Full wwPDB X-ray Structure Validation Report (i)

Mar 27, 2025 – 10:12 AM EDT

PDB ID	:	7I2C
Title	:	Group deposition for crystallographic fragment screening of the NS5 RNA-dependent RNA polymerase from Dengue virus serotype 2 – Crystal structure of the NS5 RNA-dependent RNA polymerase from Dengue virus serotype 2 in complex with Z71308235 (DNV2_NS5A-x0253)
Authors	:	Aschenbrenner, J.C.; Saini, M.; Chopra, A.; Marples, P.G.; Balcomb, B.H.; Lithgo, R.M.; Fearon, D.; von Delft, F.; Ruiz, F.X.; Arnold, E.
Deposited on	:	2025-03-06
Resolution	:	1.63 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 (i) 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 (i)) were used in the production of this report:

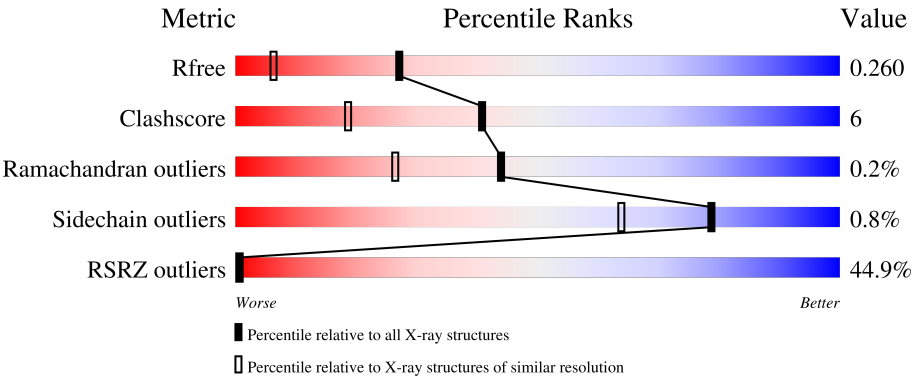
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.63 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	1015 (1.64-1.64)
Clashscore	180529	1093 (1.64-1.64)
Ramachandran outliers	177936	1077 (1.64-1.64)
Sidechain outliers	177891	1077 (1.64-1.64)
RSRZ outliers	164620	1015 (1.64-1.64)

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 <=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	637	40% 78% 11% 10%

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:

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	PO4	A	1008	-	X	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5216 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 NS5 RNA-dependent RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	573	4736	2982	849	871	34	0	7	0

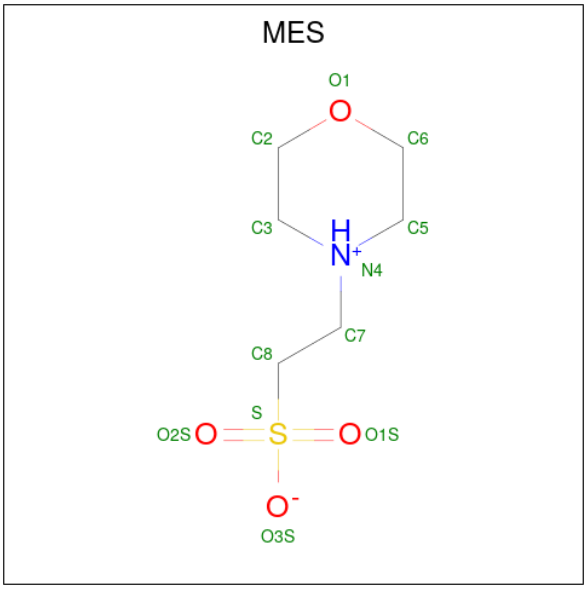
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	264	GLY	-	expression tag	UNP Q91H74
A	265	PRO	-	expression tag	UNP Q91H74

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

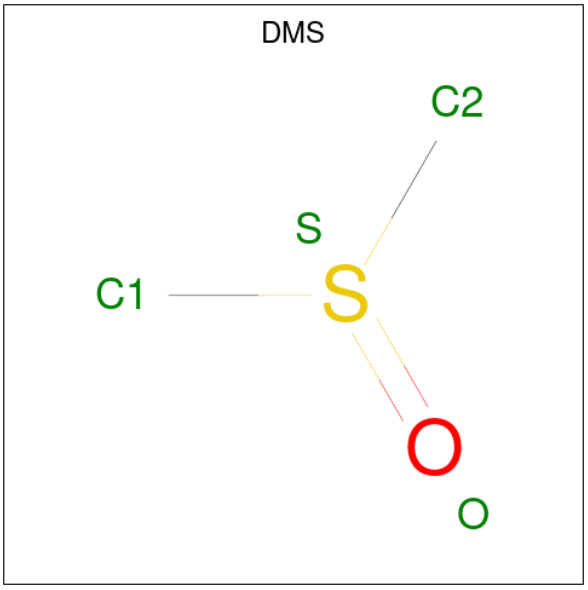
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	2	2	2	0	0

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



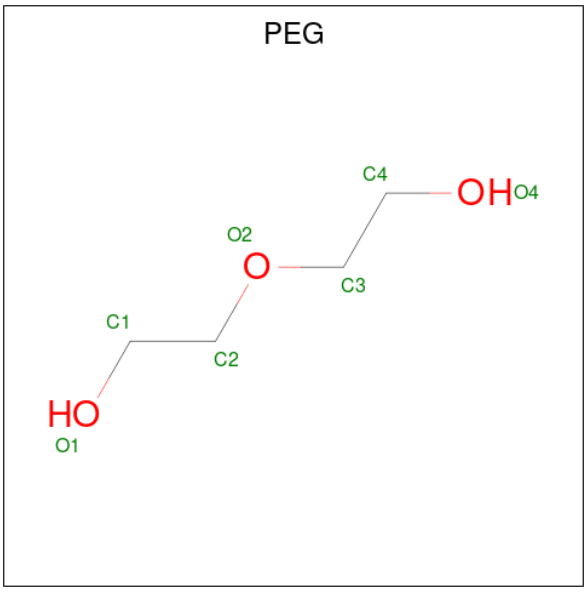
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

- Molecule 4 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



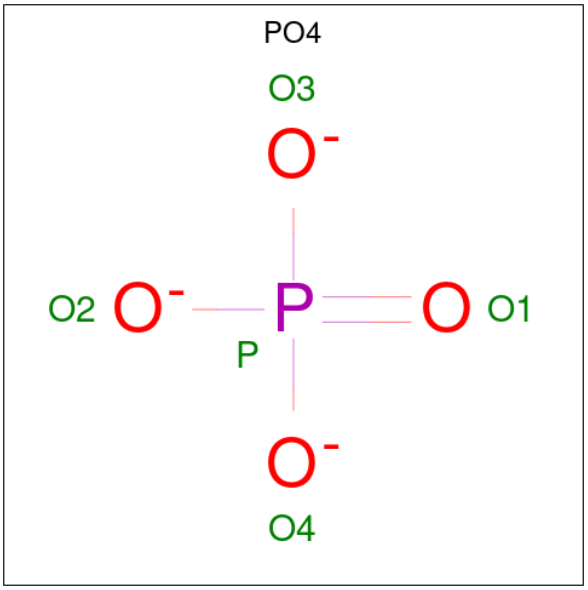
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	O	S		0	0
			4	2	1	1			
4	A	1	Total	C	O	S		0	0
			4	2	1	1			
4	A	1	Total	C	O	S		0	0
			4	2	1	1			

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



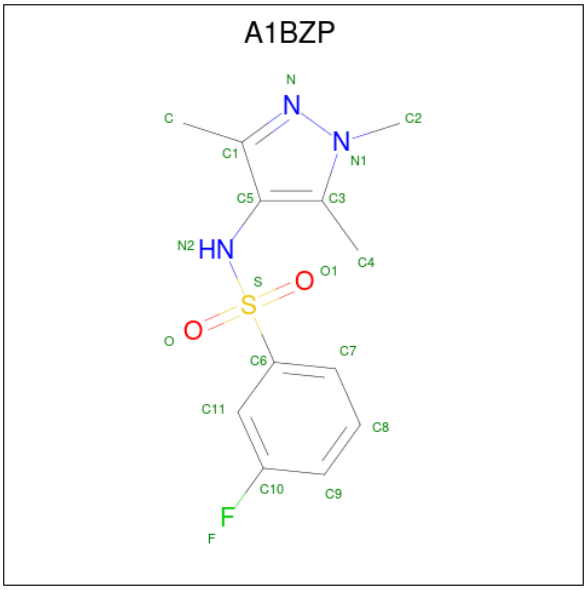
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0
6	A	1	Total O P 5 4 1	0	0

- Molecule 7 is 3-fluoro-N-(1,3,5-trimethyl-1H-pyrazol-4-yl)benzene-1-sulfonamide (three-letter code: A1BZP) (formula: $C_{12}H_{14}FN_3O_2S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C F N O S 19 12 1 3 2 1	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 9 is water.

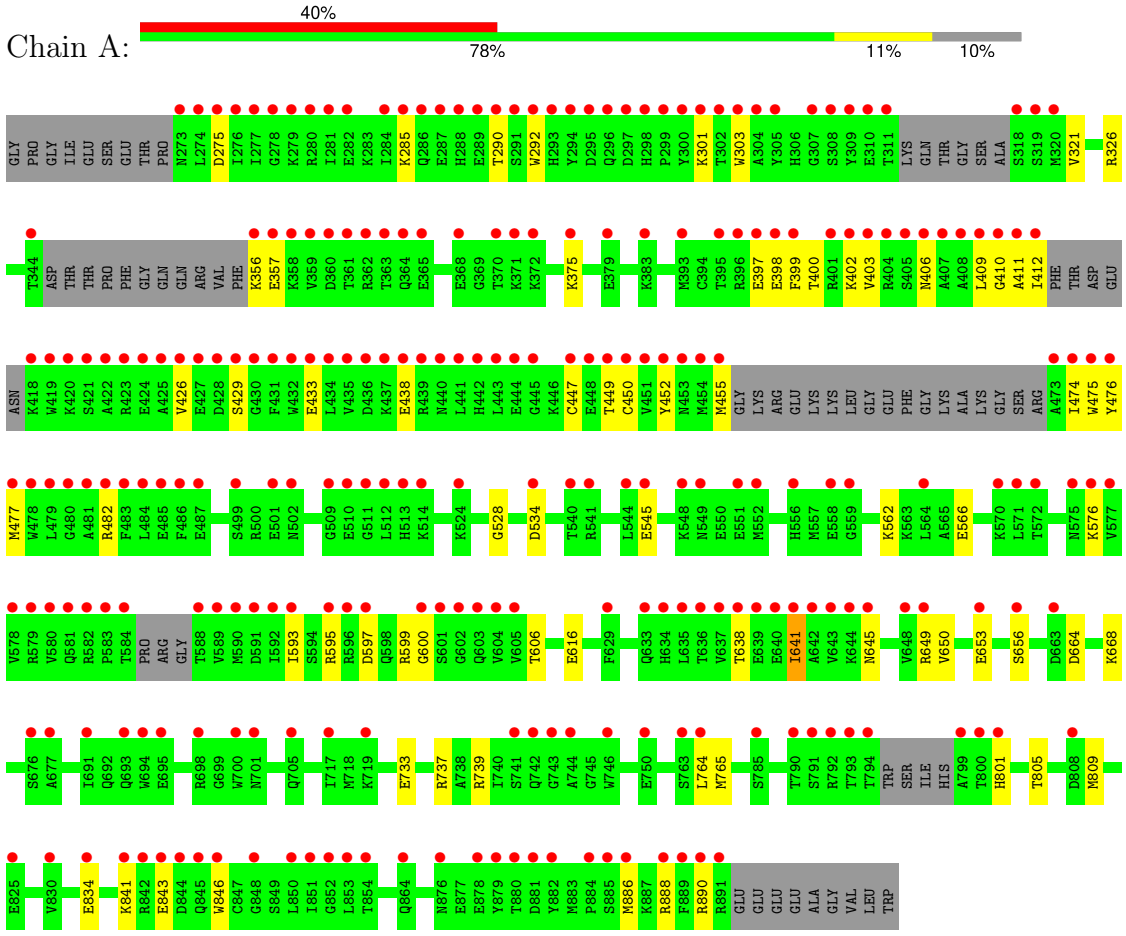
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	398	Total O 398 398	0	0

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: NS5 RNA-dependent RNA polymerase

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	82.64Å 117.01Å 149.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.55 – 1.63 74.55 – 1.63	Depositor EDS
% Data completeness (in resolution range)	97.7 (74.55-1.63) 97.7 (74.55-1.63)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.01 (at 1.63Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC5	Depositor
R, R_{free}	0.193 , 0.226 0.236 , 0.260	Depositor DCC
R_{free} test set	4581 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	30.0	Xtriage
Anisotropy	0.165	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 76.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5216	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, PEG, DMS, PO4, A1BZP, MES, ZN

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.75	1/4841 (0.0%)	0.82	1/6528 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	616	GLU	CD-OE2	5.11	1.31	1.25

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	739	ARG	NE-CZ-NH1	5.66	123.13	120.30

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	4736	0	4640	58	0
2	A	2	0	0	0	0
3	A	24	0	26	0	0
4	A	12	0	18	2	0
5	A	14	0	20	0	0
6	A	10	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	A	19	0	0	2	0
8	A	1	0	0	0	0
9	A	398	0	0	9	1
All	All	5216	0	4704	61	1

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 6.

All (61) 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:638:THR:O	1:A:641:ILE:HG23	1.77	0.84
1:A:403:VAL:HG21	1:A:426:VAL:HG21	1.59	0.83
1:A:638:THR:O	1:A:641:ILE:CG2	2.27	0.82
1:A:664:ASP:OD1	6:A:1008:PO4:O4	2.00	0.79
1:A:409:LEU:O	1:A:482:ARG:HD3	1.84	0.77
1:A:375:LYS:HD2	9:A:1101:HOH:O	1.83	0.77
1:A:595:ARG:NE	1:A:597:ASP:OD1	2.19	0.76
7:A:1011:A1BZP:N2	9:A:1103:HOH:O	2.30	0.64
1:A:356:LYS:HG2	1:A:357:GLU:H	1.63	0.63
1:A:398:GLU:O	1:A:402:LYS:HG3	2.02	0.60
1:A:375:LYS:CD	9:A:1101:HOH:O	2.42	0.60
1:A:375:LYS:HZ3	1:A:545:GLU:CD	2.07	0.58
1:A:638:THR:O	1:A:641:ILE:HG22	2.02	0.57
1:A:397:GLU:OE1	1:A:397:GLU:N	2.30	0.56
1:A:801[B]:HIS:H	1:A:801[B]:HIS:CD2	2.22	0.56
1:A:664:ASP:OD1	6:A:1008:PO4:P	2.63	0.56
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.47	0.55
1:A:357:GLU:N	1:A:357:GLU:OE2	2.40	0.55
1:A:733:GLU:O	1:A:737:ARG:HG3	2.07	0.55
1:A:653:GLU:O	1:A:656:SER:OG	2.21	0.54
1:A:534:ASP:OD1	6:A:1008:PO4:O4	2.26	0.53
1:A:400:THR:HG23	1:A:426:VAL:HG11	1.92	0.52
1:A:438:GLU:HG3	1:A:449:THR:OG1	2.09	0.52
1:A:764:LEU:HG	1:A:765:MET:CE	2.41	0.51
1:A:303:TRP:CE3	1:A:593:ILE:HD12	2.45	0.51
1:A:474:ILE:HD12	1:A:474:ILE:N	2.27	0.50
4:A:1004:DMS:C1	9:A:1245:HOH:O	2.59	0.50
1:A:411:ALA:HA	1:A:477:MET:O	2.12	0.49
1:A:399:PHE:O	1:A:403:VAL:HG13	2.13	0.49
1:A:764:LEU:HG	1:A:765:MET:HE3	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:649:ARG:NH1	9:A:1104:HOH:O	2.33	0.48
1:A:475:TRP:CD1	1:A:475:TRP:N	2.82	0.48
1:A:843:GLU:HA	1:A:846:TRP:CE3	2.49	0.48
1:A:357:GLU:N	1:A:357:GLU:CD	2.68	0.47
1:A:834:GLU:OE2	1:A:890:ARG:NE	2.44	0.47
1:A:429:SER:O	1:A:433:GLU:HG3	2.14	0.46
1:A:475:TRP:HZ3	1:A:576:LYS:HD3	1.81	0.46
1:A:452:TYR:CZ	1:A:600:GLY:O	2.68	0.46
1:A:528:GLY:O	1:A:668:LYS:HE3	2.15	0.46
1:A:375:LYS:NZ	1:A:545:GLU:OE2	2.36	0.46
1:A:886:MET:CE	9:A:1234:HOH:O	2.62	0.46
1:A:275:ASP:N	1:A:275:ASP:OD1	2.48	0.46
1:A:638:THR:HA	1:A:641:ILE:CG2	2.46	0.46
1:A:285:LYS:HG3	1:A:292:TRP:CE2	2.51	0.46
1:A:641:ILE:HD11	1:A:645:ASN:ND2	2.31	0.45
1:A:410:GLY:O	1:A:476:TYR:HA	2.16	0.45
1:A:841:LYS:HD2	7:A:1011:A1BZP:O1	2.17	0.45
1:A:599:ARG:HG2	1:A:606:THR:HG23	1.99	0.44
1:A:562:LYS:NZ	9:A:1110:HOH:O	2.41	0.44
1:A:649:ARG:HG2	1:A:650:VAL:HG13	2.00	0.43
1:A:400:THR:HG23	1:A:426:VAL:CG1	2.49	0.43
1:A:805:THR:CG2	1:A:809:MET:HE1	2.49	0.42
1:A:888:ARG:HD2	9:A:1268:HOH:O	2.18	0.42
1:A:375:LYS:NZ	1:A:545:GLU:CD	2.71	0.42
4:A:1004:DMS:H11	9:A:1245:HOH:O	2.18	0.41
1:A:412:ILE:O	1:A:412:ILE:HG13	2.20	0.41
1:A:638:THR:HA	1:A:641:ILE:HG22	2.02	0.41
1:A:412:ILE:HG23	1:A:476:TYR:HB3	2.02	0.41
1:A:321:VAL:HG11	1:A:326:ARG:CZ	2.51	0.41
1:A:534:ASP:OD1	6:A:1008:PO4:P	2.78	0.41
1:A:562:LYS:HE3	1:A:566:GLU:OE2	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1175:HOH:O	9:A:1175:HOH:O[2_445]	1.68	0.52

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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	566/637 (89%)	545 (96%)	20 (4%)	1 (0%)	44 26

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	ASN

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	509/554 (92%)	505 (99%)	4 (1%)	79 64

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	290	THR
1	A	301	LYS
1	A	455	MET
1	A	641	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	603	GLN

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Mol	Chain	Res	Type
1	A	645	ASN

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

Of 13 ligands modelled in this entry, 3 are monoatomic - leaving 10 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	$\#\|Z\| > 2$
4	DMS	A	1004	-	3,3,3	0.91	0	3,3,3	0.54	0
3	MES	A	1003[B]	-	12,12,12	0.70	0	15,16,16	0.32	0
4	DMS	A	1005	-	3,3,3	0.46	0	3,3,3	0.14	0
6	PO4	A	1008	-	4,4,4	5.36	4 (100%)	6,6,6	0.96	0
7	A1BZP	A	1011	-	19,20,20	0.81	1 (5%)	23,30,30	0.47	0
6	PO4	A	1009	-	4,4,4	1.58	1 (25%)	6,6,6	0.54	0
5	PEG	A	1007	-	6,6,6	0.22	0	5,5,5	0.11	0
3	MES	A	1003[A]	-	12,12,12	0.91	0	15,16,16	0.67	0
4	DMS	A	1006	-	3,3,3	0.28	0	3,3,3	0.27	0
5	PEG	A	1010	-	6,6,6	0.13	0	5,5,5	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
3	MES	A	1003[B]	-	-	5/6/14/14	0/1/1/1
7	A1BZP	A	1011	-	-	0/9/11/11	0/2/2/2
5	PEG	A	1007	-	-	1/4/4/4	-
3	MES	A	1003[A]	-	-	0/6/14/14	0/1/1/1
5	PEG	A	1010	-	-	2/4/4/4	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1008	PO4	P-O1	8.30	1.69	1.50
6	A	1008	PO4	P-O2	4.98	1.69	1.54
6	A	1008	PO4	P-O3	3.86	1.65	1.54
6	A	1009	PO4	P-O1	2.74	1.57	1.50
6	A	1008	PO4	P-O4	-2.56	1.47	1.54
7	A	1011	A1BZP	C3-N1	-2.21	1.34	1.37

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003[B]	MES	C8-C7-N4-C3
3	A	1003[B]	MES	C7-C8-S-O3S
5	A	1007	PEG	O2-C3-C4-O4
5	A	1010	PEG	O2-C3-C4-O4
3	A	1003[B]	MES	C8-C7-N4-C5
3	A	1003[B]	MES	C7-C8-S-O1S
3	A	1003[B]	MES	C7-C8-S-O2S
5	A	1010	PEG	C4-C3-O2-C2

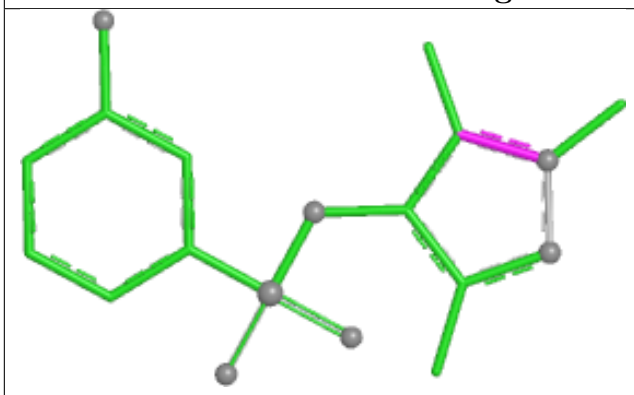
There are no ring outliers.

3 monomers are involved in 8 short contacts:

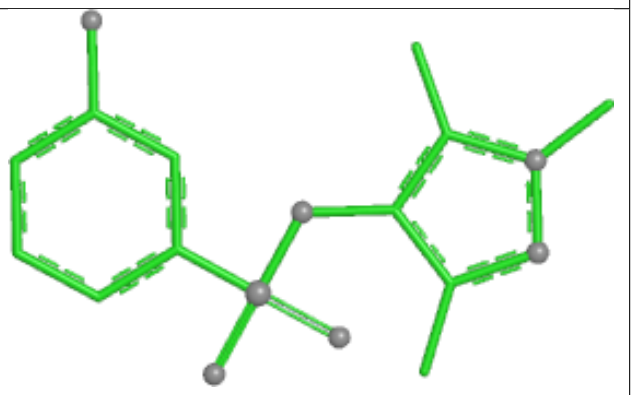
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	DMS	2	0
6	A	1008	PO4	4	0
7	A	1011	A1BZP	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 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.

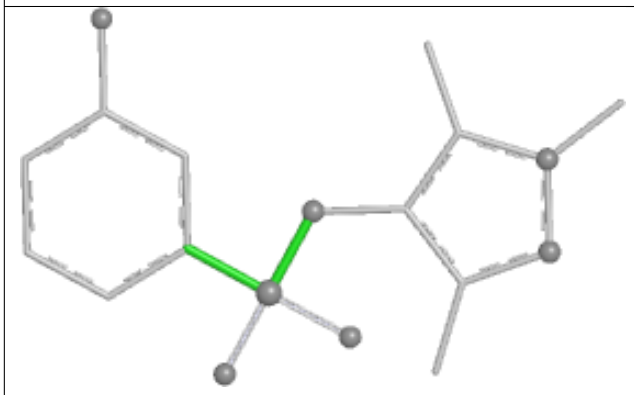
Ligand A1BZP A 1011



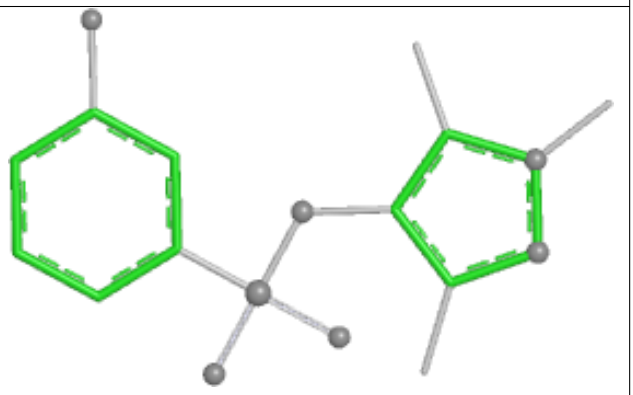
Bond lengths



Bond angles



Torsions



Rings

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^{th} 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	573/637 (89%)	2.94	257 (44%)	1	0	6, 33, 82, 158	135 (23%)

All (257) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	850	LEU	16.2
1	A	846	TRP	15.2
1	A	853	LEU	15.1
1	A	851	ILE	14.4
1	A	854	THR	13.6
1	A	852	GLY	13.3
1	A	848	GLY	12.8
1	A	512[A]	LEU	11.9
1	A	303	TRP	11.8
1	A	304	ALA	11.8
1	A	641	ILE	11.6
1	A	844	ASP	11.6
1	A	409	LEU	11.4
1	A	411	ALA	11.4
1	A	700	TRP	11.4
1	A	801[A]	HIS	11.4
1	A	719[A]	LYS	11.3
1	A	478	TRP	11.0
1	A	580	VAL	11.0
1	A	281	ILE	10.9
1	A	426	VAL	10.9
1	A	589	VAL	10.7
1	A	399	PHE	10.7
1	A	309	TYR	10.6
1	A	451	VAL	10.3
1	A	588	THR	10.0
1	A	475	TRP	10.0

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Mol	Chain	Res	Type	RSRZ
1	A	274	LEU	9.8
1	A	600	GLY	9.7
1	A	403	VAL	9.6
1	A	511	GLY	9.2
1	A	601	SER	9.1
1	A	800	THR	8.9
1	A	474	ILE	8.9
1	A	308	SER	8.9
1	A	429	SER	8.8
1	A	743	GLY	8.7
1	A	841	LYS	8.6
1	A	842	ARG	8.5
1	A	845	GLN	8.4
1	A	311	THR	8.4
1	A	843	GLU	8.4
1	A	476	TYR	8.4
1	A	656	SER	8.3
1	A	410	GLY	8.3
1	A	277	ILE	8.3
1	A	638	THR	8.3
1	A	408	ALA	8.3
1	A	359	VAL	8.2
1	A	544	LEU	8.2
1	A	412	ILE	8.1
1	A	602	GLY	8.1
1	A	741[A]	SER	8.0
1	A	480	GLY	7.9
1	A	513	HIS	7.9
1	A	422	ALA	7.9
1	A	276	ILE	7.9
1	A	319	SER	7.9
1	A	575	ASN	7.8
1	A	473	ALA	7.8
1	A	280	ARG	7.7
1	A	481	ALA	7.7
1	A	499	SER	7.7
1	A	509	GLY	7.7
1	A	552	MET	7.6
1	A	576	LYS	7.6
1	A	549	ASN	7.5
1	A	421	SER	7.5
1	A	540	THR	7.4

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Mol	Chain	Res	Type	RSRZ
1	A	419	TRP	7.4
1	A	785[A]	SER	7.3
1	A	484	LEU	7.3
1	A	356	LYS	7.3
1	A	402	LYS	7.3
1	A	763[A]	SER	7.3
1	A	425	ALA	7.2
1	A	375	LYS	7.2
1	A	479	LEU	7.1
1	A	423	ARG	7.1
1	A	273	ASN	7.1
1	A	649	ARG	7.0
1	A	453	ASN	6.9
1	A	742	GLN	6.9
1	A	864[A]	GLN	6.9
1	A	371	LYS	6.9
1	A	320	MET	6.9
1	A	372	LYS	6.9
1	A	541	ARG	6.9
1	A	279	LYS	6.8
1	A	401	ARG	6.8
1	A	595	ARG	6.8
1	A	639	GLU	6.8
1	A	485	GLU	6.7
1	A	302	THR	6.7
1	A	361	THR	6.7
1	A	318	SER	6.7
1	A	358	LYS	6.7
1	A	294	TYR	6.7
1	A	300	TYR	6.6
1	A	640	GLU	6.6
1	A	514	LYS	6.6
1	A	428	ASP	6.6
1	A	502	ASN	6.5
1	A	582	ARG	6.4
1	A	794	THR	6.3
1	A	477	MET	6.3
1	A	441	LEU	6.3
1	A	551	GLU	6.3
1	A	305	TYR	6.3
1	A	292	TRP	6.3
1	A	591	ASP	6.2

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Mol	Chain	Res	Type	RSRZ
1	A	705	GLN	6.2
1	A	482	ARG	6.1
1	A	635	LEU	6.1
1	A	791	SER	6.0
1	A	590	MET	6.0
1	A	397	GLU	5.9
1	A	597	ASP	5.9
1	A	284	ILE	5.9
1	A	298	HIS	5.9
1	A	548	LYS	5.8
1	A	362	ARG	5.8
1	A	363	THR	5.8
1	A	698	ARG	5.8
1	A	581	GLN	5.8
1	A	287	GLU	5.8
1	A	889	PHE	5.7
1	A	282	GLU	5.7
1	A	880	THR	5.7
1	A	644	LYS	5.7
1	A	431	PHE	5.6
1	A	407	ALA	5.6
1	A	793	THR	5.5
1	A	888	ARG	5.5
1	A	297	ASP	5.4
1	A	418	LYS	5.4
1	A	275	ASP	5.4
1	A	634	HIS	5.4
1	A	510	GLU	5.4
1	A	290	THR	5.3
1	A	596	ARG	5.3
1	A	487	GLU	5.3
1	A	501	GLU	5.3
1	A	379	GLU	5.2
1	A	364	GLN	5.2
1	A	357	GLU	5.2
1	A	442	HIS	5.2
1	A	398	GLU	5.2
1	A	286	GLN	5.1
1	A	653	GLU	5.1
1	A	583	PRO	5.1
1	A	420	LYS	5.0
1	A	310	GLU	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	444	GLU	4.9
1	A	545	GLU	4.9
1	A	434	LEU	4.9
1	A	645	ASN	4.9
1	A	289	GLU	4.9
1	A	293	HIS	4.9
1	A	424	GLU	4.9
1	A	360	ASP	4.9
1	A	790	THR	4.8
1	A	603	GLN	4.7
1	A	799	ALA	4.6
1	A	452	TYR	4.6
1	A	890	ARG	4.5
1	A	427	GLU	4.5
1	A	288	HIS	4.4
1	A	299	PRO	4.4
1	A	629	PHE	4.3
1	A	435	VAL	4.2
1	A	556	HIS	4.1
1	A	430	GLY	4.1
1	A	564	LEU	4.1
1	A	886	MET	4.1
1	A	881	ASP	4.1
1	A	584	THR	3.9
1	A	571	LEU	3.8
1	A	604	VAL	3.8
1	A	882	TYR	3.8
1	A	404	ARG	3.8
1	A	792	ARG	3.7
1	A	448	GLU	3.7
1	A	891	ARG	3.7
1	A	637	VAL	3.6
1	A	406	ASN	3.6
1	A	443	LEU	3.6
1	A	694	TRP	3.6
1	A	825	GLU	3.6
1	A	368	GLU	3.4
1	A	445	GLY	3.3
1	A	291	SER	3.3
1	A	344	THR	3.3
1	A	592	ILE	3.2
1	A	455	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	439	ARG	3.1
1	A	593	ILE	3.1
1	A	677	ALA	3.1
1	A	750	GLU	3.1
1	A	746	TRP	3.0
1	A	296	GLN	3.0
1	A	884	PRO	3.0
1	A	570	LYS	3.0
1	A	695	GLU	3.0
1	A	437	LYS	2.9
1	A	301	LYS	2.9
1	A	432	TRP	2.9
1	A	307	GLY	2.9
1	A	744	ALA	2.8
1	A	438	GLU	2.8
1	A	834	GLU	2.7
1	A	396	ARG	2.7
1	A	436	ASP	2.7
1	A	876	ASN	2.7
1	A	285	LYS	2.6
1	A	524	LYS	2.5
1	A	558	GLU	2.5
1	A	764	LEU	2.5
1	A	440	ASN	2.5
1	A	717	ILE	2.5
1	A	830	VAL	2.5
1	A	693	GLN	2.5
1	A	393	MET	2.5
1	A	559	GLY	2.5
1	A	454	MET	2.4
1	A	648	VAL	2.4
1	A	579	ARG	2.4
1	A	295	ASP	2.4
1	A	633	GLN	2.4
1	A	433	GLU	2.4
1	A	572	THR	2.3
1	A	643	VAL	2.3
1	A	691	ILE	2.3
1	A	370	THR	2.3
1	A	577	VAL	2.3
1	A	642	ALA	2.2
1	A	578	VAL	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	605	VAL	2.2
1	A	808	ASP	2.2
1	A	450	CYS	2.2
1	A	486	PHE	2.2
1	A	405	SER	2.2
1	A	534	ASP	2.2
1	A	278	GLY	2.2
1	A	447	CYS	2.1
1	A	676	SER	2.1
1	A	885	SER	2.1
1	A	449	THR	2.1
1	A	701	ASN	2.1
1	A	483	PHE	2.1
1	A	878	GLU	2.1
1	A	879	TYR	2.1
1	A	636	THR	2.0
1	A	383	LYS	2.0
1	A	365	GLU	2.0
1	A	395	THR	2.0
1	A	663	ASP	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, 95^{th} 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
7	A1BZP	A	1011	19/19	0.48	0.40	45,48,51,52	19
6	PO4	A	1009	5/5	0.54	0.20	66,70,79,108	0
5	PEG	A	1007	7/7	0.54	0.24	91,101,108,109	0

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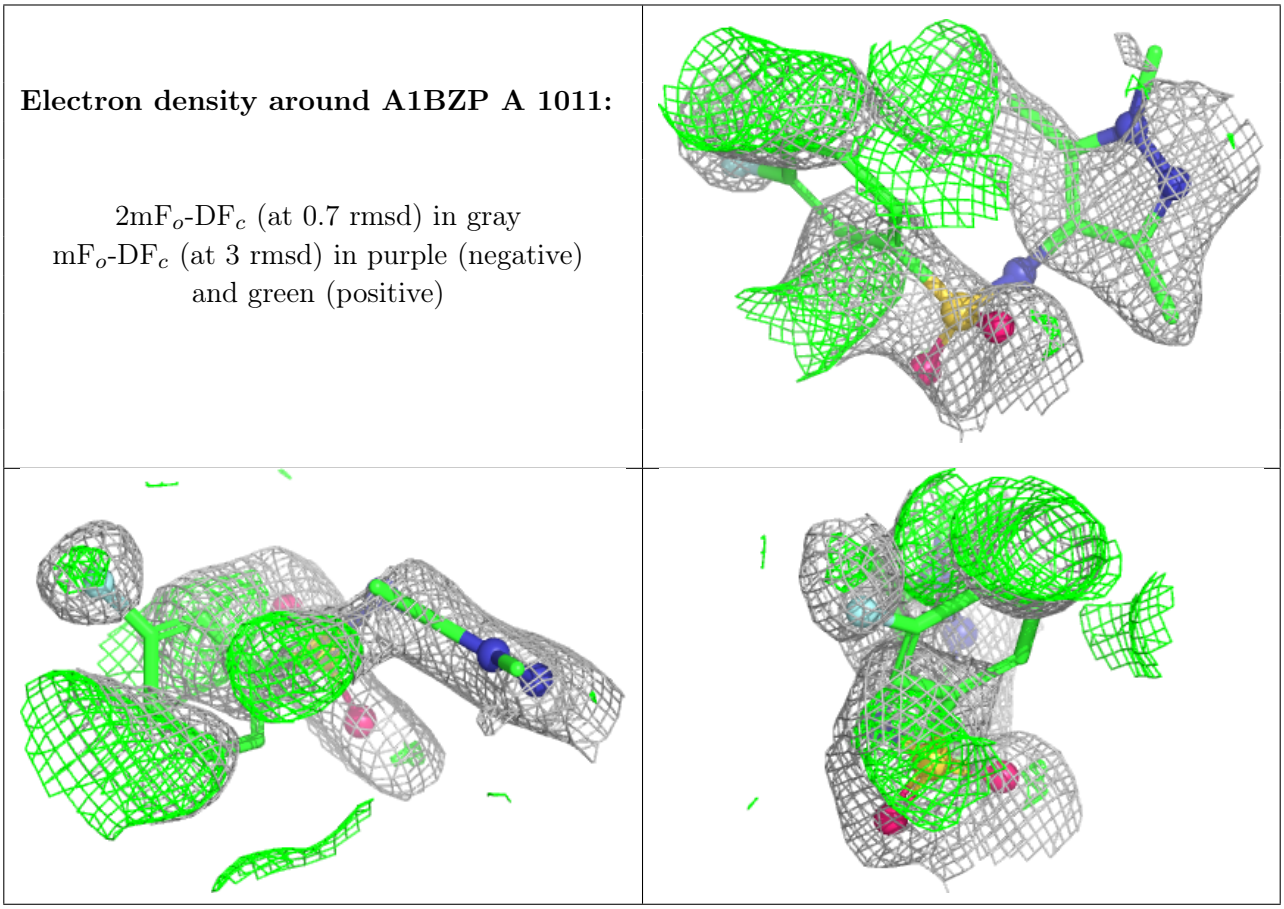
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	DMS	A	1005	4/4	0.60	0.34	70,95,99,119	0
6	PO4	A	1008	5/5	0.72	0.17	36,37,55,58	0
5	PEG	A	1010	7/7	0.81	0.19	65,68,75,76	0
4	DMS	A	1006	4/4	0.91	0.14	45,54,61,62	0
4	DMS	A	1004	4/4	0.91	0.17	39,46,50,51	0
3	MES	A	1003[A]	12/12	0.97	0.32	21,25,29,30	12
3	MES	A	1003[B]	12/12	0.97	0.32	621,639,661,664	12
2	ZN	A	1002	1/1	0.98	0.06	50,50,50,50	0
8	CL	A	1012	1/1	0.98	0.06	40,40,40,40	0
2	ZN	A	1001	1/1	1.00	0.01	21,21,21,21	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 A1BZP A 1011:

$2mF_o$-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

There are no such residues in this entry.