Full wwPDB X-ray Structure Validation Report ⓘ

May 20, 2024 – 03:00 AM JST

PDB ID	:	8HJF
Title	:	Crystal structure of glycosyltransferase SgUGT94-289-3 in complex with M5, state 2
Authors	:	Li, M.; Zhang, S.; Cui, S.
Deposited on	:	2022-11-23
Resolution	:	2.00 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:

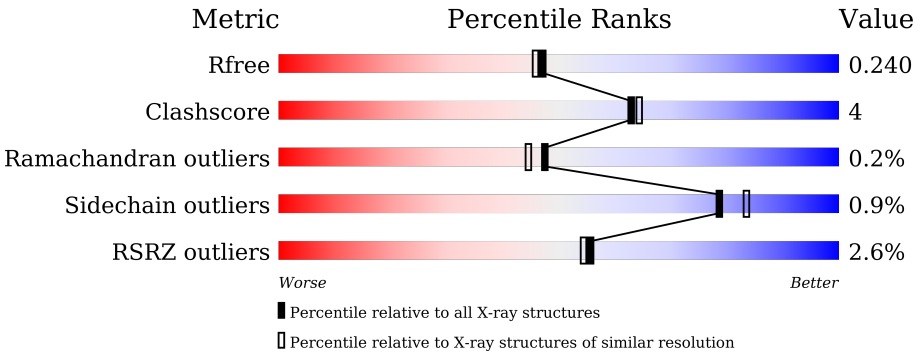
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.2

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 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	459	3% 84% 10% 6%
1	B	459	2% 84% 10% 6%

2 Entry composition

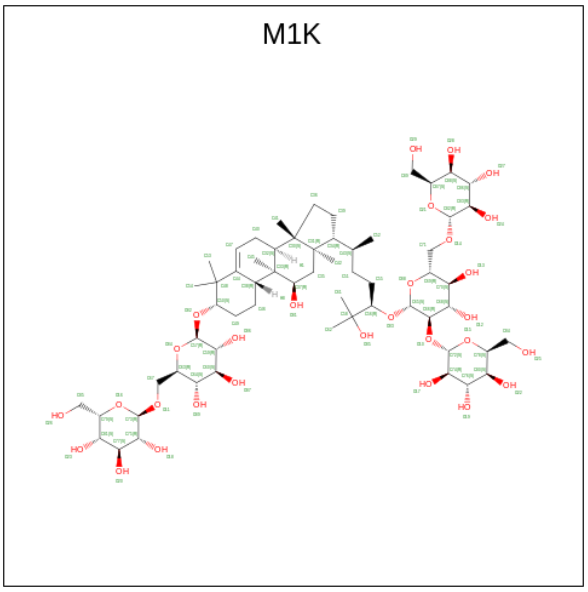
There are 6 unique types of molecules in this entry. The entry contains 7723 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 glycosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	431	Total	C	N	O	S	8	0	0
			3408	2204	577	611	16			
1	B	431	Total	C	N	O	S	5	0	0
			3405	2202	576	611	16			

- Molecule 2 is (2S,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[[(2R,3S,4S,5R,6R)-6-[[(3S,8S,9R,10R,11R,13R,14S,17R)-17-[(2S,5R)-5-[(2S,3R,4S,5S,6R)-3-[(2R,3R,4S,5S,6S)-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-6-[[(2R,3R,4S,5S,6S)-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxymethyl]-4,5-bis(oxidanyl)oxan-2-yl]oxy-6-methyl-6-oxidanyl-heptan-2-yl]-4,4,9,13,14-pentamethyl-11-oxidanyl-2,3,7,8,10,11,12,15,16,17-decahydro-1H-cyclopenta[a]phenanthren-3-yl]oxy]-3,4,5-tris(oxidanyl)oxan-2-yl]methoxy]oxane-3,4,5-triol (three-letter code: M1K) (formula: $C_{60}H_{102}O_{29}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	1	0
			89	60	29		

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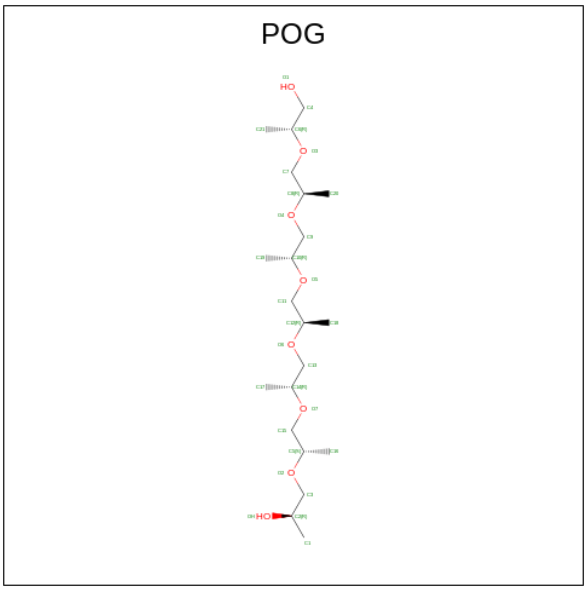
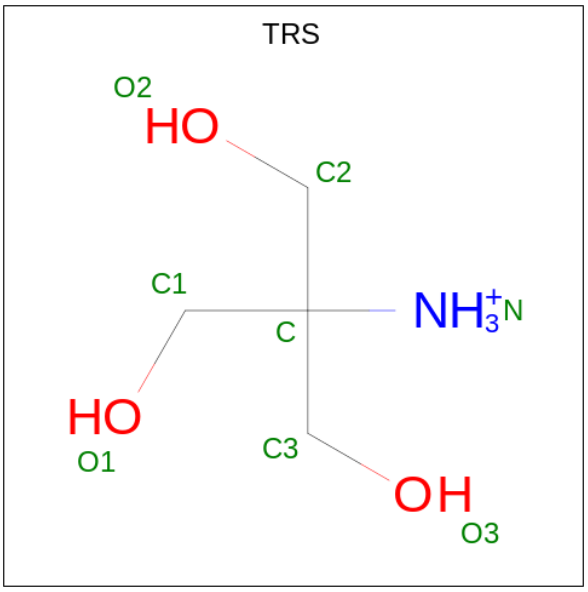
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total C O 89 60 29	1	0

- Molecule 3 is (20S)-2,5,8,11,14,17-HEXAMETHYL-3,6,9,12,15,18-HEXAOXAHENICOSANE-1,20-DIOL (three-letter code: POG) (formula: $C_{21}H_{44}O_8$).



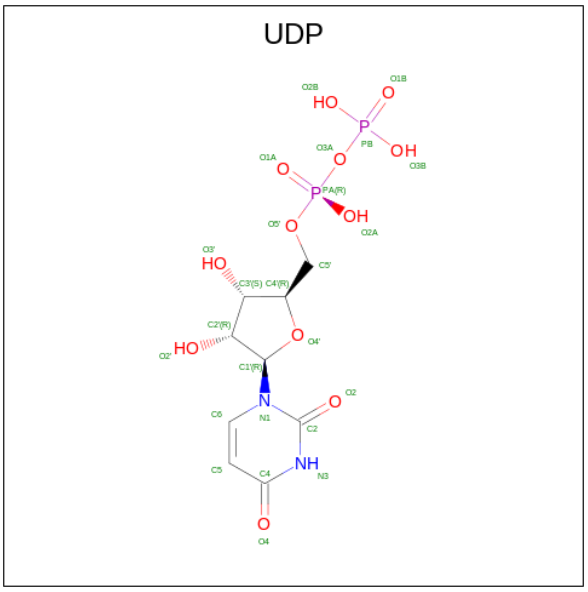
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 21 15 6	0	0
3	B	1	Total C O 13 9 4	0	0

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		
4	B	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 6 is water.

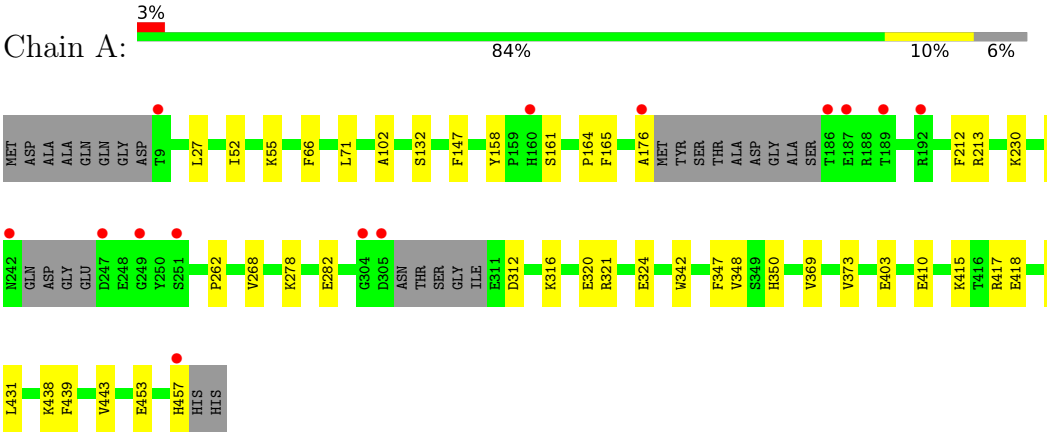
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	278	Total	O	0	0
			278	278		
6	B	354	Total	O	0	0
			354	354		

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.

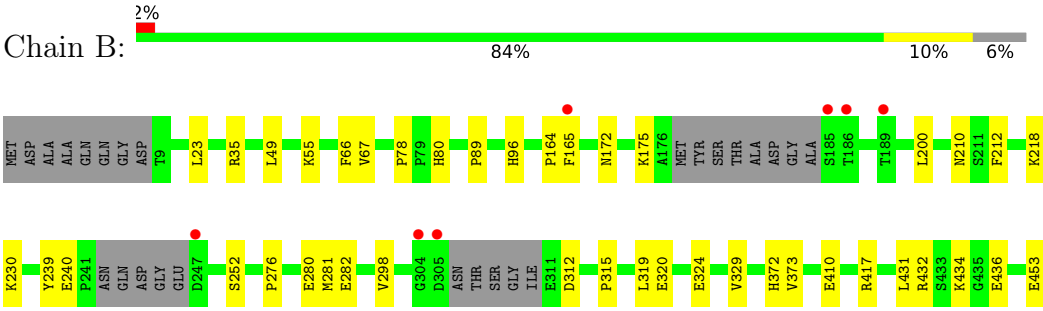
• Molecule 1: glycosyltransferase

Chain A:



• Molecule 1: glycosyltransferase

Chain B:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.95Å 76.81Å 81.46Å 90.00° 93.25° 90.00°	Depositor
Resolution (Å)	19.66 – 2.00 19.95 – 1.57	Depositor EDS
% Data completeness (in resolution range)	99.6 (19.66-2.00) 71.9 (19.95-1.57)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.05 (at 1.56Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.198 , 0.240 0.198 , 0.240	Depositor DCC
R_{free} test set	5113 reflections (5.27%)	wwPDB-VP
Wilson B-factor (Å^2)	24.0	Xtriage
Anisotropy	0.158	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 32.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.011 for l,-k,h	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	7723	wwPDB-VP
Average B, all atoms (Å^2)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.80% 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: TRS, UDP, POG, M1K

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	0.32	0/3506	0.48	0/4754
1	B	0.32	0/3503	0.49	0/4750
All	All	0.32	0/7009	0.49	0/9504

There are no bond length outliers.

There are no bond angle outliers.

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	3408	0	3354	31	1
1	B	3405	0	3351	28	0
2	A	89	0	0	0	0
2	B	89	0	0	0	0
3	A	21	0	31	1	1
3	B	13	0	18	1	0
4	A	8	0	12	0	0
4	B	8	0	12	0	0
5	A	25	0	11	0	0
5	B	25	0	11	0	0
6	A	278	0	0	13	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	354	0	0	11	0
All	All	7723	0	6800	60	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 4.

All (60) 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:282:GLU:OE1	6:A:601:HOH:O	2.02	0.76
1:B:96:HIS:HD2	6:B:617:HOH:O	1.68	0.76
1:B:35:ARG:NH1	6:B:603:HOH:O	2.19	0.73
1:B:280:GLU:OE2	6:B:601:HOH:O	2.05	0.73
1:A:415:LYS:HB3	1:A:421:ARG:NE	2.04	0.71
1:B:436:GLU:OE2	6:B:602:HOH:O	2.08	0.71
1:A:324:GLU:OE2	6:A:602:HOH:O	2.10	0.69
1:A:176:ALA:O	6:A:603:HOH:O	2.13	0.65
1:A:158:TYR:HB3	1:A:161:SER:OG	1.97	0.65
1:B:218:LYS:HE3	6:B:872:HOH:O	1.99	0.62
1:B:172:ASN:HA	1:B:175:LYS:HG3	1.81	0.62
1:A:415:LYS:HB3	1:A:421:ARG:HE	1.64	0.62
1:A:421:ARG:NH1	6:A:611:HOH:O	2.34	0.59
1:B:164:PRO:HG2	1:B:165:PHE:CE2	2.38	0.59
1:A:410:GLU:OE1	6:A:604:HOH:O	2.17	0.59
1:A:235:GLY:HA3	1:A:438:LYS:HD3	1.84	0.58
1:B:230:LYS:NZ	6:B:613:HOH:O	2.32	0.58
1:A:71:LEU:HD12	1:A:102:ALA:HB2	1.89	0.55
1:B:324:GLU:HG2	6:B:700:HOH:O	2.07	0.55
1:B:410:GLU:HB3	1:B:417:ARG:HG2	1.89	0.54
1:B:453:GLU:HB3	1:B:457:HIS:CE1	2.43	0.53
1:A:429:GLU:OE1	6:A:606:HOH:O	2.19	0.52
1:A:312:ASP:N	1:A:312:ASP:OD1	2.39	0.52
1:A:213:ARG:NH1	6:A:605:HOH:O	2.18	0.51
1:B:282:GLU:HG3	1:B:315:PRO:HG3	1.93	0.51
1:B:434:LYS:HD2	6:B:901:HOH:O	2.11	0.50
1:A:230:LYS:HE3	6:A:610:HOH:O	2.12	0.50
1:B:55:LYS:HE2	1:B:239:TYR:CD2	2.48	0.49
1:A:439:PHE:O	1:A:443:VAL:HG23	2.14	0.47
1:A:230:LYS:NZ	6:A:621:HOH:O	2.47	0.47
1:A:403:GLU:HG2	6:A:613:HOH:O	2.13	0.47
1:A:55:LYS:HE3	1:A:239:TYR:CD2	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:320:GLU:HA	1:B:320:GLU:OE1	2.15	0.46
1:A:147:PHE:HB3	6:A:715:HOH:O	2.14	0.46
1:A:417:ARG:NH1	6:A:604:HOH:O	2.25	0.46
1:A:164:PRO:HG2	1:A:165:PHE:CD1	2.50	0.46
1:A:453:GLU:HB3	1:A:457:HIS:CE1	2.51	0.45
3:A:502:POG:H202	3:A:502:POG:H91	1.61	0.45
1:A:262:PRO:HB3	1:A:342:TRP:CD1	2.52	0.45
1:A:213:ARG:HD3	6:A:605:HOH:O	2.16	0.44
1:B:89:PRO:HD2	6:B:912:HOH:O	2.17	0.44
1:A:268:VAL:HG22	1:A:348:VAL:HB	2.00	0.44
1:B:200:LEU:HD23	1:B:227:LEU:HD11	2.00	0.44
1:A:212:PHE:CZ	1:A:431:LEU:HD21	2.53	0.44
1:A:418:GLU:HB3	1:A:421:ARG:NH2	2.34	0.43
1:B:240:GLU:OE1	1:B:432:ARG:NH1	2.51	0.43
1:B:276:PRO:HG2	1:B:281:MET:SD	2.59	0.43
1:B:276:PRO:O	6:B:605:HOH:O	2.21	0.43
1:B:210:ASN:ND2	6:B:604:HOH:O	2.20	0.43
1:A:316:LYS:HA	1:A:316:LYS:HD2	1.94	0.42
1:A:320:GLU:HG3	1:A:321:ARG:N	2.33	0.42
1:B:49:LEU:HD13	1:B:66:PHE:HB3	2.01	0.42
1:B:78:PRO:HG2	1:B:80:HIS:CE1	2.54	0.42
1:B:212:PHE:CZ	1:B:431:LEU:HD21	2.55	0.42
1:B:229:LYS:HB2	1:B:229:LYS:HE2	1.83	0.42
1:B:67:VAL:HG22	3:B:501:POG:H182	2.02	0.41
1:B:319:LEU:HD23	1:B:319:LEU:HA	1.92	0.41
1:A:350:HIS:HA	1:A:369:VAL:O	2.21	0.41
1:B:298:VAL:HA	1:B:329:VAL:O	2.21	0.41
1:A:27:LEU:HD22	1:A:52:ILE:HG13	2.03	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)
1:A:66:PHE:O	3:A:502:POG:C4[2_656]	2.19	0.01

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	423/459 (92%)	410 (97%)	12 (3%)	1 (0%)	47 44
1	B	423/459 (92%)	415 (98%)	7 (2%)	1 (0%)	47 44
All	All	846/918 (92%)	825 (98%)	19 (2%)	2 (0%)	47 44

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	373	VAL
1	B	373	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	372/399 (93%)	369 (99%)	3 (1%)	81 86
1	B	372/399 (93%)	368 (99%)	4 (1%)	73 78
All	All	744/798 (93%)	737 (99%)	7 (1%)	78 83

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	SER
1	A	278	LYS
1	A	347	PHE
1	B	23	LEU

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Mol	Chain	Res	Type
1	B	252	SER
1	B	312	ASP
1	B	372	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	157	HIS
1	A	286	HIS
1	A	372	HIS
1	B	157	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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	UDP	A	504	-	24,26,26	0.66	0	37,40,40	0.65	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	M1K	A	501	-	97,97,97	2.71	32 (32%)	147,153,153	1.87	35 (23%)
4	TRS	A	503	-	7,7,7	0.35	0	9,9,9	0.43	0
2	M1K	B	502	-	97,97,97	2.71	32 (32%)	147,153,153	2.15	39 (26%)
4	TRS	B	503	-	7,7,7	0.34	0	9,9,9	0.48	0
5	UDP	B	504	-	24,26,26	0.61	0	37,40,40	0.62	0
3	POG	B	501	-	9,12,28	1.16	1 (11%)	10,14,34	1.11	1 (10%)
3	POG	A	502	-	15,20,28	1.22	2 (13%)	18,24,34	1.00	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
5	UDP	A	504	-	-	2/16/32/32	0/2/2/2
2	M1K	A	501	-	-	19/43/219/219	0/9/9/9
4	TRS	A	503	-	-	3/9/9/9	-
2	M1K	B	502	-	-	15/43/219/219	0/9/9/9
4	TRS	B	503	-	-	4/9/9/9	-
5	UDP	B	504	-	-	2/16/32/32	0/2/2/2
3	POG	B	501	-	-	5/12/12/32	-
3	POG	A	502	-	-	8/22/22/32	-

All (67) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	M1K	O02-C50	9.87	1.58	1.45
2	B	502	M1K	O02-C50	9.86	1.58	1.45
2	A	501	M1K	C48-C44	-7.91	1.42	1.54
2	B	502	M1K	C48-C44	-7.77	1.43	1.54
2	A	501	M1K	C48-C50	-7.52	1.41	1.54
2	B	502	M1K	C48-C50	-7.47	1.41	1.54
2	B	502	M1K	C60-C59	6.90	1.69	1.52
2	A	501	M1K	C47-C44	6.85	1.46	1.33
2	A	501	M1K	C60-C59	6.83	1.69	1.52
2	B	502	M1K	C47-C44	6.70	1.46	1.33
2	B	502	M1K	C31-C30	-6.45	1.45	1.56
2	A	501	M1K	C31-C30	-6.16	1.45	1.56
2	B	502	M1K	O14-C71	5.91	1.54	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	M1K	O14-C71	5.51	1.53	1.43
2	A	501	M1K	O16-C79	5.47	1.57	1.44
2	B	502	M1K	O16-C79	5.43	1.57	1.44
2	B	502	M1K	C58-C56	5.41	1.63	1.53
2	A	501	M1K	C58-C56	5.26	1.63	1.53
2	A	501	M1K	C81-C79	-5.12	1.42	1.53
2	B	502	M1K	C81-C79	-4.97	1.42	1.53
2	B	502	M1K	O02-C57	4.45	1.54	1.41
2	A	501	M1K	O02-C57	4.29	1.53	1.41
2	A	501	M1K	O11-C67	4.03	1.51	1.43
2	B	502	M1K	O11-C67	3.87	1.50	1.43
2	B	502	M1K	C41-C30	3.62	1.61	1.54
2	A	501	M1K	C41-C30	3.52	1.61	1.54
2	A	501	M1K	O04-C63	3.42	1.52	1.44
2	B	502	M1K	O04-C63	3.35	1.52	1.44
2	A	501	M1K	C54-C48	-3.13	1.47	1.54
2	B	502	M1K	C54-C48	-3.05	1.47	1.54
2	A	501	M1K	C55-C56	2.99	1.59	1.51
2	B	502	M1K	C55-C56	2.98	1.59	1.51
2	B	502	M1K	O06-C59	2.90	1.49	1.43
2	B	502	M1K	C40-C47	-2.82	1.44	1.50
2	A	501	M1K	C49-C50	-2.82	1.46	1.51
2	B	502	M1K	C49-C50	-2.78	1.46	1.51
2	A	501	M1K	O06-C59	2.78	1.49	1.43
2	A	501	M1K	C33-C38	-2.74	1.51	1.56
2	A	501	M1K	C40-C47	-2.67	1.44	1.50
2	A	501	M1K	C39-C34	2.60	1.59	1.54
2	B	502	M1K	C64-C63	-2.58	1.47	1.53
2	A	501	M1K	O15-C72	2.57	1.48	1.41
2	A	501	M1K	C85-C79	2.57	1.60	1.51
2	B	502	M1K	C85-C79	2.56	1.60	1.51
2	B	502	M1K	O25-C84	2.54	1.53	1.42
2	A	501	M1K	O25-C84	2.51	1.53	1.42
2	B	502	M1K	O14-C82	2.48	1.44	1.40
2	B	502	M1K	C33-C38	-2.39	1.51	1.56
2	B	502	M1K	C39-C34	2.32	1.59	1.54
2	A	501	M1K	C71-C69	2.31	1.58	1.51
2	A	501	M1K	C64-C63	-2.27	1.48	1.53
2	B	502	M1K	O08-C69	-2.26	1.38	1.44
2	B	502	M1K	C71-C69	2.25	1.58	1.51
2	A	501	M1K	C30-C32	-2.24	1.52	1.56
3	A	502	POG	O5-C11	-2.23	1.39	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	502	M1K	C40-C32	2.22	1.57	1.53
3	A	502	POG	O4-C9	-2.21	1.39	1.43
2	B	502	M1K	O15-C72	2.20	1.47	1.41
3	B	501	POG	O7-C15	-2.19	1.39	1.43
2	B	502	M1K	C72-C74	2.17	1.58	1.52
2	A	501	M1K	O14-C82	2.15	1.43	1.40
2	A	501	M1K	C40-C32	2.13	1.57	1.53
2	A	501	M1K	C72-C74	2.11	1.58	1.52
2	B	502	M1K	C30-C32	-2.10	1.53	1.56
2	A	501	M1K	O08-C69	-2.09	1.39	1.44
2	A	501	M1K	C88-C87	-2.06	1.48	1.53
2	B	502	M1K	C57-C59	-2.02	1.46	1.52

All (75) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	502	M1K	C48-C44-C38	6.94	122.33	115.91
2	B	502	M1K	O03-C56-C58	6.63	114.75	106.42
2	B	502	M1K	C48-C44-C47	-6.61	118.07	122.08
2	A	501	M1K	C49-C50-C48	-6.12	108.68	113.28
2	B	502	M1K	C40-C32-C30	-5.68	109.34	114.69
2	B	502	M1K	C49-C50-C48	-5.65	109.03	113.28
2	A	501	M1K	C48-C44-C38	5.39	120.89	115.91
2	A	501	M1K	C33-C38-C44	5.34	121.92	113.47
2	B	502	M1K	C33-C38-C44	5.32	121.88	113.47
2	B	502	M1K	C55-C56-C58	-5.27	106.82	115.49
2	B	502	M1K	O15-C78-C80	4.81	118.42	109.69
2	B	502	M1K	C32-C40-C47	4.80	121.97	113.02
2	A	501	M1K	C40-C32-C30	-4.77	110.19	114.69
2	A	501	M1K	C55-C56-C58	-4.65	107.84	115.49
2	B	502	M1K	C41-C30-C32	4.55	117.77	111.44
2	A	501	M1K	C48-C44-C47	-4.44	119.39	122.08
2	A	501	M1K	C32-C40-C47	4.40	121.23	113.02
2	B	502	M1K	C49-C46-C38	-4.30	101.18	112.03
2	A	501	M1K	O03-C56-C58	4.16	111.64	106.42
2	B	502	M1K	C31-C34-C43	4.13	124.65	119.30
2	B	502	M1K	C52-C43-C34	4.01	119.06	112.92
2	B	502	M1K	C40-C47-C44	-3.95	117.65	125.07
2	B	502	M1K	C45-C33-C32	-3.77	103.24	112.73
2	A	501	M1K	C40-C47-C44	-3.71	118.11	125.07
2	B	502	M1K	O14-C82-C83	3.69	114.06	108.30
2	A	501	M1K	C45-C33-C32	-3.66	103.51	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	501	M1K	O15-C78-C80	3.63	116.29	109.69
2	A	501	M1K	C49-C46-C38	-3.54	103.09	112.03
2	B	502	M1K	C57-O02-C50	-3.49	109.51	115.08
2	B	502	M1K	C72-O15-C78	3.45	120.47	113.69
2	A	501	M1K	C41-C30-C32	3.39	116.16	111.44
2	A	501	M1K	C57-O02-C50	-3.31	109.80	115.08
2	A	501	M1K	C52-C43-C34	3.30	117.98	112.92
2	B	502	M1K	C88-C86-C83	-3.19	105.25	110.82
2	B	502	M1K	C67-O11-C73	-3.07	107.74	113.74
2	B	502	M1K	C42-C31-C30	-3.07	107.32	112.39
2	A	501	M1K	O08-C69-C71	2.98	112.67	106.67
2	B	502	M1K	C41-C30-C31	-2.98	107.47	112.39
2	A	501	M1K	C31-C34-C43	2.97	123.15	119.30
2	A	501	M1K	C72-O10-C66	-2.97	110.62	117.96
2	A	501	M1K	C31-C30-C32	2.91	112.86	109.92
2	A	501	M1K	C41-C30-C31	-2.89	107.61	112.39
2	A	501	M1K	C45-C33-C38	-2.88	103.32	110.13
3	B	501	POG	C15-O7-C14	-2.79	110.86	115.02
2	B	502	M1K	C46-C38-C44	-2.79	103.39	111.28
2	A	501	M1K	C46-C38-C44	-2.78	103.40	111.28
2	A	501	M1K	C67-O11-C73	-2.77	108.33	113.74
2	A	501	M1K	O14-C82-C83	2.76	112.61	108.30
2	B	502	M1K	C76-C80-C78	2.73	115.11	110.24
2	B	502	M1K	C31-C30-C32	2.71	112.66	109.92
2	B	502	M1K	C39-C34-C31	-2.70	100.10	103.73
2	A	501	M1K	O08-C69-C70	-2.66	104.86	109.69
2	A	501	M1K	C88-C86-C83	-2.66	106.18	110.82
2	B	502	M1K	O08-C69-C70	-2.66	104.87	109.69
2	A	501	M1K	O04-C63-C67	2.60	111.91	106.67
2	B	502	M1K	C55-C51-C43	-2.59	108.57	115.34
2	B	502	M1K	C40-C32-C33	2.48	113.42	110.41
2	B	502	M1K	C45-C33-C38	-2.38	104.50	110.13
2	A	501	M1K	C39-C34-C31	-2.36	100.56	103.73
2	B	502	M1K	C41-C30-C36	-2.34	103.30	111.86
2	B	502	M1K	O08-C69-C71	2.30	111.32	106.67
2	A	501	M1K	C55-C51-C43	-2.29	109.36	115.34
2	A	501	M1K	O10-C66-C68	2.29	113.36	107.28
2	A	501	M1K	C42-C31-C30	-2.27	108.64	112.39
2	A	501	M1K	C72-O15-C78	2.24	118.08	113.69
2	B	502	M1K	O04-C63-C67	2.22	111.15	106.67
2	B	502	M1K	O05-C58-C56	2.22	113.23	107.89
2	A	501	M1K	C41-C30-C36	-2.21	103.77	111.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	502	M1K	O01-C37-C33	2.20	114.75	111.03
2	B	502	M1K	O21-C87-C88	2.18	113.64	109.69
2	A	501	M1K	C57-O04-C63	-2.11	109.54	113.69
2	B	502	M1K	C46-C49-C50	2.08	114.51	110.81
2	B	502	M1K	C89-C87-C88	-2.05	108.19	113.00
2	A	501	M1K	C89-C87-C88	-2.04	108.23	113.00
2	B	502	M1K	C72-O10-C66	-2.03	112.94	117.96

There are no chirality outliers.

All (58) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	M1K	C58-C56-O03-C65
2	A	501	M1K	C83-C82-O14-C71
2	A	501	M1K	O21-C82-O14-C71
2	B	502	M1K	C31-C34-C43-C51
2	B	502	M1K	C39-C34-C43-C51
2	B	502	M1K	C58-C56-O03-C65
2	B	502	M1K	C83-C82-O14-C71
2	B	502	M1K	O21-C82-O14-C71
3	A	502	POG	C21-C6-O3-C7
3	A	502	POG	O3-C7-C8-O4
3	A	502	POG	O3-C7-C8-C20
3	A	502	POG	C20-C8-O4-C9
3	A	502	POG	O5-C10-C9-O4
3	B	501	POG	C18-C12-O6-C13
5	A	504	UDP	PB-O3A-PA-O5'
2	B	502	M1K	C39-C34-C43-C52
2	A	501	M1K	C31-C34-C43-C52
2	B	502	M1K	C31-C34-C43-C52
2	A	501	M1K	C39-C34-C43-C51
2	A	501	M1K	C31-C34-C43-C51
2	A	501	M1K	O08-C69-C71-O14
2	B	502	M1K	O08-C69-C71-O14
2	A	501	M1K	O16-C79-C85-O26
2	B	502	M1K	C70-C69-C71-O14
2	A	501	M1K	C39-C34-C43-C52
2	A	501	M1K	C81-C79-C85-O26
2	A	501	M1K	O15-C78-C84-O25
2	B	502	M1K	O16-C79-C85-O26
2	B	502	M1K	C81-C79-C85-O26
2	A	501	M1K	C70-C69-C71-O14

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Mol	Chain	Res	Type	Atoms
2	A	501	M1K	C43-C51-C55-C56
2	B	502	M1K	C43-C51-C55-C56
2	A	501	M1K	C80-C78-C84-O25
2	B	502	M1K	O21-C87-C89-O29
2	A	501	M1K	O21-C87-C89-O29
3	A	502	POG	C19-C10-C9-O4
3	B	501	POG	O6-C13-C14-O7
5	B	504	UDP	PB-O3A-PA-O5'
3	B	501	POG	O5-C11-C12-O6
4	A	503	TRS	N-C-C1-O1
4	B	503	TRS	C3-C-C1-O1
4	B	503	TRS	N-C-C2-O2
3	B	501	POG	O5-C11-C12-C18
2	A	501	M1K	O04-C63-C67-O11
2	A	501	M1K	C68-C66-O10-C72
2	A	501	M1K	C64-C63-C67-O11
3	A	502	POG	C18-C12-O6-C13
2	A	501	M1K	O03-C56-C58-C62
2	B	502	M1K	O03-C56-C58-C62
5	A	504	UDP	O4'-C4'-C5'-O5'
5	B	504	UDP	O4'-C4'-C5'-O5'
4	A	503	TRS	C2-C-C1-O1
4	A	503	TRS	C3-C-C1-O1
4	B	503	TRS	C2-C-C1-O1
3	A	502	POG	O1-C4-C6-O3
3	B	501	POG	C17-C14-O7-C15
4	B	503	TRS	N-C-C1-O1
2	B	502	M1K	O04-C63-C67-O11

There are no ring outliers.

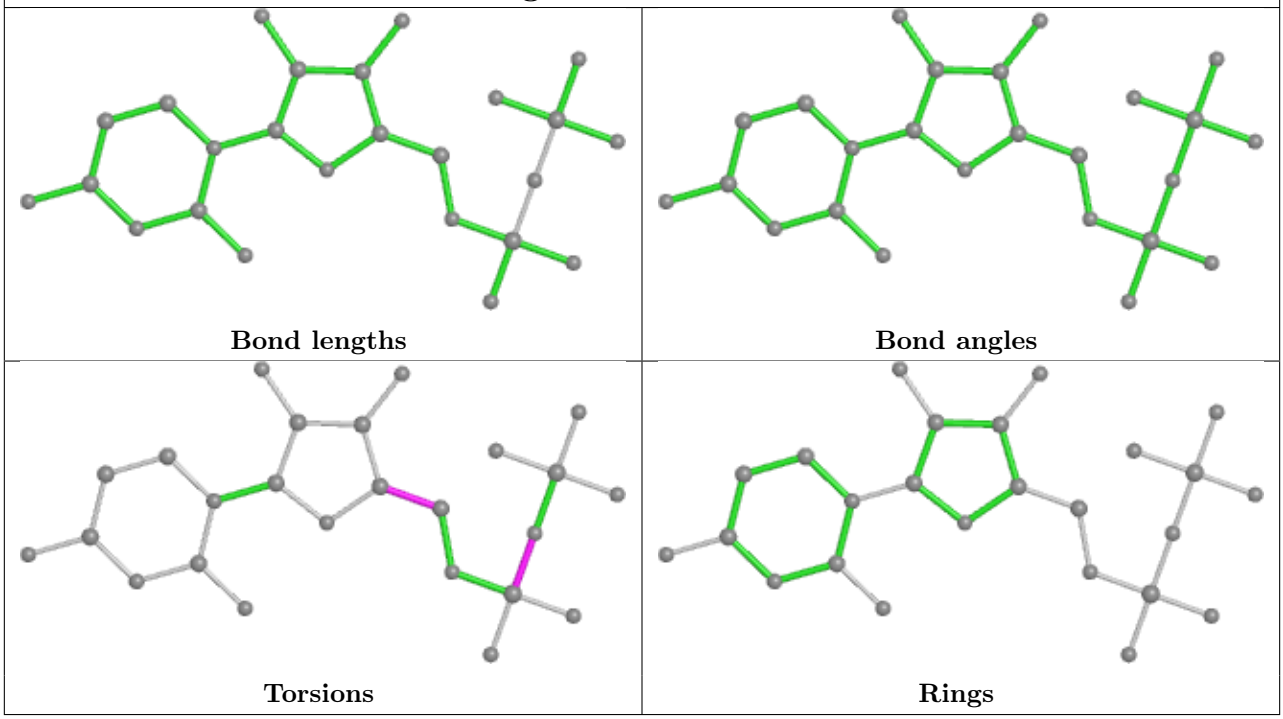
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	POG	1	0
3	A	502	POG	1	1

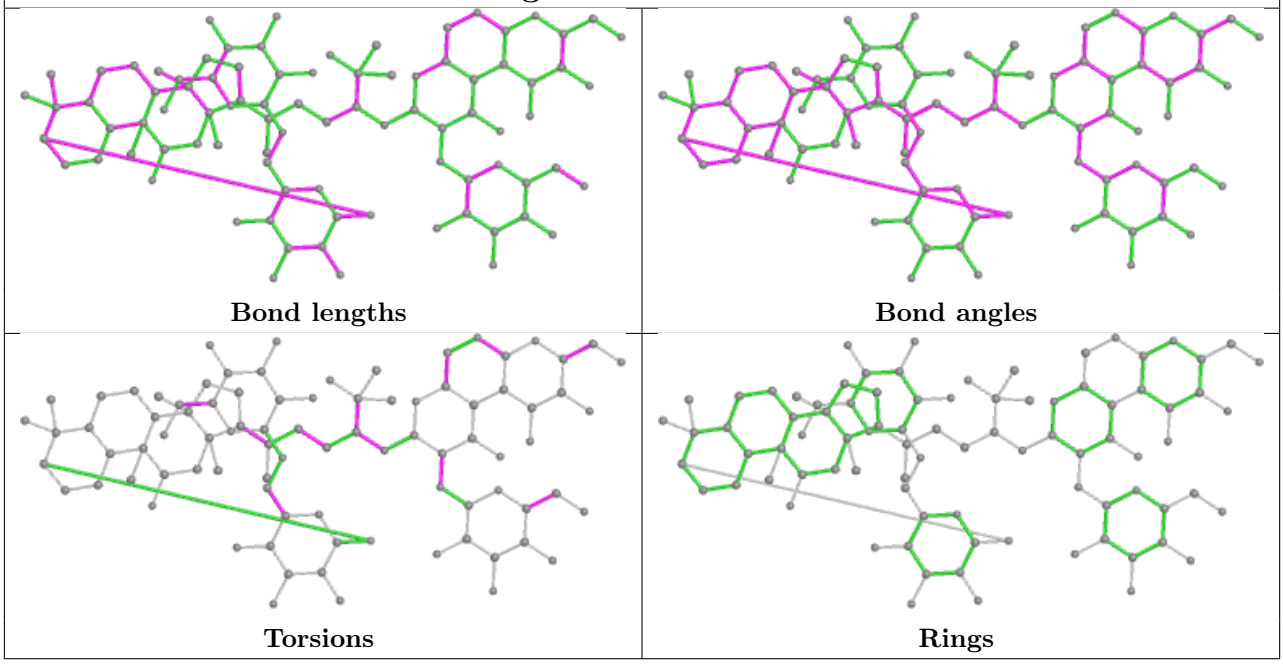
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

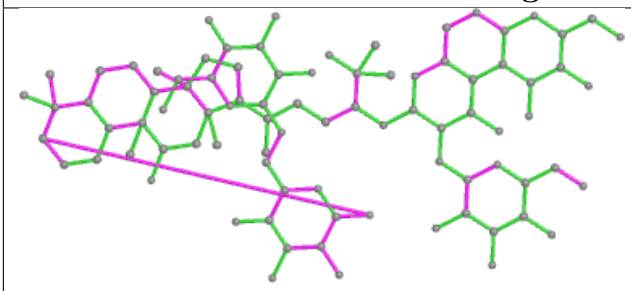
Ligand UDP A 504



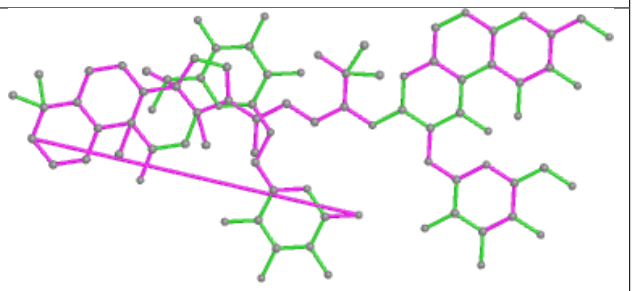
Ligand M1K A 501



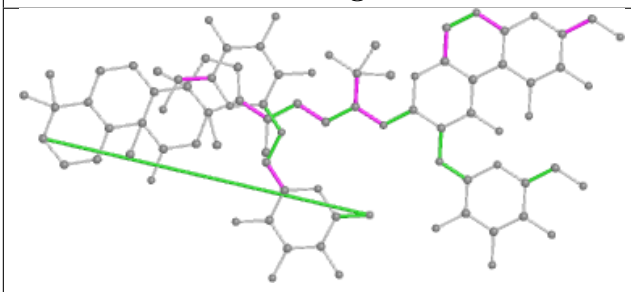
Ligand M1K B 502



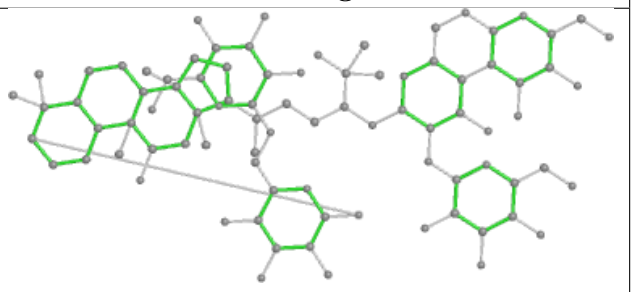
Bond lengths



Bond angles

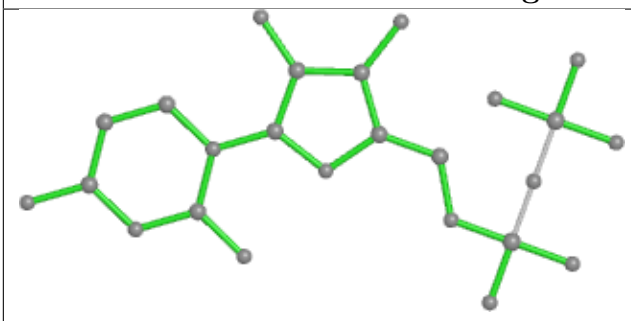


Torsions

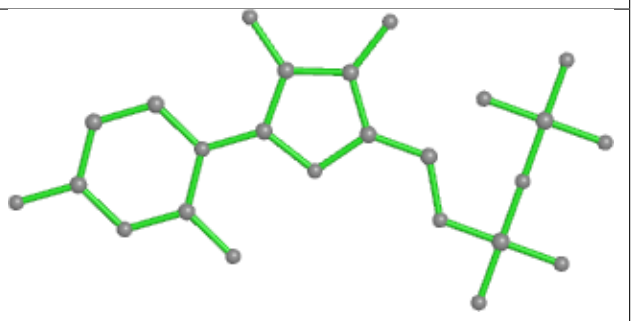


Rings

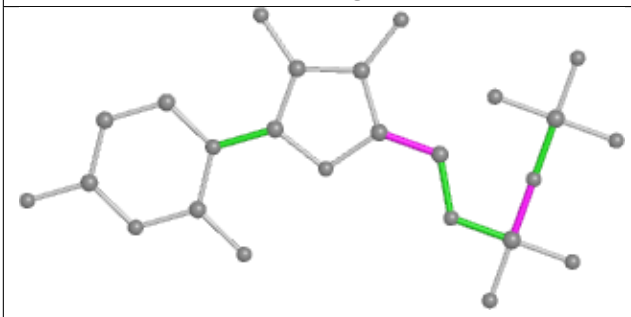
Ligand UDP B 504



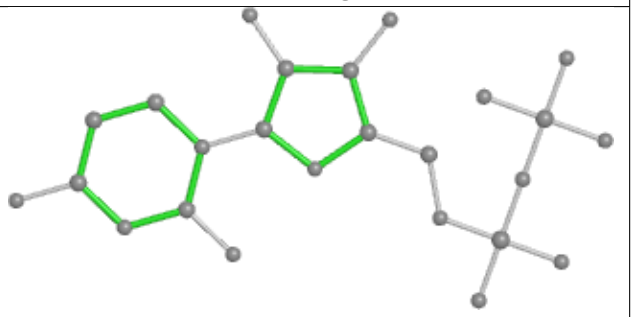
Bond lengths



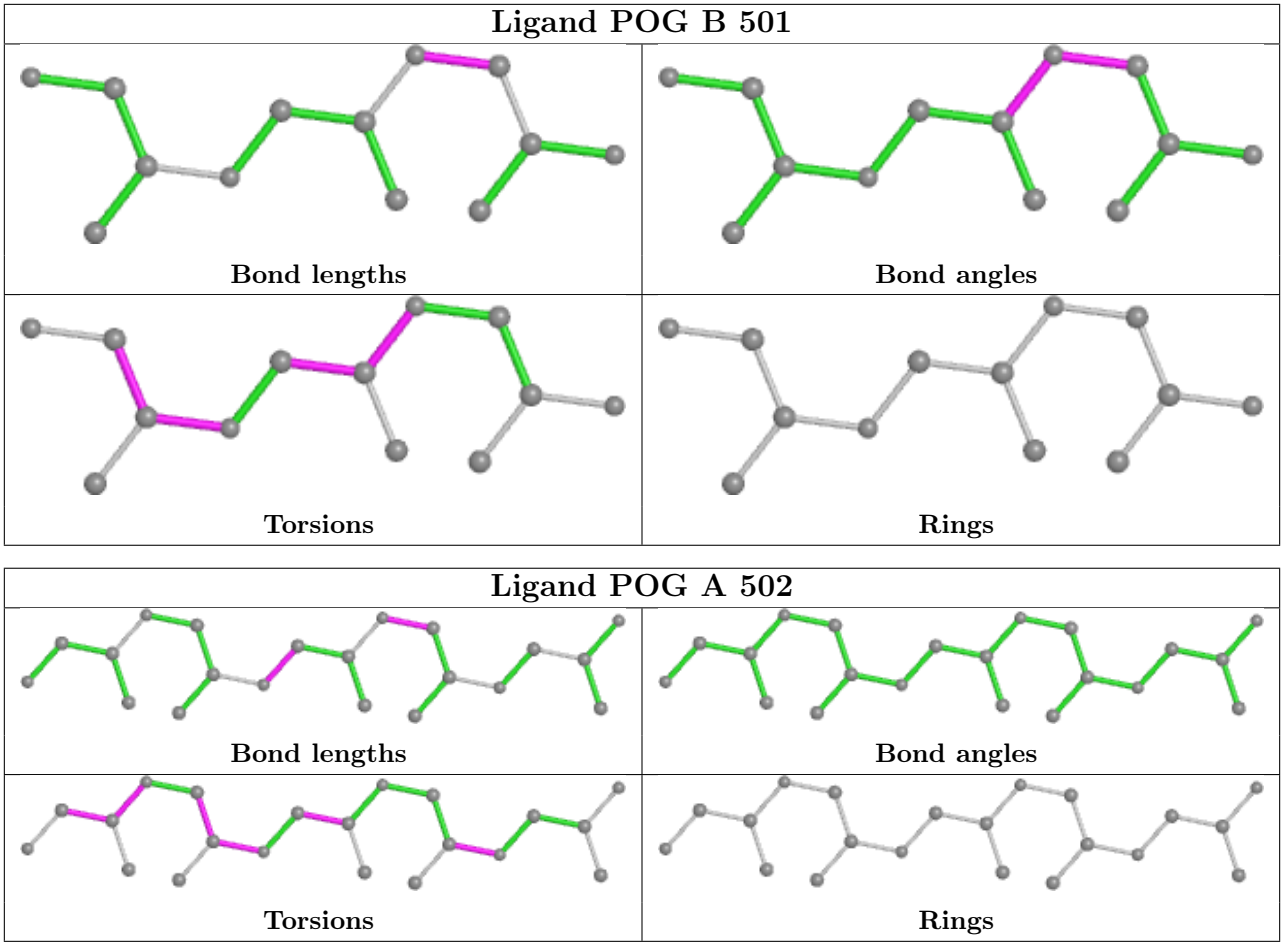
Bond angles



Torsions



Rings



5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	431/459 (93%)	-0.31	14 (3%) 47 46	17, 26, 43, 66	145 (33%)
1	B	431/459 (93%)	-0.45	8 (1%) 66 65	15, 24, 41, 67	129 (29%)
All	All	862/918 (93%)	-0.38	22 (2%) 56 54	15, 25, 42, 67	274 (31%)

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	186	THR	6.3
1	B	185	SER	5.6
1	A	247	ASP	5.0
1	A	176	ALA	4.7
1	B	305	ASP	4.4
1	B	304	GLY	4.1
1	A	187	GLU	4.1
1	A	186	THR	3.9
1	A	189	THR	3.7
1	A	304	GLY	3.4
1	A	305	ASP	3.2
1	A	457	HIS	3.1
1	B	457	HIS	3.1
1	B	247	ASP	2.8
1	A	249	GLY	2.7
1	A	9	THR	2.3
1	B	189	THR	2.3
1	A	242	ASN	2.2
1	A	251	SER	2.1
1	A	160	HIS	2.1
1	A	192	ARG	2.0
1	B	165	PHE	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)

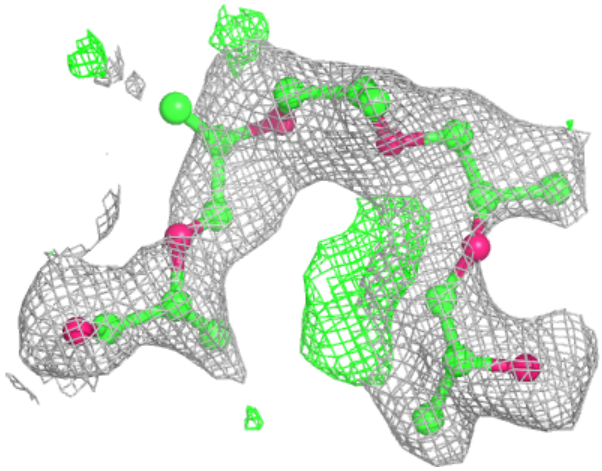
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

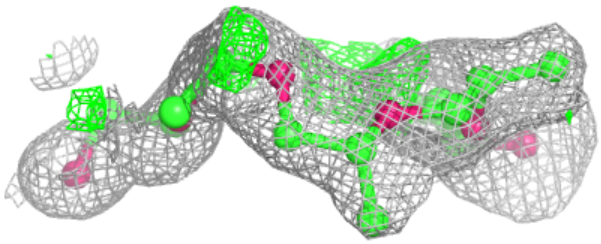
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	POG	A	502	21/29	0.77	0.20	24,33,40,43	12
2	M1K	B	502	89/89	0.83	0.13	19,27,38,42	28
3	POG	B	501	13/29	0.85	0.23	22,25,30,31	9
2	M1K	A	501	89/89	0.88	0.11	19,27,38,42	28
4	TRS	B	503	8/8	0.88	0.16	17,25,25,29	0
4	TRS	A	503	8/8	0.94	0.14	22,25,27,28	0
5	UDP	A	504	25/25	0.97	0.07	18,21,26,30	0
5	UDP	B	504	25/25	0.97	0.06	16,19,22,30	0

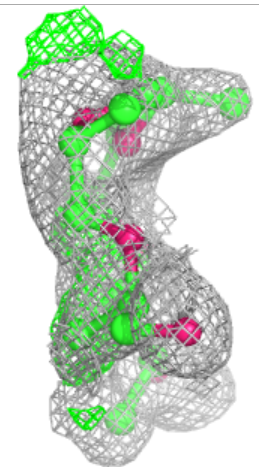
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around POG A 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

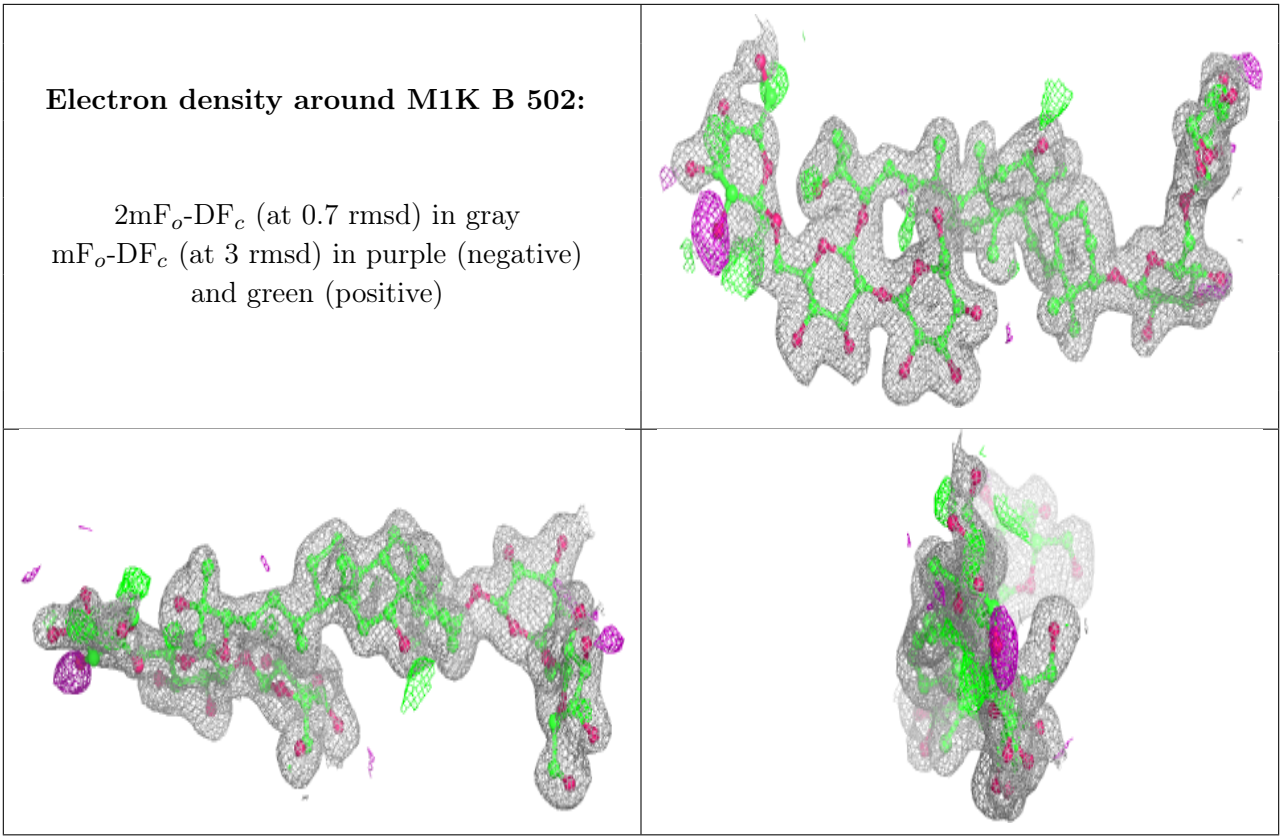






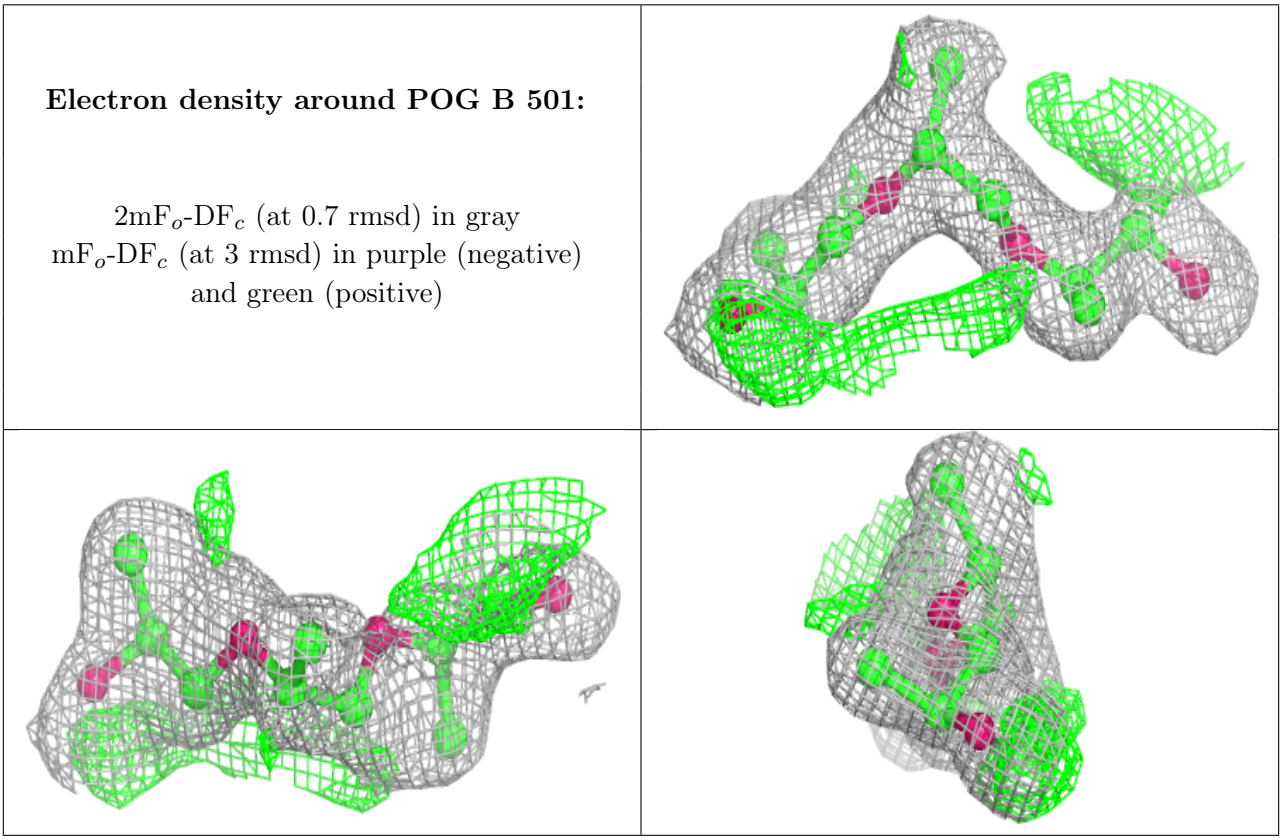
Electron density around M1K B 502:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



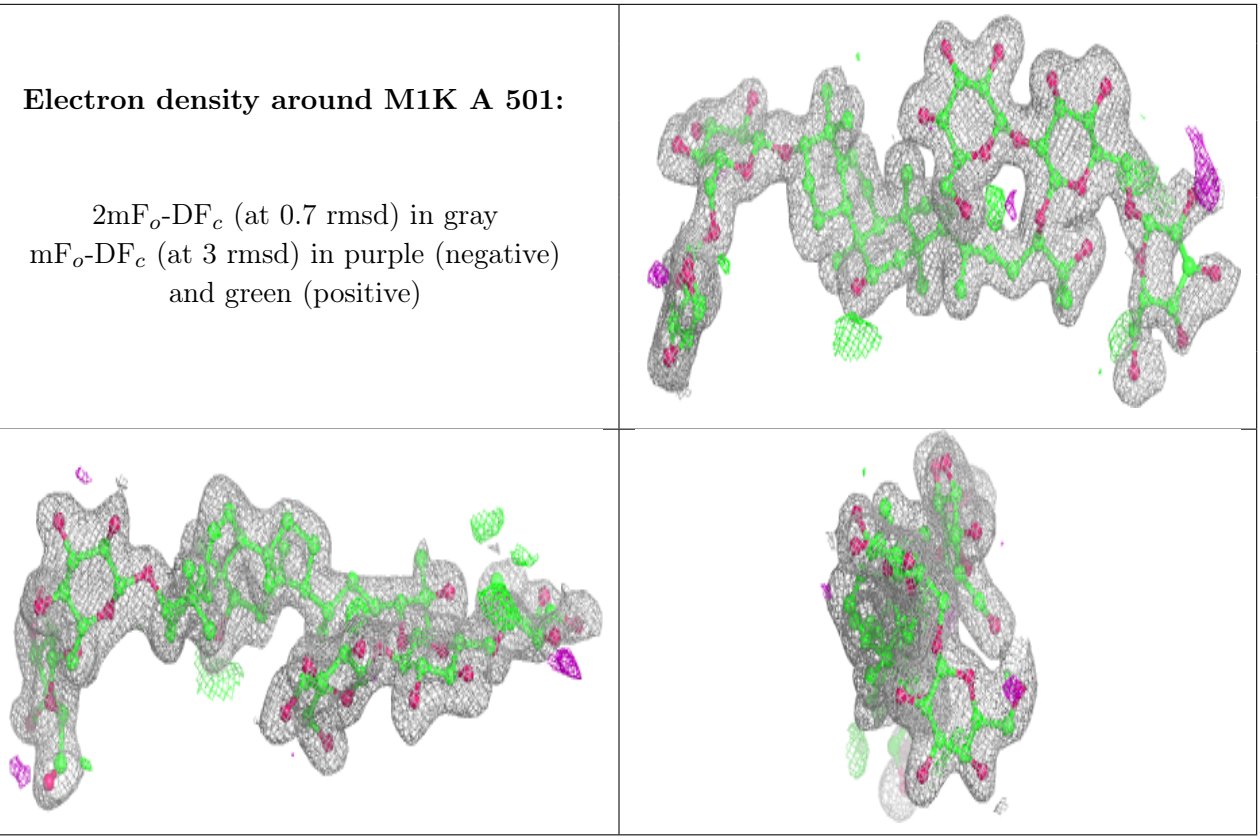
Electron density around POG B 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



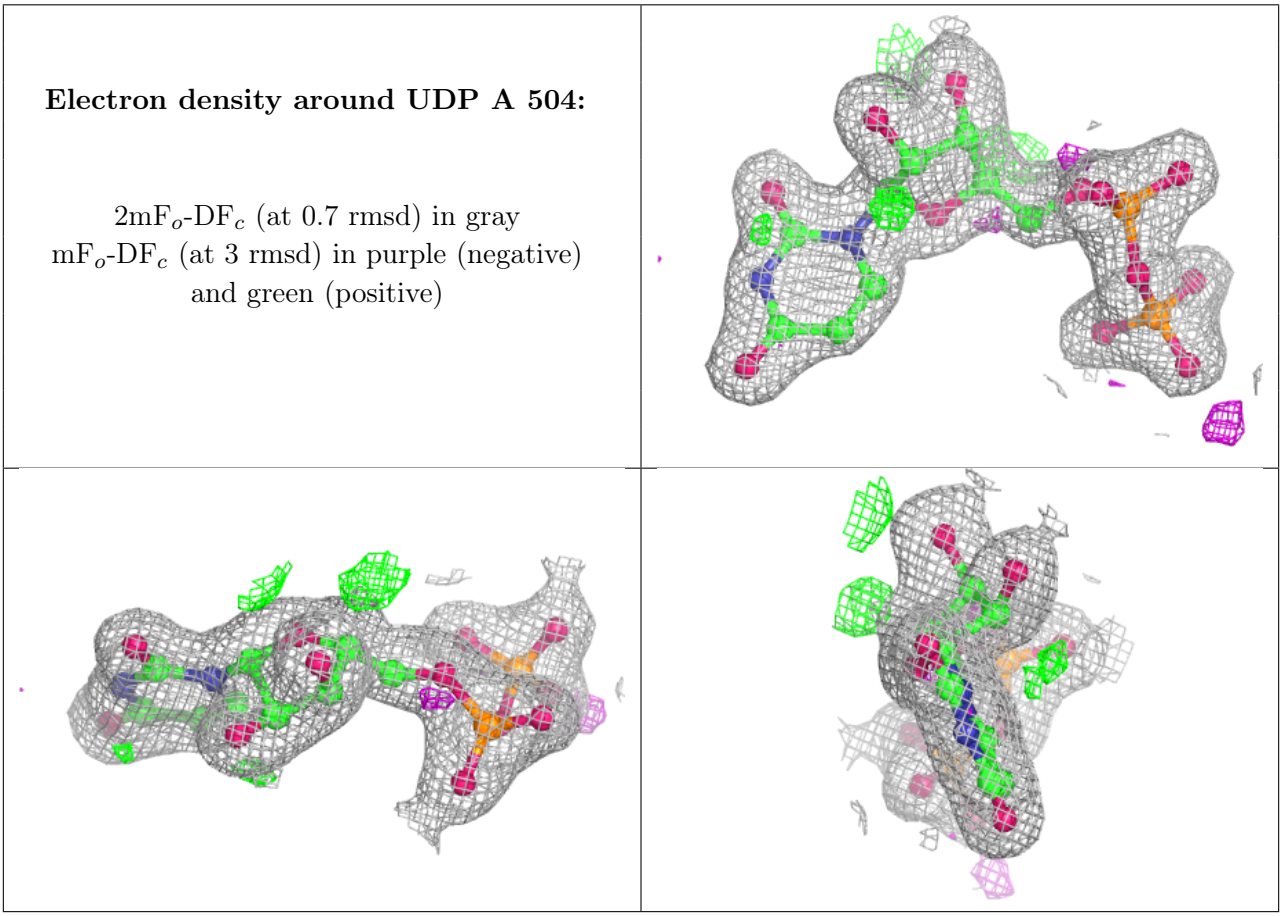
Electron density around M1K A 501:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



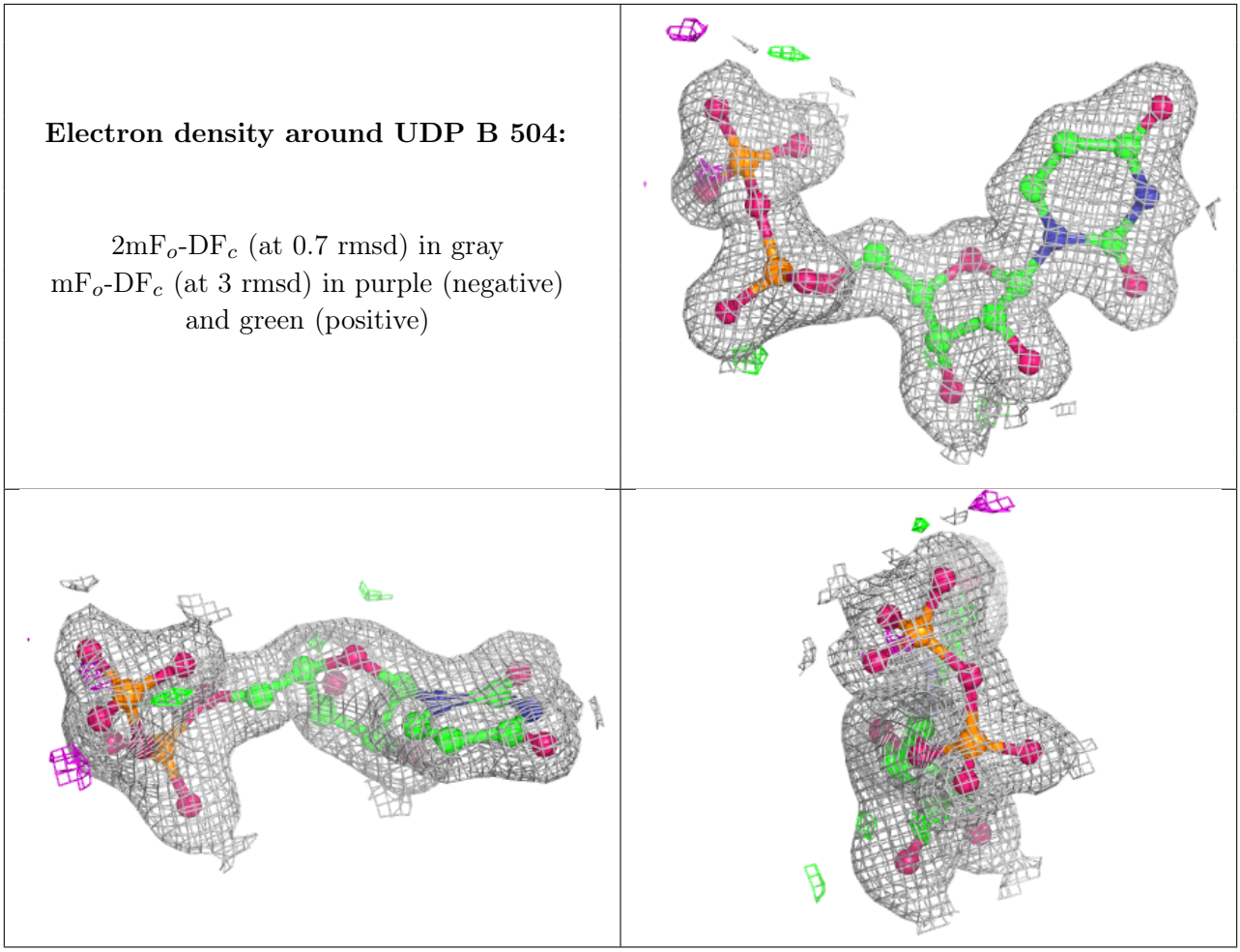
Electron density around UDP A 504:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around UDP B 504:

$2mF_o$-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.