



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 3, 2025 – 03:10 pm GMT

PDB ID : 8S77
Title : Soluble epoxide hydrolase in complex with PROTAC JSF234
Authors : Kumar, A.; Schoenfeld, J.; Hiesinger, K.; Lillich, F.; Proschak, E.; Knapp, S.;
Structural Genomics Consortium (SGC)
Deposited on : 2024-02-29
Resolution : 1.36 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

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A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, 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

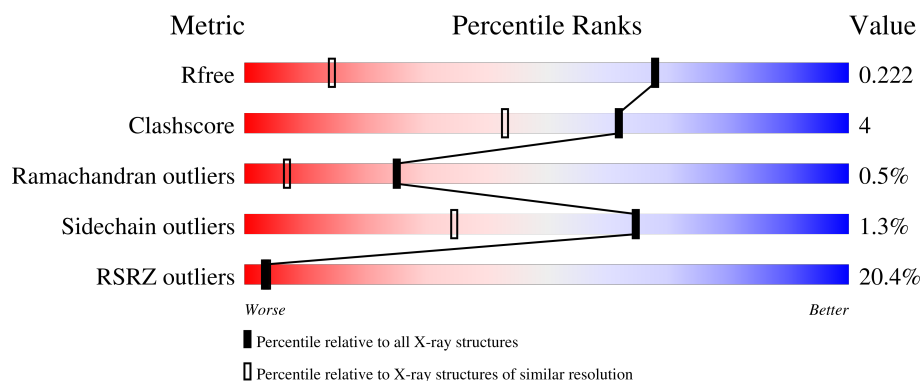
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.36 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	1089 (1.36-1.36)
Clashscore	180529	1157 (1.36-1.36)
Ramachandran outliers	177936	1146 (1.36-1.36)
Sidechain outliers	177891	1146 (1.36-1.36)
RSRZ outliers	164620	1088 (1.36-1.36)

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	 11% 78% 10% 13%
1	B	367	 25% 79% 8% 13%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 5725 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	12	0
			2624	1685	444	472	23			
1	B	321	Total	C	N	O	S	0	14	0
			2631	1685	449	474	23			

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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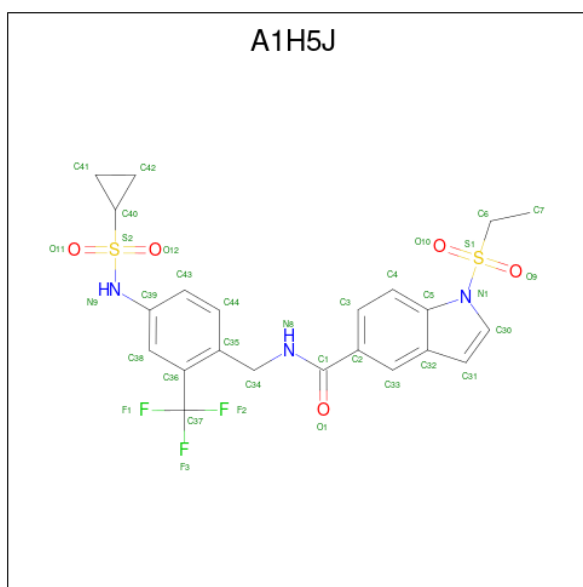
Chain	Residue	Modelled	Actual	Comment	Reference
A	557	LEU	-	expression tag	UNP P34913
A	558	GLU	-	expression tag	UNP P34913
A	559	HIS	-	expression tag	UNP P34913
A	560	HIS	-	expression tag	UNP P34913
A	561	HIS	-	expression tag	UNP P34913
A	562	HIS	-	expression tag	UNP P34913
A	563	HIS	-	expression tag	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 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

- Molecule 3 is {N}-[[4-(cyclopropylsulfonylamino)-2-(trifluoromethyl)phenyl]methyl]-1-e thylsulfonyl-indole-5-carboxamide (three-letter code: A1H5J) (formula: C₂₂H₂₂F₃N₃O₅S₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	F	N	O	S	0	0
			35	22	3	3	5	2		
3	B	1	Total	C	F	N	O	S	0	0
			35	22	3	3	5	2		

- Molecule 4 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

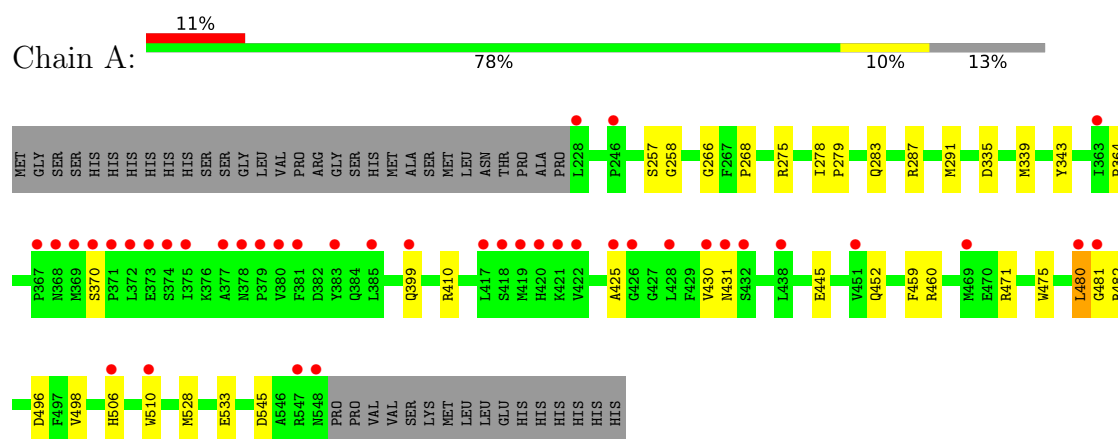
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	242	Total 242	O 242	0	0
5	B	123	Total 123	O 123	0	0

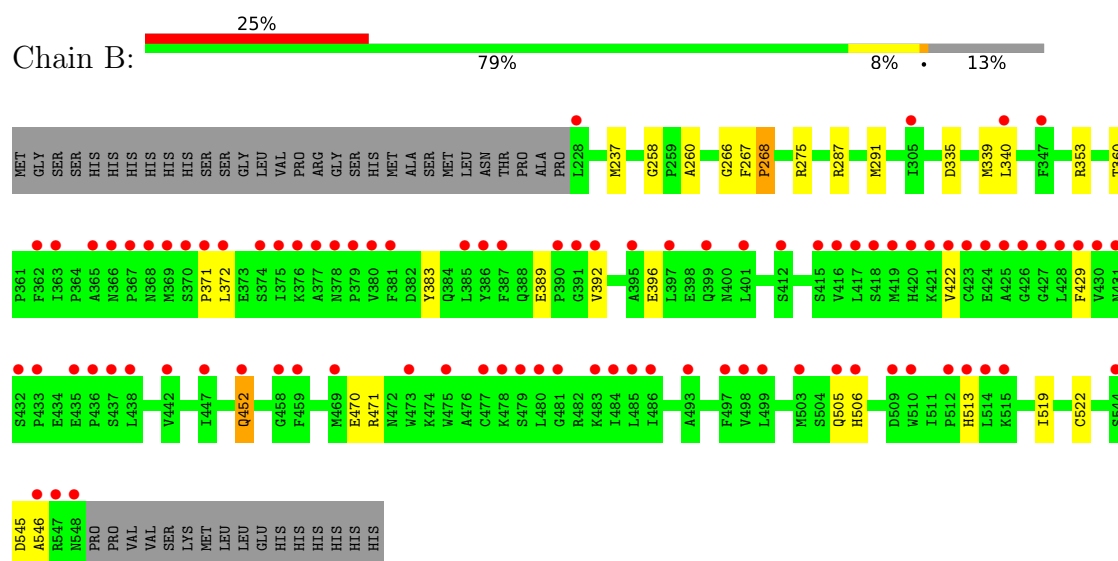
3 Residue-property plots [i](#)

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: 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, α , β , γ	47.28Å 80.34Å 89.25Å 90.00° 91.87° 90.00°	Depositor
Resolution (Å)	47.30 – 1.36 47.30 – 1.36	Depositor EDS
% Data completeness (in resolution range)	98.8 (47.30-1.36) 98.8 (47.30-1.36)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.61 (at 1.36Å)	Xtriage
Refinement program	REFMAC 5.8.0425	Depositor
R, R_{free}	0.194 , 0.215 0.204 , 0.222	Depositor DCC
R_{free} test set	7016 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.469	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.063 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5725	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 6.16% 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: EDO, A1H5J, PEG

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	0.59	0/2701	1.01	7/3672 (0.2%)
1	B	0.47	0/2706	0.88	4/3677 (0.1%)
All	All	0.54	0/5407	0.95	11/7349 (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	2
1	B	0	1
All	All	0	3

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	287	ARG	NE-CZ-NH2	-9.75	115.42	120.30
1	A	410	ARG	NE-CZ-NH2	9.02	124.81	120.30
1	B	275	ARG	NE-CZ-NH1	6.28	123.44	120.30
1	A	471	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	A	459	PHE	CB-CG-CD2	-5.70	116.81	120.80
1	B	237	MET	CG-SD-CE	5.38	108.81	100.20
1	B	471	ARG	N-CA-CB	-5.30	101.05	110.60
1	A	275	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	A	445	GLU	CG-CD-OE2	5.24	128.77	118.30
1	A	459	PHE	CB-CG-CD1	5.18	124.42	120.80
1	A	533	GLU	CG-CD-OE1	5.03	128.35	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	291	MET	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	2624	0	2498	26	0
1	B	2631	0	2497	16	0
2	A	24	0	36	4	0
2	B	4	0	6	0	0
3	A	35	0	0	2	0
3	B	35	0	0	0	0
4	B	7	0	10	3	0
5	A	242	0	0	10	0
5	B	123	0	0	4	0
All	All	5725	0	5047	42	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 4.

All (42) 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:A:528:MET:CE	5:A:750:HOH:O	2.37	0.73
1:B:396:GLU:OE2	1:B:429:PHE:N	2.21	0.69
1:A:528:MET:HE1	5:A:750:HOH:O	1.95	0.64
1:B:470:GLU:HB2	5:B:770:HOH:O	1.98	0.64
1:A:370:SER:CB	5:A:726:HOH:O	2.48	0.62
1:A:425:ALA:HB1	1:A:430:VAL:HG21	1.83	0.60
1:A:287:ARG:HD3	2:A:606:EDO:H21	1.84	0.60
1:B:258:GLY:O	4:B:601:PEG:H11	2.03	0.59
1:A:283:GLN:HG2	5:A:771:HOH:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:383:TYR:HB3	1:B:422:VAL:HG21	1.88	0.55
1:A:399:GLN:HG2	5:A:767:HOH:O	2.06	0.55
1:B:372:LEU:CB	5:B:810:HOH:O	2.55	0.55
1:A:498:VAL:HG23	3:A:605:A1H5J:O11	2.08	0.53
1:A:480:LEU:HD12	1:A:482:ARG:HH21	1.74	0.53
1:A:460:ARG:HD3	5:A:927:HOH:O	2.09	0.53
1:B:266:GLY:HA3	1:B:335:ASP:HB3	1.92	0.51
1:A:339[A]:MET:HE3	5:A:902:HOH:O	2.09	0.51
1:A:283:GLN:OE1	2:A:602:EDO:H22	2.11	0.50
1:A:266:GLY:HA3	1:A:335:ASP:HB3	1.95	0.49
1:A:364:PRO:HG2	1:A:510:TRP:NE1	2.27	0.49
1:A:339[A]:MET:CE	5:A:902:HOH:O	2.60	0.49
1:B:452[A]:GLN:HG3	5:B:815:HOH:O	2.13	0.49
1:A:528:MET:HE2	5:A:750:HOH:O	2.07	0.47
1:A:343[B]:TYR:CD1	1:A:475:TRP:CZ3	3.03	0.46
1:B:353:ARG:NH2	1:B:546:ALA:O	2.48	0.46
1:A:278:ILE:HB	1:A:279:PRO:HD3	1.98	0.45
1:B:260:ALA:CB	4:B:601:PEG:H31	2.46	0.45
1:B:340:LEU:C	1:B:340:LEU:HD23	2.36	0.45
1:A:430:VAL:HG23	1:A:431:ASN:ND2	2.31	0.45
1:A:496:ASP:HA	3:A:605:A1H5J:C41	2.47	0.45
1:A:364:PRO:CG	1:A:510:TRP:NE1	2.81	0.44
1:A:339[A]:MET:CE	1:A:339[A]:MET:HA	2.48	0.44
1:B:339[A]:MET:HE2	1:B:360:THR:CG2	2.49	0.43
2:A:607:EDO:H11	1:B:258:GLY:HA2	2.01	0.43
1:B:505:GLN:O	1:B:506:HIS:HB2	2.19	0.42
1:A:506:HIS:HD2	5:A:907:HOH:O	2.02	0.42
1:A:258:GLY:O	2:A:606:EDO:H12	2.20	0.42
1:A:257:SER:HB2	4:B:601:PEG:H12	2.01	0.42
1:B:519:ILE:HG22	1:B:522:CYS:HB2	2.02	0.41
1:B:513:HIS:HB3	5:B:818:HOH:O	2.20	0.41
1:A:339[A]:MET:HA	1:A:339[A]:MET:HE2	2.03	0.40
1:B:267:PHE:HA	1:B:268:PRO:HA	1.97	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	331/367 (90%)	321 (97%)	9 (3%)	1 (0%)	37	17
1	B	333/367 (91%)	320 (96%)	11 (3%)	2 (1%)	22	6
All	All	664/734 (90%)	641 (96%)	20 (3%)	3 (0%)	25	7

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	392	VAL
1	A	268	PRO
1	B	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	276/323 (85%)	272 (99%)	4 (1%)	62	33
1	B	275/323 (85%)	270 (98%)	5 (2%)	54	23
All	All	551/646 (85%)	542 (98%)	9 (2%)	65	27

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	452[A]	GLN
1	A	452[B]	GLN
1	A	480	LEU

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Mol	Chain	Res	Type
1	A	545	ASP
1	B	371	PRO
1	B	389	GLU
1	B	452[A]	GLN
1	B	452[B]	GLN
1	B	545	ASP

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

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	A1H5J	B	603	-	33,38,38	0.60	0	42,59,59	1.06	2 (4%)
2	EDO	A	603	-	3,3,3	0.09	0	2,2,2	0.29	0
2	EDO	A	607	-	3,3,3	0.30	0	2,2,2	0.28	0
2	EDO	A	604	-	3,3,3	0.42	0	2,2,2	0.67	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	A	606	-	3,3,3	0.53	0	2,2,2	0.69	0
3	A1H5J	A	605	-	33,38,38	0.86	1 (3%)	42,59,59	1.11	2 (4%)
2	EDO	A	602	-	3,3,3	0.13	0	2,2,2	0.19	0
2	EDO	A	601	-	3,3,3	0.14	0	2,2,2	0.02	0
2	EDO	B	602	-	3,3,3	0.51	0	2,2,2	0.33	0
4	PEG	B	601	-	6,6,6	0.52	0	5,5,5	0.45	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	A1H5J	B	603	-	-	7/27/37/37	0/4/4/4
2	EDO	A	603	-	-	1/1/1/1	-
2	EDO	A	607	-	-	1/1/1/1	-
2	EDO	A	604	-	-	1/1/1/1	-
2	EDO	A	606	-	-	1/1/1/1	-
3	A1H5J	A	605	-	-	5/27/37/37	0/4/4/4
2	EDO	A	602	-	-	1/1/1/1	-
2	EDO	A	601	-	-	0/1/1/1	-
2	EDO	B	602	-	-	0/1/1/1	-
4	PEG	B	601	-	-	3/4/4/4	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	605	A1H5J	S2-N9	3.24	1.69	1.62

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	605	A1H5J	O10-S1-C6	4.11	115.65	108.55
3	B	603	A1H5J	O10-S1-C6	2.91	113.58	108.55
3	B	603	A1H5J	O9-S1-C6	-2.85	103.64	108.55
3	A	605	A1H5J	C3-C4-C5	-2.02	116.60	119.70

There are no chirality outliers.

All (20) torsion outliers are listed below:

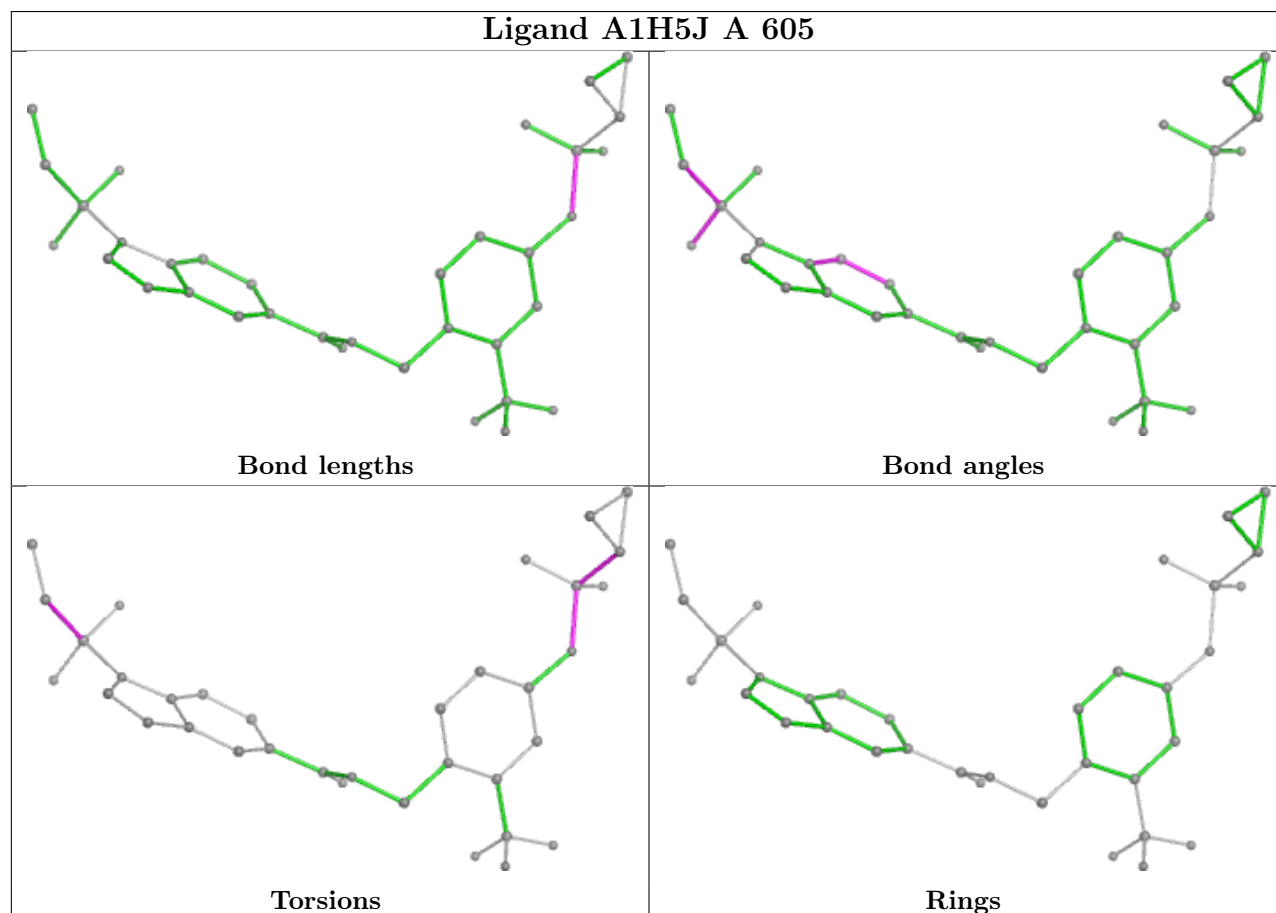
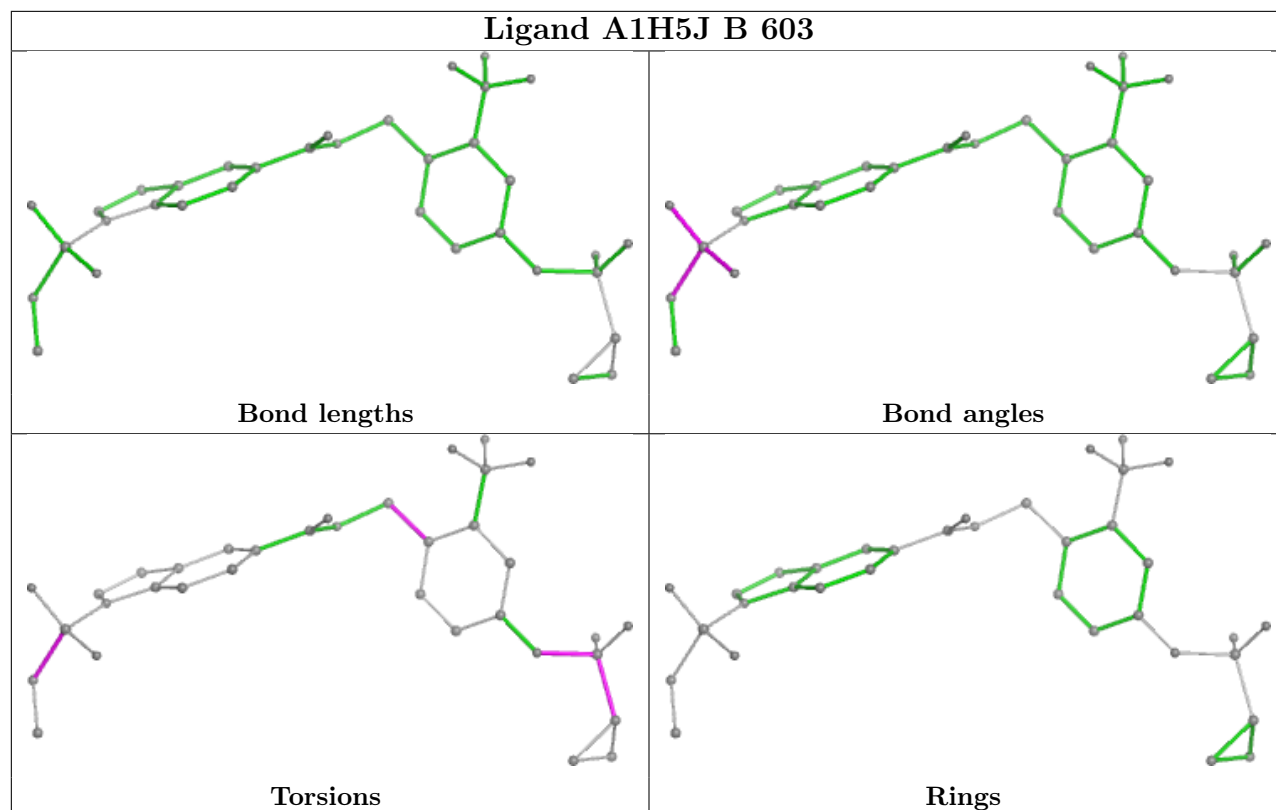
Mol	Chain	Res	Type	Atoms
3	A	605	A1H5J	C7-C6-S1-N1
3	A	605	A1H5J	C7-C6-S1-O10
3	B	603	A1H5J	C7-C6-S1-N1
3	B	603	A1H5J	C7-C6-S1-O9
3	B	603	A1H5J	C7-C6-S1-O10
3	B	603	A1H5J	C39-N9-S2-C40
3	B	603	A1H5J	C39-N9-S2-O11
3	B	603	A1H5J	C42-C40-S2-O11
4	B	601	PEG	O2-C3-C4-O4
2	A	606	EDO	O1-C1-C2-O2
3	A	605	A1H5J	C39-N9-S2-O12
4	B	601	PEG	C4-C3-O2-C2
4	B	601	PEG	O1-C1-C2-O2
3	A	605	A1H5J	C39-N9-S2-C40
2	A	604	EDO	O1-C1-C2-O2
2	A	607	EDO	O1-C1-C2-O2
3	A	605	A1H5J	C41-C40-S2-O12
2	A	602	EDO	O1-C1-C2-O2
2	A	603	EDO	O1-C1-C2-O2
3	B	603	A1H5J	N8-C34-C35-C44

There are no ring outliers.

5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	607	EDO	1	0
2	A	606	EDO	2	0
3	A	605	A1H5J	2	0
2	A	602	EDO	1	0
4	B	601	PEG	3	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%)	0.76	41 (12%)	9 11	8, 19, 55, 81	12 (3%)
1	B	321/367 (87%)	1.62	90 (28%)	2 2	8, 29, 73, 89	14 (4%)
All	All	642/734 (87%)	1.19	131 (20%)	3 4	8, 23, 65, 89	26 (4%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	480	LEU	8.1
1	B	548	ASN	6.5
1	B	368	ASN	6.2
1	B	546	ALA	6.0
1	B	420	HIS	5.8
1	B	417	LEU	5.6
1	B	422	VAL	5.6
1	A	372	LEU	5.4
1	B	547[A]	ARG	5.4
1	B	380	VAL	5.4
1	B	479	SER	5.4
1	B	375	ILE	5.1
1	A	548	ASN	5.1
1	A	381	PHE	5.0
1	B	377	ALA	4.9
1	B	428	LEU	4.8
1	B	421	LYS	4.8
1	B	363[A]	ILE	4.7
1	A	547[A]	ARG	4.7
1	B	430	VAL	4.7
1	B	416	VAL	4.6
1	B	370	SER	4.6
1	A	380	VAL	4.6
1	B	365	ALA	4.5

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Mol	Chain	Res	Type	RSRZ
1	B	371	PRO	4.5
1	B	381	PHE	4.3
1	B	418	SER	4.3
1	B	385	LEU	4.2
1	B	378	ASN	4.1
1	A	418	SER	4.1
1	B	347	PHE	4.0
1	B	481	GLY	4.0
1	B	510	TRP	3.9
1	B	425	ALA	3.9
1	A	506	HIS	3.9
1	A	377	ALA	3.9
1	B	392	VAL	3.8
1	A	370	SER	3.8
1	B	506	HIS	3.8
1	B	485	LEU	3.7
1	B	362	PHE	3.6
1	A	417	LEU	3.6
1	A	375	ILE	3.6
1	A	430	VAL	3.6
1	B	305	ILE	3.6
1	B	423	CYS	3.5
1	B	429	PHE	3.5
1	B	379	PRO	3.5
1	A	385[A]	LEU	3.5
1	A	368	ASN	3.5
1	A	419	MET	3.5
1	A	379	PRO	3.5
1	B	367	PRO	3.5
1	B	493	ALA	3.4
1	A	421	LYS	3.4
1	A	481	GLY	3.4
1	B	391	GLY	3.4
1	B	473	TRP	3.4
1	B	395	ALA	3.4
1	A	374	SER	3.4
1	A	428	LEU	3.4
1	B	372	LEU	3.4
1	B	374	SER	3.4
1	B	228	LEU	3.3
1	B	514	LEU	3.3
1	B	458	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	505	GLN	3.3
1	A	510	TRP	3.3
1	A	420	HIS	3.3
1	B	438	LEU	3.2
1	B	412[A]	SER	3.2
1	B	426	GLY	3.2
1	A	228	LEU	3.2
1	B	437	SER	3.2
1	A	480	LEU	3.1
1	A	369	MET	3.0
1	A	431	ASN	3.0
1	B	415	SER	3.0
1	B	544	SER	3.0
1	B	397	LEU	3.0
1	B	442	VAL	3.0
1	B	475	TRP	2.9
1	A	383	TYR	2.9
1	A	425	ALA	2.9
1	B	512	PRO	2.9
1	A	422	VAL	2.9
1	B	477	CYS	2.8
1	B	469	MET	2.8
1	B	497	PHE	2.8
1	A	367	PRO	2.8
1	A	371	PRO	2.8
1	B	483	LYS	2.8
1	B	431	ASN	2.8
1	A	426	GLY	2.8
1	B	515	LYS	2.7
1	A	373	GLU	2.7
1	B	390	PRO	2.7
1	B	436	PRO	2.7
1	B	399	GLN	2.7
1	B	369	MET	2.6
1	B	427	GLY	2.6
1	B	484	ILE	2.6
1	B	386	TYR	2.6
1	B	401	LEU	2.5
1	A	378	ASN	2.5
1	B	452[A]	GLN	2.5
1	B	513	HIS	2.5
1	B	433	PRO	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	469	MET	2.4
1	B	435	GLU	2.4
1	A	246	PRO	2.4
1	B	478	LYS	2.4
1	A	438	LEU	2.4
1	B	387	PHE	2.4
1	B	376	LYS	2.4
1	B	419	MET	2.4
1	B	366	ASN	2.3
1	A	363[A]	ILE	2.3
1	B	340	LEU	2.3
1	B	509	ASP	2.3
1	B	424	GLU	2.3
1	B	498	VAL	2.2
1	B	499	LEU	2.2
1	B	486	ILE	2.2
1	A	399	GLN	2.1
1	B	447	ILE	2.1
1	A	451	VAL	2.1
1	B	432[A]	SER	2.1
1	B	503	MET	2.0
1	B	459	PHE	2.0
1	A	432[A]	SER	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

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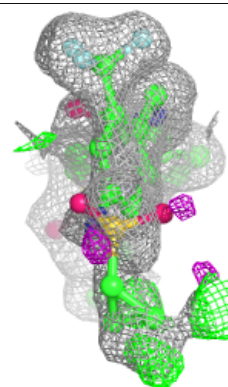
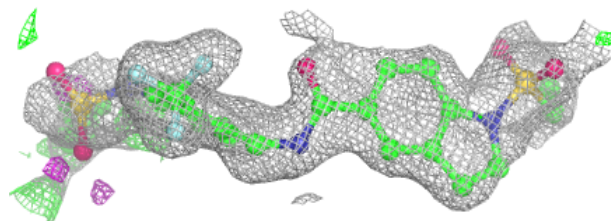
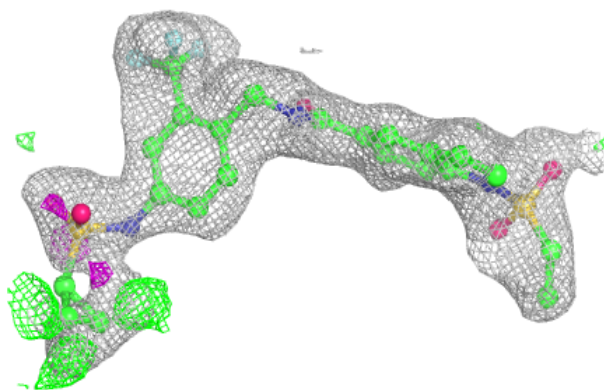
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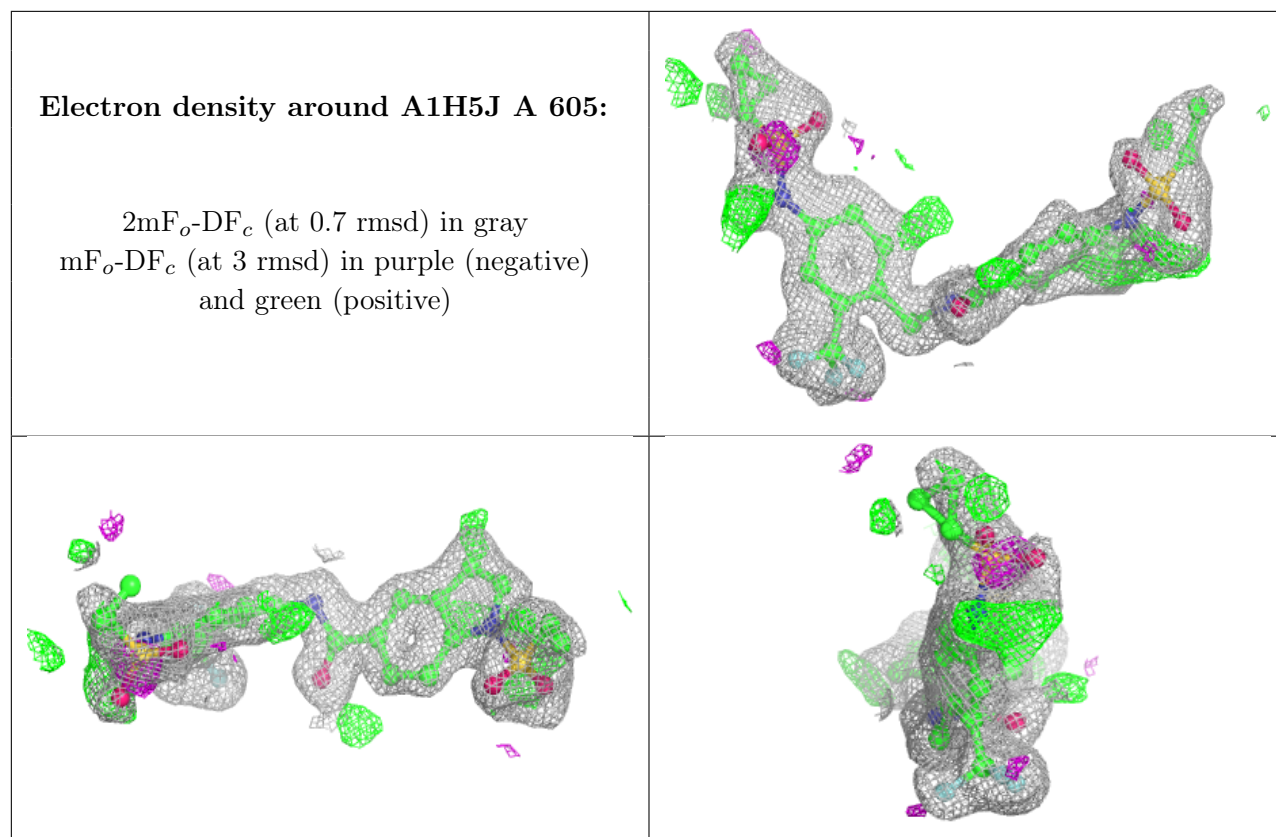
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	EDO	A	607	4/4	0.73	0.17	33,36,40,41	0
3	A1H5J	B	603	35/35	0.74	0.19	35,45,70,72	35
2	EDO	A	602	4/4	0.80	0.16	36,41,41,42	0
2	EDO	A	603	4/4	0.80	0.15	42,48,50,58	0
3	A1H5J	A	605	35/35	0.83	0.17	20,26,46,53	35
2	EDO	A	604	4/4	0.88	0.11	24,27,27,28	0
4	PEG	B	601	7/7	0.88	0.15	26,38,41,43	0
2	EDO	A	606	4/4	0.89	0.11	22,24,29,30	0
2	EDO	B	602	4/4	0.92	0.10	25,27,31,31	0
2	EDO	A	601	4/4	0.94	0.08	24,27,29,29	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 A1H5J B 603:

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.