



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2025 – 10:25 AM EDT

PDB ID : 7I2K
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 Z1343518214 (DNV2_NS5A-x0503)
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Deposited on : 2025-03-06
Resolution : 1.90 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	:	4.02b-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)

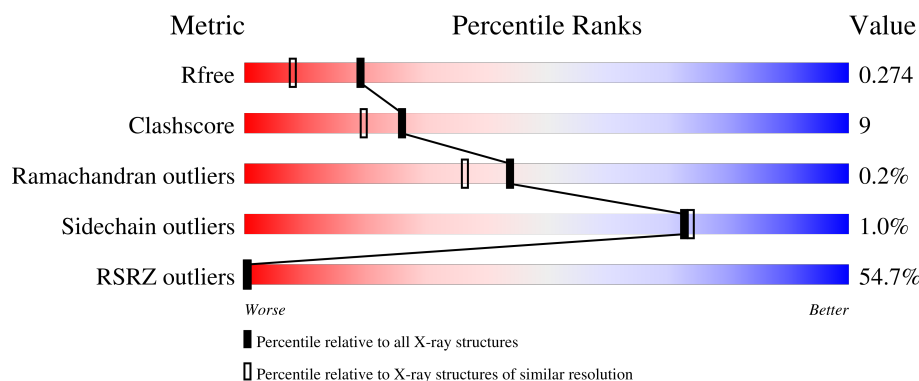
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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	637	

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
5	PO4	A	1006	-	-	X	-
8	A1BFU	A	1010	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5133 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
1	A	572	Total	C	N	O	S	0	7	0
			4731	2982	846	869	34			

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
2	A	2	Total	Zn	0	0
			2	2		

- Molecule 3 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



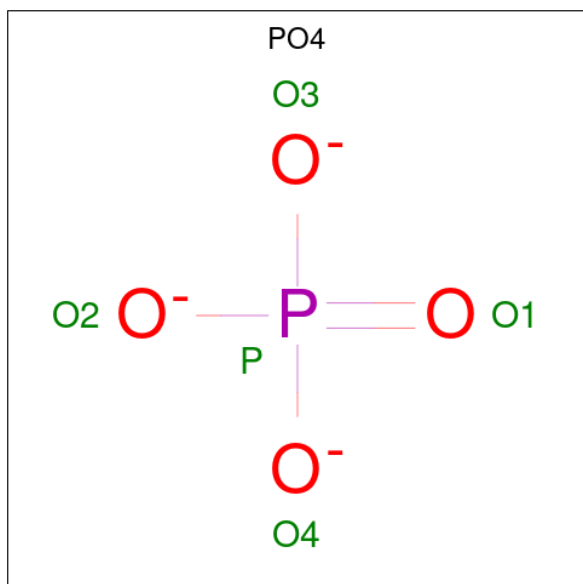
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

- 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		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).

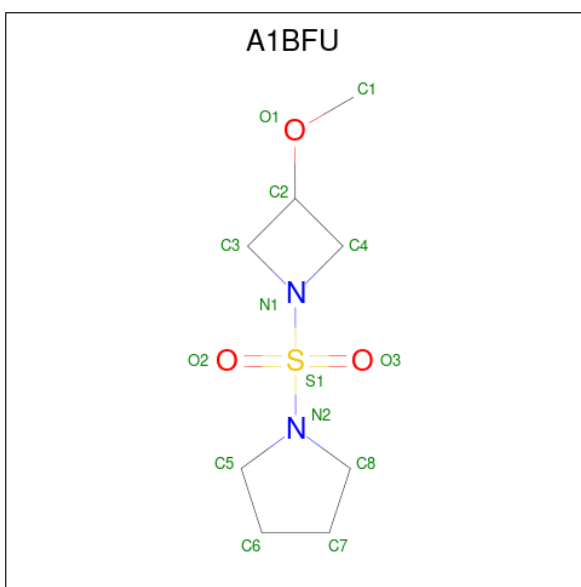


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			7	4	3		

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Cl	0	0
			2	2		

- Molecule 8 is 1-(3-methoxyazetidine-1-sulfonyl)pyrrolidine (three-letter code: A1BFU) (formula: C₈H₁₆N₂O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	S	0	0
			14	8	2	3	1		

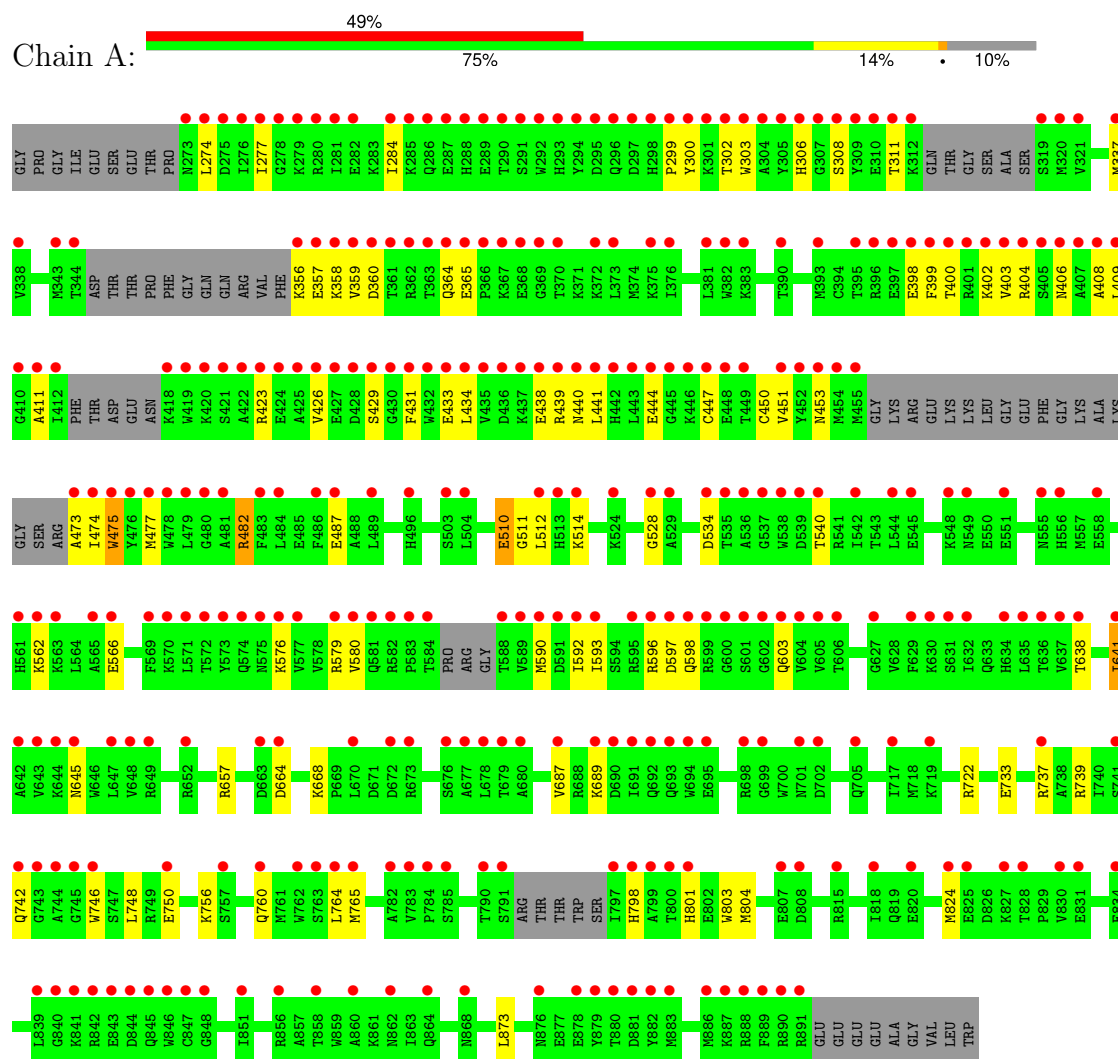
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	335	Total	O	0	0
			335	335		

3 Residue-property plots

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



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	82.28Å 116.04Å 147.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.30 – 1.90 91.30 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.2 (91.30-1.90) 99.2 (91.30-1.90)	Depositor EDS
R_{merge}	0.25	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.09 (at 1.90Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.197 , 0.240 0.247 , 0.274	Depositor DCC
R_{free} test set	2881 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 163.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	5133	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.23% 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: CL, A1BFU, PEG, MES, DMS, PO4, 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	0.73	1/4836 (0.0%)	0.82	2/6520 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	510	GLU	CD-OE2	7.18	1.33	1.25

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	739	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	657	ARG	CG-CD-NE	-5.55	100.14	111.80

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	4731	0	4638	85	0
2	A	2	0	0	0	0
3	A	24	0	26	2	0
4	A	8	0	12	3	0
5	A	10	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	7	0	10	0	0
7	A	2	0	0	0	0
8	A	14	0	0	0	0
9	A	335	0	0	5	0
All	All	5133	0	4686	88	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 9.

All (88) 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:356:LYS:HZ3	1:A:473:ALA:N	1.38	1.22
1:A:302:THR:OG1	1:A:360:ASP:OD1	1.57	1.19
1:A:514:LYS:HE2	9:A:1291:HOH:O	1.73	0.88
1:A:664:ASP:OD1	5:A:1006:PO4:O4	1.93	0.86
1:A:356:LYS:NZ	1:A:473:ALA:N	2.26	0.82
1:A:562:LYS:O	1:A:566:GLU:HG3	1.86	0.75
1:A:311:THR:HG21	1:A:590:MET:HB2	1.71	0.73
1:A:764:LEU:HG	1:A:765:MET:HE3	1.73	0.71
1:A:534:ASP:OD1	5:A:1006:PO4:O4	2.08	0.70
1:A:423:ARG:O	1:A:426:VAL:HG22	1.92	0.69
1:A:356:LYS:HD3	1:A:473:ALA:HB2	1.76	0.68
1:A:400:THR:O	1:A:403:VAL:HG22	1.94	0.66
1:A:439:ARG:NH1	1:A:487:GLU:OE1	2.28	0.66
1:A:364:GLN:CG	1:A:365:GLU:H	2.09	0.65
1:A:364:GLN:HG2	1:A:365:GLU:N	2.11	0.65
1:A:400:THR:O	1:A:404:ARG:HG2	1.96	0.65
1:A:411:ALA:HA	1:A:477:MET:O	1.97	0.64
1:A:356:LYS:CD	1:A:473:ALA:HB2	2.27	0.64
1:A:562:LYS:NZ	1:A:566:GLU:OE2	2.22	0.63
1:A:357:GLU:H	1:A:357:GLU:CD	2.02	0.62
1:A:308:SER:HA	1:A:590:MET:O	1.98	0.62
4:A:1004:DMS:H11	9:A:1364:HOH:O	1.98	0.62
1:A:311:THR:CG2	1:A:590:MET:HB2	2.29	0.61
1:A:764:LEU:HG	1:A:765:MET:CE	2.30	0.61
1:A:364:GLN:CG	1:A:365:GLU:N	2.64	0.60
1:A:438:GLU:O	1:A:441:LEU:HB2	2.00	0.60
1:A:580:VAL:HG21	1:A:593:ILE:HD11	1.84	0.60
1:A:477:MET:SD	1:A:482:ARG:NH1	2.75	0.60
1:A:337:MET:HG2	9:A:1314:HOH:O	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:403:VAL:HG21	1:A:426:VAL:HG11	1.84	0.59
1:A:475:TRP:CD1	1:A:475:TRP:N	2.68	0.59
1:A:664:ASP:OD1	5:A:1006:PO4:P	2.61	0.58
1:A:364:GLN:HG2	1:A:365:GLU:H	1.67	0.57
1:A:638:THR:O	1:A:641:ILE:HG23	2.05	0.57
1:A:733:GLU:O	1:A:737:ARG:HG3	2.05	0.57
1:A:597:ASP:O	1:A:598:GLN:HB2	2.05	0.56
1:A:764:LEU:C	1:A:765:MET:HE3	2.25	0.56
1:A:439:ARG:CZ	1:A:487:GLU:OE1	2.54	0.56
1:A:510:GLU:O	1:A:514:LYS:HG3	2.06	0.56
4:A:1004:DMS:C1	9:A:1364:HOH:O	2.53	0.55
1:A:311:THR:HG21	1:A:590:MET:HE2	1.89	0.55
1:A:357:GLU:CD	1:A:357:GLU:N	2.59	0.55
1:A:311:THR:HG21	1:A:590:MET:CE	2.37	0.54
1:A:399:PHE:O	1:A:403:VAL:HG13	2.09	0.53
1:A:429:SER:O	1:A:433:GLU:HG3	2.09	0.53
1:A:638:THR:HA	1:A:641:ILE:CG2	2.39	0.53
1:A:756:LYS:O	1:A:760:GLN:HG3	2.10	0.51
1:A:408:ALA:HB1	1:A:603:GLN:OE1	2.11	0.51
1:A:303:TRP:CE3	1:A:593:ILE:HD12	2.46	0.51
1:A:303:TRP:HZ2	1:A:359:VAL:CG2	2.23	0.51
1:A:760:GLN:NE2	1:A:803:TRP:O	2.45	0.50
1:A:431:PHE:O	1:A:434:LEU:HB2	2.12	0.50
1:A:303:TRP:CD2	1:A:593:ILE:HD12	2.47	0.49
1:A:580:VAL:CG2	1:A:593:ILE:HD11	2.43	0.48
1:A:511:GLY:N	1:A:798:HIS:O	2.43	0.48
1:A:748:LEU:HD13	3:A:1003[B]:MES:H61	1.94	0.48
1:A:764:LEU:O	1:A:765:MET:HE2	2.14	0.48
4:A:1004:DMS:H12	9:A:1263:HOH:O	2.14	0.47
1:A:576:LYS:NZ	1:A:596:ARG:O	2.47	0.47
1:A:453:ASN:O	1:A:475:TRP:HA	2.15	0.47
1:A:409:LEU:O	1:A:482:ARG:HG2	2.16	0.46
1:A:398:GLU:O	1:A:402:LYS:HG3	2.15	0.46
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.56	0.46
1:A:440:ASN:O	1:A:444:GLU:N	2.41	0.45
1:A:746:TRP:CE3	1:A:750[A]:GLU:HG2	2.51	0.45
1:A:801:HIS:HB3	1:A:804:MET:HG2	1.97	0.45
1:A:431:PHE:HA	1:A:434:LEU:HD12	1.98	0.45
1:A:438:GLU:OE2	1:A:438:GLU:HA	2.17	0.44
1:A:764:LEU:O	1:A:765:MET:CE	2.66	0.44
1:A:274:LEU:HA	1:A:277:ILE:HG12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:358:LYS:HG3	1:A:540:THR:HG21	1.99	0.44
1:A:474:ILE:HD12	1:A:474:ILE:N	2.32	0.43
1:A:356:LYS:HE2	1:A:473:ALA:CB	2.48	0.43
1:A:284:ILE:HD11	1:A:451:VAL:HG21	2.00	0.42
1:A:453:ASN:OD1	1:A:453:ASN:N	2.52	0.42
1:A:306:HIS:HB2	1:A:592:ILE:O	2.18	0.42
1:A:475:TRP:HZ3	1:A:576:LYS:HD3	1.85	0.42
1:A:512[A]:LEU:HD12	1:A:512[A]:LEU:HA	1.88	0.42
1:A:356:LYS:O	1:A:359:VAL:HG12	2.20	0.41
1:A:299:PRO:HD2	1:A:300:TYR:CE2	2.56	0.41
1:A:689:LYS:HB3	1:A:689:LYS:HE2	1.82	0.41
1:A:453:ASN:ND2	1:A:579:ARG:HD2	2.36	0.41
1:A:722:ARG:HB3	1:A:824:MET:SD	2.61	0.41
1:A:873:LEU:HD13	3:A:1003[A]:MES:H62	2.03	0.41
1:A:303:TRP:CZ2	1:A:359:VAL:HG22	2.56	0.41
1:A:528:GLY:O	1:A:668:LYS:HE3	2.21	0.40
1:A:356:LYS:CE	1:A:473:ALA:HB2	2.50	0.40
1:A:742:GLN:HA	1:A:742:GLN:OE1	2.21	0.40

There are no symmetry-related clashes.

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	565/637 (89%)	538 (95%)	26 (5%)	1 (0%)	44 36

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	508/554 (92%)	503 (99%)	5 (1%)	73	74

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	475	TRP
1	A	482	ARG
1	A	641	ILE
1	A	645	ASN
1	A	687	VAL

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	298	HIS
1	A	645	ASN

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

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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
3	MES	A	1003[A]	-	12,12,12	0.70	0	15,16,16	0.29	0
4	DMS	A	1005	-	3,3,3	0.28	0	3,3,3	0.06	0
5	PO4	A	1006	-	4,4,4	3.46	3 (75%)	6,6,6	0.77	0
3	MES	A	1003[B]	-	12,12,12	0.73	0	15,16,16	0.73	0
5	PO4	A	1007	-	4,4,4	1.11	1 (25%)	6,6,6	0.38	0
8	A1BFU	A	1010	-	11,15,15	0.18	0	16,22,22	2.85	4 (25%)
6	PEG	A	1008	-	6,6,6	0.11	0	5,5,5	0.11	0
4	DMS	A	1004	-	3,3,3	0.45	0	3,3,3	0.32	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	A1BFU	A	1010	-	-	3/10/29/29	0/2/2/2
6	PEG	A	1008	-	-	3/4/4/4	-
3	MES	A	1003[A]	-	-	3/6/14/14	0/1/1/1
3	MES	A	1003[B]	-	-	5/6/14/14	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1006	PO4	P-O1	5.68	1.63	1.50
5	A	1006	PO4	P-O4	-2.72	1.46	1.54
5	A	1006	PO4	P-O2	2.40	1.61	1.54
5	A	1007	PO4	P-O1	2.17	1.55	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	1010	A1BFU	C4-N1-S1	7.18	135.15	123.66
8	A	1010	A1BFU	C3-N1-S1	6.37	133.85	123.66
8	A	1010	A1BFU	C2-C4-N1	-4.19	83.62	87.75
8	A	1010	A1BFU	C2-C3-N1	-4.12	83.69	87.75

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1003[A]	MES	C7-C8-S-O2S
3	A	1003[B]	MES	C8-C7-N4-C3
3	A	1003[B]	MES	C7-C8-S-O1S
8	A	1010	A1BFU	C4-C2-O1-C1
8	A	1010	A1BFU	C3-C2-O1-C1
8	A	1010	A1BFU	C8-N2-S1-O2
6	A	1008	PEG	O2-C3-C4-O4
3	A	1003[A]	MES	C7-C8-S-O3S
3	A	1003[B]	MES	C7-C8-S-O3S
3	A	1003[A]	MES	C7-C8-S-O1S
3	A	1003[B]	MES	C7-C8-S-O2S
6	A	1008	PEG	C4-C3-O2-C2
3	A	1003[B]	MES	C8-C7-N4-C5
6	A	1008	PEG	O1-C1-C2-O2

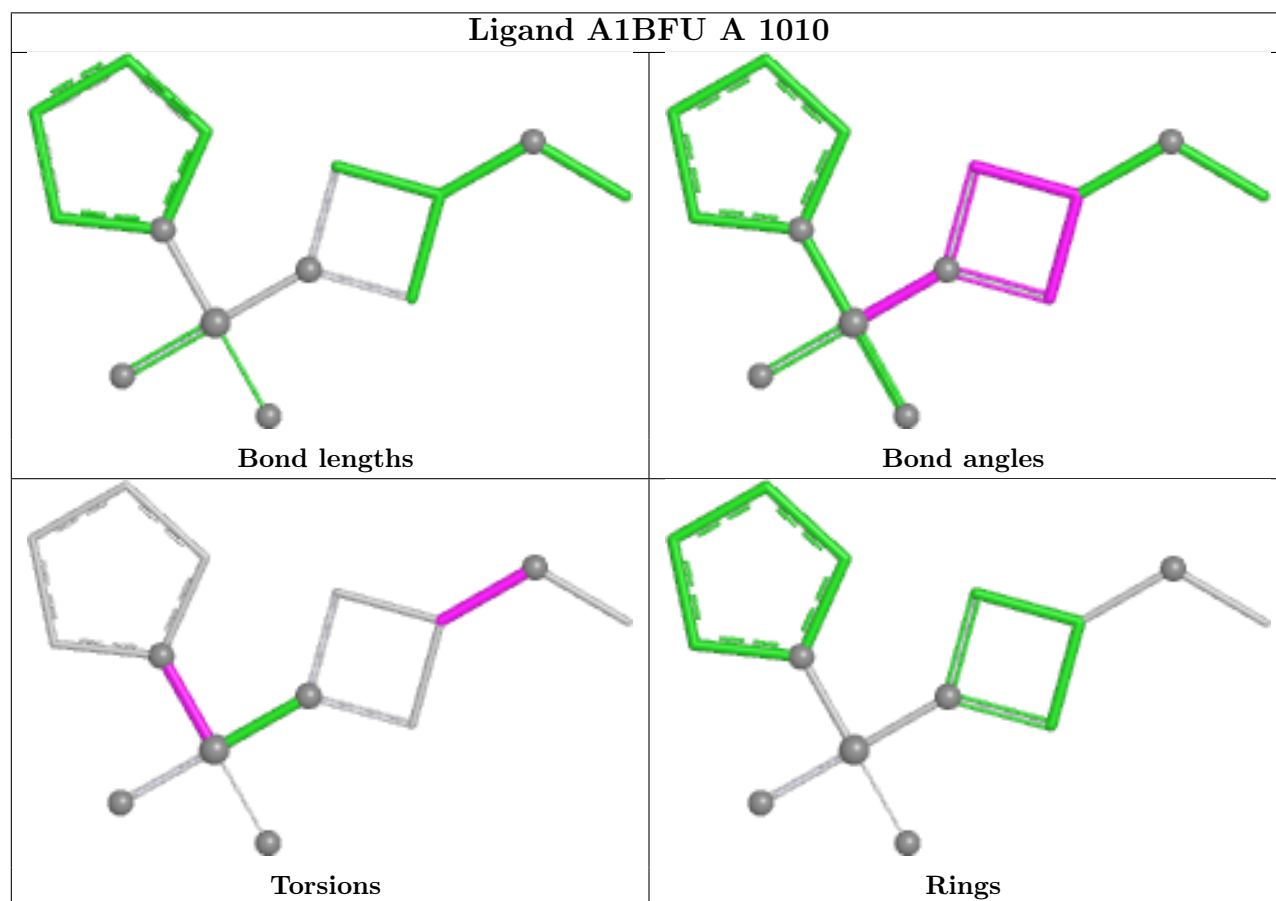
There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003[A]	MES	1	0
5	A	1006	PO4	3	0
3	A	1003[B]	MES	1	0
4	A	1004	DMS	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	572/637 (89%)	3.59	313 (54%) 0 0	6, 35, 74, 121	167 (29%)

All (313) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	409	LEU	16.3
1	A	889	PHE	14.5
1	A	419	TRP	13.9
1	A	410	GLY	13.5
1	A	411	ALA	13.3
1	A	637	VAL	13.0
1	A	580	VAL	12.5
1	A	589	VAL	12.4
1	A	431	PHE	12.4
1	A	408	ALA	12.3
1	A	304	ALA	12.0
1	A	292	TRP	12.0
1	A	303	TRP	11.9
1	A	474	ILE	11.6
1	A	785[A]	SER	11.6
1	A	309	TYR	11.3
1	A	407	ALA	11.3
1	A	475	TRP	11.3
1	A	412	ILE	11.1
1	A	404	ARG	11.0
1	A	799	ALA	11.0
1	A	512[A]	LEU	10.9
1	A	762	TRP	10.6
1	A	359	VAL	10.6
1	A	797	ILE	10.4
1	A	403	VAL	10.4
1	A	800	THR	10.4

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Mol	Chain	Res	Type	RSRZ
1	A	305	TYR	10.3
1	A	641	ILE	10.2
1	A	476	TYR	10.2
1	A	573	TYR	10.2
1	A	478	TRP	10.1
1	A	300	TYR	10.0
1	A	428	ASP	10.0
1	A	400	THR	10.0
1	A	719[A]	LYS	9.8
1	A	424	GLU	9.7
1	A	846	TRP	9.7
1	A	504	LEU	9.7
1	A	888	ARG	9.6
1	A	588	THR	9.6
1	A	798	HIS	9.5
1	A	503	SER	9.5
1	A	741[A]	SER	9.5
1	A	851	ILE	9.3
1	A	632	ILE	9.3
1	A	291	SER	9.2
1	A	363	THR	9.2
1	A	299	PRO	9.1
1	A	801	HIS	9.1
1	A	605	VAL	9.1
1	A	847	CYS	9.1
1	A	430	GLY	8.9
1	A	308	SER	8.9
1	A	443	LEU	8.8
1	A	301	LYS	8.8
1	A	405	SER	8.7
1	A	420	LYS	8.7
1	A	839	LEU	8.6
1	A	606	THR	8.6
1	A	856	ARG	8.5
1	A	406	ASN	8.4
1	A	601	SER	8.4
1	A	423	ARG	8.3
1	A	273	ASN	8.3
1	A	595	ARG	8.3
1	A	590	MET	8.3
1	A	840	GLY	8.3
1	A	418	LYS	8.3

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Mol	Chain	Res	Type	RSRZ
1	A	562	LYS	8.3
1	A	890	ARG	8.3
1	A	848	GLY	8.2
1	A	887	LYS	8.1
1	A	298	HIS	8.1
1	A	745	GLY	8.1
1	A	477	MET	8.0
1	A	302	THR	8.0
1	A	514	LYS	7.9
1	A	581	GLN	7.9
1	A	791	SER	7.9
1	A	321	VAL	7.8
1	A	445	GLY	7.8
1	A	361	THR	7.8
1	A	757	SER	7.8
1	A	366	PRO	7.8
1	A	631	SER	7.7
1	A	886	MET	7.7
1	A	290	THR	7.7
1	A	441	LEU	7.6
1	A	764	LEU	7.6
1	A	513	HIS	7.6
1	A	763[A]	SER	7.5
1	A	356	LYS	7.5
1	A	575	ASN	7.5
1	A	582	ARG	7.5
1	A	576	LYS	7.5
1	A	311	THR	7.4
1	A	287	GLU	7.4
1	A	473	ALA	7.4
1	A	596	ARG	7.4
1	A	427	GLU	7.4
1	A	599	ARG	7.3
1	A	572	THR	7.2
1	A	602	GLY	7.2
1	A	570	LYS	7.1
1	A	274	LEU	7.1
1	A	765	MET	7.1
1	A	312	LYS	7.1
1	A	790	THR	7.1
1	A	687	VAL	7.0
1	A	649	ARG	7.0

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Mol	Chain	Res	Type	RSRZ
1	A	598	GLN	6.9
1	A	597	ASP	6.9
1	A	540	THR	6.8
1	A	429	SER	6.8
1	A	600	GLY	6.8
1	A	630	LYS	6.8
1	A	438	GLU	6.8
1	A	286	GLN	6.7
1	A	591	ASP	6.7
1	A	844	ASP	6.7
1	A	281	ILE	6.7
1	A	295	ASP	6.6
1	A	574	GLN	6.5
1	A	284	ILE	6.5
1	A	744	ALA	6.5
1	A	539	ASP	6.5
1	A	566	GLU	6.5
1	A	743	GLY	6.4
1	A	367	LYS	6.4
1	A	634	HIS	6.4
1	A	750[A]	GLU	6.4
1	A	358	LYS	6.4
1	A	644	LYS	6.4
1	A	319	SER	6.3
1	A	446	LYS	6.3
1	A	402	LYS	6.3
1	A	289	GLU	6.3
1	A	535	THR	6.2
1	A	277	ILE	6.2
1	A	401	ARG	6.2
1	A	275	ASP	6.2
1	A	841	LYS	6.1
1	A	842	ARG	6.1
1	A	645	ASN	6.0
1	A	864[A]	GLN	6.0
1	A	742	GLN	6.0
1	A	689	LYS	6.0
1	A	603	GLN	6.0
1	A	442	HIS	5.9
1	A	439	ARG	5.9
1	A	453	ASN	5.9
1	A	368	GLU	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	422	ALA	5.8
1	A	760	GLN	5.8
1	A	487	GLU	5.8
1	A	676	SER	5.8
1	A	584	THR	5.7
1	A	293	HIS	5.7
1	A	296	GLN	5.7
1	A	393	MET	5.6
1	A	845	GLN	5.6
1	A	320	MET	5.6
1	A	583	PRO	5.6
1	A	629	PHE	5.5
1	A	638	THR	5.5
1	A	288	HIS	5.5
1	A	357	GLU	5.5
1	A	297	ASP	5.5
1	A	843	GLU	5.4
1	A	360	ASP	5.3
1	A	705	GLN	5.3
1	A	448	GLU	5.3
1	A	436	ASP	5.3
1	A	433	GLU	5.2
1	A	880	THR	5.2
1	A	451	VAL	5.2
1	A	362	ARG	5.2
1	A	677	ALA	5.2
1	A	635	LEU	5.1
1	A	437	LYS	5.1
1	A	891	ARG	5.1
1	A	692	GLN	5.1
1	A	690	ASP	5.0
1	A	558	GLU	4.9
1	A	746	TRP	4.9
1	A	693	GLN	4.9
1	A	481	ALA	4.8
1	A	310	GLU	4.8
1	A	479	LEU	4.8
1	A	383	LYS	4.7
1	A	365	GLU	4.7
1	A	452	TYR	4.7
1	A	627	GLY	4.5
1	A	486	PHE	4.5

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Mol	Chain	Res	Type	RSRZ
1	A	278	GLY	4.4
1	A	882	TYR	4.4
1	A	398	GLU	4.4
1	A	294	TYR	4.4
1	A	280	ARG	4.2
1	A	593	ILE	4.2
1	A	529	ALA	4.2
1	A	435	VAL	4.2
1	A	648	VAL	4.2
1	A	881	ASP	4.1
1	A	364	GLN	4.0
1	A	397	GLU	3.9
1	A	285	LYS	3.9
1	A	396	ARG	3.9
1	A	808	ASP	3.9
1	A	534	ASP	3.8
1	A	440	ASN	3.8
1	A	344	THR	3.7
1	A	375	LYS	3.7
1	A	449	THR	3.7
1	A	694	TRP	3.6
1	A	426	VAL	3.6
1	A	399	PHE	3.6
1	A	434	LEU	3.5
1	A	282	GLU	3.5
1	A	592	ILE	3.5
1	A	306	HIS	3.5
1	A	834	GLU	3.5
1	A	556	HIS	3.4
1	A	876	ASN	3.4
1	A	455	MET	3.4
1	A	604	VAL	3.4
1	A	496	HIS	3.4
1	A	524	LYS	3.3
1	A	544	LEU	3.3
1	A	670	LEU	3.3
1	A	868	ASN	3.3
1	A	425	ALA	3.3
1	A	563	LYS	3.3
1	A	483	PHE	3.3
1	A	444	GLU	3.2
1	A	538	TRP	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	421	SER	3.2
1	A	858	THR	3.2
1	A	571	LEU	3.1
1	A	337	MET	3.1
1	A	825	GLU	3.1
1	A	372	LYS	3.1
1	A	484	LEU	3.0
1	A	830	VAL	3.0
1	A	454	MET	3.0
1	A	579	ARG	3.0
1	A	536	ALA	3.0
1	A	701	ASN	2.9
1	A	307	GLY	2.9
1	A	548	LYS	2.9
1	A	276	ILE	2.9
1	A	807	GLU	2.9
1	A	699	GLY	2.8
1	A	643	VAL	2.8
1	A	279	LYS	2.8
1	A	636	THR	2.8
1	A	698	ARG	2.8
1	A	717	ILE	2.8
1	A	878	GLU	2.8
1	A	432	TRP	2.8
1	A	818	ILE	2.8
1	A	390	THR	2.7
1	A	447	CYS	2.7
1	A	480	GLY	2.7
1	A	551	GLU	2.7
1	A	831	GLU	2.7
1	A	784	PRO	2.7
1	A	678	LEU	2.7
1	A	652	ARG	2.6
1	A	828	THR	2.6
1	A	879	TYR	2.6
1	A	663	ASP	2.6
1	A	577	VAL	2.6
1	A	545	GLU	2.6
1	A	820	GLU	2.6
1	A	489	LEU	2.5
1	A	827	LYS	2.5
1	A	555	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	691	ILE	2.5
1	A	395	THR	2.5
1	A	672	ASP	2.4
1	A	737	ARG	2.4
1	A	673	ARG	2.4
1	A	783	VAL	2.4
1	A	369	GLY	2.4
1	A	680	ALA	2.4
1	A	373	LEU	2.3
1	A	883	MET	2.3
1	A	382	TRP	2.3
1	A	782	ALA	2.3
1	A	702	ASP	2.3
1	A	824	MET	2.2
1	A	561	HIS	2.2
1	A	565	ALA	2.2
1	A	862	ASN	2.2
1	A	343	MET	2.2
1	A	338	VAL	2.2
1	A	528	GLY	2.2
1	A	376	ILE	2.2
1	A	542	ILE	2.2
1	A	370	THR	2.1
1	A	815	ARG	2.1
1	A	695	GLU	2.1
1	A	537	GLY	2.1
1	A	569	PHE	2.1
1	A	642	ALA	2.1
1	A	664	ASP	2.1
1	A	679	THR	2.1
1	A	381	LEU	2.0
1	A	647	LEU	2.0
1	A	860	ALA	2.0
1	A	549	ASN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

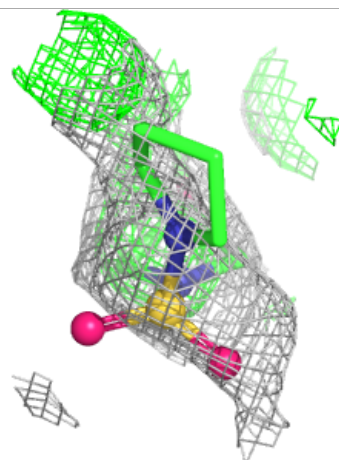
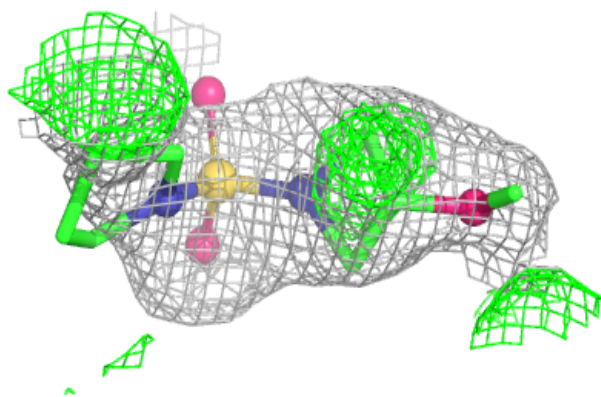
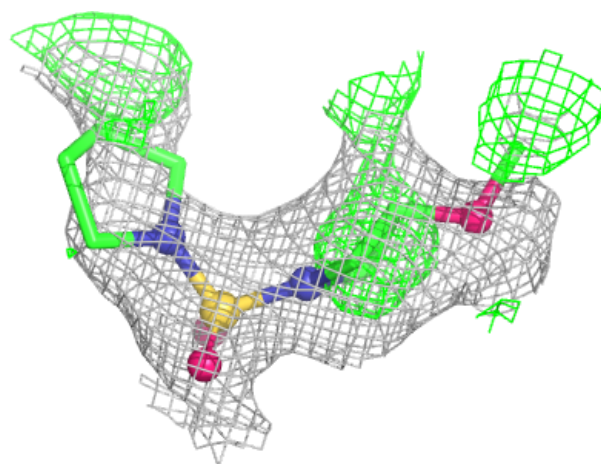
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	A1BFU	A	1010	14/14	0.66	0.45	75,84,90,91	14
5	PO4	A	1007	5/5	0.76	0.14	79,91,99,115	0
6	PEG	A	1008	7/7	0.82	0.22	66,71,81,82	0
4	DMS	A	1005	4/4	0.82	0.23	78,91,96,100	0
5	PO4	A	1006	5/5	0.83	0.12	36,42,50,67	0
4	DMS	A	1004	4/4	0.94	0.17	43,44,47,49	0
3	MES	A	1003[A]	12/12	0.94	0.23	686,701,724,735	12
3	MES	A	1003[B]	12/12	0.94	0.23	31,33,34,37	12
7	CL	A	1011	1/1	0.95	0.23	34,34,34,34	1
7	CL	A	1009	1/1	0.98	0.05	44,44,44,44	0
2	ZN	A	1001	1/1	0.99	0.04	25,25,25,25	0
2	ZN	A	1002	1/1	0.99	0.04	53,53,53,53	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 A1BFU A 1010:

$2mF_o-DF_c$ (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.