Full wwPDB X-ray Structure Validation Report (i)

Mar 27, 2025 – 10:05 AM EDT

PDB ID	:	7I2R
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 Z31432226 (DNV2_NS5A-x0759)
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Deposited on	:	2025-03-06
Resolution	:	1.80 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 (i) 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 (i)) were used in the production of this report:

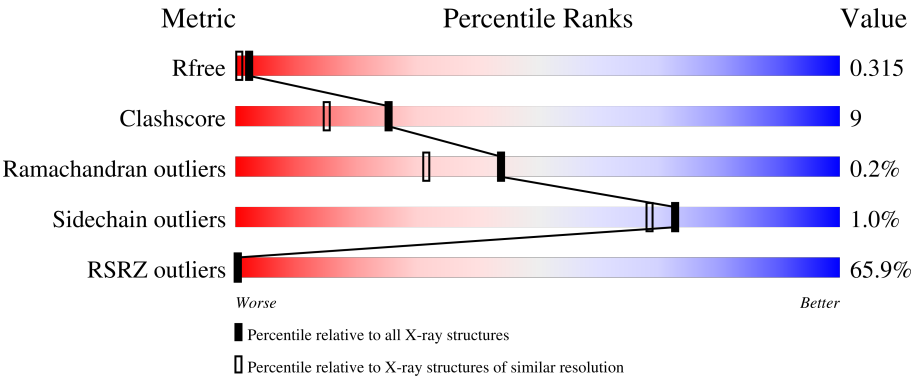
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (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 1.80 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	7108 (1.80-1.80)
Clashscore	180529	8162 (1.80-1.80)
Ramachandran outliers	177936	8077 (1.80-1.80)
Sidechain outliers	177891	8076 (1.80-1.80)
RSRZ outliers	164620	7108 (1.80-1.80)

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	58% 73% 15% 12%

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	1006	-	-	X	-
5	PO4	A	1007	-	-	-	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5014 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	560	4641	2924	829	854	34	0	6	0

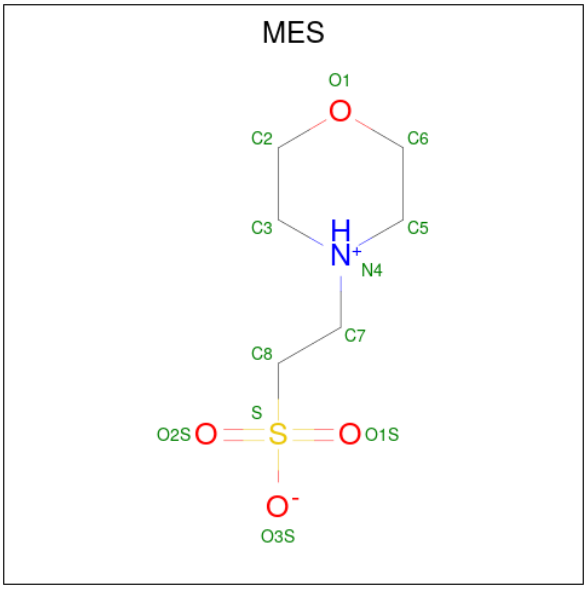
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	264	GLY	-	expression tag	UNP Q91H74
A	265	PRO	-	expression tag	UNP Q91H74

- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

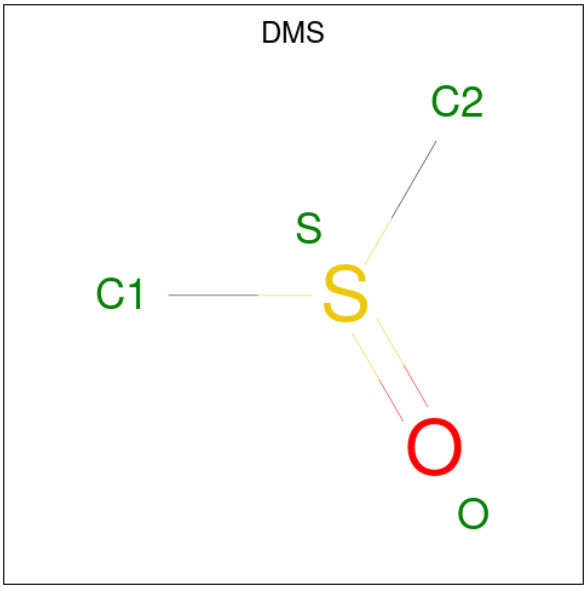
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	2	2	2	0	0

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



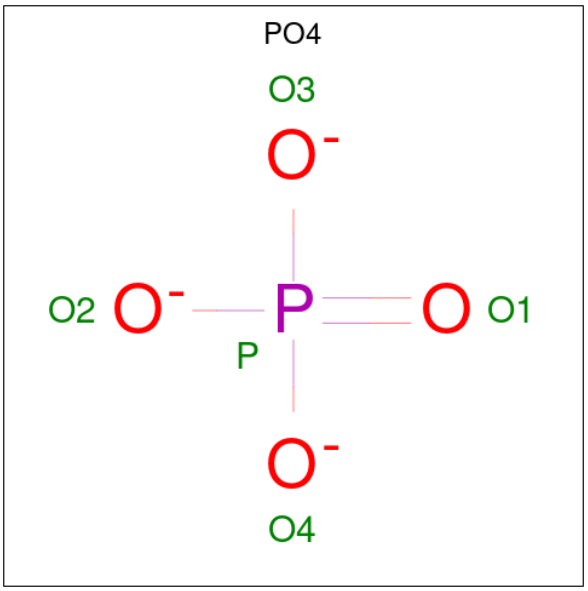
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			24	12	2	8	2		

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



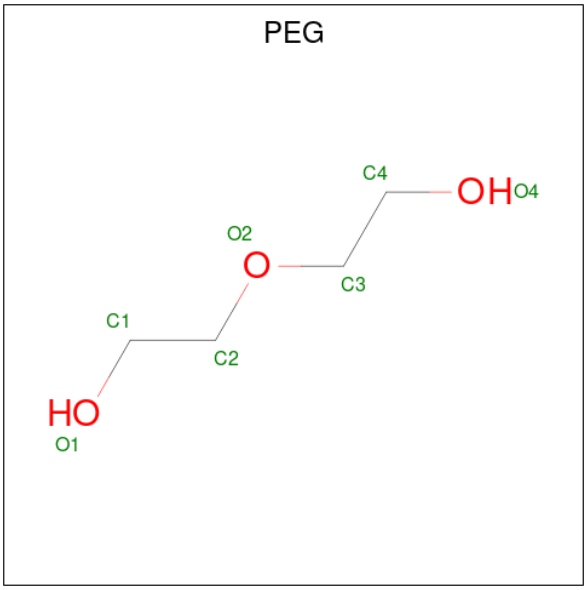
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	S	0	0
			4	2	1	1		
4	A	1	Total	C	O	S	0	0
			4	2	1	1		

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



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

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

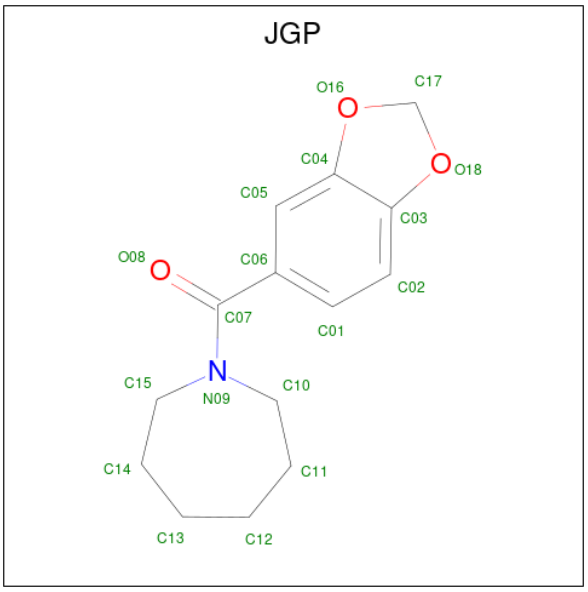


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 7 4 3	0	0

- Molecule 7 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 8 is (azepan-1-yl)(2H-1,3-benzodioxol-5-yl)methanone (three-letter code: JGP) (formula: $C_{14}H_{17}NO_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C N O 18 14 1 3	0	0

- Molecule 9 is water.

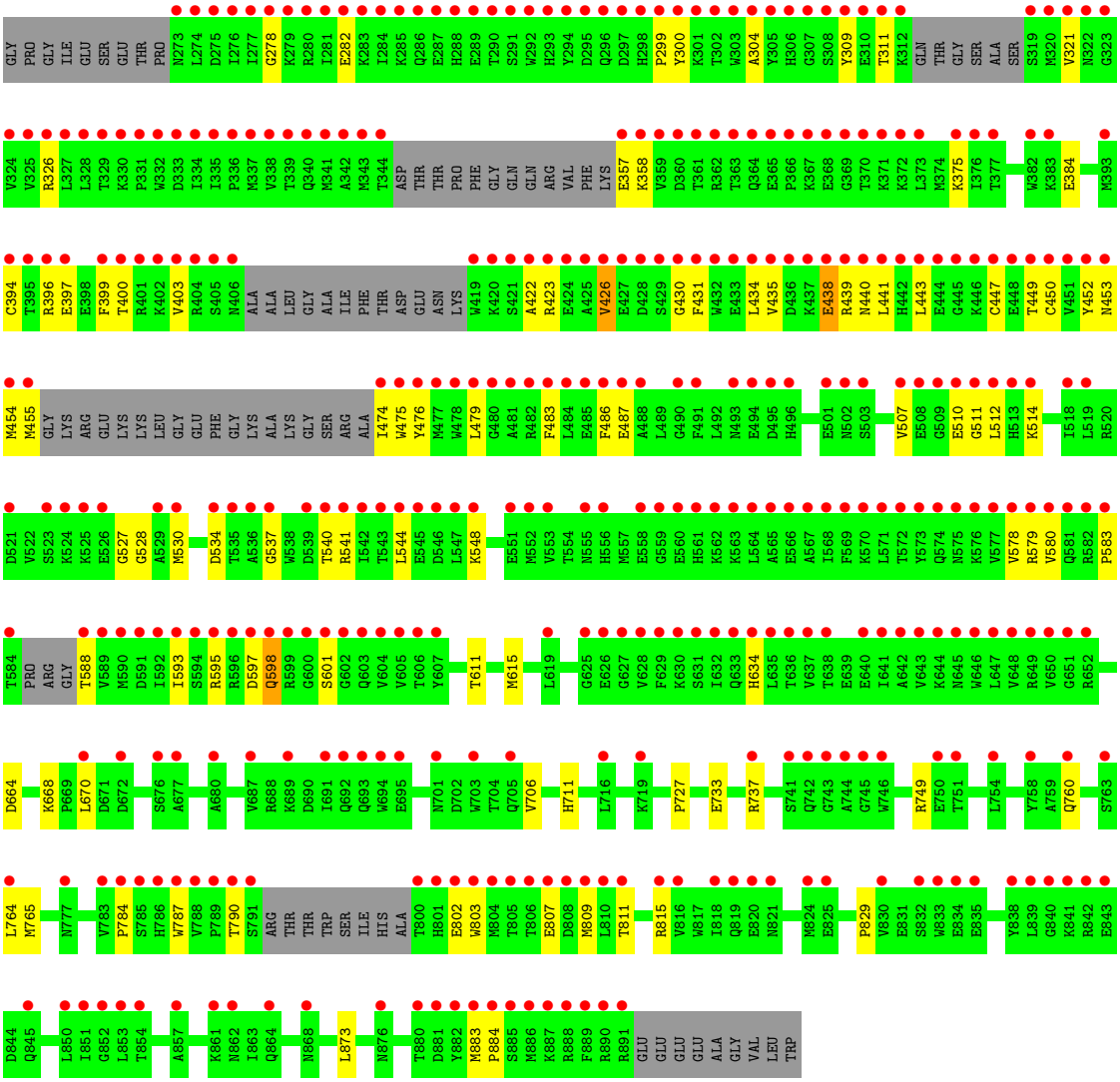
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	303	Total O 303 303	0	0

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	81.93Å 115.96Å 148.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.75 – 1.80 45.75 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.6 (45.75-1.80) 97.6 (45.75-1.80)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	0.96 (at 1.79Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.209 , 0.246 0.285 , 0.315	Depositor DCC
R_{free} test set	3391 reflections (5.16%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.317	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 194.8	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	0.85	EDS
Total number of atoms	5014	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.89% 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: PO4, JGP, DMS, CL, ZN, 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	0.68	0/4745	0.75	1/6398 (0.0%)

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	4

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	815	ARG	NE-CZ-NH2	-5.50	117.55	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	511	GLY	Mainchain
1	A	784	PRO	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	4641	0	4539	86	0
2	A	2	0	0	0	0
3	A	24	0	26	2	0
4	A	8	0	12	2	0
5	A	10	0	0	3	0
6	A	7	0	10	0	0
7	A	1	0	0	0	0
8	A	18	0	0	0	0
9	A	303	0	0	14	2
All	All	5014	0	4587	88	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 9.

All (88) 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:454:MET:HE2	1:A:475:TRP:HE1	1.22	1.02
1:A:790:THR:HG21	9:A:1340:HOH:O	1.67	0.95
1:A:807:GLU:HG3	9:A:1201:HOH:O	1.67	0.93
1:A:454:MET:O	1:A:455:MET:SD	2.26	0.92
1:A:452:TYR:HB2	1:A:578:VAL:HG22	1.63	0.78
1:A:487:GLU:OE1	9:A:1101:HOH:O	2.03	0.77
1:A:454:MET:CE	1:A:475:TRP:HE1	1.98	0.76
1:A:454:MET:HE2	1:A:475:TRP:NE1	2.00	0.74
1:A:440:ASN:HA	1:A:443:LEU:HD12	1.71	0.72
1:A:790:THR:HG22	9:A:1383:HOH:O	1.90	0.71
1:A:597:ASP:O	1:A:598:GLN:HB2	1.92	0.69
1:A:664:ASP:OD1	5:A:1006:PO4:O4	2.10	0.68
1:A:438:GLU:HG3	1:A:449:THR:OG1	1.94	0.68
1:A:454:MET:C	1:A:455:MET:SD	2.72	0.67
1:A:453:ASN:HA	1:A:579:ARG:HG2	1.77	0.66
1:A:454:MET:HG2	1:A:455:MET:H	1.60	0.66
1:A:601:SER:HB3	9:A:1123:HOH:O	1.95	0.66
1:A:438:GLU:O	1:A:441:LEU:HB2	1.96	0.66
1:A:580:VAL:HG21	1:A:593:ILE:HD11	1.78	0.65
1:A:454:MET:CE	1:A:475:TRP:NE1	2.58	0.65
1:A:873:LEU:HD13	3:A:1003[A]:MES:H62	1.82	0.60
1:A:764:LEU:HG	1:A:765:MET:HE3	1.84	0.59
1:A:802:GLU:HG2	9:A:1382:HOH:O	2.03	0.58
1:A:453:ASN:OD1	1:A:579:ARG:HD2	2.04	0.58
1:A:664:ASP:OD1	5:A:1006:PO4:P	2.62	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:453:ASN:OD1	1:A:579:ARG:CD	2.52	0.57
1:A:452:TYR:O	1:A:578:VAL:HA	2.06	0.55
1:A:454:MET:HG2	1:A:455:MET:N	2.22	0.55
4:A:1004:DMS:C1	9:A:1305:HOH:O	2.55	0.55
1:A:733:GLU:O	1:A:737:ARG:HG3	2.08	0.54
1:A:510:GLU:O	1:A:514:LYS:HG3	2.08	0.53
1:A:396:ARG:HG2	1:A:483:PHE:CZ	2.44	0.53
1:A:358:LYS:HG3	1:A:540:THR:HG21	1.93	0.51
1:A:438:GLU:HA	1:A:441:LEU:HD12	1.91	0.51
1:A:534:ASP:OD1	5:A:1006:PO4:O4	2.29	0.50
1:A:530:MET:HE2	1:A:706:VAL:HG21	1.93	0.50
1:A:583:PRO:O	1:A:588:THR:HA	2.11	0.50
1:A:537:GLY:O	1:A:541:ARG:HG2	2.11	0.50
1:A:430:GLY:O	1:A:434:LEU:HG	2.13	0.49
1:A:439:ARG:NH1	1:A:487:GLU:OE1	2.45	0.49
1:A:423:ARG:O	1:A:426:VAL:HG12	2.13	0.48
1:A:579:ARG:O	1:A:579:ARG:HG3	2.13	0.48
1:A:278:GLY:O	1:A:282:GLU:HG3	2.14	0.48
1:A:453:ASN:OD1	1:A:579:ARG:NE	2.46	0.47
1:A:304:ALA:O	1:A:593:ILE:HA	2.14	0.47
1:A:438:GLU:CG	1:A:449:THR:OG1	2.62	0.47
1:A:453:ASN:N	1:A:476:TYR:O	2.38	0.47
1:A:474:ILE:HG23	1:A:474:ILE:O	2.14	0.47
1:A:400:THR:HA	1:A:426:VAL:HG21	1.97	0.47
1:A:544:LEU:HD11	1:A:548:LYS:HE3	1.96	0.47
1:A:760:GLN:NE2	1:A:803:TRP:O	2.47	0.47
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.55	0.46
1:A:452:TYR:HB3	1:A:475:TRP:HB3	1.97	0.46
1:A:595:ARG:NH2	1:A:597:ASP:OD2	2.47	0.46
1:A:512[A]:LEU:HG	1:A:727:PRO:HB3	1.98	0.46
1:A:580:VAL:CG2	1:A:593:ILE:HD11	2.43	0.45
1:A:873:LEU:HD13	3:A:1003[B]:MES:H51	1.98	0.45
1:A:829:PRO:O	9:A:1103:HOH:O	2.21	0.45
1:A:394:CYS:HB3	1:A:486:PHE:CE2	2.52	0.44
1:A:512[A]:LEU:HG	1:A:727:PRO:CB	2.47	0.44
1:A:422:ALA:HB1	1:A:479:LEU:HD22	2.00	0.44
1:A:601:SER:CB	9:A:1123:HOH:O	2.59	0.44
1:A:595:ARG:HG2	1:A:597:ASP:O	2.17	0.44
1:A:528:GLY:O	1:A:668:LYS:HE3	2.18	0.44
1:A:431:PHE:O	1:A:435:VAL:HG23	2.18	0.44
1:A:399:PHE:O	1:A:403:VAL:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:749:ARG:HG3	1:A:787:TRP:CZ3	2.53	0.43
1:A:811:THR:OG1	9:A:1104:HOH:O	2.21	0.43
1:A:309:TYR:CE1	1:A:311:THR:HG23	2.53	0.43
1:A:397:GLU:H	1:A:397:GLU:CD	2.21	0.43
1:A:299:PRO:HD2	1:A:300:TYR:CE2	2.53	0.43
1:A:384:GLU:HG2	9:A:1107:HOH:O	2.18	0.43
1:A:807:GLU:OE2	9:A:1102:HOH:O	2.21	0.43
1:A:790:THR:CG2	9:A:1383:HOH:O	2.59	0.43
1:A:809:MET:CE	1:A:809:MET:HA	2.49	0.42
1:A:397:GLU:CD	1:A:397:GLU:N	2.72	0.42
1:A:512[A]:LEU:HD21	1:A:711:HIS:NE2	2.35	0.42
1:A:455:MET:SD	1:A:476:TYR:HD2	2.42	0.42
1:A:597:ASP:O	1:A:598:GLN:CB	2.65	0.41
1:A:507:VAL:O	1:A:510:GLU:HG2	2.20	0.41
1:A:400:THR:O	1:A:403:VAL:HG22	2.19	0.41
1:A:809:MET:HA	1:A:809:MET:HE2	2.02	0.41
1:A:611:THR:O	1:A:615:MET:HG3	2.20	0.41
4:A:1004:DMS:H11	9:A:1305:HOH:O	2.16	0.41
1:A:527:GLY:HA2	1:A:670:LEU:O	2.21	0.41
1:A:580:VAL:HG21	1:A:593:ILE:CD1	2.49	0.40
1:A:883:MET:N	1:A:884:PRO:CD	2.84	0.40
1:A:321:VAL:HG11	1:A:326:ARG:CZ	2.52	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:1248:HOH:O	9:A:1342:HOH:O[2_545]	1.84	0.36
9:A:1131:HOH:O	9:A:1131:HOH:O[2_445]	1.98	0.22

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	552/637 (87%)	534 (97%)	17 (3%)	1 (0%)	44 31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	598	GLN

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	501/554 (90%)	496 (99%)	5 (1%)	73 68

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

Mol	Chain	Res	Type
1	A	357	GLU
1	A	375	LYS
1	A	426	VAL
1	A	438	GLU
1	A	634	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	298	HIS
1	A	603	GLN

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 11 ligands modelled in this entry, 3 are monoatomic - leaving 8 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	$\#\|Z\| > 2$
3	MES	A	1003[A]	-	12,12,12	0.70	0	15,16,16	0.30	0
5	PO4	A	1007	-	4,4,4	0.71	0	6,6,6	0.46	0
6	PEG	A	1008	-	6,6,6	0.14	0	5,5,5	0.08	0
5	PO4	A	1006	-	4,4,4	4.05	3 (75%)	6,6,6	0.92	0
4	DMS	A	1005	-	3,3,3	0.22	0	3,3,3	0.07	0
3	MES	A	1003[B]	-	12,12,12	0.70	0	15,16,16	0.29	0
8	JGP	A	1010	-	20,20,20	0.30	0	27,27,27	0.51	0
4	DMS	A	1004	-	3,3,3	0.38	0	3,3,3	0.58	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]	-	-	0/6/14/14	0/1/1/1
6	PEG	A	1008	-	-	2/4/4/4	-
3	MES	A	1003[A]	-	-	0/6/14/14	0/1/1/1
8	JGP	A	1010	-	-	0/8/23/23	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1006	PO4	P-O1	7.07	1.67	1.50
5	A	1006	PO4	P-O2	2.71	1.62	1.54
5	A	1006	PO4	P-O4	-2.42	1.47	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1008	PEG	O2-C3-C4-O4
6	A	1008	PEG	C4-C3-O2-C2

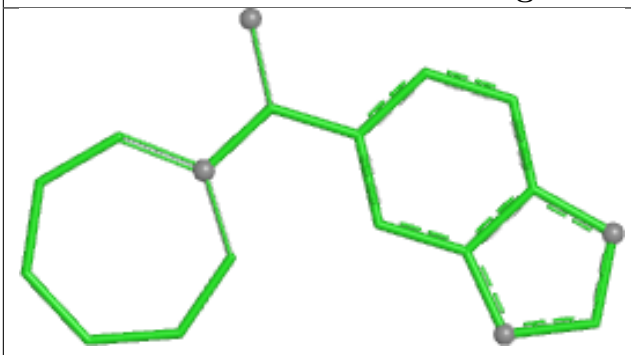
There are no ring outliers.

4 monomers are involved in 7 short contacts:

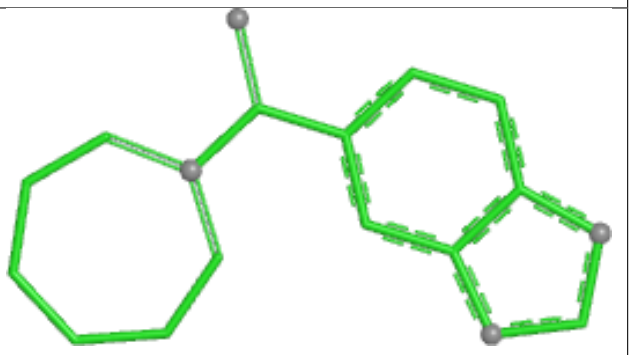
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003[A]	MES	1	0
5	A	1006	PO4	3	0
3	A	1003[B]	MES	1	0
4	A	1004	DMS	2	0

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.

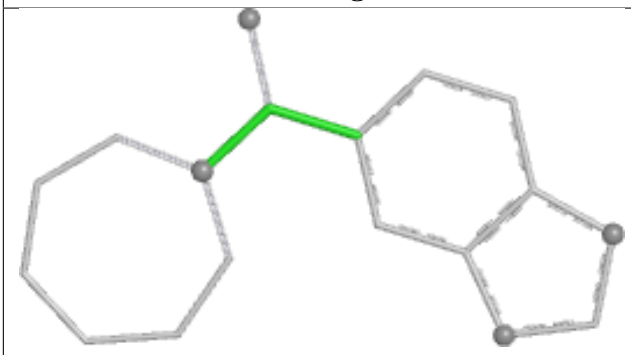
Ligand JGP A 1010



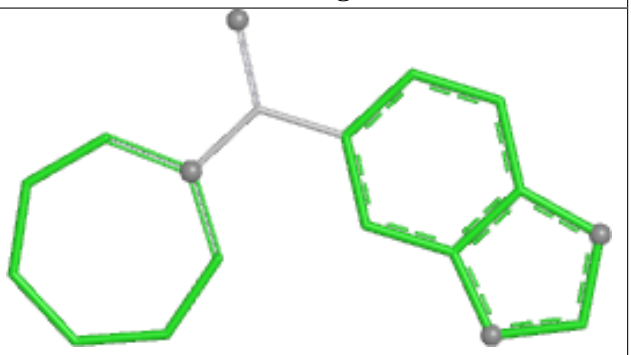
Bond lengths



Bond angles



Torsions



Rings

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	560/637 (87%)	4.41	369 (65%)	0	0	5, 35, 63, 111	263 (46%)

All (369) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	TRP	12.9
1	A	403	VAL	12.7
1	A	290	THR	12.7
1	A	512[A]	LEU	12.7
1	A	600	GLY	12.6
1	A	300	TYR	11.9
1	A	476	TYR	11.8
1	A	589	VAL	11.8
1	A	478	TRP	11.8
1	A	542	ILE	11.7
1	A	299	PRO	11.7
1	A	293	HIS	11.6
1	A	763[A]	SER	11.5
1	A	294	TYR	11.2
1	A	431	PHE	11.1
1	A	309	TYR	11.0
1	A	641	ILE	10.8
1	A	291	SER	10.8
1	A	441	LEU	10.7
1	A	764	LEU	10.3
1	A	785[A]	SER	10.2
1	A	628	VAL	10.0
1	A	744	ALA	9.9
1	A	426	VAL	9.9
1	A	637	VAL	9.9
1	A	274	LEU	9.8
1	A	281	ILE	9.8

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Mol	Chain	Res	Type	RSRZ
1	A	363	THR	9.7
1	A	838	TYR	9.6
1	A	425	ALA	9.6
1	A	791	SER	9.5
1	A	305	TYR	9.4
1	A	480	GLY	9.3
1	A	578	VAL	9.3
1	A	367	LYS	9.2
1	A	583	PRO	9.2
1	A	479	LEU	9.1
1	A	359	VAL	9.1
1	A	277	ILE	9.1
1	A	298	HIS	9.1
1	A	435	VAL	9.0
1	A	575	ASN	9.0
1	A	276	ILE	9.0
1	A	366	PRO	8.9
1	A	788	VAL	8.9
1	A	839	LEU	8.9
1	A	443	LEU	8.8
1	A	629	PHE	8.8
1	A	636	THR	8.8
1	A	519	LEU	8.8
1	A	854	THR	8.8
1	A	789	PRO	8.7
1	A	719[A]	LYS	8.7
1	A	311	THR	8.7
1	A	453	ASN	8.7
1	A	518	ILE	8.7
1	A	474	ILE	8.7
1	A	423	ARG	8.6
1	A	325	VAL	8.6
1	A	742	GLN	8.6
1	A	475	TRP	8.6
1	A	635	LEU	8.5
1	A	551	GLU	8.5
1	A	810	LEU	8.4
1	A	541	ARG	8.4
1	A	530	MET	8.4
1	A	606	THR	8.3
1	A	790	THR	8.3
1	A	486	PHE	8.3

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Mol	Chain	Res	Type	RSRZ
1	A	419	TRP	8.2
1	A	809	MET	8.2
1	A	741[A]	SER	8.2
1	A	803	TRP	8.1
1	A	627	GLY	8.1
1	A	565	ALA	8.1
1	A	604	VAL	8.1
1	A	432	TRP	8.1
1	A	364	GLN	8.0
1	A	279	LYS	8.0
1	A	490	GLY	8.0
1	A	477	MET	8.0
1	A	571	LEU	8.0
1	A	584	THR	8.0
1	A	850	LEU	8.0
1	A	544	LEU	7.9
1	A	885	SER	7.9
1	A	580	VAL	7.9
1	A	601	SER	7.9
1	A	301	LYS	7.9
1	A	607	TYR	7.9
1	A	687	VAL	7.9
1	A	321	VAL	7.8
1	A	334	ILE	7.8
1	A	511	GLY	7.8
1	A	581	GLN	7.8
1	A	800	THR	7.8
1	A	552	MET	7.8
1	A	484	LEU	7.7
1	A	455	MET	7.7
1	A	808	ASP	7.7
1	A	596	ARG	7.7
1	A	864[A]	GLN	7.6
1	A	332	TRP	7.6
1	A	889	PHE	7.6
1	A	296	GLN	7.6
1	A	327	LEU	7.6
1	A	297	ASP	7.5
1	A	525	LYS	7.5
1	A	582	ARG	7.5
1	A	488	ALA	7.5
1	A	401	ARG	7.5

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Mol	Chain	Res	Type	RSRZ
1	A	599	ARG	7.5
1	A	328	LEU	7.5
1	A	588	THR	7.5
1	A	543	THR	7.4
1	A	745	GLY	7.4
1	A	579	ARG	7.4
1	A	884	PRO	7.4
1	A	452	TYR	7.4
1	A	853	LEU	7.4
1	A	342	ALA	7.4
1	A	852	GLY	7.3
1	A	312	LYS	7.3
1	A	851	ILE	7.3
1	A	481	ALA	7.2
1	A	372	LYS	7.2
1	A	323	GLY	7.2
1	A	406	ASN	7.2
1	A	338	VAL	7.2
1	A	597	ASP	7.2
1	A	405	SER	7.2
1	A	358	LYS	7.2
1	A	434	LEU	7.2
1	A	802	GLU	7.1
1	A	306	HIS	7.0
1	A	598	GLN	7.0
1	A	285	LYS	7.0
1	A	572	THR	7.0
1	A	422	ALA	7.0
1	A	567	ALA	7.0
1	A	645	ASN	7.0
1	A	564	LEU	7.0
1	A	649	ARG	6.9
1	A	638	THR	6.9
1	A	439	ARG	6.9
1	A	746	TRP	6.9
1	A	524	LYS	6.9
1	A	335	ILE	6.9
1	A	449	THR	6.8
1	A	811	THR	6.8
1	A	368	GLU	6.8
1	A	886	MET	6.8
1	A	626	GLU	6.7

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Mol	Chain	Res	Type	RSRZ
1	A	324	VAL	6.7
1	A	319	SER	6.6
1	A	343	MET	6.6
1	A	360	ASP	6.6
1	A	805	THR	6.6
1	A	806	THR	6.6
1	A	743	GLY	6.6
1	A	303	TRP	6.6
1	A	308	SER	6.6
1	A	424	GLU	6.6
1	A	632	ILE	6.5
1	A	329	THR	6.5
1	A	344	THR	6.5
1	A	446	LYS	6.5
1	A	737	ARG	6.4
1	A	887	LYS	6.4
1	A	331	PRO	6.4
1	A	801	HIS	6.4
1	A	322	ASN	6.3
1	A	562	LYS	6.3
1	A	320	MET	6.3
1	A	521	ASP	6.3
1	A	845	GLN	6.2
1	A	361	THR	6.2
1	A	556	HIS	6.2
1	A	548	LYS	6.2
1	A	555	ASN	6.2
1	A	280	ARG	6.2
1	A	396	ARG	6.2
1	A	830	VAL	6.2
1	A	437	LYS	6.2
1	A	339	THR	6.2
1	A	602	GLY	6.1
1	A	483	PHE	6.1
1	A	428	ASP	6.1
1	A	526	GLU	6.1
1	A	545	GLU	6.1
1	A	454	MET	6.1
1	A	427	GLU	6.1
1	A	275	ASP	6.1
1	A	393	MET	6.1
1	A	513	HIS	6.0

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Mol	Chain	Res	Type	RSRZ
1	A	284	ILE	6.0
1	A	450	CYS	6.0
1	A	333	ASP	6.0
1	A	421	SER	6.0
1	A	295	ASP	5.9
1	A	451	VAL	5.9
1	A	840	GLY	5.9
1	A	330	LYS	5.9
1	A	326	ARG	5.9
1	A	440	ASN	5.9
1	A	890	ARG	5.9
1	A	336	PRO	5.9
1	A	634	HIS	5.8
1	A	283	LYS	5.8
1	A	289	GLU	5.8
1	A	841	LYS	5.8
1	A	705	GLN	5.8
1	A	304	ALA	5.7
1	A	341	MET	5.7
1	A	482	ARG	5.7
1	A	509	GLY	5.7
1	A	694	TRP	5.7
1	A	842	ARG	5.7
1	A	307	GLY	5.7
1	A	442	HIS	5.7
1	A	561	HIS	5.6
1	A	760	GLN	5.6
1	A	404	ARG	5.6
1	A	357	GLU	5.6
1	A	508	GLU	5.6
1	A	883	MET	5.6
1	A	595	ARG	5.6
1	A	485	GLU	5.6
1	A	286	GLN	5.6
1	A	537	GLY	5.6
1	A	448	GLU	5.5
1	A	430	GLY	5.5
1	A	445	GLY	5.5
1	A	630	LYS	5.4
1	A	523	SER	5.4
1	A	282	GLU	5.4
1	A	310	GLU	5.4

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Mol	Chain	Res	Type	RSRZ
1	A	689	LYS	5.4
1	A	577	VAL	5.4
1	A	540	THR	5.4
1	A	337	MET	5.3
1	A	880	THR	5.3
1	A	514	LYS	5.3
1	A	891	ARG	5.3
1	A	288	HIS	5.3
1	A	546	ASP	5.3
1	A	365	GLU	5.2
1	A	494	GLU	5.2
1	A	383	LYS	5.2
1	A	397	GLU	5.2
1	A	278	GLY	5.2
1	A	438	GLU	5.2
1	A	568	ILE	5.2
1	A	843	GLU	5.1
1	A	825	GLU	5.1
1	A	340	GLN	5.1
1	A	302	THR	5.1
1	A	576	LYS	5.1
1	A	362	ARG	5.0
1	A	429	SER	5.0
1	A	563	LYS	5.0
1	A	882	TYR	4.9
1	A	559	GLY	4.9
1	A	888	ARG	4.9
1	A	804	MET	4.8
1	A	273	ASN	4.8
1	A	287	GLU	4.8
1	A	433	GLU	4.8
1	A	881	ASP	4.7
1	A	487	GLU	4.7
1	A	566	GLU	4.7
1	A	590	MET	4.6
1	A	591	ASP	4.6
1	A	510	GLU	4.6
1	A	693	GLN	4.6
1	A	593	ILE	4.5
1	A	501	GLU	4.5
1	A	648	VAL	4.4
1	A	820	GLU	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	436	ASP	4.4
1	A	807	GLU	4.4
1	A	876	ASN	4.3
1	A	647	LEU	4.3
1	A	400	THR	4.3
1	A	691	ILE	4.2
1	A	784	PRO	4.2
1	A	369	GLY	4.2
1	A	633	GLN	4.2
1	A	818	ILE	4.1
1	A	750	GLU	4.1
1	A	605	VAL	4.1
1	A	394	CYS	4.1
1	A	558	GLU	4.1
1	A	644	LYS	3.9
1	A	815	ARG	3.8
1	A	676	SER	3.8
1	A	819	GLN	3.7
1	A	640	GLU	3.7
1	A	399	PHE	3.7
1	A	695	GLU	3.6
1	A	677	ALA	3.6
1	A	547	LEU	3.6
1	A	603	GLN	3.6
1	A	373	LEU	3.5
1	A	670	LEU	3.5
1	A	493	ASN	3.4
1	A	529	ALA	3.4
1	A	534	ASP	3.4
1	A	420	LYS	3.3
1	A	402	LYS	3.3
1	A	376	ILE	3.3
1	A	370	THR	3.2
1	A	444	GLU	3.2
1	A	701	ASN	3.2
1	A	503	SER	3.2
1	A	861	LYS	3.1
1	A	821	ASN	3.1
1	A	377	THR	3.1
1	A	835	GLU	3.1
1	A	652	ARG	3.1
1	A	592	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	536	ALA	2.9
1	A	447	CYS	2.9
1	A	716	LEU	2.8
1	A	824	MET	2.8
1	A	560	GLU	2.8
1	A	495	ASP	2.8
1	A	833	TRP	2.8
1	A	786	HIS	2.8
1	A	570	LYS	2.8
1	A	569	PHE	2.7
1	A	680	ALA	2.7
1	A	754	LEU	2.7
1	A	646	TRP	2.6
1	A	642	ALA	2.6
1	A	787	TRP	2.6
1	A	783	VAL	2.6
1	A	816	VAL	2.6
1	A	507	VAL	2.6
1	A	496	HIS	2.5
1	A	491	PHE	2.5
1	A	573	TYR	2.5
1	A	692	GLN	2.5
1	A	868	ASN	2.5
1	A	703	TRP	2.5
1	A	672	ASP	2.5
1	A	375	LYS	2.4
1	A	395	THR	2.4
1	A	539	ASP	2.3
1	A	631	SER	2.3
1	A	535	THR	2.3
1	A	574	GLN	2.3
1	A	502	ASN	2.3
1	A	862	ASN	2.3
1	A	619	LEU	2.3
1	A	651	GLY	2.3
1	A	758	TYR	2.2
1	A	553	VAL	2.2
1	A	777	ASN	2.2
1	A	857	ALA	2.2
1	A	751	THR	2.1
1	A	643	VAL	2.1
1	A	834	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	832	SER	2.1
1	A	625	GLY	2.1
1	A	594	SER	2.1
1	A	371	LYS	2.1
1	A	650	VAL	2.0
1	A	382	TRP	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)

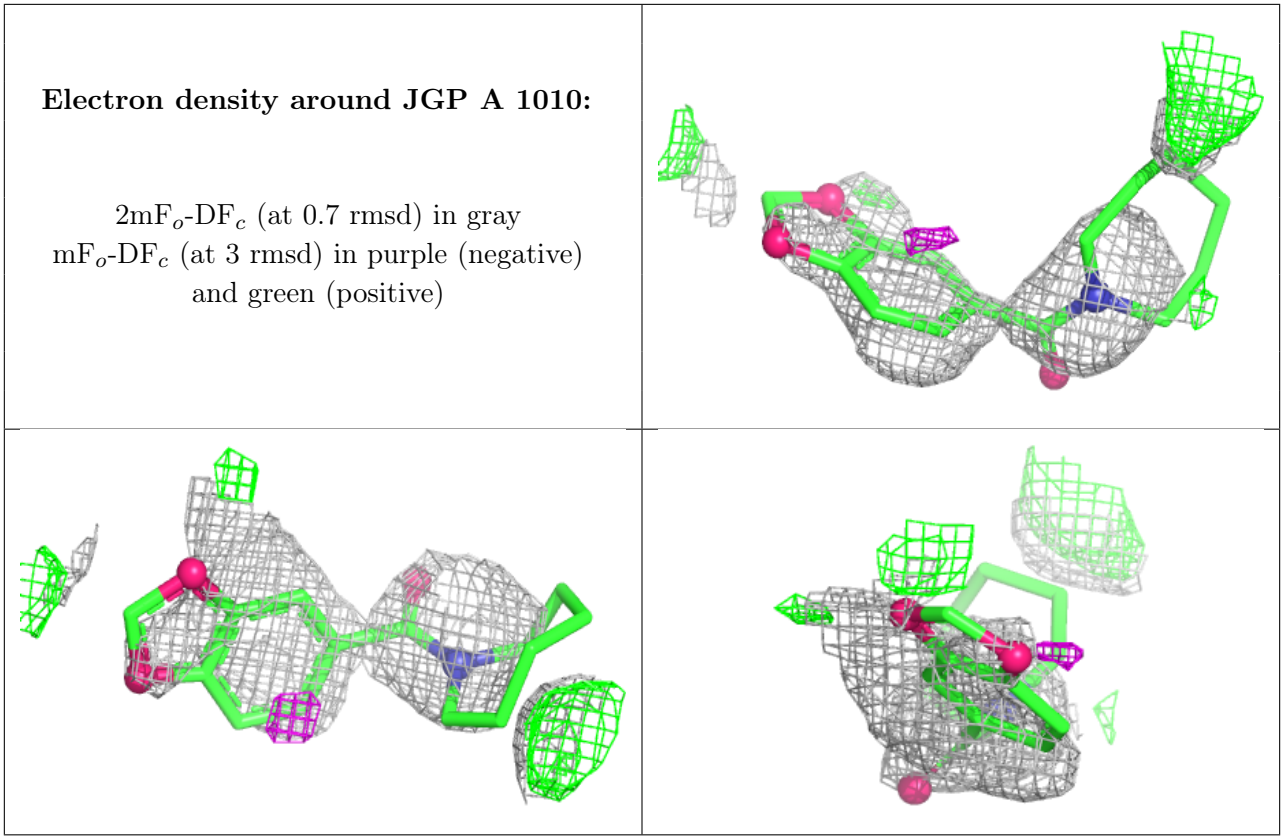
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
8	JGP	A	1010	18/18	0.61	0.37	57,64,67,69	18
5	PO4	A	1007	5/5	0.62	0.51	175,179,185,185	5
6	PEG	A	1008	7/7	0.73	0.30	54,59,61,61	7
5	PO4	A	1006	5/5	0.84	0.14	37,41,48,68	0
4	DMS	A	1005	4/4	0.85	0.44	93,95,98,99	4
3	MES	A	1003[B]	12/12	0.86	0.41	22,27,38,39	12
3	MES	A	1003[A]	12/12	0.86	0.41	744,999,999,999	12
4	DMS	A	1004	4/4	0.90	0.15	51,57,58,60	0
7	CL	A	1009	1/1	0.97	0.08	44,44,44,44	0
2	ZN	A	1002	1/1	0.99	0.06	58,58,58,58	0
2	ZN	A	1001	1/1	1.00	0.03	28,28,28,28	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 JGP 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.