



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 06:43 PM EDT

PDB ID : 5PZK
Title : CRYSTAL STRUCTURE OF THE HEPATITIS C VIRUS NS5B RNA-DEPENDENT RNA POLYMERASE IN COMPLEX WITH 2-(4-FLUOROPHENYL)-N-METHYL-6-[(METHYLSULFONYL)AMINO]-5-(PROPAN-2-YLOXY)-1-BENZOFURAN-3-CARBOXAMIDE
Authors : Sheriff, S.
Deposited on : 2017-02-27
Resolution : 2.20 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](#) ①) 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)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

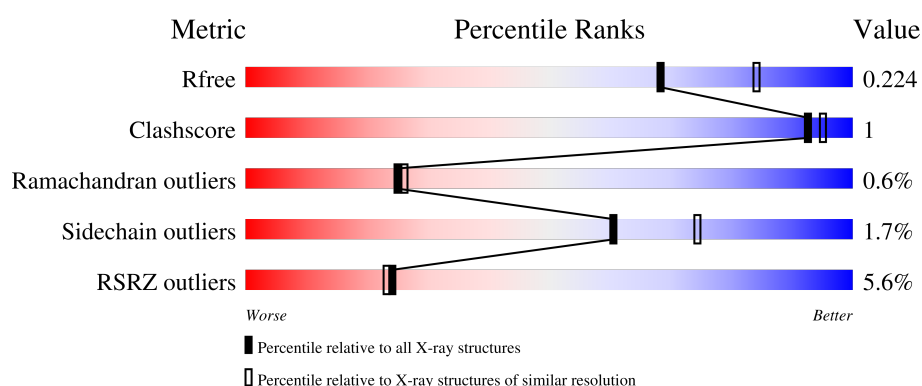
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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>4%</div> <div>90%</div> <div>6%</div> </div>
1	B	574	<div> <div>6%</div> <div>89%</div> <div>5%</div> <div>6%</div> </div>

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 9211 atoms, of which 118 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.

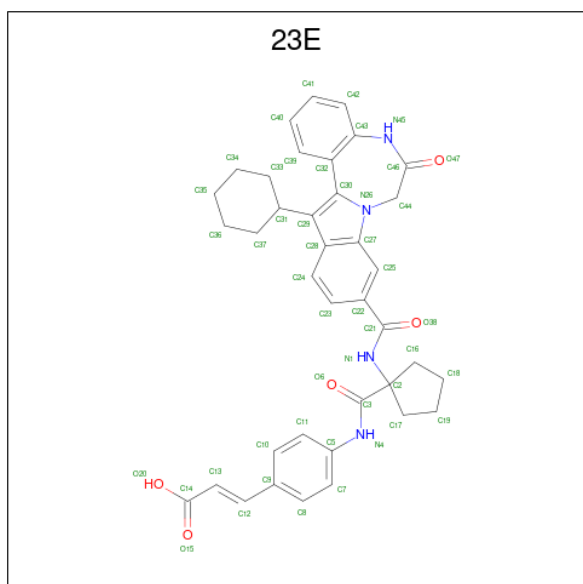
- Molecule 1 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	541	Total	C	N	O	S	0	1	0
			4176	2633	736	775	32			
1	B	542	Total	C	N	O	S	0	3	0
			4188	2637	741	777	33			

There are 2 discrepancies between the modelled and reference sequences:

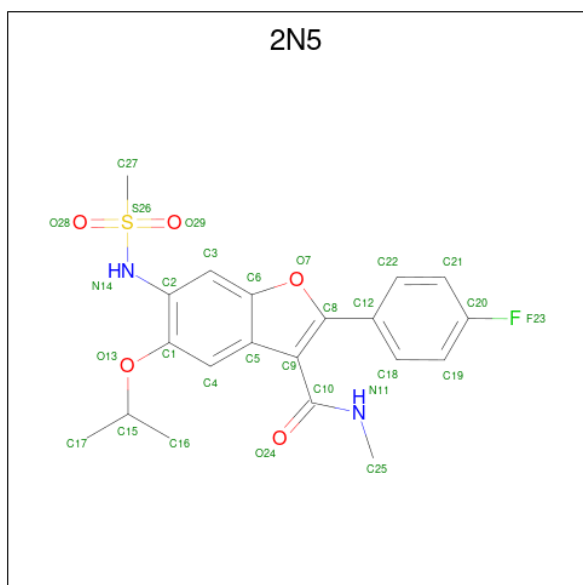
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP Q9WMX2
B	0	MET	-	expression tag	UNP Q9WMX2

- 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
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-6-[(methylsulfonyl)amino]-5-(propan-2-yloxy)-1-benzofuran-3-carboxamide (three-letter code: 2N5) (formula: C₂₀H₂₁FN₂O₅S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	F	H	N	O	S	21	0
			50	20	1	21	2	5	1		
3	B	1	Total	C	F	H	N	O	S	21	0
			50	20	1	21	2	5	1		

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



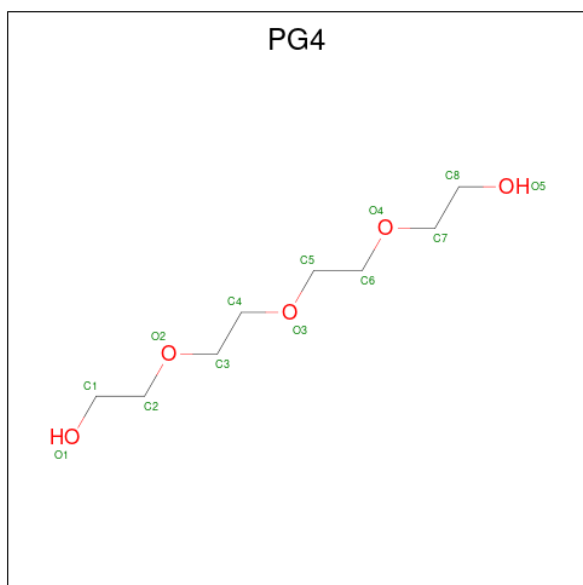
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	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	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 TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	8	5		

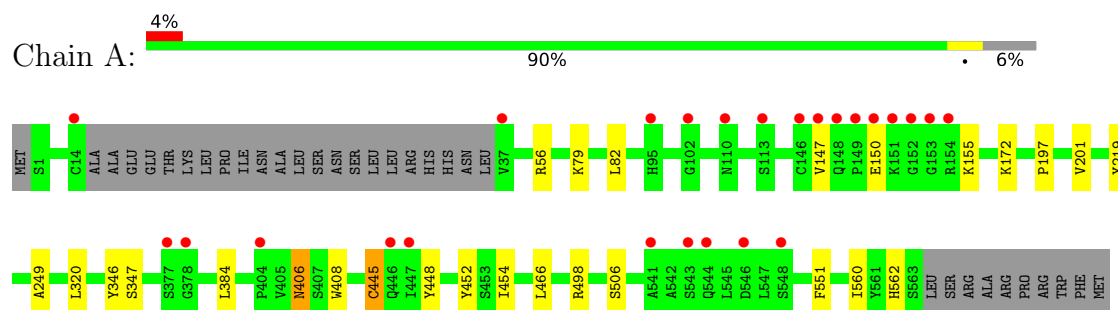
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	251	Total	O	0	0
			251	251		
7	B	229	Total	O	0	0
			229	229		

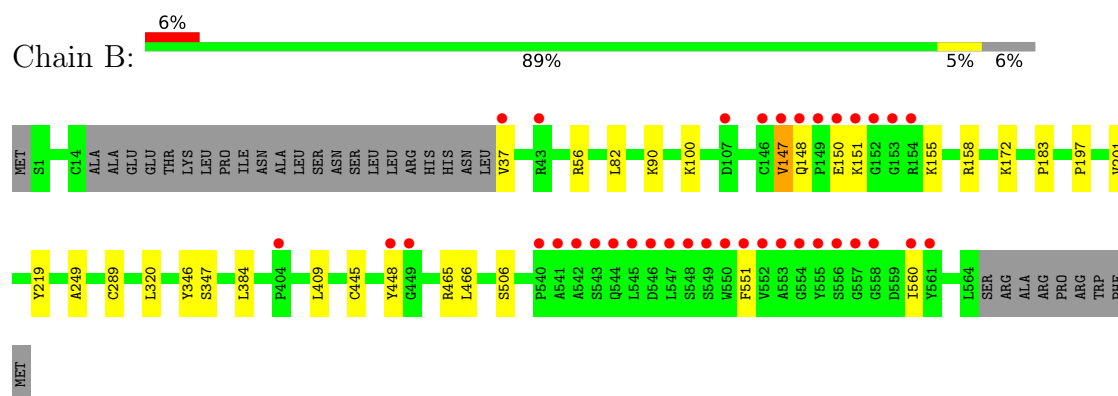
3 Residue-property plots [i](#)

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	75.40Å 90.00Å 231.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	32.21 – 2.20 45.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (32.21-2.20) 99.8 (45.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.71 (at 2.20Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.201 , 0.224 0.198 , 0.224	Depositor DCC
R_{free} test set	1200 reflections (1.49%)	wwPDB-VP
Wilson B-factor (Å ²)	23.0	Xtriage
Anisotropy	0.505	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 48.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	9211	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.51% 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: PG4, GOL, 23E, 2N5, SO4

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	0.50	0/4271	0.62	0/5797
1	B	0.49	0/4293	0.63	0/5826
All	All	0.50	0/8564	0.62	0/11623

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	4176	0	4164	13	0
1	B	4188	0	4162	12	0
2	A	47	38	37	0	0
2	B	47	38	37	0	0
3	A	29	21	21	0	0
3	B	29	21	21	0	0
4	A	25	0	0	0	0
4	B	35	0	0	0	0
5	A	18	0	24	1	0
5	B	6	0	8	0	0
6	A	13	0	18	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	251	0	0	0	0
7	B	229	0	0	0	0
All	All	9093	118	8492	25	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 1.

All (25) 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:172:LYS:HE3	1:B:560:ILE:HD13	1.81	0.63
1:B:197:PRO:O	1:B:201:VAL:HG23	1.99	0.61
1:A:197:PRO:O	1:A:201:VAL:HG23	2.00	0.61
1:B:466:LEU:HD22	1:B:551:PHE:HE2	1.66	0.58
1:A:219:TYR:HB3	1:A:320:LEU:HD23	1.85	0.58
1:A:172:LYS:HE3	1:A:560:ILE:HD13	1.86	0.58
1:B:219:TYR:HB3	1:B:320:LEU:HD23	1.86	0.57
1:B:409:LEU:HD23	1:B:445[B]:CYS:SG	2.44	0.56
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.88	0.56
1:B:82:LEU:HD13	1:B:249:ALA:HB2	1.88	0.54
1:A:197:PRO:HD2	1:A:466:LEU:HB3	1.90	0.52
1:A:466:LEU:HD22	1:A:551:PHE:HE2	1.76	0.50
1:B:197:PRO:HD2	1:B:466:LEU:HB3	1.93	0.50
1:B:466:LEU:HD22	1:B:551:PHE:CE2	2.46	0.49
1:B:346:TYR:O	1:B:347:SER:HB3	2.13	0.48
1:A:346:TYR:O	1:A:347:SER:HB3	2.14	0.48
1:B:37:VAL:CB	1:B:147:VAL:H	2.27	0.47
1:A:452:TYR:HA	1:A:562:HIS:O	2.14	0.47
1:A:445:CYS:SG	1:A:454:ILE:HD12	2.57	0.44
1:A:406:ASN:HB2	1:A:408:TRP:NE1	2.33	0.44
1:A:406:ASN:HB2	1:A:408:TRP:CD1	2.54	0.43
1:A:201:VAL:HG22	1:A:384:LEU:HG	2.02	0.41
1:B:183:PRO:HG3	1:B:289:CYS:SG	2.60	0.41
1:B:201:VAL:HG22	1:B:384:LEU:HG	2.03	0.40
1:A:79:LYS:NZ	5:A:610:GOL:H11	2.36	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	538/574 (94%)	526 (98%)	9 (2%)	3 (1%)	25	26
1	B	541/574 (94%)	525 (97%)	13 (2%)	3 (1%)	25	26
All	All	1079/1148 (94%)	1051 (97%)	22 (2%)	6 (1%)	25	26

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	GLU
1	A	448	TYR
1	B	150	GLU
1	B	448	TYR
1	A	147	VAL
1	B	147	VAL

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	449/486 (92%)	443 (99%)	6 (1%)	69	81
1	B	449/486 (92%)	440 (98%)	9 (2%)	55	69
All	All	898/972 (92%)	883 (98%)	15 (2%)	60	74

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

Mol	Chain	Res	Type
1	A	56	ARG
1	A	155	LYS
1	A	406	ASN
1	A	445	CYS
1	A	498	ARG
1	A	506	SER
1	B	56	ARG
1	B	90	LYS
1	B	100	LYS
1	B	148	GLN
1	B	151	LYS
1	B	155	LYS
1	B	158	ARG
1	B	465	ARG
1	B	506	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	273	ASN
1	A	436	GLN
1	A	446	GLN
1	B	309	GLN
1	B	406	ASN
1	B	436	GLN

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

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	$\# Z > 2$
4	SO4	B	607	-	4,4,4	0.14	0	6,6,6	0.17	0
5	GOL	A	610	-	5,5,5	0.16	0	5,5,5	0.16	0
4	SO4	B	605	-	4,4,4	0.20	0	6,6,6	0.33	0
3	2N5	A	602	-	27,31,31	0.74	1 (3%)	37,46,46	1.46	5 (13%)
4	SO4	B	604	-	4,4,4	0.20	0	6,6,6	0.21	0
4	SO4	B	606	-	4,4,4	0.23	0	6,6,6	0.11	0
4	SO4	A	603	-	4,4,4	0.20	0	6,6,6	0.18	0
4	SO4	A	606	-	4,4,4	0.24	0	6,6,6	0.19	0
4	SO4	B	603	-	4,4,4	0.23	0	6,6,6	0.19	0
5	GOL	B	610	-	5,5,5	0.23	0	5,5,5	0.46	0
2	23E	B	601	-	46,53,53	0.86	1 (2%)	60,77,77	0.65	0
6	PG4	A	611	-	12,12,12	0.15	0	11,11,11	0.21	0
4	SO4	A	605	-	4,4,4	0.31	0	6,6,6	0.19	0
5	GOL	A	609	-	5,5,5	0.07	0	5,5,5	0.12	0
2	23E	A	601	-	46,53,53	0.83	1 (2%)	60,77,77	0.62	0
4	SO4	A	604	-	4,4,4	0.22	0	6,6,6	0.38	0
3	2N5	B	602	-	27,31,31	0.72	1 (3%)	37,46,46	1.43	5 (13%)
4	SO4	B	609	-	4,4,4	0.16	0	6,6,6	0.15	0
4	SO4	B	608	-	4,4,4	0.13	0	6,6,6	0.27	0
5	GOL	A	608	-	5,5,5	0.23	0	5,5,5	0.20	0
4	SO4	A	607	-	4,4,4	0.20	0	6,6,6	0.09	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
2	23E	B	601	-	-	0/24/57/57	0/6/7/7
5	GOL	A	610	-	-	0/4/4/4	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PG4	A	611	-	-	2/10/10/10	-
5	GOL	A	609	-	-	0/4/4/4	-
2	23E	A	601	-	-	0/24/57/57	0/6/7/7
3	2N5	A	602	-	-	8/13/19/19	0/3/3/3
5	GOL	B	610	-	-	2/4/4/4	-
3	2N5	B	602	-	-	8/13/19/19	0/3/3/3
5	GOL	A	608	-	-	0/4/4/4	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	23E	C29-C28	4.24	1.45	1.40
2	A	601	23E	C29-C28	3.97	1.44	1.40
3	A	602	2N5	C5-C6	-2.04	1.39	1.43
3	B	602	2N5	C5-C6	-2.00	1.39	1.43

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	602	2N5	C12-C8-C9	5.40	134.85	127.13
3	A	602	2N5	C12-C8-C9	5.37	134.81	127.13
3	B	602	2N5	O13-C15-C16	3.54	120.33	107.93
3	A	602	2N5	O13-C15-C16	3.52	120.27	107.93
3	A	602	2N5	C5-C9-C10	-3.44	120.39	125.83
3	B	602	2N5	C5-C9-C10	-3.18	120.81	125.83
3	A	602	2N5	C2-C3-C6	-2.18	117.38	119.46
3	B	602	2N5	C1-O13-C15	2.16	123.69	119.53
3	A	602	2N5	C1-O13-C15	2.11	123.59	119.53
3	B	602	2N5	C2-C3-C6	-2.09	117.47	119.46

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	602	2N5	C16-C15-O13-C1
3	B	602	2N5	C16-C15-O13-C1
3	A	602	2N5	C17-C15-O13-C1
3	B	602	2N5	C17-C15-O13-C1
5	B	610	GOL	O1-C1-C2-C3
3	B	602	2N5	C2-N14-S26-O28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	610	GOL	O1-C1-C2-O2
3	A	602	2N5	C2-N14-S26-O28
3	A	602	2N5	C2-N14-S26-O29
3	B	602	2N5	C2-N14-S26-O29
3	A	602	2N5	C18-C12-C8-C9
3	A	602	2N5	C22-C12-C8-C9
3	B	602	2N5	C18-C12-C8-C9
3	B	602	2N5	C22-C12-C8-C9
6	A	611	PG4	O2-C3-C4-O3
6	A	611	PG4	C8-C7-O4-C6
3	A	602	2N5	C2-N14-S26-C27
3	B	602	2N5	C2-N14-S26-C27
3	A	602	2N5	C4-C1-O13-C15
3	B	602	2N5	C4-C1-O13-C15

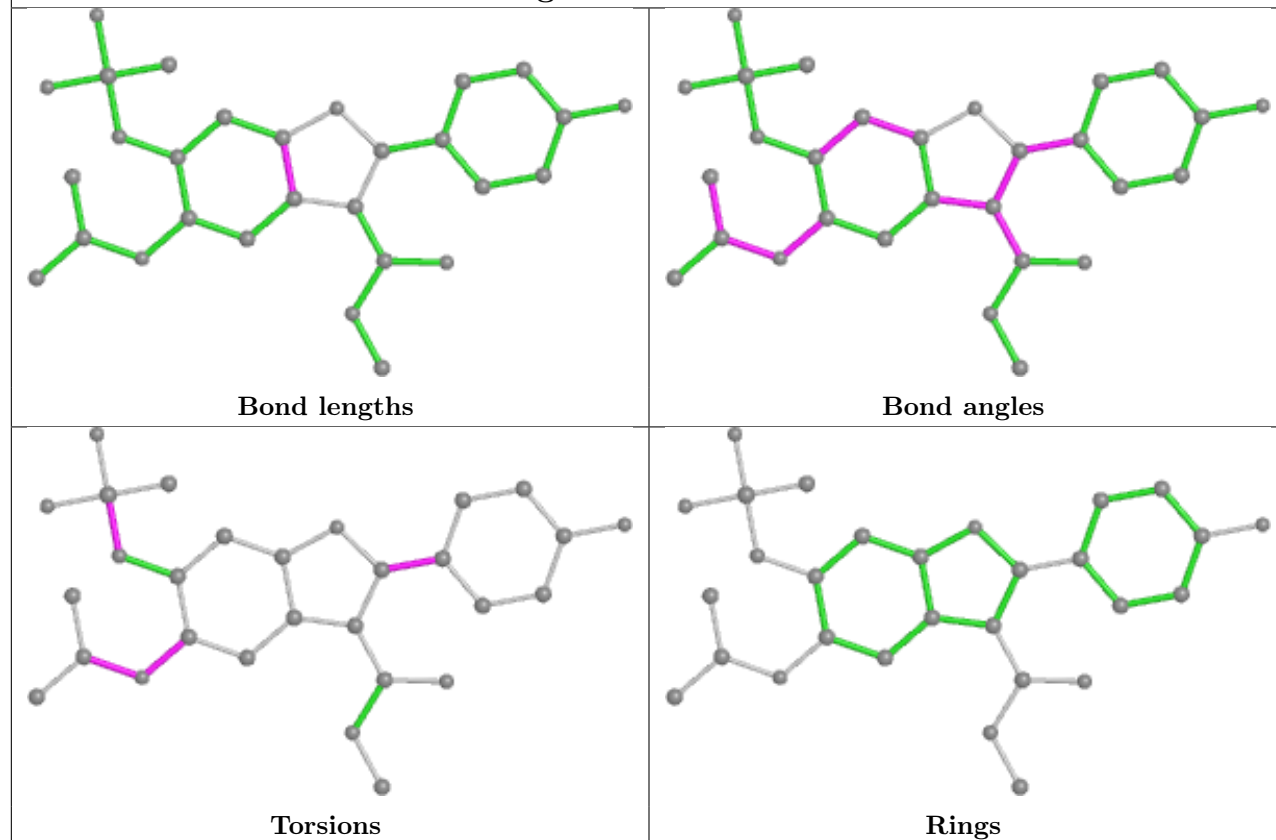
There are no ring outliers.

1 monomer is involved in 1 short contact:

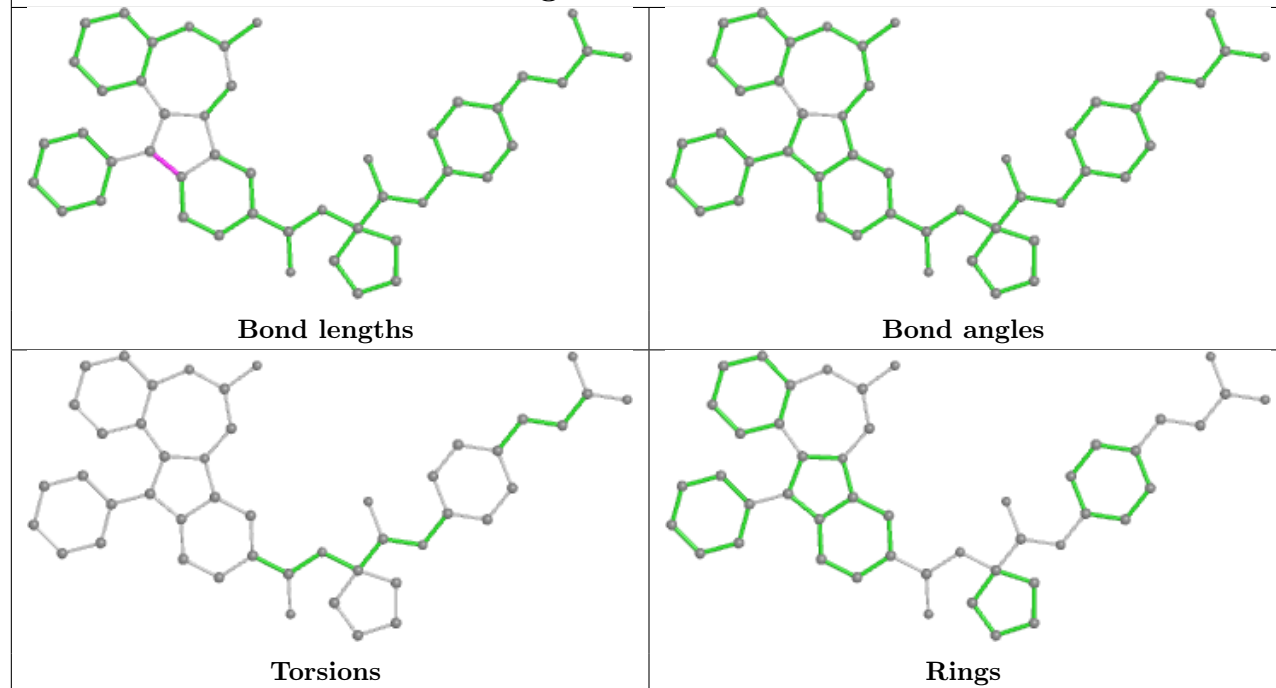
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	610	GOL	1	0

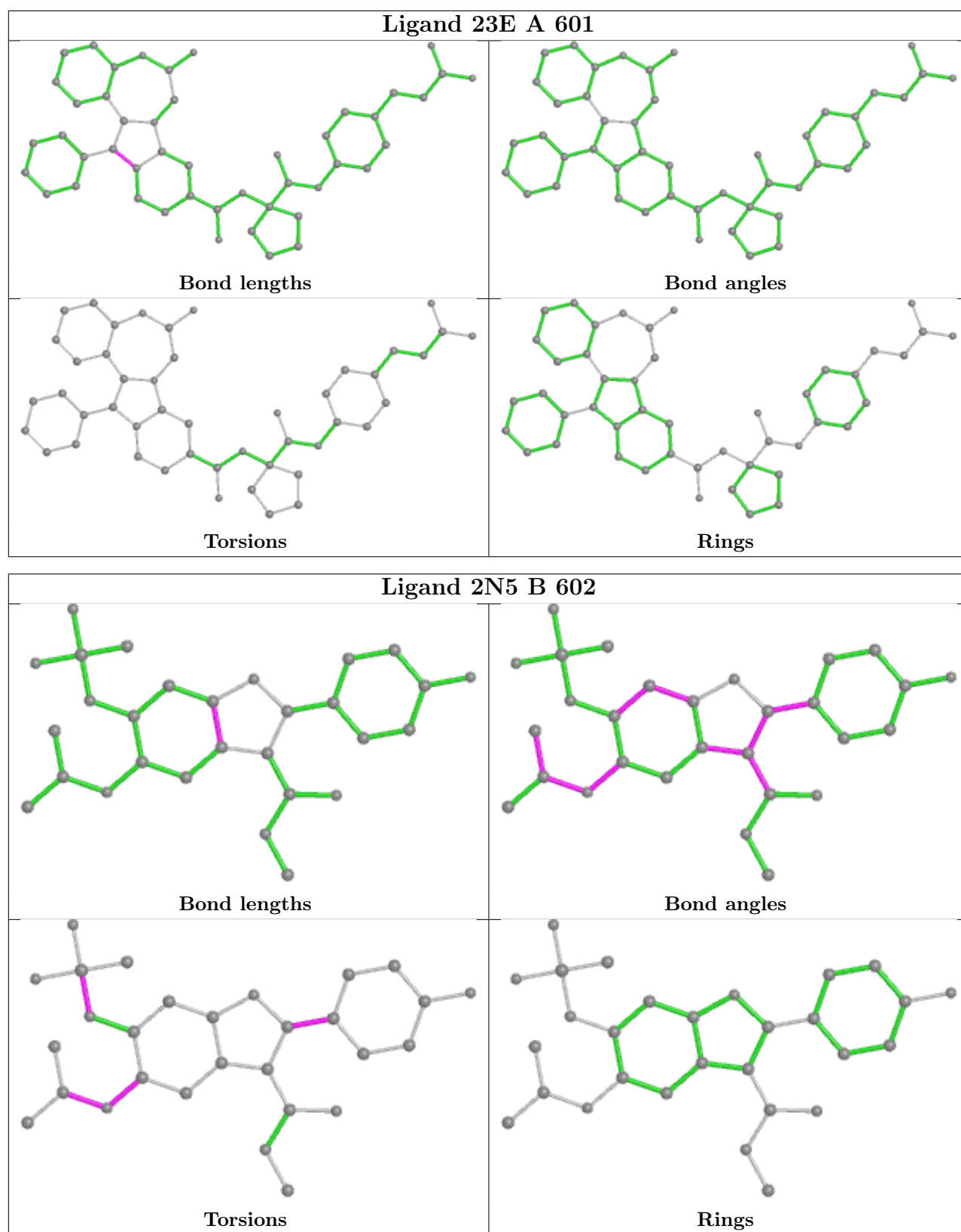
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand 2N5 A 602



Ligand 23E B 601





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	541/574 (94%)	-0.03	25 (4%) 32 31	13, 24, 52, 100	0
1	B	542/574 (94%)	0.19	36 (6%) 18 17	13, 25, 74, 115	0
All	All	1083/1148 (94%)	0.08	61 (5%) 24 23	13, 24, 64, 115	0

All (61) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	149	PRO	13.8
1	B	550	TRP	11.8
1	A	148	GLN	10.7
1	A	150	GLU	10.7
1	B	150	GLU	10.0
1	B	149	PRO	9.9
1	B	147	VAL	8.2
1	B	543	SER	8.1
1	B	552	VAL	7.8
1	B	544	GLN	7.5
1	A	152	GLY	7.3
1	A	151	LYS	7.0
1	B	541	ALA	6.8
1	B	546	ASP	6.7
1	B	548	SER	6.7
1	B	153	GLY	6.7
1	B	545	LEU	6.7
1	B	404	PRO	6.4
1	B	555	TYR	6.1
1	B	152	GLY	5.8
1	B	542	ALA	5.6
1	B	148	GLN	5.5
1	B	557	GLY	5.5
1	B	540	PRO	5.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	151	LYS	5.2
1	B	549	SER	5.2
1	A	147	VAL	5.2
1	B	556	SER	4.6
1	A	37	VAL	4.5
1	B	554	GLY	4.3
1	A	153	GLY	4.2
1	B	551	PHE	4.2
1	B	37	VAL	4.0
1	A	541	ALA	3.8
1	B	154	ARG	3.6
1	B	558	GLY	3.6
1	A	546	ASP	3.6
1	B	560	ILE	3.2
1	B	547	LEU	3.1
1	A	548	SER	3.0
1	A	404	PRO	2.9
1	A	544	GLN	2.9
1	A	113	SER	2.8
1	A	543	SER	2.7
1	A	447	ILE	2.7
1	B	553	ALA	2.6
1	A	154	ARG	2.4
1	A	110	ASN	2.4
1	B	146	CYS	2.4
1	B	448	TYR	2.3
1	A	14	CYS	2.3
1	A	378	GLY	2.2
1	A	95	HIS	2.1
1	B	561	TYR	2.1
1	B	449	GLY	2.1
1	A	446	GLN	2.1
1	A	102	GLY	2.0
1	A	377	SER	2.0
1	B	107	ASP	2.0
1	A	146	CYS	2.0
1	B	43	ARG	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 monosaccharides in this entry.

6.4 Ligands [i](#)

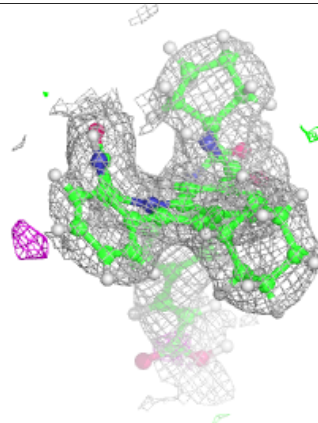
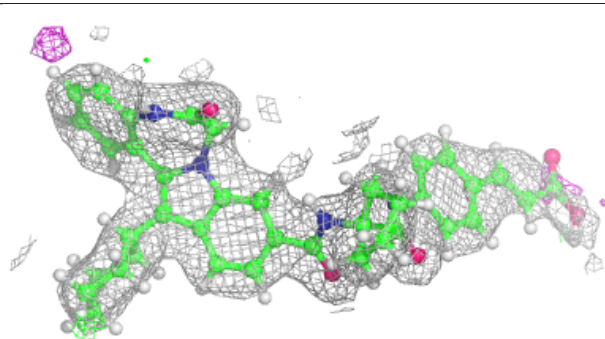
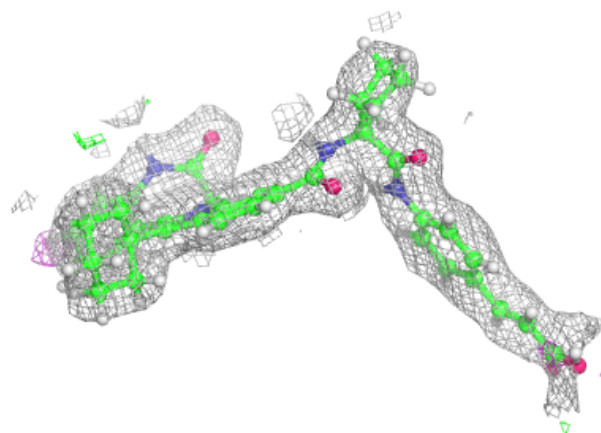
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	SO4	A	607	5/5	0.85	0.28	83,84,86,87	0
4	SO4	B	609	5/5	0.87	0.21	96,97,97,98	0
5	GOL	B	610	6/6	0.89	0.15	31,37,38,38	0
6	PG4	A	611	13/13	0.89	0.16	43,46,62,64	0
4	SO4	B	608	5/5	0.90	0.14	80,81,81,82	0
5	GOL	A	610	6/6	0.90	0.22	35,46,49,49	0
4	SO4	B	606	5/5	0.91	0.16	71,73,74,75	0
4	SO4	B	607	5/5	0.92	0.30	83,83,85,86	0
2	23E	A	601	47/47	0.92	0.12	13,19,48,61	38
5	GOL	A	609	6/6	0.93	0.18	28,38,41,42	0
5	GOL	A	608	6/6	0.93	0.12	24,29,34,37	0
4	SO4	A	606	5/5	0.94	0.15	68,68,69,71	0
2	23E	B	601	47/47	0.94	0.12	15,21,38,47	38
4	SO4	B	604	5/5	0.94	0.32	67,70,71,72	0
3	2N5	A	602	29/29	0.94	0.14	15,29,43,47	21
4	SO4	B	605	5/5	0.95	0.10	50,53,54,57	0
4	SO4	B	603	5/5	0.97	0.11	43,44,47,49	0
3	2N5	B	602	29/29	0.97	0.12	13,21,26,30	21
4	SO4	A	605	5/5	0.97	0.12	48,51,55,55	0
4	SO4	A	604	5/5	0.98	0.10	27,28,32,33	0
4	SO4	A	603	5/5	0.99	0.08	29,29,33,37	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.

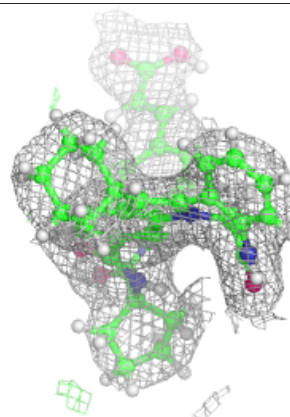
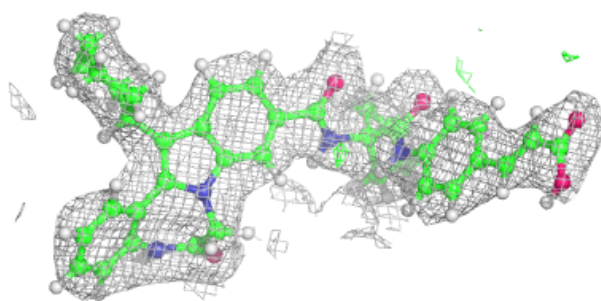
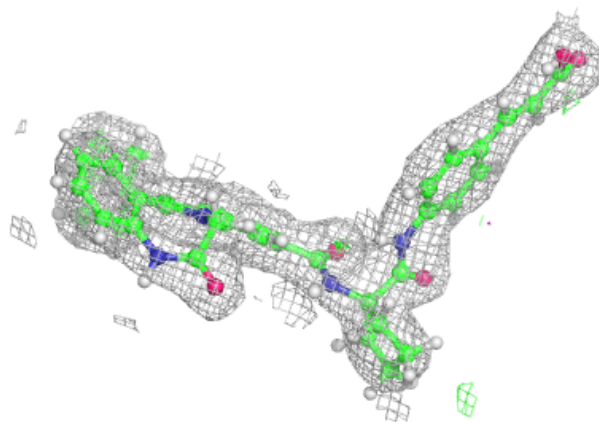
Electron density around 23E A 601:

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



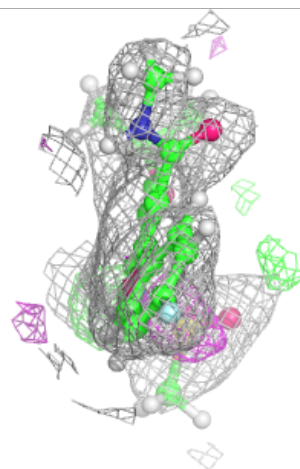
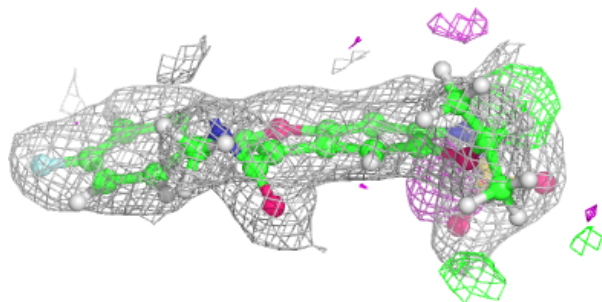
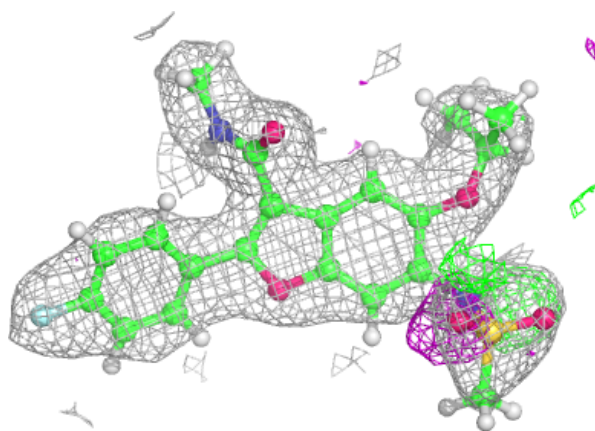
Electron density around 23E B 601:

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



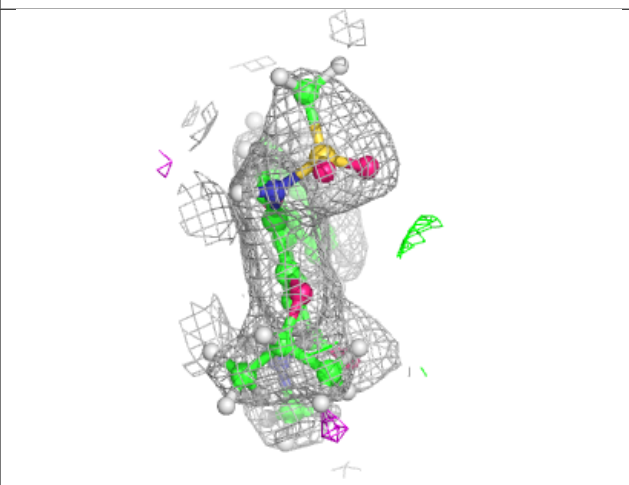
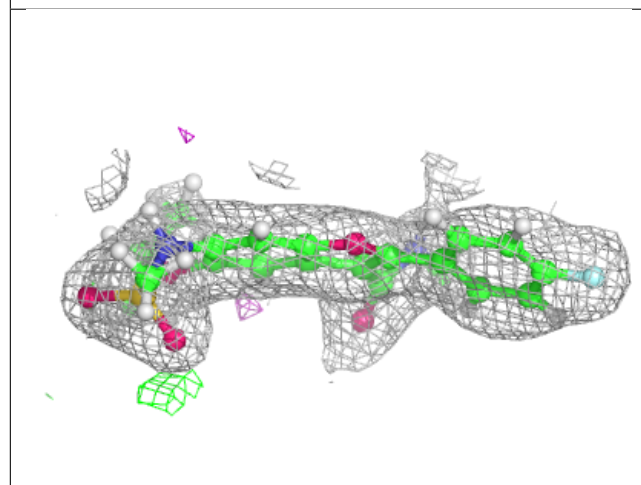
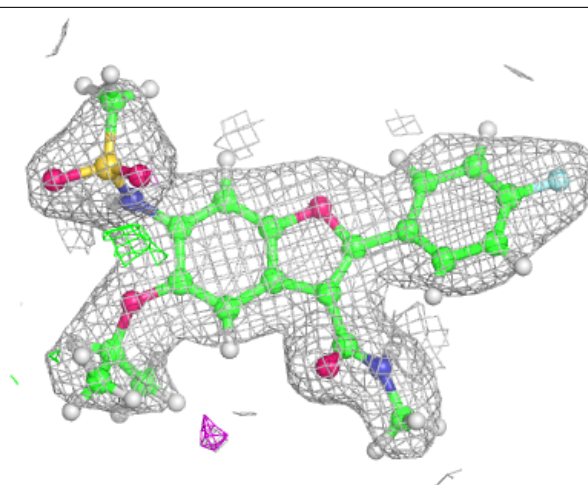
Electron density around 2N5 A 602:

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



Electron density around 2N5 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.