



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2025 – 10:41 AM EDT

PDB ID : 7I2M
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 Z1639162606 (DNV2_NS5A-x0567)
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Deposited on : 2025-03-06
Resolution : 1.78 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)

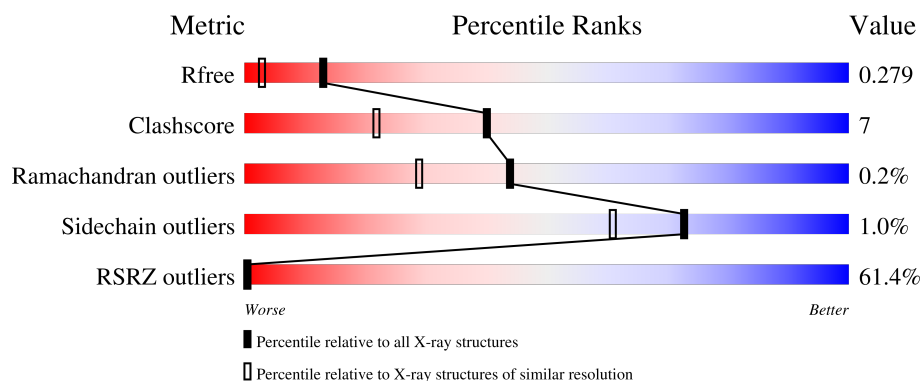
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	1191 (1.78-1.78)
Clashscore	180529	1282 (1.78-1.78)
Ramachandran outliers	177936	1270 (1.78-1.78)
Sidechain outliers	177891	1270 (1.78-1.78)
RSRZ outliers	164620	1191 (1.78-1.78)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	637	<div> <div>55%</div> <div>78%</div> <div>12%</div> <div>10%</div> </div>

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	X	-
7	PK4	A	1010	-	-	-	X

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5118 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	4739	2983	852	870	34	0	7	0

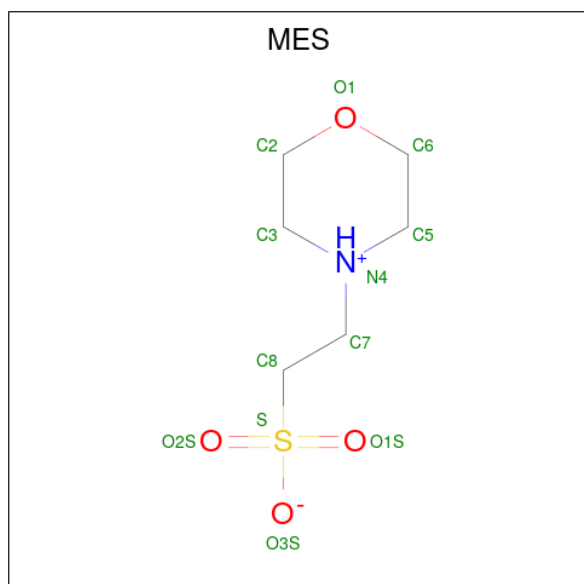
There are 2 discrepancies between the modelled and reference sequences:

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).

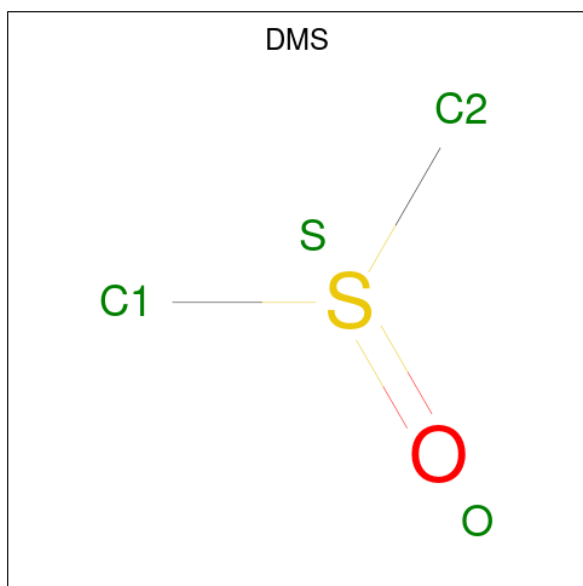
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		

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



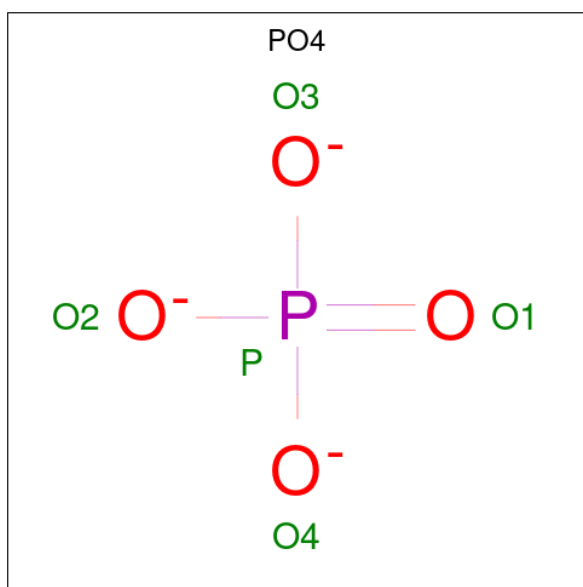
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

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



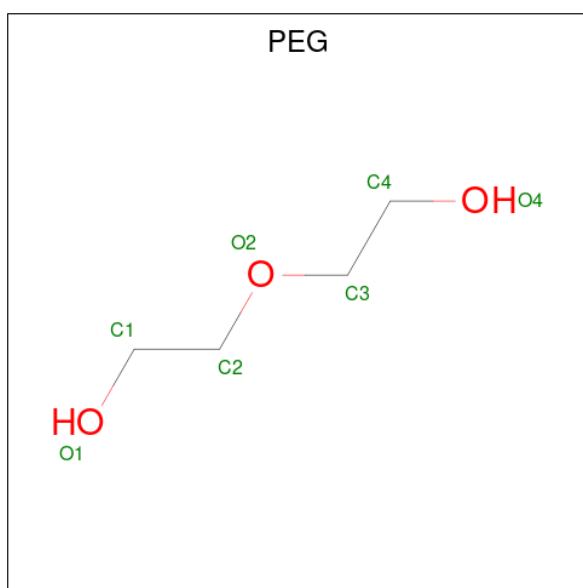
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

- 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		

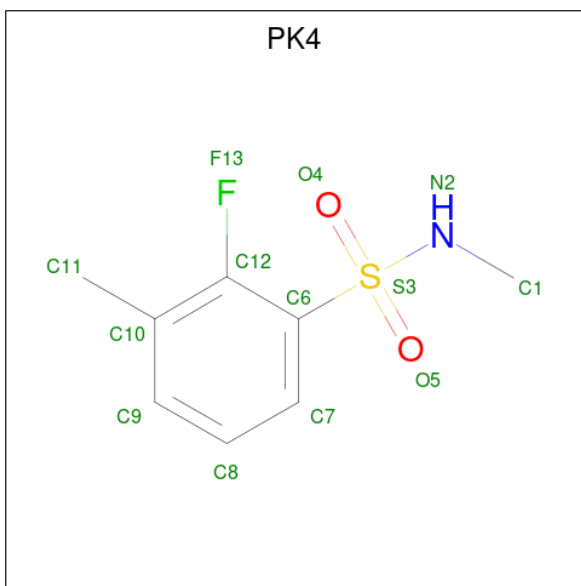
- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 7 is 2-fluoro-N,3-dimethylbenzene-1-sulfonamide (three-letter code: PK4) (formula:

C₈H₁₀FNO₂S (labeled as "Ligand of Interest" by depositor).



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

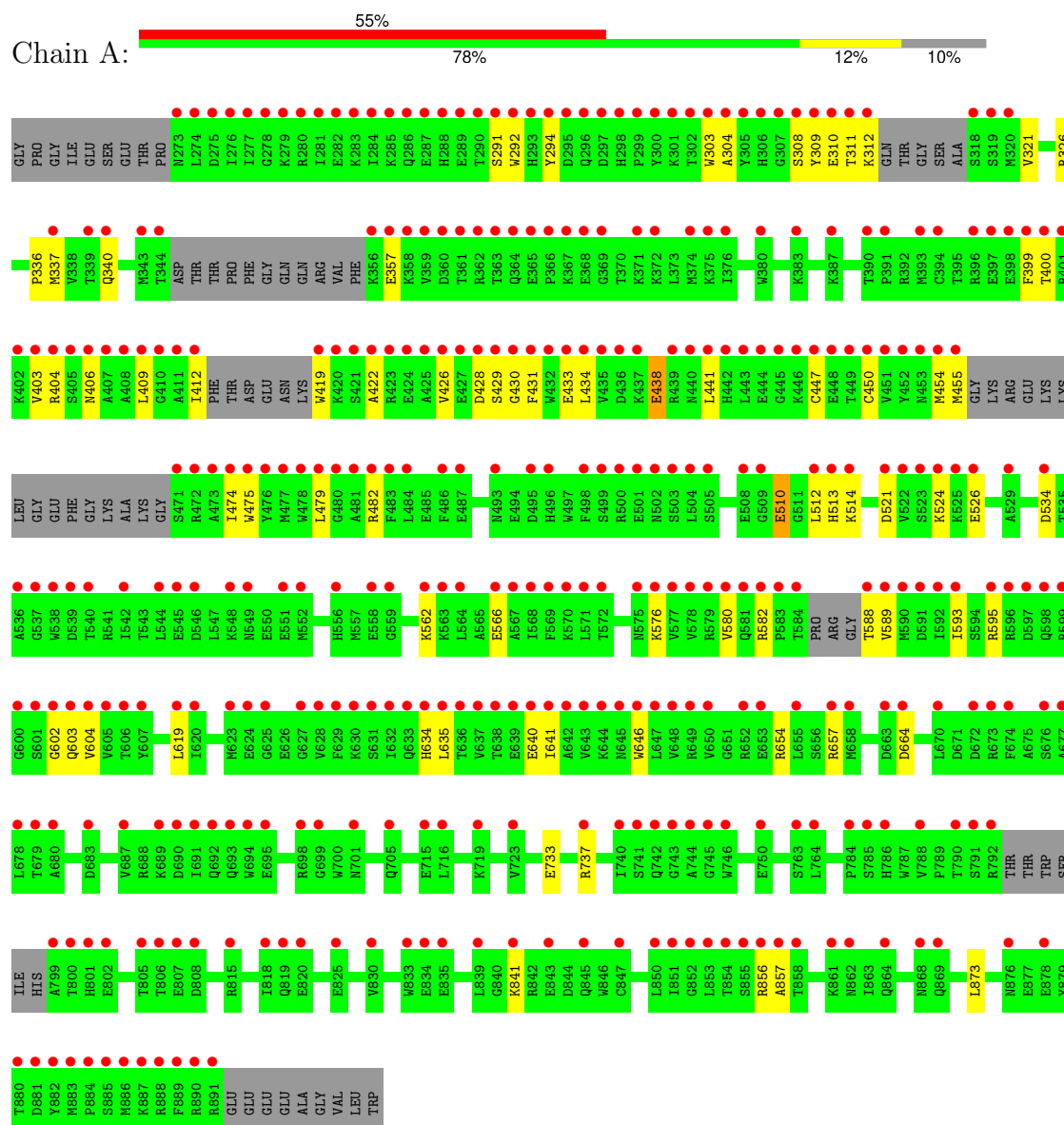
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	310	Total	O	0	0
			310	310		

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	82.36Å 115.81Å 147.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	73.55 – 1.78 73.55 – 1.78	Depositor EDS
% Data completeness (in resolution range)	98.0 (73.55-1.78) 98.0 (73.55-1.78)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.78Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.196 , 0.235 0.261 , 0.279	Depositor DCC
R_{free} test set	3472 reflections (5.15%)	wwPDB-VP
Wilson B-factor (Å ²)	33.6	Xtriage
Anisotropy	0.272	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 136.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	5118	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.55% 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: PEG, MES, CL, ZN, DMS, PK4, 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	2/4844 (0.0%)	0.79	0/6530

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	510	GLU	CD-OE2	7.12	1.33	1.25
1	A	513	HIS	C-O	5.51	1.33	1.23

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4739	0	4644	60	0
2	A	2	0	0	0	0
3	A	24	0	26	1	0
4	A	12	0	18	2	0
5	A	10	0	0	3	0
6	A	7	0	10	0	0
7	A	13	0	0	2	0
8	A	1	0	0	0	0
9	A	310	0	0	5	2

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5118	0	4698	62	2

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 7.

All (62) 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:412:ILE:O	1:A:412:ILE:HG13	1.68	0.91
1:A:857:ALA:HA	7:A:1010:PK4:C1	2.06	0.85
1:A:409:LEU:O	9:A:1101:HOH:O	1.98	0.81
1:A:664:ASP:OD1	5:A:1007:PO4:O4	1.99	0.81
1:A:311:THR:O	1:A:312:LYS:HG3	1.82	0.80
1:A:602:GLY:HA3	9:A:1156:HOH:O	1.81	0.80
1:A:400:THR:HG23	1:A:426:VAL:HG11	1.65	0.76
1:A:400:THR:O	1:A:403:VAL:HG22	1.85	0.75
1:A:635:LEU:HD23	1:A:640:GLU:HG2	1.72	0.71
1:A:534:ASP:OD1	5:A:1007:PO4:O4	2.13	0.67
1:A:510:GLU:O	1:A:514:LYS:HG3	1.96	0.65
1:A:474:ILE:HD12	1:A:474:ILE:N	2.12	0.64
1:A:526:GLU:O	1:A:657:ARG:NH2	2.26	0.64
1:A:431:PHE:O	1:A:434:LEU:HB2	1.98	0.64
1:A:357:GLU:N	1:A:357:GLU:OE2	2.32	0.63
1:A:400:THR:HG23	1:A:426:VAL:CG1	2.32	0.59
1:A:309:TYR:CE1	1:A:311:THR:HG23	2.38	0.58
1:A:430:GLY:O	1:A:434:LEU:HG	2.04	0.58
1:A:429:SER:O	1:A:433:GLU:HG3	2.05	0.57
1:A:412:ILE:O	1:A:412:ILE:CG1	2.44	0.56
1:A:562:LYS:HE3	1:A:566:GLU:OE2	2.05	0.56
1:A:664:ASP:OD1	5:A:1007:PO4:P	2.64	0.55
1:A:337:MET:HG2	9:A:1317:HOH:O	2.05	0.55
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.47	0.55
1:A:336:PRO:O	1:A:340:GLN:HG2	2.07	0.54
4:A:1004:DMS:C1	9:A:1182:HOH:O	2.56	0.54
1:A:475:TRP:HZ3	1:A:576:LYS:HD3	1.75	0.51
1:A:399:PHE:O	1:A:403:VAL:HG13	2.11	0.51
1:A:438:GLU:O	1:A:441:LEU:HB2	2.13	0.49
1:A:294:TYR:CD1	1:A:294:TYR:O	2.64	0.49
1:A:431:PHE:HA	1:A:434:LEU:HD12	1.94	0.49
1:A:422:ALA:HB1	1:A:479:LEU:CD2	2.43	0.49
1:A:582:ARG:O	1:A:588:THR:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:303:TRP:CE3	1:A:593:ILE:HD12	2.48	0.48
1:A:309:TYR:HE1	1:A:311:THR:HG23	1.79	0.47
1:A:292:TRP:HA	1:A:308:SER:O	2.15	0.47
1:A:856:ARG:HH11	7:A:1010:PK4:C1	2.28	0.46
1:A:873:LEU:HD13	3:A:1003[A]:MES:H62	1.97	0.46
1:A:422:ALA:HB1	1:A:479:LEU:HD22	1.98	0.46
1:A:521:ASP:O	1:A:524:LYS:HB2	2.15	0.46
1:A:454:MET:O	1:A:455:MET:HG3	2.16	0.45
1:A:291:SER:HB3	1:A:310:GLU:H	1.82	0.45
1:A:311:THR:O	1:A:312:LYS:CG	2.59	0.45
1:A:733:GLU:O	1:A:737:ARG:HG3	2.17	0.45
1:A:454:MET:HB3	1:A:580:VAL:HG13	1.99	0.44
1:A:291:SER:HB3	1:A:310:GLU:HG3	1.99	0.44
1:A:419:TRP:NE1	1:A:428:ASP:OD2	2.36	0.43
1:A:321:VAL:HG11	1:A:326:ARG:CZ	2.49	0.43
1:A:474:ILE:HD12	1:A:474:ILE:H	1.82	0.43
4:A:1004:DMS:H13	9:A:1182:HOH:O	2.16	0.43
1:A:304:ALA:O	1:A:593:ILE:HA	2.19	0.42
1:A:474:ILE:N	1:A:474:ILE:CD1	2.82	0.42
1:A:646:TRP:CZ2	1:A:654:ARG:HG3	2.53	0.42
1:A:400:THR:O	1:A:404:ARG:HG3	2.19	0.42
1:A:589:VAL:HG23	1:A:589:VAL:O	2.19	0.42
1:A:603:GLN:HG3	1:A:604:VAL:N	2.34	0.42
1:A:562:LYS:O	1:A:566:GLU:HG3	2.20	0.42
1:A:619:LEU:HD23	1:A:619:LEU:HA	1.89	0.42
1:A:580:VAL:HG21	1:A:593:ILE:HD11	2.02	0.42
1:A:303:TRP:CZ2	1:A:595:ARG:HD2	2.55	0.41
1:A:512[B]:LEU:HD23	1:A:512[B]:LEU:HA	1.90	0.41
1:A:311:THR:HB	1:A:312:LYS:H	1.80	0.40

All (2) 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:1269:HOH:O	9:A:1345:HOH:O[2_545]	1.88	0.32
9:A:1119:HOH:O	9:A:1119:HOH:O[2_445]	1.91	0.29

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%)	542 (96%)	23 (4%)	1 (0%)	44	29

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%)	504 (99%)	5 (1%)	73	61

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

Mol	Chain	Res	Type
1	A	438	GLU
1	A	482	ARG
1	A	634	HIS
1	A	641	ILE
1	A	841	LYS

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 ⓘ

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 12 ligands modelled in this entry, 3 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	$\# Z > 2$
5	PO4	A	1008	-	4,4,4	1.07	1 (25%)	6,6,6	0.38	0
3	MES	A	1003[A]	-	12,12,12	0.71	0	15,16,16	0.31	0
7	PK4	A	1010	-	12,13,13	0.17	0	15,19,19	0.65	1 (6%)
4	DMS	A	1006	-	3,3,3	0.23	0	3,3,3	0.29	0
4	DMS	A	1005	-	3,3,3	0.24	0	3,3,3	0.06	0
4	DMS	A	1004	-	3,3,3	0.44	0	3,3,3	0.35	0
6	PEG	A	1009	-	6,6,6	0.17	0	5,5,5	0.11	0
3	MES	A	1003[B]	-	12,12,12	0.68	0	15,16,16	0.51	0
5	PO4	A	1007	-	4,4,4	4.74	4 (100%)	6,6,6	0.76	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]	-	-	1/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	PK4	A	1010	-	-	8/9/9/9	0/1/1/1
3	MES	A	1003[A]	-	-	3/6/14/14	0/1/1/1
6	PEG	A	1009	-	-	2/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1007	PO4	P-O1	8.00	1.69	1.50
5	A	1007	PO4	P-O4	-3.57	1.44	1.54
5	A	1007	PO4	P-O2	2.94	1.63	1.54
5	A	1007	PO4	P-O3	2.17	1.61	1.54
5	A	1008	PO4	P-O1	2.12	1.55	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	1010	PK4	C12-C6-S3	2.25	122.97	121.28

There are no chirality outliers.

All (14) torsion outliers are listed below:

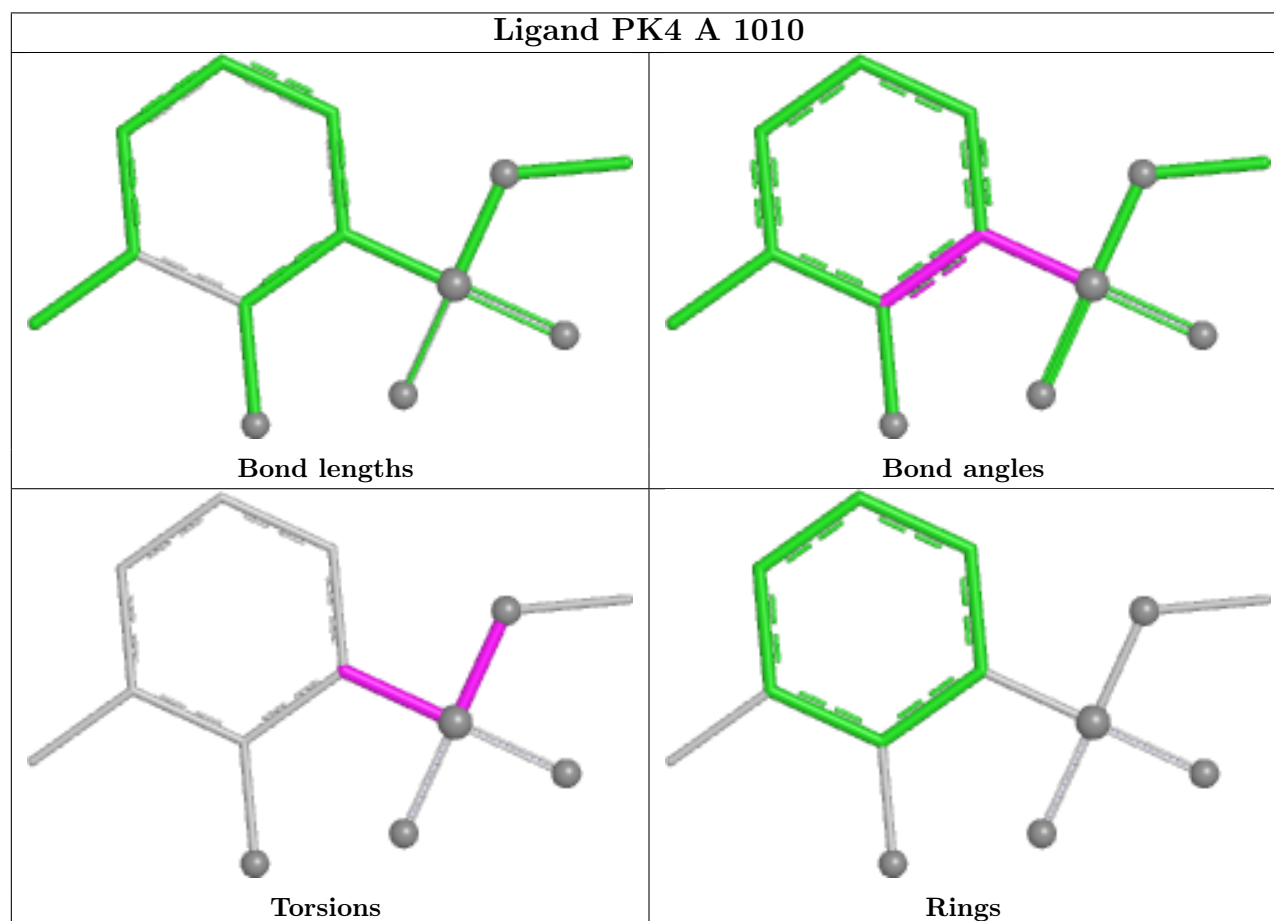
Mol	Chain	Res	Type	Atoms
3	A	1003[B]	MES	C8-C7-N4-C3
7	A	1010	PK4	C12-C6-S3-O5
7	A	1010	PK4	C1-N2-S3-C6
7	A	1010	PK4	C1-N2-S3-O4
7	A	1010	PK4	C1-N2-S3-O5
7	A	1010	PK4	C7-C6-S3-O5
6	A	1009	PEG	O2-C3-C4-O4
7	A	1010	PK4	C7-C6-S3-N2
7	A	1010	PK4	C12-C6-S3-N2
7	A	1010	PK4	C12-C6-S3-O4
3	A	1003[A]	MES	C7-C8-S-O3S
3	A	1003[A]	MES	C7-C8-S-O1S
3	A	1003[A]	MES	C7-C8-S-O2S
6	A	1009	PEG	C4-C3-O2-C2

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
7	A	1010	PK4	2	0
4	A	1004	DMS	2	0
5	A	1007	PO4	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	573/637 (89%)	4.09	352 (61%) 0 0	5, 37, 83, 162	187 (32%)

All (352) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	889	PHE	19.3
1	A	839	LEU	15.8
1	A	785[A]	SER	14.2
1	A	592	ILE	13.3
1	A	475	TRP	13.3
1	A	850	LEU	13.0
1	A	858	THR	13.0
1	A	719[A]	LYS	12.7
1	A	589	VAL	12.4
1	A	412	ILE	11.7
1	A	763[A]	SER	11.6
1	A	431	PHE	11.5
1	A	474	ILE	11.5
1	A	888	ARG	11.5
1	A	864[A]	GLN	11.3
1	A	593	ILE	11.2
1	A	432	TRP	11.0
1	A	851	ILE	10.9
1	A	855	SER	10.9
1	A	577	VAL	10.9
1	A	637	VAL	10.9
1	A	403	VAL	10.8
1	A	580	VAL	10.8
1	A	411	ALA	10.8
1	A	854	THR	10.7
1	A	399	PHE	10.7
1	A	853	LEU	10.6

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Mol	Chain	Res	Type	RSRZ
1	A	628	VAL	10.6
1	A	648	VAL	10.5
1	A	407	ALA	10.5
1	A	886	MET	10.5
1	A	409	LEU	10.4
1	A	292	TRP	10.4
1	A	835	GLU	10.3
1	A	293	HIS	10.3
1	A	801[A]	HIS	10.2
1	A	294	TYR	10.2
1	A	705	GLN	10.1
1	A	304	ALA	10.0
1	A	542	ILE	10.0
1	A	856	ARG	9.9
1	A	588	THR	9.9
1	A	646	TRP	9.9
1	A	632	ILE	9.9
1	A	852	GLY	9.9
1	A	512[A]	LEU	9.9
1	A	619	LEU	9.9
1	A	498	PHE	9.7
1	A	620	ILE	9.6
1	A	452	TYR	9.6
1	A	476	TYR	9.6
1	A	600	GLY	9.6
1	A	522	VAL	9.5
1	A	303	TRP	9.5
1	A	400	THR	9.5
1	A	434	LEU	9.4
1	A	538	TRP	9.4
1	A	307	GLY	9.4
1	A	655	LEU	9.3
1	A	575	ASN	9.3
1	A	435	VAL	9.2
1	A	635	LEU	9.2
1	A	449	THR	9.2
1	A	410	GLY	9.2
1	A	281	ILE	9.1
1	A	890	ARG	9.1
1	A	290	THR	9.0
1	A	309	TYR	9.0
1	A	845	GLN	9.0

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Mol	Chain	Res	Type	RSRZ
1	A	834	GLU	8.9
1	A	282	GLU	8.9
1	A	741[A]	SER	8.9
1	A	799	ALA	8.9
1	A	602	GLY	8.8
1	A	430	GLY	8.8
1	A	299	PRO	8.8
1	A	606	THR	8.8
1	A	887	LYS	8.8
1	A	636	THR	8.7
1	A	647	LEU	8.7
1	A	601	SER	8.7
1	A	642	ALA	8.7
1	A	641	ILE	8.6
1	A	643	VAL	8.6
1	A	361	THR	8.6
1	A	274	LEU	8.5
1	A	359	VAL	8.5
1	A	421	SER	8.5
1	A	504	LEU	8.5
1	A	419	TRP	8.5
1	A	513	HIS	8.4
1	A	311	THR	8.4
1	A	363	THR	8.3
1	A	843	GLU	8.3
1	A	841	LYS	8.2
1	A	582	ARG	8.1
1	A	277	ILE	8.0
1	A	509	GLY	7.9
1	A	505	SER	7.9
1	A	375	LYS	7.9
1	A	679	THR	7.8
1	A	631	SER	7.8
1	A	406	ASN	7.7
1	A	715	GLU	7.7
1	A	534	ASP	7.7
1	A	366	PRO	7.7
1	A	364	GLN	7.7
1	A	629	PHE	7.6
1	A	861	LYS	7.6
1	A	649	ARG	7.5
1	A	305	TYR	7.5

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Mol	Chain	Res	Type	RSRZ
1	A	404	ARG	7.4
1	A	514	LYS	7.4
1	A	405	SER	7.4
1	A	521	ASP	7.4
1	A	383	LYS	7.4
1	A	429	SER	7.3
1	A	746	TRP	7.2
1	A	596	ARG	7.2
1	A	548	LYS	7.2
1	A	591	ASP	7.2
1	A	455	MET	7.2
1	A	426	VAL	7.1
1	A	312	LYS	7.1
1	A	576	LYS	7.1
1	A	657	ARG	7.1
1	A	291	SER	7.0
1	A	436	ASP	7.0
1	A	638	THR	7.0
1	A	358	LYS	7.0
1	A	603	GLN	7.0
1	A	356	LYS	6.9
1	A	300	TYR	6.9
1	A	546	ASP	6.9
1	A	742	GLN	6.9
1	A	286	GLN	6.8
1	A	525	LYS	6.8
1	A	298	HIS	6.8
1	A	437	LYS	6.7
1	A	744	ALA	6.7
1	A	627	GLY	6.7
1	A	428	ASP	6.7
1	A	551	GLU	6.7
1	A	423	ARG	6.7
1	A	422	ALA	6.6
1	A	745	GLY	6.6
1	A	454	MET	6.6
1	A	523	SER	6.6
1	A	499	SER	6.6
1	A	302	THR	6.6
1	A	597	ASP	6.5
1	A	453	ASN	6.5
1	A	526	GLU	6.5

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Mol	Chain	Res	Type	RSRZ
1	A	698	ARG	6.5
1	A	502	ASN	6.5
1	A	360	ASP	6.4
1	A	595	ARG	6.4
1	A	891	ARG	6.4
1	A	308	SER	6.3
1	A	402	LYS	6.3
1	A	524	LYS	6.3
1	A	441	LEU	6.3
1	A	584	THR	6.3
1	A	288	HIS	6.2
1	A	590	MET	6.2
1	A	448	GLU	6.1
1	A	880	THR	6.1
1	A	693	GLN	6.1
1	A	653	GLU	6.0
1	A	583	PRO	6.0
1	A	658	MET	6.0
1	A	306	HIS	6.0
1	A	289	GLU	6.0
1	A	287	GLU	6.0
1	A	401	ARG	5.9
1	A	424	GLU	5.9
1	A	598	GLN	5.9
1	A	692	GLN	5.9
1	A	645	ASN	5.9
1	A	357	GLU	5.8
1	A	500	ARG	5.8
1	A	478	TRP	5.8
1	A	644	LYS	5.8
1	A	536	ALA	5.7
1	A	501	GLU	5.6
1	A	433	GLU	5.6
1	A	581	GLN	5.6
1	A	640	GLU	5.5
1	A	486	PHE	5.5
1	A	599	ARG	5.5
1	A	568	ILE	5.4
1	A	284	ILE	5.4
1	A	471	SER	5.3
1	A	473	ALA	5.3
1	A	362	ARG	5.3

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Mol	Chain	Res	Type	RSRZ
1	A	791	SER	5.3
1	A	623	MET	5.3
1	A	694	TRP	5.3
1	A	481	ALA	5.2
1	A	790	THR	5.2
1	A	882	TYR	5.2
1	A	800	THR	5.2
1	A	278	GLY	5.2
1	A	445	GLY	5.1
1	A	408	ALA	5.1
1	A	420	LYS	5.0
1	A	539	ASP	5.0
1	A	503	SER	5.0
1	A	443	LEU	4.9
1	A	508	GLU	4.9
1	A	295	ASP	4.8
1	A	563	LYS	4.8
1	A	639	GLU	4.8
1	A	451	VAL	4.8
1	A	633	GLN	4.7
1	A	569	PHE	4.7
1	A	479	LEU	4.7
1	A	398	GLU	4.7
1	A	792	ARG	4.7
1	A	427	GLU	4.7
1	A	634	HIS	4.6
1	A	572	THR	4.6
1	A	310	GLU	4.6
1	A	444	GLU	4.6
1	A	446	LYS	4.6
1	A	537	GLY	4.5
1	A	279	LYS	4.5
1	A	630	LYS	4.5
1	A	365	GLU	4.5
1	A	442	HIS	4.4
1	A	484	LEU	4.4
1	A	318	SER	4.3
1	A	301	LYS	4.3
1	A	701	ASN	4.2
1	A	885	SER	4.1
1	A	529	ALA	4.1
1	A	297	ASP	4.1

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Mol	Chain	Res	Type	RSRZ
1	A	472	ARG	4.1
1	A	743	GLY	4.1
1	A	544	LEU	4.1
1	A	545	GLU	4.1
1	A	691	ILE	4.0
1	A	699	GLY	4.0
1	A	396	ARG	4.0
1	A	280	ARG	4.0
1	A	559	GLY	3.9
1	A	558	GLU	3.9
1	A	578	VAL	3.9
1	A	750	GLU	3.8
1	A	372	LYS	3.7
1	A	670	LEU	3.7
1	A	830	VAL	3.7
1	A	881	ASP	3.7
1	A	344	THR	3.7
1	A	570	LYS	3.7
1	A	764	LEU	3.7
1	A	275	ASP	3.6
1	A	690	ASP	3.6
1	A	818	ILE	3.6
1	A	723	VAL	3.6
1	A	425	ALA	3.6
1	A	604	VAL	3.5
1	A	680	ALA	3.5
1	A	440	ASN	3.5
1	A	687	VAL	3.5
1	A	788	VAL	3.5
1	A	807	GLU	3.5
1	A	571	LEU	3.5
1	A	439	ARG	3.5
1	A	393	MET	3.4
1	A	482	ARG	3.4
1	A	296	GLN	3.4
1	A	847	CYS	3.4
1	A	273	ASN	3.4
1	A	319	SER	3.4
1	A	340	GLN	3.4
1	A	833	TRP	3.4
1	A	285	LYS	3.4
1	A	371	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	663	ASP	3.3
1	A	477	MET	3.3
1	A	556	HIS	3.3
1	A	825	GLU	3.3
1	A	683	ASP	3.2
1	A	276	ILE	3.2
1	A	857	ALA	3.2
1	A	676	SER	3.1
1	A	820	GLU	3.1
1	A	876	ASN	3.1
1	A	884	PRO	3.0
1	A	483	PHE	3.0
1	A	802	GLU	3.0
1	A	343	MET	3.0
1	A	367	LYS	3.0
1	A	716	LEU	2.9
1	A	579	ARG	2.9
1	A	368	GLU	2.9
1	A	808	ASP	2.9
1	A	447	CYS	2.8
1	A	652	ARG	2.8
1	A	450	CYS	2.8
1	A	566	GLU	2.8
1	A	376	ILE	2.7
1	A	380	TRP	2.7
1	A	496	HIS	2.7
1	A	664	ASP	2.6
1	A	390	THR	2.6
1	A	806	THR	2.6
1	A	784	PRO	2.6
1	A	689	LYS	2.6
1	A	695	GLU	2.6
1	A	650	VAL	2.6
1	A	805	THR	2.6
1	A	487	GLU	2.5
1	A	677	ALA	2.5
1	A	394	CYS	2.5
1	A	320	MET	2.5
1	A	552	MET	2.5
1	A	480	GLY	2.5
1	A	625	GLY	2.5
1	A	737	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	878	GLU	2.5
1	A	549	ASN	2.4
1	A	868	ASN	2.4
1	A	283	LYS	2.4
1	A	815	ARG	2.4
1	A	337	MET	2.4
1	A	493	ASN	2.4
1	A	564	LEU	2.4
1	A	540	THR	2.3
1	A	673	ARG	2.3
1	A	819	GLN	2.3
1	A	869	GLN	2.3
1	A	397	GLU	2.3
1	A	567	ALA	2.3
1	A	339	THR	2.3
1	A	607	TYR	2.3
1	A	674	PHE	2.2
1	A	562	LYS	2.2
1	A	862	ASN	2.2
1	A	369	GLY	2.2
1	A	740	ILE	2.2
1	A	391	PRO	2.2
1	A	678	LEU	2.2
1	A	786	HIS	2.2
1	A	374	MET	2.2
1	A	387	LYS	2.2
1	A	495	ASP	2.2
1	A	624	GLU	2.1
1	A	605	VAL	2.1
1	A	672	ASP	2.1
1	A	883	MET	2.1

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 ⓘ

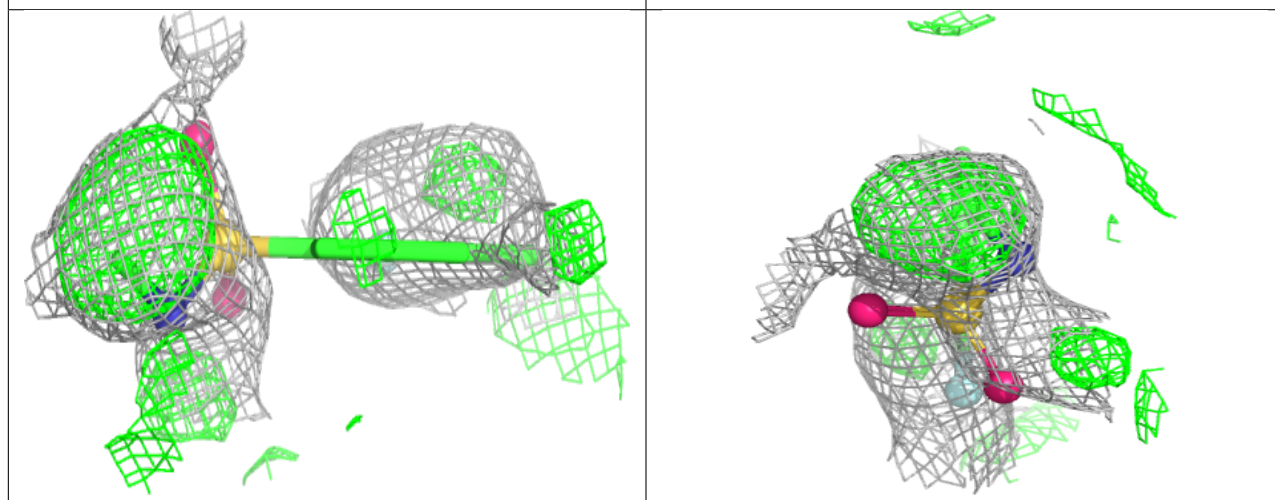
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	PK4	A	1010	13/13	0.41	0.45	50,53,55,56	13
5	PO4	A	1008	5/5	0.74	0.17	97,97,108,121	0
6	PEG	A	1009	7/7	0.81	0.19	74,75,90,92	0
4	DMS	A	1005	4/4	0.83	0.19	81,95,103,103	0
5	PO4	A	1007	5/5	0.84	0.12	36,38,48,65	0
4	DMS	A	1006	4/4	0.92	0.14	60,62,65,65	0
4	DMS	A	1004	4/4	0.93	0.15	49,49,51,52	0
3	MES	A	1003[B]	12/12	0.94	0.25	33,40,47,50	12
3	MES	A	1003[A]	12/12	0.94	0.25	543,557,597,602	12
2	ZN	A	1002	1/1	0.99	0.06	58,58,58,58	0
8	CL	A	1011	1/1	0.99	0.15	17,17,17,17	1
2	ZN	A	1001	1/1	1.00	0.04	26,26,26,26	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 PK4 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.