Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2025 – 10:34 AM EDT

PDB ID	:	7I2A
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 Z54226095 (DNV2_NS5A-x0176)
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	:	1.51 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:

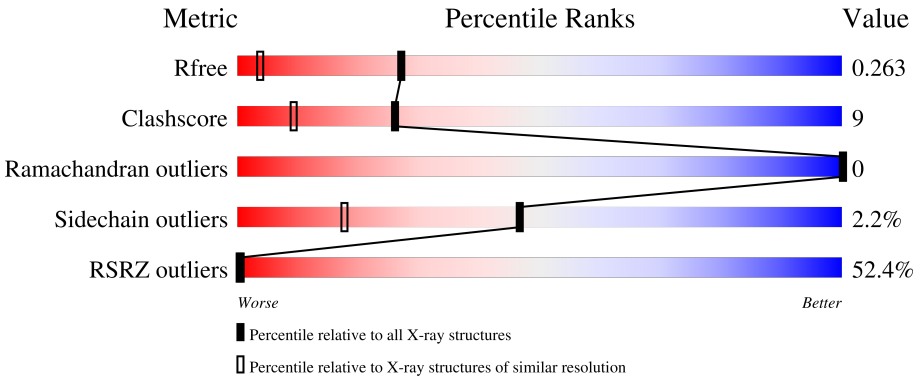
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (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 1.51 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	5293 (1.54-1.50)
Clashscore	180529	5759 (1.54-1.50)
Ramachandran outliers	177936	5653 (1.54-1.50)
Sidechain outliers	177891	5650 (1.54-1.50)
RSRZ outliers	164620	5293 (1.54-1.50)

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 <=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	47% 75% 14% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41.4

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	DMS	A	1004	-	-	X	-
4	DMS	A	1005	-	-	-	X
6	PO4	A	1007	-	-	X	-
7	WLJ	A	1010	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5244 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	574	4743	2989	848	872	34	0	7	0

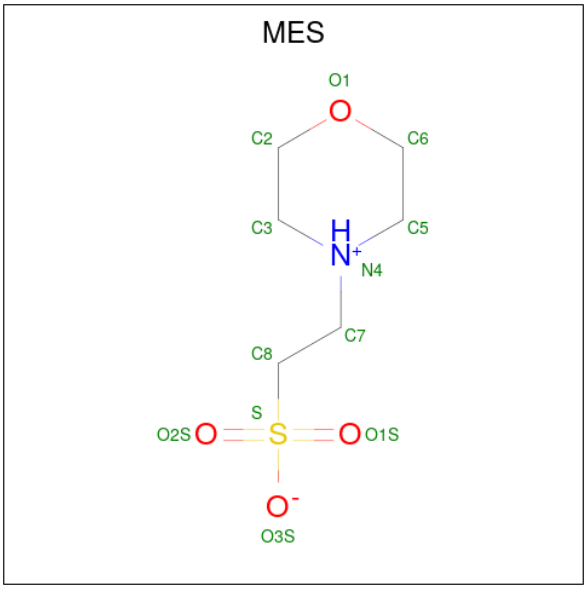
There are 2 discrepancies between the modelled and reference sequences:

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).

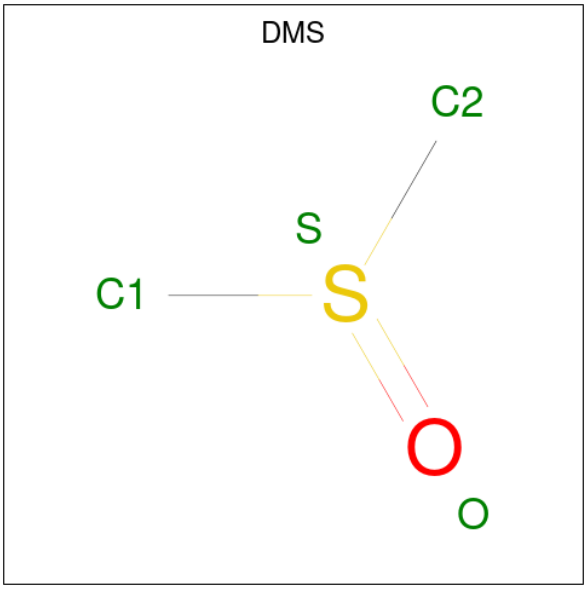
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	2	2	2	0	0

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



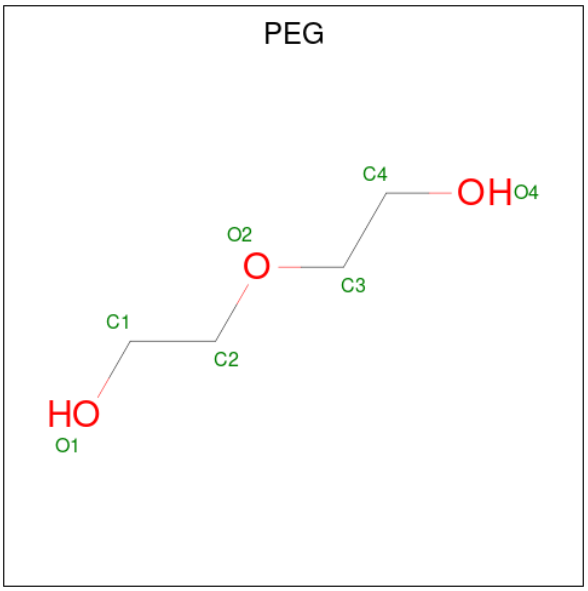
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

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



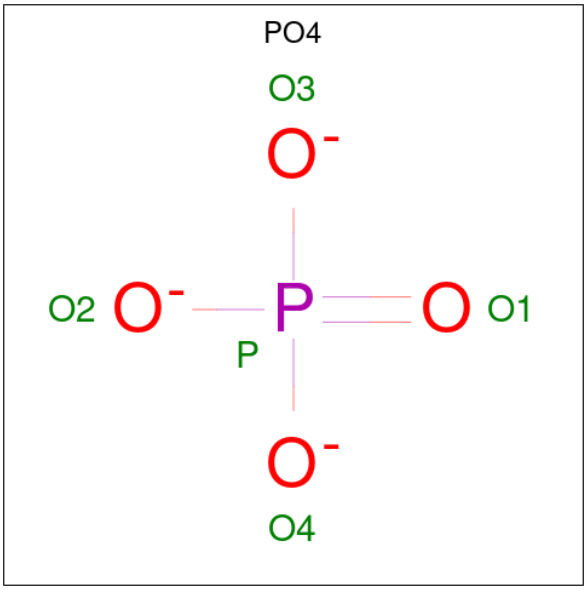
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	O	S		0	0
			4	2	1	1			
4	A	1	Total	C	O	S		0	0
			4	2	1	1			

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



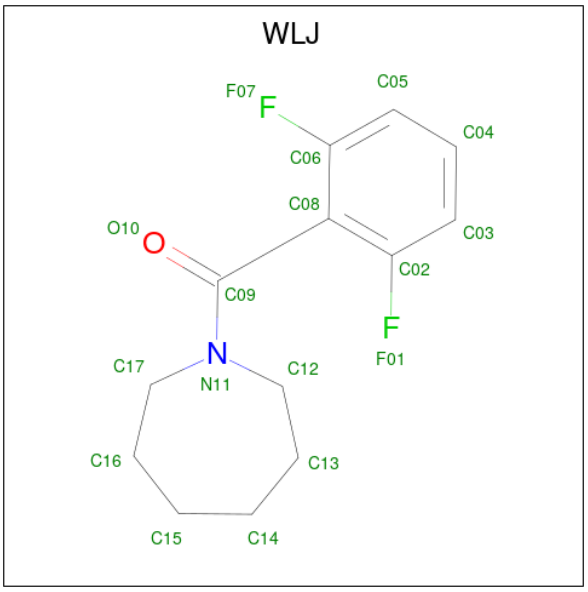
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 7 4 3	0	0
5	A	1	Total C O 7 4 3	0	0

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



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

- Molecule 7 is (azepan-1-yl)(2,6-difluorophenyl)methanone (three-letter code: WLJ) (formula: $C_{13}H_{15}F_2NO$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C F N O 17 13 2 1 1	0	0

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

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

- Molecule 9 is water.

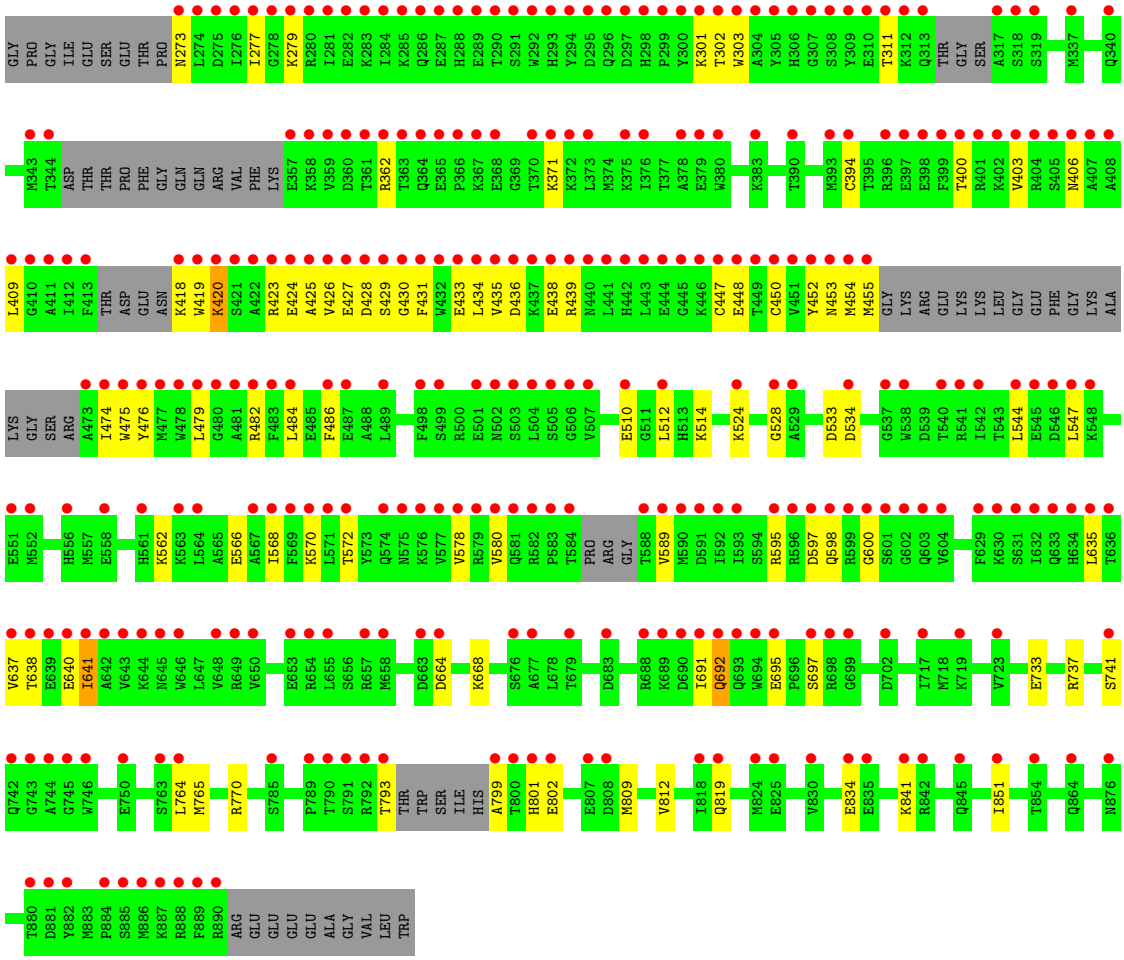
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	425	Total O 425 425	0	0

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	82.48Å 116.71Å 148.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	74.06 – 1.51 74.06 – 1.51	Depositor EDS
% Data completeness (in resolution range)	96.2 (74.06-1.51) 96.3 (74.06-1.51)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.95 (at 1.51Å)	Xtriage
Refinement program	REFMAC 5.8.0267, REFMAC5	Depositor
R, R_{free}	0.202 , 0.231 0.243 , 0.263	Depositor DCC
R_{free} test set	5681 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å^2)	25.8	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 106.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	5244	wwPDB-VP
Average B, all atoms (Å^2)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% 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: DMS, ZN, WLJ, CL, PO4, PEG, MES

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	0.75	0/4849	0.77	0/6539

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	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	741[B]	SER	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	4743	0	4642	85	0
2	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	24	0	26	0	0
4	A	8	0	12	4	0
5	A	14	0	20	2	0
6	A	10	0	0	4	0
7	A	17	0	0	0	0
8	A	1	0	0	0	0
9	A	425	0	0	11	1
All	All	5244	0	4700	89	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 (89) 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:429:SER:O	1:A:433:GLU:HG3	1.26	1.27
1:A:638:THR:O	1:A:641:ILE:HG23	1.41	1.17
1:A:425:ALA:HB1	1:A:431:PHE:CD1	1.95	1.02
1:A:303:TRP:CZ2	1:A:595:ARG:HD2	2.03	0.92
1:A:429:SER:O	1:A:433:GLU:CG	2.19	0.89
1:A:664:ASP:OD1	6:A:1007:PO4:O4	1.93	0.85
1:A:637:VAL:O	1:A:641:ILE:HG22	1.79	0.83
1:A:303:TRP:CE2	1:A:595:ARG:HD2	2.18	0.78
1:A:303:TRP:NE1	1:A:595:ARG:NH1	2.32	0.78
1:A:425:ALA:HB1	1:A:431:PHE:CG	2.18	0.78
1:A:544:LEU:HA	1:A:547:LEU:HD12	1.66	0.78
1:A:801[B]:HIS:CD2	5:A:1006:PEG:H42	2.19	0.77
1:A:425:ALA:O	1:A:431:PHE:HB3	1.86	0.75
1:A:428:ASP:OD1	1:A:430:GLY:N	2.19	0.75
1:A:474:ILE:HG12	1:A:476:TYR:CZ	2.21	0.74
1:A:664:ASP:OD1	6:A:1007:PO4:P	2.46	0.73
1:A:273:ASN:OD1	1:A:277:ILE:HD11	1.88	0.72
1:A:435:VAL:HG13	1:A:484:LEU:HD21	1.71	0.71
1:A:692:GLN:HG3	1:A:695:GLU:OE1	1.91	0.71
1:A:303:TRP:CD1	1:A:595:ARG:NH1	2.59	0.70
1:A:524:LYS:NZ	9:A:1104:HOH:O	2.27	0.67
1:A:303:TRP:HH2	1:A:475:TRP:CH2	2.14	0.66
1:A:425:ALA:HB1	1:A:431:PHE:CE1	2.30	0.66
1:A:635:LEU:HD23	1:A:640:GLU:HG2	1.77	0.66
1:A:279:LYS:HE3	1:A:448:GLU:HB2	1.77	0.65
1:A:452:TYR:HB2	1:A:578:VAL:HG22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:764:LEU:HG	1:A:765:MET:HE3	1.80	0.64
1:A:638:THR:O	1:A:641:ILE:CG2	2.32	0.63
1:A:455:MET:C	1:A:474:ILE:HG23	2.19	0.62
1:A:454:MET:O	1:A:455:MET:HG3	2.00	0.62
1:A:436:ASP:HA	1:A:439:ARG:HB3	1.82	0.61
1:A:534:ASP:OD1	6:A:1007:PO4:O4	2.17	0.61
1:A:764:LEU:HG	1:A:765:MET:CE	2.31	0.61
1:A:273:ASN:O	1:A:277:ILE:HG12	2.01	0.61
1:A:403:VAL:HG21	1:A:426:VAL:HG11	1.82	0.61
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.43	0.58
1:A:435:VAL:CG1	1:A:484:LEU:HD21	2.32	0.58
1:A:454:MET:HB3	1:A:580:VAL:HG22	1.85	0.58
1:A:425:ALA:O	1:A:431:PHE:CB	2.53	0.57
1:A:400:THR:O	1:A:403:VAL:HG22	2.05	0.56
1:A:420:LYS:O	1:A:420:LYS:HG2	2.04	0.56
1:A:303:TRP:CZ2	1:A:595:ARG:CD	2.84	0.56
1:A:409:LEU:O	1:A:482:ARG:HG2	2.06	0.56
1:A:406:ASN:OD1	1:A:423:ARG:NH1	2.34	0.56
1:A:423:ARG:O	1:A:427:GLU:HG3	2.07	0.55
1:A:474:ILE:HG12	1:A:476:TYR:CE1	2.42	0.54
1:A:371:LYS:O	9:A:1101:HOH:O	2.18	0.52
1:A:638:THR:C	1:A:641:ILE:HG23	2.24	0.52
4:A:1004:DMS:C1	9:A:1289:HOH:O	2.58	0.51
1:A:528:GLY:O	1:A:668:LYS:HE3	2.12	0.50
1:A:431:PHE:CZ	1:A:479:LEU:HD23	2.47	0.50
1:A:455:MET:C	1:A:474:ILE:CG2	2.79	0.49
1:A:770:ARG:HD2	1:A:851:ILE:HD13	1.94	0.49
1:A:428:ASP:OD1	1:A:428:ASP:C	2.51	0.49
1:A:428:ASP:OD1	1:A:430:GLY:CA	2.62	0.48
1:A:430:GLY:O	1:A:434:LEU:HG	2.12	0.48
1:A:733:GLU:O	1:A:737:ARG:HG3	2.13	0.48
1:A:809:MET:HA	1:A:809:MET:HE2	1.94	0.48
1:A:691:ILE:HD11	1:A:695:GLU:HG2	1.95	0.47
1:A:597:ASP:O	1:A:598:GLN:HB2	2.15	0.47
1:A:419:TRP:HB3	1:A:424:GLU:CB	2.45	0.47
1:A:809:MET:HE1	1:A:812:VAL:HG21	1.97	0.47
1:A:841:LYS:HE3	9:A:1474:HOH:O	2.15	0.47
1:A:801[B]:HIS:CD2	5:A:1006:PEG:C4	2.98	0.45
1:A:303:TRP:CH2	1:A:475:TRP:CH2	3.00	0.45
1:A:394:CYS:HB3	1:A:486:PHE:CE2	2.52	0.45
1:A:419:TRP:HB3	1:A:424:GLU:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:475:TRP:CD1	1:A:475:TRP:N	2.86	0.44
1:A:510:GLU:OE1	1:A:510:GLU:HA	2.17	0.44
1:A:512[B]:LEU:HD23	1:A:512[B]:LEU:HA	1.90	0.44
1:A:453:ASN:HB3	1:A:455:MET:CE	2.48	0.44
1:A:301:LYS:HD2	1:A:301:LYS:HA	1.71	0.43
1:A:302:THR:O	1:A:362:ARG:NH1	2.51	0.43
1:A:474:ILE:HG23	1:A:474:ILE:O	2.17	0.43
1:A:568:ILE:O	1:A:572:THR:OG1	2.22	0.43
1:A:638:THR:HA	1:A:641:ILE:CG2	2.49	0.43
1:A:819:GLN:NE2	9:A:1109:HOH:O	2.40	0.43
4:A:1004:DMS:H12	9:A:1292:HOH:O	2.19	0.42
1:A:514:LYS:NZ	9:A:1121:HOH:O	2.49	0.42
1:A:533:ASP:OD2	1:A:697:SER:OG	2.30	0.42
1:A:474:ILE:HG23	1:A:476:TYR:CE2	2.55	0.42
1:A:764:LEU:CG	1:A:765:MET:HE3	2.50	0.41
1:A:562:LYS:NZ	9:A:1127:HOH:O	2.53	0.41
1:A:534:ASP:OD1	6:A:1007:PO4:P	2.78	0.41
1:A:562:LYS:HE3	1:A:566:GLU:OE2	2.20	0.41
4:A:1004:DMS:H11	9:A:1289:HOH:O	2.17	0.41
1:A:799:ALA:N	9:A:1129:HOH:O	2.54	0.40
4:A:1004:DMS:H13	9:A:1289:HOH:O	2.19	0.40
1:A:475:TRP:CE3	1:A:600:GLY:HA3	2.56	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)
9:A:1159:HOH:O	9:A:1159:HOH:O[2_445]	1.60	0.60

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	567/637 (89%)	548 (97%)	19 (3%)	0	100 100

There are no Ramachandran outliers to report.

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%)	498 (98%)	11 (2%)	47 18

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	311	THR
1	A	418	LYS
1	A	420	LYS
1	A	438	GLU
1	A	570	LYS
1	A	589	VAL
1	A	641	ILE
1	A	692	GLN
1	A	793	THR
1	A	802	GLU
1	A	834	GLU

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

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	$\#\|Z\| > 2$
7	WLJ	A	1010	-	18,18,18	0.13	0	24,24,24	0.58	1 (4%)
5	PEG	A	1006	-	6,6,6	0.15	0	5,5,5	0.12	0
4	DMS	A	1005	-	3,3,3	0.21	0	3,3,3	0.09	0
3	MES	A	1003[A]	-	12,12,12	0.76	0	15,16,16	0.96	1 (6%)
3	MES	A	1003[B]	-	12,12,12	0.71	0	15,16,16	0.30	0
4	DMS	A	1004	-	3,3,3	0.75	0	3,3,3	0.55	0
6	PO4	A	1008	-	4,4,4	0.56	0	6,6,6	0.55	0
6	PO4	A	1007	-	4,4,4	5.89	3 (75%)	6,6,6	0.96	0
5	PEG	A	1009	-	6,6,6	0.15	0	5,5,5	0.07	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	WLJ	A	1010	-	-	0/8/17/17	0/2/2/2
5	PEG	A	1006	-	-	3/4/4/4	-
3	MES	A	1003[A]	-	-	3/6/14/14	0/1/1/1
3	MES	A	1003[B]	-	-	5/6/14/14	0/1/1/1
5	PEG	A	1009	-	-	2/4/4/4	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	1007	PO4	P-O1	9.26	1.72	1.50
6	A	1007	PO4	P-O2	6.07	1.72	1.54
6	A	1007	PO4	P-O3	3.80	1.65	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1010	WLJ	C06-C08-C09	2.30	125.02	121.54
3	A	1003[A]	MES	O1S-S-C8	-2.26	103.31	106.73

There are no chirality outliers.

All (13) torsion outliers are listed below:

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

There are no ring outliers.

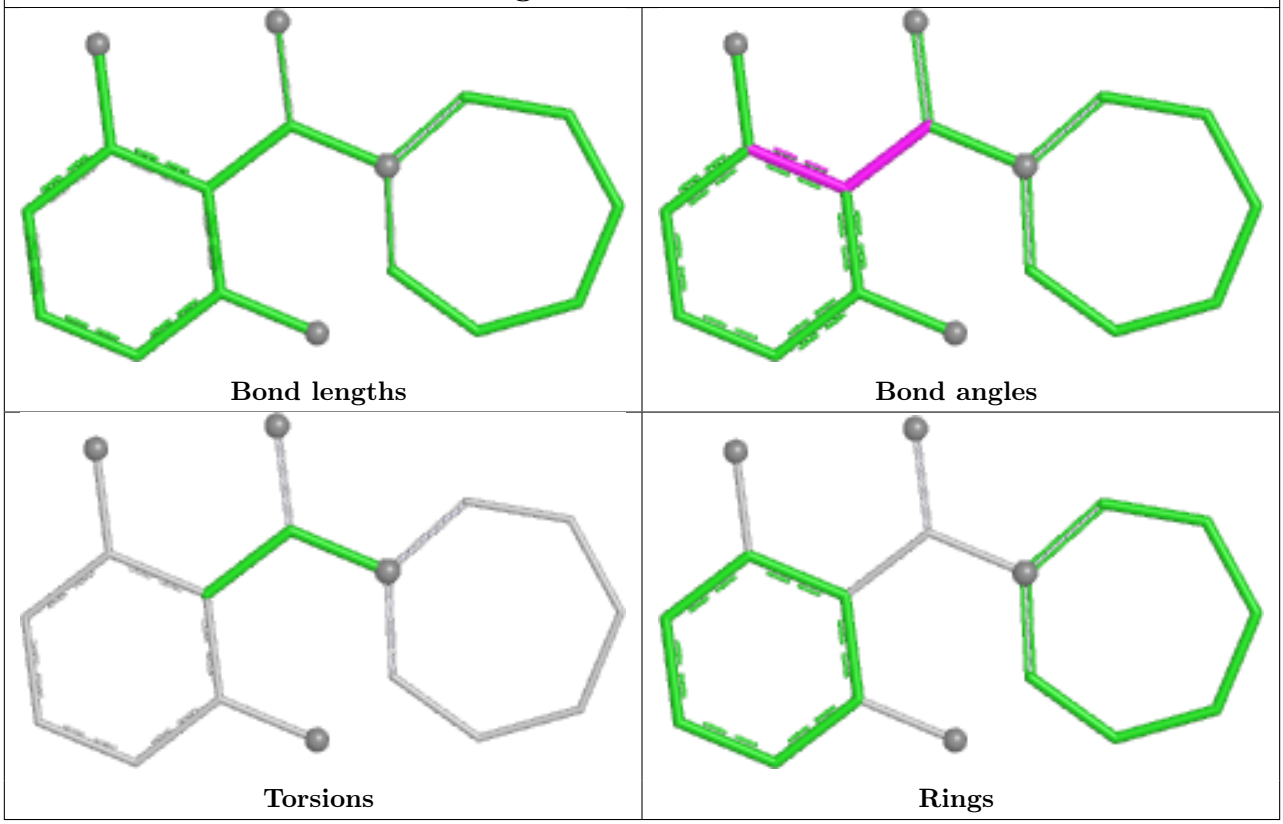
3 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1006	PEG	2	0
4	A	1004	DMS	4	0
6	A	1007	PO4	4	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.

Ligand WLJ A 1010



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	574/637 (90%)	3.50	301 (52%)	0	0	3, 27, 60, 116	192 (33%)

All (301) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	589	VAL	15.3
1	A	851	ILE	14.5
1	A	884	PRO	13.4
1	A	885	SER	13.3
1	A	719[A]	LYS	13.3
1	A	763[A]	SER	12.6
1	A	512[A]	LEU	12.4
1	A	294	TYR	12.2
1	A	435	VAL	12.0
1	A	886	MET	12.0
1	A	412	ILE	12.0
1	A	800	THR	11.9
1	A	407	ALA	11.8
1	A	635	LEU	11.7
1	A	319	SER	11.2
1	A	604	VAL	11.1
1	A	284	ILE	10.9
1	A	637	VAL	10.8
1	A	380	TRP	10.6
1	A	411	ALA	10.5
1	A	318	SER	10.5
1	A	413	PHE	10.5
1	A	864[A]	GLN	10.4
1	A	478	TRP	10.4
1	A	304	ALA	10.2
1	A	281	ILE	10.2
1	A	547	LEU	10.2

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Mol	Chain	Res	Type	RSRZ
1	A	292	TRP	10.2
1	A	431	PHE	10.2
1	A	311	THR	10.1
1	A	441	LEU	10.1
1	A	303	TRP	10.1
1	A	432	TRP	10.0
1	A	582	ARG	10.0
1	A	578	VAL	9.9
1	A	842	ARG	9.8
1	A	451	VAL	9.8
1	A	475	TRP	9.7
1	A	835	GLU	9.6
1	A	887	LYS	9.6
1	A	600	GLY	9.5
1	A	409	LEU	9.5
1	A	434	LEU	9.5
1	A	274	LEU	9.4
1	A	655	LEU	9.4
1	A	845	GLN	9.4
1	A	641	ILE	9.3
1	A	452	TYR	9.3
1	A	305	TYR	9.3
1	A	636	THR	9.2
1	A	694	TRP	9.1
1	A	544	LEU	9.1
1	A	888	ARG	9.1
1	A	276	ILE	8.9
1	A	317	ALA	8.9
1	A	498	PHE	8.9
1	A	834	GLU	8.8
1	A	510	GLU	8.8
1	A	801[A]	HIS	8.7
1	A	448	GLU	8.7
1	A	841	LYS	8.7
1	A	277	ILE	8.7
1	A	293	HIS	8.6
1	A	359	VAL	8.6
1	A	506	GLY	8.5
1	A	479	LEU	8.4
1	A	742	GLN	8.3
1	A	741[A]	SER	8.3
1	A	799	ALA	8.3

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Mol	Chain	Res	Type	RSRZ
1	A	638	THR	8.2
1	A	473	ALA	8.2
1	A	629	PHE	8.2
1	A	697	SER	8.1
1	A	588	THR	8.1
1	A	298	HIS	8.0
1	A	542	ILE	8.0
1	A	476	TYR	8.0
1	A	419	TRP	7.9
1	A	474	ILE	7.9
1	A	400	THR	7.8
1	A	645	ASN	7.8
1	A	300	TYR	7.7
1	A	602	GLY	7.7
1	A	744	ALA	7.7
1	A	283	LYS	7.7
1	A	299	PRO	7.7
1	A	484	LEU	7.5
1	A	453	ASN	7.5
1	A	309	TYR	7.5
1	A	785[A]	SER	7.4
1	A	679	THR	7.4
1	A	363	THR	7.3
1	A	505	SER	7.3
1	A	890	ARG	7.2
1	A	601	SER	7.2
1	A	403	VAL	7.2
1	A	789	PRO	7.2
1	A	426	VAL	7.1
1	A	290	THR	7.1
1	A	634	HIS	7.1
1	A	504	LEU	7.1
1	A	402	LYS	7.1
1	A	572	THR	7.0
1	A	691	ILE	7.0
1	A	631	SER	6.9
1	A	575	ASN	6.8
1	A	439	ARG	6.8
1	A	401	ARG	6.8
1	A	405	SER	6.8
1	A	430	GLY	6.7
1	A	291	SER	6.7

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Mol	Chain	Res	Type	RSRZ
1	A	499	SER	6.7
1	A	275	ASP	6.7
1	A	425	ALA	6.7
1	A	524	LYS	6.6
1	A	576	LYS	6.6
1	A	551	GLU	6.6
1	A	408	ALA	6.6
1	A	437	LYS	6.5
1	A	422	ALA	6.4
1	A	396	ARG	6.4
1	A	410	GLY	6.4
1	A	455	MET	6.4
1	A	438	GLU	6.4
1	A	282	GLU	6.4
1	A	436	ASP	6.4
1	A	280	ARG	6.4
1	A	584	THR	6.3
1	A	454	MET	6.3
1	A	595	ARG	6.3
1	A	406	ASN	6.3
1	A	791	SER	6.3
1	A	482	ARG	6.3
1	A	429	SER	6.3
1	A	583	PRO	6.2
1	A	658	MET	6.2
1	A	654	ARG	6.2
1	A	372	LYS	6.2
1	A	296	GLN	6.2
1	A	657	ARG	6.1
1	A	692	GLN	6.1
1	A	597	ASP	6.1
1	A	790	THR	6.1
1	A	288	HIS	6.1
1	A	301	LYS	6.1
1	A	793	THR	6.1
1	A	279	LYS	6.0
1	A	640	GLU	6.0
1	A	579	ARG	6.0
1	A	295	ASP	5.9
1	A	302	THR	5.9
1	A	358	LYS	5.9
1	A	548	LYS	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	599	ARG	5.9
1	A	591	ASP	5.8
1	A	630	LYS	5.8
1	A	397	GLU	5.7
1	A	477	MET	5.7
1	A	644	LYS	5.7
1	A	603	GLN	5.7
1	A	361	THR	5.7
1	A	273	ASN	5.7
1	A	433	GLU	5.7
1	A	580	VAL	5.6
1	A	423	ARG	5.6
1	A	442	HIS	5.6
1	A	503	SER	5.6
1	A	593	ILE	5.6
1	A	689	LYS	5.6
1	A	598	GLN	5.6
1	A	889	PHE	5.6
1	A	688	ARG	5.6
1	A	364	GLN	5.5
1	A	570	LYS	5.5
1	A	802	GLU	5.5
1	A	421	SER	5.4
1	A	633	GLN	5.4
1	A	310	GLU	5.4
1	A	375	LYS	5.4
1	A	366	PRO	5.3
1	A	574	GLN	5.3
1	A	297	ASP	5.3
1	A	399	PHE	5.3
1	A	344	THR	5.2
1	A	285	LYS	5.2
1	A	362	ARG	5.2
1	A	502	ASN	5.1
1	A	312	LYS	5.1
1	A	541	ARG	5.1
1	A	286	GLN	5.1
1	A	367	LYS	5.0
1	A	590	MET	5.0
1	A	695	GLU	5.0
1	A	596	ARG	4.9
1	A	564	LEU	4.9

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Mol	Chain	Res	Type	RSRZ
1	A	371	LYS	4.9
1	A	278	GLY	4.7
1	A	446	LYS	4.7
1	A	653	GLU	4.7
1	A	698	ARG	4.7
1	A	443	LEU	4.6
1	A	746	TRP	4.6
1	A	428	ASP	4.6
1	A	501	GLU	4.6
1	A	357	GLU	4.6
1	A	632	ILE	4.5
1	A	571	LEU	4.5
1	A	289	GLU	4.5
1	A	581	GLN	4.5
1	A	745	GLY	4.5
1	A	449	THR	4.4
1	A	404	ARG	4.4
1	A	424	GLU	4.4
1	A	313	GLN	4.3
1	A	308	SER	4.3
1	A	639	GLU	4.3
1	A	563	LYS	4.2
1	A	444	GLU	4.2
1	A	379	GLU	4.2
1	A	825	GLU	4.2
1	A	287	GLU	4.1
1	A	445	GLY	4.0
1	A	420	LYS	4.0
1	A	693	GLN	3.9
1	A	882	TYR	3.9
1	A	393	MET	3.9
1	A	418	LYS	3.8
1	A	481	ALA	3.8
1	A	538	TRP	3.7
1	A	390	THR	3.7
1	A	880	THR	3.6
1	A	545	GLU	3.6
1	A	486	PHE	3.6
1	A	360	ASP	3.5
1	A	398	GLU	3.5
1	A	556	HIS	3.5
1	A	568	ILE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	440	ASN	3.3
1	A	365	GLU	3.3
1	A	592	ILE	3.3
1	A	427	GLU	3.3
1	A	717	ILE	3.3
1	A	792	ARG	3.2
1	A	643	VAL	3.2
1	A	764	LEU	3.2
1	A	690	ASP	3.1
1	A	370	THR	3.1
1	A	743	GLY	3.1
1	A	676	SER	3.1
1	A	376	ILE	3.1
1	A	677	ALA	3.0
1	A	881	ASP	3.0
1	A	723	VAL	3.0
1	A	807	GLU	3.0
1	A	487	GLU	3.0
1	A	373	LEU	2.9
1	A	649	ARG	2.9
1	A	561	HIS	2.9
1	A	528	GLY	2.9
1	A	552	MET	2.9
1	A	569	PHE	2.9
1	A	577	VAL	2.9
1	A	480	GLY	2.9
1	A	483	PHE	2.8
1	A	450	CYS	2.8
1	A	824	MET	2.8
1	A	307	GLY	2.7
1	A	368	GLU	2.7
1	A	854	THR	2.7
1	A	394	CYS	2.7
1	A	383	LYS	2.7
1	A	750	GLU	2.6
1	A	830	VAL	2.6
1	A	683	ASP	2.6
1	A	337	MET	2.5
1	A	540	THR	2.4
1	A	819	GLN	2.4
1	A	699	GLY	2.4
1	A	447	CYS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	534	ASP	2.4
1	A	558	GLU	2.3
1	A	876	ASN	2.3
1	A	378	ALA	2.3
1	A	340	GLN	2.2
1	A	567	ALA	2.2
1	A	489	LEU	2.2
1	A	546	ASP	2.2
1	A	664	ASP	2.2
1	A	702	ASP	2.2
1	A	529	ALA	2.2
1	A	663	ASP	2.1
1	A	808	ASP	2.1
1	A	646	TRP	2.1
1	A	537	GLY	2.1
1	A	650	VAL	2.1
1	A	642	ALA	2.1
1	A	306	HIS	2.1
1	A	818	ILE	2.1
1	A	648	VAL	2.0
1	A	343	MET	2.0
1	A	507	VAL	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
6	PO4	A	1008	5/5	0.47	0.32	46,47,54,56	5

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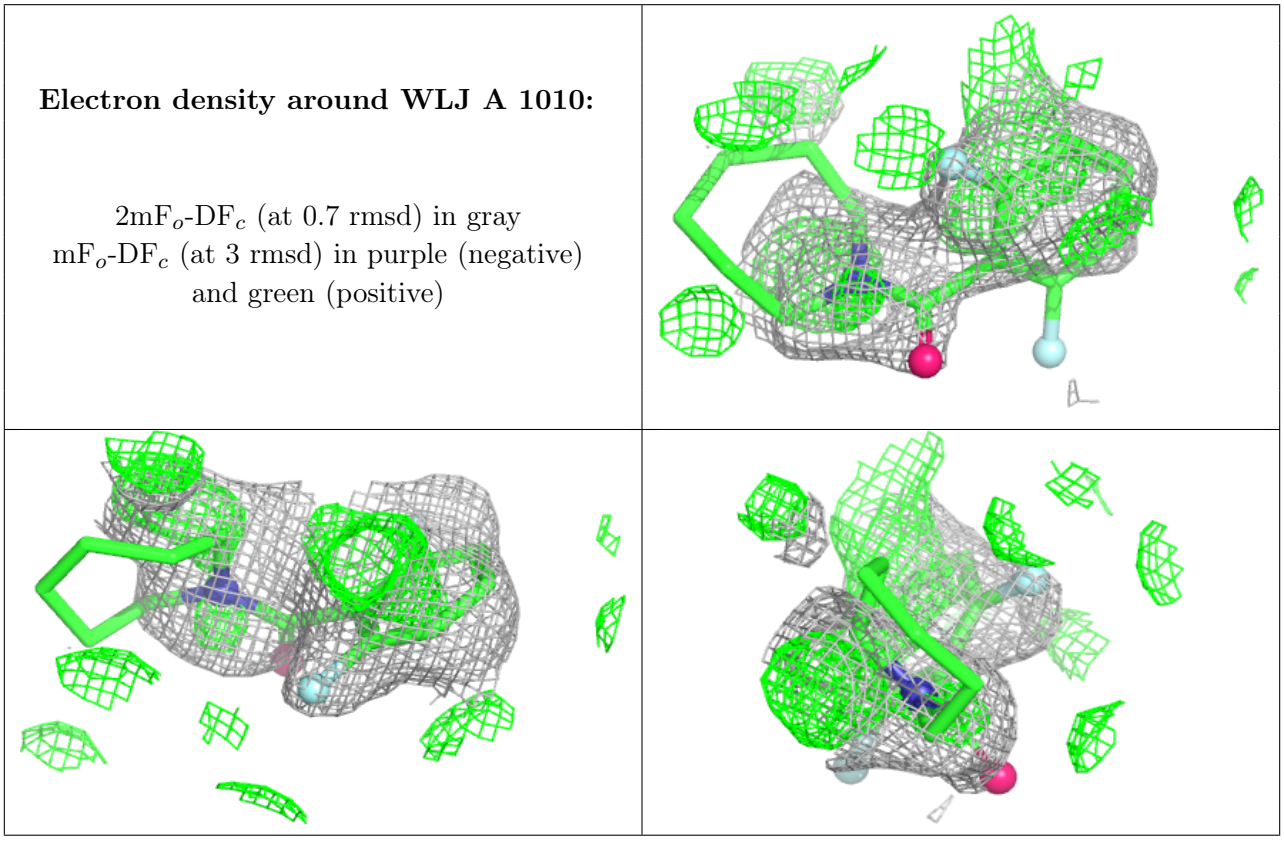
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	WLJ	A	1010	17/17	0.64	0.46	41,49,51,52	17
4	DMS	A	1005	4/4	0.75	0.61	68,70,72,73	4
6	PO4	A	1007	5/5	0.76	0.18	30,31,44,59	0
5	PEG	A	1006	7/7	0.79	0.19	47,47,47,48	7
5	PEG	A	1009	7/7	0.83	0.17	61,68,72,75	0
4	DMS	A	1004	4/4	0.87	0.18	38,40,42,45	0
3	MES	A	1003[B]	12/12	0.96	0.32	502,519,540,541	12
3	MES	A	1003[A]	12/12	0.96	0.32	19,23,25,27	12
2	ZN	A	1002	1/1	0.98	0.06	45,45,45,45	0
8	CL	A	1011	1/1	0.98	0.09	34,34,34,34	0
2	ZN	A	1001	1/1	1.00	0.02	18,18,18,18	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 WLJ 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.