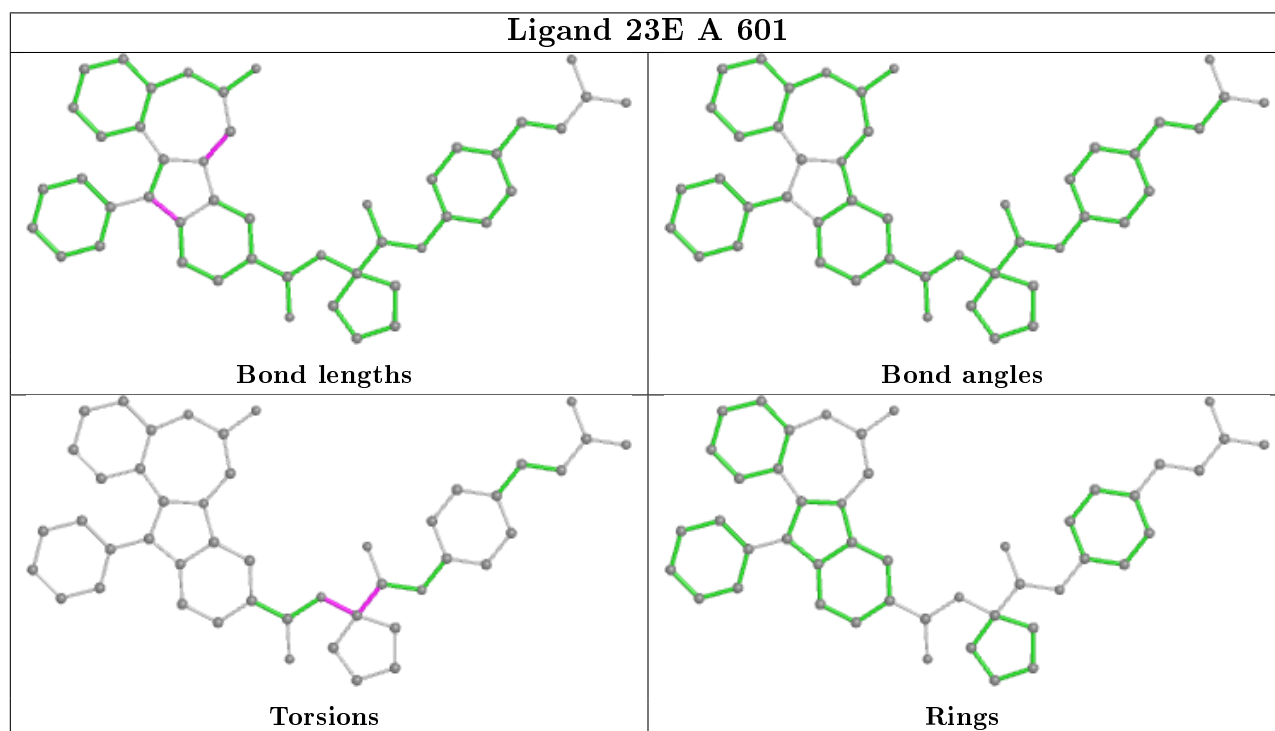
Mol	Chain	Res	Type	Atoms
2	A	601	23E	C17-C2-C3-O6
3	B	602	8XJ	C8-C11-N13-C14
5	A	607	GOL	O1-C1-C2-C3
2	B	601	23E	C16-C2-C3-O6
3	B	602	8XJ	C9-C11-N13-C14

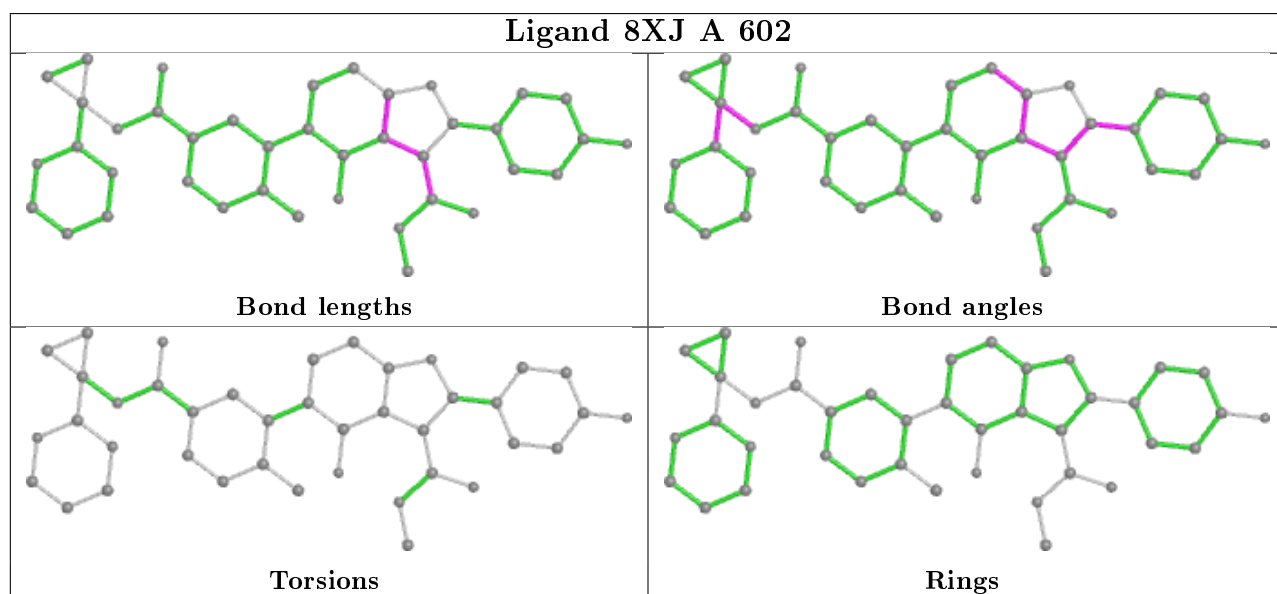
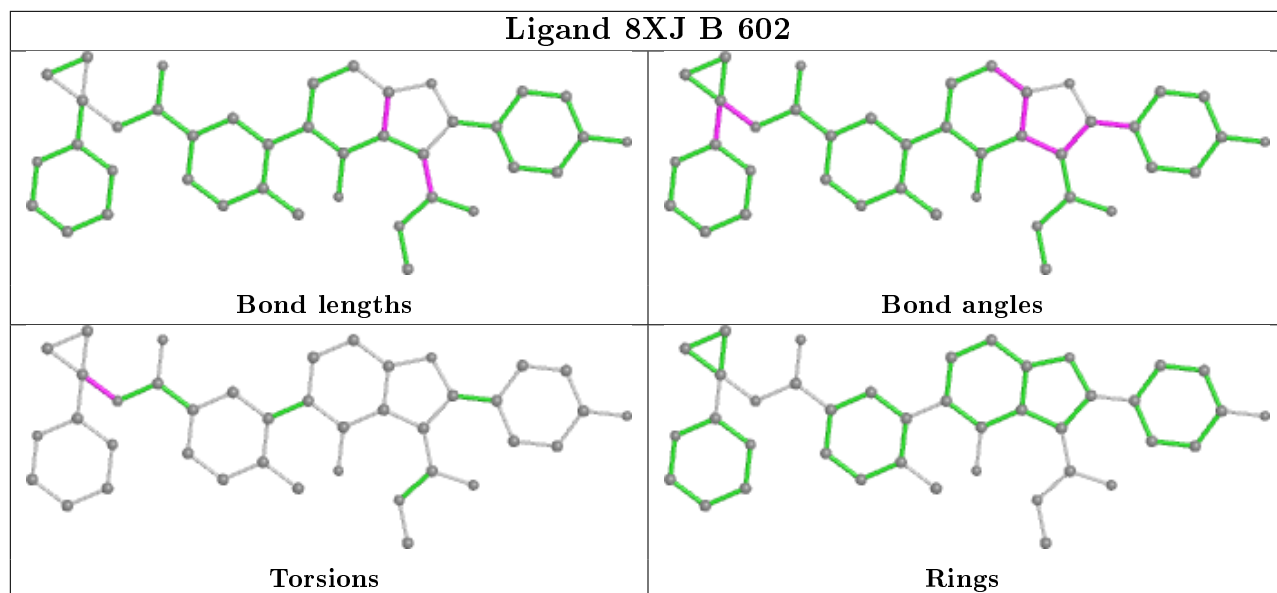
There are no ring outliers.

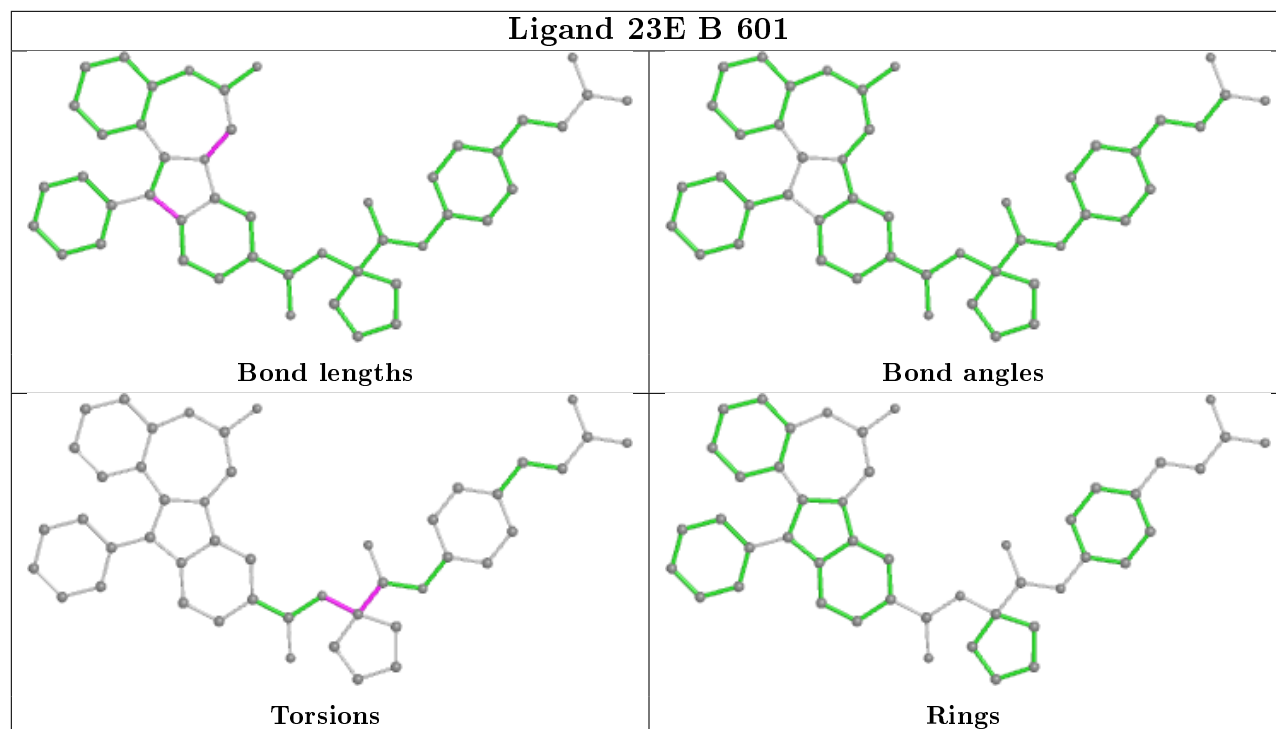
1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	609	GOL	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	545/574 (94%)	0.52	57 (10%) 6 4	27, 56, 112, 152	0
1	B	535/574 (93%)	0.89	88 (16%) 1 1	37, 64, 145, 168	0
All	All	1080/1148 (94%)	0.70	145 (13%) 3 1	27, 60, 137, 168	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	14	CYS	13.5
1	B	41	THR	13.4
1	B	556	SER	9.4
1	A	12	THR	9.4
1	A	14	CYS	9.2
1	B	39	ALA	9.1
1	B	561	TYR	9.1
1	A	567	ALA	8.7
1	A	147	VAL	8.1
1	A	13	PRO	8.1
1	B	557	GLY	7.5
1	B	149	PRO	7.1
1	B	42	SER	6.9
1	B	44	SER	6.9
1	B	145	PHE	6.6
1	A	149	PRO	6.6
1	A	40	THR	6.5
1	B	11	ILE	6.4
1	B	544	GLN	6.4
1	A	38	TYR	6.3
1	B	12	THR	6.3
1	B	156	PRO	6.1
1	A	41	THR	6.1
1	B	6	TRP	6.1

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Mol	Chain	Res	Type	RSRZ
1	B	142	ASN	6.0
1	B	40	THR	6.0
1	A	10	LEU	5.9
1	B	157	ALA	5.7
1	B	13	PRO	5.7
1	B	545	LEU	5.7
1	B	8	GLY	5.7
1	B	268	ASN	5.6
1	B	10	LEU	5.6
1	B	147	VAL	5.6
1	B	540	PRO	5.3
1	B	9	ALA	5.3
1	B	43	ARG	5.3
1	B	146	CYS	4.9
1	A	103	TYR	4.9
1	B	553	ALA	4.8
1	B	46	SER	4.7
1	B	148	GLN	4.7
1	A	156	PRO	4.7
1	B	47	LEU	4.7
1	A	566	ARG	4.6
1	B	144	VAL	4.5
1	A	111	LEU	4.5
1	B	554	GLY	4.5
1	B	103	TYR	4.5
1	B	552	VAL	4.4
1	A	146	CYS	4.3
1	A	44	SER	4.3
1	A	269	SER	4.2
1	A	43	ARG	4.1
1	B	7	THR	4.1
1	A	11	ILE	4.0
1	B	138	ILE	4.0
1	B	401	ARG	4.0
1	A	272	GLN	4.0
1	A	157	ALA	3.9
1	A	48	ARG	3.9
1	A	42	SER	3.9
1	A	270	LYS	3.9
1	B	274	CYS	3.8
1	B	49	GLN	3.8
1	A	110	ASN	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	8	GLY	3.7
1	A	148	GLN	3.7
1	B	535	LYS	3.7
1	B	558	GLY	3.7
1	B	548	SER	3.7
1	B	38	TYR	3.6
1	B	272	GLN	3.6
1	B	551	PHE	3.6
1	B	560	ILE	3.5
1	B	534	LEU	3.4
1	B	55	ASP	3.4
1	A	544	GLN	3.4
1	A	108	VAL	3.3
1	A	116	VAL	3.3
1	B	543	SER	3.3
1	B	539	ILE	3.3
1	B	269	SER	3.2
1	A	107	ASP	3.1
1	A	86	GLU	3.1
1	B	108	VAL	3.0
1	A	145	PHE	3.0
1	B	53	THR	3.0
1	B	563	SER	3.0
1	B	155	LYS	3.0
1	B	59	VAL	2.9
1	A	112	SER	2.9
1	A	102	GLY	2.9
1	B	93	PRO	2.9
1	B	270	LYS	2.9
1	B	2	MET	2.9
1	A	114	LYS	2.8
1	A	268	ASN	2.8
1	B	111	LEU	2.8
1	B	97	ALA	2.8
1	B	212	LYS	2.8
1	B	143	GLU	2.8
1	B	546	ASP	2.8
1	A	568	ARG	2.7
1	B	45	ALA	2.7
1	A	115	ALA	2.7
1	B	89	CYS	2.7
1	B	266	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	222	ARG	2.6
1	B	98	ARG	2.6
1	B	107	ASP	2.6
1	A	554	GLY	2.6
1	B	54	PHE	2.6
1	A	545	LEU	2.5
1	A	113	SER	2.5
1	A	273	ASN	2.5
1	A	330	GLN	2.5
1	B	95	HIS	2.5
1	B	102	GLY	2.5
1	B	139	MET	2.5
1	A	267	THR	2.5
1	A	39	ALA	2.5
1	B	549	SER	2.4
1	B	86	GLU	2.4
1	A	555	TYR	2.3
1	A	556	SER	2.3
1	B	51	LYS	2.3
1	B	267	THR	2.3
1	B	516	GLY	2.3
1	A	119	ILE	2.3
1	B	96	SER	2.3
1	B	114	LYS	2.2
1	A	45	ALA	2.2
1	A	101	PHE	2.2
1	A	9	ALA	2.2
1	B	490	ARG	2.2
1	A	541	ALA	2.1
1	A	118	HIS	2.1
1	A	305	ALA	2.1
1	A	565	SER	2.1
1	B	3	SER	2.1
1	B	112	SER	2.1
1	A	155	LYS	2.1
1	B	4	TYR	2.0
1	B	214	PRO	2.0

6.2 Non-standard residues in protein, DNA, RNA chains

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](#)

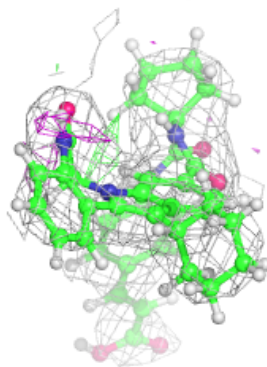
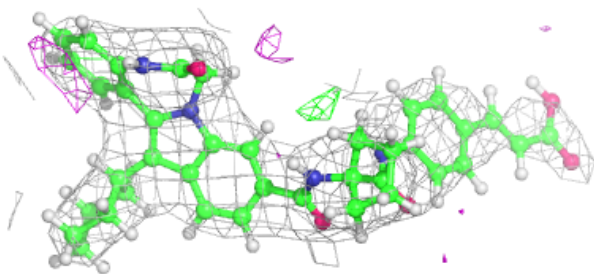
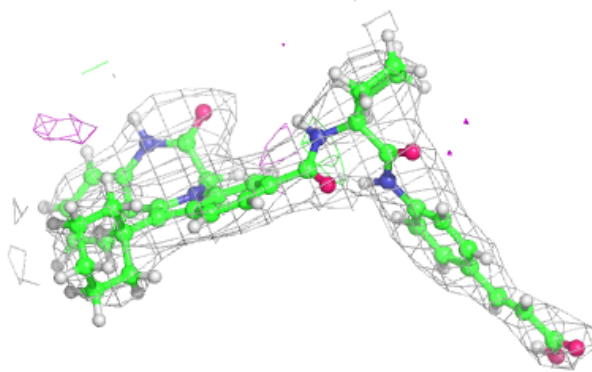
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	A	609	6/6	0.82	0.22	87,90,93,95	0
4	SO4	A	605	5/5	0.83	0.27	117,121,121,122	0
4	SO4	A	606	5/5	0.85	0.27	126,129,129,130	0
4	SO4	B	606	5/5	0.85	0.27	117,119,120,120	0
4	SO4	B	605	5/5	0.85	0.18	112,112,113,114	0
5	GOL	B	607	6/6	0.87	0.36	65,68,70,71	0
4	SO4	B	603	5/5	0.89	0.13	119,120,121,122	0
5	GOL	A	608	6/6	0.91	0.23	55,64,70,70	0
5	GOL	A	607	6/6	0.92	0.21	68,69,74,76	0
4	SO4	A	604	5/5	0.94	0.27	92,95,96,97	0
2	23E	B	601	47/47	0.95	0.20	45,49,70,80	38
3	8XJ	B	602	40/40	0.95	0.20	43,49,54,59	24
4	SO4	B	604	5/5	0.96	0.13	83,84,87,87	0
2	23E	A	601	47/47	0.96	0.18	32,42,56,72	38
3	8XJ	A	602	40/40	0.97	0.19	33,46,57,58	24
4	SO4	A	603	5/5	0.99	0.12	63,64,65,67	0

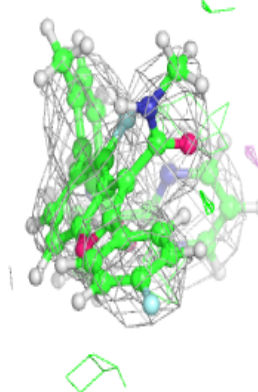
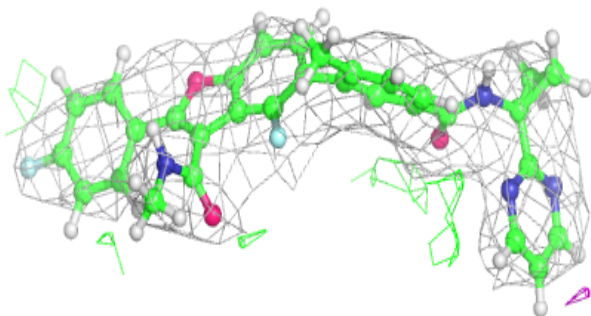
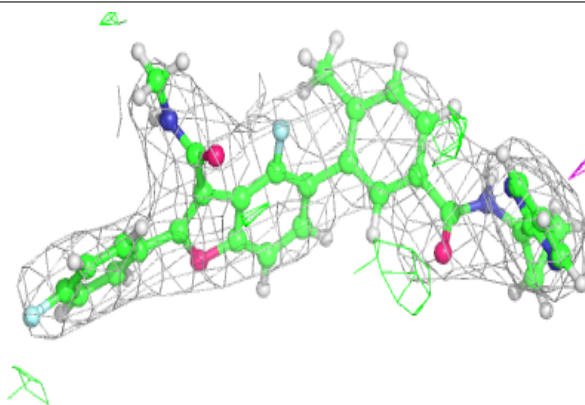
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 23E B 601:

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

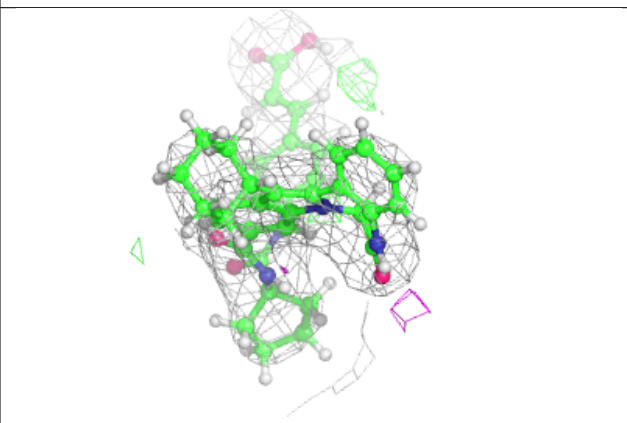
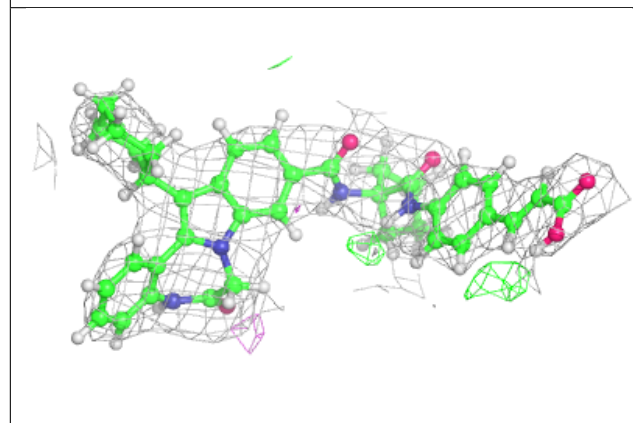
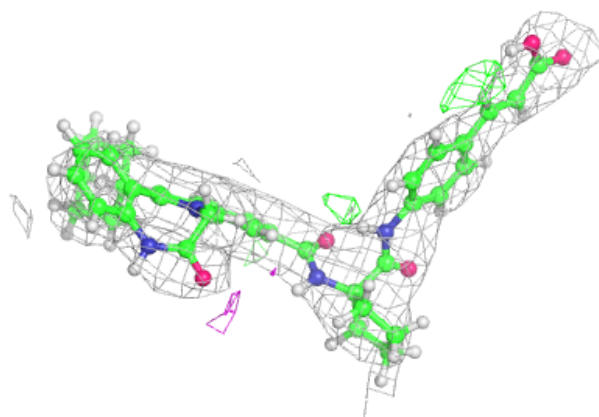
**Electron density around 8XJ B 602:**

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

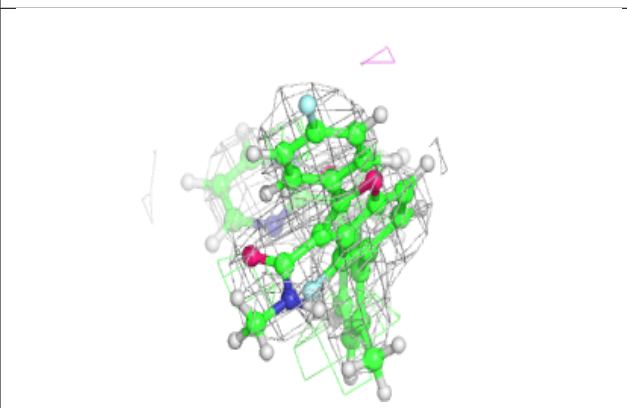
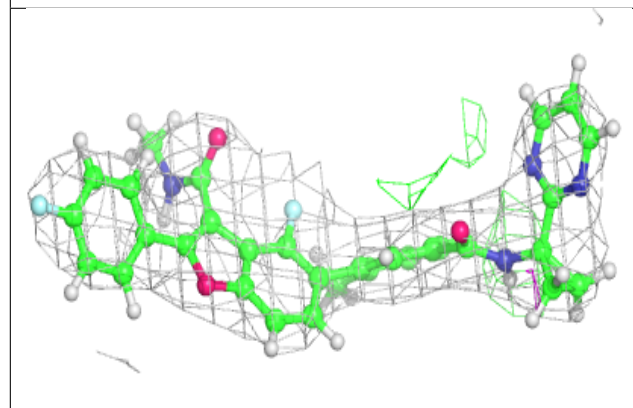
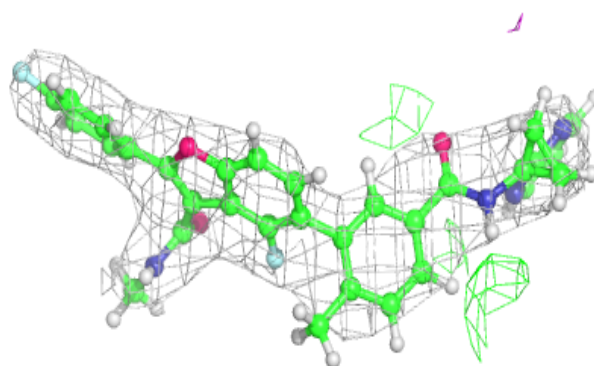


Electron density around 23E A 601:

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

**Electron density around 8XJ A 602:**

$2mF_o-DF_c$ (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.