



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2025 – 11:46 AM EDT

PDB ID : 7I28  
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 Z45527714 (DNV2\_NS5A-x0153)  
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](mailto: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)

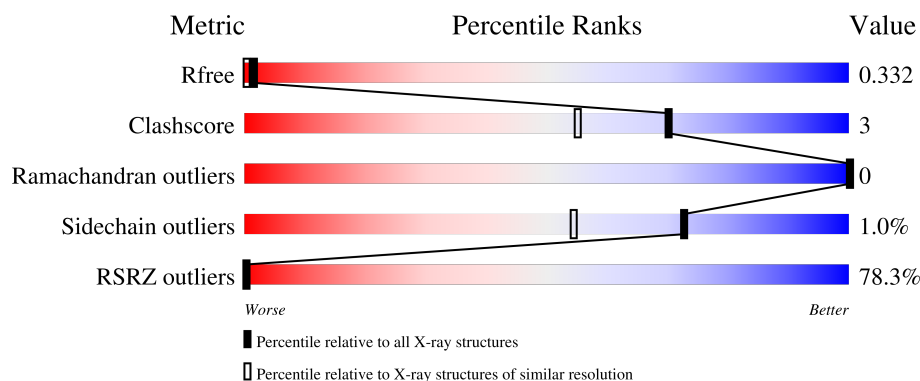
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.63 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  $\geq 3$ , 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
4	DMS	A	1004	-	-	-	X
6	PO4	A	1007	-	-	X	-

## 2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5083 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	571	Total	C	N	O	S	0	6	0
			4710	2966	844	866	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: C<sub>6</sub>H<sub>13</sub>NO<sub>4</sub>S).



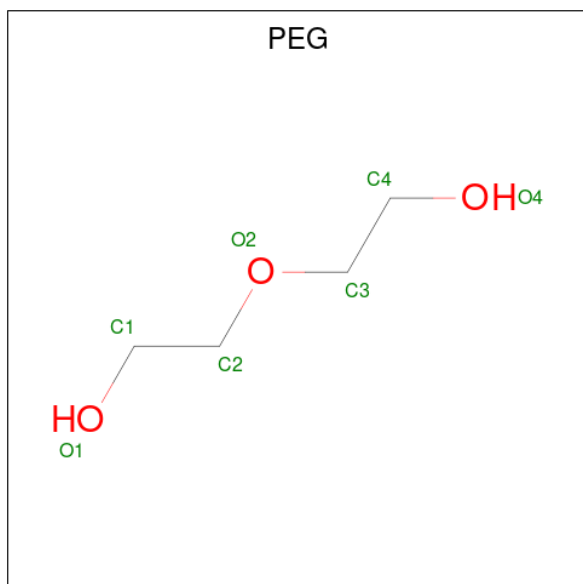
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

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



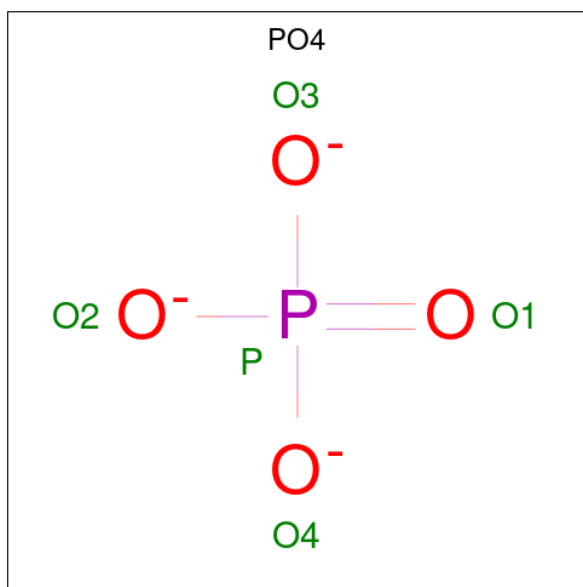
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

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



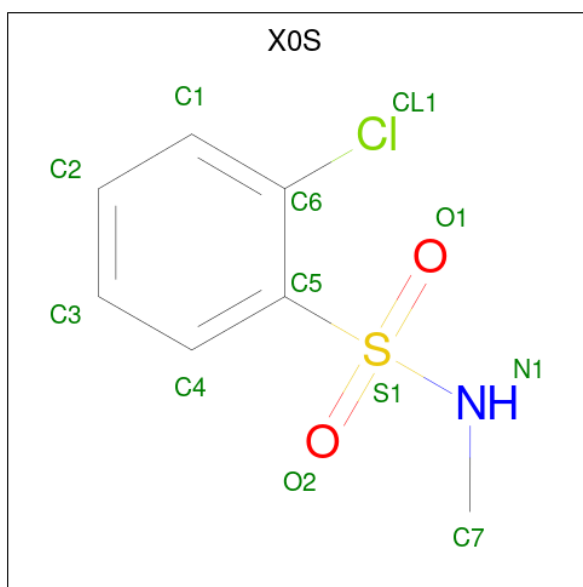
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		

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



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

- Molecule 7 is 2-chloro-N-methylbenzene-1-sulfonamide (three-letter code: X0S) (formula:  $C_7H_8ClNO_2S$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
7	A	1	Total	C	Cl	N	O	S	0	0
			12	7	1	1	2	1		
7	A	1	Total	C	Cl	N	O	S	0	1
			24	14	2	2	4	2		

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

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

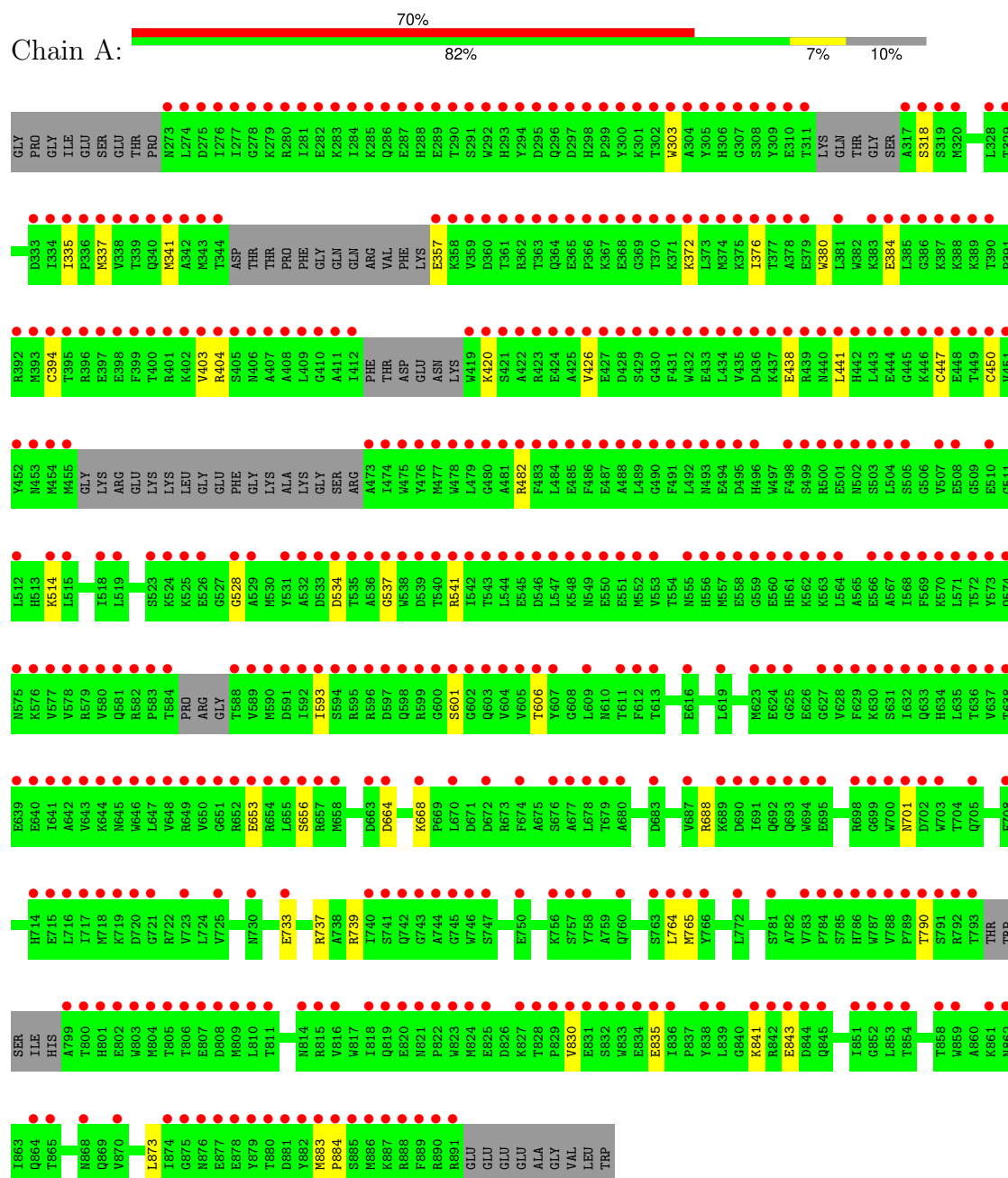
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	290	Total	O	0	0
			290	290		

### 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, $\alpha$ , $\beta$ , $\gamma$	82.56Å 117.17Å 148.29Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.15 – 1.63 74.15 – 1.63	Depositor EDS
% Data completeness (in resolution range)	94.1 (74.15-1.63) 94.1 (74.15-1.63)	Depositor EDS
$R_{merge}$	0.13	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	0.95 (at 1.63Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, $R_{free}$	0.217 , 0.250 0.318 , 0.332	Depositor DCC
$R_{free}$ test set	4556 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	26.3	Xtriage
Anisotropy	0.393	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 441.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.82	EDS
Total number of atoms	5083	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: DMS, X0S, MES, PEG, PO4, ZN, CL

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	0.78	0/4815	0.81	2/6495 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	739	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	A	688	ARG	NE-CZ-NH2	-5.49	117.56	120.30

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	4710	0	4608	30	0
2	A	2	0	0	0	0
3	A	12	0	13	1	0
4	A	8	0	12	0	0
5	A	14	0	20	0	0
6	A	10	0	0	3	0
7	A	36	0	0	3	0
8	A	1	0	0	0	0
9	A	290	0	0	7	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5083	0	4653	31	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 3.

All (31) 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:841:LYS:HD3	7:A:1011[B]:X0S:CL1	2.03	0.95
1:A:653:GLU:O	1:A:656:SER:OG	2.02	0.76
1:A:601:SER:HG	1:A:606:THR:HG1	1.40	0.69
1:A:394:CYS:SG	9:A:1221:HOH:O	2.52	0.68
1:A:534:ASP:OD1	6:A:1007:PO4:O2	2.15	0.65
1:A:318:SER:O	9:A:1101:HOH:O	2.16	0.62
1:A:733:GLU:O	1:A:737:ARG:HG3	2.03	0.58
1:A:843:GLU:OE2	9:A:1102:HOH:O	2.17	0.58
1:A:664:ASP:OD1	6:A:1007:PO4:O2	2.22	0.57
1:A:380:TRP:O	1:A:384:GLU:HG2	2.06	0.56
1:A:528:GLY:O	1:A:668:LYS:HE3	2.08	0.54
1:A:830:VAL:HG13	1:A:835:GLU:HB2	1.90	0.53
1:A:841:LYS:CD	7:A:1011[B]:X0S:CL1	2.88	0.53
1:A:303:TRP:CE3	1:A:593:ILE:HD12	2.45	0.51
1:A:873:LEU:HD13	3:A:1003:MES:H62	1.92	0.50
1:A:737:ARG:HB3	9:A:1354:HOH:O	2.11	0.50
1:A:790:THR:HG21	9:A:1366:HOH:O	2.13	0.48
1:A:664:ASP:OD1	6:A:1007:PO4:P	2.72	0.48
1:A:372:LYS:HD2	1:A:376:ILE:HD11	1.96	0.48
1:A:537:GLY:O	1:A:541:ARG:HG2	2.14	0.48
1:A:337:MET:O	1:A:341:MET:HG3	2.15	0.47
1:A:701:ASN:ND2	9:A:1108:HOH:O	2.29	0.46
1:A:403:VAL:HG21	1:A:426:VAL:HG21	1.98	0.46
1:A:438:GLU:O	1:A:441:LEU:HB2	2.17	0.44
1:A:514:LYS:HE3	9:A:1292:HOH:O	2.17	0.44
1:A:764:LEU:HG	1:A:765:MET:HE3	2.00	0.44
7:A:1011[B]:X0S:CL1	7:A:1011[B]:X0S:O2	2.75	0.41
1:A:733:GLU:O	1:A:737:ARG:CG	2.69	0.41
1:A:883:MET:N	1:A:884:PRO:CD	2.84	0.41
1:A:303:TRP:CD2	1:A:593:ILE:HD12	2.55	0.41
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.60	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	563/637 (88%)	542 (96%)	21 (4%)	0	100	100

There are no Ramachandran outliers to report.

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	505/554 (91%)	500 (99%)	5 (1%)	73	54

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

Mol	Chain	Res	Type
1	A	335	ILE
1	A	357	GLU
1	A	404	ARG
1	A	420	LYS
1	A	482	ARG

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

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

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$
5	PEG	A	1006	-	6,6,6	0.19	0	5,5,5	0.13	0
7	X0S	A	1011[A]	-	12,12,12	0.31	0	16,17,17	0.36	0
3	MES	A	1003	-	12,12,12	0.72	0	15,16,16	0.30	0
6	PO4	A	1007	-	4,4,4	2.05	1 (25%)	6,6,6	0.66	0
6	PO4	A	1008	-	4,4,4	0.62	0	6,6,6	0.45	0
4	DMS	A	1004	-	3,3,3	0.24	0	3,3,3	0.13	0
5	PEG	A	1009	-	6,6,6	0.15	0	5,5,5	0.10	0
7	X0S	A	1010	-	12,12,12	0.18	0	16,17,17	0.27	0
7	X0S	A	1011[B]	-	12,12,12	0.13	0	16,17,17	0.40	0
4	DMS	A	1005	-	3,3,3	0.13	0	3,3,3	0.11	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
5	PEG	A	1006	-	-	3/4/4/4	-
7	X0S	A	1011[A]	-	-	0/9/9/9	0/1/1/1
3	MES	A	1003	-	-	0/6/14/14	0/1/1/1
5	PEG	A	1009	-	-	1/4/4/4	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	X0S	A	1010	-	-	2/9/9/9	0/1/1/1
7	X0S	A	1011[B]	-	-	8/9/9/9	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1007	PO4	P-O1	3.90	1.59	1.50

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	1011[B]	X0S	C6-C5-S1-N1
7	A	1011[B]	X0S	C6-C5-S1-O1
7	A	1011[B]	X0S	C7-N1-S1-C5
7	A	1011[B]	X0S	C7-N1-S1-O1
7	A	1011[B]	X0S	C7-N1-S1-O2
7	A	1011[B]	X0S	C4-C5-S1-O1
7	A	1011[B]	X0S	C4-C5-S1-N1
5	A	1006	PEG	O2-C3-C4-O4
5	A	1009	PEG	O2-C3-C4-O4
7	A	1011[B]	X0S	C6-C5-S1-O2
5	A	1006	PEG	O1-C1-C2-O2
7	A	1010	X0S	C7-N1-S1-O1
7	A	1010	X0S	C7-N1-S1-O2
5	A	1006	PEG	C4-C3-O2-C2

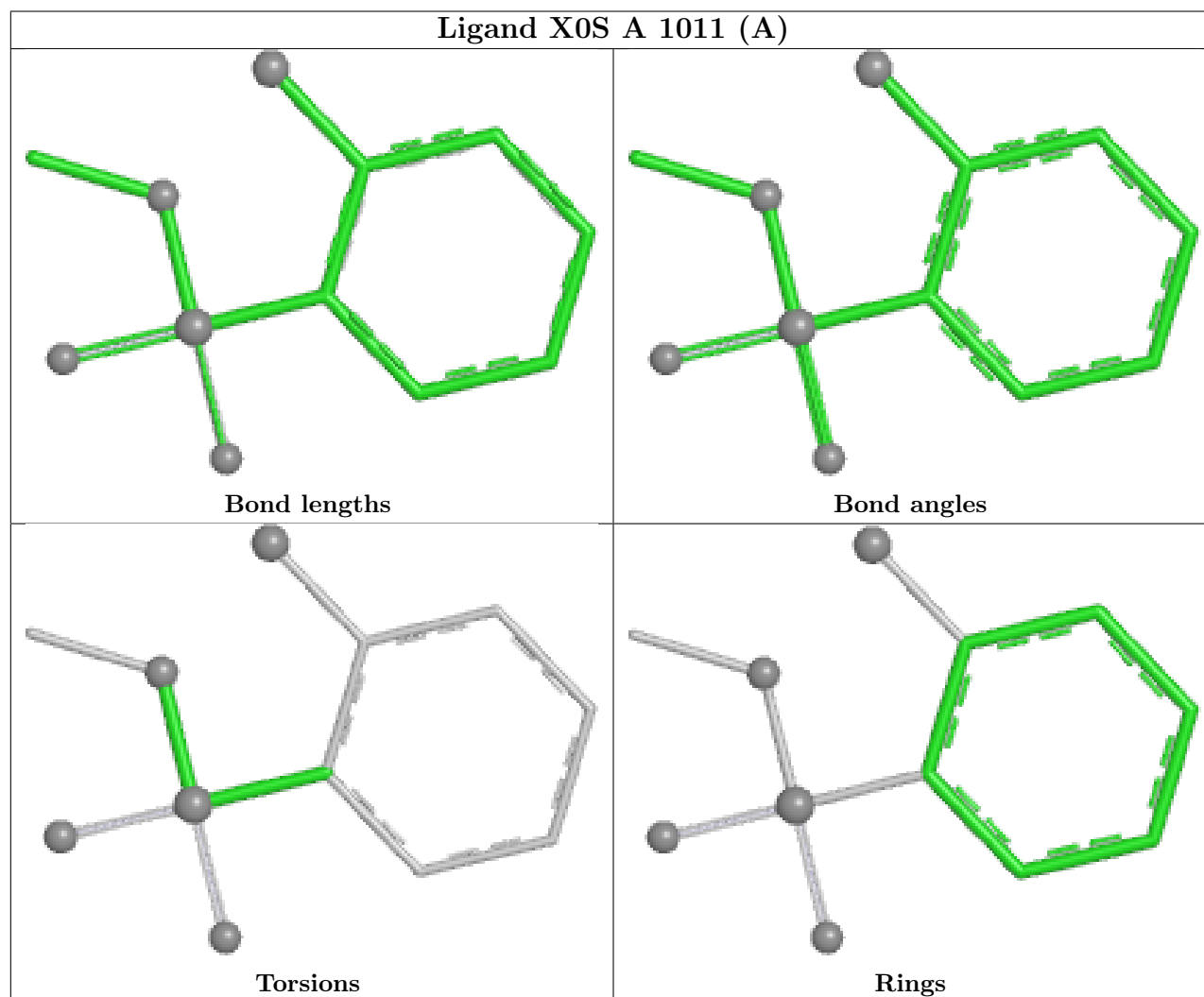
There are no ring outliers.

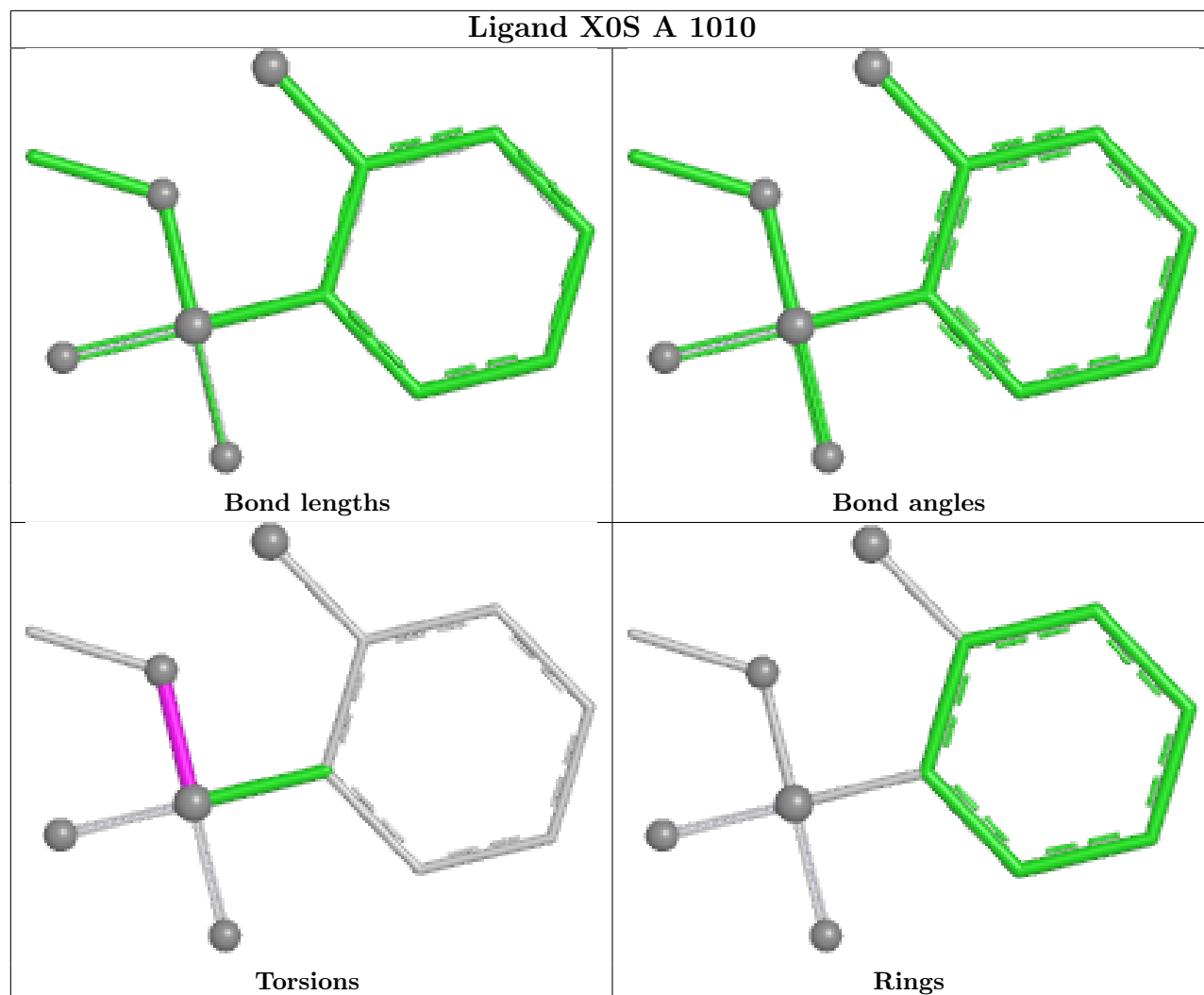
3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003	MES	1	0
6	A	1007	PO4	3	0
7	A	1011[B]	X0S	3	0

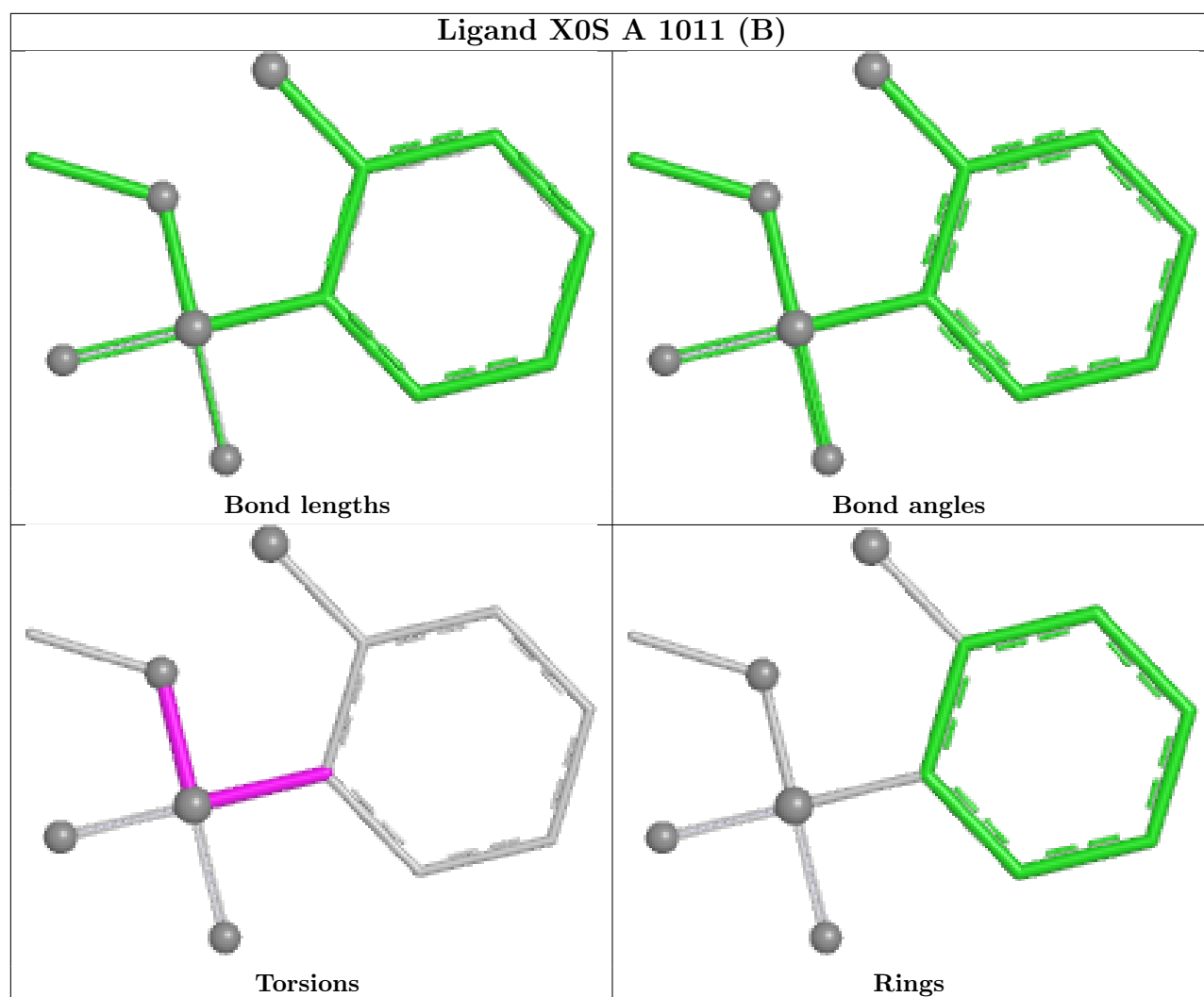
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	571/637 (89%)	6.35	447 (78%) <b>0</b> <b>0</b>	5, 26, 65, 131	291 (50%)

All (447) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	277	ILE	19.2
1	A	284	ILE	18.9
1	A	474	ILE	18.7
1	A	311	THR	18.2
1	A	359	VAL	17.8
1	A	411	ALA	17.7
1	A	281	ILE	17.2
1	A	412	ILE	17.0
1	A	403	VAL	16.8
1	A	800	THR	16.5
1	A	589	VAL	16.4
1	A	441	LEU	16.2
1	A	286	GLN	16.1
1	A	292	TRP	15.9
1	A	584	THR	15.6
1	A	641	ILE	15.5
1	A	274	LEU	15.5
1	A	276	ILE	15.2
1	A	304	ALA	14.6
1	A	409	LEU	14.4
1	A	435	VAL	14.2
1	A	305	TYR	14.0
1	A	452	TYR	14.0
1	A	290	THR	14.0
1	A	580	VAL	13.9
1	A	405	SER	13.9
1	A	283	LYS	13.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	294	TYR	13.6
1	A	282	GLU	13.5
1	A	884	PRO	13.2
1	A	299	PRO	13.2
1	A	478	TRP	13.2
1	A	436	ASP	13.1
1	A	475	TRP	13.1
1	A	291	SER	13.0
1	A	309	TYR	12.9
1	A	476	TYR	12.9
1	A	450	CYS	12.9
1	A	650	VAL	12.8
1	A	455	MET	12.7
1	A	799	ALA	12.7
1	A	637	VAL	12.7
1	A	285	LYS	12.5
1	A	479	LEU	12.5
1	A	279	LYS	12.5
1	A	577	VAL	12.4
1	A	434	LEU	12.4
1	A	642	ALA	12.3
1	A	358	LYS	12.3
1	A	432	TRP	12.3
1	A	636	THR	12.2
1	A	830	VAL	12.2
1	A	431	PHE	12.2
1	A	293	HIS	12.2
1	A	564	LEU	12.2
1	A	453	ASN	12.1
1	A	449	THR	12.1
1	A	278	GLY	12.1
1	A	648	VAL	12.0
1	A	882	TYR	12.0
1	A	400	THR	12.0
1	A	422	ALA	12.0
1	A	638	THR	11.9
1	A	288	HIS	11.9
1	A	746	TRP	11.8
1	A	803	TRP	11.8
1	A	384	GLU	11.7
1	A	512[A]	LEU	11.7
1	A	280	ARG	11.7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	362	ARG	11.7
1	A	880	THR	11.7
1	A	376	ILE	11.7
1	A	483	PHE	11.5
1	A	543	THR	11.4
1	A	308	SER	11.4
1	A	451	VAL	11.4
1	A	592	ILE	11.4
1	A	406	ASN	11.4
1	A	645	ASN	11.2
1	A	572	THR	11.2
1	A	408	ALA	11.1
1	A	879	TYR	11.1
1	A	578	VAL	11.1
1	A	600	GLY	11.1
1	A	787	TRP	11.0
1	A	357	GLU	11.0
1	A	791	SER	11.0
1	A	790	THR	10.9
1	A	788	VAL	10.9
1	A	612	PHE	10.8
1	A	883	MET	10.8
1	A	605	VAL	10.8
1	A	480	GLY	10.8
1	A	885	SER	10.7
1	A	547	LEU	10.7
1	A	404	ARG	10.7
1	A	582	ARG	10.7
1	A	289	GLU	10.7
1	A	789	PRO	10.6
1	A	307	GLY	10.6
1	A	481	ALA	10.5
1	A	583	PRO	10.5
1	A	334	ILE	10.5
1	A	425	ALA	10.5
1	A	419	TRP	10.5
1	A	743	GLY	10.4
1	A	338	VAL	10.4
1	A	805	THR	10.4
1	A	810	LEU	10.3
1	A	399	PHE	10.3
1	A	828	THR	10.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	371	LYS	10.3
1	A	407	ALA	10.3
1	A	836	ILE	10.3
1	A	519	LEU	10.3
1	A	375	LYS	10.2
1	A	426	VAL	10.2
1	A	397	GLU	10.1
1	A	891	ARG	10.1
1	A	868	ASN	10.1
1	A	335	ILE	10.0
1	A	410	GLY	10.0
1	A	486	PHE	9.9
1	A	491	PHE	9.9
1	A	421	SER	9.8
1	A	861	LYS	9.8
1	A	563	LYS	9.7
1	A	454	MET	9.7
1	A	402	LYS	9.7
1	A	385	LEU	9.7
1	A	604	VAL	9.7
1	A	793	THR	9.6
1	A	833	TRP	9.6
1	A	588	THR	9.5
1	A	562	LYS	9.5
1	A	649	ARG	9.4
1	A	822	PRO	9.4
1	A	275	ASP	9.4
1	A	606	THR	9.4
1	A	573	TYR	9.4
1	A	420	LYS	9.4
1	A	655	LEU	9.4
1	A	499	SER	9.4
1	A	717	ILE	9.3
1	A	504	LEU	9.3
1	A	401	ARG	9.3
1	A	372	LYS	9.3
1	A	287	GLU	9.3
1	A	574	GLN	9.3
1	A	742	GLN	9.3
1	A	886	MET	9.3
1	A	336	PRO	9.3
1	A	851	ILE	9.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	317	ALA	9.2
1	A	764	LEU	9.2
1	A	716	LEU	9.1
1	A	423	ARG	9.1
1	A	339	THR	9.1
1	A	792	ARG	9.1
1	A	498	PHE	9.0
1	A	639	GLU	9.0
1	A	551	GLU	9.0
1	A	839	LEU	9.0
1	A	561	HIS	9.0
1	A	446	LYS	9.0
1	A	319	SER	8.9
1	A	570	LYS	8.9
1	A	538	TRP	8.9
1	A	298	HIS	8.9
1	A	473	ALA	8.9
1	A	273	ASN	8.8
1	A	581	GLN	8.8
1	A	559	GLY	8.8
1	A	484	LEU	8.8
1	A	310	GLU	8.8
1	A	801[A]	HIS	8.8
1	A	806	THR	8.8
1	A	430	GLY	8.8
1	A	556	HIS	8.8
1	A	881	ASP	8.7
1	A	297	ASP	8.7
1	A	535	THR	8.6
1	A	303	TRP	8.6
1	A	541	ARG	8.5
1	A	781	SER	8.5
1	A	537	GLY	8.5
1	A	300	TYR	8.5
1	A	576	LYS	8.5
1	A	644	LYS	8.5
1	A	804	MET	8.5
1	A	747	SER	8.4
1	A	477	MET	8.4
1	A	888	ARG	8.4
1	A	429	SER	8.4
1	A	505	SER	8.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	320	MET	8.3
1	A	889	PHE	8.3
1	A	424	GLU	8.3
1	A	302	THR	8.3
1	A	635	LEU	8.3
1	A	306	HIS	8.2
1	A	599	ARG	8.2
1	A	296	GLN	8.1
1	A	834	GLU	8.1
1	A	757	SER	8.1
1	A	701	ASN	8.1
1	A	487	GLU	8.1
1	A	802	GLU	8.0
1	A	363	THR	8.0
1	A	295	ASP	7.9
1	A	337	MET	7.9
1	A	809	MET	7.9
1	A	389	LYS	7.9
1	A	640	GLU	7.9
1	A	656	SER	7.9
1	A	741[A]	SER	7.9
1	A	820	GLU	7.8
1	A	714	HIS	7.8
1	A	689	LYS	7.8
1	A	383	LYS	7.8
1	A	507	VAL	7.8
1	A	448	GLU	7.8
1	A	744	ALA	7.7
1	A	862	ASN	7.7
1	A	668	LYS	7.7
1	A	428	ASP	7.7
1	A	364	GLN	7.7
1	A	536	ALA	7.7
1	A	784	PRO	7.6
1	A	510	GLU	7.6
1	A	333	ASP	7.6
1	A	361	THR	7.6
1	A	814	ASN	7.6
1	A	493	ASN	7.6
1	A	829	PRO	7.6
1	A	721	GLY	7.5
1	A	318	SER	7.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	786	HIS	7.4
1	A	575	ASN	7.4
1	A	745	GLY	7.4
1	A	598	GLN	7.4
1	A	514	LYS	7.3
1	A	427	GLU	7.3
1	A	392	ARG	7.3
1	A	591	ASP	7.3
1	A	597	ASP	7.2
1	A	616	GLU	7.2
1	A	386	GLY	7.1
1	A	785[A]	SER	7.1
1	A	808	ASP	7.1
1	A	657	ARG	7.1
1	A	546	ASP	7.0
1	A	702	ASP	7.0
1	A	890	ARG	7.0
1	A	495	ASP	7.0
1	A	807	GLU	6.9
1	A	763	SER	6.9
1	A	765	MET	6.9
1	A	558	GLU	6.8
1	A	387	LYS	6.8
1	A	433	GLU	6.8
1	A	718	MET	6.8
1	A	832	SER	6.8
1	A	694	TRP	6.8
1	A	388	LYS	6.7
1	A	443	LEU	6.7
1	A	539	ASP	6.7
1	A	658	MET	6.7
1	A	690	ASP	6.6
1	A	720	ASP	6.6
1	A	503	SER	6.6
1	A	390	THR	6.6
1	A	654	ARG	6.6
1	A	301	LYS	6.5
1	A	445	GLY	6.5
1	A	634	HIS	6.5
1	A	482	ARG	6.5
1	A	601	SER	6.4
1	A	560	GLU	6.4

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	825	GLU	6.4
1	A	632	ILE	6.3
1	A	393	MET	6.3
1	A	629	PHE	6.3
1	A	603	GLN	6.3
1	A	525	LYS	6.3
1	A	523	SER	6.3
1	A	845	GLN	6.2
1	A	876	ASN	6.2
1	A	590	MET	6.2
1	A	643	VAL	6.2
1	A	360	ASP	6.2
1	A	887	LYS	6.1
1	A	750	GLU	6.1
1	A	340	GLN	6.0
1	A	756	LYS	6.0
1	A	500	ARG	6.0
1	A	835	GLU	6.0
1	A	719[A]	LYS	5.9
1	A	875	GLY	5.9
1	A	864[A]	GLN	5.9
1	A	715	GLU	5.9
1	A	652	ARG	5.8
1	A	571	LEU	5.8
1	A	502	ASN	5.8
1	A	579	ARG	5.8
1	A	379	GLU	5.8
1	A	540	THR	5.7
1	A	494	GLU	5.7
1	A	544	LEU	5.6
1	A	524	LYS	5.6
1	A	440	ASN	5.5
1	A	365	GLU	5.5
1	A	552	MET	5.4
1	A	439	ARG	5.4
1	A	595	ARG	5.3
1	A	693	GLN	5.3
1	A	815	ARG	5.3
1	A	567	ALA	5.2
1	A	370	THR	5.2
1	A	508	GLU	5.2
1	A	398	GLU	5.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	854	THR	5.2
1	A	526	GLU	5.1
1	A	396	ARG	5.1
1	A	653	GLU	5.1
1	A	760	GLN	5.0
1	A	569	PHE	5.0
1	A	842	ARG	5.0
1	A	593	ILE	5.0
1	A	367	LYS	5.0
1	A	841	LYS	4.9
1	A	843	GLU	4.9
1	A	442	HIS	4.9
1	A	676	SER	4.9
1	A	555	ASN	4.8
1	A	695	GLU	4.8
1	A	831	GLU	4.8
1	A	368	GLU	4.8
1	A	596	ARG	4.7
1	A	602	GLY	4.7
1	A	670	LEU	4.7
1	A	819	GLN	4.7
1	A	630	LYS	4.6
1	A	501	GLU	4.6
1	A	878	GLU	4.6
1	A	568	ILE	4.5
1	A	663	ASP	4.5
1	A	818	ILE	4.4
1	A	877	GLU	4.4
1	A	447	CYS	4.4
1	A	366	PRO	4.4
1	A	633	GLN	4.4
1	A	698	ARG	4.4
1	A	692	GLN	4.3
1	A	489	LEU	4.3
1	A	758	TYR	4.3
1	A	485	GLU	4.3
1	A	699	GLY	4.3
1	A	548	LYS	4.3
1	A	344	THR	4.2
1	A	646	TRP	4.1
1	A	651	GLY	4.1
1	A	549	ASN	4.1

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	678	LEU	4.1
1	A	545	GLU	4.0
1	A	687	VAL	4.0
1	A	628	VAL	3.9
1	A	438	GLU	3.9
1	A	740	ILE	3.9
1	A	631	SER	3.9
1	A	373	LEU	3.8
1	A	647	LEU	3.8
1	A	343	MET	3.8
1	A	625	GLY	3.8
1	A	496	HIS	3.8
1	A	534	ASP	3.8
1	A	488	ALA	3.7
1	A	674	PHE	3.7
1	A	619	LEU	3.6
1	A	444	GLU	3.6
1	A	683	ASP	3.5
1	A	381	LEU	3.5
1	A	627	GLY	3.4
1	A	725	VAL	3.4
1	A	529	ALA	3.3
1	A	394	CYS	3.3
1	A	853	LEU	3.3
1	A	672	ASP	3.2
1	A	613	THR	3.2
1	A	341	MET	3.2
1	A	691	ILE	3.2
1	A	378	ALA	3.2
1	A	858	THR	3.2
1	A	821	ASN	3.1
1	A	824	MET	3.0
1	A	328	LEU	2.9
1	A	532	ALA	2.9
1	A	677	ALA	2.9
1	A	611	THR	2.9
1	A	703	TRP	2.8
1	A	772	LEU	2.8
1	A	874	ILE	2.8
1	A	437	LYS	2.8
1	A	557	MET	2.8
1	A	664	ASP	2.8

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	607	TYR	2.8
1	A	490	GLY	2.7
1	A	708	PHE	2.7
1	A	859	TRP	2.7
1	A	723	VAL	2.7
1	A	374	MET	2.6
1	A	766	TYR	2.6
1	A	342	ALA	2.6
1	A	533	ASP	2.6
1	A	528	GLY	2.5
1	A	377	THR	2.5
1	A	679	THR	2.5
1	A	783	VAL	2.5
1	A	531	TYR	2.5
1	A	811	THR	2.5
1	A	844	ASP	2.5
1	A	680	ALA	2.5
1	A	542	ILE	2.4
1	A	865	THR	2.4
1	A	329	THR	2.3
1	A	395	THR	2.3
1	A	553	VAL	2.3
1	A	609	LEU	2.3
1	A	594	SER	2.3
1	A	518	ILE	2.3
1	A	705	GLN	2.3
1	A	515	LEU	2.3
1	A	623	MET	2.2
1	A	566	GLU	2.2
1	A	816	VAL	2.2
1	A	492	LEU	2.2
1	A	624	GLU	2.2
1	A	700	TRP	2.2
1	A	827	LYS	2.2
1	A	550	GLU	2.2
1	A	733	GLU	2.2
1	A	852	GLY	2.2
1	A	823	TRP	2.1
1	A	870	VAL	2.1
1	A	369	GLY	2.1
1	A	838	TYR	2.1
1	A	730	ASN	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](#)

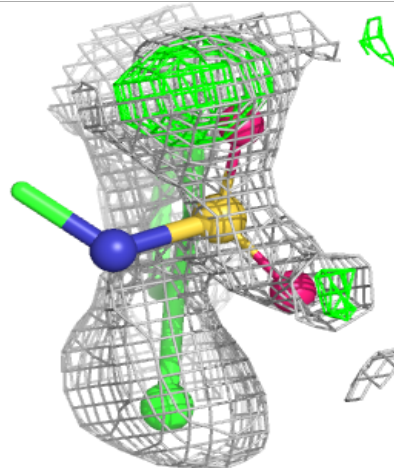
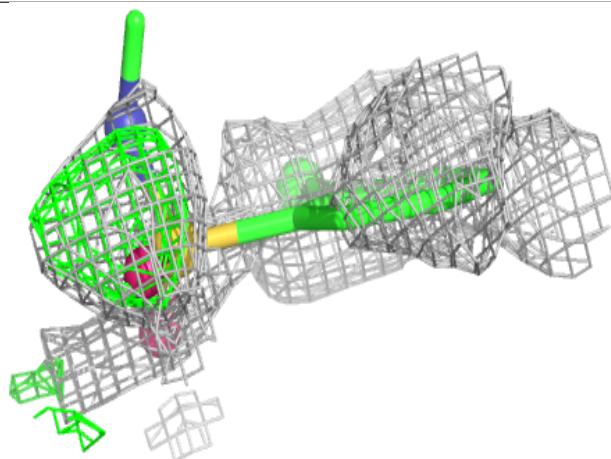
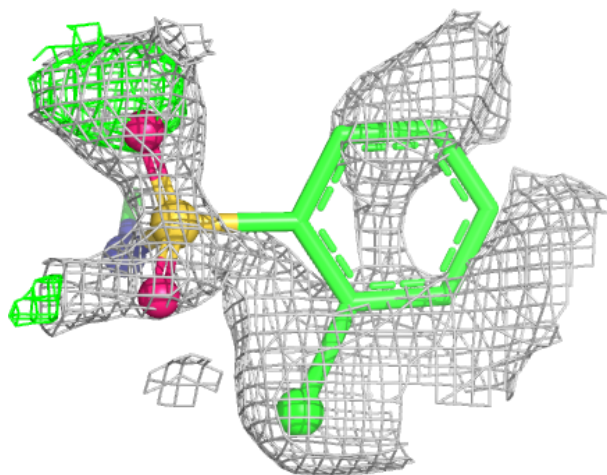
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	X0S	A	1011[A]	12/12	0.40	0.37	33,34,36,37	12
7	X0S	A	1011[B]	12/12	0.40	0.37	32,44,50,52	12
6	PO4	A	1008	5/5	0.41	0.32	57,63,66,66	5
5	PEG	A	1006	7/7	0.60	0.30	49,51,52,52	7
6	PO4	A	1007	5/5	0.64	0.27	29,30,32,35	5
4	DMS	A	1004	4/4	0.67	0.63	91,97,98,99	4
7	X0S	A	1010	12/12	0.69	0.36	44,47,53,56	12
5	PEG	A	1009	7/7	0.81	0.32	42,45,48,49	7
4	DMS	A	1005	4/4	0.88	0.34	43,47,48,48	4
3	MES	A	1003	12/12	0.92	0.24	14,24,35,412	12
8	CL	A	1012	1/1	0.93	0.08	18,18,18,18	1
2	ZN	A	1002	1/1	0.96	0.08	49,49,49,49	0
2	ZN	A	1001	1/1	1.00	0.06	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.

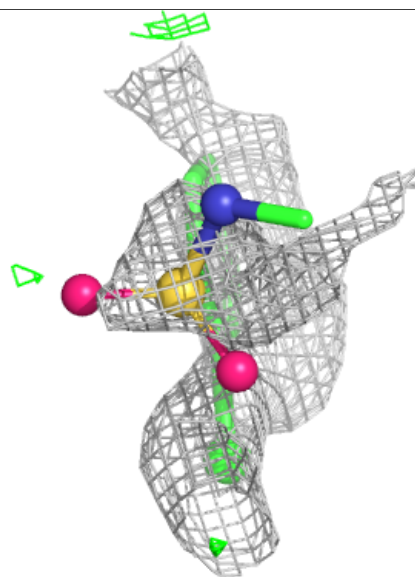
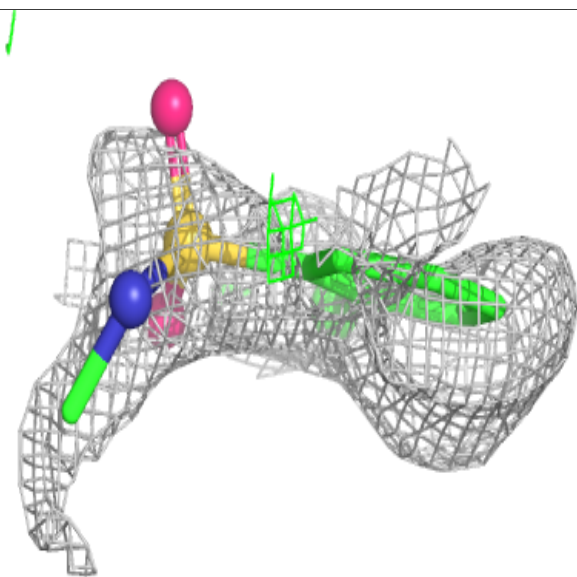
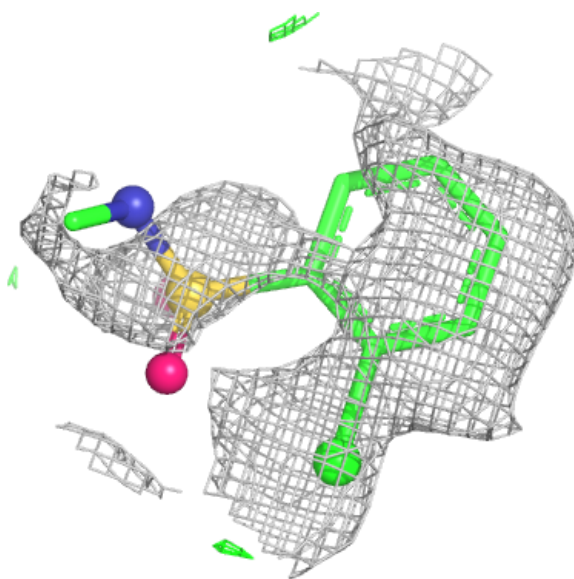
**Electron density around X0S A 1011 (A):**

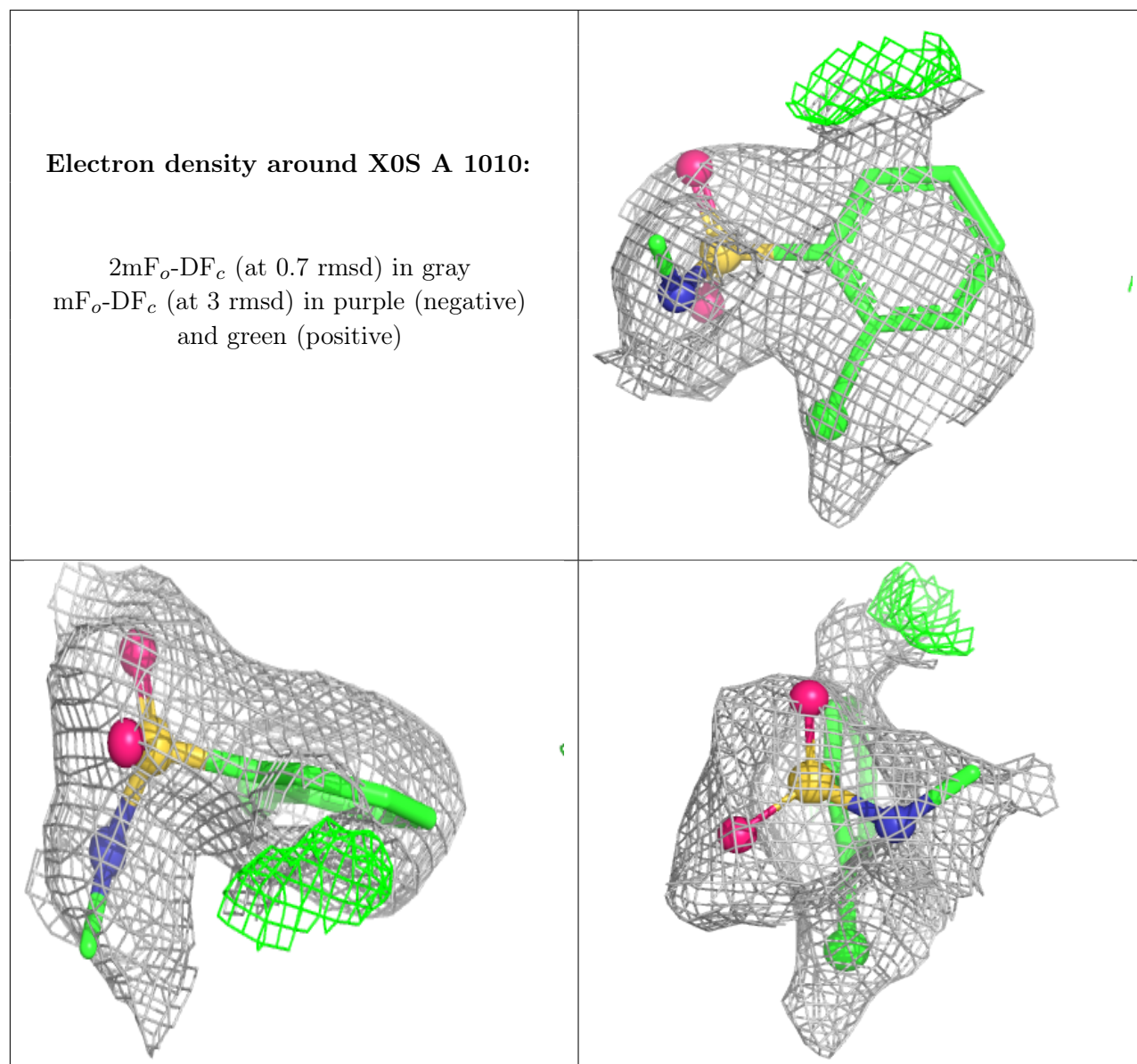
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around X0S A 1011 (B):**

$2mF_o-DF_c$  (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.