



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 02:29 AM EDT

PDB ID : 8S76 / pdb_00008s76
Title : Soluble epoxide hydrolase in complex with PROTAC JSF67
Authors : Kumar, A.; Schoenfeld, J.; Hiesinger, K.; Lillich, F.; Proschak, E.; Knapp, S.;
Structural Genomics Consortium (SGC)
Deposited on : 2024-02-29
Resolution : 1.48 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	:	4-5-2 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

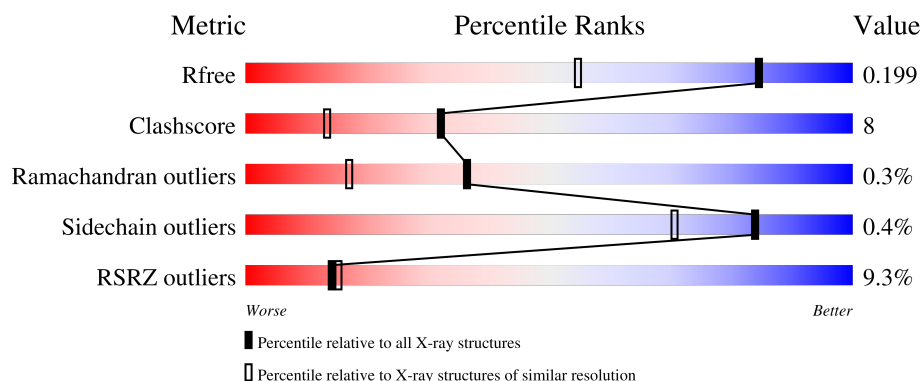
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.48 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	6779 (1.50-1.46)
Clashscore	190562	7025 (1.50-1.46)
Ramachandran outliers	187476	6917 (1.50-1.46)
Sidechain outliers	187428	6914 (1.50-1.46)
RSRZ outliers	180081	6781 (1.50-1.46)

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	367	5% 77% 10% 13%
1	B	367	12% 76% 11% 13%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	PEG	A	610	-	-	X	-
4	PEG	B	605	-	-	X	-
4	PEG	B	606	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5852 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Bifunctional epoxide hydrolase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	321	Total	C	N	O	S	0	19	0
			2681	1721	454	481	25			
1	B	321	Total	C	N	O	S	0	13	0
			2623	1687	443	469	24			

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	198	MET	-	initiating methionine	UNP P34913
A	199	GLY	-	expression tag	UNP P34913
A	200	SER	-	expression tag	UNP P34913
A	201	SER	-	expression tag	UNP P34913
A	202	HIS	-	expression tag	UNP P34913
A	203	HIS	-	expression tag	UNP P34913
A	204	HIS	-	expression tag	UNP P34913
A	205	HIS	-	expression tag	UNP P34913
A	206	HIS	-	expression tag	UNP P34913
A	207	HIS	-	expression tag	UNP P34913
A	208	SER	-	expression tag	UNP P34913
A	209	SER	-	expression tag	UNP P34913
A	210	GLY	-	expression tag	UNP P34913
A	211	LEU	-	expression tag	UNP P34913
A	212	VAL	-	expression tag	UNP P34913
A	213	PRO	-	expression tag	UNP P34913
A	214	ARG	-	expression tag	UNP P34913
A	215	GLY	-	expression tag	UNP P34913
A	216	SER	-	expression tag	UNP P34913
A	217	HIS	-	expression tag	UNP P34913
A	218	MET	-	expression tag	UNP P34913
A	219	ALA	-	expression tag	UNP P34913
A	220	SER	-	expression tag	UNP P34913
A	221	MET	-	expression tag	UNP P34913
A	556	LEU	-	expression tag	UNP P34913

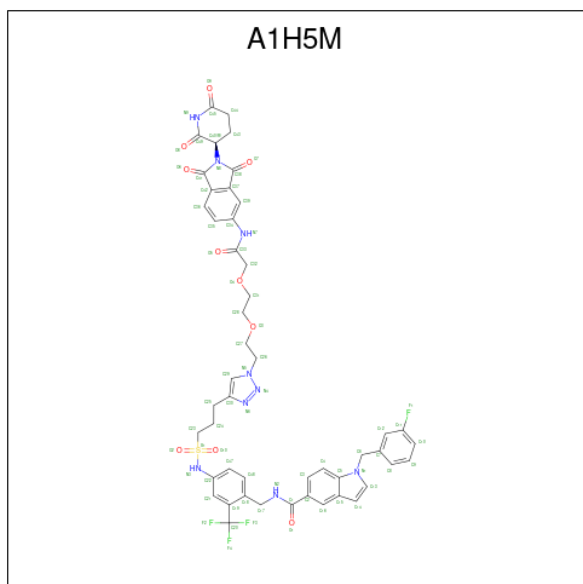
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Chain	Residue	Modelled	Actual	Comment	Reference
A	557	LEU	-	expression tag	UNP P34913
A	558	GLU	-	expression tag	UNP P34913
A	559	HIS	-	expression tag	UNP P34913
A	560	HIS	-	expression tag	UNP P34913
A	561	HIS	-	expression tag	UNP P34913
A	562	HIS	-	expression tag	UNP P34913
A	563	HIS	-	expression tag	UNP P34913
A	564	HIS	-	expression tag	UNP P34913
B	198	MET	-	initiating methionine	UNP P34913
B	199	GLY	-	expression tag	UNP P34913
B	200	SER	-	expression tag	UNP P34913
B	201	SER	-	expression tag	UNP P34913
B	202	HIS	-	expression tag	UNP P34913
B	203	HIS	-	expression tag	UNP P34913
B	204	HIS	-	expression tag	UNP P34913
B	205	HIS	-	expression tag	UNP P34913
B	206	HIS	-	expression tag	UNP P34913
B	207	HIS	-	expression tag	UNP P34913
B	208	SER	-	expression tag	UNP P34913
B	209	SER	-	expression tag	UNP P34913
B	210	GLY	-	expression tag	UNP P34913
B	211	LEU	-	expression tag	UNP P34913
B	212	VAL	-	expression tag	UNP P34913
B	213	PRO	-	expression tag	UNP P34913
B	214	ARG	-	expression tag	UNP P34913
B	215	GLY	-	expression tag	UNP P34913
B	216	SER	-	expression tag	UNP P34913
B	217	HIS	-	expression tag	UNP P34913
B	218	MET	-	expression tag	UNP P34913
B	219	ALA	-	expression tag	UNP P34913
B	220	SER	-	expression tag	UNP P34913
B	221	MET	-	expression tag	UNP P34913
B	556	LEU	-	expression tag	UNP P34913
B	557	LEU	-	expression tag	UNP P34913
B	558	GLU	-	expression tag	UNP P34913
B	559	HIS	-	expression tag	UNP P34913
B	560	HIS	-	expression tag	UNP P34913
B	561	HIS	-	expression tag	UNP P34913
B	562	HIS	-	expression tag	UNP P34913
B	563	HIS	-	expression tag	UNP P34913
B	564	HIS	-	expression tag	UNP P34913

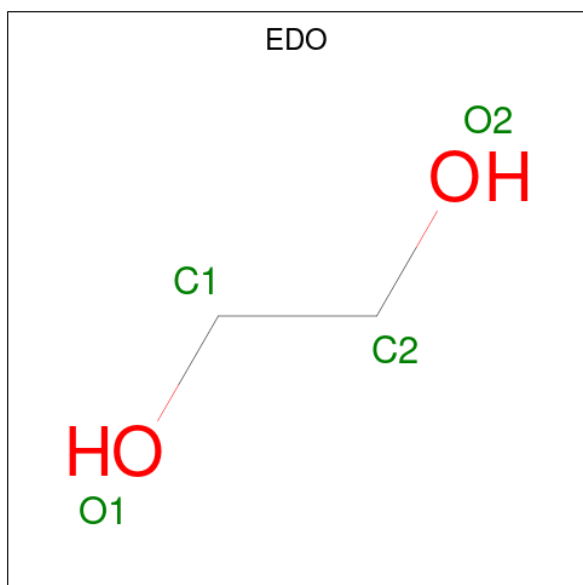
- Molecule 2 is {N}-[[4-[3-[1-[2-[2-[2-[[2-[2,6-bis(oxidanylidene)piperidin-3-yl]-1,3-bis(oxidany

lidene)isoindol-5-yl]amino]-2-oxidanylidene-ethoxy]ethoxy]ethyl]-1,2,3-triazol-4-yl]propylsulfonamido]-2-(trifluoromethyl)phenyl]methyl]-1-[(3-fluorophenyl)methyl]indole-5-carboxamide (CCD ID: A1H5M) (formula: $C_{48}H_{45}F_4N_9O_{10}S$) (labeled as "Ligand of Interest" by depositor).



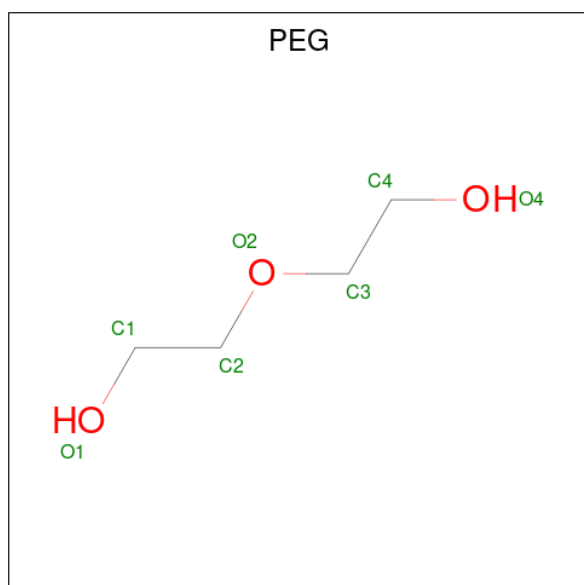
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			36	25	4	3	3	1		
2	B	1	Total	C	F	N	O	S	0	0
			36	25	4	3	3	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	A	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0

- Molecule 4 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 7 4 3	0	0
4	A	1	Total C O 7 4 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			7	4	3		
4	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	269	Total	O	0	0
			269	269		
5	B	139	Total	O	0	0
			139	139		

- Molecule 1: Bifunctional epoxide hydrolase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	47.40Å 80.36Å 90.22Å 90.00° 92.17° 90.00°	Depositor
Resolution (Å)	47.41 – 1.48 47.41 – 1.48	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.41-1.48) 99.3 (47.41-1.48)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 1.48Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.166 , 0.199 0.166 , 0.199	Depositor DCC
R_{free} test set	5464 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	19.6	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.027 for h,-k,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5852	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.05% 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: PEG, A1H5M, EDO

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	0.75	0/2777	1.09	3/3771 (0.1%)
1	B	0.71	0/2707	1.09	8/3679 (0.2%)
All	All	0.73	0/5484	1.09	11/7450 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	1
All	All	0	5

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	245	LYS	O-C-N	-6.49	116.91	121.65
1	B	438	LEU	N-CA-CB	-5.64	101.21	109.95
1	A	480	LEU	N-CA-CB	5.54	118.19	110.04
1	A	302	PRO	O-C-N	-5.46	118.80	121.31
1	B	467	ARG	CD-NE-CZ	5.34	131.88	124.40
1	B	359	ASN	CA-CB-CG	5.26	117.86	112.60
1	A	292	ASP	CA-CB-CG	5.22	117.82	112.60
1	B	516	ARG	CA-C-N	5.21	126.06	121.58
1	B	516	ARG	C-N-CA	5.21	126.06	121.58
1	B	245	LYS	CB-CA-C	-5.14	102.00	109.97
1	B	405	PHE	CA-CB-CG	-5.04	108.76	113.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	MET	Peptide
1	A	353[A]	ARG	Sidechain
1	A	479	SER	Peptide
1	A	481	GLY	Peptide
1	B	291	MET	Peptide

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	2681	0	2596	39	0
1	B	2623	0	2516	38	0
2	A	36	0	0	11	0
2	B	36	0	0	5	0
3	A	28	0	42	3	0
3	B	12	0	17	4	0
4	A	14	0	20	8	0
4	B	14	0	20	18	0
5	A	269	0	0	5	0
5	B	139	0	0	9	0
All	All	5852	0	5211	86	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 8.

All (86) 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:471[B]:ARG:HG3	1:B:471[B]:ARG:HH11	1.09	1.09
1:A:383:TYR:OH	2:A:601:A1H5M:O1	1.70	1.08
1:A:383:TYR:HH	2:A:601:A1H5M:C1	1.73	1.02
1:A:260:ALA:H	4:A:610:PEG:H32	1.29	0.97
1:B:471[B]:ARG:HH11	1:B:471[B]:ARG:CG	1.78	0.92
1:B:327[B]:SER:OG	4:B:606:PEG:C2	2.20	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:327[B]:SER:OG	4:B:606:PEG:H22	1.74	0.87
1:B:471[B]:ARG:HG3	1:B:471[B]:ARG:NH1	1.73	0.85
1:B:471[B]:ARG:NH1	5:B:701:HOH:O	2.10	0.84
1:A:316:GLU:OE2	3:A:602:EDO:O2	1.98	0.81
1:A:528:MET:HE2	5:A:728:HOH:O	1.81	0.81
1:B:287:ARG:HD3	4:B:605:PEG:H12	1.70	0.74
1:A:383:TYR:CZ	2:A:601:A1H5M:O1	2.41	0.73
1:A:503:MET:HE1	2:A:601:A1H5M:F1	1.79	0.72
1:B:327[B]:SER:OG	4:B:606:PEG:H21	1.87	0.71
1:A:383:TYR:OH	2:A:601:A1H5M:C3	2.39	0.69
1:A:258:GLY:O	4:A:610:PEG:C1	2.42	0.68
1:B:396:GLU:OE2	1:B:429:PHE:N	2.21	0.65
1:B:327[A]:SER:OG	4:B:606:PEG:H32	1.96	0.64
1:A:317:MET:SD	3:A:602:EDO:H11	2.37	0.64
4:B:606:PEG:O2	5:B:702:HOH:O	2.15	0.64
1:B:258:GLY:O	4:B:605:PEG:H21	1.97	0.64
1:A:258:GLY:O	4:A:610:PEG:H11	1.98	0.64
1:A:293:MET:HE1	1:A:340[B]:LEU:HD23	1.81	0.62
1:B:317:MET:SD	3:B:604:EDO:H11	2.41	0.61
4:B:606:PEG:H11	5:B:702:HOH:O	1.99	0.61
1:A:471[A]:ARG:HD3	5:A:887:HOH:O	2.02	0.60
4:B:606:PEG:H22	5:B:746:HOH:O	2.03	0.58
1:B:260:ALA:H	4:B:605:PEG:H31	1.67	0.58
1:B:287:ARG:CD	4:B:605:PEG:H12	2.33	0.57
1:B:383:TYR:OH	2:B:601:A1H5M:O1	2.21	0.57
1:A:260:ALA:N	4:A:610:PEG:H32	2.12	0.55
1:B:310:MET:HE3	1:B:336:TRP:CZ3	2.44	0.53
1:A:383:TYR:CE2	2:A:601:A1H5M:O1	2.62	0.53
1:A:503:MET:CE	2:A:601:A1H5M:F1	2.44	0.53
1:B:471[A]:ARG:HD3	5:B:832:HOH:O	2.07	0.53
1:B:287:ARG:HH11	4:B:605:PEG:C1	2.22	0.52
1:B:327[B]:SER:HB2	4:B:606:PEG:HO4	1.74	0.51
1:B:500:VAL:HG22	1:B:503:MET:HG3	1.93	0.51
1:B:468:ASN:HA	1:B:471[B]:ARG:HH12	1.76	0.51
1:A:293:MET:HE1	1:A:340[B]:LEU:CD2	2.41	0.50
2:A:601:A1H5M:C23	5:A:903:HOH:O	2.58	0.50
1:A:515:LYS:HB3	3:A:605:EDO:H21	1.95	0.49
1:B:327[B]:SER:HB2	4:B:606:PEG:H32	1.95	0.49
1:A:502[A]:GLN:H	1:A:502[A]:GLN:CD	2.21	0.49
2:B:601:A1H5M:C23	5:B:703:HOH:O	2.60	0.48
1:B:419:MET:HA	1:B:422:VAL:CG2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:325:GLY:HA3	3:B:602:EDO:H21	1.95	0.48
2:B:601:A1H5M:C23	5:B:808:HOH:O	2.62	0.47
4:B:606:PEG:C1	5:B:702:HOH:O	2.61	0.47
4:B:606:PEG:C2	5:B:746:HOH:O	2.60	0.47
1:A:249[B]:ARG:HB3	1:A:249[B]:ARG:NH2	2.30	0.47
1:B:420:HIS:O	1:B:421:LYS:C	2.56	0.47
1:A:339:MET:CE	2:A:601:A1H5M:C13	2.93	0.46
1:B:317:MET:SD	3:B:604:EDO:C1	3.04	0.46
1:A:254:GLU:HA	1:A:288:VAL:O	2.16	0.45
1:B:266:GLY:HA3	1:B:335:ASP:HB3	1.98	0.45
1:A:335:ASP:OD1	2:A:601:A1H5M:N2	2.50	0.45
1:A:266:GLY:HA3	1:A:335:ASP:HB3	1.99	0.45
1:A:420:HIS:O	1:A:421:LYS:C	2.59	0.45
1:A:353[A]:ARG:NE	5:A:709:HOH:O	2.49	0.44
1:B:310:MET:HE3	1:B:336:TRP:CE3	2.52	0.44
1:A:502[A]:GLN:CD	1:A:502[A]:GLN:N	2.76	0.44
1:A:503:MET:HE1	2:A:601:A1H5M:C11	2.48	0.44
4:B:605:PEG:H42	4:B:606:PEG:O4	2.18	0.44
1:B:325:GLY:CA	3:B:602:EDO:H21	2.48	0.44
1:B:396:GLU:OE1	1:B:428:LEU:N	2.47	0.44
4:A:609:PEG:O4	4:B:605:PEG:H22	2.17	0.43
1:A:254:GLU:OE1	1:B:254:GLU:OE1	2.37	0.43
1:B:383:TYR:HH	2:B:601:A1H5M:C1	2.30	0.43
1:B:254:GLU:HA	1:B:288:VAL:O	2.19	0.42
1:A:306:GLU:H	1:A:306:GLU:CD	2.28	0.42
1:A:260:ALA:H	4:A:610:PEG:C3	2.16	0.42
1:B:278:ILE:HB	1:B:279:PRO:HD3	2.02	0.41
1:A:260:ALA:HB2	4:A:610:PEG:H31	2.01	0.41
1:B:479:SER:O	1:B:482:ARG:HB2	2.20	0.41
1:A:378:ASN:HA	1:A:379:PRO:HD2	1.94	0.41
1:A:536:GLN:HG3	5:A:895:HOH:O	2.21	0.41
1:A:277:GLN:HG3	1:A:535:ASN:OD1	2.20	0.41
1:A:353[A]:ARG:HH21	4:A:610:PEG:H41	1.86	0.41
1:B:293:MET:HE1	1:B:340[B]:LEU:HD23	2.02	0.41
1:B:386:TYR:CE1	1:B:392:VAL:HG12	2.56	0.41
1:A:502[B]:GLN:O	1:A:502[B]:GLN:HG2	2.21	0.40
1:A:355:VAL:O	1:A:488:ALA:HA	2.21	0.40
1:A:408:LEU:HD23	1:A:417:LEU:HD11	2.02	0.40
1:B:339:MET:CE	2:B:601:A1H5M:C13	2.99	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	338/367 (92%)	332 (98%)	5 (2%)	1 (0%)	36	17
1	B	332/367 (90%)	325 (98%)	6 (2%)	1 (0%)	36	17
All	All	670/734 (91%)	657 (98%)	11 (2%)	2 (0%)	36	17

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	268	PRO
1	A	268	PRO

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	291/323 (90%)	289 (99%)	2 (1%)	76	56
1	B	279/323 (86%)	279 (100%)	0	100	100
All	All	570/646 (88%)	568 (100%)	2 (0%)	84	70

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	306	GLU
1	A	445	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	384	GLN
1	A	388	GLN
1	A	513	HIS
1	B	384	GLN
1	B	388	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 ⓘ

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	$\# Z > 2$
3	EDO	B	603	-	3,3,3	0.62	0	2,2,2	0.42	0
3	EDO	B	604	-	3,3,3	1.09	0	2,2,2	0.22	0
3	EDO	A	603	-	3,3,3	0.65	0	2,2,2	0.74	0
2	A1H5M	B	601	-	39,39,79	0.43	0	56,58,114	0.84	2 (3%)
4	PEG	B	605	-	6,6,6	0.72	0	5,5,5	0.35	0
4	PEG	B	606	-	6,6,6	0.36	0	5,5,5	0.48	0
3	EDO	A	605	-	3,3,3	0.21	0	2,2,2	0.15	0
4	PEG	A	610	-	6,6,6	0.52	0	5,5,5	0.58	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1H5M	A	601	-	39,39,79	0.66	0	56,58,114	0.70	1 (1%)
3	EDO	A	607	-	3,3,3	0.08	0	2,2,2	0.06	0
3	EDO	B	602	-	3,3,3	0.50	0	2,2,2	0.51	0
4	PEG	A	609	-	6,6,6	0.28	0	5,5,5	0.19	0
3	EDO	A	602	-	3,3,3	0.55	0	2,2,2	0.54	0
3	EDO	A	604	-	3,3,3	0.61	0	2,2,2	0.41	0
3	EDO	A	606	-	3,3,3	0.11	0	2,2,2	0.45	0
3	EDO	A	608	-	3,3,3	0.10	0	2,2,2	0.21	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	EDO	B	603	-	-	0/1/1/1	-
3	EDO	B	604	-	-	0/1/1/1	-
3	EDO	A	603	-	-	0/1/1/1	-
2	A1H5M	B	601	-	-	4/24/24/78	0/4/4/8
4	PEG	B	605	-	-	2/4/4/4	-
4	PEG	B	606	-	-	3/4/4/4	-
3	EDO	A	605	-	-	1/1/1/1	-
4	PEG	A	610	-	-	3/4/4/4	-
2	A1H5M	A	601	-	-	2/24/24/78	0/4/4/8
3	EDO	A	607	-	-	1/1/1/1	-
3	EDO	B	602	-	-	0/1/1/1	-
4	PEG	A	609	-	-	3/4/4/4	-
3	EDO	A	602	-	-	1/1/1/1	-
3	EDO	A	604	-	-	0/1/1/1	-
3	EDO	A	606	-	-	0/1/1/1	-
3	EDO	A	608	-	-	0/1/1/1	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	A1H5M	O10-S1-N3	2.70	112.50	107.10
2	A	601	A1H5M	C18-C17-N2	-2.06	109.00	113.15
2	B	601	A1H5M	O2-S1-N3	-2.02	103.06	107.10

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	601	A1H5M	C22-N3-S1-C23
2	A	601	A1H5M	C22-N3-S1-O10
2	B	601	A1H5M	C22-N3-S1-O2
2	B	601	A1H5M	C22-N3-S1-C23
4	A	609	PEG	O1-C1-C2-O2
4	B	605	PEG	O2-C3-C4-O4
4	B	606	PEG	O2-C3-C4-O4
4	A	610	PEG	O1-C1-C2-O2
4	B	605	PEG	O1-C1-C2-O2
4	A	609	PEG	O2-C3-C4-O4
4	A	610	PEG	O2-C3-C4-O4
4	B	606	PEG	O1-C1-C2-O2
3	A	605	EDO	O1-C1-C2-O2
4	A	609	PEG	C4-C3-O2-C2
4	B	606	PEG	C4-C3-O2-C2
3	A	602	EDO	O1-C1-C2-O2
4	A	610	PEG	C4-C3-O2-C2
3	A	607	EDO	O1-C1-C2-O2
2	B	601	A1H5M	N1-C6-C7-C12
2	B	601	A1H5M	N1-C6-C7-C8

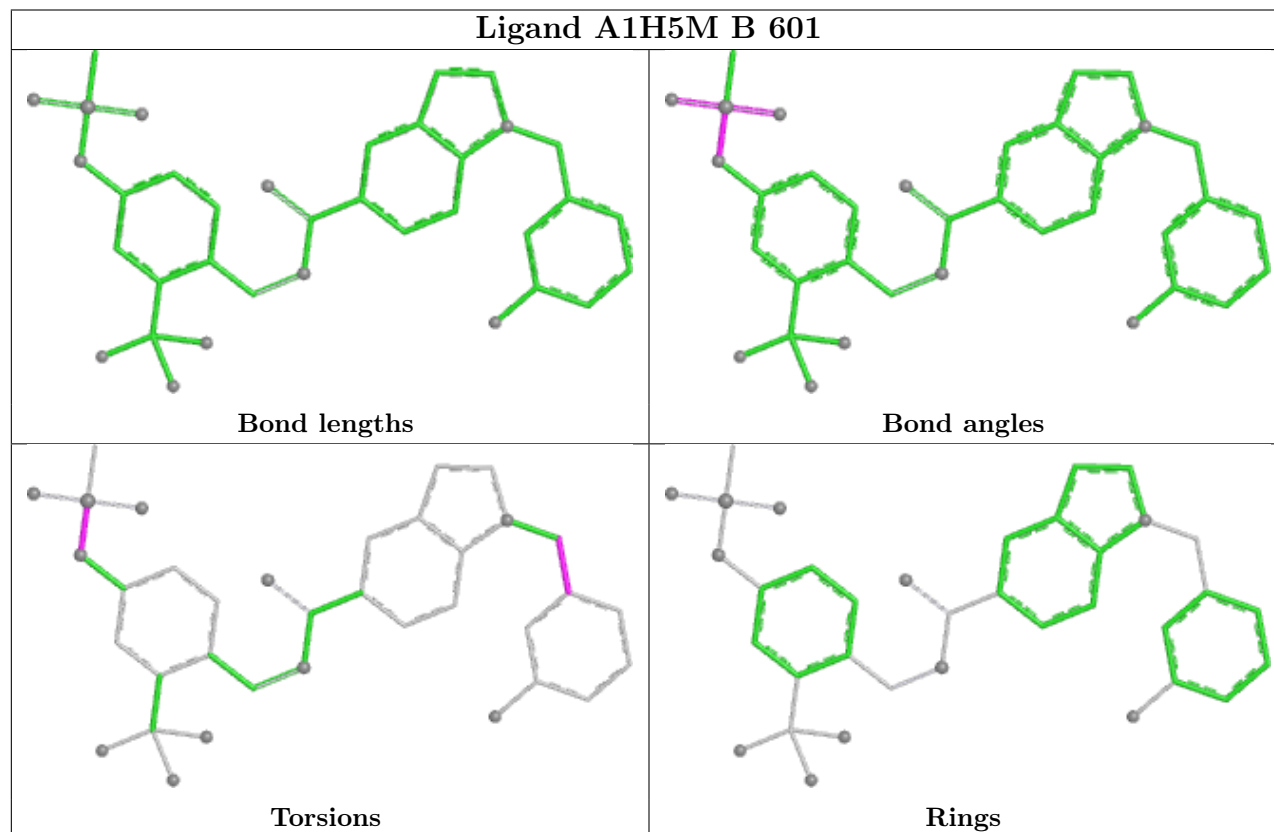
There are no ring outliers.

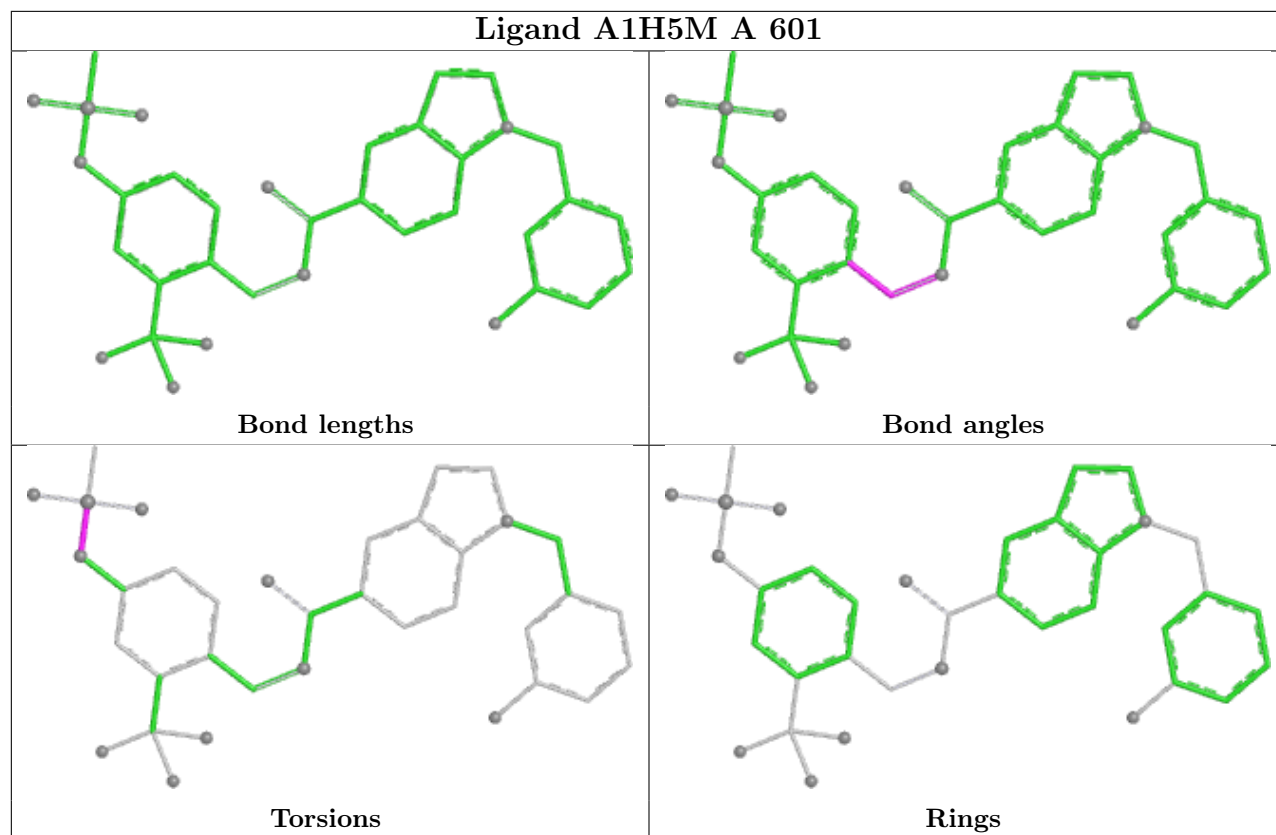
10 monomers are involved in 48 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	604	EDO	2	0
2	B	601	A1H5M	5	0
4	B	605	PEG	7	0
4	B	606	PEG	12	0
3	A	605	EDO	1	0
4	A	610	PEG	7	0
2	A	601	A1H5M	11	0
3	B	602	EDO	2	0
4	A	609	PEG	1	0
3	A	602	EDO	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.





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	321/367 (87%)	0.13	17 (5%) 32 35	7, 19, 48, 63	19 (5%)
1	B	321/367 (87%)	0.73	43 (13%) 7 7	9, 28, 61, 82	13 (4%)
All	All	642/734 (87%)	0.43	60 (9%) 14 15	7, 23, 58, 82	32 (4%)

All (60) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	426	GLY	5.0
1	B	430	VAL	4.4
1	B	425	ALA	4.2
1	A	380	VAL	4.1
1	B	416	VAL	4.1
1	A	227	PRO	4.0
1	B	422	VAL	3.7
1	B	412[A]	SER	3.7
1	B	227	PRO	3.7
1	A	481	GLY	3.6
1	A	422[A]	VAL	3.5
1	B	385	LEU	3.5
1	B	421	LYS	3.4
1	B	428	LEU	3.4
1	B	546	ALA	3.4
1	B	391	GLY	3.2
1	A	381	PHE	3.1
1	A	430	VAL	3.1
1	B	423	CYS	3.1
1	B	392	VAL	3.0
1	B	368	ASN	3.0
1	B	547	ARG	3.0
1	B	417	LEU	2.9
1	B	380	VAL	2.9

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Mol	Chain	Res	Type	RSRZ
1	B	506	HIS	2.9
1	B	510	TRP	2.9
1	B	420	HIS	2.9
1	B	363[A]	ILE	2.8
1	B	429	PHE	2.8
1	B	478	LYS	2.7
1	A	368	ASN	2.7
1	B	505[A]	GLN	2.7
1	A	510	TRP	2.6
1	A	372	LEU	2.6
1	B	427	GLY	2.6
1	B	432	SER	2.6
1	B	377	ALA	2.5
1	B	228	LEU	2.5
1	A	421	LYS	2.5
1	A	423[A]	CYS	2.5
1	B	473	TRP	2.5
1	B	379	PRO	2.5
1	B	480	LEU	2.4
1	B	481	GLY	2.4
1	A	419	MET	2.4
1	A	480	LEU	2.4
1	B	372	LEU	2.4
1	A	547	ARG	2.3
1	B	395	ALA	2.3
1	B	419	MET	2.3
1	A	425	ALA	2.3
1	B	369	MET	2.3
1	A	426	GLY	2.3
1	B	424	GLU	2.3
1	B	386	TYR	2.3
1	B	375	ILE	2.2
1	B	485	LEU	2.0
1	B	433	PRO	2.0
1	A	546	ALA	2.0
1	B	362	PHE	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

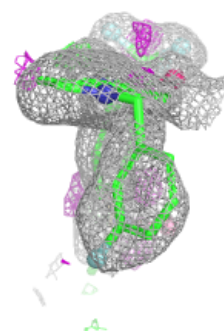
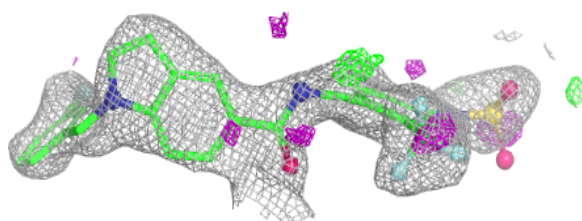
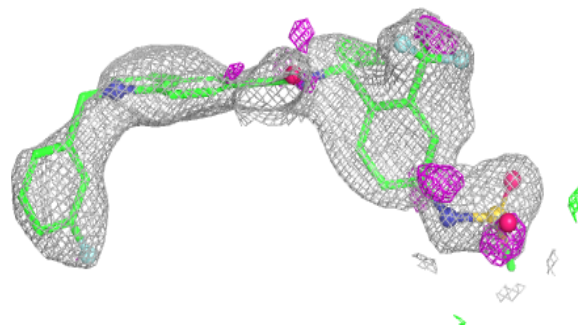
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	PEG	B	606	7/7	0.70	0.18	32,41,45,47	7
4	PEG	A	610	7/7	0.75	0.20	23,30,37,37	7
4	PEG	A	609	7/7	0.76	0.18	43,52,60,62	0
3	EDO	A	608	4/4	0.79	0.18	56,57,59,60	0
3	EDO	A	606	4/4	0.80	0.14	39,40,41,45	0
2	A1H5M	B	601	36/72	0.82	0.15	47,58,85,103	0
2	A1H5M	A	601	36/72	0.82	0.16	27,35,74,78	36
4	PEG	B	605	7/7	0.83	0.14	24,27,33,34	7
3	EDO	A	607	4/4	0.83	0.13	38,41,44,51	0
3	EDO	B	602	4/4	0.84	0.13	38,42,44,47	0
3	EDO	A	605	4/4	0.88	0.13	34,34,44,50	0
3	EDO	B	603	4/4	0.90	0.11	27,32,33,35	0
3	EDO	A	603	4/4	0.91	0.14	23,24,25,28	0
3	EDO	A	602	4/4	0.93	0.09	22,23,31,39	0
3	EDO	A	604	4/4	0.93	0.09	24,28,30,30	0
3	EDO	B	604	4/4	0.95	0.09	28,30,33,40	0

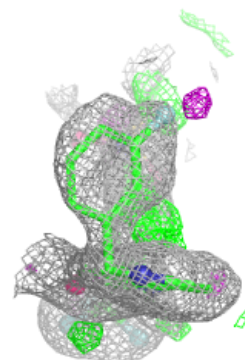
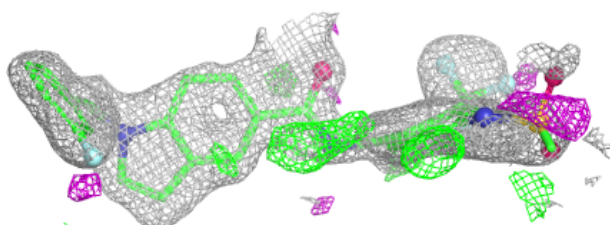
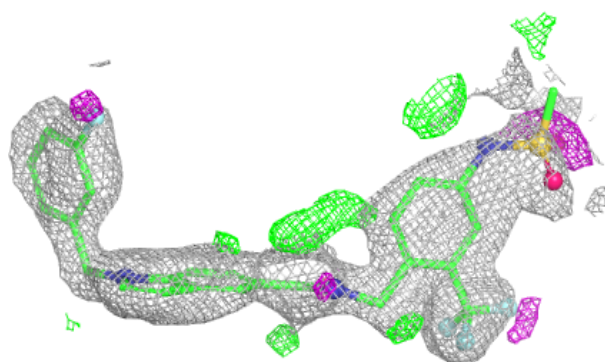
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around A1H5M 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 A1H5M 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.