



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 08:14 PM EDT

PDB ID : 5PZO
Title : CRYSTAL STRUCTURE OF THE HEPATITIS C VIRUS NS5B RNA-DEPENDENT RNA POLYMERASE C316N IN COMPLEX WITH 2-(4-F LUOROPHENYL)-N-METHYL-5-[3-({2-METHYL-1-OXO-1-[(1,3,4-THIAD IAZOL-2-YL)AMINO]PROPAN-2-YL}CARBAMOYL)PHENYL]-1-BENZO FURAN-3-CARBOXAMIDE
Authors : Sheriff, S.
Deposited on : 2017-02-27
Resolution : 2.80 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
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)

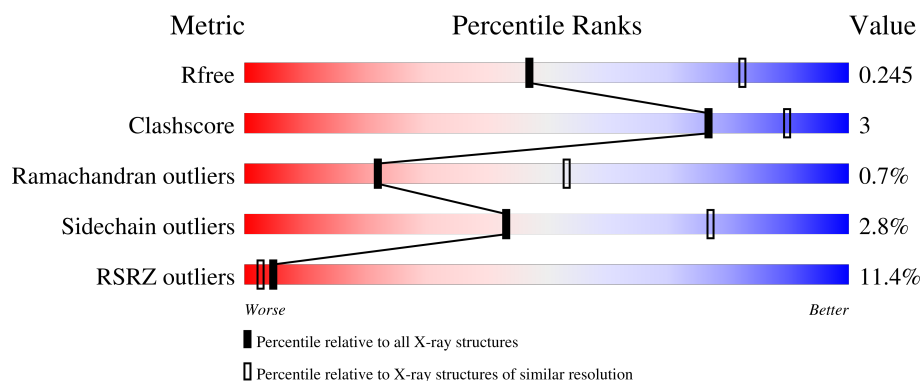
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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	574	<div> <div>9%</div> <div>85%</div> <div>10%</div> <div>• •</div> </div>
1	B	574	<div> <div>12%</div> <div>83%</div> <div>9%</div> <div>• 8%</div> </div>

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 8759 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.

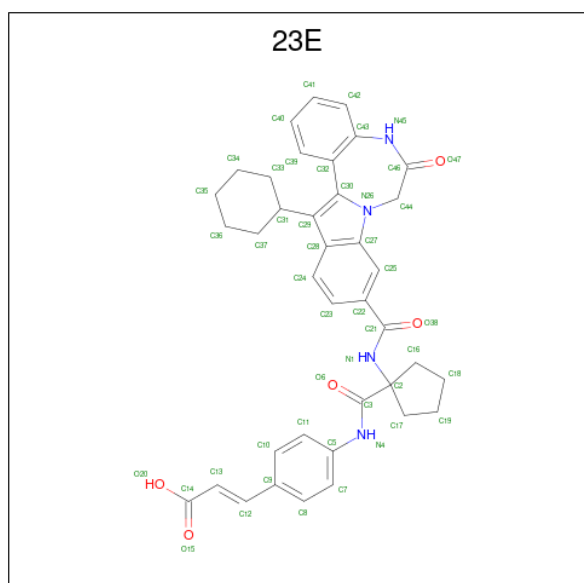
- Molecule 1 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	550	Total	C	N	O	S	0	2	0
			4262	2686	759	785	32			
1	B	529	Total	C	N	O	S	0	0	0
			4049	2551	716	752	30			

There are 4 discrepancies between the modelled and reference sequences:

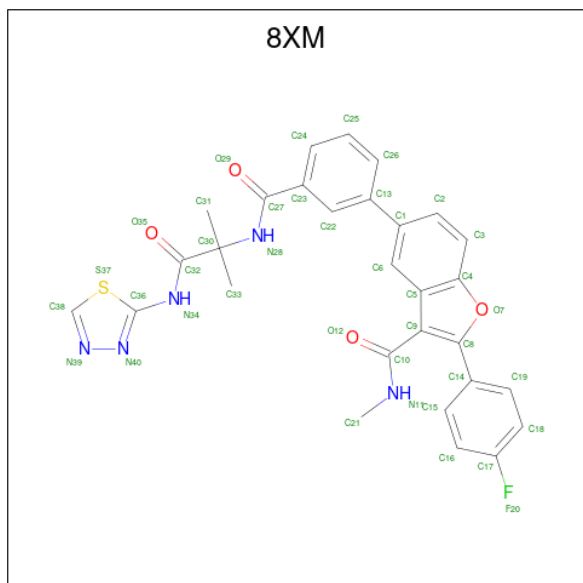
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP Q9WMX2
A	316	ASN	CYS	engineered mutation	UNP Q9WMX2
B	0	MET	-	expression tag	UNP Q9WMX2
B	316	ASN	CYS	engineered mutation	UNP Q9WMX2

- 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
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 2-(4-fluorophenyl)-N-methyl-5-[3-(2-methyl-1-oxo-1-[(1,3,4-thiadiazol-2-yl)amino]propan-2-yl}carbamoyl)phenyl]-1-benzofuran-3-carboxamide (three-letter code: 8XM) (formula: C₂₉H₂₄FN₅O₄S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total 64	C 29	F 1	H 24	N 5	O 4	S 1	24	0
3	B	1	Total 64	C 29	F 1	H 24	N 5	O 4	S 1	24	0

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



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

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



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

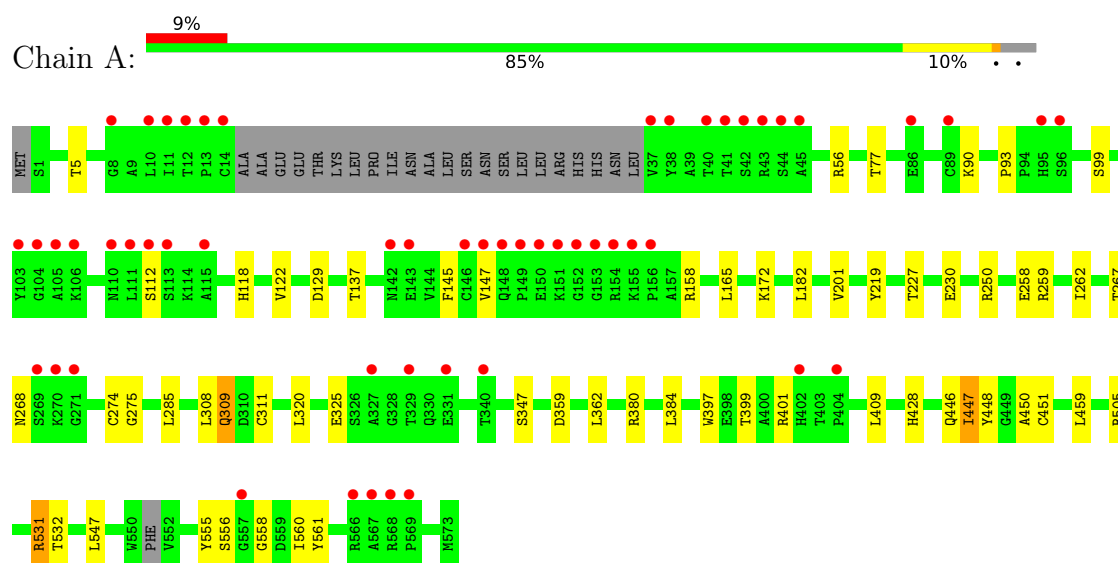
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	39	Total O 39 39	0	0
6	B	17	Total O 17 17	0	0

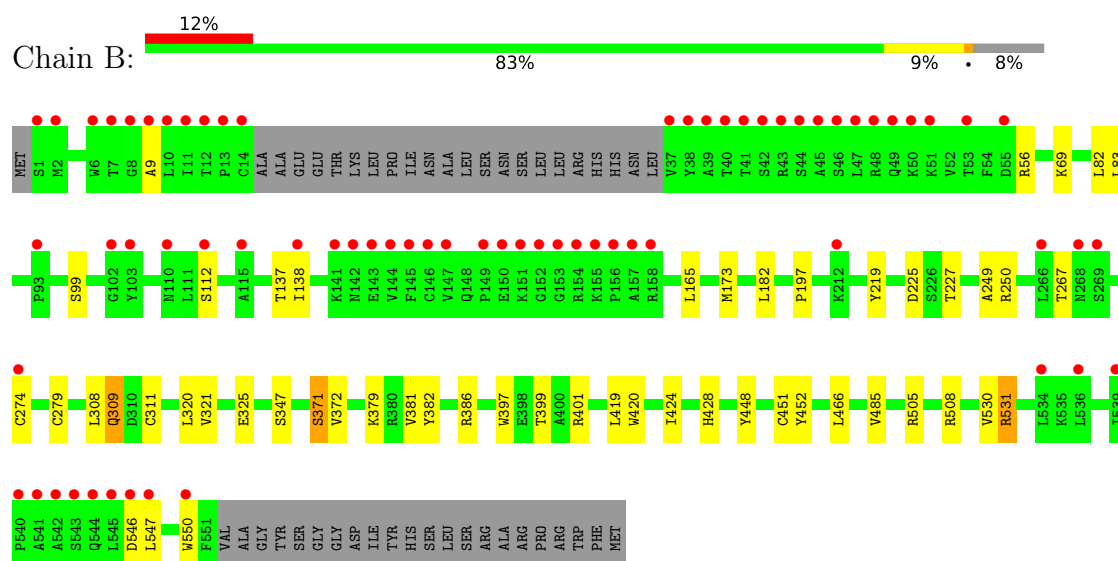
3 Residue-property plots [i](#)

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: 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 90.30Å 234.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.23 – 2.80 49.23 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (49.23-2.80) 99.5 (49.23-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.38 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.200 , 0.243 0.203 , 0.245	Depositor DCC
R_{free} test set	1086 reflections (3.11%)	wwPDB-VP
Wilson B-factor (Å ²)	55.9	Xtriage
Anisotropy	0.665	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 69.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	8759	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.86% 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: SO4, GOL, 8XM, 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	0/4357	0.70	0/5914
1	B	0.52	0/4135	0.68	0/5621
All	All	0.53	0/8492	0.69	0/11535

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	4262	0	4219	24	0
1	B	4049	0	3997	26	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	2	0
4	A	20	0	0	0	0
4	B	20	0	0	0	0
5	A	30	0	40	1	0
5	B	24	0	32	2	0
6	A	39	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	17	0	0	0	0
All	All	8635	124	8362	50	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 (50) 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:386:ARG:HH22	5:B:610:GOL:H12	1.61	0.66
1:B:399:THR:HG21	1:B:428:HIS:NE2	2.11	0.66
1:A:399:THR:HG21	1:A:428:HIS:NE2	2.11	0.65
1:B:219:TYR:HB3	1:B:320:LEU:HD23	1.81	0.63
1:A:219:TYR:HB3	1:A:320:LEU:HD23	1.82	0.62
1:B:197:PRO:HD2	1:B:466:LEU:HB3	1.82	0.61
1:A:172:LYS:HE2	1:A:560:ILE:HD13	1.90	0.54
1:A:77:THR:HA	1:B:69:LYS:HD3	1.91	0.53
1:A:505:ARG:HH12	1:A:531:ARG:HG2	1.76	0.51
1:B:386:ARG:HH12	5:B:610:GOL:H32	1.76	0.50
1:B:9:ALA:HB3	1:B:274:CYS:HA	1.94	0.49
1:A:285:LEU:HA	1:A:558:GLY:HA2	1.95	0.48
1:B:451:CYS:O	1:B:550:TRP:HE3	1.95	0.48
1:A:93:PRO:HA	1:A:561:TYR:HB2	1.95	0.48
1:B:227:THR:HB	1:B:347:SER:O	2.14	0.47
1:B:309:GLN:HG3	1:B:325:GLU:HB3	1.96	0.47
1:B:508:ARG:NH1	1:B:530:VAL:HG11	2.30	0.46
1:A:145:PHE:HE1	5:A:610:GOL:H11	1.79	0.46
1:B:372:VAL:HA	1:B:381:VAL:O	2.15	0.46
1:B:397:TRP:CZ2	1:B:401:ARG:HD2	2.51	0.46
1:B:83:LEU:HB2	1:B:173:MET:HA	1.97	0.46
1:A:309:GLN:HG3	1:A:325:GLU:HB3	1.98	0.45
1:A:227:THR:HB	1:A:347:SER:O	2.17	0.45
1:B:419:LEU:HD23	1:B:485:VAL:HG21	1.99	0.45
1:B:452:TYR:CD2	1:B:550:TRP:HB3	2.52	0.44
1:A:308:LEU:HB2	1:A:311:CYS:SG	2.57	0.44
3:B:602:8XM:O35	3:B:602:8XM:S37	2.76	0.43
1:A:93:PRO:CA	1:A:561:TYR:HB2	2.48	0.43
1:A:555:TYR:CD1	1:A:560:ILE:HG13	2.52	0.43
1:B:99:SER:HB2	1:B:165:LEU:HB3	2.00	0.43
1:A:118[A]:HIS:O	1:A:122:VAL:HG23	2.19	0.43
1:A:137:THR:HA	1:A:267:THR:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:397:TRP:CZ2	1:A:401:ARG:HD2	2.53	0.43
1:B:82:LEU:HD13	1:B:249:ALA:HB2	2.00	0.43
1:A:99:SER:HB2	1:A:165:LEU:HB3	2.01	0.43
1:A:201:VAL:HG23	1:A:384:LEU:HG	2.00	0.42
1:B:505:ARG:HH22	1:B:531:ARG:HG3	1.84	0.42
1:A:359:ASP:HB2	1:A:362:LEU:HD12	2.02	0.42
1:B:225:ASP:O	1:B:279:CYS:HB2	2.19	0.42
1:B:420:TRP:HA	1:B:424:ILE:HD12	2.02	0.42
1:A:230:GLU:HG3	1:A:262:ILE:HB	2.02	0.42
1:B:321:VAL:HG21	3:B:602:8XM:C18	2.50	0.41
1:B:397:TRP:CE2	1:B:401:ARG:HD2	2.54	0.41
1:B:137:THR:HA	1:B:267:THR:O	2.21	0.41
1:B:371:SER:O	1:B:382:TYR:HA	2.20	0.41
1:A:5:THR:O	1:A:275:GLY:HA3	2.21	0.40
1:A:268:ASN:HB3	1:A:274:CYS:SG	2.61	0.40
1:A:129:ASP:HB3	1:A:259:ARG:NH1	2.36	0.40
1:B:308:LEU:HB2	1:B:311:CYS:SG	2.61	0.40
1:A:409:LEU:HD11	1:A:459:LEU:HD21	2.04	0.40

There are no symmetry-related clashes.

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	546/574 (95%)	523 (96%)	18 (3%)	5 (1%)	17	46
1	B	525/574 (92%)	507 (97%)	16 (3%)	2 (0%)	34	66
All	All	1071/1148 (93%)	1030 (96%)	34 (3%)	7 (1%)	22	53

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	447	ILE
1	A	448	TYR
1	A	450	ALA
1	A	147	VAL
1	A	446	GLN
1	B	546	ASP
1	B	448	TYR

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	453/486 (93%)	438 (97%)	15 (3%)	38	72
1	B	427/486 (88%)	417 (98%)	10 (2%)	50	82
All	All	880/972 (90%)	855 (97%)	25 (3%)	43	77

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ARG
1	A	90	LYS
1	A	112	SER
1	A	158	ARG
1	A	182	LEU
1	A	250	ARG
1	A	258	GLU
1	A	309	GLN
1	A	380	ARG
1	A	447	ILE
1	A	451	CYS
1	A	531	ARG
1	A	532	THR
1	A	547	LEU
1	A	556	SER
1	B	56	ARG
1	B	112	SER

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Mol	Chain	Res	Type
1	B	138	ILE
1	B	182	LEU
1	B	250	ARG
1	B	309	GLN
1	B	371	SER
1	B	379	LYS
1	B	531	ARG
1	B	547	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	B	110	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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

21 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
5	GOL	B	608	-	5,5,5	0.31	0	5,5,5	0.63	0
5	GOL	A	610	-	5,5,5	0.10	0	5,5,5	0.25	0
5	GOL	A	607	-	5,5,5	0.44	0	5,5,5	1.18	1 (20%)
5	GOL	B	607	-	5,5,5	0.07	0	5,5,5	0.35	0
3	8XM	B	602	-	36,44,44	0.67	1 (2%)	46,64,64	0.96	1 (2%)
5	GOL	A	609	-	5,5,5	0.15	0	5,5,5	0.28	0
4	SO4	A	603	-	4,4,4	0.17	0	6,6,6	0.13	0
4	SO4	B	603	-	4,4,4	0.29	0	6,6,6	0.18	0
4	SO4	B	605	-	4,4,4	0.30	0	6,6,6	0.23	0
2	23E	B	601	-	46,53,53	0.88	2 (4%)	60,77,77	0.68	0
5	GOL	A	611	-	5,5,5	0.08	0	5,5,5	0.14	0
4	SO4	B	606	-	4,4,4	0.27	0	6,6,6	0.34	0
5	GOL	B	610	-	5,5,5	0.08	0	5,5,5	0.28	0
4	SO4	A	606	-	4,4,4	0.25	0	6,6,6	0.15	0
5	GOL	A	608	-	5,5,5	0.05	0	5,5,5	0.19	0
2	23E	A	601	-	46,53,53	0.83	1 (2%)	60,77,77	0.61	0
3	8XM	A	602	-	36,44,44	0.94	2 (5%)	46,64,64	0.99	1 (2%)
4	SO4	A	605	-	4,4,4	0.39	0	6,6,6	0.24	0
4	SO4	B	604	-	4,4,4	0.31	0	6,6,6	0.15	0
5	GOL	B	609	-	5,5,5	0.07	0	5,5,5	0.27	0
4	SO4	A	604	-	4,4,4	0.11	0	6,6,6	0.19	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	-	-	0/4/4/4	-
5	GOL	B	610	-	-	0/4/4/4	-
5	GOL	B	608	-	-	0/4/4/4	-
5	GOL	A	608	-	-	0/4/4/4	-
5	GOL	A	610	-	-	0/4/4/4	-
2	23E	B	601	-	-	1/24/57/57	0/6/7/7
5	GOL	B	609	-	-	0/4/4/4	-
5	GOL	B	607	-	-	0/4/4/4	-
5	GOL	A	607	-	-	2/4/4/4	-
2	23E	A	601	-	-	2/24/57/57	0/6/7/7
5	GOL	A	611	-	-	2/4/4/4	-
3	8XM	A	602	-	-	6/25/33/33	0/5/5/5

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	8XM	B	602	-	-	3/25/33/33	0/5/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	8XM	C9-C10	-4.09	1.45	1.51
2	B	601	23E	C29-C28	4.07	1.45	1.40
2	A	601	23E	C29-C28	3.82	1.44	1.40
2	B	601	23E	C44-N26	-2.07	1.46	1.48
3	B	602	8XM	C5-C4	-2.04	1.39	1.43
3	A	602	8XM	C5-C4	-2.04	1.39	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	8XM	C14-C8-C9	5.58	135.11	127.13
3	A	602	8XM	C14-C8-C9	5.43	134.89	127.13
5	A	607	GOL	C3-C2-C1	2.28	120.57	111.70

There are no chirality outliers.

All (16) torsion outliers are listed below:

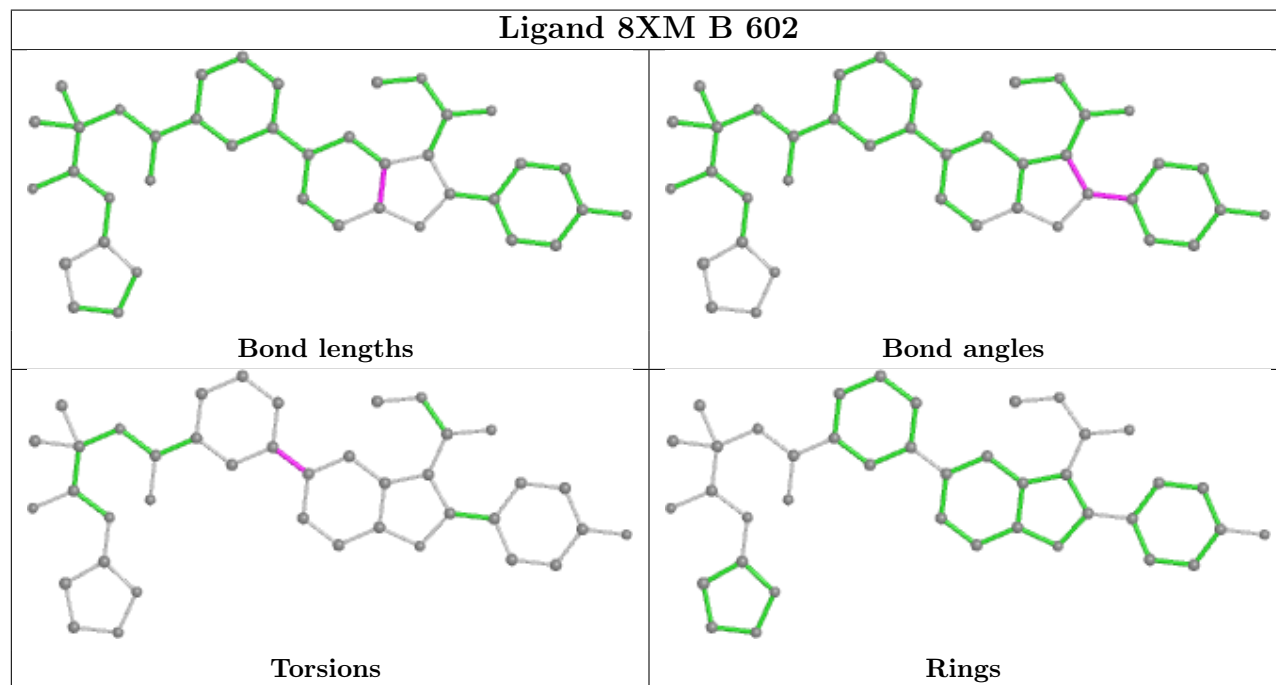
Mol	Chain	Res	Type	Atoms
5	A	607	GOL	C1-C2-C3-O3
5	A	611	GOL	C1-C2-C3-O3
5	A	607	GOL	O2-C2-C3-O3
5	A	611	GOL	O2-C2-C3-O3
3	A	602	8XM	C6-C1-C13-C26
2	A	601	23E	C17-C2-C3-O6
3	A	602	8XM	C6-C1-C13-C22
2	A	601	23E	N1-C2-C3-O6
3	B	602	8XM	C6-C1-C13-C26
3	A	602	8XM	C2-C1-C13-C26
3	A	602	8XM	C2-C1-C13-C22
3	B	602	8XM	C6-C1-C13-C22
3	B	602	8XM	C2-C1-C13-C26
3	A	602	8XM	C15-C14-C8-C9
3	A	602	8XM	C19-C14-C8-C9
2	B	601	23E	C16-C2-N1-C21

There are no ring outliers.

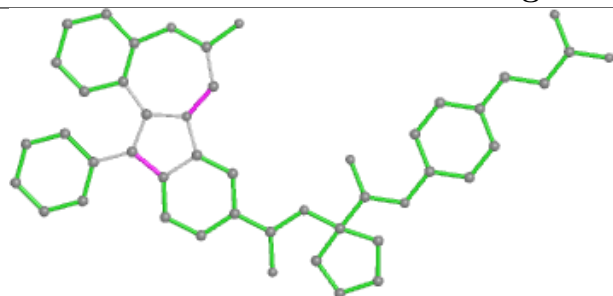
3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	610	GOL	1	0
3	B	602	8XM	2	0
5	B	610	GOL	2	0

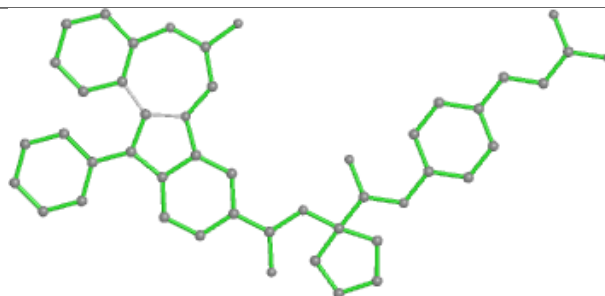
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



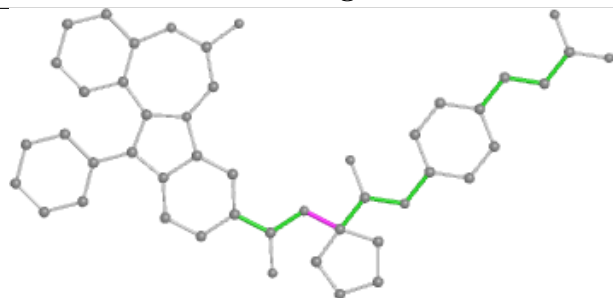
Ligand 23E B 601



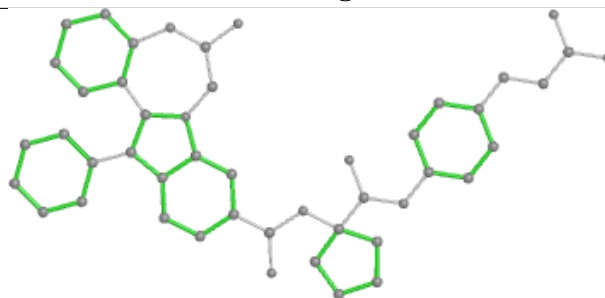
Bond lengths



Bond angles

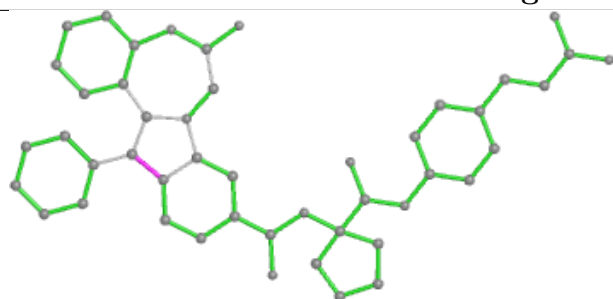


Torsions

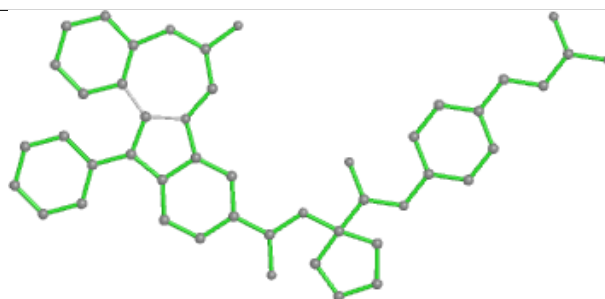


Rings

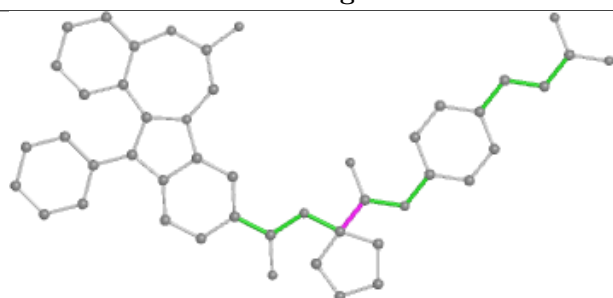
Ligand 23E A 601



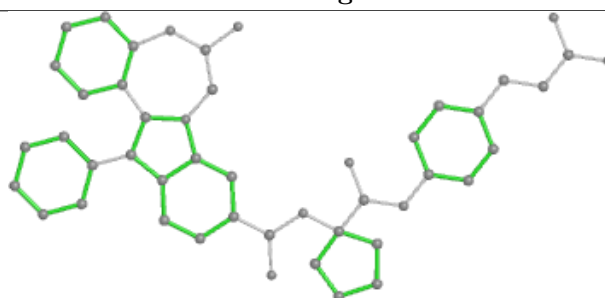
Bond lengths



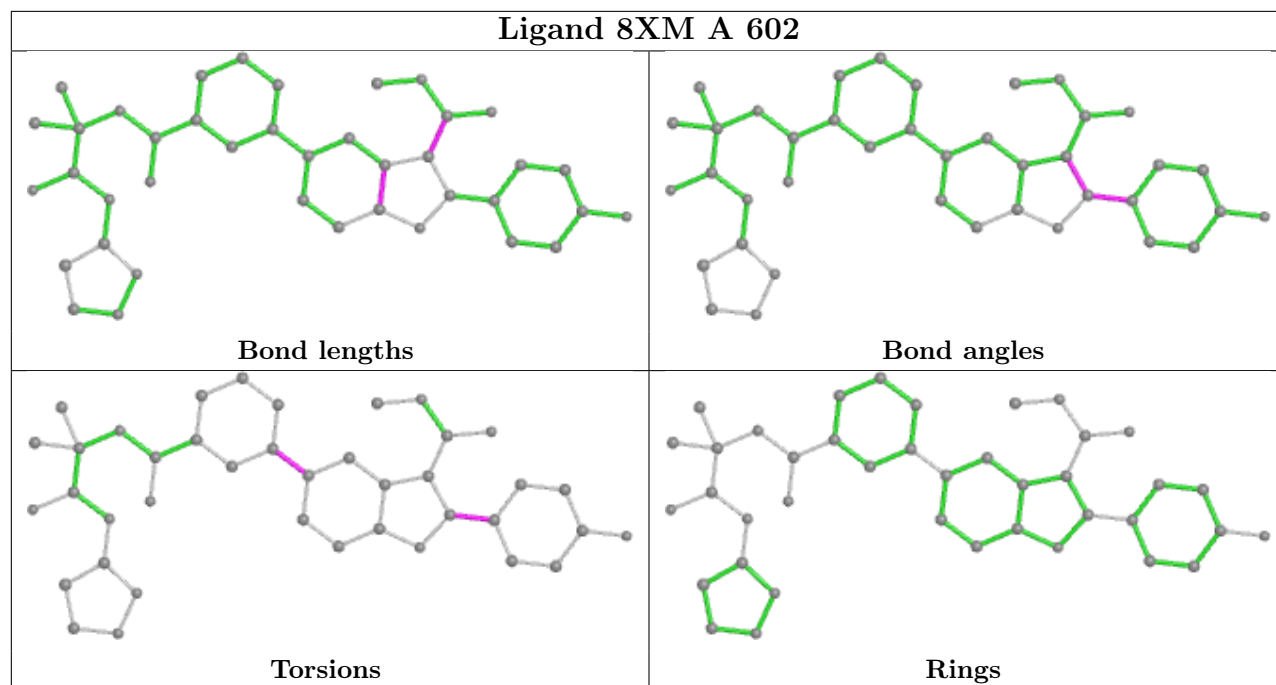
Bond angles



Torsions



Rings



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	550/574 (95%)	0.51	54 (9%) 7 4	30, 57, 113, 160	0
1	B	529/574 (92%)	0.66	69 (13%) 3 2	38, 62, 141, 176	0
All	All	1079/1148 (93%)	0.58	123 (11%) 5 3	30, 60, 126, 176	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	39	ALA	13.0
1	B	41	THR	12.0
1	B	152	GLY	11.7
1	B	14	CYS	10.8
1	B	153	GLY	9.8
1	A	41	THR	9.7
1	A	152	GLY	9.4
1	A	149	PRO	9.1
1	B	44	SER	8.4
1	B	42	SER	8.3
1	B	154	ARG	8.1
1	A	567	ALA	8.0
1	A	40	THR	8.0
1	B	13	PRO	7.8
1	B	156	PRO	7.4
1	A	12	THR	7.2
1	B	149	PRO	7.1
1	A	150	GLU	7.0
1	A	154	ARG	6.9
1	B	40	THR	6.8
1	A	153	GLY	6.7
1	B	43	ARG	6.7
1	B	145	PHE	6.7
1	B	47	LEU	6.4

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Mol	Chain	Res	Type	RSRZ
1	B	10	LEU	6.3
1	B	38	TYR	6.2
1	B	144	VAL	6.2
1	B	142	ASN	6.1
1	B	46	SER	5.9
1	B	12	THR	5.9
1	B	37	VAL	5.9
1	A	42	SER	5.8
1	A	148	GLN	5.6
1	A	151	LYS	5.4
1	B	155	LYS	5.4
1	B	540	PRO	5.4
1	A	155	LYS	5.2
1	A	270	LYS	5.1
1	B	150	GLU	5.1
1	A	13	PRO	5.1
1	A	14	CYS	4.9
1	B	151	LYS	4.7
1	A	10	LEU	4.6
1	B	143	GLU	4.4
1	A	37	VAL	4.3
1	B	9	ALA	4.3
1	A	44	SER	4.3
1	A	156	PRO	4.2
1	B	11	ILE	4.2
1	B	274	CYS	4.1
1	A	143	GLU	4.1
1	B	157	ALA	4.1
1	A	89	CYS	4.0
1	A	569	PRO	4.0
1	B	6	TRP	3.9
1	A	147	VAL	3.9
1	A	142	ASN	3.8
1	B	48	ARG	3.8
1	A	568	ARG	3.8
1	B	8	GLY	3.8
1	B	545	LEU	3.7
1	B	544	GLN	3.6
1	B	158	ARG	3.6
1	A	269	SER	3.6
1	B	268	ASN	3.5
1	B	53	THR	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	38	TYR	3.5
1	B	49	GLN	3.4
1	B	45	ALA	3.3
1	A	146	CYS	3.3
1	B	7	THR	3.2
1	A	115	ALA	3.2
1	A	86	GLU	3.2
1	B	112	SER	3.1
1	B	50	LYS	3.1
1	A	110	ASN	3.1
1	B	110	ASN	3.1
1	A	43	ARG	3.0
1	A	103	TYR	3.0
1	A	111	LEU	3.0
1	A	271	GLY	2.9
1	B	547	LEU	2.9
1	B	51	LYS	2.9
1	B	269	SER	2.8
1	A	113	SER	2.8
1	B	147	VAL	2.7
1	A	45	ALA	2.7
1	B	115	ALA	2.7
1	B	212	LYS	2.7
1	B	539	ILE	2.7
1	A	557	GLY	2.6
1	A	329	THR	2.6
1	B	542	ALA	2.6
1	A	340	THR	2.6
1	B	534	LEU	2.5
1	B	2	MET	2.5
1	B	543	SER	2.5
1	B	55	ASP	2.5
1	A	566	ARG	2.5
1	A	8	GLY	2.5
1	A	331	GLU	2.5
1	A	95	HIS	2.4
1	A	404	PRO	2.4
1	A	106	LYS	2.4
1	A	327	ALA	2.4
1	A	11	ILE	2.3
1	B	102	GLY	2.3
1	B	541	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	402	HIS	2.3
1	B	146	CYS	2.3
1	A	96	SER	2.3
1	B	550	TRP	2.2
1	A	112	SER	2.2
1	B	1	SER	2.2
1	B	93	PRO	2.2
1	A	104	GLY	2.1
1	A	105	ALA	2.1
1	B	103	TYR	2.1
1	B	546	ASP	2.1
1	B	266	LEU	2.1
1	B	138	ILE	2.0
1	B	141	LYS	2.0
1	B	536	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no 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.

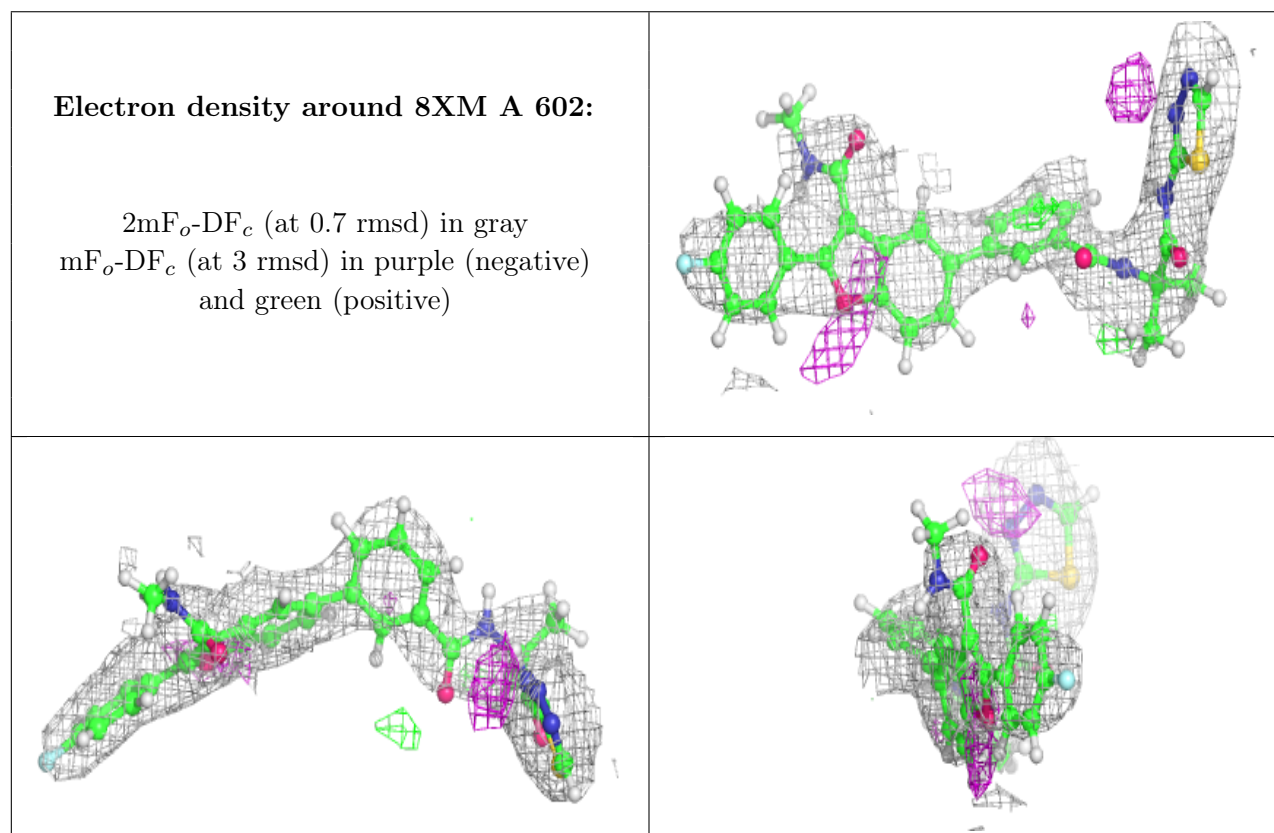
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	GOL	B	608	6/6	0.80	0.28	62,71,75,78	0
4	SO4	B	605	5/5	0.82	0.23	130,131,132,132	0
5	GOL	A	610	6/6	0.83	0.41	76,81,82,83	0
4	SO4	A	604	5/5	0.83	0.24	134,134,136,137	0
5	GOL	B	609	6/6	0.83	0.31	72,73,75,75	0
5	GOL	A	609	6/6	0.84	0.29	73,80,83,83	0
5	GOL	A	611	6/6	0.84	0.50	78,81,82,85	0
5	GOL	A	607	6/6	0.87	0.23	44,47,47,50	0

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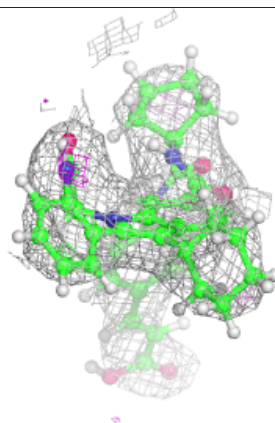
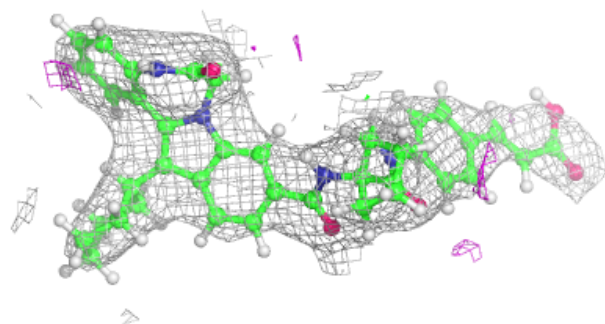
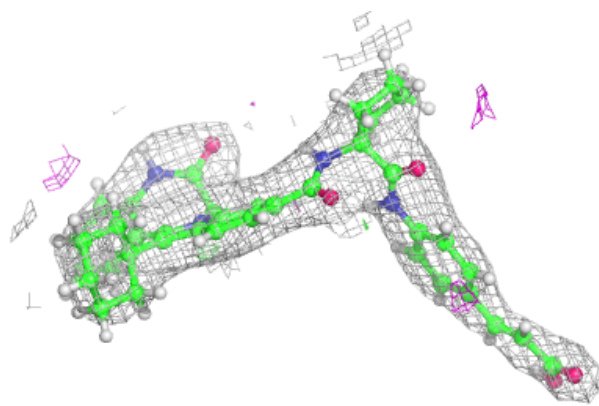
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	GOL	B	610	6/6	0.87	0.24	74,79,83,85	0
5	GOL	B	607	6/6	0.88	0.23	83,84,85,86	0
4	SO4	B	603	5/5	0.89	0.15	117,118,121,121	0
4	SO4	B	606	5/5	0.89	0.24	55,56,58,59	5
4	SO4	A	603	5/5	0.91	0.11	142,142,143,143	0
5	GOL	A	608	6/6	0.92	0.29	87,88,88,91	0
3	8XM	A	602	40/40	0.93	0.22	58,63,69,77	24
2	23E	B	601	47/47	0.95	0.18	39,46,69,79	38
4	SO4	A	606	5/5	0.95	0.21	107,109,109,113	0
4	SO4	B	604	5/5	0.96	0.15	84,88,89,91	0
2	23E	A	601	47/47	0.96	0.17	34,41,61,71	38
3	8XM	B	602	40/40	0.96	0.15	35,53,62,65	24
4	SO4	A	605	5/5	0.98	0.10	61,62,64,64	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.



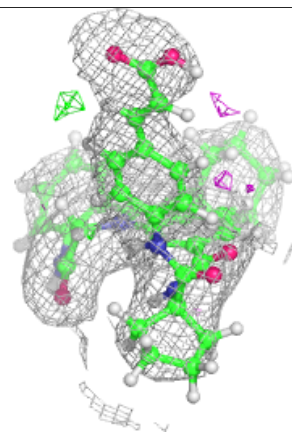
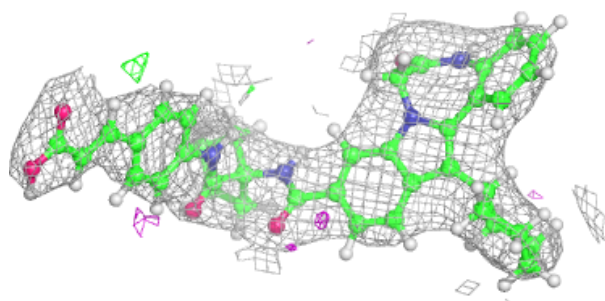
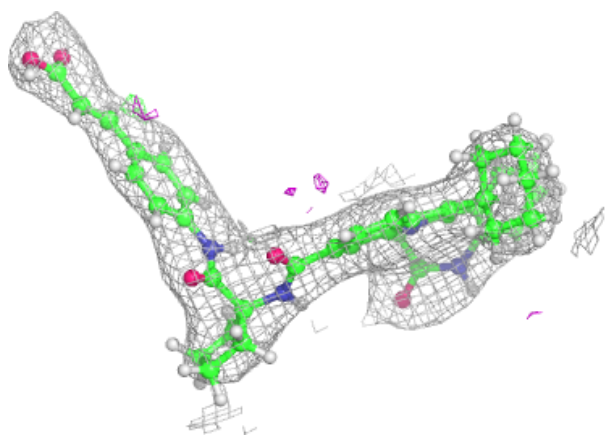
Electron density around 23E B 601:

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

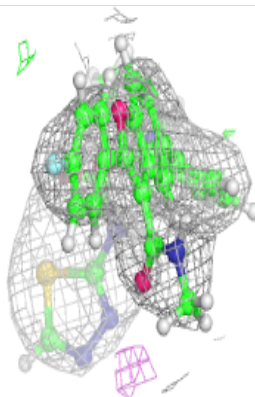
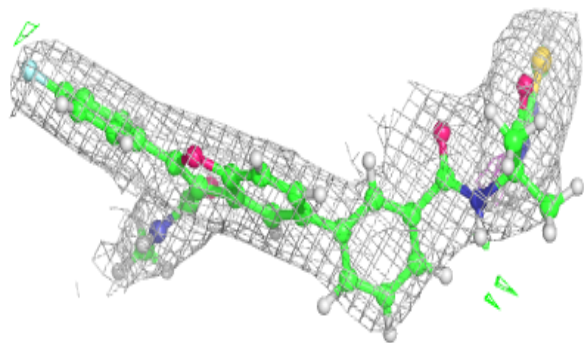
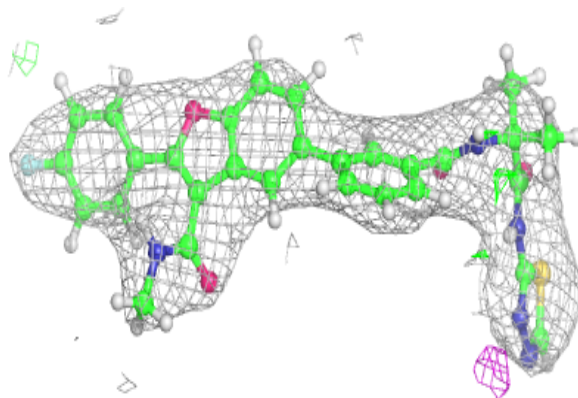


Electron density around 23E A 601:

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

**Electron density around 8XM 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.