



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 3, 2025 – 03:19 pm GMT

PDB ID : 8S76  
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](mailto: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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 3.0  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.41

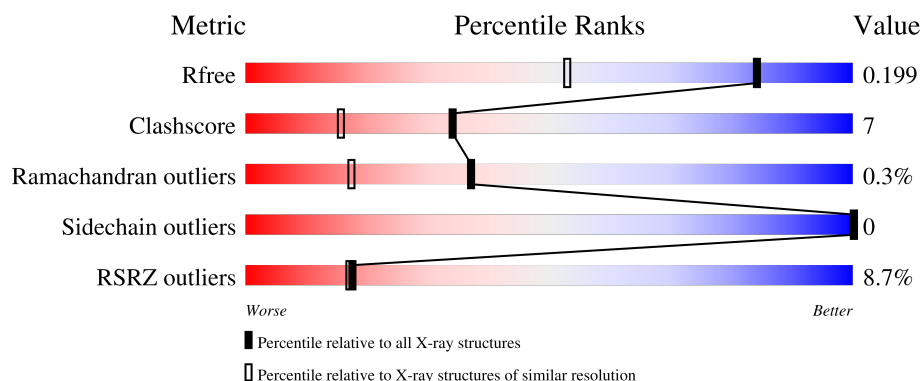
# 1 Overall quality at a glance

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))
$R_{free}$	164625	6131 (1.50-1.46)
Clashscore	180529	6623 (1.50-1.46)
Ramachandran outliers	177936	6521 (1.50-1.46)
Sidechain outliers	177891	6518 (1.50-1.46)
RSRZ outliers	164620	6132 (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  $\geq 3$ , 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	<div> <div>4%</div> <div>78%</div> <div>8%</div> <div>13%</div> </div>
1	B	367	<div> <div>11%</div> <div>78%</div> <div>10%</div> <div>13%</div> </div>

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

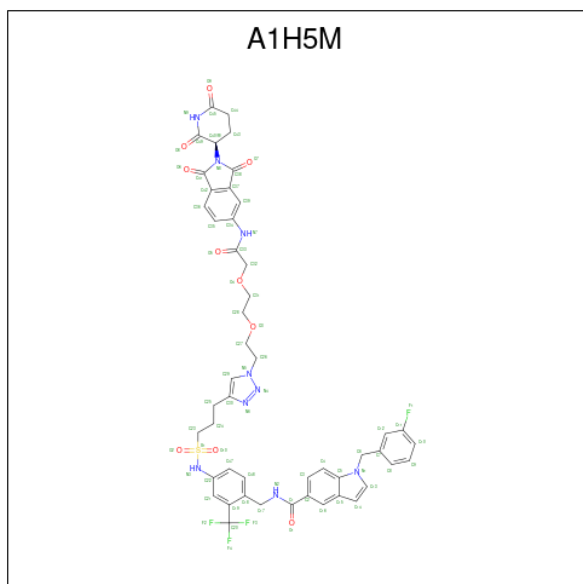
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Chain	Residue	Modelled	Actual	Comment	Reference
A	557	LEU	-	expression tag	UNP P34913
A	558	GLU	-	expression tag	UNP P34913
A	559	HIS	-	expression tag	UNP P34913
A	560	HIS	-	expression tag	UNP P34913
A	561	HIS	-	expression tag	UNP P34913
A	562	HIS	-	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

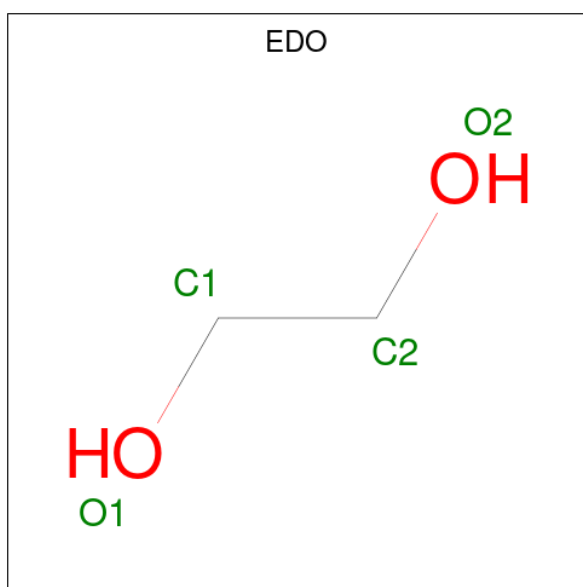
- Molecule 2 is {N}-[[4-[3-[1-[2-[2-[2-[2-[2,6-bis(oxidanylidene)piperidin-3-yl]-1,3-bis(oxidanyl

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



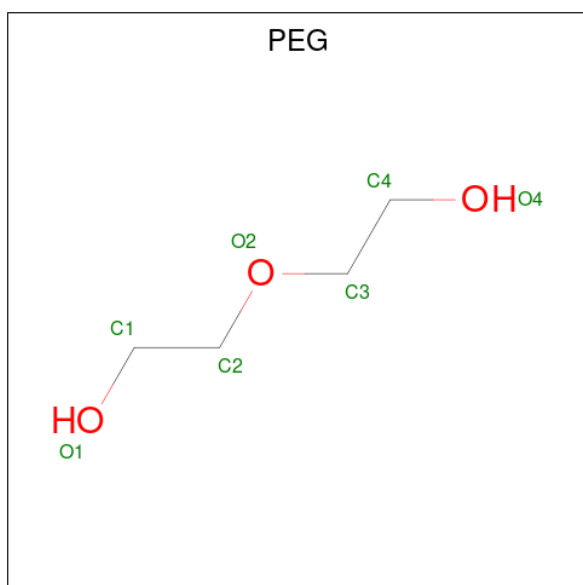
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			36	25	4	3	3	1		
2	B	1	Total	C	F	N	O	S	0	0
			36	25	4	3	3	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: 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 (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



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.

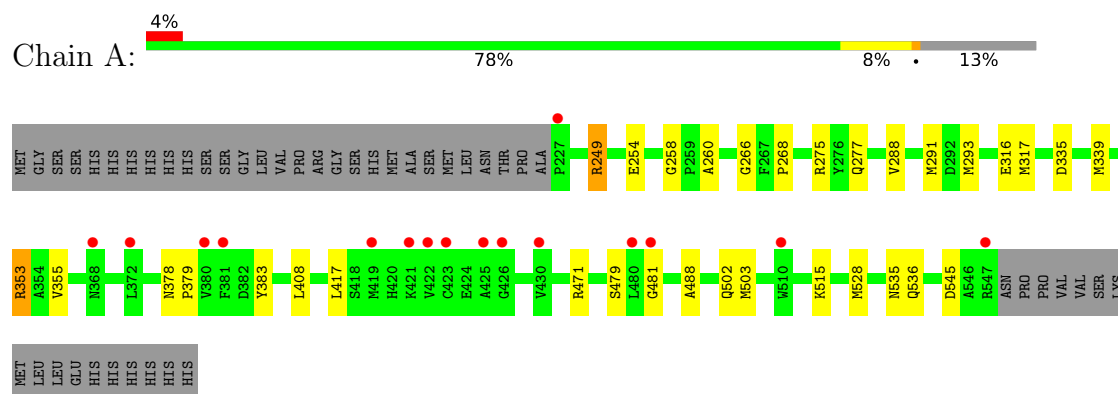
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	269	Total	O	0	0
			269	269		
5	B	139	Total	O	0	0
			139	139		



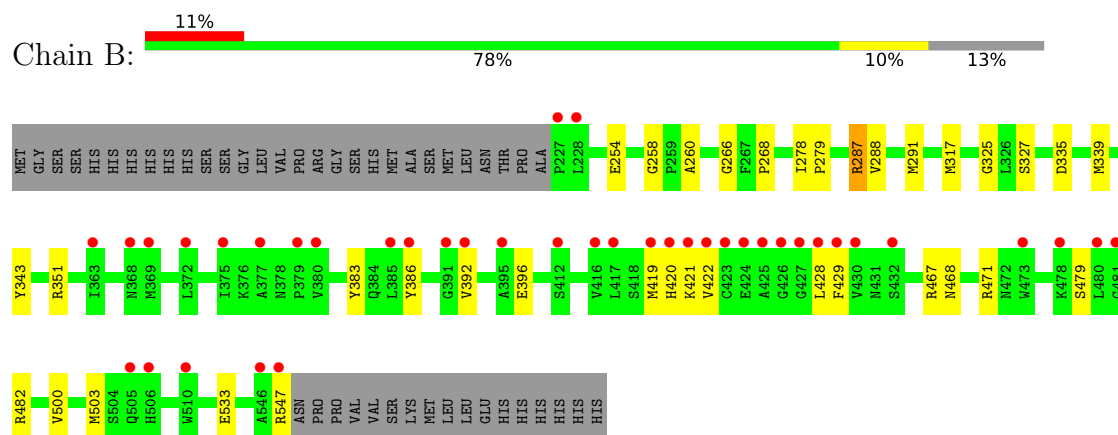
### 3 Residue-property plots [i](#)

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: Bifunctional epoxide hydrolase 2



#### • 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, $\alpha$ , $\beta$ , $\gamma$	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
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	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	5504 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.6	Xtriage
Anisotropy	0.414	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 38.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	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 <sup>2</sup> )	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: EDO, PEG, A1H5M

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	0.58	0/2777	0.98	4/3771 (0.1%)
1	B	0.53	0/2707	0.92	7/3679 (0.2%)
All	All	0.55	0/5484	0.95	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	A	249[A]	ARG	NE-CZ-NH1	-9.38	115.61	120.30
1	A	249[B]	ARG	NE-CZ-NH1	-9.38	115.61	120.30
1	B	287	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	275	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	B	351	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	B	467	ARG	CD-NE-CZ	5.91	131.88	123.60
1	B	547	ARG	NE-CZ-NH1	5.86	123.23	120.30
1	A	293	MET	CG-SD-CE	-5.74	91.02	100.20
1	B	343[A]	TYR	CA-CB-CG	-5.74	102.50	113.40
1	B	343[B]	TYR	CA-CB-CG	-5.74	102.50	113.40
1	B	533	GLU	CG-CD-OE1	5.17	128.63	118.30

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	36	0
1	B	2623	0	2516	35	0
2	A	36	0	0	12	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	80	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 7.

All (80) 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: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:B:327[B]:SER:OG	4:B:606:PEG:H21	1.87	0.71
1:A:528:MET:HE2	5:A:728:HOH:O	1.92	0.69
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: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:A:503:MET:CE	2:A:601:A1H5M:F1	2.44	0.55
1:A:383:TYR:CE2	2:A:601:A1H5M:O1	2.62	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	1.73	0.52
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
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
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
1:B:325:GLY:HA3	3:B:602:EDO:H21	1.95	0.48
1:A:503:MET:HE2	2:A:601:A1H5M:F1	2.04	0.47
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:249[B]:ARG:HB3	1:A:249[B]:ARG:NH2	2.30	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:503:MET:HE1	2:A:601:A1H5M:F1	2.06	0.45
1:A:515:LYS:NZ	1:A:545:ASP:OD1	2.37	0.45
1:A:353[A]:ARG:NE	5:A:709:HOH:O	2.49	0.44
1:A:502[A]:GLN:H	1:A:502[A]:GLN:CD	2.21	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:420:HIS:O	1:B:421:LYS:C	2.56	0.43
1:B:254:GLU:HA	1:B:288:VAL:O	2.19	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:339:MET:HE3	2:A:601:A1H5M:C13	2.50	0.41
1:A:353[A]:ARG:HH21	4:A:610:PEG:H41	1.86	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%)	37	17
1	B	332/367 (90%)	325 (98%)	6 (2%)	1 (0%)	37	17
All	All	670/734 (91%)	657 (98%)	11 (2%)	2 (0%)	37	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%)	291 (100%)	0	100	100
1	B	279/323 (86%)	279 (100%)	0	100	100
All	All	570/646 (88%)	570 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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	$\# Z  > 2$
4	PEG	B	606	-	6,6,6	0.35	0	5,5,5	0.49	0
3	EDO	A	603	-	3,3,3	0.68	0	2,2,2	0.83	0
3	EDO	A	605	-	3,3,3	0.22	0	2,2,2	0.17	0
3	EDO	A	604	-	3,3,3	0.61	0	2,2,2	0.49	0
3	EDO	B	602	-	3,3,3	0.50	0	2,2,2	0.54	0
2	A1H5M	B	601	-	39,39,79	0.59	0	53,58,114	0.89	1 (1%)
3	EDO	A	607	-	3,3,3	0.08	0	2,2,2	0.13	0
4	PEG	A	609	-	6,6,6	0.27	0	5,5,5	0.19	0
2	A1H5M	A	601	-	39,39,79	0.74	0	53,58,114	0.77	0
3	EDO	A	606	-	3,3,3	0.11	0	2,2,2	0.42	0
3	EDO	A	602	-	3,3,3	0.57	0	2,2,2	0.62	0
3	EDO	B	603	-	3,3,3	0.62	0	2,2,2	0.51	0
3	EDO	A	608	-	3,3,3	0.11	0	2,2,2	0.29	0
3	EDO	B	604	-	3,3,3	1.08	0	2,2,2	0.22	0
4	PEG	A	610	-	6,6,6	0.53	0	5,5,5	0.59	0
4	PEG	B	605	-	6,6,6	0.71	0	5,5,5	0.36	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
4	PEG	B	606	-	-	3/4/4/4	-
3	EDO	A	603	-	-	0/1/1/1	-
3	EDO	A	605	-	-	1/1/1/1	-
3	EDO	A	604	-	-	0/1/1/1	-
3	EDO	B	602	-	-	0/1/1/1	-
2	A1H5M	B	601	-	-	4/24/24/78	0/4/4/8
3	EDO	A	607	-	-	1/1/1/1	-
4	PEG	A	609	-	-	3/4/4/4	-
2	A1H5M	A	601	-	-	4/24/24/78	0/4/4/8
3	EDO	A	606	-	-	0/1/1/1	-
3	EDO	A	602	-	-	1/1/1/1	-
3	EDO	B	603	-	-	0/1/1/1	-
3	EDO	A	608	-	-	0/1/1/1	-
3	EDO	B	604	-	-	0/1/1/1	-
4	PEG	A	610	-	-	3/4/4/4	-
4	PEG	B	605	-	-	2/4/4/4	-

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	A1H5M	O10-S1-N3	2.65	112.50	107.10

There are no chirality outliers.

All (22) 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	606	PEG	O2-C3-C4-O4
4	B	605	PEG	O1-C1-C2-O2
4	B	605	PEG	O2-C3-C4-O4
4	A	609	PEG	O2-C3-C4-O4

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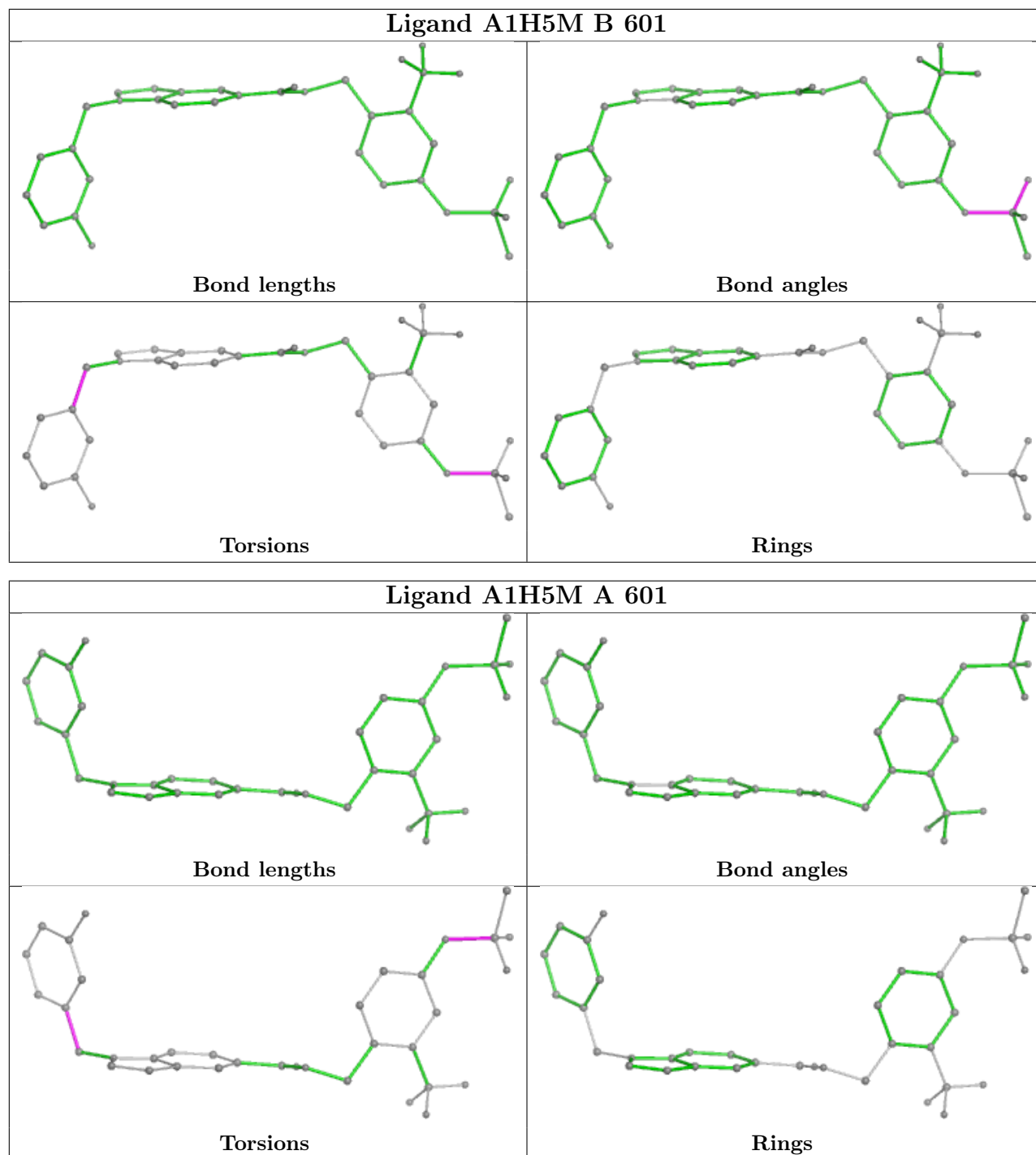
Mol	Chain	Res	Type	Atoms
4	A	610	PEG	O1-C1-C2-O2
4	A	610	PEG	O2-C3-C4-O4
3	A	605	EDO	O1-C1-C2-O2
2	B	601	A1H5M	N1-C6-C7-C12
4	B	606	PEG	O1-C1-C2-O2
2	B	601	A1H5M	N1-C6-C7-C8
2	A	601	A1H5M	N1-C6-C7-C12
3	A	602	EDO	O1-C1-C2-O2
4	A	609	PEG	C4-C3-O2-C2
2	A	601	A1H5M	N1-C6-C7-C8
4	B	606	PEG	C4-C3-O2-C2
4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

There are no ring outliers.

10 monomers are involved in 49 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	606	PEG	12	0
3	A	605	EDO	1	0
3	B	602	EDO	2	0
2	B	601	A1H5M	5	0
4	A	609	PEG	1	0
2	A	601	A1H5M	12	0
3	A	602	EDO	2	0
3	B	604	EDO	2	0
4	A	610	PEG	7	0
4	B	605	PEG	7	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	321/367 (87%)	0.08	16 (4%) 35 37	7, 19, 48, 63	19 (5%)
1	B	321/367 (87%)	0.68	40 (12%) 9 8	9, 28, 61, 82	13 (4%)
All	All	642/734 (87%)	0.38	56 (8%) 17 17	7, 23, 58, 82	32 (4%)

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	426	GLY	4.9
1	B	430	VAL	4.2
1	A	380	VAL	4.0
1	B	416	VAL	4.0
1	B	425	ALA	4.0
1	A	227	PRO	3.9
1	B	422	VAL	3.6
1	B	412[A]	SER	3.6
1	B	227	PRO	3.5
1	A	481	GLY	3.5
1	A	422[A]	VAL	3.4
1	B	421	LYS	3.4
1	B	385	LEU	3.3
1	B	428	LEU	3.3
1	B	546	ALA	3.3
1	B	391	GLY	3.1
1	A	381	PHE	3.1
1	A	430	VAL	3.0
1	B	423	CYS	3.0
1	B	392	VAL	2.9
1	B	368	ASN	2.9
1	B	547	ARG	2.9
1	B	417	LEU	2.8
1	B	506	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	B	380	VAL	2.8
1	B	420	HIS	2.8
1	B	510	TRP	2.8
1	B	478	LYS	2.7
1	B	363[A]	ILE	2.7
1	B	429	PHE	2.7
1	A	368	ASN	2.6
1	B	505[A]	GLN	2.6
1	A	510	TRP	2.5
1	A	372	LEU	2.5
1	A	421	LYS	2.5
1	B	427	GLY	2.5
1	B	432	SER	2.5
1	B	228	LEU	2.4
1	B	377	ALA	2.4
1	A	423[A]	CYS	2.4
1	B	473	TRP	2.4
1	A	419	MET	2.4
1	B	379	PRO	2.4
1	B	480	LEU	2.3
1	B	481	GLY	2.3
1	A	547	ARG	2.3
1	B	419	MET	2.3
1	A	480	LEU	2.3
1	B	372	LEU	2.3
1	B	369	MET	2.3
1	B	395	ALA	2.2
1	B	424	GLU	2.2
1	A	425	ALA	2.2
1	A	426	GLY	2.2
1	B	386	TYR	2.2
1	B	375	ILE	2.1

## 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 ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

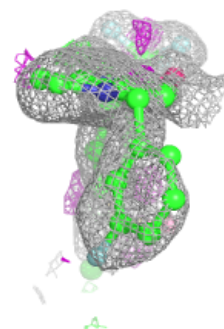
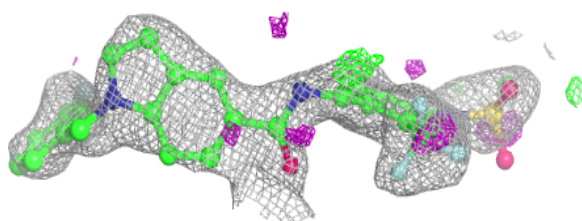
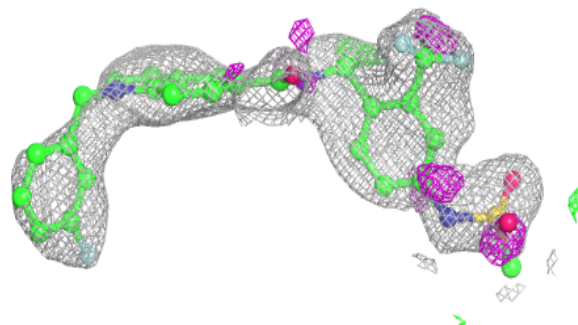
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	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

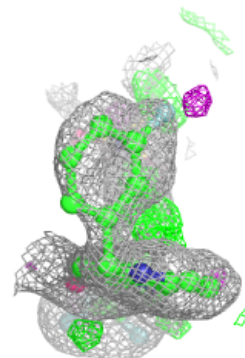
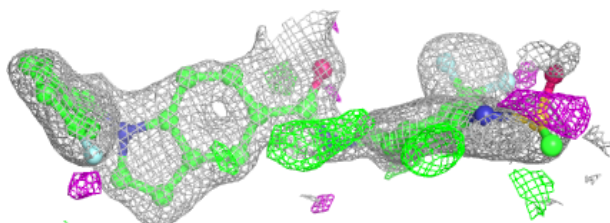
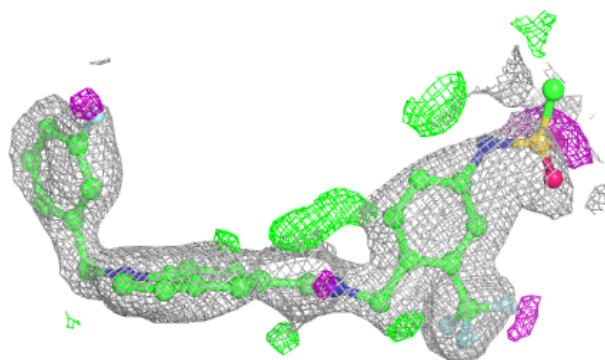
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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