



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 02:29 PM UTC

PDB ID : 6ZM2 / pdb_00006zm2
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 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

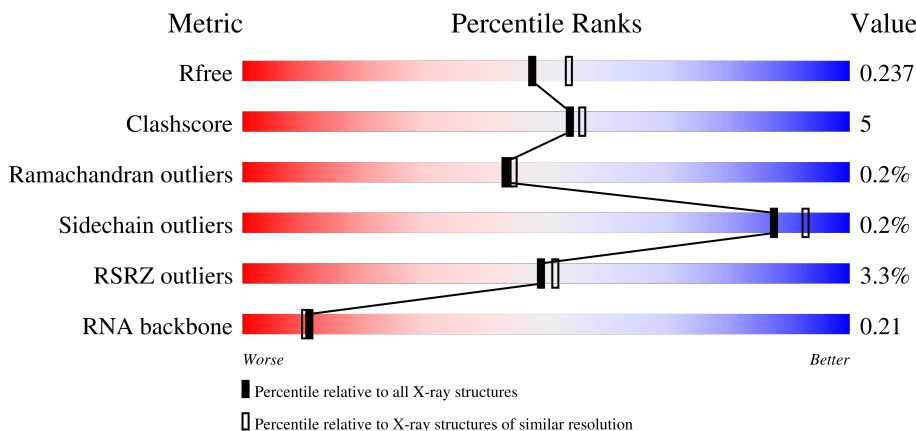
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)
RNA backbone	3983	1006 (2.42-1.78)

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	3% 89% 10%
2	B	8	12% 38% 38% 25%

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.

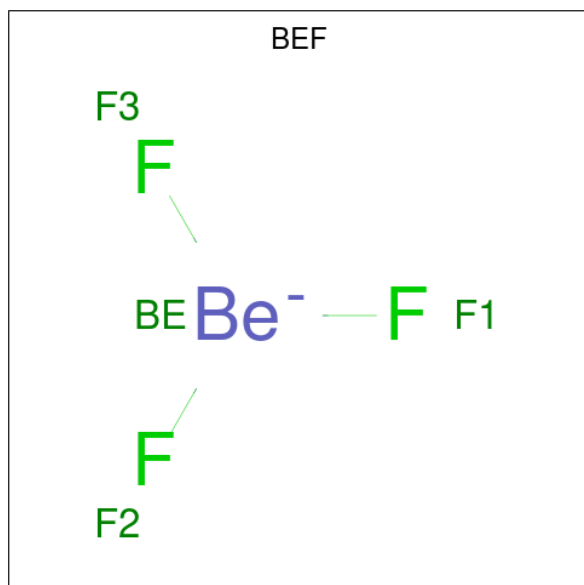
- Molecule 1 is a protein called Putative mRNA splicing factor.

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

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

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

- Molecule 3 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃).



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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).

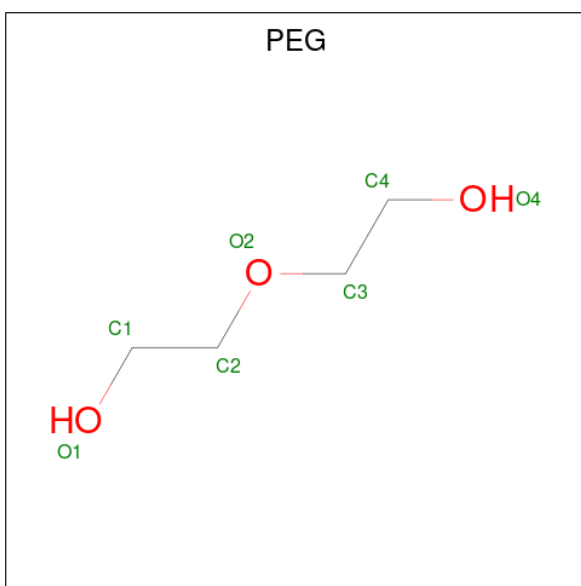


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



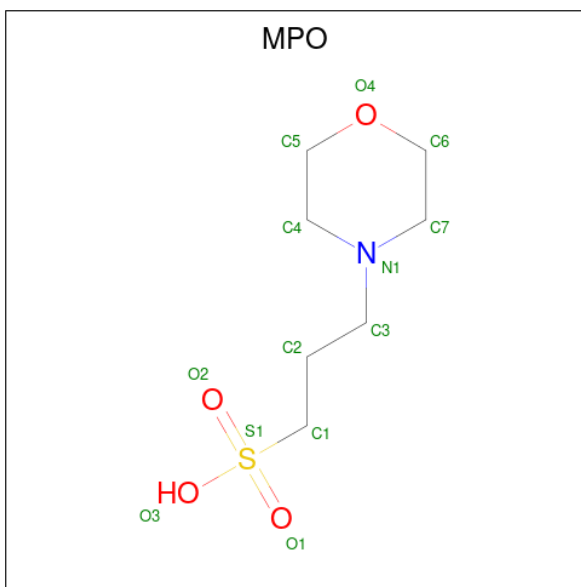
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is GLYCEROL (CCD ID: 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 (CCD ID: MPO) (formula: $C_7H_{15}NO_4S$).

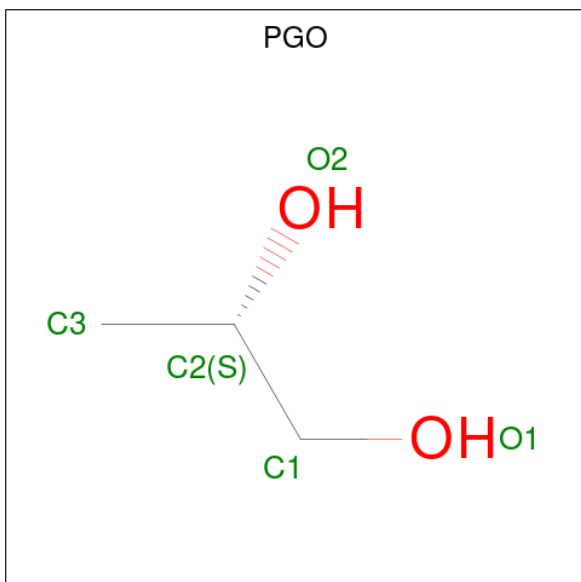


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		
8	A	1	Total	C	N	O	S	0	0
			13	7	1	4	1		

- Molecule 9 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

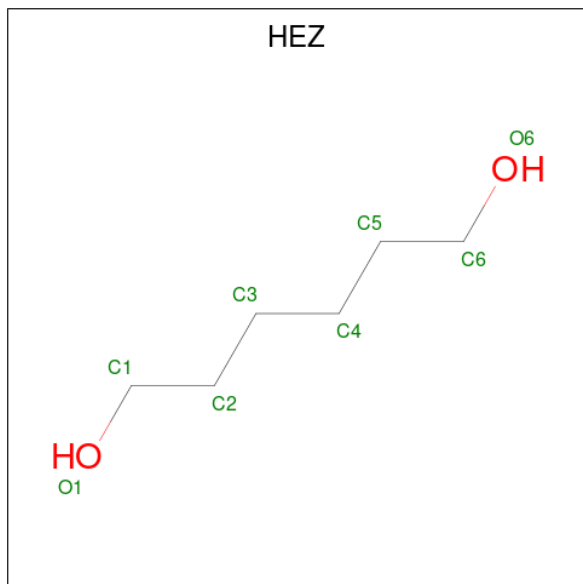
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	Cl	0	0
			1	1		

- Molecule 10 is S-1,2-PROPANEDIOL (CCD ID: PGO) (formula: C₃H₈O₂).



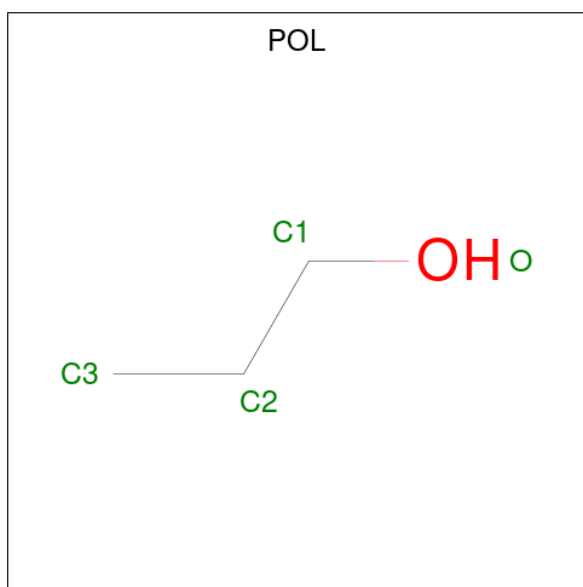
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			5	3	2		
10	A	1	Total	C	O	0	0
			5	3	2		
10	A	1	Total	C	O	0	0
			5	3	2		

- Molecule 11 is HEXANE-1,6-DIOL (CCD ID: 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 (CCD ID: 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 (CCD ID: 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		

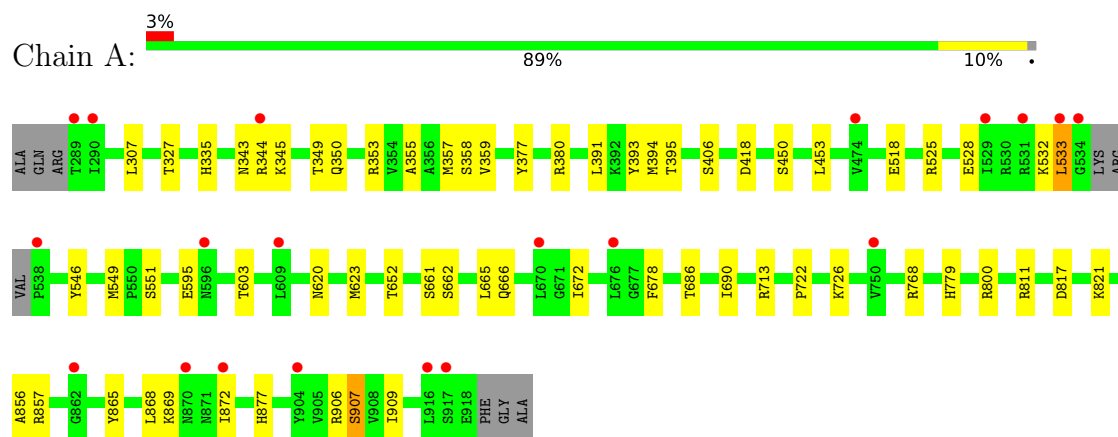
- Molecule 14 is water.

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

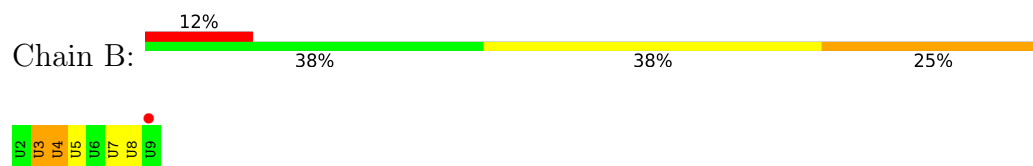
3 Residue-property plots [i](#)

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 0.189 , 0.237	Depositor DCC
R_{free} test set	2051 reflections (4.98%)	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 , 52.4	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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEZ, CL, GOL, POL, PEG, MPO, CSO, MG, ADP, BEF, PGO, 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	0.15	0/4947	0.40	0/6725
2	B	0.28	0/148	0.60	0/227
All	All	0.16	0/5095	0.40	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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4851	0	4861	49	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	1	0
14	A	187	0	0	4	0
14	B	13	0	0	0	0
All	All	5355	0	5149	50	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 5.

All (50) 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:800:ARG:HD3	1:A:800:ARG:C	2.26	0.60
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:345:LYS:NZ	14:A:1205:HOH:O	2.38	0.57
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:357:MET:HE1	1:A:551:SER:HB2	1.88	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:620:ASN:HA	1:A:623:MET:HE2	1.96	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
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:907:SER:H	13:A:1125:EDO:HO2	1.61	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%)	43	44

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%)	521 (100%)	1 (0%)	87 93

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	533	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	332	GLN
1	A	606	GLN
1	A	871	ASN

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 ⓘ

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	0.72	0	1,6,8	0.12	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
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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
12	POL	A	1124	-	3,3,3	0.26	0	2,2,2	0.27	0
10	PGO	A	1113	-	4,4,4	0.52	0	4,4,4	0.64	0
4	ADP	A	1102	5,3	28,29,29	1.45	5 (17%)	43,45,45	1.78	9 (20%)
3	BEF	A	1101	4	0,3,3	-	-	-	-	-
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
12	POL	A	1123	-	3,3,3	0.25	0	2,2,2	0.26	0
12	POL	A	1121	-	3,3,3	0.22	0	2,2,2	0.40	0
12	POL	A	1117	-	3,3,3	0.35	0	2,2,2	0.29	0
12	POL	A	1119	-	3,3,3	0.34	0	2,2,2	0.31	0
11	HEZ	A	1115	-	7,7,7	0.29	0	6,6,6	0.39	0
13	EDO	A	1126	-	3,3,3	0.42	0	2,2,2	0.38	0
6	PEG	A	1107	-	6,6,6	0.12	0	5,5,5	0.09	0
6	PEG	A	1105	-	6,6,6	0.12	0	5,5,5	0.08	0
13	EDO	A	1128	-	3,3,3	0.35	0	2,2,2	0.33	0
13	EDO	A	1125	-	3,3,3	0.43	0	2,2,2	0.31	0
12	POL	A	1122	-	3,3,3	0.27	0	2,2,2	0.20	0
7	GOL	A	1108	-	5,5,5	0.92	0	5,5,5	1.08	0
12	POL	A	1118	-	3,3,3	0.33	0	2,2,2	0.42	0
13	EDO	A	1127	-	3,3,3	0.42	0	2,2,2	0.38	0
12	POL	A	1116	-	3,3,3	0.35	0	2,2,2	0.30	0
12	POL	A	1120	-	3,3,3	0.28	0	2,2,2	0.23	0
8	MPO	A	1109	-	13,13,13	0.95	1 (7%)	17,17,17	1.89	4 (23%)
10	PGO	A	1112	-	4,4,4	0.53	0	4,4,4	0.64	0
8	MPO	A	1110	-	13,13,13	1.05	1 (7%)	17,17,17	1.46	3 (17%)
10	PGO	A	1114	-	4,4,4	0.52	0	4,4,4	0.67	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
12	POL	A	1124	-	-	1/1/1/1	-
10	PGO	A	1113	-	-	2/2/2/2	-
4	ADP	A	1102	5,3	-	2/16/32/32	0/3/3/3
6	PEG	A	1104	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	PEG	A	1106	-	-	0/4/4/4	-
12	POL	A	1123	-	-	1/1/1/1	-
12	POL	A	1121	-	-	0/1/1/1	-
12	POL	A	1117	-	-	0/1/1/1	-
12	POL	A	1119	-	-	0/1/1/1	-
11	HEZ	A	1115	-	-	2/5/5/5	-
13	EDO	A	1126	-	-	0/1/1/1	-
6	PEG	A	1107	-	-	1/4/4/4	-
6	PEG	A	1105	-	-	2/4/4/4	-
13	EDO	A	1128	-	-	1/1/1/1	-
13	EDO	A	1125	-	-	1/1/1/1	-
12	POL	A	1122	-	-	1/1/1/1	-
7	GOL	A	1108	-	-	0/4/4/4	-
12	POL	A	1118	-	-	0/1/1/1	-
13	EDO	A	1127	-	-	0/1/1/1	-
12	POL	A	1116	-	-	0/1/1/1	-
12	POL	A	1120	-	-	0/1/1/1	-
8	MPO	A	1109	-	-	5/7/15/15	0/1/1/1
10	PGO	A	1112	-	-	0/2/2/2	-
8	MPO	A	1110	-	-	5/7/15/15	0/1/1/1
10	PGO	A	1114	-	-	2/2/2/2	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1102	ADP	C5-C4	4.77	1.47	1.39
8	A	1110	MPO	O1-S1	3.61	1.55	1.45
8	A	1109	MPO	O2-S1	3.18	1.54	1.45
4	A	1102	ADP	C5-C6	2.69	1.48	1.41
4	A	1102	ADP	C8-N7	2.41	1.36	1.31
4	A	1102	ADP	C5-N7	-2.31	1.34	1.39
4	A	1102	ADP	PA-O3A	2.04	1.61	1.59

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1102	ADP	C5-C4-N3	-5.80	118.73	126.72
8	A	1109	MPO	C5-C4-N1	5.63	118.67	110.12
4	A	1102	ADP	N3-C4-N9	4.55	134.90	127.17
8	A	1110	MPO	O3-S1-O2	3.73	120.74	111.40
4	A	1102	ADP	C2-N3-C4	3.66	120.77	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1102	ADP	C4-C5-N7	-3.29	106.82	110.58
4	A	1102	ADP	N3-C2-N1	-3.13	123.85	128.58
8	A	1109	MPO	O4-C5-C4	2.90	118.02	111.77
8	A	1109	MPO	O3-S1-O1	2.76	118.30	111.40
8	A	1110	MPO	O1-S1-C1	-2.71	102.64	106.73
4	A	1102	ADP	C4-N9-C8	2.45	108.31	105.74
4	A	1102	ADP	C5-N7-C8	2.30	107.07	103.45
8	A	1110	MPO	O3-S1-O1	-2.17	105.97	111.40
4	A	1102	ADP	C2'-C1'-N9	-2.10	108.09	113.30
4	A	1102	ADP	O2A-PA-O3A	2.07	112.88	107.27
8	A	1109	MPO	C7-N1-C4	2.06	113.28	108.84

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	1110	MPO	C1-C2-C3-N1
8	A	1109	MPO	C2-C1-S1-O2
8	A	1110	MPO	C2-C1-S1-O1
8	A	1110	MPO	C2-C1-S1-O2
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-C1-S1-O1
12	A	1122	POL	O-C1-C2-C3
12	A	1124	POL	O-C1-C2-C3
8	A	1109	MPO	C2-C1-S1-O3
8	A	1109	MPO	C2-C3-N1-C4
6	A	1104	PEG	O2-C3-C4-O4
10	A	1114	PGO	O1-C1-C2-O2
13	A	1125	EDO	O1-C1-C2-O2

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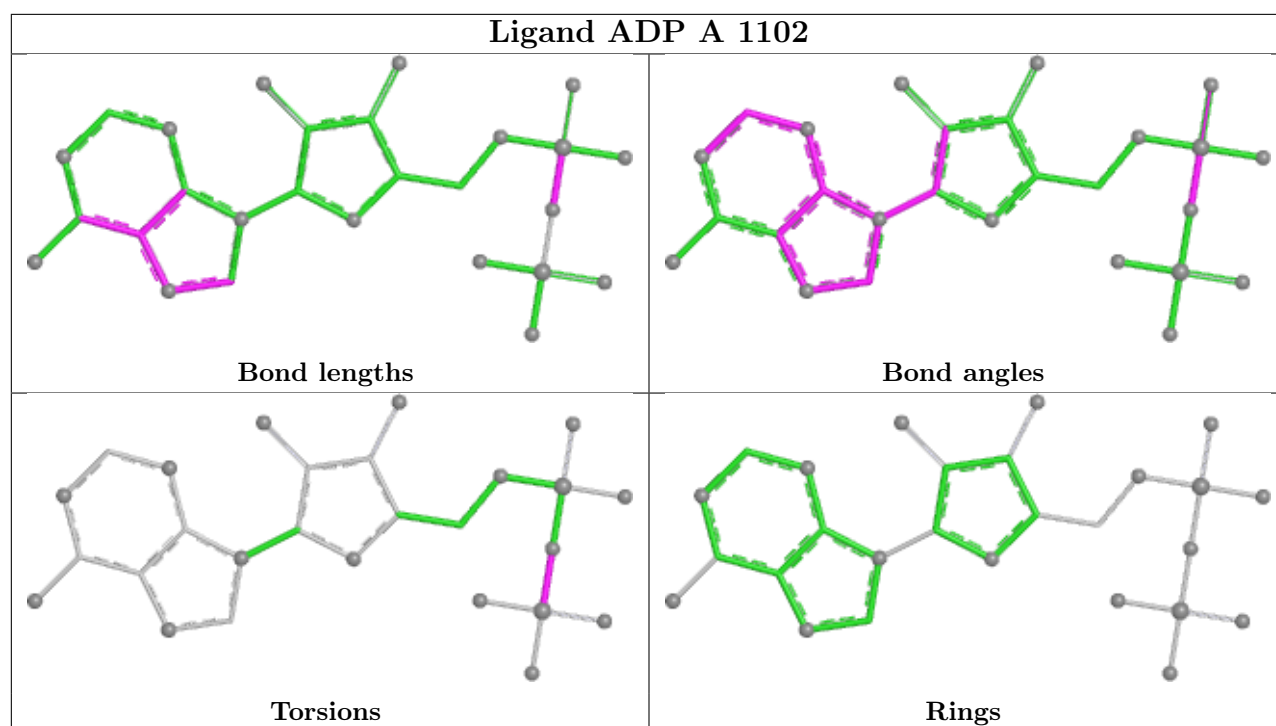
Mol	Chain	Res	Type	Atoms
12	A	1123	POL	O-C1-C2-C3
4	A	1102	ADP	PA-O3A-PB-O1B
6	A	1105	PEG	O1-C1-C2-O2

There are no ring outliers.

12 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	A	1113	PGO	2	0
12	A	1123	POL	1	0
12	A	1121	POL	3	0
11	A	1115	HEZ	2	0
6	A	1107	PEG	2	0
6	A	1105	PEG	1	0
13	A	1125	EDO	1	0
12	A	1122	POL	2	0
12	A	1118	POL	1	0
12	A	1120	POL	2	0
8	A	1110	MPO	1	0
10	A	1114	PGO	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 [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	626/636 (98%)	0.15	20 (3%) 50 53	20, 41, 70, 110	4 (0%)
2	B	8/8 (100%)	0.51	1 (12%) 8 8	41, 68, 101, 111	1 (12%)
All	All	634/644 (98%)	0.16	21 (3%) 49 51	20, 41, 71, 111	5 (0%)

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	534	GLY	3.9
1	A	862	GLY	3.4
1	A	916	LEU	3.2
2	B	9	U	3.1
1	A	533	LEU	3.0
1	A	538	PRO	3.0
1	A	609	LEU	2.9
1	A	870	ASN	2.8
1	A	344	ARG	2.6
1	A	676	LEU	2.5
1	A	872	ILE	2.5
1	A	474	VAL	2.4
1	A	596	ASN	2.3
1	A	290	ILE	2.3
1	A	904	TYR	2.3
1	A	289	THR	2.3
1	A	917	SER	2.1
1	A	529	ILE	2.1
1	A	670	LEU	2.1
1	A	750	VAL	2.1
1	A	531	ARG	2.0

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	0.97	0.06	31,38,44,59	0

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.

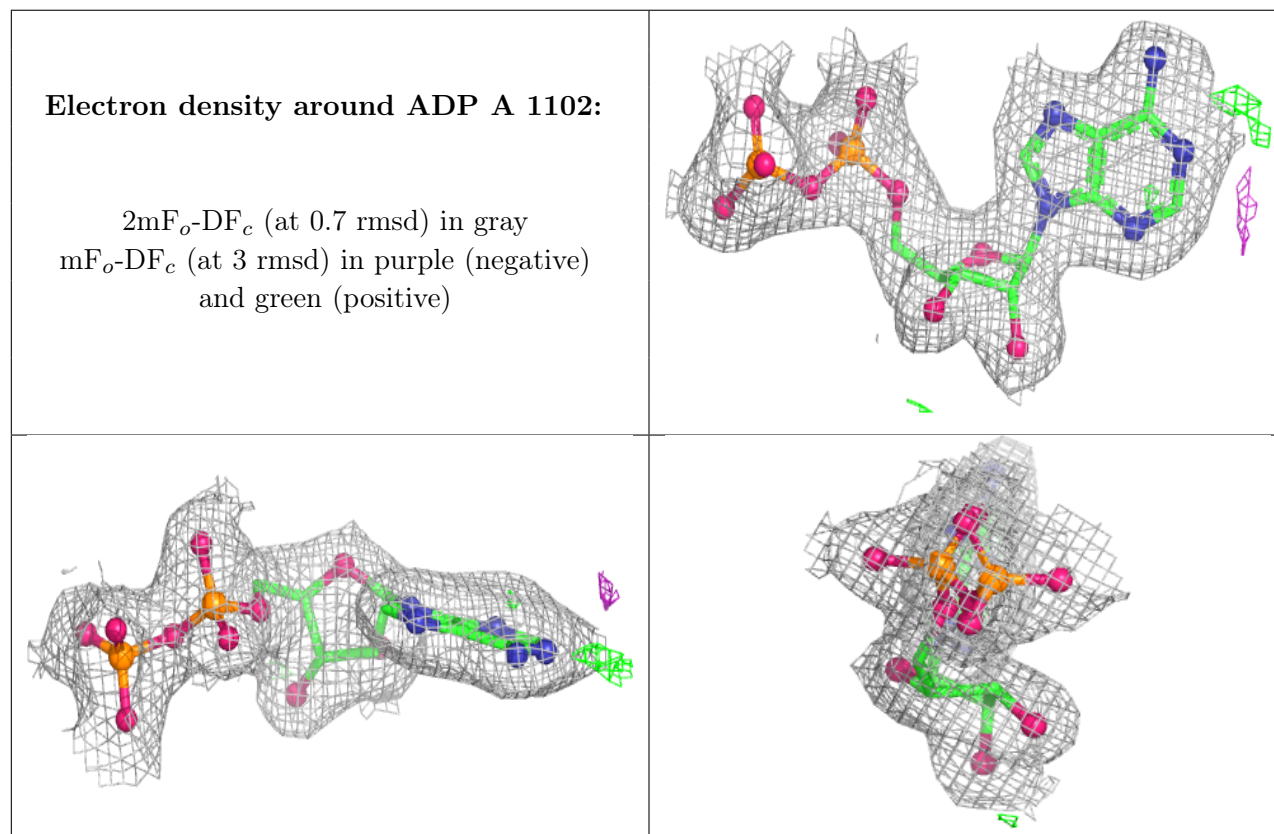
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
13	EDO	A	1128	4/4	0.63	0.18	94,96,96,96	0
12	POL	A	1118	4/4	0.69	0.25	53,55,61,64	0
10	PGO	A	1113	5/5	0.71	0.20	56,57,63,64	0
12	POL	A	1120	4/4	0.74	0.22	68,71,73,78	0
12	POL	A	1122	4/4	0.77	0.23	58,58,58,63	0
12	POL	A	1123	4/4	0.78	0.30	71,72,74,74	0
6	PEG	A	1105	7/7	0.78	0.18	68,68,76,77	0
12	POL	A	1119	4/4	0.79	0.23	74,74,75,78	0
8	MPO	A	1109	13/13	0.80	0.18	72,74,88,97	0
10	PGO	A	1112	5/5	0.82	0.19	67,71,73,75	0
13	EDO	A	1126	4/4	0.82	0.20	73,78,82,85	0
13	EDO	A	1127	4/4	0.82	0.17	61,66,66,69	0
12	POL	A	1116	4/4	0.82	0.20	72,73,74,74	0
8	MPO	A	1110	13/13	0.83	0.22	68,77,105,107	0
6	PEG	A	1107	7/7	0.83	0.15	60,62,68,71	0
6	PEG	A	1104	7/7	0.83	0.18	63,68,69,70	0
12	POL	A	1124	4/4	0.84	0.21	55,64,64,65	0
12	POL	A	1117	4/4	0.85	0.20	55,61,66,66	0
9	CL	A	1111	1/1	0.86	0.15	78,78,78,78	0
11	HEZ	A	1115	8/8	0.87	0.16	37,44,54,66	0
6	PEG	A	1106	7/7	0.87	0.15	70,75,77,78	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
12	POL	A	1121	4/4	0.88	0.25	75,76,77,79	0
10	PGO	A	1114	5/5	0.89	0.21	64,68,73,83	0
13	EDO	A	1125	4/4	0.90	0.14	39,54,58,60	0
7	GOL	A	1108	6/6	0.91	0.11	46,53,58,58	0
3	BEF	A	1101	4/4	0.96	0.07	30,32,32,33	0
5	MG	A	1103	1/1	0.97	0.06	34,34,34,34	0
4	ADP	A	1102	27/27	0.97	0.06	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 ⓘ

There are no such residues in this entry.