Full wwPDB X-ray Structure Validation Report ⓘ

Mar 7, 2026 – 03:39 AM UTC

PDB ID	:	5PZK / pdb_00005pzk
Title	:	CRYSTAL STRUCTURE OF THE HEPATITIS C VIRUS NS5B RNA-DEPENDENT RNA POLYMERASE IN COMPLEX WITH 2-(4-FLUOR OPHENYL)-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:

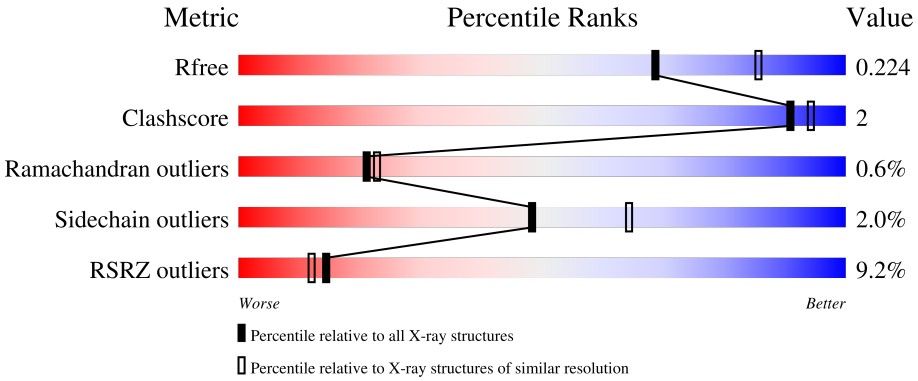
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 <=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	8% 87% 7% 6%
1	B	574	10% 87% 7% 6%

2 Entry composition

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.

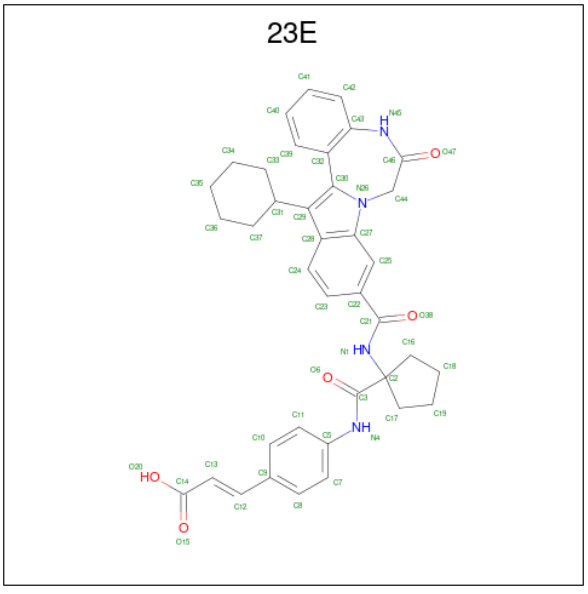
- Molecule 1 is a protein called RNA-directed RNA polymerase.

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:

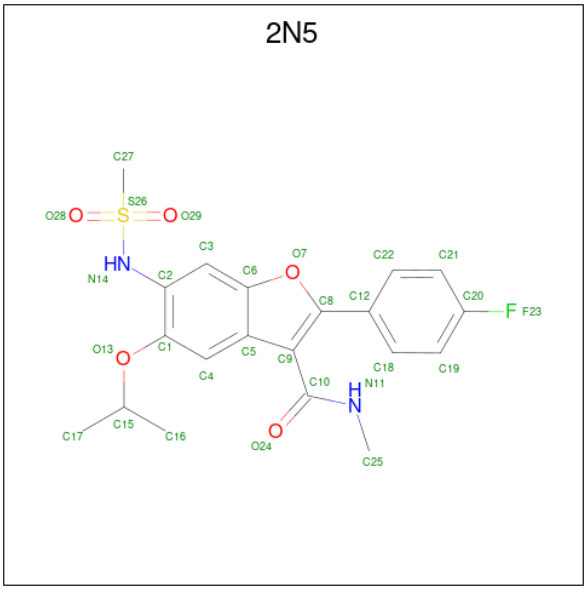
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP Q9WMX2
B	0	MET	-	expression tag	UNP Q9WMX2

- 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 (CCD ID: 23E) (formula: $C_{38}H_{38}N_4O_5$).



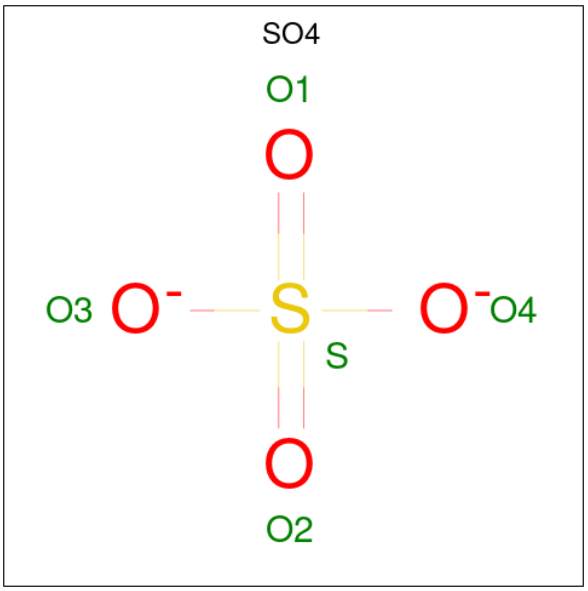
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	H	N	O	38	0
			85	38	38	4	5		
2	B	1	Total	C	H	N	O	38	0
			85	38	38	4	5		

- Molecule 3 is 2-(4-fluorophenyl)-N-methyl-6-[(methylsulfonyl)amino]-5-(propan-2-yloxy)-1-benzofuran-3-carboxamide (CCD ID: 2N5) (formula: $C_{20}H_{21}FN_2O_5S$).



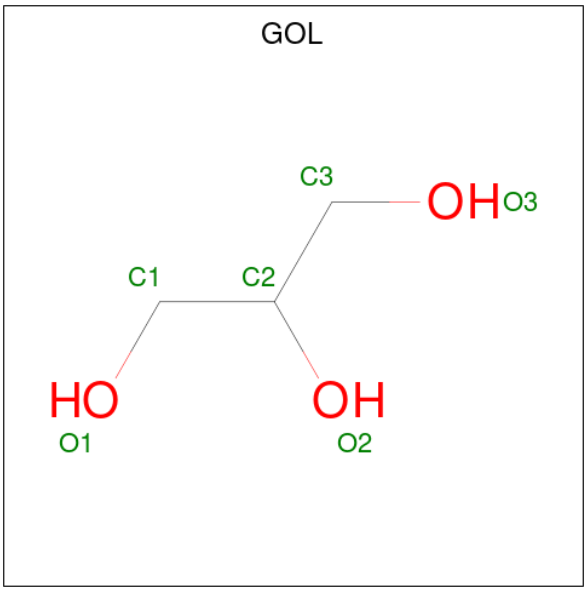
Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
3	A	1	Total	C	F	H	N	O	S	21	0
			50	20	1	21	2	5	1		
3	B	1	Total	C	F	H	N	O	S	21	0
			50	20	1	21	2	5	1		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



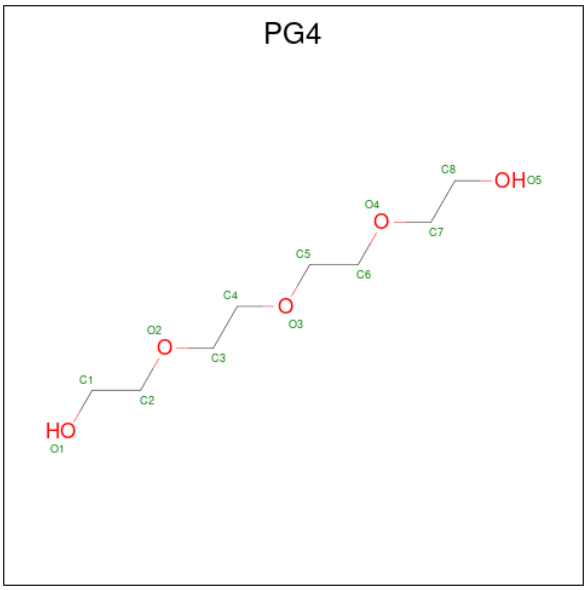
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



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	B	1	Total C O 6 3 3	0	0

- Molecule 6 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



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

- Molecule 7 is water.

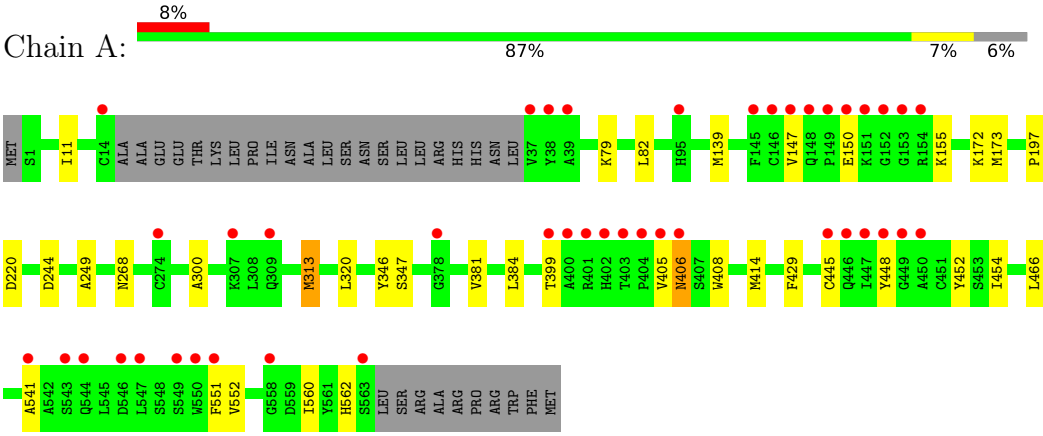
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	251	Total O 251 251	0	0
7	B	229	Total O 229 229	0	0

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.

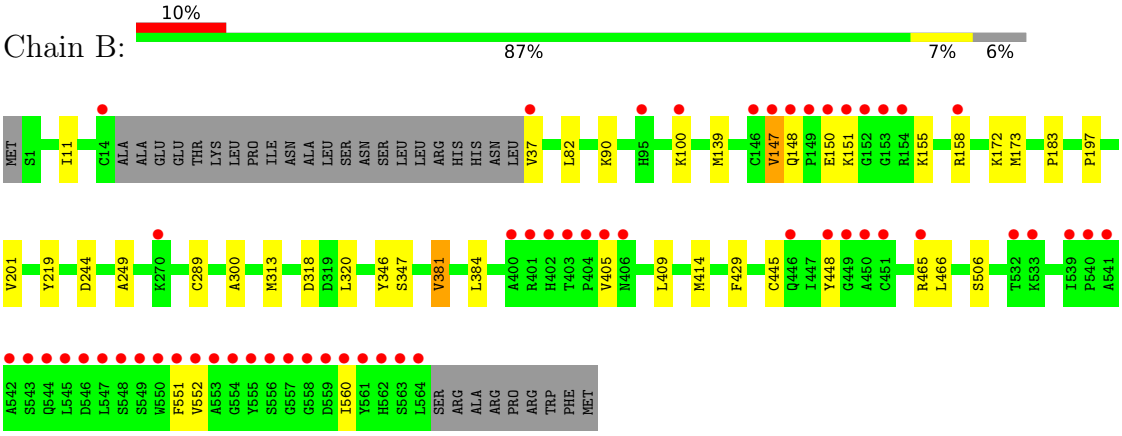
• Molecule 1: RNA-directed RNA polymerase

Chain A:



• Molecule 1: RNA-directed RNA polymerase

Chain B:



4 Data and refinement statistics (i)

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 32.21 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.8 (32.21-2.20) 99.7 (32.21-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [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)	0.37 , 44.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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, PG4, 2N5, 23E, GOL

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	0.85	2/4271 (0.0%)	1.18	9/5797 (0.2%)
1	B	0.84	1/4293 (0.0%)	1.19	6/5826 (0.1%)
All	All	0.85	3/8564 (0.0%)	1.19	15/11623 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	173	MET	SD-CE	-5.89	1.64	1.79
1	A	313	MET	SD-CE	-5.15	1.66	1.79
1	A	173	MET	SD-CE	-5.15	1.66	1.79

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	552	VAL	N-CA-C	-5.72	106.10	111.48
1	B	429	PHE	CA-CB-CG	-5.70	108.10	113.80
1	B	381	VAL	N-CA-CB	5.56	119.64	111.52
1	A	244	ASP	N-CA-C	-5.39	101.00	109.25
1	B	244	ASP	N-CA-C	-5.21	101.27	109.25
1	A	11	ILE	N-CA-C	-5.21	99.98	107.37
1	A	552	VAL	N-CA-C	-5.19	106.60	111.48
1	A	541	ALA	CA-C-N	5.15	131.38	121.54
1	A	541	ALA	C-N-CA	5.15	131.38	121.54
1	B	11	ILE	N-CA-C	-5.14	100.07	107.37
1	B	318	ASP	CA-CB-CG	5.12	117.72	112.60
1	A	399	THR	CA-C-N	5.11	127.13	120.28
1	A	399	THR	C-N-CA	5.11	127.13	120.28
1	A	429	PHE	CA-CB-CG	-5.10	108.70	113.80
1	A	268	ASN	CA-CB-CG	5.07	117.67	112.60

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	4176	0	4164	15	0
1	B	4188	0	4162	14	0
2	A	47	38	37	0	0
2	B	47	38	37	0	0
3	A	29	21	21	1	0
3	B	29	21	21	1	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
7	A	251	0	0	0	0
7	B	229	0	0	0	0
All	All	9093	118	8492	29	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 2.

All (29) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	0.47
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:300:ALA:HB2	1:A:313:MET:HE1	1.97	0.46
1:A:414:MET:HE3	3:A:602:2N5:O28	2.16	0.46
1:A:445:CYS:SG	1:A:454:ILE:HD12	2.57	0.44
1:B:414:MET:HE3	3:B:602:2N5:O28	2.18	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:B:300:ALA:HB2	1:B:313:MET:HE1	2.00	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 (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	538/574 (94%)	526 (98%)	9 (2%)	3 (1%)	21	23
1	B	541/574 (94%)	525 (97%)	13 (2%)	3 (1%)	21	23
All	All	1079/1148 (94%)	1051 (97%)	22 (2%)	6 (1%)	21	23

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 (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	449/486 (92%)	442 (98%)	7 (2%)	55 71
1	B	449/486 (92%)	438 (98%)	11 (2%)	43 58
All	All	898/972 (92%)	880 (98%)	18 (2%)	48 64

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	139	MET
1	A	155	LYS
1	A	220	ASP
1	A	381	VAL
1	A	405	VAL
1	A	406	ASN
1	A	506	SER
1	B	90	LYS
1	B	100	LYS
1	B	139	MET
1	B	148	GLN
1	B	151	LYS
1	B	155	LYS
1	B	158	ARG
1	B	381	VAL
1	B	405	VAL
1	B	465	ARG
1	B	506	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	A	184	GLN
1	A	406	ASN
1	A	436	GLN
1	A	446	GLN
1	A	502	HIS
1	B	184	GLN
1	B	309	GLN
1	B	436	GLN
1	B	446	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 oligosaccharides 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	$\#\|Z\| > 2$
6	PG4	A	611	-	12,12,12	0.14	0	11,11,11	0.21	0
4	SO4	B	604	-	4,4,4	0.31	0	6,6,6	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
4	SO4	A	606	-	4,4,4	0.35	0	6,6,6	0.22	0
4	SO4	A	605	-	4,4,4	0.42	0	6,6,6	0.20	0
5	GOL	A	609	-	5,5,5	0.08	0	5,5,5	0.15	0
4	SO4	B	609	-	4,4,4	0.27	0	6,6,6	0.17	0
4	SO4	B	603	-	4,4,4	0.34	0	6,6,6	0.21	0
4	SO4	A	607	-	4,4,4	0.30	0	6,6,6	0.08	0
3	2N5	A	602	-	31,31,31	0.37	0	43,46,46	0.79	2 (4%)
4	SO4	A	604	-	4,4,4	0.30	0	6,6,6	0.31	0
5	GOL	B	610	-	5,5,5	0.24	0	5,5,5	0.47	0
4	SO4	B	605	-	4,4,4	0.31	0	6,6,6	0.37	0
4	SO4	B	606	-	4,4,4	0.34	0	6,6,6	0.16	0
4	SO4	A	603	-	4,4,4	0.24	0	6,6,6	0.20	0
2	23E	B	601	-	52,53,53	0.40	0	68,77,77	0.55	0
5	GOL	A	610	-	5,5,5	0.16	0	5,5,5	0.18	0
3	2N5	B	602	-	31,31,31	0.37	0	43,46,46	0.78	2 (4%)
4	SO4	B	607	-	4,4,4	0.25	0	6,6,6	0.17	0
5	GOL	A	608	-	5,5,5	0.24	0	5,5,5	0.20	0
2	23E	A	601	-	52,53,53	0.36	0	68,77,77	0.51	0
4	SO4	B	608	-	4,4,4	0.24	0	6,6,6	0.28	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
3	2N5	A	602	-	-	6/19/19/19	0/3/3/3
3	2N5	B	602	-	-	6/19/19/19	0/3/3/3
5	GOL	B	610	-	-	2/4/4/4	-
6	PG4	A	611	-	-	2/10/10/10	-
2	23E	B	601	-	-	0/28/57/57	0/6/7/7
5	GOL	A	610	-	-	0/4/4/4	-
5	GOL	A	608	-	-	0/4/4/4	-
2	23E	A	601	-	-	0/28/57/57	0/6/7/7
5	GOL	A	609	-	-	0/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	602	2N5	O13-C15-C16	3.27	120.33	107.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	602	2N5	O13-C15-C16	3.25	120.27	107.89
3	B	602	2N5	C1-O13-C15	2.26	123.69	119.53
3	A	602	2N5	C1-O13-C15	2.21	123.59	119.53

There are no chirality outliers.

All (16) 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
5	B	610	GOL	O1-C1-C2-O2
3	B	602	2N5	C2-N14-S26-O28
3	A	602	2N5	C2-N14-S26-O28
3	A	602	2N5	C2-N14-S26-O29
3	B	602	2N5	C2-N14-S26-O29
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.

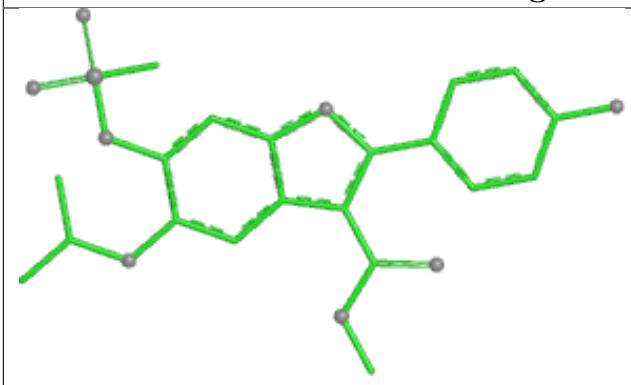
3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	2N5	1	0
5	A	610	GOL	1	0
3	B	602	2N5	1	0

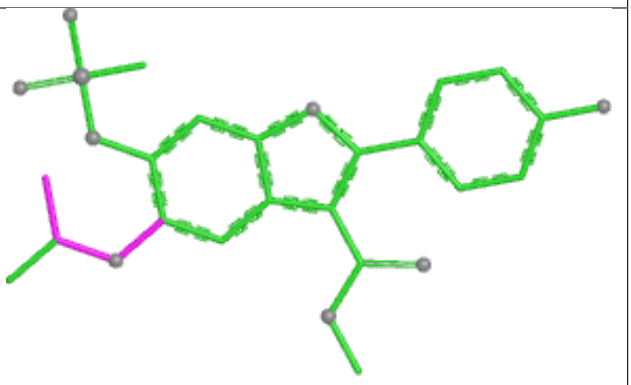
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

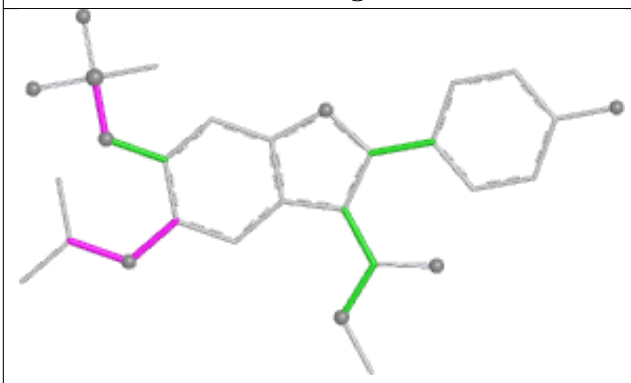
Ligand 2N5 A 602



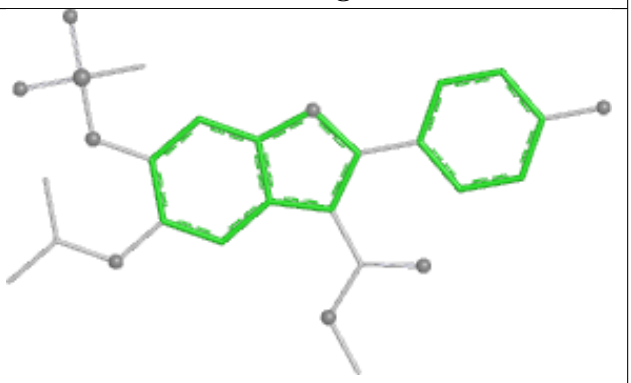
Bond lengths



Bond angles

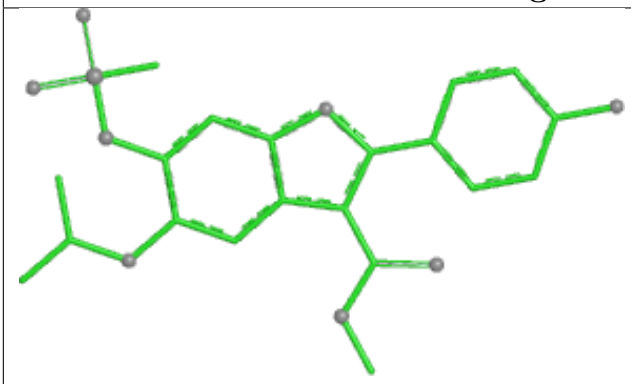


Torsions

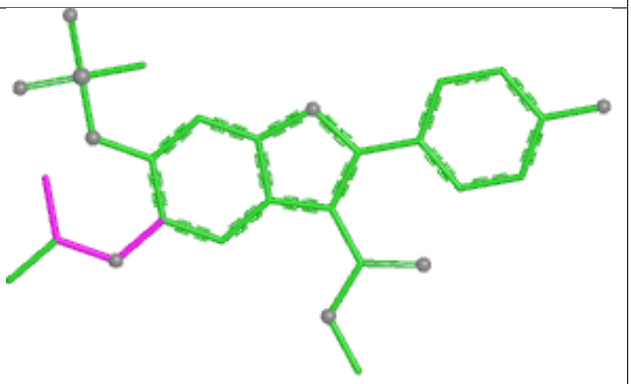


Rings

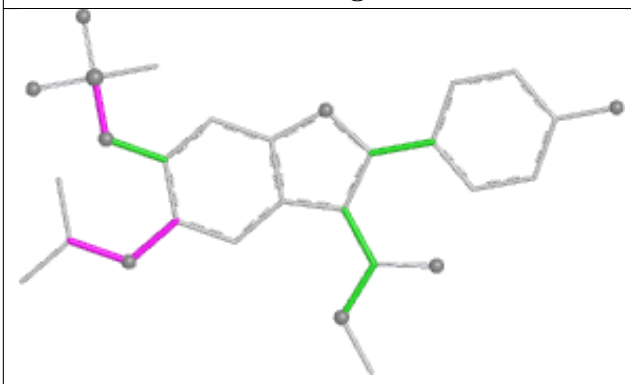
Ligand 2N5 B 602



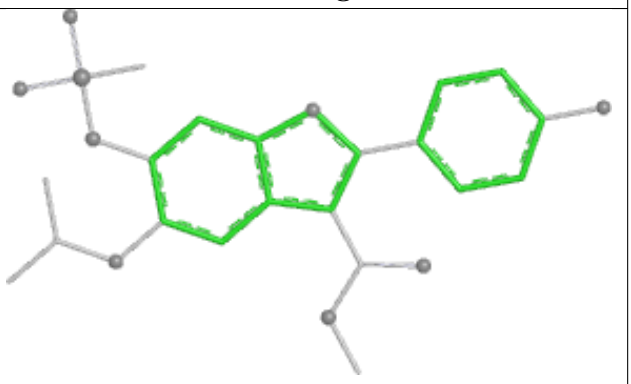
Bond lengths



Bond angles



Torsions



Rings

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, 95^{th} 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%)	0.13	44 (8%) 18 15	13, 24, 52, 100	1 (0%)
1	B	542/574 (94%)	0.39	56 (10%) 12 9	13, 25, 74, 115	3 (0%)
All	All	1083/1148 (94%)	0.26	100 (9%) 14 12	13, 24, 64, 115	4 (0%)

All (100) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	552	VAL	10.2
1	A	149	PRO	9.6
1	A	148	GLN	9.5
1	B	550	TRP	9.4
1	B	564	LEU	9.0
1	B	149	PRO	8.9
1	B	555	TYR	8.9
1	A	147	VAL	8.1
1	B	147	VAL	8.0
1	B	558	GLY	7.5
1	B	554	GLY	7.5
1	B	545	LEU	7.5
1	A	150	GLU	7.4
1	B	551	PHE	7.0
1	B	553	ALA	6.9
1	A	151	LYS	6.9
1	B	557	GLY	6.8
1	B	542	ALA	6.5
1	B	404	PRO	6.5
1	B	37	VAL	6.4
1	B	541	ALA	6.0
1	A	563	SER	5.9
1	A	37	VAL	5.7
1	B	560	ILE	5.7

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Mol	Chain	Res	Type	RSRZ
1	B	549	SER	5.7
1	B	540	PRO	5.6
1	B	151	LYS	5.6
1	B	150	GLU	5.5
1	A	152	GLY	5.4
1	B	544	GLN	5.4
1	A	541	ALA	5.3
1	A	447	ILE	5.1
1	B	546	ASP	5.1
1	B	543	SER	5.0
1	B	548	SER	4.9
1	A	446	GLN	4.8
1	B	547	LEU	4.8
1	B	148	GLN	4.8
1	B	556	SER	4.7
1	A	405	VAL	4.7
1	A	14	CYS	4.6
1	B	153	GLY	4.5
1	A	448	TYR	4.3
1	B	563	SER	4.2
1	A	404	PRO	4.2
1	B	559	ASP	4.1
1	B	146	CYS	4.1
1	B	561	TYR	4.0
1	B	449	GLY	3.9
1	A	146	CYS	3.7
1	B	402	HIS	3.7
1	A	445	CYS	3.6
1	B	562	HIS	3.6
1	B	448	TYR	3.6
1	B	154	ARG	3.5
1	A	153	GLY	3.5
1	B	446	GLN	3.5
1	B	450	ALA	3.4
1	B	14	CYS	3.4
1	A	550	TRP	3.4
1	B	405	VAL	3.4
1	A	154	ARG	3.4
1	B	539	ILE	3.4
1	A	544	GLN	3.3
1	B	152	GLY	3.3
1	B	403	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	451	CYS	3.1
1	A	402	HIS	3.1
1	B	401	ARG	3.1
1	B	406	ASN	3.0
1	A	543	SER	3.0
1	B	95	HIS	2.9
1	A	403	THR	2.8
1	A	95	HIS	2.6
1	A	400	ALA	2.6
1	A	309	GLN	2.6
1	B	270	LYS	2.5
1	A	449	GLY	2.5
1	A	38	TYR	2.4
1	A	406	ASN	2.4
1	A	307	LYS	2.4
1	B	465	ARG	2.4
1	A	558	GLY	2.3
1	A	399	THR	2.3
1	B	533	LYS	2.3
1	A	378	GLY	2.3
1	A	546	ASP	2.3
1	A	549	SER	2.2
1	A	535	LYS	2.2
1	B	400	ALA	2.2
1	B	532	THR	2.2
1	A	401	ARG	2.2
1	B	158	ARG	2.2
1	A	551	PHE	2.2
1	A	274	CYS	2.1
1	A	145	PHE	2.1
1	A	450	ALA	2.1
1	A	547	LEU	2.1
1	A	39	ALA	2.0
1	B	100	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

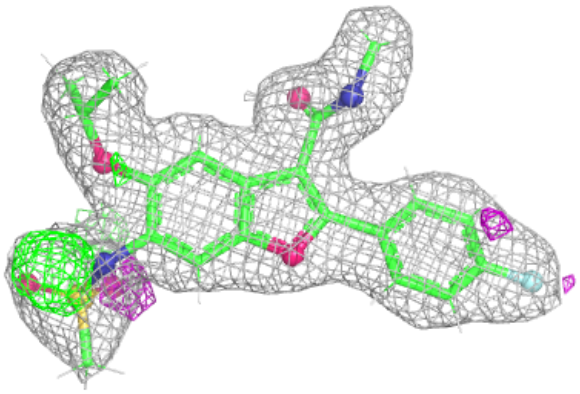
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

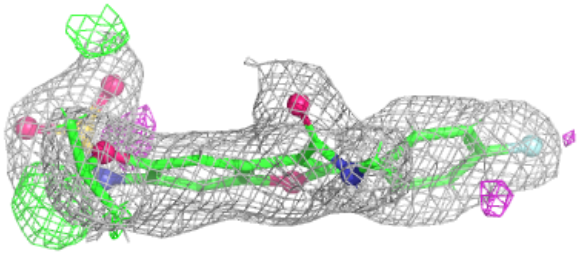
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SO4	B	609	5/5	0.65	0.20	96,97,97,98	0
4	SO4	B	608	5/5	0.79	0.16	80,81,81,82	0
4	SO4	B	606	5/5	0.82	0.13	71,73,74,75	0
4	SO4	B	604	5/5	0.83	0.14	67,70,71,72	0
6	PG4	A	611	13/13	0.83	0.16	43,46,62,64	0
4	SO4	A	607	5/5	0.84	0.16	83,84,86,87	0
4	SO4	A	606	5/5	0.85	0.13	68,68,69,71	0
5	GOL	A	610	6/6	0.86	0.18	35,46,49,49	0
4	SO4	B	607	5/5	0.86	0.15	83,83,85,86	0
5	GOL	A	609	6/6	0.87	0.14	28,38,41,42	0
5	GOL	B	610	6/6	0.89	0.12	31,37,38,38	0
5	GOL	A	608	6/6	0.89	0.10	24,29,34,37	0
4	SO4	B	605	5/5	0.92	0.10	50,53,54,57	0
3	2N5	A	602	29/29	0.93	0.09	15,29,43,47	21
2	23E	A	601	47/47	0.94	0.08	13,19,48,61	38
4	SO4	B	603	5/5	0.95	0.12	43,44,47,49	0
2	23E	B	601	47/47	0.95	0.07	15,21,38,47	38
4	SO4	A	605	5/5	0.95	0.13	48,51,55,55	0
4	SO4	A	604	5/5	0.98	0.06	27,28,32,33	0
3	2N5	B	602	29/29	0.98	0.05	13,21,26,30	21
4	SO4	A	603	5/5	0.99	0.04	29,29,33,37	0

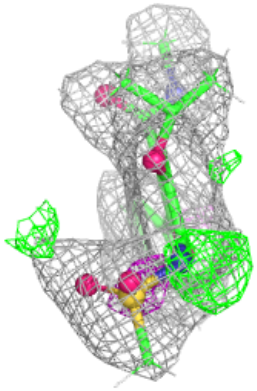
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

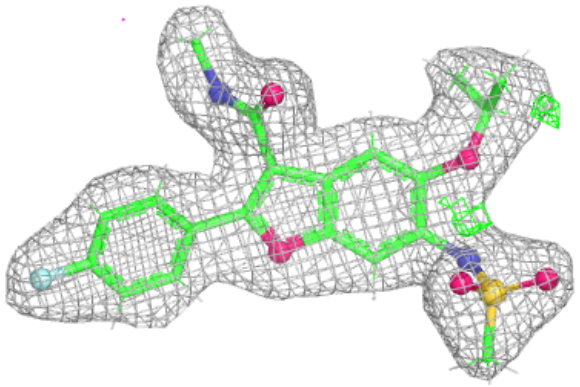


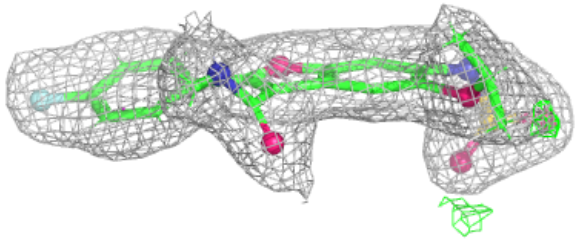


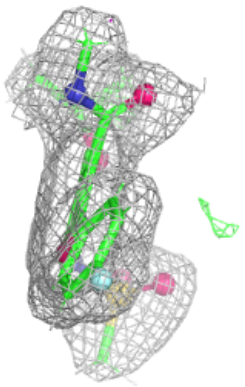


Electron density around 2N5 B 602:

$2mF_o$-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.