



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2025 – 10:46 AM EDT

PDB ID : 7I29
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 Z48847594 (DNV2_NS5A-x0162)
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 : 1.50 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)

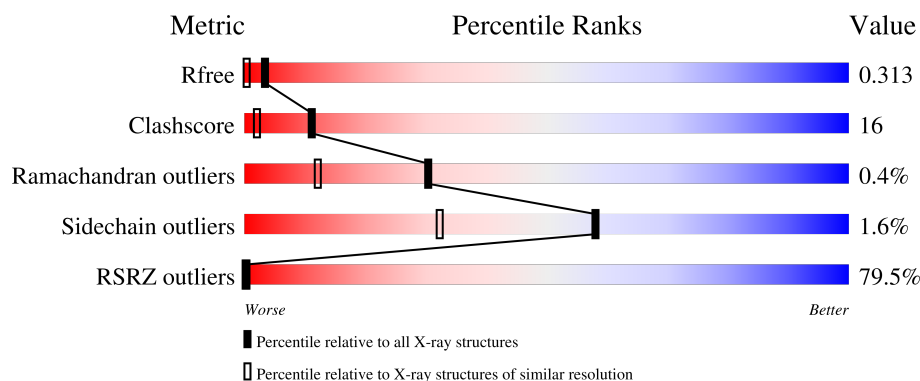
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	3717 (1.50-1.50)
Clashscore	180529	4048 (1.50-1.50)
Ramachandran outliers	177936	3970 (1.50-1.50)
Sidechain outliers	177891	3967 (1.50-1.50)
RSRZ outliers	164620	3718 (1.50-1.50)

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
4	DMS	A	1005	-	-	-	X
6	PO4	A	1007	-	-	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 5068 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	561	Total	C	N	O	S	0	7	0
			4640	2924	832	850	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).



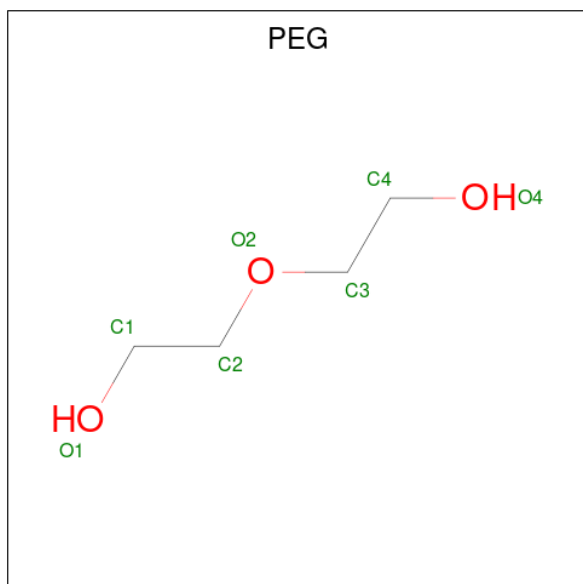
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

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



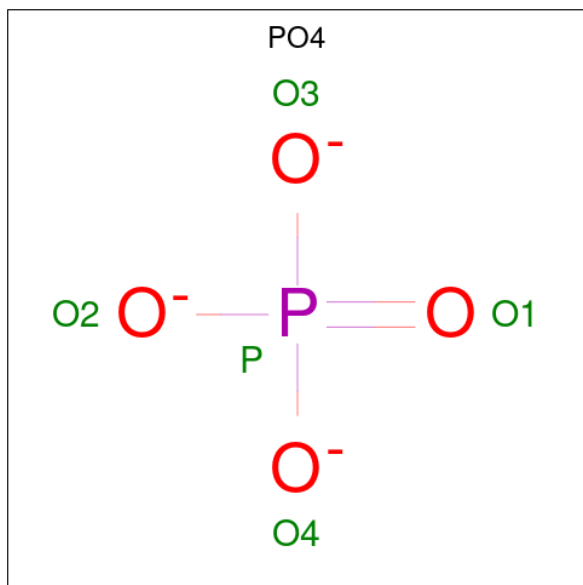
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

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



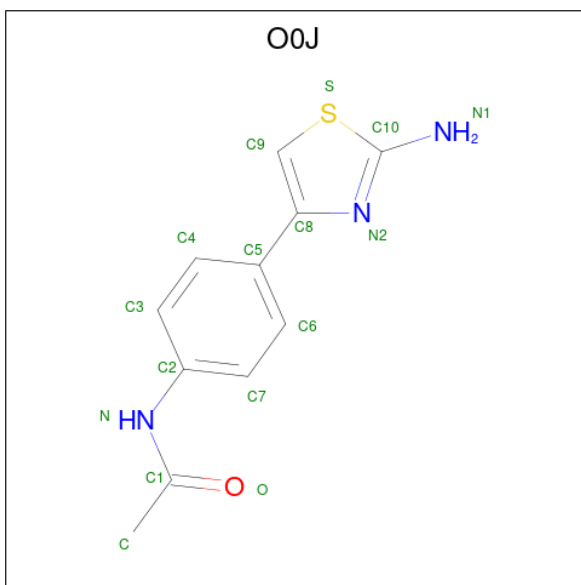
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		

- 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 N-[4-(2-amino-1,3-thiazol-4-yl)phenyl]acetamide (three-letter code: O0J) (formula: $C_{11}H_{11}N_3OS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			16	11	3	1	1		

- 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		

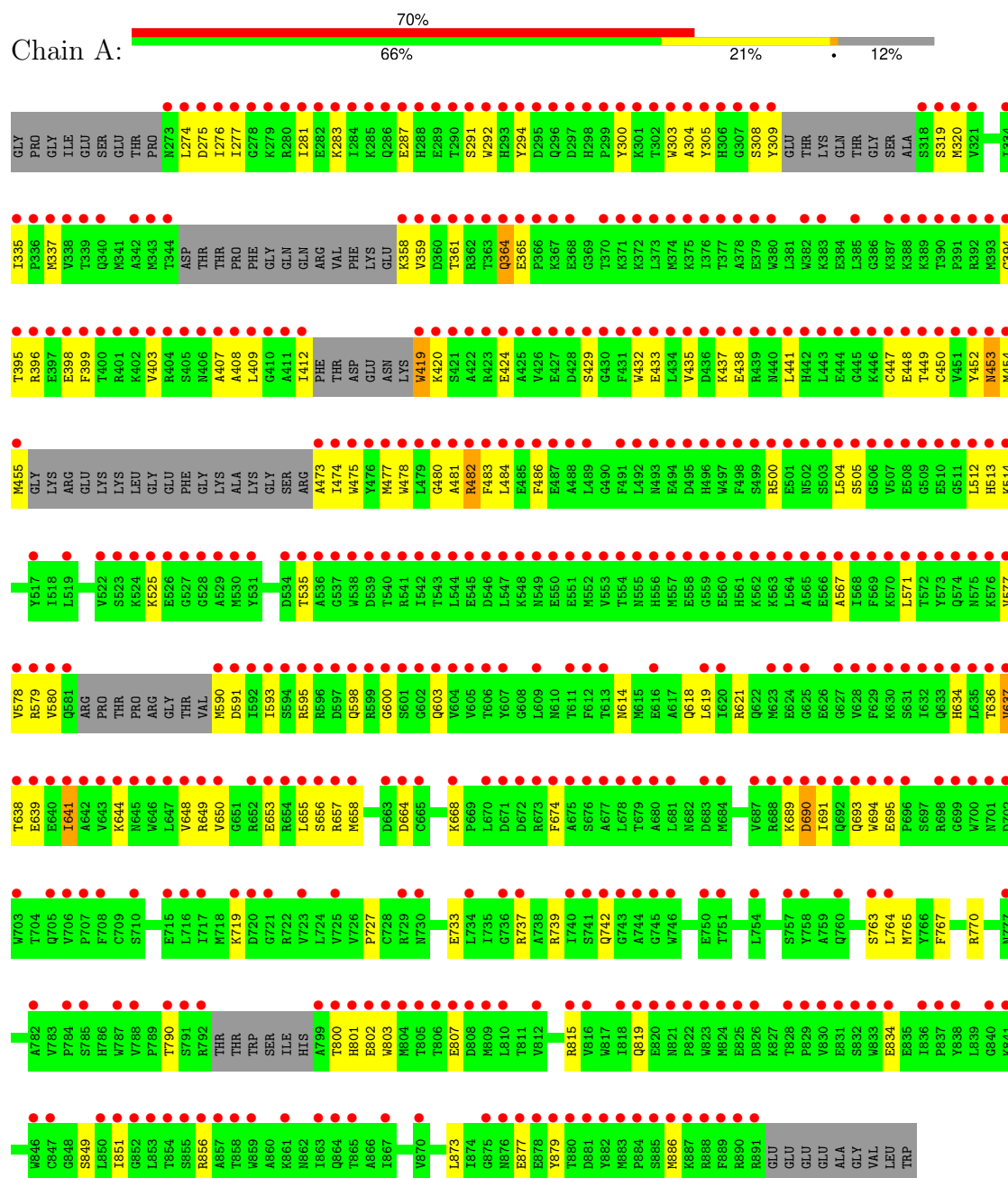
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	352	Total	O	0	1
			353	353		

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 117.42Å 148.92Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.46 – 1.50 74.46 – 1.50	Depositor EDS
% Data completeness (in resolution range)	95.1 (74.46-1.50) 95.1 (74.46-1.50)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.00 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC5	Depositor
R, R_{free}	0.255 , 0.291 0.298 , 0.313	Depositor DCC
R_{free} test set	5823 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	6.3	Xtriage
Anisotropy	1.261	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 379.0	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	0.82	EDS
Total number of atoms	5068	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.99% 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, O0J, MES, PO4, ZN, CL, DMS

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	0.77	0/4744	0.83	3/6396 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	815	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	739	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	A	815	ARG	NE-CZ-NH1	5.38	122.99	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	4640	0	4538	148	0
2	A	2	0	0	1	0
3	A	24	0	26	1	0
4	A	8	0	12	2	0
5	A	14	0	20	0	0
6	A	10	0	0	2	0
7	A	16	0	0	0	0
8	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	A	353	0	0	12	0
All	All	5068	0	4596	150	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 16.

All (150) 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:HD12	1:A:412:ILE:O	1.06	1.21
1:A:452:TYR:HB2	1:A:578:VAL:HG22	1.29	1.13
1:A:412:ILE:O	1:A:412:ILE:CD1	1.98	1.10
1:A:638:THR:O	1:A:641:ILE:HG23	1.59	1.02
1:A:653:GLU:O	1:A:656:SER:OG	1.79	0.99
1:A:505:SER:OG	1:A:655:LEU:O	1.86	0.93
1:A:480:GLY:O	1:A:484:LEU:HG	1.70	0.91
1:A:638:THR:O	1:A:641:ILE:CG2	2.18	0.90
1:A:304:ALA:O	1:A:593:ILE:HA	1.73	0.88
1:A:291:SER:O	1:A:309:TYR:HA	1.76	0.85
1:A:300:TYR:OH	1:A:591:ASP:OD2	1.95	0.85
1:A:664:ASP:OD1	6:A:1007:PO4:O2	1.99	0.80
1:A:800:THR:HB	1:A:802:GLU:OE1	1.84	0.77
1:A:800:THR:O	1:A:802:GLU:OE2	2.03	0.77
1:A:304:ALA:O	1:A:593:ILE:CB	2.33	0.77
1:A:304:ALA:O	1:A:593:ILE:CA	2.32	0.77
1:A:303:TRP:CZ3	1:A:595:ARG:HB3	2.19	0.77
1:A:800:THR:HB	1:A:802:GLU:CD	2.07	0.75
1:A:535:THR:O	9:A:1101:HOH:O	2.05	0.74
1:A:319:SER:HA	1:A:742:GLN:HE22	1.54	0.72
1:A:438:GLU:OE1	2:A:1002:ZN:ZN	1.37	0.71
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.32	0.70
1:A:693:GLN:OE1	1:A:694:TRP:NE1	2.26	0.69
1:A:274:LEU:HA	1:A:277:ILE:HG12	1.74	0.68
1:A:304:ALA:O	1:A:593:ILE:HB	1.93	0.68
1:A:409:LEU:O	1:A:482:ARG:HG2	1.93	0.68
1:A:450:CYS:HB3	1:A:477:MET:HE1	1.74	0.68
1:A:319:SER:HA	1:A:742:GLN:NE2	2.07	0.68
1:A:303:TRP:HE1	1:A:359:VAL:HG22	1.58	0.67
1:A:303:TRP:CZ2	1:A:595:ARG:HD2	2.31	0.65
1:A:807:GLU:HG3	9:A:1298:HOH:O	1.96	0.65
1:A:303:TRP:CD2	1:A:593:ILE:HD12	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:437:LYS:O	1:A:441:LEU:HG	1.97	0.64
1:A:303:TRP:CG	1:A:593:ILE:HD12	2.33	0.64
1:A:664:ASP:OD1	6:A:1007:PO4:P	2.55	0.64
1:A:396:ARG:NH1	1:A:432:TRP:HB3	2.13	0.63
1:A:452:TYR:HB3	1:A:475:TRP:HB3	1.80	0.63
1:A:770:ARG:HD2	1:A:851:ILE:HD13	1.80	0.63
1:A:455:MET:O	1:A:473:ALA:HB1	2.00	0.61
1:A:283:LYS:HD2	1:A:448:GLU:HG2	1.82	0.61
1:A:819:GLN:HG3	9:A:1421:HOH:O	1.99	0.61
1:A:849:SER:OG	1:A:851:ILE:HG12	2.02	0.59
1:A:276:ILE:O	9:A:1102:HOH:O	2.17	0.59
1:A:300:TYR:CE2	1:A:591:ASP:OD2	2.56	0.58
1:A:399:PHE:CE2	1:A:483:PHE:HB2	2.39	0.57
1:A:801[A]:HIS:HA	1:A:803:TRP:CZ3	2.40	0.57
1:A:283:LYS:O	1:A:287:GLU:HG3	2.05	0.57
1:A:475:TRP:CZ3	1:A:600:GLY:HA3	2.40	0.56
4:A:1004:DMS:C1	9:A:1271:HOH:O	2.52	0.56
1:A:737:ARG:HB3	9:A:1385:HOH:O	2.06	0.56
1:A:429:SER:O	1:A:433:GLU:HG3	2.06	0.55
1:A:595:ARG:HD3	1:A:598:GLN:HB2	1.89	0.55
1:A:638:THR:O	1:A:641:ILE:HG22	2.06	0.54
1:A:407:ALA:O	1:A:409:LEU:HG	2.08	0.54
1:A:300:TYR:CZ	1:A:591:ASP:OD2	2.60	0.54
1:A:412:ILE:HD12	1:A:412:ILE:C	2.12	0.54
1:A:337:MET:HG2	9:A:1309:HOH:O	2.08	0.54
1:A:305:TYR:HE1	1:A:308:SER:OG	1.90	0.53
1:A:319:SER:CA	1:A:742:GLN:HE22	2.20	0.53
1:A:399:PHE:CE1	1:A:483:PHE:HA	2.43	0.53
1:A:305:TYR:HA	1:A:593:ILE:HG22	1.91	0.53
1:A:580:VAL:O	1:A:590:MET:HA	2.09	0.52
1:A:483:PHE:CD2	1:A:484:LEU:HD23	2.44	0.52
1:A:733:GLU:O	1:A:737:ARG:HG3	2.10	0.51
1:A:305:TYR:CE1	1:A:308:SER:OG	2.63	0.51
1:A:408:ALA:HB3	1:A:603:GLN:HE22	1.76	0.51
1:A:452:TYR:HB2	1:A:578:VAL:CG2	2.21	0.51
1:A:396:ARG:HH12	1:A:432:TRP:HB3	1.74	0.50
1:A:856:ARG:O	1:A:856:ARG:HD3	2.11	0.50
1:A:449:THR:O	1:A:478:TRP:CD1	2.64	0.50
1:A:801[B]:HIS:HA	1:A:803:TRP:CZ3	2.46	0.50
4:A:1004:DMS:H13	9:A:1271:HOH:O	2.09	0.50
1:A:320:MET:HA	9:A:1103:HOH:O	0.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:454:MET:C	1:A:455:MET:HG3	2.32	0.50
1:A:475:TRP:CD1	1:A:475:TRP:N	2.78	0.49
1:A:764:LEU:HG	1:A:765:MET:HE3	1.93	0.49
1:A:303:TRP:HB3	1:A:593:ILE:HD12	1.93	0.49
1:A:886:MET:HE1	9:A:1207:HOH:O	2.12	0.49
1:A:395:THR:O	1:A:398:GLU:HB2	2.12	0.49
1:A:294:TYR:CE1	1:A:305:TYR:CE2	3.01	0.48
1:A:649:ARG:HG2	1:A:650:VAL:HG13	1.94	0.48
1:A:320:MET:CA	9:A:1103:HOH:O	0.83	0.48
1:A:438:GLU:OE1	1:A:447:CYS:SG	2.71	0.48
1:A:274:LEU:HD23	1:A:277:ILE:HG13	1.95	0.48
1:A:453:ASN:ND2	1:A:579:ARG:HD2	2.29	0.48
1:A:454:MET:HE1	1:A:475:TRP:CZ2	2.47	0.48
1:A:358:LYS:HG2	1:A:361:THR:OG1	2.13	0.48
1:A:621:ARG:HG2	1:A:674:PHE:CE2	2.49	0.48
1:A:303:TRP:CH2	1:A:595:ARG:HD2	2.49	0.47
1:A:283:LYS:HD2	1:A:448:GLU:CG	2.44	0.47
1:A:303:TRP:CE3	1:A:595:ARG:HB3	2.49	0.47
1:A:403:VAL:HG22	1:A:409:LEU:CD1	2.45	0.47
1:A:303:TRP:CH2	1:A:595:ARG:HG2	2.50	0.47
1:A:619:LEU:HD11	1:A:655:LEU:HD21	1.96	0.47
1:A:873:LEU:HD13	3:A:1003[A]:MES:H62	1.97	0.47
1:A:578:VAL:CG1	1:A:579:ARG:N	2.77	0.46
1:A:403:VAL:HG22	1:A:409:LEU:HD11	1.96	0.46
1:A:719[A]:LYS:NZ	1:A:834:GLU:O	2.49	0.46
1:A:275:ASP:N	1:A:275:ASP:OD1	2.49	0.46
1:A:644:LYS:O	1:A:648:VAL:HG23	2.16	0.46
1:A:689:LYS:O	1:A:690:ASP:HB2	2.17	0.45
1:A:277:ILE:HB	1:A:577:VAL:CG2	2.47	0.45
1:A:309:TYR:CD1	1:A:309:TYR:C	2.91	0.44
1:A:292:TRP:HZ3	1:A:309:TYR:HD2	1.63	0.44
1:A:454:MET:HG3	1:A:473:ALA:HB3	1.99	0.44
1:A:525:LYS:O	1:A:668:LYS:NZ	2.48	0.44
1:A:396:ARG:HD3	1:A:432:TRP:CE3	2.52	0.44
1:A:408:ALA:CB	1:A:603:GLN:HE22	2.31	0.44
1:A:514:LYS:HA	1:A:514:LYS:HD2	1.88	0.44
1:A:525:LYS:O	1:A:668:LYS:HE2	2.17	0.44
1:A:525:LYS:O	1:A:668:LYS:CE	2.66	0.44
1:A:693:GLN:CD	1:A:694:TRP:NE1	2.71	0.44
1:A:474:ILE:HD12	1:A:474:ILE:N	2.33	0.43
1:A:300:TYR:HE2	1:A:591:ASP:OD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:THR:O	1:A:398:GLU:N	2.51	0.43
1:A:453:ASN:OD1	1:A:453:ASN:N	2.52	0.43
1:A:636:THR:O	1:A:637:VAL:C	2.56	0.43
1:A:763[B]:SER:O	1:A:767:PHE:HB3	2.18	0.43
1:A:394:CYS:HB3	1:A:486:PHE:CE2	2.54	0.43
1:A:359:VAL:HG21	1:A:454:MET:HE1	1.99	0.43
1:A:790:THR:HG22	9:A:1327:HOH:O	2.18	0.43
1:A:764:LEU:HG	1:A:765:MET:CE	2.49	0.43
1:A:277:ILE:O	1:A:281:ILE:HG13	2.19	0.43
1:A:636:THR:O	1:A:639:GLU:N	2.51	0.42
1:A:500:ARG:CZ	1:A:504:LEU:O	2.68	0.42
1:A:657:ARG:HB3	1:A:668:LYS:O	2.18	0.42
1:A:737:ARG:NH2	1:A:737:ARG:HG2	2.34	0.42
1:A:419:TRP:HB3	1:A:424:GLU:HB2	2.01	0.42
1:A:454:MET:HB2	1:A:454:MET:HE2	1.93	0.42
1:A:618:GLN:HB2	1:A:658:MET:SD	2.60	0.42
1:A:614:ASN:O	1:A:618:GLN:HG2	2.19	0.42
1:A:412:ILE:O	1:A:412:ILE:CG1	2.61	0.42
1:A:364:GLN:HG3	1:A:365:GLU:N	2.35	0.42
1:A:567:ALA:HB1	1:A:571:LEU:HD12	2.02	0.42
1:A:800:THR:HB	1:A:802:GLU:OE2	2.19	0.42
1:A:512[A]:LEU:HD12	1:A:512[A]:LEU:HA	1.82	0.41
1:A:435:VAL:HG13	1:A:484:LEU:HD21	2.02	0.41
1:A:303:TRP:CE3	1:A:593:ILE:HD12	2.55	0.41
1:A:800:THR:CB	1:A:802:GLU:OE1	2.61	0.41
1:A:653:GLU:C	1:A:656:SER:OG	2.55	0.41
1:A:303:TRP:CB	1:A:593:ILE:HD12	2.51	0.40
1:A:512[A]:LEU:HG	1:A:727:PRO:CB	2.52	0.40
1:A:877:GLU:HB2	1:A:879:TYR:CE2	2.56	0.40
1:A:303:TRP:CZ3	1:A:595:ARG:CB	2.99	0.40
1:A:477:MET:SD	1:A:481:ALA:HB1	2.61	0.40
1:A:691:ILE:HG12	1:A:695:GLU:HB3	2.04	0.40
1:A:412:ILE:CD1	1:A:412:ILE:C	2.84	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	554/637 (87%)	532 (96%)	20 (4%)	2 (0%)	30	12

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	690	ASP
1	A	637	VAL

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	497/554 (90%)	489 (98%)	8 (2%)	58	32

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	335	ILE
1	A	364	GLN
1	A	419	TRP
1	A	420	LYS
1	A	453	ASN
1	A	482	ARG
1	A	634	HIS
1	A	641	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	603	GLN
1	A	742	GLN
1	A	786	HIS

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 [i](#)

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	PEG	A	1006	-	6,6,6	0.19	0	5,5,5	0.10	0
3	MES	A	1003[B]	-	12,12,12	0.71	0	15,16,16	0.30	0
6	PO4	A	1008	-	4,4,4	1.12	1 (25%)	6,6,6	0.51	0
5	PEG	A	1009	-	6,6,6	0.17	0	5,5,5	0.07	0
7	O0J	A	1010	-	14,17,17	0.41	0	17,23,23	0.72	1 (5%)
4	DMS	A	1005	-	3,3,3	0.21	0	3,3,3	0.13	0
4	DMS	A	1004	-	3,3,3	1.11	0	3,3,3	0.54	0
6	PO4	A	1007	-	4,4,4	2.29	1 (25%)	6,6,6	0.59	0
3	MES	A	1003[A]	-	12,12,12	1.09	1 (8%)	15,16,16	1.07	2 (13%)

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	-
3	MES	A	1003[B]	-	-	5/6/14/14	0/1/1/1
5	PEG	A	1009	-	-	2/4/4/4	-
7	O0J	A	1010	-	-	2/8/8/8	0/2/2/2
3	MES	A	1003[A]	-	-	0/6/14/14	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1007	PO4	P-O1	4.19	1.60	1.50
3	A	1003[A]	MES	O1S-S	-2.50	1.38	1.45
6	A	1008	PO4	P-O1	2.04	1.55	1.50

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1003[A]	MES	O2S-S-C8	-3.26	101.81	106.73
7	A	1010	O0J	C9-C8-C5	-2.65	125.76	129.44
3	A	1003[A]	MES	O3S-S-O1S	2.05	116.54	111.40

There are no chirality outliers.

All (12) torsion outliers are listed below:

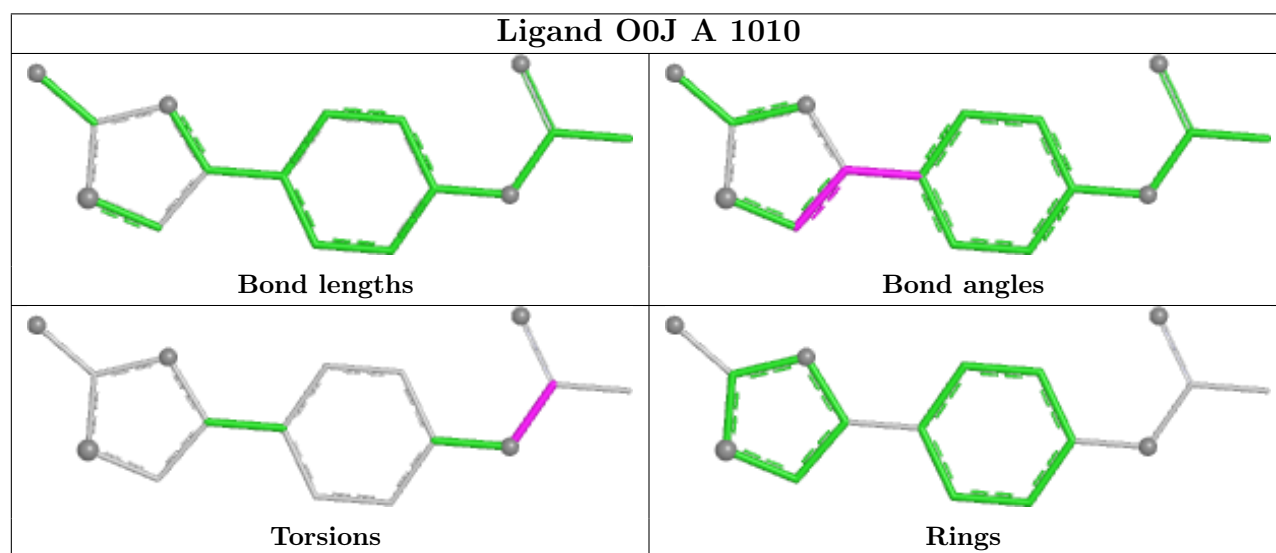
Mol	Chain	Res	Type	Atoms
3	A	1003[B]	MES	C8-C7-N4-C3
7	A	1010	O0J	C-C1-N-C2
7	A	1010	O0J	O-C1-N-C2
5	A	1006	PEG	O2-C3-C4-O4
3	A	1003[B]	MES	C7-C8-S-O3S
5	A	1009	PEG	O2-C3-C4-O4
5	A	1009	PEG	O1-C1-C2-O2
3	A	1003[B]	MES	C8-C7-N4-C5
3	A	1003[B]	MES	C7-C8-S-O1S
3	A	1003[B]	MES	C7-C8-S-O2S
5	A	1006	PEG	O1-C1-C2-O2
5	A	1006	PEG	C1-C2-O2-C3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1004	DMS	2	0
6	A	1007	PO4	2	0
3	A	1003[A]	MES	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 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	561/637 (88%)	6.28	446 (79%) 0 0	6, 30, 55, 105	245 (43%)

All (446) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	412	ILE	25.4
1	A	411	ALA	21.5
1	A	294	TYR	20.2
1	A	403	VAL	19.9
1	A	292	TRP	17.1
1	A	419	TRP	17.0
1	A	409	LEU	16.7
1	A	293	HIS	16.7
1	A	305	TYR	16.5
1	A	284	ILE	16.5
1	A	299	PRO	16.3
1	A	474	ILE	16.3
1	A	435	VAL	16.1
1	A	432	TRP	15.9
1	A	303	TRP	15.8
1	A	431	PHE	15.6
1	A	309	TYR	15.4
1	A	281	ILE	15.1
1	A	800	THR	15.0
1	A	300	TYR	15.0
1	A	426	VAL	14.9
1	A	635	LEU	14.9
1	A	277	ILE	14.5
1	A	441	LEU	14.5
1	A	592	ILE	14.4
1	A	637	VAL	14.4
1	A	375	LYS	14.3

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Mol	Chain	Res	Type	RSRZ
1	A	302	THR	14.3
1	A	593	ILE	14.3
1	A	641	ILE	14.2
1	A	399	PHE	14.1
1	A	286	GLN	14.0
1	A	604	VAL	14.0
1	A	425	ALA	14.0
1	A	359	VAL	14.0
1	A	364	GLN	13.9
1	A	291	SER	13.9
1	A	404	ARG	13.9
1	A	799	ALA	13.9
1	A	443	LEU	13.8
1	A	434	LEU	13.8
1	A	362	ARG	13.7
1	A	578	VAL	13.7
1	A	407	ALA	13.5
1	A	859	TRP	13.5
1	A	298	HIS	13.4
1	A	422	ALA	13.3
1	A	577	VAL	13.2
1	A	544	LEU	13.1
1	A	687	VAL	13.0
1	A	483	PHE	13.0
1	A	600	GLY	12.9
1	A	446	LYS	12.9
1	A	304	ALA	12.8
1	A	891	ARG	12.7
1	A	420	LYS	12.6
1	A	452	TYR	12.6
1	A	307	GLY	12.5
1	A	476	TYR	12.3
1	A	570	LYS	12.3
1	A	451	VAL	12.3
1	A	580	VAL	12.3
1	A	648	VAL	12.3
1	A	295	ASP	12.3
1	A	638	THR	12.3
1	A	803	TRP	12.3
1	A	453	ASN	12.2
1	A	402	LYS	12.2
1	A	297	ASP	12.1

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Mol	Chain	Res	Type	RSRZ
1	A	290	THR	12.1
1	A	694	TRP	12.1
1	A	636	THR	12.0
1	A	361	THR	12.0
1	A	408	ALA	11.9
1	A	575	ASN	11.9
1	A	367	LYS	11.8
1	A	405	SER	11.8
1	A	447	CYS	11.8
1	A	455	MET	11.8
1	A	889	PHE	11.8
1	A	401	ARG	11.8
1	A	288	HIS	11.7
1	A	410	GLY	11.7
1	A	406	ASN	11.7
1	A	479	LEU	11.6
1	A	850	LEU	11.6
1	A	473	ALA	11.6
1	A	319	SER	11.5
1	A	478	TRP	11.4
1	A	857	ALA	11.4
1	A	536	ALA	11.4
1	A	484	LEU	11.3
1	A	475	TRP	11.2
1	A	851	ILE	11.2
1	A	454	MET	11.2
1	A	283	LYS	11.2
1	A	400	THR	11.2
1	A	634	HIS	11.1
1	A	854	THR	11.1
1	A	512[A]	LEU	11.0
1	A	449	THR	10.9
1	A	430	GLY	10.9
1	A	421	SER	10.8
1	A	573	TYR	10.8
1	A	279	LYS	10.8
1	A	450	CYS	10.7
1	A	647	LEU	10.7
1	A	318	SER	10.7
1	A	858	THR	10.6
1	A	547	LEU	10.6
1	A	834	GLU	10.5

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Mol	Chain	Res	Type	RSRZ
1	A	320	MET	10.5
1	A	691	ILE	10.5
1	A	424	GLU	10.5
1	A	287	GLU	10.4
1	A	301	LYS	10.4
1	A	719[A]	LYS	10.3
1	A	498	PHE	10.3
1	A	274	LEU	10.2
1	A	428	ASP	10.2
1	A	363	THR	10.1
1	A	366	PRO	10.1
1	A	742	GLN	10.1
1	A	395	THR	10.1
1	A	289	GLU	10.0
1	A	853	LEU	10.0
1	A	543	THR	9.9
1	A	285	LYS	9.9
1	A	477	MET	9.8
1	A	538	TRP	9.8
1	A	480	GLY	9.7
1	A	429	SER	9.7
1	A	603	GLN	9.7
1	A	445	GLY	9.6
1	A	699	GLY	9.6
1	A	708	PHE	9.6
1	A	282	GLU	9.6
1	A	601	SER	9.6
1	A	542	ILE	9.6
1	A	643	VAL	9.5
1	A	423	ARG	9.5
1	A	344	THR	9.5
1	A	308	SER	9.5
1	A	852	GLY	9.5
1	A	744	ALA	9.5
1	A	563	LYS	9.5
1	A	763[A]	SER	9.5
1	A	296	GLN	9.4
1	A	440	ASN	9.4
1	A	602	GLY	9.4
1	A	365	GLU	9.4
1	A	321	VAL	9.3
1	A	481	ALA	9.3

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Mol	Chain	Res	Type	RSRZ
1	A	649	ARG	9.3
1	A	654	ARG	9.1
1	A	879	TYR	9.0
1	A	383	LYS	9.0
1	A	741[A]	SER	8.8
1	A	280	ARG	8.8
1	A	594	SER	8.8
1	A	801[A]	HIS	8.7
1	A	595	ARG	8.7
1	A	785[A]	SER	8.7
1	A	524	LYS	8.7
1	A	864[A]	GLN	8.6
1	A	633	GLN	8.6
1	A	655	LEU	8.6
1	A	696	PRO	8.6
1	A	596	ARG	8.6
1	A	576	LYS	8.6
1	A	607	TYR	8.5
1	A	427	GLU	8.5
1	A	540	THR	8.4
1	A	306	HIS	8.4
1	A	535	THR	8.4
1	A	439	ARG	8.4
1	A	275	ASP	8.4
1	A	278	GLY	8.3
1	A	511	GLY	8.3
1	A	581	GLN	8.3
1	A	438	GLU	8.3
1	A	884	PRO	8.2
1	A	358	LYS	8.2
1	A	564	LEU	8.1
1	A	890	ARG	8.1
1	A	396	ARG	8.1
1	A	448	GLU	8.0
1	A	791	SER	8.0
1	A	790	THR	8.0
1	A	579	ARG	8.0
1	A	656	SER	7.9
1	A	688	ARG	7.9
1	A	482	ARG	7.9
1	A	433	GLU	7.8
1	A	506	GLY	7.8

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Mol	Chain	Res	Type	RSRZ
1	A	360	ASP	7.8
1	A	273	ASN	7.7
1	A	371	LYS	7.7
1	A	645	ASN	7.7
1	A	887	LYS	7.7
1	A	397	GLU	7.6
1	A	591	ASP	7.6
1	A	507	VAL	7.6
1	A	841	LYS	7.6
1	A	640	GLU	7.5
1	A	525	LYS	7.5
1	A	668	LYS	7.5
1	A	504	LEU	7.4
1	A	437	LYS	7.4
1	A	692	GLN	7.4
1	A	398	GLU	7.3
1	A	444	GLU	7.3
1	A	689	LYS	7.2
1	A	856	ARG	7.2
1	A	436	ASP	7.1
1	A	888	ARG	7.1
1	A	702	ASP	7.1
1	A	499	SER	7.1
1	A	505	SER	7.0
1	A	680	ALA	7.0
1	A	574	GLN	7.0
1	A	639	GLU	7.0
1	A	572	THR	6.8
1	A	541	ARG	6.8
1	A	599	ARG	6.7
1	A	598	GLN	6.7
1	A	804	MET	6.7
1	A	276	ILE	6.7
1	A	590	MET	6.7
1	A	545	GLU	6.6
1	A	802	GLU	6.6
1	A	551	GLU	6.6
1	A	693	GLN	6.6
1	A	644	LYS	6.5
1	A	658	MET	6.4
1	A	500	ARG	6.4
1	A	556	HIS	6.4

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Mol	Chain	Res	Type	RSRZ
1	A	508	GLU	6.4
1	A	881	ASP	6.4
1	A	502	ASN	6.3
1	A	559	GLY	6.3
1	A	743	GLY	6.3
1	A	529	ALA	6.3
1	A	534	ASP	6.3
1	A	652	ARG	6.3
1	A	571	LEU	6.3
1	A	876	ASN	6.3
1	A	886	MET	6.3
1	A	539	ASP	6.3
1	A	562	LYS	6.3
1	A	537	GLY	6.3
1	A	690	ASP	6.2
1	A	548	LYS	6.2
1	A	509	GLY	6.2
1	A	513	HIS	6.2
1	A	657	ARG	6.1
1	A	597	ASP	6.0
1	A	550	GLU	6.0
1	A	514	LYS	6.0
1	A	629	PHE	5.9
1	A	882	TYR	5.9
1	A	376	ILE	5.9
1	A	745	GLY	5.8
1	A	885	SER	5.8
1	A	823	TRP	5.8
1	A	566	GLU	5.8
1	A	496	HIS	5.8
1	A	501	GLU	5.8
1	A	486	PHE	5.8
1	A	503	SER	5.8
1	A	630	LYS	5.7
1	A	677	ALA	5.7
1	A	558	GLU	5.7
1	A	530	MET	5.7
1	A	510	GLU	5.7
1	A	526	GLU	5.7
1	A	825	GLU	5.6
1	A	792	ARG	5.6
1	A	833	TRP	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	646	TRP	5.6
1	A	663	ASP	5.5
1	A	717	ILE	5.5
1	A	605	VAL	5.5
1	A	378	ALA	5.5
1	A	695	GLU	5.5
1	A	701	ASN	5.4
1	A	338	VAL	5.4
1	A	746	TRP	5.4
1	A	390	THR	5.3
1	A	393	MET	5.2
1	A	830	VAL	5.2
1	A	642	ALA	5.2
1	A	855	SER	5.1
1	A	561	HIS	5.1
1	A	877	GLU	5.1
1	A	489	LEU	5.1
1	A	653	GLU	5.1
1	A	442	HIS	5.1
1	A	337	MET	5.0
1	A	676	SER	5.0
1	A	683	ASP	5.0
1	A	569	PHE	5.0
1	A	880	THR	5.0
1	A	740	ILE	4.9
1	A	368	GLU	4.8
1	A	674	PHE	4.8
1	A	628	VAL	4.7
1	A	698	ARG	4.7
1	A	819	GLN	4.7
1	A	491	PHE	4.6
1	A	495	ASP	4.6
1	A	568	ILE	4.6
1	A	370	THR	4.6
1	A	485	GLU	4.6
1	A	552	MET	4.5
1	A	818	ILE	4.5
1	A	340	GLN	4.5
1	A	620	ILE	4.4
1	A	878	GLU	4.4
1	A	632	ILE	4.4
1	A	387	LYS	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	379	GLU	4.3
1	A	493	ASN	4.3
1	A	549	ASN	4.3
1	A	664	ASP	4.2
1	A	723	VAL	4.2
1	A	750	GLU	4.2
1	A	391	PRO	4.2
1	A	373	LEU	4.1
1	A	625	GLY	4.0
1	A	883	MET	4.0
1	A	555	ASN	3.9
1	A	546	ASP	3.9
1	A	815	ARG	3.9
1	A	807	GLU	3.9
1	A	494	GLU	3.9
1	A	820	GLU	3.9
1	A	700	TRP	3.8
1	A	720	ASP	3.8
1	A	497	TRP	3.8
1	A	670	LEU	3.8
1	A	528	GLY	3.7
1	A	678	LEU	3.7
1	A	565	ALA	3.7
1	A	808	ASP	3.7
1	A	334	ILE	3.7
1	A	560	GLU	3.6
1	A	831	GLU	3.6
1	A	806	THR	3.6
1	A	631	SER	3.6
1	A	679	THR	3.6
1	A	828	THR	3.5
1	A	810	LEU	3.5
1	A	821	ASN	3.5
1	A	627	GLY	3.5
1	A	554	THR	3.5
1	A	826	ASP	3.5
1	A	764	LEU	3.4
1	A	703	TRP	3.4
1	A	737	ARG	3.4
1	A	829	PRO	3.4
1	A	816	VAL	3.4
1	A	716	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	488	ALA	3.3
1	A	377	THR	3.3
1	A	567	ALA	3.3
1	A	673	ARG	3.3
1	A	527	GLY	3.2
1	A	619	LEU	3.2
1	A	788	VAL	3.2
1	A	342	ALA	3.2
1	A	870	VAL	3.2
1	A	336	PRO	3.2
1	A	650	VAL	3.2
1	A	389	LYS	3.1
1	A	861	LYS	3.1
1	A	846	TRP	3.1
1	A	487	GLU	3.1
1	A	531	TYR	3.1
1	A	523	SER	3.0
1	A	832	SER	3.0
1	A	707	PRO	3.0
1	A	557	MET	3.0
1	A	380	TRP	3.0
1	A	665	CYS	3.0
1	A	372	LYS	2.9
1	A	836	ILE	2.9
1	A	343	MET	2.9
1	A	681	LEU	2.9
1	A	706	VAL	2.8
1	A	840	GLY	2.8
1	A	824	MET	2.8
1	A	335	ILE	2.8
1	A	606	THR	2.8
1	A	613	THR	2.7
1	A	838	TYR	2.7
1	A	392	ARG	2.7
1	A	624	GLU	2.7
1	A	822	PRO	2.7
1	A	710	SER	2.7
1	A	623	MET	2.7
1	A	374	MET	2.6
1	A	867	ILE	2.6
1	A	725	VAL	2.6
1	A	684	MET	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	616	GLU	2.6
1	A	705	GLN	2.6
1	A	754	LEU	2.5
1	A	388	LYS	2.5
1	A	715	GLU	2.5
1	A	760	GLN	2.5
1	A	809	MET	2.5
1	A	784	PRO	2.5
1	A	721	GLY	2.5
1	A	492	LEU	2.4
1	A	612	PHE	2.4
1	A	757	SER	2.4
1	A	382	TRP	2.4
1	A	385	LEU	2.4
1	A	672	ASP	2.4
1	A	875	GLY	2.3
1	A	609	LEU	2.3
1	A	777	ASN	2.3
1	A	758	TYR	2.3
1	A	522	VAL	2.3
1	A	671	ASP	2.3
1	A	394	CYS	2.2
1	A	611	THR	2.2
1	A	553	VAL	2.2
1	A	837	PRO	2.2
1	A	730	ASN	2.2
1	A	734	LEU	2.2
1	A	805	THR	2.1
1	A	736	GLY	2.1
1	A	847	CYS	2.1
1	A	339	THR	2.1
1	A	519	LEU	2.1
1	A	751	THR	2.1
1	A	865	THR	2.1
1	A	517	TYR	2.1
1	A	782	ALA	2.0
1	A	863	ILE	2.0
1	A	787	TRP	2.0
1	A	675	ALA	2.0
1	A	812	VAL	2.0
1	A	729	ARG	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 ⓘ

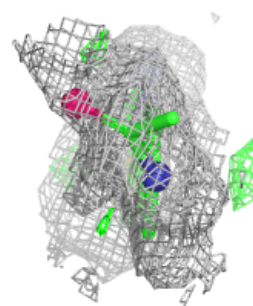
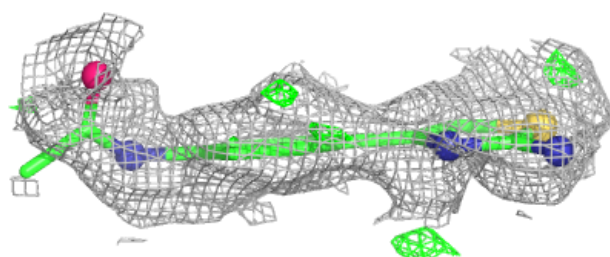
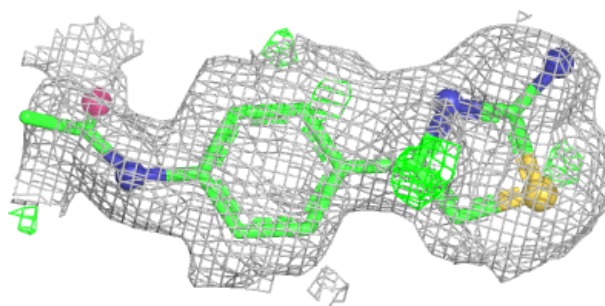
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	DMS	A	1005	4/4	0.53	0.64	52,57,58,58	4
6	PO4	A	1008	5/5	0.57	0.20	72,81,89,108	0
5	PEG	A	1006	7/7	0.58	0.36	46,48,50,50	7
7	O0J	A	1010	16/16	0.70	0.32	39,45,47,47	16
6	PO4	A	1007	5/5	0.72	0.23	28,29,33,36	5
5	PEG	A	1009	7/7	0.76	0.23	60,67,71,72	0
4	DMS	A	1004	4/4	0.88	0.18	41,46,47,52	0
2	ZN	A	1002	1/1	0.91	0.13	36,36,36,36	1
3	MES	A	1003[B]	12/12	0.96	0.31	504,516,534,537	12
3	MES	A	1003[A]	12/12	0.96	0.31	24,25,28,29	12
8	CL	A	1011	1/1	0.96	0.08	38,38,38,38	0
2	ZN	A	1001	1/1	1.00	0.04	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 O0J 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.