



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 13, 2021 – 11:11 am BST

PDB ID : 6ZM2
Title : Crystal structure of the DEAH-box ATPase Prp2 in complex with ADP-BeF3 and ssRNA
Authors : Hamann, F.; Ficner, R.
Deposited on : 2020-07-01
Resolution : 2.10 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.18
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.18

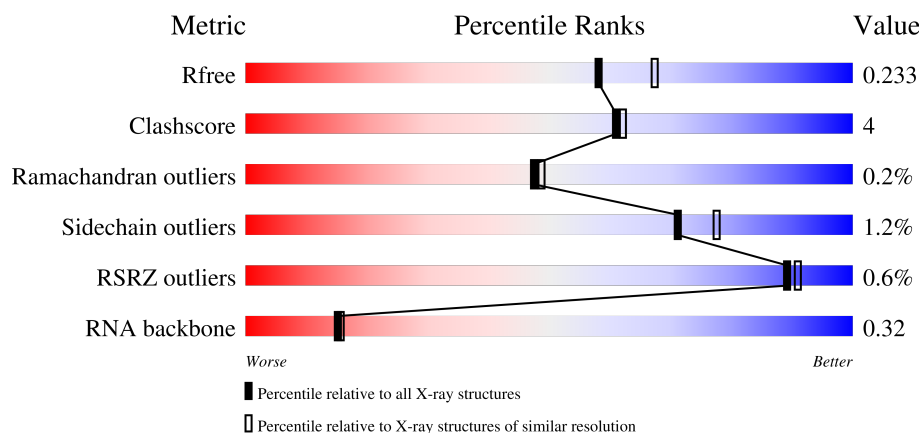
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


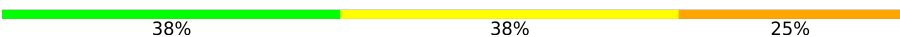
The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5197 (2.10-2.10)
Clashscore	141614	5710 (2.10-2.10)
Ramachandran outliers	138981	5647 (2.10-2.10)
Sidechain outliers	138945	5648 (2.10-2.10)
RSRZ outliers	127900	5083 (2.10-2.10)
RNA backbone	3102	1000 (2.54-1.66)

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	636	
2	B	8	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
12	POL	A	1118	-	-	-	X

2 Entry composition [i](#)

There are 14 unique types of molecules in this entry. The entry contains 5355 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.

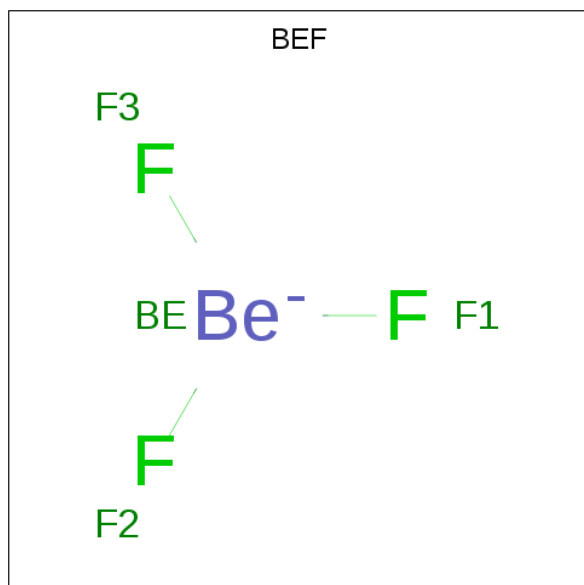
- Molecule 1 is a protein called Putative mRNA splicing factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	627	4851	3080	829	917	25	1	3	0

- Molecule 2 is a RNA chain called RNA (5'-R(P*UP*UP*UP*UP*UP*U)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	B	8	136	59	12	57	8	0	0	0

- Molecule 3 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	Be	F		
3	A	1	4	1	3	0	0

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:

The image displays the chemical structure of Adenosine Diphosphate (ADP). It consists of an adenine base (a purine ring system with an amino group at C6) attached to a ribose sugar (a five-membered ring). The ribose sugar is linked to a diphosphate group (two phosphate groups connected by an oxygen atom). The atoms are labeled with their respective element symbols and numbers: N1, N3, N7, N9 for the nitrogen atoms in the adenine base; C2, C4, C5, C6, C8 for the carbon atoms in the adenine base; C1', C2', C3', C4', C5' for the carbon atoms in the ribose sugar; and O1A, O2A, O3A, O4A, O5A, O1B, O2B, O3B, O4B, O5B for the oxygen atoms in the phosphate groups. The structure is shown in a 3D representation with wedges and dashes indicating stereochemistry.

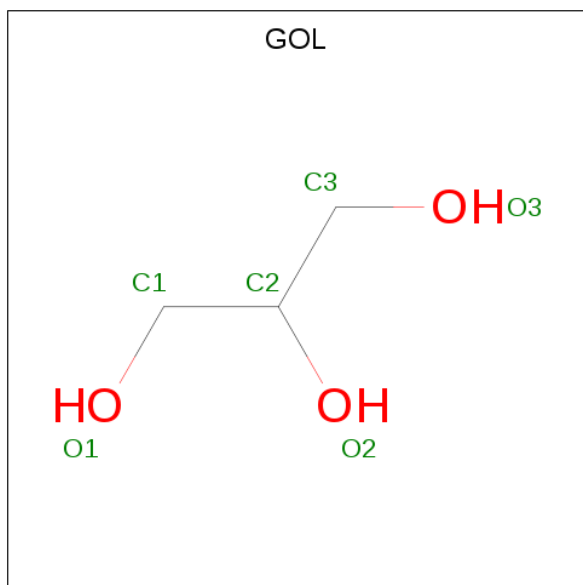
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 5 | A | 1 | Total Mg
1 1 | 0 | 0 |

-
- The diagram illustrates the chemical structure of Polyethylene Glycol (PEG), a linear polymer. It shows a repeating unit consisting of carbon (C) and oxygen (O) atoms. The structure is labeled with green text: C1, C2, C3, C4 for carbon atoms and O1, O2 for oxygen atoms. The terminal groups are hydroxyl (OH) groups, also labeled with green text. The structure is shown in a zig-zag conformation, with the terminal OH groups at the ends of the chain.

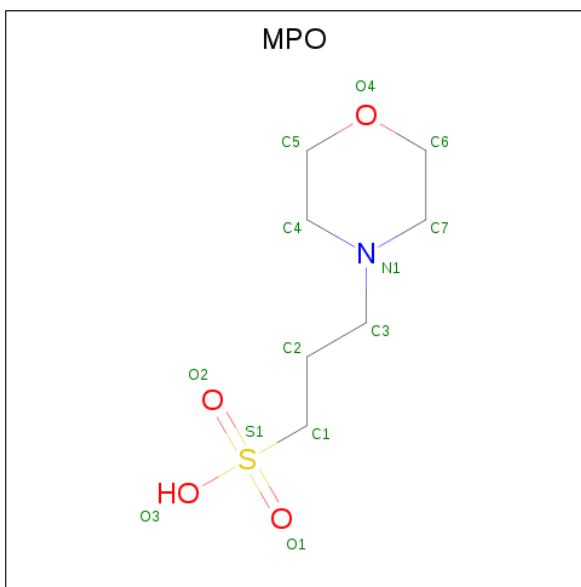
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: $C_7H_{15}NO_4S$).

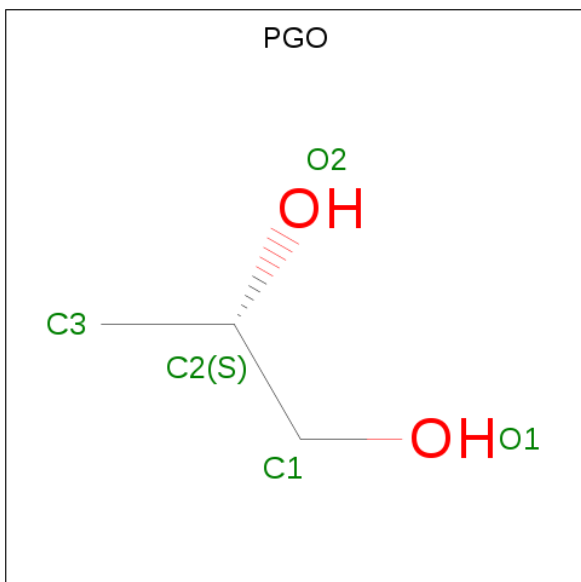


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
8	A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 9 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

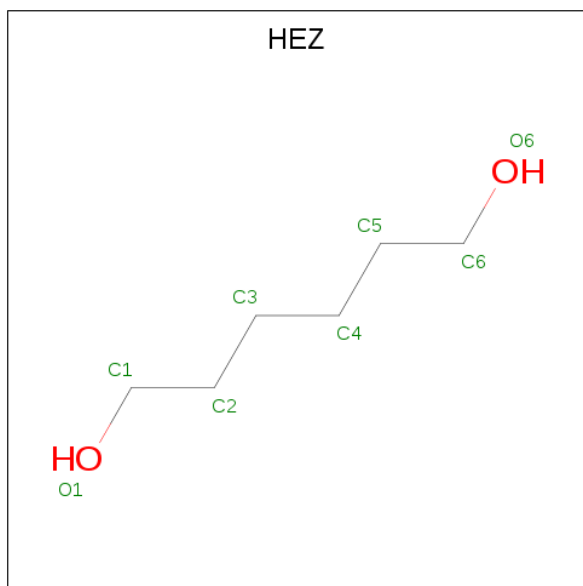
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Cl	0	0
			1	1		

- Molecule 10 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: C₃H₈O₂).



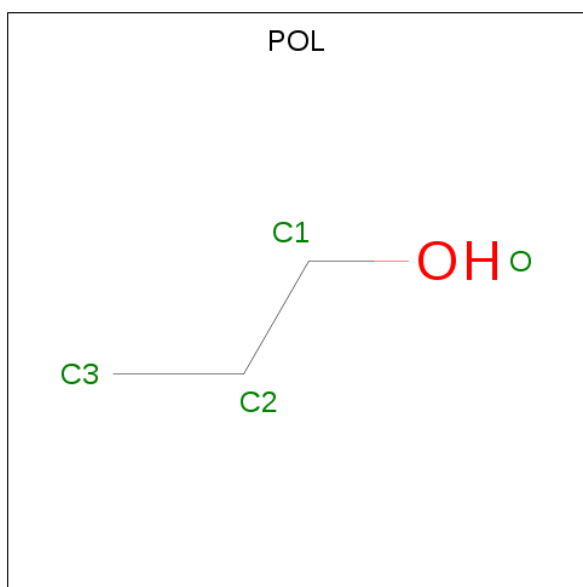
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			5	3	2		
10	A	1	Total	C	O	0	0
			5	3	2		
10	A	1	Total	C	O	0	0
			5	3	2		

- Molecule 11 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 12 is N-PROPANOL (three-letter code: POL) (formula: C_3H_8O).



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

- Molecule 13 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



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

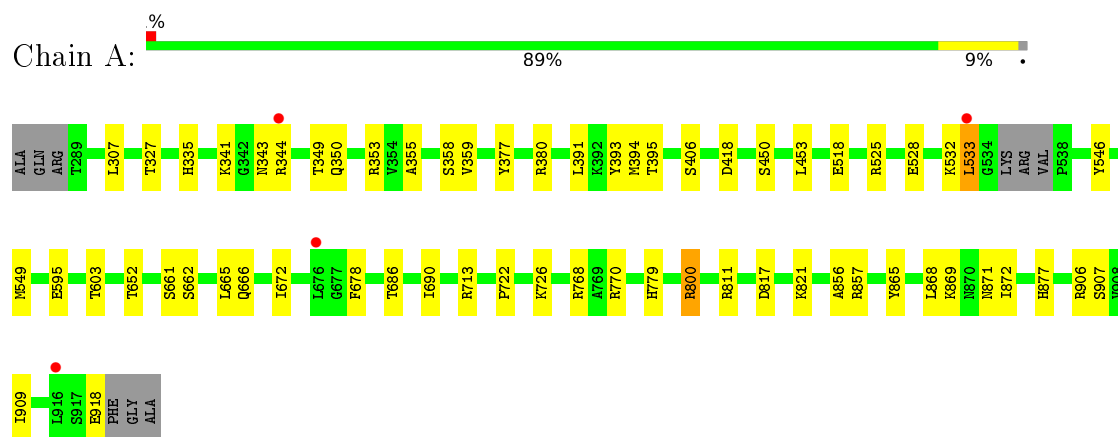
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	184	Total	O	0	3
			187	187		
14	B	13	Total	O	0	0
			13	13		

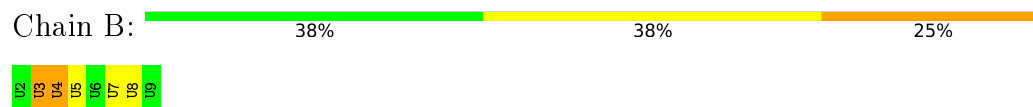
3 Residue-property plots [i](#)

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: Putative mRNA splicing factor



- Molecule 2: RNA (5'-R(P*UP*UP*UP*UP*UP*UP*U)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	48.66Å 100.41Å 140.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	81.78 – 2.10 81.78 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.5 (81.78-2.10) 99.5 (81.78-2.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.20 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.185 , 0.233 0.187 , 0.233	Depositor DCC
R_{free} test set	2051 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	36.4	Xtriage
Anisotropy	0.535	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 56.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5355	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: GOL, CL, PEG, EDO, POL, HEZ, BEF, MG, MPO, ADP, CSO, PGO

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	0.27	0/4947	0.47	0/6725
2	B	0.33	0/148	1.01	0/227
All	All	0.27	0/5095	0.50	0/6952

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4851	0	4861	45	0
2	B	136	0	66	3	0
3	A	4	0	0	0	0
4	A	27	0	12	0	0
5	A	1	0	0	0	0
6	A	28	0	40	3	0
7	A	6	0	8	0	0
8	A	26	0	28	1	0
9	A	1	0	0	0	0
10	A	15	0	24	3	0
11	A	8	0	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
12	A	36	0	72	9	0
13	A	16	0	24	0	0
14	A	187	0	0	3	0
14	B	13	0	0	0	0
All	All	5355	0	5149	46	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 (46) 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:713:ARG:HD2	12:A:1120:POL:H12	1.66	0.78
1:A:532:LYS:HB3	1:A:533:LEU:HD22	1.76	0.68
1:A:603:THR:H	10:A:1113:PGO:H2	1.61	0.65
1:A:450:SER:HB3	1:A:453:LEU:HB2	1.78	0.64
1:A:877:HIS:CD2	1:A:906:ARG:HD3	2.35	0.62
1:A:307:LEU:HB3	12:A:1118:POL:H11	1.82	0.61
1:A:661:SER:HB3	1:A:722:PRO:HG2	1.82	0.60
1:A:726:LYS:HE3	6:A:1107:PEG:H31	1.83	0.58
1:A:869:LYS:HE3	6:A:1105:PEG:H31	1.86	0.58
1:A:595:GLU:OE2	12:A:1121:POL:H21	2.05	0.56
1:A:652:THR:H	12:A:1121:POL:H22	1.70	0.56
1:A:768:ARG:NH2	10:A:1114:PGO:O1	2.38	0.56
1:A:800:ARG:HD3	1:A:800:ARG:C	2.26	0.55
1:A:406:SER:HB2	8:A:1110:MPO:H71	1.90	0.53
1:A:327:THR:OG1	1:A:418:ASP:OD2	2.25	0.53
1:A:872:ILE:HD12	10:A:1113:PGO:H31	1.91	0.53
1:A:343:ASN:ND2	14:A:1205:HOH:O	2.41	0.53
1:A:857:ARG:HG3	1:A:868:LEU:HD21	1.92	0.52
1:A:358[A]:SER:HA	11:A:1115:HEZ:H11	1.91	0.52
1:A:358[B]:SER:HA	11:A:1115:HEZ:H11	1.91	0.51
2:B:3:U:O2'	2:B:4:U:H5''	2.10	0.51
1:A:549[A]:MET:HA	12:A:1122:POL:H11	1.93	0.50
1:A:353:ARG:HG3	2:B:7:U:H5''	1.94	0.49
1:A:380:ARG:HD2	2:B:8:U:H2'	1.95	0.48
1:A:344:ARG:HG2	14:A:1353:HOH:O	2.12	0.48
1:A:672:ILE:HD13	1:A:678:PHE:CE1	2.48	0.48
1:A:377:TYR:HA	1:A:393:TYR:O	2.13	0.48
1:A:355:ALA:O	1:A:359:VAL:HG22	2.15	0.47
1:A:652:THR:H	12:A:1121:POL:C2	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:THR:HA	1:A:394:MET:O	2.16	0.46
1:A:713:ARG:CD	12:A:1120:POL:H12	2.42	0.45
1:A:549[B]:MET:HA	12:A:1122:POL:H11	1.97	0.45
1:A:779:HIS:ND1	1:A:909:ILE:HG23	2.32	0.45
1:A:335:HIS:HB2	1:A:391:LEU:HD11	1.99	0.44
1:A:546:TYR:O	1:A:549[A]:MET:HG2	2.19	0.43
1:A:686:THR:O	1:A:690:ILE:HG12	2.18	0.43
1:A:811:ARG:HH11	12:A:1123:POL:H21	1.83	0.42
1:A:518:GLU:HG2	14:A:1329:HOH:O	2.19	0.42
1:A:662:SER:O	1:A:666:GLN:HG3	2.20	0.42
1:A:726:LYS:CE	6:A:1107:PEG:H31	2.49	0.42
1:A:525:ARG:NH1	1:A:528:GLU:OE1	2.50	0.42
1:A:665:LEU:HD23	1:A:665:LEU:HA	1.90	0.42
1:A:350:GLN:O	1:A:395:THR:HA	2.20	0.41
1:A:856:ALA:HB1	1:A:865:TYR:HB3	2.03	0.41
1:A:546:TYR:O	1:A:549[B]:MET:HG2	2.21	0.41
1:A:817:ASP:O	1:A:821:LYS:HG2	2.21	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	625/636 (98%)	610 (98%)	14 (2%)	1 (0%)	47 49

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	907	SER

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	522/538 (97%)	516 (99%)	6 (1%)	73	79

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	341	LYS
1	A	533	LEU
1	A	770	ARG
1	A	800	ARG
1	A	871	ASN
1	A	918	GLU

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

5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	6/8 (75%)	3 (50%)	0

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	3	U
2	B	4	U
2	B	5	U

There are no RNA pucker outliers to report.

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

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
1	CSO	A	384	1	3,6,7	0.70	0	0,6,8	0.00	-

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
1	CSO	A	384	1	-	0/1/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 28 ligands modelled in this entry, 2 are monoatomic - leaving 26 for Mogul analysis.

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
8	MPO	A	1110	-	13,13,13	1.04	1 (7%)	17,17,17	1.59	3 (17%)
12	POL	A	1116	-	3,3,3	0.36	0	2,2,2	0.29	0
10	PGO	A	1113	-	3,4,4	0.15	0	1,4,4	0.22	0
6	PEG	A	1105	-	6,6,6	0.12	0	5,5,5	0.08	0
6	PEG	A	1104	-	6,6,6	0.12	0	5,5,5	0.08	0
6	PEG	A	1106	-	6,6,6	0.16	0	5,5,5	0.10	0
10	PGO	A	1112	-	3,4,4	0.15	0	1,4,4	0.03	0
12	POL	A	1117	-	3,3,3	0.36	0	2,2,2	0.28	0
13	EDO	A	1126	-	3,3,3	0.46	0	2,2,2	0.34	0
6	PEG	A	1107	-	6,6,6	0.12	0	5,5,5	0.09	0
12	POL	A	1124	-	3,3,3	0.27	0	2,2,2	0.26	0
11	HEZ	A	1115	-	7,7,7	0.30	0	6,6,6	0.39	0
12	POL	A	1120	-	3,3,3	0.29	0	2,2,2	0.23	0
7	GOL	A	1108	-	5,5,5	0.88	0	5,5,5	1.00	0
3	BEF	A	1101	4	0,3,3	0.00	-	-	-	-
13	EDO	A	1127	-	3,3,3	0.45	0	2,2,2	0.34	0
12	POL	A	1119	-	3,3,3	0.35	0	2,2,2	0.30	0
13	EDO	A	1128	-	3,3,3	0.38	0	2,2,2	0.28	0
4	ADP	A	1102	3,5	24,29,29	1.02	2 (8%)	29,45,45	1.22	3 (10%)
8	MPO	A	1109	-	13,13,13	0.94	1 (7%)	17,17,17	1.94	4 (23%)
10	PGO	A	1114	-	3,4,4	0.19	0	1,4,4	0.00	0
12	POL	A	1121	-	3,3,3	0.23	0	2,2,2	0.38	0
12	POL	A	1122	-	3,3,3	0.27	0	2,2,2	0.19	0
12	POL	A	1118	-	3,3,3	0.34	0	2,2,2	0.40	0
12	POL	A	1123	-	3,3,3	0.26	0	2,2,2	0.25	0
13	EDO	A	1125	-	3,3,3	0.46	0	2,2,2	0.27	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
8	MPO	A	1110	-	-	5/7/15/15	0/1/1/1
12	POL	A	1116	-	-	0/1/1/1	-
10	PGO	A	1113	-	-	2/2/2/2	-
6	PEG	A	1105	-	-	2/4/4/4	-
6	PEG	A	1104	-	-	3/4/4/4	-
6	PEG	A	1106	-	-	0/4/4/4	-
10	PGO	A	1112	-	-	0/2/2/2	-
12	POL	A	1117	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
13	EDO	A	1126	-	-	0/1/1/1	-
6	PEG	A	1107	-	-	1/4/4/4	-
12	POL	A	1124	-	-	1/1/1/1	-
11	HEZ	A	1115	-	-	2/5/5/5	-
12	POL	A	1120	-	-	0/1/1/1	-
7	GOL	A	1108	-	-	0/4/4/4	-
13	EDO	A	1127	-	-	0/1/1/1	-
12	POL	A	1119	-	-	0/1/1/1	-
13	EDO	A	1128	-	-	1/1/1/1	-
4	ADP	A	1102	3,5	-	2/12/32/32	0/3/3/3
8	MPO	A	1109	-	-	5/7/15/15	0/1/1/1
10	PGO	A	1114	-	-	2/2/2/2	-
12	POL	A	1121	-	-	0/1/1/1	-
12	POL	A	1122	-	-	1/1/1/1	-
12	POL	A	1118	-	-	0/1/1/1	-
12	POL	A	1123	-	-	1/1/1/1	-
13	EDO	A	1125	-	-	1/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1110	MPO	O1-S1	3.48	1.55	1.45
8	A	1109	MPO	O2-S1	3.07	1.54	1.45
4	A	1102	ADP	C5-C4	2.52	1.47	1.40
4	A	1102	ADP	O4'-C1'	2.02	1.43	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1109	MPO	C5-C4-N1	5.65	118.67	110.10
8	A	1110	MPO	O3-S1-O2	3.87	120.74	111.27
8	A	1110	MPO	O1-S1-C1	-3.55	102.64	106.92
4	A	1102	ADP	N3-C2-N1	-3.09	123.85	128.68
8	A	1109	MPO	O3-S1-O1	2.87	118.30	111.27
8	A	1109	MPO	O4-C5-C4	2.83	118.02	111.80
8	A	1109	MPO	O2-S1-C1	-2.61	103.77	106.92
4	A	1102	ADP	C4-C5-N7	-2.47	106.82	109.40
4	A	1102	ADP	PA-O3A-PB	-2.40	124.59	132.83
8	A	1110	MPO	O3-S1-O1	-2.17	105.97	111.27

There are no chirality outliers.

All (29) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1102	ADP	PA-O3A-PB-O2B
8	A	1110	MPO	S1-C1-C2-C3
10	A	1113	PGO	O1-C1-C2-C3
10	A	1113	PGO	O1-C1-C2-O2
8	A	1110	MPO	C2-C1-S1-O3
6	A	1107	PEG	O2-C3-C4-O4
8	A	1109	MPO	C1-C2-C3-N1
6	A	1104	PEG	O1-C1-C2-O2
6	A	1105	PEG	O2-C3-C4-O4
11	A	1115	HEZ	C4-C5-C6-O6
8	A	1109	MPO	C2-C1-S1-O2
8	A	1110	MPO	C2-C1-S1-O1
8	A	1110	MPO	C2-C1-S1-O2
10	A	1114	PGO	O1-C1-C2-O2
8	A	1110	MPO	C1-C2-C3-N1
11	A	1115	HEZ	O1-C1-C2-C3
10	A	1114	PGO	O1-C1-C2-C3
6	A	1104	PEG	C1-C2-O2-C3
13	A	1128	EDO	O1-C1-C2-O2
8	A	1109	MPO	C2-C3-N1-C4
8	A	1109	MPO	C2-C1-S1-O1
12	A	1122	POL	O-C1-C2-C3
12	A	1124	POL	O-C1-C2-C3
6	A	1104	PEG	O2-C3-C4-O4
8	A	1109	MPO	C2-C1-S1-O3
13	A	1125	EDO	O1-C1-C2-O2
12	A	1123	POL	O-C1-C2-C3
6	A	1105	PEG	O1-C1-C2-O2
4	A	1102	ADP	PA-O3A-PB-O1B

There are no ring outliers.

11 monomers are involved in 18 short contacts:

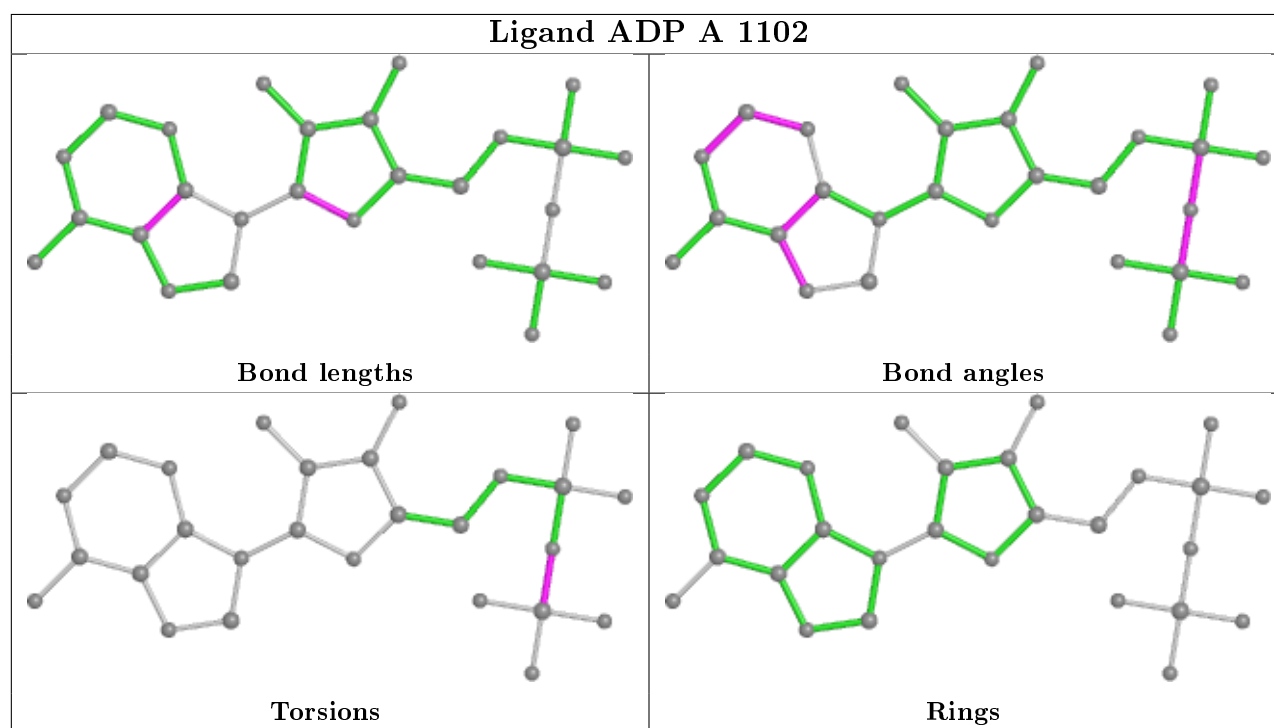
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1110	MPO	1	0
10	A	1113	PGO	2	0
6	A	1105	PEG	1	0
6	A	1107	PEG	2	0
11	A	1115	HEZ	2	0
12	A	1120	POL	2	0
10	A	1114	PGO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
12	A	1121	POL	3	0
12	A	1122	POL	2	0
12	A	1118	POL	1	0
12	A	1123	POL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	626/636 (98%)	-0.01	4 (0%) 89 91	27, 41, 70, 110	1 (0%)
2	B	8/8 (100%)	-0.18	0 100 100	41, 68, 101, 111	1 (12%)
All	All	634/644 (98%)	-0.01	4 (0%) 89 91	27, 41, 71, 111	2 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	533	LEU	2.9
1	A	676	LEU	2.5
1	A	916	LEU	2.3
1	A	344	ARG	2.3

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
1	CSO	A	384	7/8	0.96	0.11	31,38,44,59	0

6.3 Carbohydrates [i](#)

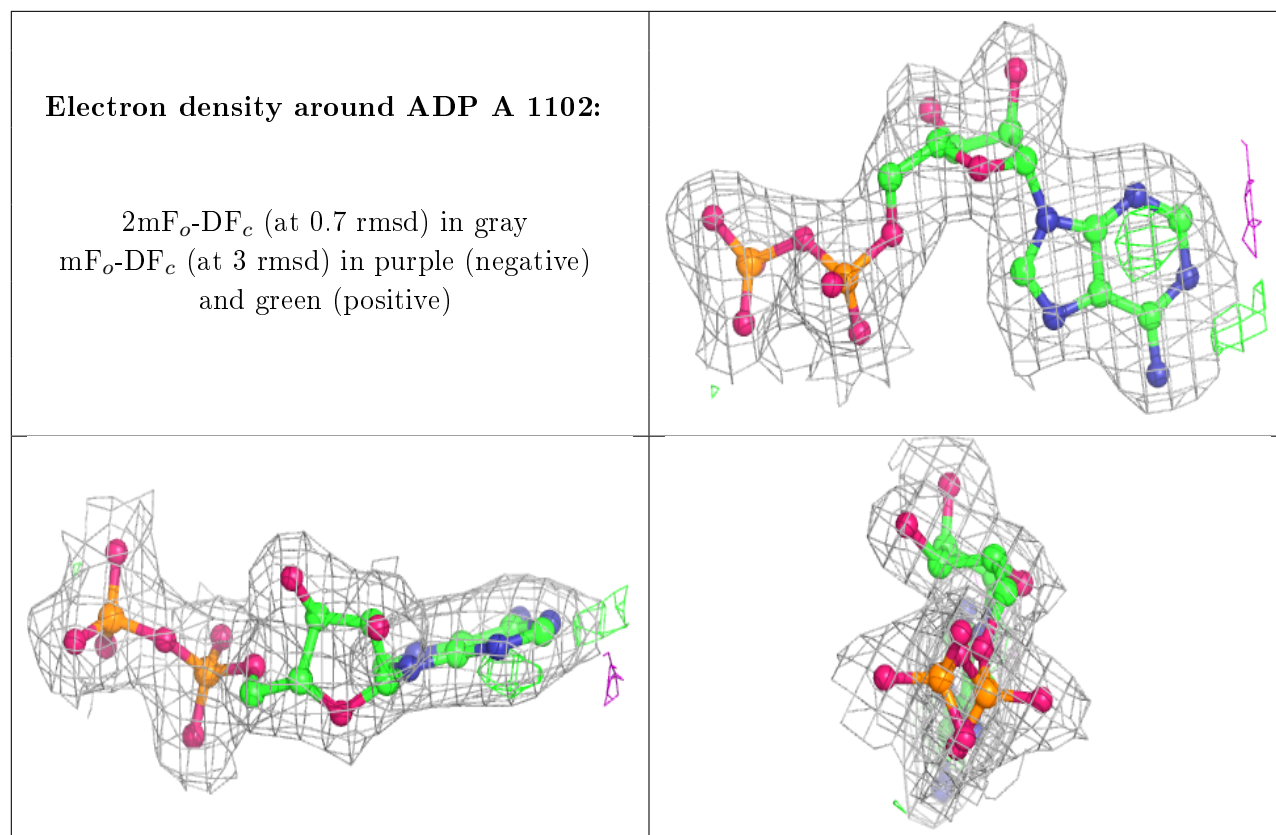
There are no monosaccharides in this entry.

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, 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(Å ²)	Q<0.9
13	EDO	A	1128	4/4	0.42	0.27	94,96,96,96	0
12	POL	A	1118	4/4	0.63	0.40	53,55,61,64	0
12	POL	A	1122	4/4	0.66	0.21	58,58,58,63	0
6	PEG	A	1105	7/7	0.71	0.21	68,68,76,77	0
9	CL	A	1111	1/1	0.73	0.12	78,78,78,78	0
12	POL	A	1124	4/4	0.74	0.21	55,64,64,65	0
12	POL	A	1120	4/4	0.80	0.18	68,71,73,78	0
12	POL	A	1119	4/4	0.80	0.20	74,74,75,78	0
6	PEG	A	1107	7/7	0.81	0.21	60,62,68,71	0
8	MPO	A	1109	13/13	0.82	0.21	72,74,88,97	0
10	PGO	A	1114	5/5	0.82	0.33	64,68,73,83	0
6	PEG	A	1104	7/7	0.83	0.15	63,68,69,70	0
6	PEG	A	1106	7/7	0.84	0.17	70,75,77,78	0
8	MPO	A	1110	13/13	0.84	0.32	68,77,105,107	0
12	POL	A	1116	4/4	0.85	0.20	72,73,74,74	0
13	EDO	A	1126	4/4	0.87	0.18	73,78,82,85	0
12	POL	A	1121	4/4	0.89	0.22	75,76,77,79	0
13	EDO	A	1125	4/4	0.89	0.26	39,54,58,60	0
11	HEZ	A	1115	8/8	0.89	0.19	37,44,54,66	0
12	POL	A	1123	4/4	0.89	0.15	71,72,74,74	0
10	PGO	A	1113	5/5	0.90	0.29	56,57,63,64	0
12	POL	A	1117	4/4	0.91	0.23	55,61,66,66	0
7	GOL	A	1108	6/6	0.92	0.15	46,53,58,58	0
5	MG	A	1103	1/1	0.93	0.13	34,34,34,34	0
10	PGO	A	1112	5/5	0.94	0.14	67,71,73,75	0
13	EDO	A	1127	4/4	0.95	0.15	61,66,66,69	0
3	BEF	A	1101	4/4	0.97	0.12	30,32,32,33	0
4	ADP	A	1102	27/27	0.97	0.12	29,33,37,40	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.