Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2025 – 11:49 AM EDT

PDB ID	:	7I2N
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 Z1685106505 (DNV2_NS5A-x0571)
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Deposited on	:	2025-03-06
Resolution	:	1.92 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:

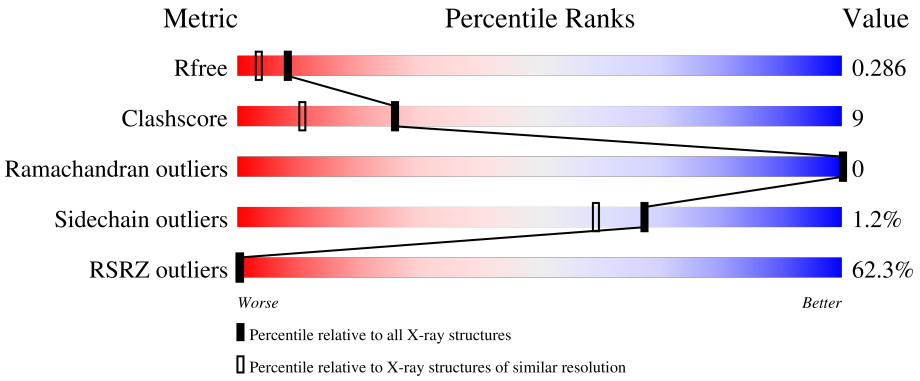
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.92 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	1028 (1.92-1.92)
Clashscore	180529	1100 (1.92-1.92)
Ramachandran outliers	177936	1087 (1.92-1.92)
Sidechain outliers	177891	1087 (1.92-1.92)
RSRZ outliers	164620	1028 (1.92-1.92)

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	55% 76% 12% • 11%

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	1007	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5034 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	565	4673	2945	836	858	34	0	6	0

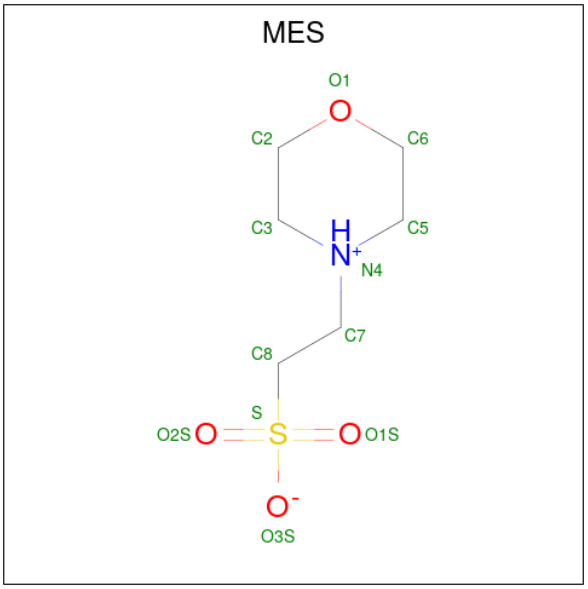
There are 2 discrepancies between the modelled and reference sequences:

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).

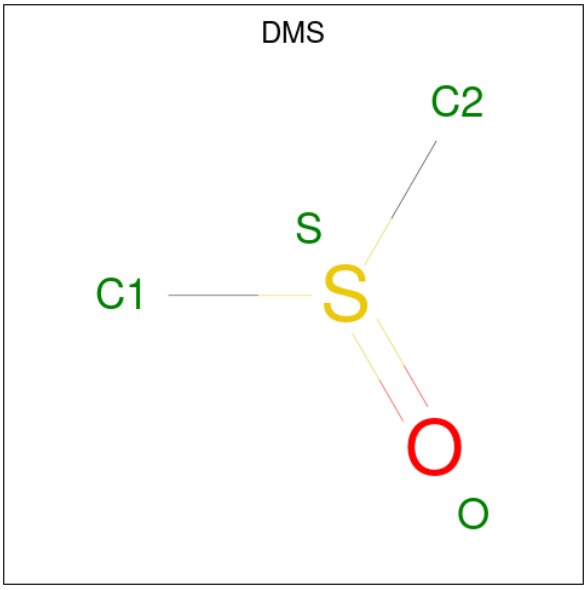
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	2	2	2	0	0

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



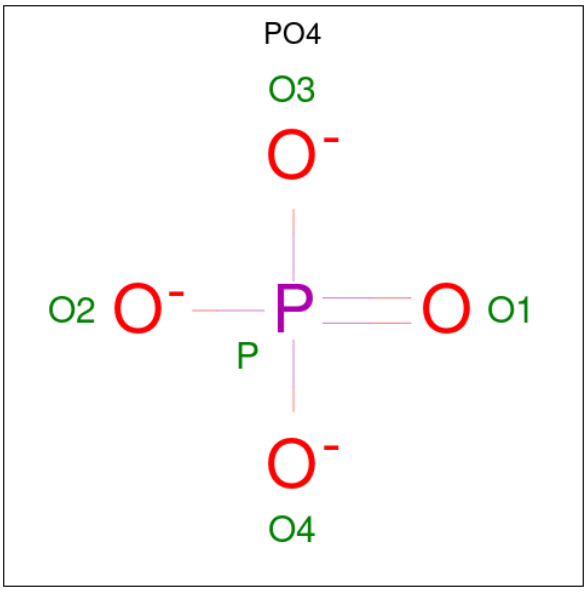
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

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



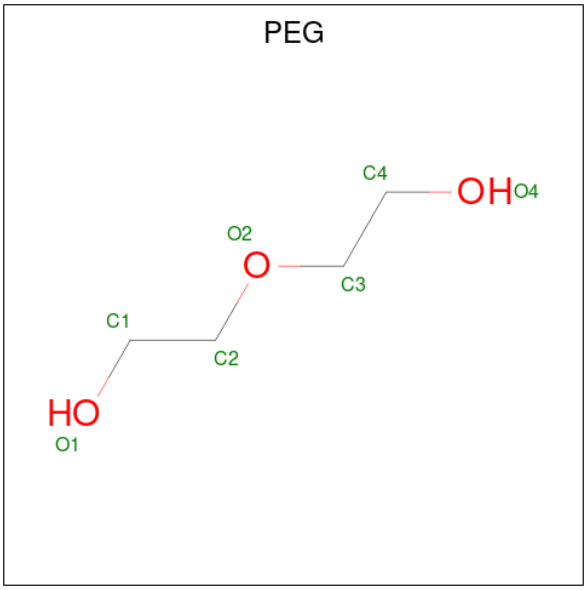
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	O	S		0	0
			4	2	1	1			
4	A	1	Total	C	O	S		0	0
			4	2	1	1			
4	A	1	Total	C	O	S		0	0
			4	2	1	1			

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



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

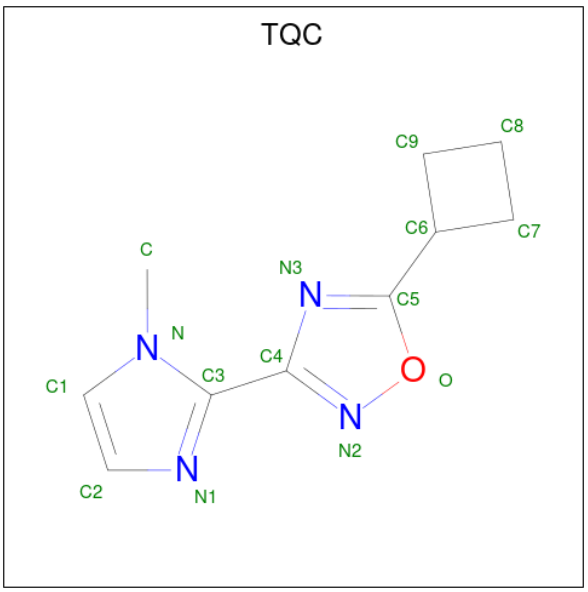
- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 7 is (3M)-5-cyclobutyl-3-(1-methyl-1H-imidazol-2-yl)-1,2,4-oxadiazole (three-letter

code: TQC) (formula: $C_{10}H_{12}N_4O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 15 10 4 1	0	0

- Molecule 8 is water.

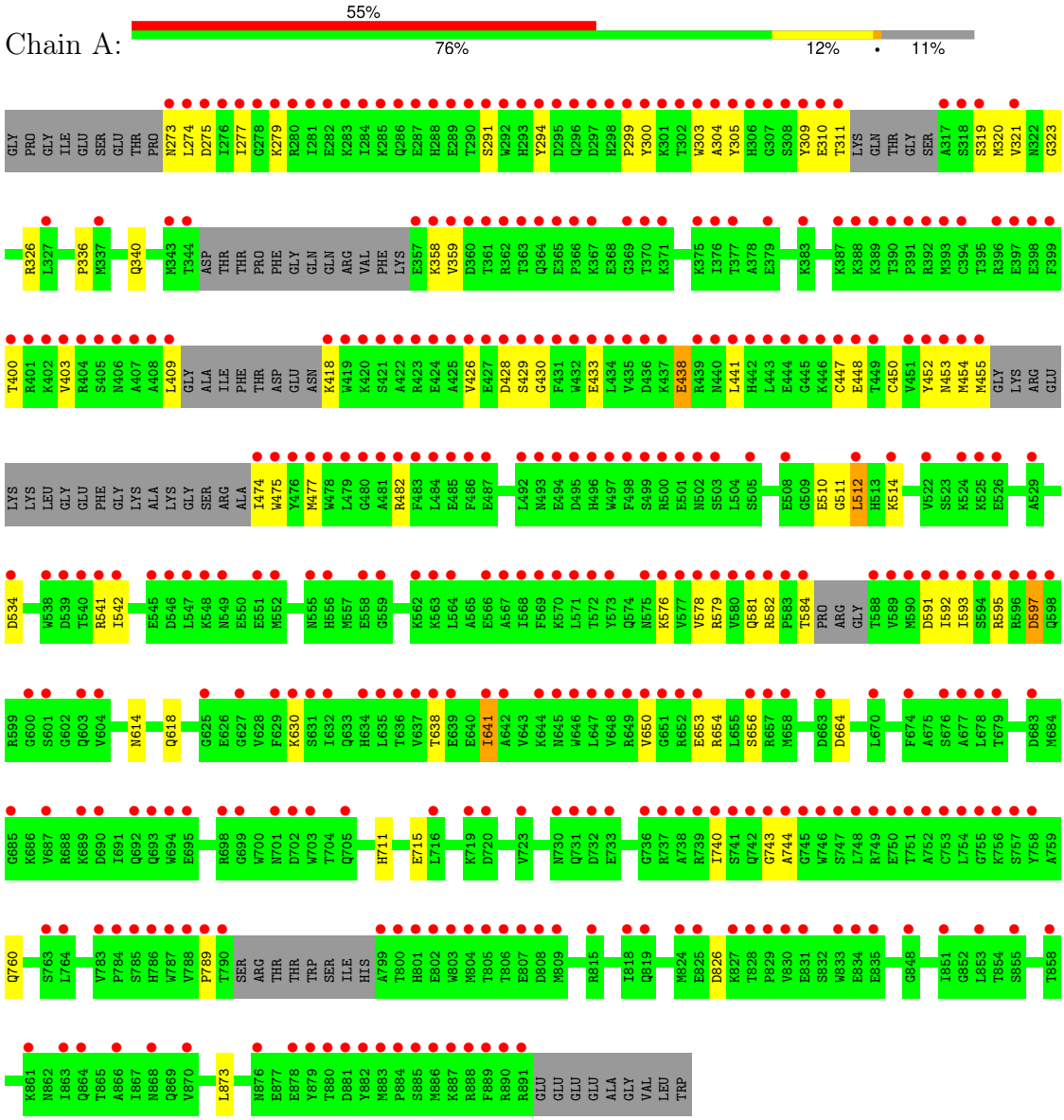
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	291	Total O 291 291	0	0

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	82.76Å 116.49Å 147.36Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.39 – 1.92 91.39 – 1.92	Depositor EDS
% Data completeness (in resolution range)	98.1 (91.39-1.92) 98.2 (91.39-1.92)	Depositor EDS
R_{merge}	0.19	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.02 (at 1.92Å)	Xtriage
Refinement program	REFMAC5	Depositor
R, R_{free}	0.200 , 0.247 0.273 , 0.286	Depositor DCC
R_{free} test set	2809 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å^2)	38.6	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 321.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.84	EDS
Total number of atoms	5034	wwPDB-VP
Average B, all atoms (Å^2)	57.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.01% 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: MES, TQC, PEG, DMS, ZN, PO4

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	0.72	0/4778	0.81	0/6444

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	511	GLY	Mainchain
1	A	512[B]	LEU	Mainchain

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	4673	0	4572	86	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	2	0	0	0	0
3	A	24	0	26	2	0
4	A	12	0	18	1	0
5	A	10	0	0	3	0
6	A	7	0	10	0	0
7	A	15	0	0	0	0
8	A	291	0	0	5	1
All	All	5034	0	4626	87	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 9.

All (87) 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:453:ASN:ND2	1:A:579:ARG:HD2	1.58	1.18
1:A:454:MET:O	1:A:455:MET:HG3	1.50	1.11
1:A:400:THR:O	1:A:403:VAL:HG22	1.68	0.92
1:A:630:LYS:HD2	8:A:1148:HOH:O	1.74	0.86
1:A:595:ARG:NH2	1:A:597:ASP:OD1	2.11	0.82
1:A:429:SER:O	1:A:433:GLU:HG3	1.80	0.81
1:A:400:THR:HG23	1:A:426:VAL:HG11	1.62	0.80
1:A:664:ASP:OD1	5:A:1007:PO4:O4	2.00	0.78
1:A:452:TYR:O	1:A:578:VAL:HA	1.83	0.78
1:A:323:GLY:HA3	3:A:1003[B]:MES:H71	1.66	0.77
1:A:638:THR:O	1:A:641:ILE:HG22	1.85	0.76
1:A:454:MET:C	1:A:455:MET:HG3	2.06	0.75
1:A:291:SER:O	1:A:309:TYR:HA	1.86	0.74
1:A:453:ASN:CG	1:A:579:ARG:HD2	2.13	0.69
1:A:418:LYS:O	1:A:418:LYS:HD3	1.93	0.68
1:A:452:TYR:HB2	1:A:578:VAL:HG22	1.77	0.66
1:A:453:ASN:HD21	1:A:579:ARG:HD2	1.60	0.66
1:A:304:ALA:O	1:A:593:ILE:HA	1.95	0.65
1:A:303:TRP:HE1	1:A:359:VAL:HG22	1.62	0.65
1:A:403:VAL:HG21	1:A:426:VAL:HG21	1.78	0.64
1:A:595:ARG:NE	1:A:597:ASP:OD1	2.32	0.63
1:A:664:ASP:OD1	5:A:1007:PO4:P	2.57	0.62
1:A:454:MET:O	1:A:455:MET:CG	2.39	0.61
1:A:400:THR:HG23	1:A:426:VAL:CG1	2.29	0.61
1:A:474:ILE:HD12	1:A:474:ILE:N	2.16	0.60
1:A:744:ALA:C	8:A:1133:HOH:O	2.40	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:TRP:CE3	1:A:593:ILE:HD12	2.38	0.59
1:A:591:ASP:O	1:A:592:ILE:HD13	2.02	0.59
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.43	0.58
1:A:303:TRP:NE1	1:A:359:VAL:HG22	2.21	0.56
1:A:510:GLU:O	1:A:514:LYS:HG3	2.05	0.56
1:A:303:TRP:CZ2	1:A:595:ARG:HD2	2.41	0.56
1:A:303:TRP:CD2	1:A:593:ILE:HD12	2.41	0.55
1:A:452:TYR:O	1:A:578:VAL:HG13	2.06	0.55
1:A:452:TYR:CE2	1:A:477:MET:CE	2.90	0.55
1:A:595:ARG:CZ	1:A:597:ASP:OD1	2.56	0.54
1:A:299:PRO:HD3	1:A:582:ARG:CZ	2.38	0.53
1:A:452:TYR:CD2	1:A:477:MET:HE3	2.43	0.53
1:A:873:LEU:HD13	3:A:1003[B]:MES:H62	1.91	0.53
1:A:512[B]:LEU:HD11	1:A:711:HIS:CE1	2.44	0.52
1:A:452:TYR:CE2	1:A:477:MET:HE1	2.44	0.52
1:A:428:ASP:OD1	1:A:430:GLY:N	2.41	0.51
1:A:409:LEU:HD22	8:A:1389:HOH:O	2.11	0.51
1:A:319:SER:HB2	1:A:740:ILE:HG23	1.92	0.51
1:A:303:TRP:HH2	1:A:475:TRP:CH2	2.29	0.51
1:A:336:PRO:O	1:A:340:GLN:HG2	2.11	0.50
1:A:299:PRO:HD2	1:A:300:TYR:CE2	2.47	0.49
1:A:579:ARG:O	1:A:579:ARG:HG3	2.12	0.49
1:A:310:GLU:O	1:A:311:THR:HG23	2.13	0.49
1:A:305:TYR:CE1	1:A:591:ASP:OD1	2.65	0.49
4:A:1004:DMS:H11	8:A:1158:HOH:O	2.11	0.49
1:A:428:ASP:OD1	1:A:428:ASP:C	2.52	0.48
1:A:576:LYS:NZ	1:A:597:ASP:O	2.34	0.48
1:A:826:ASP:OD1	1:A:826:ASP:C	2.52	0.48
1:A:294:TYR:CD1	1:A:305:TYR:HE2	2.33	0.47
1:A:274:LEU:HA	1:A:277:ILE:CG1	2.45	0.47
1:A:274:LEU:HA	1:A:277:ILE:HG12	1.97	0.47
1:A:579:ARG:HA	1:A:591:ASP:O	2.15	0.46
1:A:438:GLU:HG2	8:A:1327:HOH:O	2.15	0.45
1:A:452:TYR:CE2	1:A:477:MET:HE3	2.50	0.45
1:A:438:GLU:O	1:A:441:LEU:HB2	2.16	0.45
1:A:512[A]:LEU:HD21	1:A:711:HIS:NE2	2.31	0.45
1:A:273:ASN:N	1:A:275:ASP:OD1	2.50	0.44
1:A:303:TRP:CE2	1:A:595:ARG:HD2	2.53	0.44
1:A:653:GLU:O	1:A:656:SER:OG	2.29	0.44
1:A:358:LYS:NZ	1:A:541:ARG:HH21	2.15	0.44
1:A:614:ASN:O	1:A:618:GLN:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:TRP:CZ3	1:A:576:LYS:HD3	2.54	0.43
1:A:534:ASP:OD1	5:A:1007:PO4:O4	2.36	0.43
1:A:321:VAL:HG11	1:A:326:ARG:CZ	2.49	0.43
1:A:760:GLN:NE2	1:A:789:PRO:HG3	2.34	0.43
1:A:279:LYS:HE3	1:A:448:GLU:HB2	2.01	0.42
1:A:592:ILE:HG22	1:A:592:ILE:O	2.18	0.42
1:A:273:ASN:O	1:A:277:ILE:HG12	2.19	0.42
1:A:453:ASN:CG	1:A:579:ARG:CD	2.86	0.42
1:A:474:ILE:N	1:A:474:ILE:CD1	2.81	0.42
1:A:582:ARG:HG2	1:A:584:THR:OG1	2.19	0.42
1:A:452:TYR:CZ	1:A:477:MET:CE	3.02	0.42
1:A:542:ILE:HD13	1:A:542:ILE:HA	1.94	0.41
1:A:305:TYR:HE1	1:A:591:ASP:OD1	2.04	0.41
1:A:426:VAL:CG1	1:A:426:VAL:O	2.68	0.41
1:A:299:PRO:HD3	1:A:582:ARG:NH1	2.35	0.41
1:A:650:VAL:O	1:A:654:ARG:HG2	2.20	0.40
1:A:320:MET:HG3	1:A:743:GLY:O	2.21	0.40
1:A:303:TRP:HH2	1:A:475:TRP:HH2	1.67	0.40
1:A:438:GLU:OE1	1:A:450:CYS:SG	2.79	0.40
1:A:275:ASP:OD1	1:A:275:ASP:N	2.54	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)
8:A:1279:HOH:O	8:A:1279:HOH:O[4_545]	2.16	0.04

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	557/637 (87%)	524 (94%)	33 (6%)	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	502/554 (91%)	496 (99%)	6 (1%)	67 59

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

Mol	Chain	Res	Type
1	A	438	GLU
1	A	482	ARG
1	A	581	GLN
1	A	597	ASP
1	A	641	ILE
1	A	715	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	819	GLN

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 (i)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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	$\#\|Z\| > 2$
7	TQC	A	1010	-	11,17,17	0.62	0	17,24,24	1.24	0
3	MES	A	1003[B]	-	12,12,12	0.70	0	15,16,16	0.28	0
5	PO4	A	1007	-	4,4,4	2.77	2 (50%)	6,6,6	0.89	0
5	PO4	A	1008	-	4,4,4	0.83	0	6,6,6	0.43	0
4	DMS	A	1005	-	3,3,3	0.30	0	3,3,3	0.06	0
4	DMS	A	1004	-	3,3,3	0.21	0	3,3,3	0.14	0
3	MES	A	1003[A]	-	12,12,12	0.72	0	15,16,16	0.29	0
4	DMS	A	1006	-	3,3,3	0.18	0	3,3,3	0.29	0
6	PEG	A	1009	-	6,6,6	0.17	0	5,5,5	0.14	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
7	TQC	A	1010	-	-	1/3/14/14	0/3/3/3
3	MES	A	1003[A]	-	-	0/6/14/14	0/1/1/1
3	MES	A	1003[B]	-	-	0/6/14/14	0/1/1/1
6	PEG	A	1009	-	-	3/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1007	PO4	P-O1	4.18	1.60	1.50
5	A	1007	PO4	P-O2	2.94	1.63	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

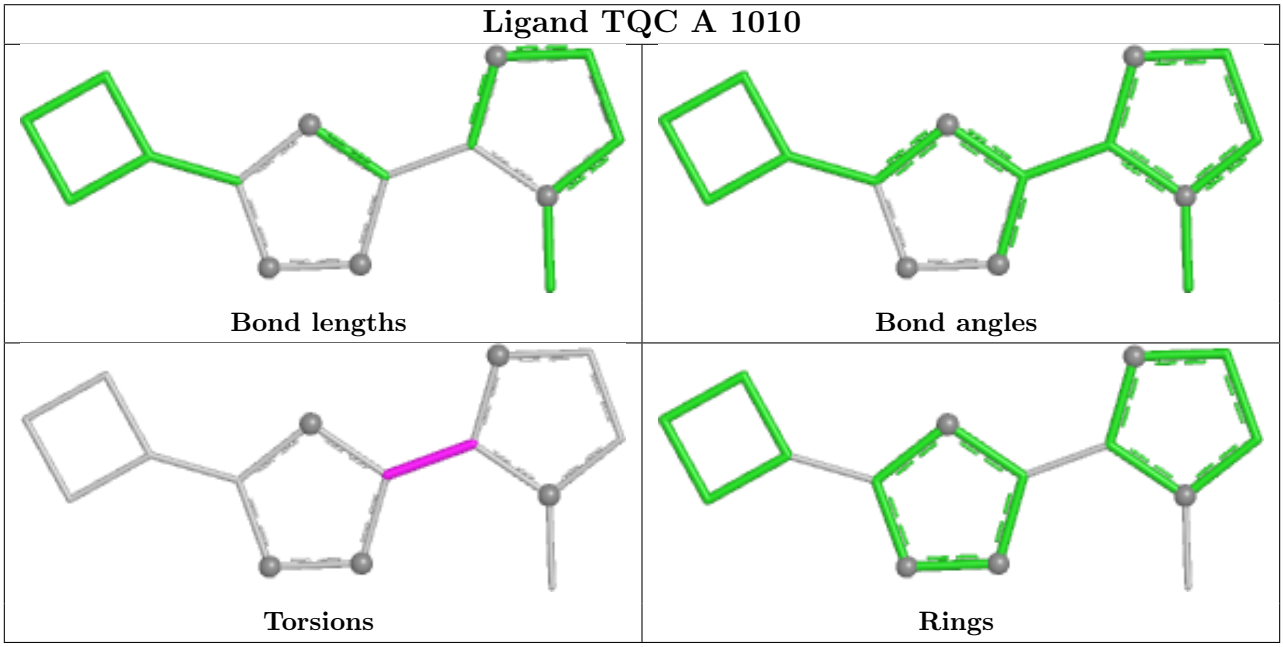
Mol	Chain	Res	Type	Atoms
6	A	1009	PEG	O2-C3-C4-O4
7	A	1010	TQC	N-C3-C4-N3
6	A	1009	PEG	C4-C3-O2-C2
6	A	1009	PEG	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003[B]	MES	2	0
5	A	1007	PO4	3	0
4	A	1004	DMS	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 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.



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	565/637 (88%)	4.68	352 (62%)	0	0	6, 41, 99, 141	158 (27%)

All (352) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	309	TYR	16.5
1	A	284	ILE	16.3
1	A	292	TRP	15.8
1	A	425	ALA	15.8
1	A	426	VAL	15.5
1	A	592	ILE	15.2
1	A	801[A]	HIS	15.0
1	A	403	VAL	14.6
1	A	478	TRP	14.4
1	A	431	PHE	14.4
1	A	593	ILE	14.3
1	A	787	TRP	14.2
1	A	748	LEU	14.2
1	A	790	THR	14.0
1	A	303	TRP	13.7
1	A	311	THR	13.7
1	A	763[A]	SER	13.6
1	A	409	LEU	13.5
1	A	443	LEU	13.5
1	A	785[A]	SER	13.3
1	A	430	GLY	13.3
1	A	736	GLY	13.3
1	A	419	TRP	13.2
1	A	805	THR	13.2
1	A	578	VAL	13.1
1	A	400	THR	13.1
1	A	746	TRP	13.0

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Mol	Chain	Res	Type	RSRZ
1	A	486	PHE	12.8
1	A	758	TYR	12.6
1	A	294	TYR	12.6
1	A	738	ALA	12.6
1	A	589	VAL	12.4
1	A	755	GLY	12.4
1	A	321	VAL	12.4
1	A	359	VAL	12.3
1	A	452	TYR	12.2
1	A	474	ILE	12.2
1	A	542	ILE	12.2
1	A	283	LYS	12.0
1	A	291	SER	12.0
1	A	391	PRO	12.0
1	A	293	HIS	12.0
1	A	319	SER	11.8
1	A	583	PRO	11.8
1	A	367	LYS	11.8
1	A	808	ASP	11.7
1	A	747	SER	11.6
1	A	806	THR	11.6
1	A	740	ILE	11.6
1	A	757	SER	11.5
1	A	751	THR	11.4
1	A	512[A]	LEU	11.3
1	A	788	VAL	11.3
1	A	600	GLY	11.3
1	A	752	ALA	11.2
1	A	591	ASP	11.2
1	A	809	MET	11.2
1	A	445	GLY	11.1
1	A	753	CYS	11.1
1	A	505	SER	11.1
1	A	475	TRP	11.1
1	A	731	GLN	11.1
1	A	789	PRO	11.1
1	A	402	LYS	11.0
1	A	366	PRO	10.9
1	A	732	ASP	10.9
1	A	804	MET	10.8
1	A	318	SER	10.8
1	A	754	LEU	10.7

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Mol	Chain	Res	Type	RSRZ
1	A	387	LYS	10.7
1	A	594	SER	10.7
1	A	540	THR	10.6
1	A	302	THR	10.6
1	A	388	LYS	10.5
1	A	575	ASN	10.5
1	A	603	GLN	10.5
1	A	401	ARG	10.3
1	A	880	THR	10.3
1	A	305	TYR	10.3
1	A	499	SER	10.3
1	A	454	MET	10.2
1	A	739	ARG	10.2
1	A	595	ARG	10.2
1	A	304	ALA	10.1
1	A	498	PHE	10.1
1	A	656	SER	10.1
1	A	576	LYS	10.1
1	A	477	MET	10.0
1	A	485	GLU	10.0
1	A	453	ASN	10.0
1	A	636	THR	9.9
1	A	800	THR	9.9
1	A	306	HIS	9.9
1	A	737	ARG	9.9
1	A	392	ARG	9.8
1	A	807	GLU	9.6
1	A	481	ALA	9.6
1	A	802	GLU	9.5
1	A	424	GLU	9.5
1	A	500	ARG	9.5
1	A	541	ARG	9.4
1	A	389	LYS	9.4
1	A	745	GLY	9.4
1	A	429	SER	9.4
1	A	694	TRP	9.3
1	A	539	ASP	9.3
1	A	298	HIS	9.3
1	A	584	THR	9.3
1	A	749	ARG	9.2
1	A	358	LYS	9.2
1	A	733	GLU	9.2

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Mol	Chain	Res	Type	RSRZ
1	A	730	ASN	9.2
1	A	476	TYR	9.2
1	A	448	GLU	9.1
1	A	744	ALA	9.1
1	A	428	ASP	9.1
1	A	282	GLU	9.0
1	A	548	LYS	9.0
1	A	551	GLU	8.9
1	A	295	ASP	8.9
1	A	433	GLU	8.9
1	A	484	LEU	8.9
1	A	657	ARG	8.8
1	A	799	ALA	8.8
1	A	406	ASN	8.7
1	A	285	LYS	8.7
1	A	393	MET	8.6
1	A	719[A]	LYS	8.5
1	A	503	SER	8.5
1	A	317	ALA	8.5
1	A	364	GLN	8.5
1	A	635	LEU	8.5
1	A	290	THR	8.5
1	A	756	LYS	8.4
1	A	365	GLU	8.3
1	A	487	GLU	8.3
1	A	658	MET	8.3
1	A	741	SER	8.2
1	A	705	GLN	8.2
1	A	596	ARG	8.2
1	A	598	GLN	8.2
1	A	525	LYS	8.2
1	A	404	ARG	8.2
1	A	408	ALA	8.0
1	A	344	THR	8.0
1	A	502	ASN	7.9
1	A	884	PRO	7.9
1	A	423	ARG	7.8
1	A	441	LEU	7.8
1	A	286	GLN	7.7
1	A	310	GLU	7.7
1	A	455	MET	7.6
1	A	390	THR	7.6

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Mol	Chain	Res	Type	RSRZ
1	A	579	ARG	7.6
1	A	693	GLN	7.5
1	A	362	ARG	7.3
1	A	275	ASP	7.3
1	A	405	SER	7.3
1	A	882	TYR	7.3
1	A	287	GLU	7.1
1	A	446	LYS	7.1
1	A	300	TYR	7.1
1	A	690	ASP	7.1
1	A	864[A]	GLN	7.1
1	A	420	LYS	6.9
1	A	418	LYS	6.9
1	A	743	GLY	6.9
1	A	296	GLN	6.8
1	A	449	THR	6.8
1	A	422	ALA	6.7
1	A	639	GLU	6.7
1	A	649	ARG	6.7
1	A	597	ASP	6.6
1	A	653	GLU	6.6
1	A	750	GLU	6.6
1	A	297	ASP	6.5
1	A	692	GLN	6.4
1	A	891	ARG	6.4
1	A	274	LEU	6.4
1	A	299	PRO	6.3
1	A	427	GLU	6.2
1	A	279	LYS	6.2
1	A	742	GLN	6.1
1	A	289	GLU	6.1
1	A	881	ASP	6.1
1	A	588	THR	5.9
1	A	288	HIS	5.8
1	A	357	GLU	5.8
1	A	301	LYS	5.8
1	A	281	ILE	5.8
1	A	582	ARG	5.7
1	A	277	ILE	5.7
1	A	630	LYS	5.6
1	A	637	VAL	5.6
1	A	883	MET	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	407	ALA	5.6
1	A	641	ILE	5.5
1	A	648	VAL	5.5
1	A	701	ASN	5.5
1	A	568	ILE	5.4
1	A	363	THR	5.3
1	A	678	LEU	5.3
1	A	890	ARG	5.3
1	A	889	PHE	5.3
1	A	444	GLU	5.2
1	A	887	LYS	5.2
1	A	888	ARG	5.1
1	A	501	GLU	5.0
1	A	435	VAL	5.0
1	A	276	ILE	4.9
1	A	885	SER	4.9
1	A	563	LYS	4.9
1	A	644	LYS	4.8
1	A	571	LEU	4.8
1	A	825	GLU	4.8
1	A	564	LEU	4.7
1	A	434	LEU	4.7
1	A	570	LYS	4.6
1	A	440	ASN	4.6
1	A	555	ASN	4.6
1	A	534	ASP	4.5
1	A	876	ASN	4.5
1	A	494	GLU	4.5
1	A	396	ARG	4.4
1	A	677	ALA	4.4
1	A	879	TYR	4.3
1	A	558	GLU	4.2
1	A	830	VAL	4.2
1	A	634	HIS	4.1
1	A	670	LEU	4.1
1	A	886	MET	4.1
1	A	572	THR	4.0
1	A	689	LYS	3.9
1	A	432	TRP	3.8
1	A	480	GLY	3.8
1	A	383	LYS	3.7
1	A	360	ASP	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	642	ALA	3.7
1	A	833	TRP	3.6
1	A	307	GLY	3.6
1	A	853	LEU	3.6
1	A	549	ASN	3.6
1	A	421	SER	3.6
1	A	398	GLU	3.6
1	A	601	SER	3.6
1	A	647	LEU	3.5
1	A	835	GLU	3.5
1	A	878	GLU	3.5
1	A	577	VAL	3.5
1	A	538	TRP	3.4
1	A	399	PHE	3.4
1	A	273	ASN	3.4
1	A	308	SER	3.4
1	A	590	MET	3.4
1	A	663	ASP	3.4
1	A	834	GLU	3.3
1	A	815	ARG	3.3
1	A	361	THR	3.3
1	A	855	SER	3.3
1	A	524	LYS	3.3
1	A	638	THR	3.3
1	A	581	GLN	3.3
1	A	683	ASP	3.2
1	A	861	LYS	3.2
1	A	442	HIS	3.2
1	A	479	LEU	3.2
1	A	703	TRP	3.2
1	A	828	THR	3.2
1	A	629	PHE	3.2
1	A	343	MET	3.1
1	A	439	ARG	3.1
1	A	529	ALA	3.1
1	A	559	GLY	3.1
1	A	562	LYS	3.1
1	A	625	GLY	3.1
1	A	764	LEU	3.1
1	A	545	GLU	3.1
1	A	451	VAL	3.1
1	A	631	SER	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	370	THR	3.0
1	A	870	VAL	3.0
1	A	824	MET	3.0
1	A	394	CYS	3.0
1	A	278	GLY	2.9
1	A	699	GLY	2.9
1	A	604	VAL	2.9
1	A	369	GLY	2.9
1	A	556	HIS	2.9
1	A	698	ARG	2.9
1	A	508	GLU	2.9
1	A	379	GLU	2.8
1	A	566	GLU	2.8
1	A	514	LYS	2.8
1	A	493	ASN	2.8
1	A	547	LEU	2.8
1	A	674	PHE	2.8
1	A	375	LYS	2.7
1	A	803	TRP	2.7
1	A	337	MET	2.7
1	A	831	GLU	2.7
1	A	377	THR	2.7
1	A	863	ILE	2.7
1	A	580	VAL	2.6
1	A	632	ILE	2.6
1	A	492	LEU	2.6
1	A	818	ILE	2.6
1	A	397	GLU	2.6
1	A	695	GLU	2.6
1	A	627	GLY	2.5
1	A	436	ASP	2.5
1	A	437	LYS	2.5
1	A	496	HIS	2.5
1	A	646	TRP	2.5
1	A	645	ASN	2.5
1	A	376	ILE	2.5
1	A	819	GLN	2.5
1	A	868	ASN	2.5
1	A	784	PRO	2.4
1	A	482	ARG	2.4
1	A	866	ALA	2.4
1	A	526	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	569	PHE	2.4
1	A	447	CYS	2.4
1	A	497	TRP	2.4
1	A	676	SER	2.4
1	A	522	VAL	2.4
1	A	679	THR	2.4
1	A	652	ARG	2.3
1	A	829	PRO	2.3
1	A	573	TYR	2.3
1	A	851	ILE	2.2
1	A	827	LYS	2.2
1	A	327	LEU	2.2
1	A	858	THR	2.2
1	A	702	ASP	2.2
1	A	650	VAL	2.2
1	A	567	ALA	2.2
1	A	552	MET	2.2
1	A	720	ASP	2.2
1	A	280	ARG	2.2
1	A	687	VAL	2.1
1	A	651	GLY	2.1
1	A	786	HIS	2.1
1	A	716	LEU	2.1
1	A	495	ASP	2.1
1	A	685	GLY	2.1
1	A	848	GLY	2.1
1	A	546	ASP	2.1
1	A	371	LYS	2.1
1	A	783	VAL	2.0
1	A	723	VAL	2.0
1	A	483	PHE	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)

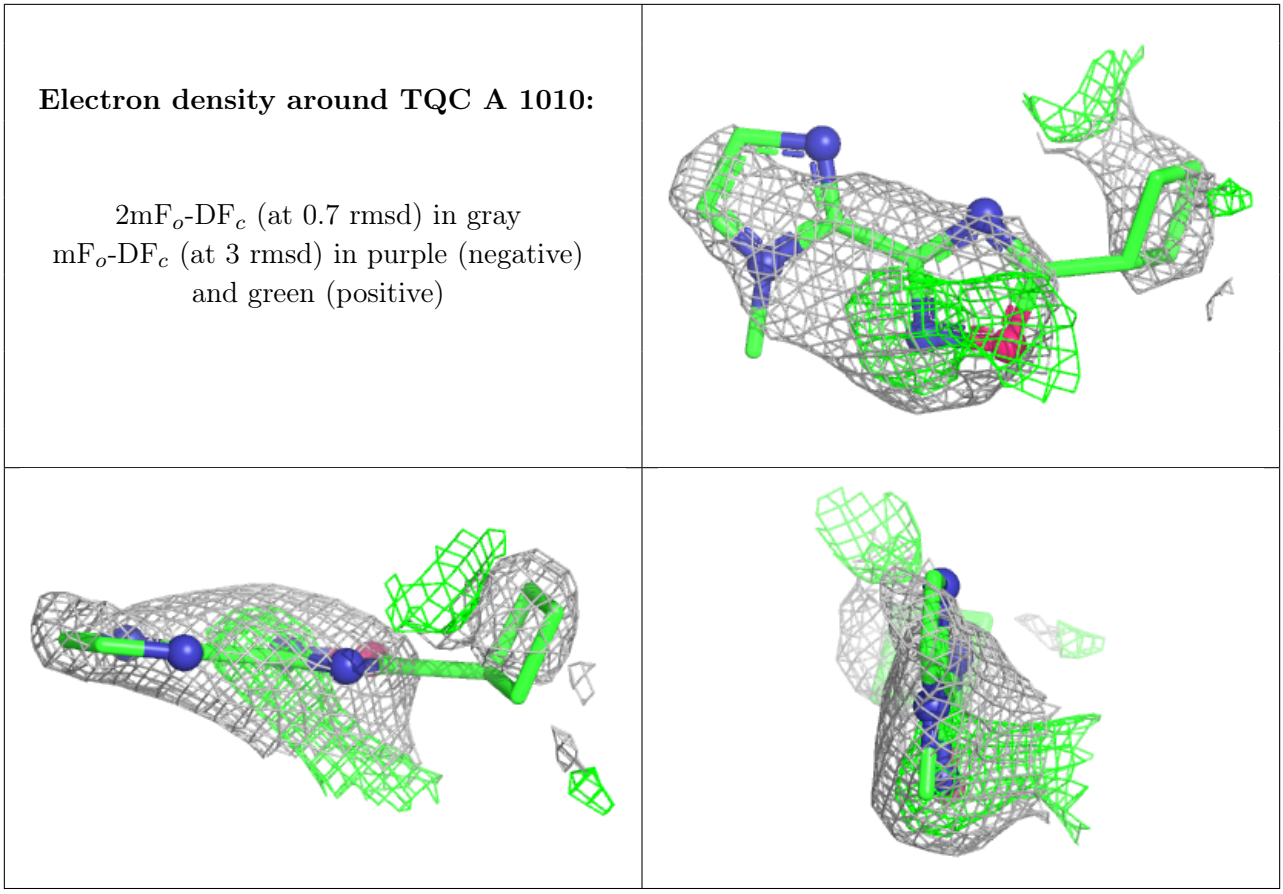
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
5	PO4	A	1008	5/5	0.69	0.18	94,100,113,122	0
7	TQC	A	1010	15/15	0.74	0.37	47,49,50,52	15
4	DMS	A	1005	4/4	0.78	0.30	103,118,121,134	0
5	PO4	A	1007	5/5	0.79	0.17	48,51,74,88	0
6	PEG	A	1009	7/7	0.83	0.18	65,76,85,86	0
4	DMS	A	1006	4/4	0.89	0.14	65,72,72,80	0
3	MES	A	1003[A]	12/12	0.90	0.28	81,101,574,578	12
3	MES	A	1003[B]	12/12	0.90	0.28	3,27,40,45	12
4	DMS	A	1004	4/4	0.91	0.18	82,86,86,105	0
2	ZN	A	1002	1/1	0.99	0.03	64,64,64,64	0
2	ZN	A	1001	1/1	1.00	0.03	29,29,29,29	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 TQC 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

There are no such residues in this entry.