Full wwPDB X-ray Structure Validation Report ⓘ

Mar 27, 2025 – 11:12 AM EDT

PDB ID	:	7I2J
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 Z1269139261 (DNV2_NS5A-x0479)
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	:	1.98 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

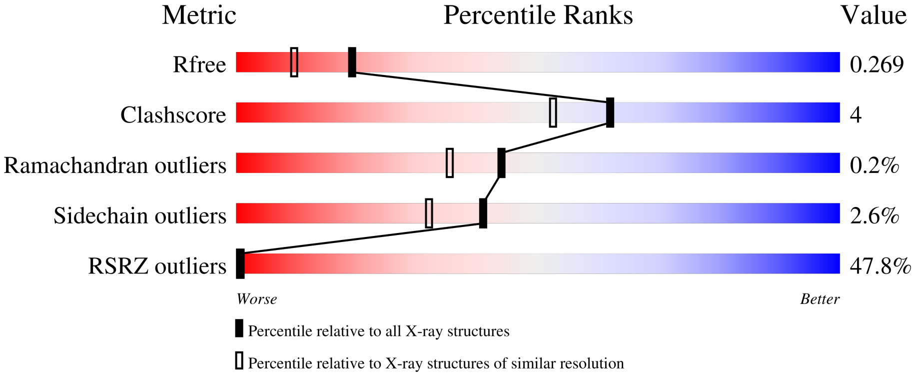
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.006 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance ⓘ

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

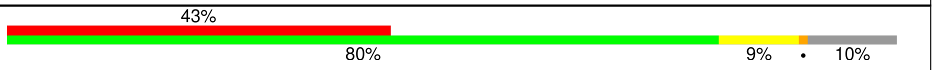
The reported resolution of this entry is 1.98 Å.

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	1356 (1.98-1.98)
Clashscore	180529	1437 (1.98-1.98)
Ramachandran outliers	177936	1426 (1.98-1.98)
Sidechain outliers	177891	1426 (1.98-1.98)
RSRZ outliers	164620	1356 (1.98-1.98)

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	

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

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PO4	A	1007	-	-	X	-

2 Entry composition (i)

There are 9 unique types of molecules in this entry. The entry contains 5194 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	571	4731	2979	848	870	34	0	8	0

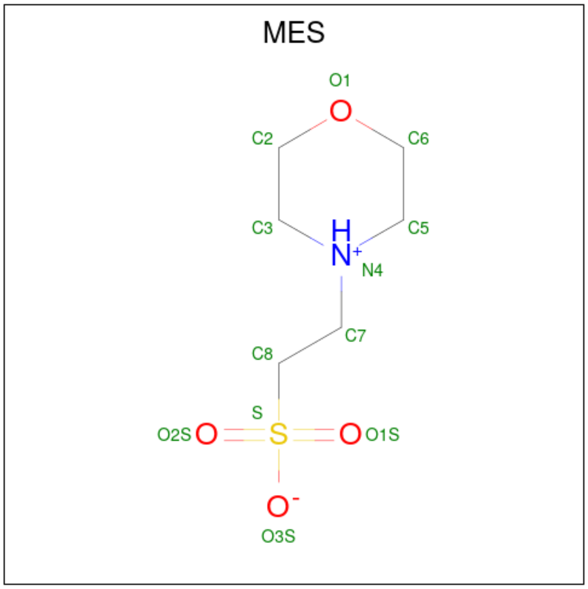
There are 2 discrepancies between the modelled and reference sequences:

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).

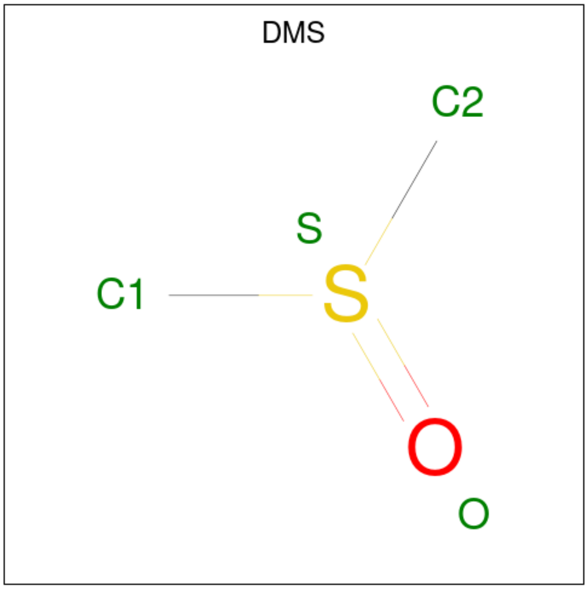
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Zn		
2	A	2	2	2	0	0

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



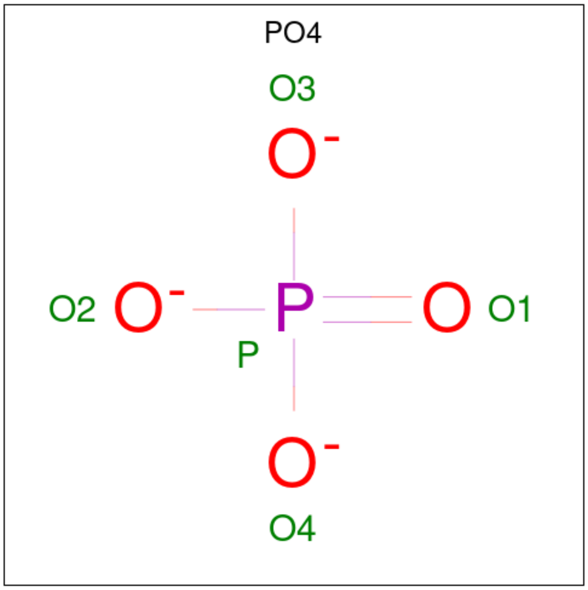
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
3	A	1	24	12	2	8	2	0	1

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



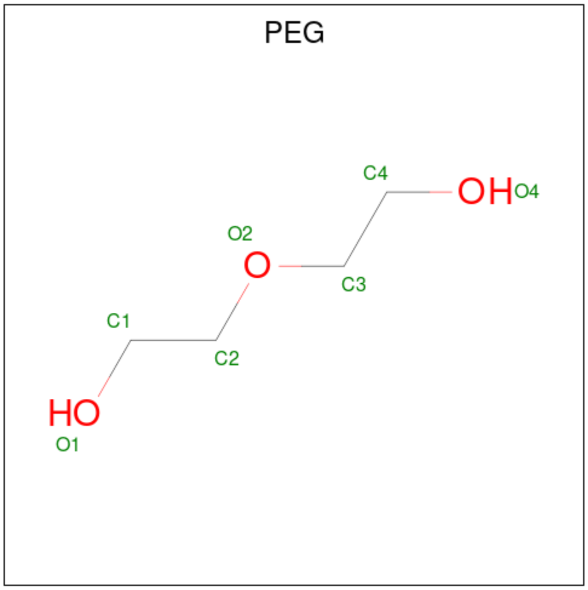
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	O	S		
4	A	1	4	2	1	1	0	0
4	A	1	4	2	1	1	0	0
4	A	1	4	2	1	1	0	0

- 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

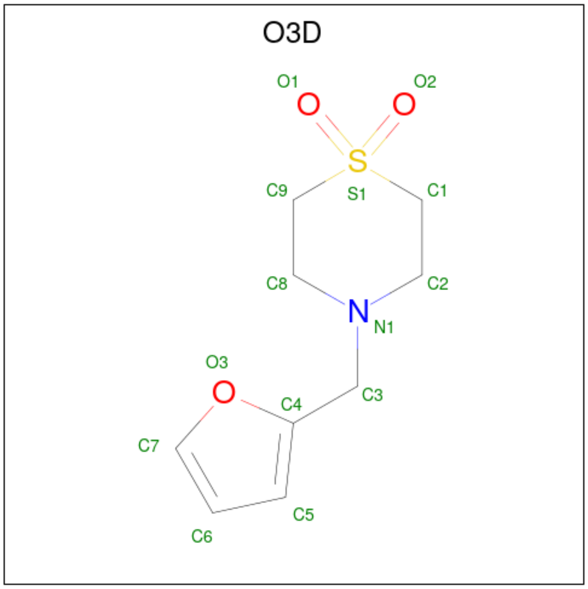
- Molecule 6 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 7 is 4-[(furan-2-yl)methyl]-1lambda 6 ,4-thiazinane-1,1-dione (three-letter code:

O3D) (formula: $C_9H_{13}NO_3S$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O S 14 9 1 3 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

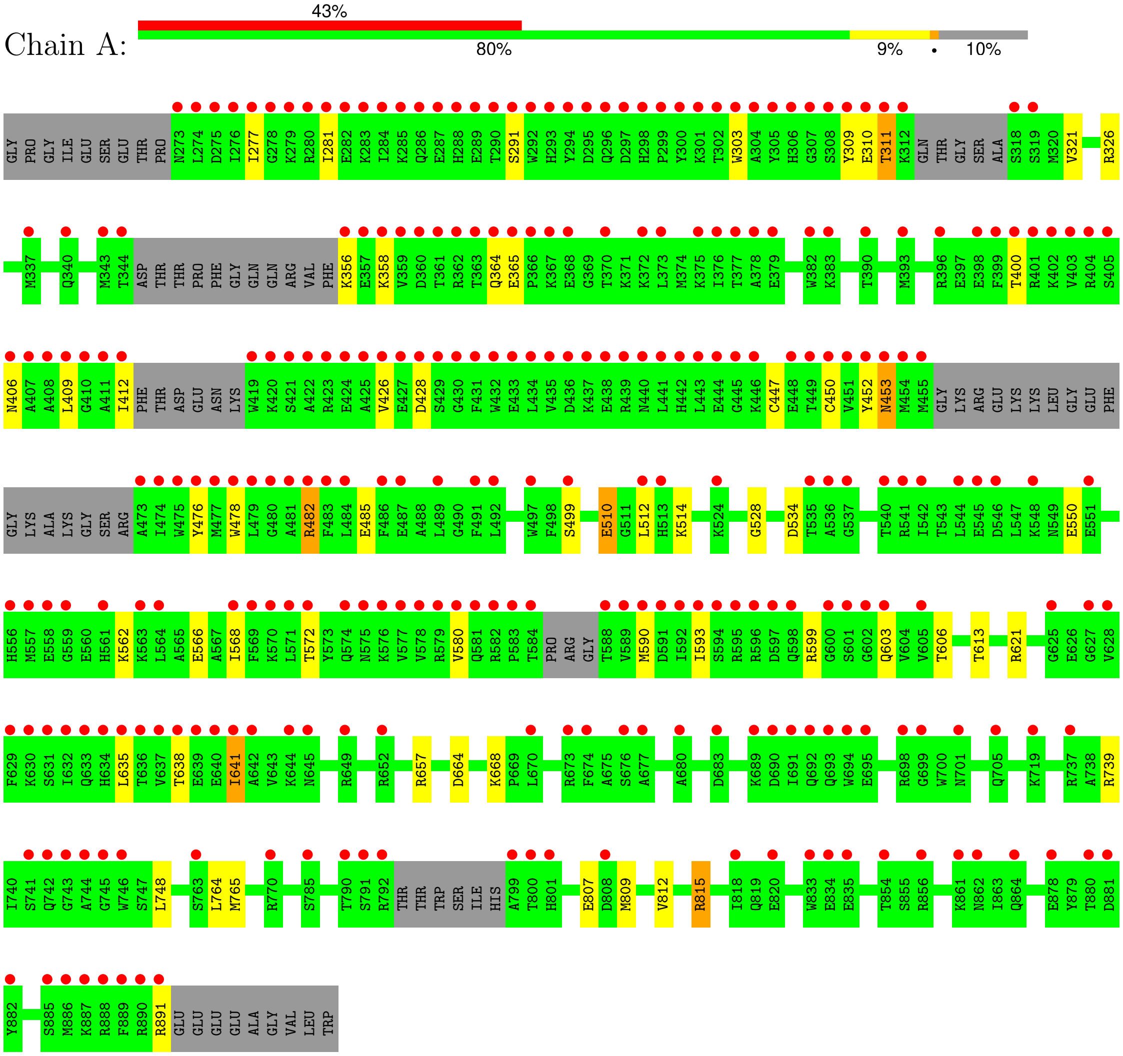
- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	393	Total O 393 393	0	0

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	82.42Å 116.07Å 148.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	72.00 – 1.98 72.00 – 1.98	Depositor EDS
% Data completeness (in resolution range)	96.7 (72.00-1.98) 96.8 (72.00-1.98)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.88 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.183 , 0.227 0.244 , 0.269	Depositor DCC
R_{free} test set	2546 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	32.7	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 171.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.88	EDS
Total number of atoms	5194	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.77% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: ZN, O3D, MES, DMS, PEG, CL, PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#|Z| > 5$	RMSZ	$\#|Z| > 5$
1	A	0.78	1/4836 (0.0%)	0.86	5/6520 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	510	GLU	CD-OE2	7.75	1.34	1.25

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	815	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	A	621	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	A	657	ARG	CG-CD-NE	-6.24	98.69	111.80
1	A	621	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	A	739	ARG	NE-CZ-NH1	5.84	123.22	120.30

There are no chirality outliers.

There are no planarity outliers.

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	4731	0	4631	35	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	1	0
4	A	12	0	18	3	0
5	A	10	0	0	4	0
6	A	7	0	10	0	0
7	A	14	0	0	0	0
8	A	1	0	0	0	0
9	A	393	0	0	5	3
All	All	5194	0	4685	38	3

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 4.

All (38) 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:534:ASP:OD1	5:A:1007:PO4:O4	1.79	1.00
1:A:664:ASP:OD1	5:A:1007:PO4:O4	1.98	0.81
4:A:1004:DMS:C1	9:A:1264:HOH:O	2.45	0.64
1:A:809:MET:HA	1:A:809:MET:HE2	1.79	0.64
1:A:664:ASP:OD1	5:A:1007:PO4:P	2.57	0.62
1:A:599:ARG:HG2	1:A:606:THR:HG23	1.90	0.53
1:A:534:ASP:OD1	5:A:1007:PO4:P	2.67	0.53
1:A:453:ASN:HB2	1:A:476:TYR:HB2	1.90	0.53
1:A:364:GLN:HG2	1:A:365:GLU:N	2.23	0.52
1:A:311:THR:HG21	1:A:590:MET:HB2	1.92	0.52
4:A:1004:DMS:H11	9:A:1264:HOH:O	2.06	0.51
1:A:562:LYS:O	1:A:566:GLU:HG3	2.11	0.51
1:A:580:VAL:HG21	1:A:593:ILE:HD11	1.94	0.50
1:A:291:SER:HB3	1:A:310:GLU:H	1.77	0.50
1:A:815:ARG:HD2	9:A:1224:HOH:O	2.13	0.48
1:A:568:ILE:O	1:A:572:THR:OG1	2.22	0.47
1:A:638:THR:HA	1:A:641:ILE:HG22	1.95	0.47
4:A:1004:DMS:H13	9:A:1264:HOH:O	2.11	0.47
1:A:809:MET:HE1	1:A:812:VAL:HG21	1.95	0.46
1:A:748:LEU:HD13	3:A:1003[B]:MES:H61	1.98	0.45
1:A:447:CYS:SG	1:A:450:CYS:HB2	2.56	0.45
1:A:482:ARG:NH1	1:A:485:GLU:OE2	2.31	0.45
1:A:428:ASP:OD1	1:A:428:ASP:C	2.55	0.45
1:A:400:THR:HG23	1:A:426:VAL:CG1	2.47	0.44
1:A:303:TRP:CE3	1:A:593:ILE:HD12	2.52	0.44
1:A:452:TYR:C	1:A:453:ASN:HD22	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:321:VAL:HG11	1:A:326:ARG:CZ	2.48	0.43
1:A:807:GLU:HG3	9:A:1304:HOH:O	2.17	0.43
1:A:510:GLU:O	1:A:514:LYS:HG3	2.18	0.43
1:A:309:TYR:CE1	1:A:311:THR:HG23	2.54	0.43
1:A:528:GLY:O	1:A:668:LYS:HE3	2.20	0.42
1:A:453:ASN:HD22	1:A:453:ASN:N	2.18	0.42
1:A:512[B]:LEU:HD23	1:A:512[B]:LEU:HA	1.92	0.42
1:A:277:ILE:HD12	1:A:281:ILE:HD11	2.02	0.41
1:A:400:THR:HG23	1:A:426:VAL:HG11	2.02	0.41
1:A:550:GLU:OE2	1:A:613:THR:OG1	2.33	0.41
1:A:764:LEU:HG	1:A:765:MET:HE3	2.02	0.41
1:A:291:SER:CB	1:A:310:GLU:H	2.33	0.41

All (3) 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:1147:HOH:O	9:A:1147:HOH:O[2_445]	1.44	0.76
9:A:1331:HOH:O	9:A:1331:HOH:O[4_545]	2.10	0.10
9:A:1349:HOH:O	9:A:1414:HOH:O[2_545]	2.12	0.08

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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	565/637 (89%)	539 (95%)	25 (4%)	1 (0%)	44 35

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	406	ASN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	508/554 (92%)	495 (97%)	13 (3%)	41 32

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	311	THR
1	A	356	LYS
1	A	358	LYS
1	A	409	LEU
1	A	412	ILE
1	A	453	ASN
1	A	478	TRP
1	A	482	ARG
1	A	499	SER
1	A	603	GLN
1	A	635	LEU
1	A	641	ILE
1	A	891	ARG

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	556	HIS
1	A	862	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 12 ligands modelled in this entry, 3 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	MES	A	1003[A]	-	12,12,12	0.73	0	15,16,16	0.34	0
4	DMS	A	1005	-	3,3,3	0.29	0	3,3,3	0.06	0
6	PEG	A	1009	-	6,6,6	0.16	0	5,5,5	0.06	0
3	MES	A	1003[B]	-	12,12,12	0.84	0	15,16,16	0.65	0
4	DMS	A	1004	-	3,3,3	0.43	0	3,3,3	0.59	0
4	DMS	A	1006	-	3,3,3	0.15	0	3,3,3	0.62	0
7	O3D	A	1010	-	12,15,15	1.38	2 (16%)	15,21,21	1.07	1 (6%)
5	PO4	A	1008	-	4,4,4	1.49	1 (25%)	6,6,6	0.36	0
5	PO4	A	1007	-	4,4,4	3.69	2 (50%)	6,6,6	0.60	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]	-	-	2/6/14/14	0/1/1/1
7	O3D	A	1010	-	-	1/3/16/16	0/2/2/2
3	MES	A	1003[A]	-	-	3/6/14/14	0/1/1/1
6	PEG	A	1009	-	-	2/4/4/4	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1007	PO4	P-O1	6.73	1.66	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1010	O3D	C5-C4	-4.07	1.34	1.39
5	A	1008	PO4	P-O1	2.96	1.57	1.50
5	A	1007	PO4	P-O2	2.39	1.61	1.54
7	A	1010	O3D	C3-C4	-2.23	1.49	1.51

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	A	1010	O3D	C3-C4-C5	2.80	133.56	129.06

There are no chirality outliers.

All (8) 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-O3S
3	A	1003[B]	MES	C8-C7-N4-C3
7	A	1010	O3D	C4-C3-N1-C2
6	A	1009	PEG	O2-C3-C4-O4
3	A	1003[B]	MES	C8-C7-N4-C5
3	A	1003[A]	MES	C7-C8-S-O2S
6	A	1009	PEG	C4-C3-O2-C2

There are no ring outliers.

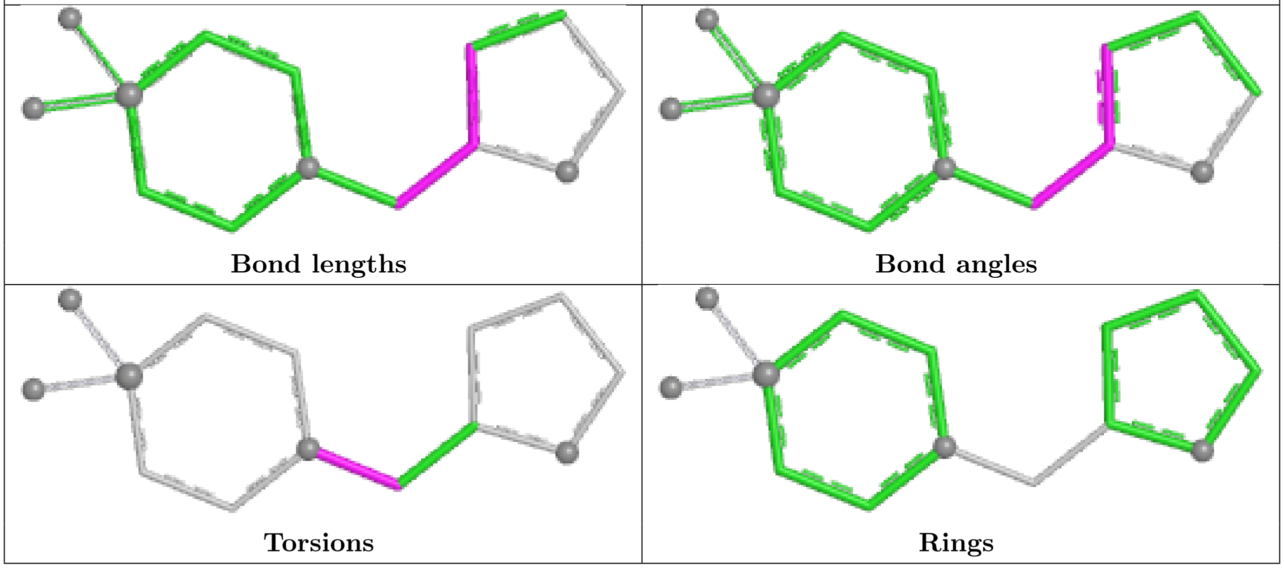
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1003[B]	MES	1	0
4	A	1004	DMS	3	0
5	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 O3D 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, 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	571/637 (89%)	3.52	273 (47%)	0	1	6, 33, 69, 123	157 (27%)

All (273) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	292	TRP	16.6
1	A	600	GLY	16.3
1	A	741[A]	SER	14.7
1	A	366	PRO	14.0
1	A	294	TYR	13.9
1	A	635	LEU	13.7
1	A	305	TYR	13.4
1	A	637	VAL	13.2
1	A	304	ALA	13.1
1	A	281	ILE	13.1
1	A	303	TRP	13.0
1	A	403	VAL	12.9
1	A	641	ILE	12.9
1	A	632	ILE	12.7
1	A	409	LEU	12.7
1	A	801[A]	HIS	12.7
1	A	431	PHE	12.5
1	A	407	ALA	12.5
1	A	425	ALA	12.4
1	A	638	THR	12.4
1	A	359	VAL	12.0
1	A	426	VAL	12.0
1	A	478	TRP	12.0
1	A	435	VAL	11.9
1	A	449	THR	11.7
1	A	691	ILE	11.6
1	A	535	THR	11.5

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Mol	Chain	Res	Type	RSRZ
1	A	367	LYS	11.5
1	A	592	ILE	11.5
1	A	284	ILE	11.4
1	A	577	VAL	11.4
1	A	422	ALA	11.3
1	A	636	THR	11.3
1	A	373	LEU	11.1
1	A	300	TYR	11.1
1	A	580	VAL	11.0
1	A	542	ILE	11.0
1	A	411	ALA	11.0
1	A	601	SER	10.8
1	A	439	ARG	10.8
1	A	412	ILE	10.7
1	A	476	TYR	10.7
1	A	482	ARG	10.5
1	A	450	CYS	10.4
1	A	578	VAL	10.4
1	A	640	GLU	10.4
1	A	593	ILE	10.3
1	A	410	GLY	10.2
1	A	290	THR	10.2
1	A	274	LEU	10.2
1	A	309	TYR	10.1
1	A	307	GLY	10.1
1	A	363	THR	10.0
1	A	551[A]	GLU	9.9
1	A	639	GLU	9.8
1	A	421	SER	9.8
1	A	475	TRP	9.8
1	A	536	ALA	9.8
1	A	299	PRO	9.8
1	A	276	ILE	9.8
1	A	477	MET	9.7
1	A	401	ARG	9.7
1	A	649	ARG	9.7
1	A	306	HIS	9.7
1	A	631	SER	9.7
1	A	644	LYS	9.6
1	A	293	HIS	9.6
1	A	512[A]	LEU	9.5
1	A	645	ASN	9.4

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Mol	Chain	Res	Type	RSRZ
1	A	402	LYS	9.4
1	A	583	PRO	9.3
1	A	408	ALA	9.3
1	A	308	SER	9.2
1	A	474	ILE	9.2
1	A	375	LYS	9.1
1	A	541	ARG	9.0
1	A	575	ASN	9.0
1	A	280	ARG	8.9
1	A	419	TRP	8.8
1	A	372	LYS	8.8
1	A	365	GLU	8.7
1	A	438	GLU	8.7
1	A	311	THR	8.6
1	A	719[A]	LYS	8.6
1	A	473	ALA	8.5
1	A	695	GLU	8.5
1	A	548	LYS	8.4
1	A	451	VAL	8.4
1	A	453	ASN	8.3
1	A	406	ASN	8.3
1	A	452	TYR	8.3
1	A	291	SER	8.2
1	A	279	LYS	8.0
1	A	356	LYS	8.0
1	A	763[A]	SER	7.9
1	A	405	SER	7.9
1	A	283	LYS	7.9
1	A	591	ASP	7.8
1	A	692	GLN	7.7
1	A	273	ASN	7.7
1	A	589	VAL	7.7
1	A	582	ARG	7.7
1	A	745	GLY	7.6
1	A	277	ILE	7.6
1	A	576	LYS	7.6
1	A	705	GLN	7.6
1	A	634	HIS	7.5
1	A	423	ARG	7.5
1	A	441	LEU	7.5
1	A	448	GLU	7.5
1	A	379	GLU	7.4

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Mol	Chain	Res	Type	RSRZ
1	A	744	ALA	7.4
1	A	437	LYS	7.4
1	A	295	ASP	7.4
1	A	302	THR	7.4
1	A	581	GLN	7.4
1	A	455	MET	7.4
1	A	785[A]	SER	7.3
1	A	424	GLU	7.2
1	A	689	LYS	7.2
1	A	698	ARG	7.2
1	A	834	GLU	7.2
1	A	358	LYS	7.2
1	A	598	GLN	7.1
1	A	298	HIS	7.1
1	A	499	SER	7.1
1	A	404	ARG	7.0
1	A	799	ALA	6.9
1	A	584	THR	6.9
1	A	427	GLU	6.9
1	A	454	MET	6.9
1	A	301	LYS	6.9
1	A	513	HIS	6.8
1	A	286	GLN	6.8
1	A	288	HIS	6.8
1	A	436	ASP	6.8
1	A	420	LYS	6.8
1	A	885	SER	6.8
1	A	835	GLU	6.7
1	A	312	LYS	6.7
1	A	595	ARG	6.6
1	A	446	LYS	6.6
1	A	484	LEU	6.5
1	A	864[A]	GLN	6.5
1	A	596	ARG	6.5
1	A	275	ASP	6.4
1	A	287	GLU	6.2
1	A	856	ARG	6.1
1	A	886	MET	6.0
1	A	737	ARG	6.0
1	A	481	ALA	6.0
1	A	770	ARG	6.0
1	A	597	ASP	5.9

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Mol	Chain	Res	Type	RSRZ
1	A	693	GLN	5.9
1	A	579	ARG	5.8
1	A	588	THR	5.8
1	A	357	GLU	5.6
1	A	479	LEU	5.6
1	A	285	LYS	5.6
1	A	310	GLU	5.6
1	A	282	GLU	5.5
1	A	800	THR	5.5
1	A	791	SER	5.4
1	A	296	GLN	5.4
1	A	399	PHE	5.2
1	A	289	GLU	5.1
1	A	428	ASP	5.1
1	A	318	SER	5.1
1	A	362	ARG	4.9
1	A	489	LEU	4.9
1	A	690	ASP	4.8
1	A	569	PHE	4.8
1	A	746	TRP	4.7
1	A	572	THR	4.6
1	A	890	ARG	4.6
1	A	605	VAL	4.5
1	A	297	ASP	4.5
1	A	888	ARG	4.5
1	A	887	LYS	4.4
1	A	699	GLY	4.2
1	A	364	GLN	4.2
1	A	590	MET	4.2
1	A	429	SER	4.2
1	A	278	GLY	4.2
1	A	568	ILE	4.1
1	A	337	MET	4.1
1	A	742	GLN	4.0
1	A	701	ASN	4.0
1	A	361	THR	4.0
1	A	880	THR	4.0
1	A	396	ARG	3.9
1	A	440	ASN	3.9
1	A	629	PHE	3.9
1	A	891	ARG	3.8
1	A	808	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	878	GLU	3.4
1	A	694	TRP	3.3
1	A	432	TRP	3.3
1	A	393	MET	3.3
1	A	627	GLY	3.3
1	A	680	ALA	3.3
1	A	444	GLU	3.3
1	A	556	HIS	3.2
1	A	743	GLY	3.2
1	A	861	LYS	3.2
1	A	564	LEU	3.2
1	A	790	THR	3.2
1	A	630	LYS	3.1
1	A	545	GLU	3.1
1	A	862	ASN	3.0
1	A	445	GLY	3.0
1	A	383	LYS	3.0
1	A	676	SER	3.0
1	A	443	LEU	3.0
1	A	677	ALA	3.0
1	A	442	HIS	2.9
1	A	571	LEU	2.9
1	A	360	ASP	2.9
1	A	497	TRP	2.9
1	A	652	ARG	2.9
1	A	319	SER	2.9
1	A	882	TYR	2.8
1	A	340	GLN	2.8
1	A	492	LEU	2.8
1	A	792	ARG	2.8
1	A	398	GLU	2.8
1	A	537	GLY	2.8
1	A	483	PHE	2.7
1	A	558	GLU	2.7
1	A	390	THR	2.7
1	A	480	GLY	2.7
1	A	433	GLU	2.7
1	A	833	TRP	2.6
1	A	594	SER	2.6
1	A	544	LEU	2.6
1	A	820	GLU	2.5
1	A	344	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	570	LYS	2.5
1	A	642	ALA	2.5
1	A	889	PHE	2.5
1	A	430	GLY	2.5
1	A	563	LYS	2.4
1	A	628	VAL	2.4
1	A	673	ARG	2.4
1	A	561	HIS	2.4
1	A	674	PHE	2.4
1	A	540	THR	2.4
1	A	546	ASP	2.4
1	A	683	ASP	2.4
1	A	559	GLY	2.4
1	A	370	THR	2.3
1	A	368	GLU	2.3
1	A	377	THR	2.3
1	A	486	PHE	2.3
1	A	524	LYS	2.3
1	A	376	ILE	2.3
1	A	487	GLU	2.3
1	A	633	GLN	2.3
1	A	434	LEU	2.3
1	A	881	ASP	2.2
1	A	378	ALA	2.2
1	A	818	ILE	2.2
1	A	400	THR	2.2
1	A	382	TRP	2.2
1	A	670	LEU	2.2
1	A	854	THR	2.1
1	A	602	GLY	2.1
1	A	557	MET	2.1
1	A	491	PHE	2.1
1	A	603	GLN	2.1
1	A	574	GLN	2.1
1	A	625	GLY	2.1
1	A	343	MET	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 ⓘ

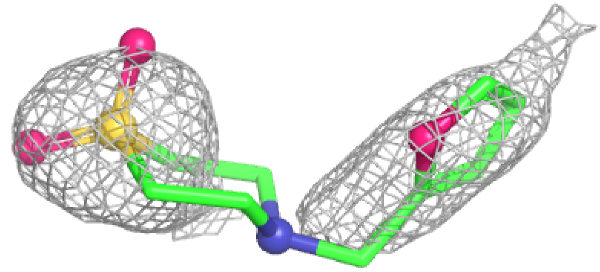
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

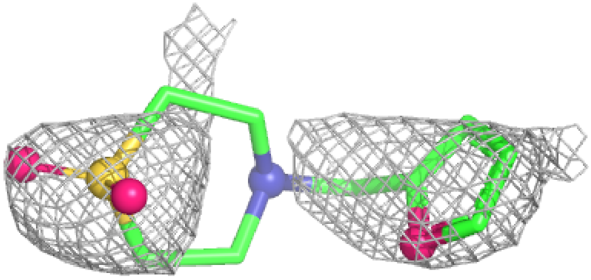
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
5	PO4	A	1008	5/5	0.72	0.21	71,91,98,120	0
7	O3D	A	1010	14/14	0.77	0.24	51,52,55,55	14
6	PEG	A	1009	7/7	0.80	0.20	61,66,84,85	0
5	PO4	A	1007	5/5	0.80	0.14	35,44,54,67	0
4	DMS	A	1005	4/4	0.84	0.21	81,85,93,98	0
3	MES	A	1003[B]	12/12	0.95	0.23	25,30,31,32	12
3	MES	A	1003[A]	12/12	0.95	0.23	847,863,864,864	12
4	DMS	A	1004	4/4	0.96	0.14	43,45,46,49	0
4	DMS	A	1006	4/4	0.96	0.14	51,55,56,58	0
8	CL	A	1011	1/1	0.98	0.17	17,17,17,17	1
2	ZN	A	1002	1/1	0.99	0.03	56,56,56,56	0
2	ZN	A	1001	1/1	1.00	0.01	25,25,25,25	0

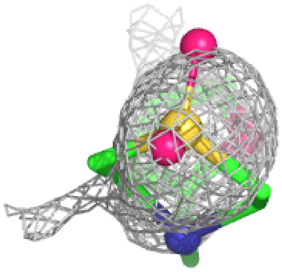
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around O3D 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.