



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 06:05 AM UTC

PDB ID : 8HJL / pdb_00008hjl
Title : Crystal structure of glycosyltransferase SgUGT94-289-3 in complex with M3E
Authors : Li, M.; Zhang, S.; Cui, S.
Deposited on : 2022-11-23
Resolution : 1.72 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

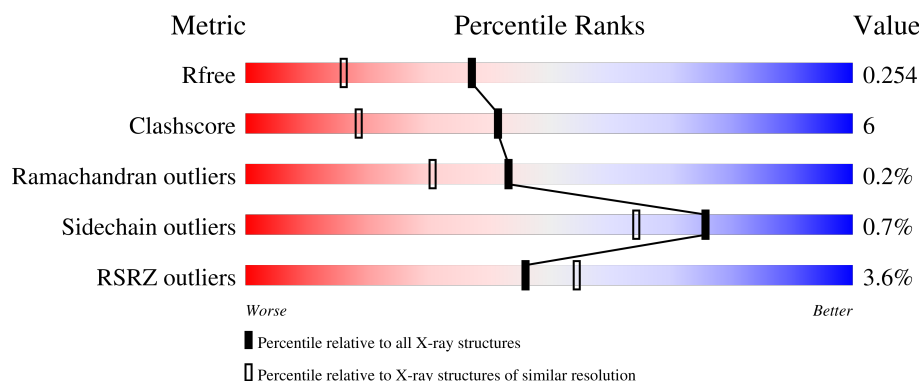
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.72 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}	180053	1039 (1.72-1.72)
Clashscore	190562	1049 (1.72-1.72)
Ramachandran outliers	187476	1041 (1.72-1.72)
Sidechain outliers	187428	1041 (1.72-1.72)
RSRZ outliers	180081	1039 (1.72-1.72)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	459	3% 81% 11% 7%
1	B	459	3% 80% 13% 7%

2 Entry composition [i](#)

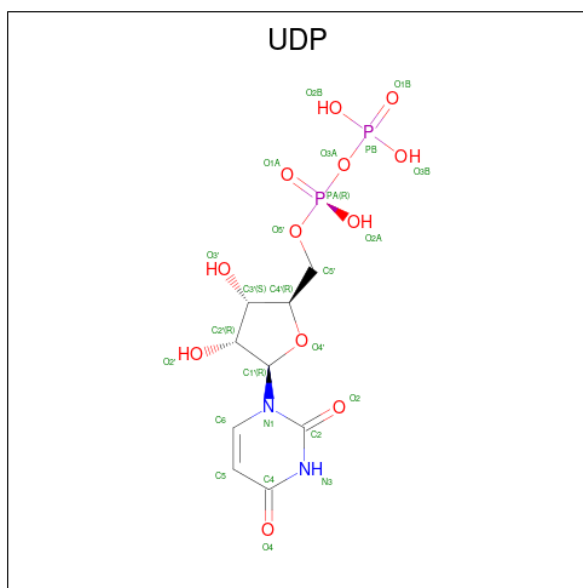
There are 6 unique types of molecules in this entry. The entry contains 8554 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

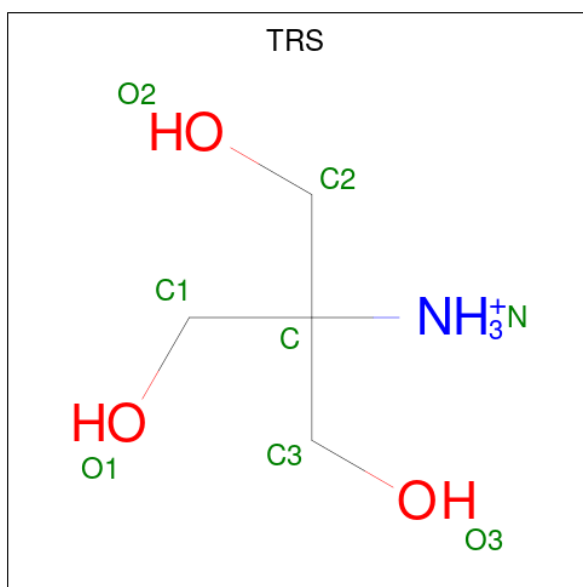
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	3	4	0
			3418	2209	580	613	16			
1	B	429	Total	C	N	O	S	11	6	0
			3448	2228	585	618	17			

- Molecule 2 is URIDINE-5'-DIPHOSPHATE (CCD ID: UDP) (formula: $C_9H_{14}N_2O_{12}P_2$) (labeled as "Ligand of Interest" by depositor).



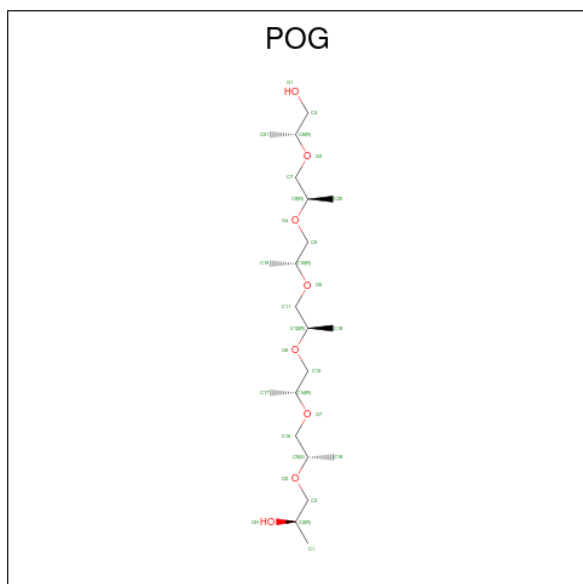
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			25	9	2	12	2		
2	B	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 3 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: $C_4H_{12}NO_3$).



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

- Molecule 4 is (2S)-2,5,8,11,14,17-HEXAMETHYL-3,6,9,12,15,18-HEXAOXAHENICOSAN E-1,20-DIOL (CCD ID: POG) (formula: $C_{21}H_{44}O_8$).



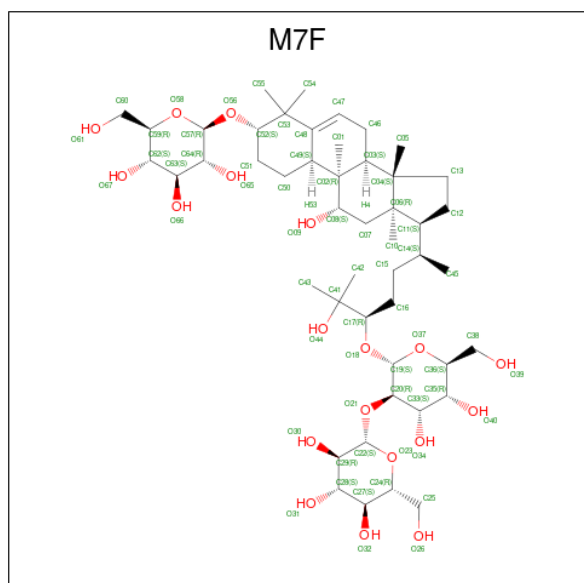
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	3	0
			29	21	8		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	1	0
			17	12	5		
4	B	1	Total	C	O	1	0
			29	21	8		
4	B	1	Total	C	O	3	0
			29	21	8		

- Molecule 5 is (2R,3S,4S,5R,6R)-2-(hydroxymethyl)-6-[[[(3S,8S,9R,10S,11S,13R,14S,17S)-17-[(2S,5R)-5-[(2S,3R,4S,5R,6S)-6-(hydroxymethyl)-3-[(2S,3R,4S,5S,6R)-6-(hydroxymethyl)-3,4,5-tris(oxidanyl)oxan-2-yl]oxy-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]oxane-3,4,5-triol (CCD ID: M7F) (formula: C₄₈H₈₂O₁₉) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			67	48	19		
5	A	1	Total	C	O	1	0
			67	48	19		
5	B	1	Total	C	O	0	0
			67	48	19		
5	B	1	Total	C	O	1	0
			67	48	19		

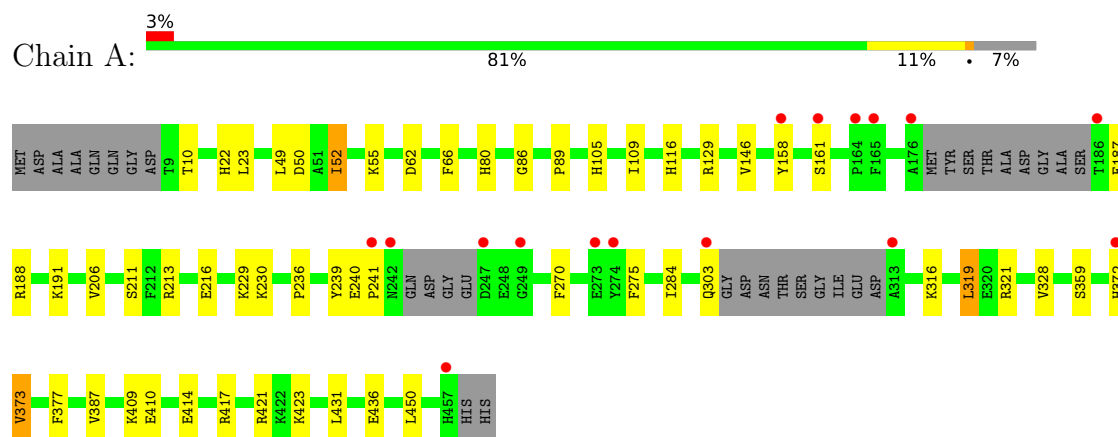
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	634	Total 634	O 634	0	0
6	B	616	Total 616	O 616	0	0

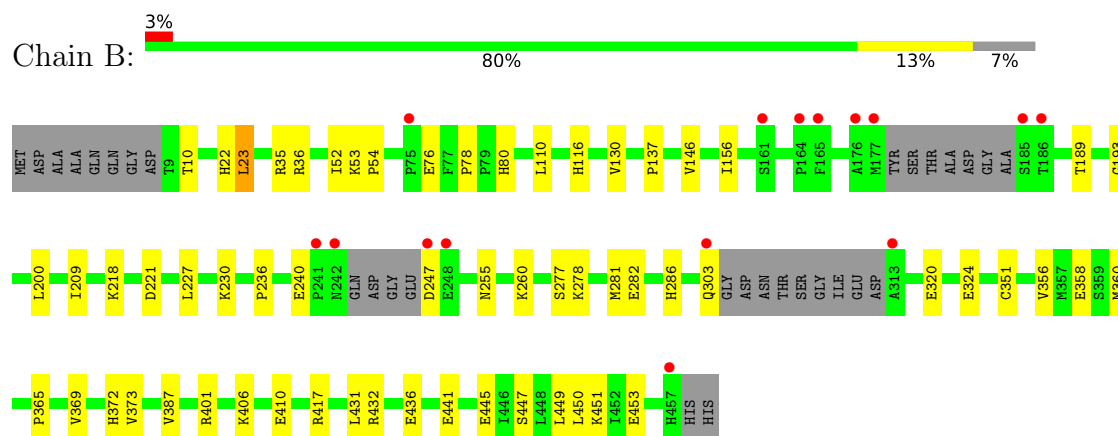
3 Residue-property plots

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: Glycosyltransferase



• Molecule 1: Glycosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	78.63Å 76.16Å 82.25Å 90.00° 92.59° 90.00°	Depositor
Resolution (Å)	24.63 – 1.72 24.63 – 1.72	Depositor EDS
% Data completeness (in resolution range)	97.7 (24.63-1.72) 98.0 (24.63-1.72)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.71 (at 1.72Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.210 , 0.255 0.210 , 0.254	Depositor DCC
R_{free} test set	4782 reflections (4.62%)	wwPDB-VP
Wilson B-factor (Å ²)	13.2	Xtriage
Anisotropy	0.576	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for k,h,-l 0.000 for -k,-h,-l 0.064 for h,-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	8554	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: POG, TRS, M7F, UDP

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	0.29	0/3524	0.48	0/4773
1	B	0.28	0/3551	0.48	0/4810
All	All	0.29	0/7075	0.48	0/9583

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 [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3418	0	3402	38	0
1	B	3448	0	3425	46	0
2	A	25	0	11	0	0
2	B	25	0	11	0	0
3	A	8	0	12	0	0
3	B	8	0	12	0	0
4	A	46	0	68	2	0
4	B	58	0	88	8	0
5	A	134	0	0	0	0
5	B	134	0	0	2	0
6	A	634	0	0	17	7

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	616	0	0	25	4
All	All	8554	0	7029	91	7

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 6.

All (91) 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:387:VAL:O	6:A:601:HOH:O	2.05	0.74
1:B:156:ILE:HD11	4:B:504:POG:H12	1.73	0.70
1:B:387:VAL:O	6:B:601:HOH:O	2.13	0.66
1:B:221:ASP:OD2	6:B:603:HOH:O	2.16	0.60
4:A:503:POG:OH	6:A:602:HOH:O	2.17	0.59
1:B:193:GLY:HA3	4:B:504:POG:H111	1.85	0.59
1:B:453:GLU:OE1	6:B:602:HOH:O	2.16	0.58
1:A:89:PRO:HD3	6:A:994:HOH:O	2.04	0.57
1:B:22:HIS:NE2	6:B:604:HOH:O	2.18	0.56
1:A:436:GLU:OE1	6:A:603:HOH:O	2.18	0.55
1:B:53:LYS:HG2	1:B:54:PRO:HD3	1.88	0.55
1:B:236:PRO:HG3	1:B:431:LEU:HD22	1.89	0.55
1:A:377:PHE:CZ	4:A:503:POG:H203	2.43	0.54
1:A:50:ASP:HB3	6:A:922:HOH:O	2.08	0.53
1:A:321:ARG:NH2	6:A:627:HOH:O	2.41	0.53
1:B:230:LYS:NZ	1:B:445:GLU:OE2	2.40	0.53
1:B:247:ASP:N	6:B:640:HOH:O	2.42	0.53
1:A:213:ARG:NH1	6:A:606:HOH:O	2.22	0.53
1:A:229:LYS:HG3	6:A:795:HOH:O	2.08	0.52
1:B:441:GLU:OE2	6:B:606:HOH:O	2.19	0.52
1:B:282:GLU:HG3	1:B:286:HIS:HD2	1.75	0.52
1:A:230:LYS:NZ	6:A:630:HOH:O	2.43	0.52
1:B:76:GLU:OE2	6:B:607:HOH:O	2.19	0.51
1:B:189:THR:O	6:B:605:HOH:O	2.18	0.51
1:B:356:VAL:HG12	1:B:360:MET:HE2	1.91	0.51
1:A:22:HIS:NE2	6:A:616:HOH:O	2.34	0.51
4:B:503:POG:H41	5:B:505:M7F:C08	2.42	0.49
1:B:137:PRO:HG3	1:B:453:GLU:HG3	1.95	0.48
1:B:282:GLU:HB2	6:B:632:HOH:O	2.13	0.48
1:A:146:VAL:HG12	1:A:216:GLU:CD	2.38	0.48
1:B:23:LEU:HB3	1:B:52[B]:ILE:HG21	1.96	0.48
1:B:255:ASN:OD1	6:B:608:HOH:O	2.20	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:409:LYS:HE3	1:A:414:GLU:CD	2.39	0.47
1:A:55[B]:LYS:HE3	1:A:239:TYR:CD2	2.50	0.47
1:B:240:GLU:OE2	1:B:432:ARG:NH1	2.45	0.47
1:B:320:GLU:HG2	6:B:961:HOH:O	2.14	0.46
1:A:211:SER:OG	1:A:216:GLU:OE1	2.29	0.46
1:B:410:GLU:HB3	1:B:417:ARG:HG2	1.98	0.46
1:A:423:LYS:HE3	6:A:1092:HOH:O	2.15	0.46
1:A:158:TYR:HB3	1:A:161:SER:OG	2.16	0.46
1:B:78:PRO:HG2	1:B:80:HIS:CE1	2.51	0.46
1:B:372:HIS:HE1	6:B:952:HOH:O	1.98	0.46
1:B:80:HIS:HD2	1:B:303:GLN:NE2	2.14	0.45
1:A:80:HIS:HD2	1:A:303:GLN:NE2	2.15	0.45
1:A:129:ARG:NH2	6:A:643:HOH:O	2.49	0.45
1:A:187:GLU:HG2	1:A:191:LYS:NZ	2.32	0.45
1:A:421:ARG:HD3	6:A:1076:HOH:O	2.17	0.45
1:B:278:LYS:HG2	6:B:632:HOH:O	2.15	0.45
1:A:52:ILE:HD12	1:A:52:ILE:HA	1.88	0.45
1:A:316:LYS:HB2	6:A:770:HOH:O	2.17	0.45
1:B:358:GLU:HG3	6:B:664:HOH:O	2.18	0.44
1:B:436:GLU:OE1	6:B:609:HOH:O	2.21	0.44
1:B:260:LYS:NZ	1:B:324:GLU:O	2.50	0.44
1:A:86:GLY:HA2	1:A:275:PHE:HZ	1.83	0.43
1:B:35:ARG:HD2	6:B:1070:HOH:O	2.18	0.43
1:A:410:GLU:HB3	1:A:417:ARG:HG2	2.01	0.43
4:B:503:POG:H202	4:B:503:POG:H92	1.77	0.43
1:B:10:THR:HA	1:B:116:HIS:ND1	2.33	0.43
1:A:270:PHE:CZ	1:A:284:ILE:HD13	2.54	0.43
1:B:369:VAL:N	6:B:661:HOH:O	2.51	0.43
1:A:206:VAL:HG12	1:A:230:LYS:HB3	2.01	0.42
1:A:229:LYS:HE2	1:A:229:LYS:HB2	1.75	0.42
1:B:110:LEU:HD12	1:B:130:VAL:HG12	2.01	0.42
1:B:406:LYS:O	1:B:410:GLU:HG3	2.19	0.42
1:B:401:ARG:NH2	6:B:660:HOH:O	2.51	0.42
1:B:277:SER:O	1:B:281[A]:MET:HG2	2.20	0.42
4:B:504:POG:H41	4:B:504:POG:H72	1.62	0.42
4:B:504:POG:H42	6:B:695:HOH:O	2.19	0.42
1:B:277:SER:O	1:B:281[B]:MET:HG3	2.20	0.42
1:B:351:CYS:SG	6:B:661:HOH:O	2.29	0.42
1:A:236:PRO:HG3	1:A:431:LEU:HD22	2.01	0.42
1:B:36:ARG:HD3	6:B:758:HOH:O	2.20	0.42
1:A:10:THR:HA	1:A:116:HIS:ND1	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:LYS:HE2	6:B:954:HOH:O	2.18	0.41
1:B:450:LEU:HB2	6:B:846:HOH:O	2.19	0.41
1:A:146:VAL:HG12	1:A:216:GLU:HB3	2.02	0.41
1:B:146:VAL:HG22	1:B:209:ILE:HD13	2.02	0.41
1:A:188:ARG:HB3	6:A:960:HOH:O	2.21	0.41
1:A:450:LEU:HB2	6:A:805:HOH:O	2.20	0.41
1:A:372:HIS:CD2	1:A:373:VAL:HG13	2.55	0.41
1:B:447:SER:OG	1:B:451:LYS:HE2	2.20	0.41
1:A:62:ASP:OD2	6:A:605:HOH:O	2.22	0.41
1:A:105:HIS:CE1	1:A:109:ILE:HD11	2.56	0.41
4:B:503:POG:H92	4:B:503:POG:H112	1.92	0.41
1:B:200:LEU:HD23	1:B:227:LEU:HD11	2.03	0.41
1:B:365:PRO:HD3	6:B:669:HOH:O	2.20	0.41
4:B:504:POG:O1	5:B:506:M7F:O39	2.37	0.41
1:A:49:LEU:HD13	1:A:66:PHE:HB3	2.02	0.40
1:A:240:GLU:HA	1:A:241:PRO:HD3	1.91	0.40
1:A:319:LEU:HD11	1:A:328:VAL:HG23	2.03	0.40
1:B:449:LEU:HB2	6:B:616:HOH:O	2.21	0.40

All (7) 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)
6:A:781:HOH:O	6:A:1056:HOH:O[2_656]	2.06	0.14
6:A:976:HOH:O	6:B:1116:HOH:O[2_646]	2.12	0.08
6:A:698:HOH:O	6:A:729:HOH:O[2_656]	2.15	0.05
6:A:1135:HOH:O	6:A:1174:HOH:O[2_656]	2.16	0.04
6:A:1119:HOH:O	6:B:1139:HOH:O[1_655]	2.17	0.03
6:A:1129:HOH:O	6:B:1213:HOH:O[1_655]	2.17	0.03
6:A:1231:HOH:O	6:B:1184:HOH:O[1_655]	2.18	0.02

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	423/459 (92%)	415 (98%)	7 (2%)	1 (0%)	43	31
1	B	427/459 (93%)	420 (98%)	6 (1%)	1 (0%)	43	31
All	All	850/918 (93%)	835 (98%)	13 (2%)	2 (0%)	43	31

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	373	VAL
1	B	373	VAL

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	379/399 (95%)	375 (99%)	4 (1%)	65	50
1	B	381/399 (96%)	380 (100%)	1 (0%)	86	79
All	All	760/798 (95%)	755 (99%)	5 (1%)	76	64

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

Mol	Chain	Res	Type
1	A	23	LEU
1	A	52	ILE
1	A	319	LEU
1	A	359	SER
1	B	23	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	70	HIS

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Mol	Chain	Res	Type
1	A	80	HIS
1	A	242	ASN
1	A	372	HIS
1	B	286	HIS
1	B	303	GLN
1	B	372	HIS
1	B	455	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

12 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	$\# Z > 2$
3	TRS	A	502	-	7,7,7	0.32	0	9,9,9	0.36	0
5	M7F	B	505	-	73,73,73	2.29	19 (26%)	111,117,117	4.03	31 (27%)
4	POG	A	503	-	28,28,28	1.56	8 (28%)	34,34,34	0.76	0
5	M7F	A	505	-	73,73,73	2.27	19 (26%)	111,117,117	4.13	34 (30%)
4	POG	A	504	-	16,16,28	1.39	4 (25%)	19,19,34	1.31	1 (5%)
5	M7F	B	506	-	73,73,73	2.24	21 (28%)	111,117,117	4.21	41 (36%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	POG	B	503	-	28,28,28	1.44	5 (17%)	34,34,34	0.71	0
5	M7F	A	506	-	73,73,73	2.25	20 (27%)	111,117,117	4.13	30 (27%)
2	UDP	B	501	-	25,26,26	3.42	13 (52%)	38,40,40	1.48	6 (15%)
4	POG	B	504	-	28,28,28	1.45	5 (17%)	34,34,34	0.81	0
3	TRS	B	502	-	7,7,7	0.31	0	9,9,9	0.47	0
2	UDP	A	501	-	25,26,26	3.42	13 (52%)	38,40,40	1.38	5 (13%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	TRS	A	502	-	-	1/9/9/9	-
5	M7F	B	505	-	-	13/33/169/169	0/7/7/7
4	POG	A	503	-	-	13/32/32/32	-
5	M7F	A	505	-	-	10/33/169/169	0/7/7/7
4	POG	A	504	-	-	10/17/17/32	-
5	M7F	B	506	-	-	10/33/169/169	0/7/7/7
4	POG	B	503	-	-	19/32/32/32	-
5	M7F	A	506	-	-	9/33/169/169	1/7/7/7
2	UDP	B	501	-	-	3/16/32/32	0/2/2/2
4	POG	B	504	-	-	13/32/32/32	-
3	TRS	B	502	-	-	0/9/9/9	-
2	UDP	A	501	-	-	3/16/32/32	0/2/2/2

All (127) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	505	M7F	C47-C48	12.60	1.55	1.33
5	B	505	M7F	C47-C48	12.48	1.55	1.33
5	A	506	M7F	C47-C48	12.14	1.55	1.33
5	B	506	M7F	C47-C48	11.95	1.54	1.33
5	B	506	M7F	O56-C52	-7.27	1.34	1.45
5	B	505	M7F	O56-C52	-6.88	1.35	1.45
5	A	505	M7F	O56-C52	-6.81	1.35	1.45
5	A	506	M7F	O56-C52	-6.75	1.35	1.45
2	B	501	UDP	O4'-C4'	6.74	1.60	1.45
2	A	501	UDP	O4'-C4'	6.70	1.59	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	UDP	C2-N1	6.24	1.48	1.38
2	B	501	UDP	C3'-C4'	-6.09	1.37	1.53
2	B	501	UDP	C2-N3	6.09	1.48	1.38
2	A	501	UDP	C3'-C4'	-6.07	1.37	1.53
2	A	501	UDP	C6-C5	5.92	1.48	1.35
2	B	501	UDP	C2-N1	5.84	1.47	1.38
2	A	501	UDP	C2-N3	5.72	1.47	1.38
2	B	501	UDP	C6-C5	5.66	1.48	1.35
2	A	501	UDP	O4'-C1'	-4.91	1.30	1.42
2	B	501	UDP	O4'-C1'	-4.86	1.30	1.42
2	B	501	UDP	PA-O3A	4.57	1.64	1.59
5	B	506	M7F	O44-C41	-4.32	1.37	1.44
2	A	501	UDP	PA-O3A	4.26	1.64	1.59
5	A	506	M7F	O44-C41	-4.23	1.37	1.44
5	B	505	M7F	O44-C41	-3.91	1.37	1.44
2	B	501	UDP	C4-N3	3.87	1.45	1.38
5	A	505	M7F	O44-C41	-3.86	1.38	1.44
2	A	501	UDP	C4-N3	3.77	1.45	1.38
5	A	506	M7F	O37-C36	3.56	1.53	1.44
5	B	505	M7F	C07-C06	3.31	1.59	1.54
5	B	506	M7F	O37-C36	3.24	1.52	1.44
5	B	505	M7F	C02-C49	3.21	1.63	1.56
5	A	505	M7F	O37-C36	3.18	1.52	1.44
5	B	505	M7F	O37-C36	3.17	1.52	1.44
2	B	501	UDP	O3'-C3'	3.11	1.50	1.43
5	A	505	M7F	C02-C49	3.10	1.62	1.56
2	B	501	UDP	O4-C4	-3.09	1.18	1.24
5	A	505	M7F	C07-C06	3.06	1.58	1.54
5	B	505	M7F	C46-C47	3.01	1.56	1.50
2	A	501	UDP	C6-N1	2.99	1.45	1.38
5	B	505	M7F	C35-C33	2.98	1.60	1.52
5	B	506	M7F	C07-C06	2.97	1.58	1.54
2	A	501	UDP	O3'-C3'	2.96	1.50	1.43
5	A	505	M7F	C35-C33	2.94	1.60	1.52
5	A	505	M7F	C46-C47	2.88	1.56	1.50
5	A	505	M7F	C16-C15	2.76	1.60	1.53
5	B	505	M7F	C16-C15	2.70	1.60	1.53
4	A	503	POG	O4-C8	-2.68	1.39	1.44
5	B	506	M7F	C02-C49	2.64	1.61	1.56
5	A	506	M7F	C07-C06	2.61	1.58	1.54
5	A	506	M7F	C19-C20	2.60	1.58	1.52
2	B	501	UDP	C6-N1	2.60	1.44	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	506	M7F	C41-C17	-2.60	1.49	1.53
5	A	505	M7F	C01-C02	2.59	1.58	1.54
2	A	501	UDP	O4-C4	-2.58	1.19	1.24
5	B	505	M7F	C01-C02	2.54	1.58	1.54
5	A	505	M7F	O31-C28	2.54	1.49	1.43
5	A	506	M7F	O31-C28	2.51	1.49	1.43
4	B	504	POG	O5-C10	-2.50	1.40	1.44
5	B	505	M7F	O31-C28	2.50	1.49	1.43
5	A	506	M7F	C01-C02	2.49	1.58	1.54
4	A	503	POG	O7-C14	-2.48	1.40	1.44
5	B	506	M7F	C46-C47	2.48	1.55	1.50
5	A	506	M7F	C35-C33	2.46	1.58	1.52
5	B	506	M7F	C35-C33	2.46	1.58	1.52
5	B	506	M7F	C19-C20	2.45	1.58	1.52
5	A	506	M7F	O18-C17	-2.45	1.41	1.45
5	B	506	M7F	O18-C17	-2.44	1.41	1.45
5	A	506	M7F	C02-C49	2.44	1.61	1.56
4	B	504	POG	O2-C5	-2.44	1.40	1.44
5	A	506	M7F	C46-C47	2.42	1.55	1.50
5	B	506	M7F	C14-C11	-2.41	1.50	1.54
2	A	501	UDP	C5-C4	2.41	1.48	1.43
5	A	505	M7F	C64-C63	2.41	1.58	1.52
5	B	506	M7F	C53-C48	-2.40	1.50	1.54
4	A	503	POG	O5-C10	-2.40	1.40	1.44
5	B	506	M7F	C41-C17	-2.40	1.49	1.53
4	A	503	POG	O6-C12	-2.38	1.40	1.44
5	B	505	M7F	C29-C28	2.36	1.58	1.52
5	B	505	M7F	C50-C49	2.36	1.57	1.53
2	A	501	UDP	O2-C2	-2.34	1.18	1.23
5	A	506	M7F	C53-C48	-2.34	1.51	1.54
5	B	505	M7F	O21-C20	-2.34	1.37	1.43
5	B	506	M7F	O31-C28	2.34	1.48	1.43
5	A	505	M7F	C63-C62	2.33	1.58	1.52
5	A	505	M7F	C50-C49	2.33	1.57	1.53
5	A	506	M7F	C29-C28	2.30	1.58	1.52
5	B	506	M7F	C16-C15	2.30	1.59	1.53
4	A	504	POG	O5-C10	-2.27	1.40	1.44
5	B	506	M7F	C64-C63	2.26	1.58	1.52
5	A	505	M7F	O21-C20	-2.26	1.38	1.43
5	A	505	M7F	C29-C28	2.25	1.58	1.52
4	A	503	POG	O2-C5	-2.24	1.40	1.44
5	B	506	M7F	C29-C28	2.23	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	506	M7F	C63-C62	2.23	1.58	1.52
4	A	503	POG	O3-C6	-2.23	1.40	1.44
5	A	506	M7F	C64-C63	2.19	1.58	1.52
5	A	506	M7F	C16-C15	2.18	1.58	1.53
4	B	503	POG	O3-C6	-2.18	1.40	1.44
5	B	505	M7F	C64-C63	2.18	1.58	1.52
4	B	503	POG	O6-C12	-2.16	1.40	1.44
4	A	504	POG	O6-C13	-2.16	1.40	1.43
4	A	503	POG	O7-C15	-2.15	1.40	1.43
2	B	501	UDP	C5-C4	2.13	1.48	1.43
5	A	505	M7F	C19-C20	2.13	1.57	1.52
4	A	503	POG	O5-C11	-2.12	1.40	1.43
4	B	503	POG	O4-C9	-2.12	1.40	1.43
4	B	504	POG	O2-C3	-2.11	1.40	1.43
5	B	506	M7F	C25-C24	2.11	1.58	1.51
5	A	505	M7F	C60-C59	2.10	1.58	1.51
5	B	505	M7F	C60-C59	2.10	1.58	1.51
5	B	505	M7F	C19-C20	2.10	1.57	1.52
5	A	506	M7F	C25-C24	2.09	1.58	1.51
4	A	504	POG	O6-C12	-2.09	1.40	1.44
5	A	505	M7F	O09-C08	2.09	1.47	1.43
5	B	505	M7F	C51-C52	2.08	1.55	1.51
5	B	506	M7F	C01-C02	2.08	1.57	1.54
4	B	504	POG	O6-C12	-2.06	1.40	1.44
5	B	506	M7F	C50-C49	2.06	1.57	1.53
2	B	501	UDP	O2-C2	-2.05	1.19	1.23
5	B	505	M7F	C25-C24	2.05	1.58	1.51
4	B	503	POG	O7-C14	-2.05	1.40	1.44
4	B	504	POG	O5-C11	-2.04	1.40	1.43
5	B	506	M7F	C63-C62	2.04	1.57	1.52
5	A	506	M7F	C14-C11	-2.04	1.50	1.54
4	B	503	POG	O4-C8	-2.02	1.40	1.44
4	A	504	POG	O7-C15	-2.01	1.40	1.43

All (148) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	506	M7F	C10-C06-C07	-23.62	78.43	111.08
5	B	506	M7F	C10-C06-C07	-23.46	78.65	111.08
5	B	505	M7F	C10-C06-C07	-23.32	78.84	111.08
5	A	505	M7F	C10-C06-C07	-23.05	79.23	111.08
5	A	506	M7F	C10-C06-C11	-17.87	77.17	111.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	505	M7F	C10-C06-C11	-17.85	77.22	111.72
5	B	506	M7F	C10-C06-C11	-17.84	77.24	111.72
5	A	505	M7F	C10-C06-C11	-17.55	77.79	111.72
5	A	505	M7F	C10-C06-C04	-17.18	84.67	112.36
5	B	506	M7F	C10-C06-C04	-16.36	85.98	112.36
5	A	506	M7F	C10-C06-C04	-16.32	86.05	112.36
5	B	505	M7F	C10-C06-C04	-16.22	86.20	112.36
5	A	505	M7F	C05-C04-C06	-12.72	91.85	112.36
5	B	506	M7F	C05-C04-C06	-12.63	91.99	112.36
5	B	505	M7F	C05-C04-C06	-12.58	92.09	112.36
5	A	506	M7F	C05-C04-C06	-11.79	93.35	112.36
5	A	505	M7F	C06-C04-C03	7.97	117.75	109.86
5	B	506	M7F	C49-C48-C47	-7.66	109.74	121.46
5	A	505	M7F	C49-C48-C47	-7.45	110.06	121.46
5	A	506	M7F	C13-C04-C03	7.39	127.73	113.94
5	B	506	M7F	C06-C04-C03	7.20	116.98	109.86
5	A	506	M7F	C46-C03-C04	-7.19	108.28	114.70
5	A	505	M7F	C46-C03-C04	-7.12	108.35	114.70
5	B	506	M7F	C13-C04-C03	7.12	127.21	113.94
5	B	505	M7F	C06-C04-C03	7.07	116.86	109.86
5	B	505	M7F	C49-C48-C47	-6.86	110.96	121.46
5	B	506	M7F	C46-C47-C48	-6.82	113.01	125.14
5	B	505	M7F	C13-C04-C03	6.78	126.59	113.94
5	A	506	M7F	C46-C47-C48	-6.73	113.18	125.14
5	A	506	M7F	C06-C11-C14	-6.71	111.38	119.28
5	A	506	M7F	C49-C48-C47	-6.61	111.35	121.46
5	A	506	M7F	C06-C04-C03	6.58	116.37	109.86
5	A	505	M7F	C13-C04-C03	6.48	126.02	113.94
5	A	505	M7F	O18-C17-C41	6.35	114.13	106.43
5	A	505	M7F	C46-C47-C48	-6.33	113.88	125.14
5	B	506	M7F	C06-C11-C14	-6.04	112.17	119.28
5	B	505	M7F	C46-C47-C48	-5.89	114.67	125.14
5	B	506	M7F	C46-C03-C04	-5.82	109.51	114.70
5	A	506	M7F	C16-C17-C41	-5.68	107.04	115.45
5	B	506	M7F	C53-C48-C47	-5.61	118.75	122.07
5	B	505	M7F	C05-C04-C13	-5.57	91.11	111.63
5	A	506	M7F	C05-C04-C13	-5.47	91.49	111.63
5	A	505	M7F	C05-C04-C13	-5.40	91.76	111.63
5	B	506	M7F	C16-C17-C41	-5.36	107.51	115.45
5	B	506	M7F	C05-C04-C13	-5.35	91.92	111.63
5	B	505	M7F	C46-C03-C04	-5.29	109.98	114.70
5	B	505	M7F	O18-C17-C41	4.63	112.05	106.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	505	M7F	C07-C06-C11	4.61	133.11	117.43
5	B	506	M7F	C01-C02-C03	-4.55	101.97	112.81
5	A	505	M7F	C07-C06-C11	4.55	132.90	117.43
5	B	505	M7F	C43-C41-C42	-4.43	104.06	110.52
5	A	506	M7F	C03-C46-C47	4.42	121.09	112.99
5	A	505	M7F	C53-C48-C47	-4.29	119.53	122.07
5	B	506	M7F	C03-C46-C47	4.22	120.73	112.99
5	B	506	M7F	C01-C02-C49	-4.20	100.51	110.17
5	B	506	M7F	C07-C06-C11	4.19	131.66	117.43
5	A	505	M7F	C01-C02-C49	-4.09	100.75	110.17
2	A	501	UDP	C4-N3-C2	-4.03	121.61	126.61
5	A	506	M7F	C13-C04-C06	4.03	106.62	101.83
5	B	505	M7F	C13-C04-C06	4.01	106.61	101.83
5	B	505	M7F	C06-C11-C14	-3.96	114.62	119.28
5	B	505	M7F	C01-C02-C49	-3.93	101.13	110.17
5	B	506	M7F	C51-C52-C53	-3.85	110.38	113.28
5	A	506	M7F	C04-C06-C11	3.82	109.32	100.94
5	A	506	M7F	C01-C02-C03	-3.78	103.81	112.81
5	B	506	M7F	C13-C04-C06	3.75	106.29	101.83
5	A	506	M7F	C07-C06-C11	3.73	130.10	117.43
5	A	505	M7F	C13-C04-C06	3.72	106.26	101.83
5	B	506	M7F	C16-C15-C14	-3.66	105.98	115.37
5	A	506	M7F	C16-C15-C14	-3.65	106.02	115.37
2	A	501	UDP	C5-C4-N3	3.63	119.89	114.80
5	A	505	M7F	C16-C17-C41	-3.61	110.10	115.45
5	A	506	M7F	C01-C02-C49	-3.59	101.91	110.17
2	B	501	UDP	C5-C4-N3	3.56	119.79	114.80
2	B	501	UDP	C4-N3-C2	-3.56	122.19	126.61
5	A	506	M7F	C53-C48-C47	-3.56	119.96	122.07
5	B	505	M7F	C50-C51-C52	3.47	117.10	110.79
5	B	505	M7F	C01-C02-C03	-3.45	104.60	112.81
5	B	506	M7F	C04-C06-C11	3.31	108.20	100.94
5	B	506	M7F	O18-C17-C41	3.23	110.35	106.43
2	B	501	UDP	O4-C4-C5	-3.21	119.63	125.16
5	A	505	M7F	C03-C46-C47	3.13	118.74	112.99
5	A	505	M7F	C06-C11-C14	-3.09	115.64	119.28
4	A	504	POG	C13-O6-C12	3.09	119.61	115.05
5	B	505	M7F	C03-C46-C47	3.08	118.64	112.99
5	A	506	M7F	O18-C17-C41	3.08	110.17	106.43
5	B	505	M7F	C05-C04-C03	3.07	115.58	111.49
5	A	505	M7F	C01-C02-C03	-3.02	105.63	112.81
5	B	506	M7F	O58-C59-C60	2.99	113.86	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	505	M7F	C53-C48-C47	-2.94	120.33	122.07
5	A	505	M7F	C50-C49-C02	-2.86	109.48	114.64
5	A	505	M7F	C05-C04-C03	2.78	115.20	111.49
5	A	505	M7F	C04-C06-C11	2.78	107.04	100.94
5	B	505	M7F	C50-C49-C02	-2.77	109.65	114.64
5	A	505	M7F	C12-C11-C14	-2.75	108.02	112.18
5	A	506	M7F	C43-C41-C17	-2.73	105.80	110.58
2	B	501	UDP	O2-C2-N1	-2.73	119.25	122.80
5	B	505	M7F	C16-C17-C41	-2.70	111.46	115.45
2	A	501	UDP	O4-C4-C5	-2.68	120.54	125.16
5	B	505	M7F	C04-C06-C11	2.65	106.76	100.94
5	B	506	M7F	C57-C64-C63	2.63	115.55	110.01
5	A	505	M7F	O09-C08-C07	-2.62	104.08	110.11
5	A	506	M7F	C03-C02-C08	2.62	112.47	107.52
5	B	506	M7F	C19-O18-C17	-2.60	110.29	114.92
5	B	506	M7F	C03-C02-C08	2.59	112.42	107.52
5	A	506	M7F	C57-O58-C59	-2.58	108.67	113.72
5	B	506	M7F	C57-O58-C59	2.56	118.72	113.72
5	B	506	M7F	C64-C63-C62	2.55	115.31	110.83
5	A	505	M7F	C19-O37-C36	2.54	118.68	113.72
5	A	506	M7F	O09-C08-C07	-2.52	104.33	110.11
5	A	506	M7F	O37-C19-C20	2.46	114.27	109.49
5	A	505	M7F	C50-C51-C52	2.44	115.24	110.79
5	B	506	M7F	O37-C19-C20	2.42	114.20	109.49
5	B	505	M7F	C12-C11-C14	-2.41	108.53	112.18
2	A	501	UDP	N3-C2-N1	2.41	118.03	114.89
5	B	505	M7F	C19-O37-C36	2.40	118.41	113.72
5	A	506	M7F	O39-C38-C36	-2.40	103.17	111.33
5	A	505	M7F	C03-C02-C08	2.39	112.04	107.52
5	A	505	M7F	O58-C59-C62	2.37	113.97	109.70
5	B	506	M7F	C63-C62-C59	2.35	114.50	110.23
5	B	506	M7F	C25-C24-C27	-2.35	107.24	113.02
5	B	506	M7F	O39-C38-C36	-2.33	103.41	111.33
5	B	505	M7F	O37-C19-C20	2.32	113.99	109.49
5	B	505	M7F	C60-C59-C62	-2.31	107.35	113.02
5	B	506	M7F	C60-C59-C62	-2.28	107.42	113.02
5	B	505	M7F	C06-C07-C08	2.27	116.46	113.20
5	A	506	M7F	C57-O56-C52	-2.27	110.89	114.92
5	A	505	M7F	C50-C49-C48	2.22	117.31	111.32
5	B	505	M7F	C03-C02-C08	2.22	111.72	107.52
5	B	505	M7F	O09-C08-C07	-2.20	105.05	110.11
5	B	506	M7F	C01-C02-C08	2.20	113.09	108.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	505	M7F	C06-C07-C08	2.19	116.35	113.20
2	B	501	UDP	C2'-C3'-C4'	2.14	106.74	102.61
5	B	506	M7F	O58-C57-C64	2.12	114.73	110.37
5	A	505	M7F	O37-C19-C20	2.12	113.61	109.49
5	B	506	M7F	O09-C08-C07	-2.12	105.25	110.11
2	B	501	UDP	O2B-PB-O3A	2.11	111.70	104.64
5	A	505	M7F	C51-C50-C49	2.11	117.34	112.06
5	A	505	M7F	C63-C62-C59	2.10	114.04	110.23
5	A	506	M7F	C50-C51-C52	2.08	114.57	110.79
5	B	506	M7F	C22-O21-C20	-2.07	113.07	117.98
5	B	506	M7F	C42-C41-C17	-2.07	106.95	110.58
5	A	506	M7F	C19-O18-C17	-2.05	111.27	114.92
5	A	505	M7F	C33-C35-C36	2.04	113.94	110.23
5	B	506	M7F	C05-C04-C03	2.04	114.21	111.49
2	A	501	UDP	O4'-C4'-C5'	-2.02	102.86	109.33
5	B	506	M7F	O66-C63-C64	-2.01	105.64	110.38
5	B	506	M7F	C12-C11-C14	-2.01	109.14	112.18

There are no chirality outliers.

All (104) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503	POG	O1-C4-C6-O3
4	A	503	POG	O1-C4-C6-C21
4	A	503	POG	O3-C7-C8-O4
4	A	503	POG	O5-C10-C9-O4
4	A	503	POG	O5-C11-C12-C18
4	A	503	POG	O6-C13-C14-O7
4	A	503	POG	O6-C13-C14-C17
4	A	504	POG	O7-C15-C5-O2
4	A	504	POG	O5-C10-C9-O4
4	A	504	POG	C19-C10-C9-O4
4	A	504	POG	C11-C12-O6-C13
4	B	503	POG	OH-C2-C3-O2
4	B	503	POG	C16-C5-O2-C3
4	B	503	POG	O1-C4-C6-O3
4	B	503	POG	O1-C4-C6-C21
4	B	503	POG	O3-C7-C8-O4
4	B	503	POG	O3-C7-C8-C20
4	B	503	POG	O5-C11-C12-O6
4	B	503	POG	O5-C11-C12-C18
4	B	503	POG	O6-C13-C14-O7

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Mol	Chain	Res	Type	Atoms
4	B	503	POG	C17-C14-O7-C15
4	B	504	POG	O1-C4-C6-O3
4	B	504	POG	O1-C4-C6-C21
4	B	504	POG	C4-C6-O3-C7
4	B	504	POG	C20-C8-O4-C9
4	B	504	POG	C19-C10-C9-O4
4	B	504	POG	C19-C10-O5-C11
5	A	505	M7F	C41-C17-O18-C19
5	B	505	M7F	C41-C17-O18-C19
5	B	506	M7F	C64-C57-O56-C52
5	B	506	M7F	O58-C57-O56-C52
5	B	505	M7F	C45-C14-C15-C16
5	B	506	M7F	O23-C24-C25-O26
5	A	505	M7F	C45-C14-C15-C16
5	A	505	M7F	O37-C36-C38-O39
5	B	506	M7F	C27-C24-C25-O26
5	B	505	M7F	O37-C36-C38-O39
5	B	506	M7F	C45-C14-C15-C16
5	A	506	M7F	C11-C14-C15-C16
5	B	506	M7F	C11-C14-C15-C16
5	A	506	M7F	O23-C24-C25-O26
5	A	505	M7F	C35-C36-C38-O39
5	B	505	M7F	C35-C36-C38-O39
5	A	505	M7F	C11-C14-C15-C16
5	A	506	M7F	C45-C14-C15-C16
5	B	505	M7F	C11-C14-C15-C16
5	B	506	M7F	C35-C36-C38-O39
5	B	506	M7F	O37-C36-C38-O39
2	A	501	UDP	C3'-C4'-C5'-O5'
5	A	506	M7F	C27-C24-C25-O26
5	B	505	M7F	C06-C11-C14-C45
5	A	505	M7F	C06-C11-C14-C45
5	A	505	M7F	C06-C11-C14-C15
5	B	505	M7F	C06-C11-C14-C15
5	A	506	M7F	C35-C36-C38-O39
5	A	506	M7F	O37-C36-C38-O39
2	A	501	UDP	O4'-C4'-C5'-O5'
4	A	504	POG	O7-C15-C5-C16
4	B	503	POG	C1-C2-C3-O2
4	B	504	POG	C17-C14-O7-C15
5	B	506	M7F	O58-C59-C60-O61
4	A	503	POG	C8-C7-O3-C6

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Mol	Chain	Res	Type	Atoms
4	B	503	POG	C2-C3-O2-C5
4	B	503	POG	C5-C15-O7-C14
4	B	504	POG	C14-C13-O6-C12
4	A	503	POG	C19-C10-C9-O4
4	A	504	POG	O6-C13-C14-C17
4	B	503	POG	O7-C15-C5-C16
4	B	504	POG	O5-C11-C12-C18
4	A	503	POG	O5-C11-C12-O6
4	A	504	POG	O6-C13-C14-O7
4	B	503	POG	O7-C15-C5-O2
4	B	504	POG	O5-C10-C9-O4
4	B	504	POG	O5-C11-C12-O6
5	B	505	M7F	O18-C17-C41-O44
2	A	501	UDP	PB-O3A-PA-O5'
2	B	501	UDP	PB-O3A-PA-O5'
5	A	505	M7F	C12-C11-C14-C45
5	B	505	M7F	C12-C11-C14-C45
5	B	505	M7F	O18-C17-C41-C42
5	B	505	M7F	O18-C17-C41-C43
5	A	505	M7F	C12-C11-C14-C15
5	B	505	M7F	C12-C11-C14-C15
5	B	505	M7F	C16-C17-C41-C42
2	B	501	UDP	O4'-C4'-C5'-O5'
4	A	504	POG	C14-C13-O6-C12
4	A	504	POG	C5-C15-O7-C14
4	B	503	POG	C8-C7-O3-C6
3	A	502	TRS	C2-C-C1-O1
2	B	501	UDP	C3'-C4'-C5'-O5'
5	A	506	M7F	C62-C59-C60-O61
4	B	504	POG	O3-C7-C8-O4
4	B	504	POG	O6-C13-C14-O7
5	A	505	M7F	C16-C17-C41-C43
4	B	503	POG	C19-C10-O5-C11
4	A	503	POG	C12-C11-O5-C10
5	A	506	M7F	O18-C17-C41-O44
5	B	506	M7F	C06-C11-C14-C45
4	A	503	POG	C11-C12-O6-C13
4	A	504	POG	C13-C14-O7-C15
4	B	503	POG	C4-C6-O3-C7
4	A	503	POG	C19-C10-O5-C11
4	B	503	POG	O6-C13-C14-C17
5	A	506	M7F	C06-C11-C14-C45

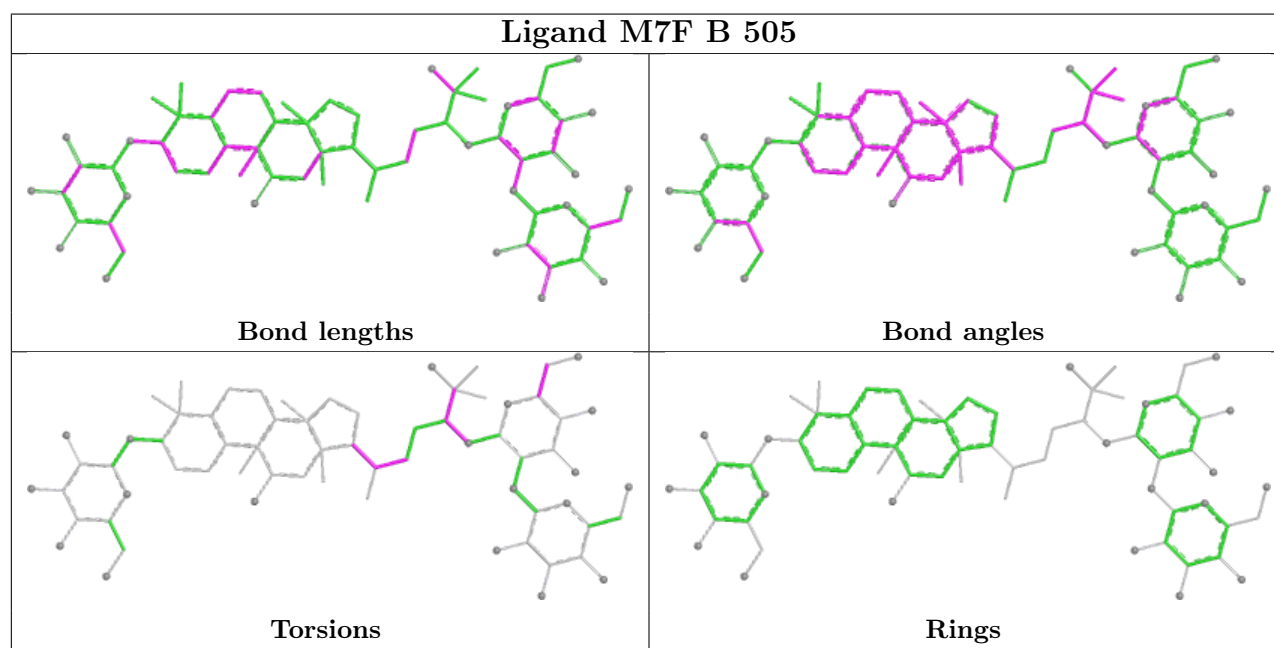
All (1) ring outliers are listed below:

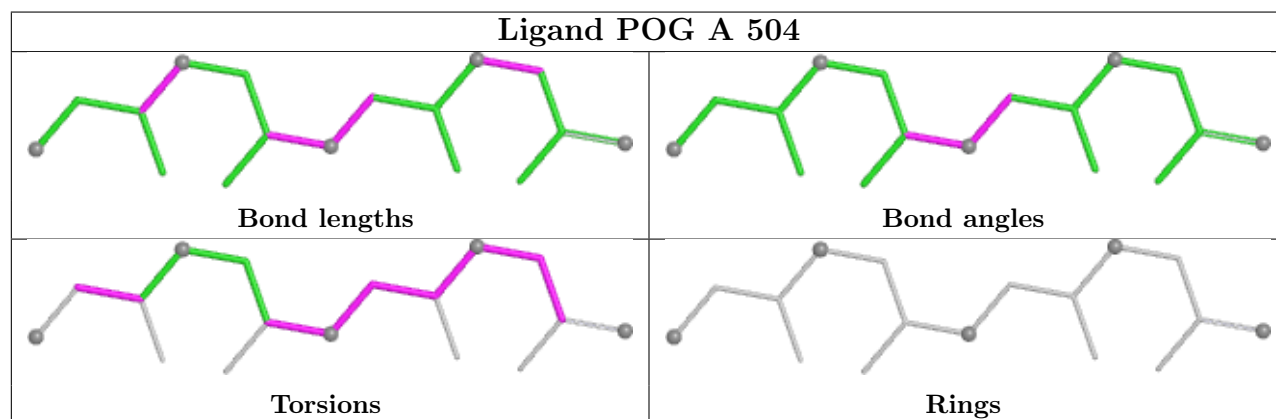
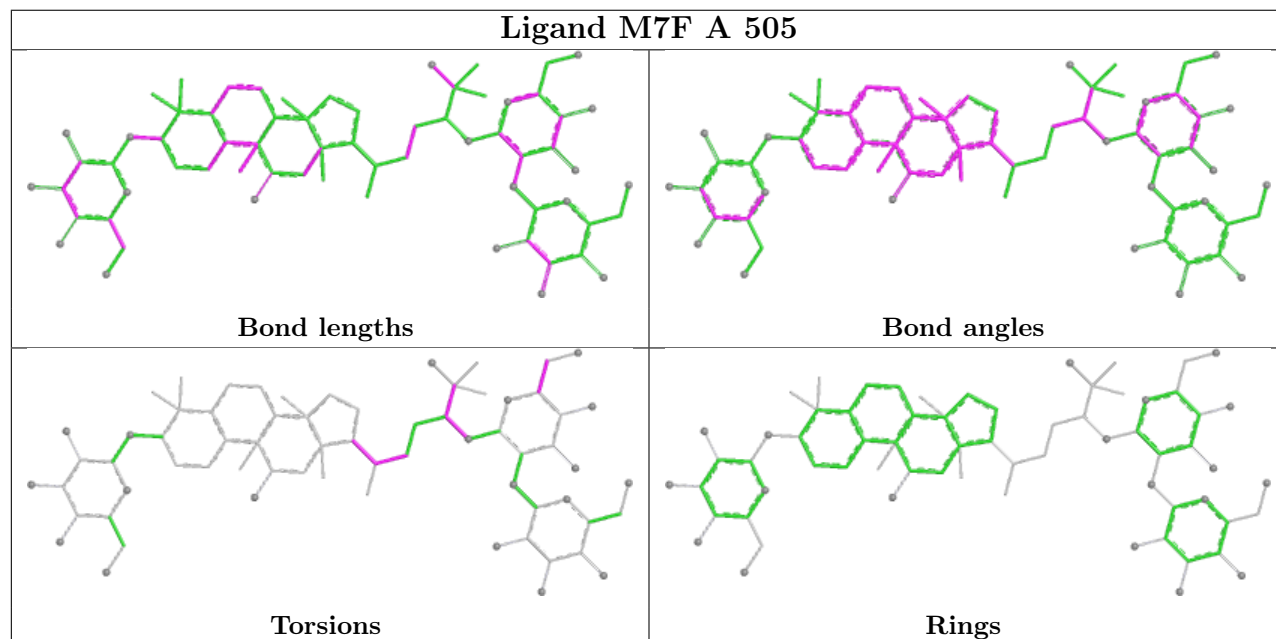
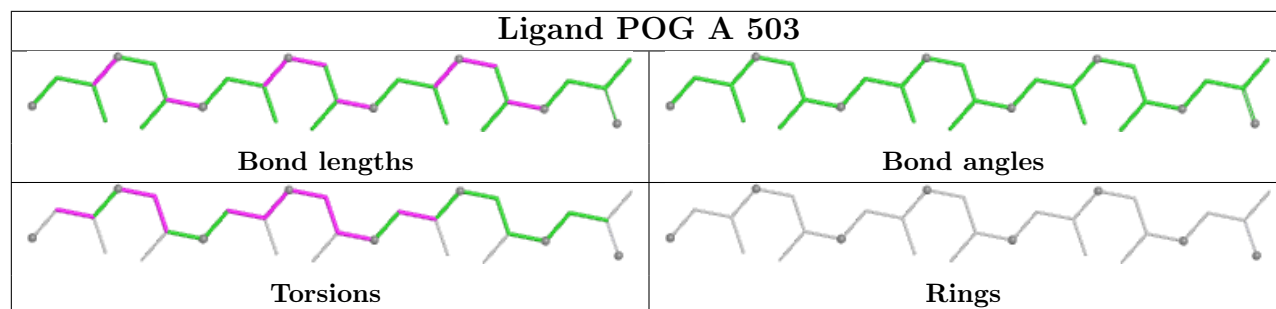
Mol	Chain	Res	Type	Atoms
5	A	506	M7F	C48-C49-C50-C51-C52-C53

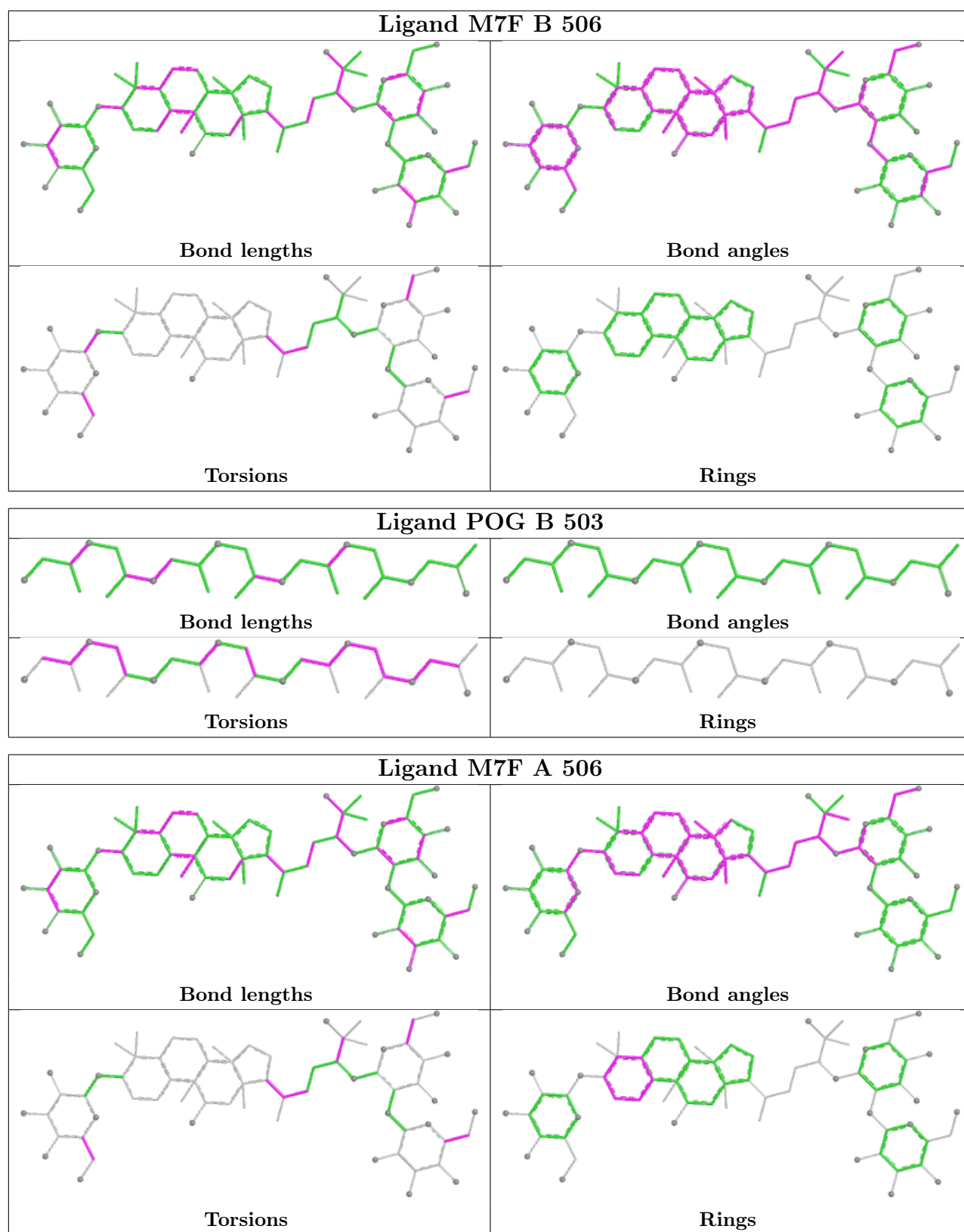
5 monomers are involved in 10 short contacts:

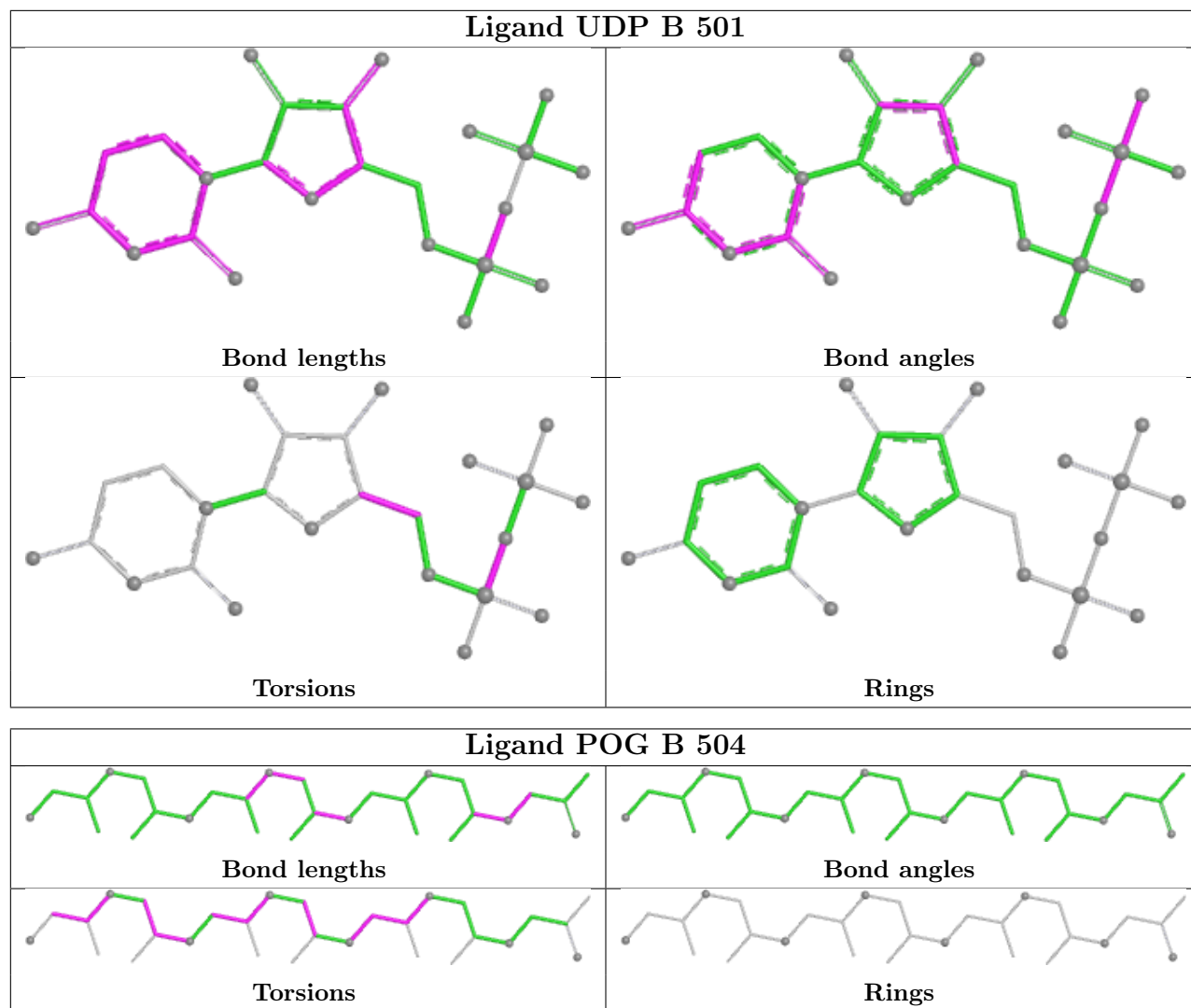
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	505	M7F	1	0
4	A	503	POG	2	0
5	B	506	M7F	1	0
4	B	503	POG	3	0
4	B	504	POG	5	0

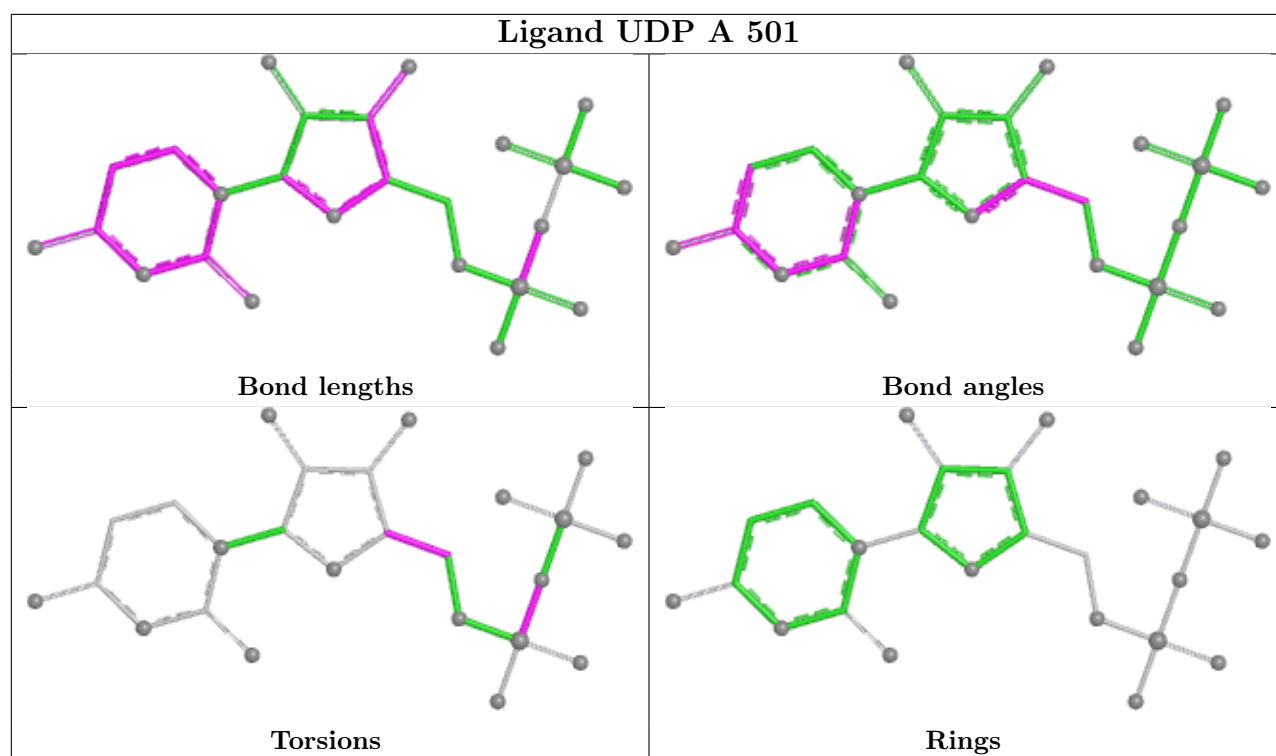
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.











5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	427/459 (93%)	0.33	16 (3%) 45 53	5, 15, 33, 58	14 (3%)
1	B	429/459 (93%)	0.44	15 (3%) 47 55	4, 16, 33, 54	17 (3%)
All	All	856/918 (93%)	0.39	31 (3%) 46 54	4, 16, 33, 58	31 (3%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	165	PHE	6.0
1	A	176	ALA	4.5
1	A	303	GLN	4.5
1	B	177	MET	4.5
1	A	165	PHE	4.0
1	B	242	ASN	4.0
1	B	185	SER	3.8
1	B	457	HIS	3.7
1	B	313	ALA	3.6
1	A	457	HIS	3.5
1	B	164	PRO	3.5
1	A	273	GLU	3.4
1	A	313	ALA	3.4
1	B	186	THR	3.3
1	B	303	GLN	3.2
1	B	176	ALA	3.2
1	A	274	TYR	3.0
1	A	164	PRO	2.9
1	A	247	ASP	2.8
1	A	372	HIS	2.5
1	B	248	GLU	2.5
1	A	241	PRO	2.5
1	A	249	GLY	2.4
1	A	158	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	186	THR	2.3
1	B	241	PRO	2.2
1	A	161	SER	2.2
1	A	242	ASN	2.2
1	B	161	SER	2.2
1	B	247	ASP	2.1
1	B	75	PRO	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

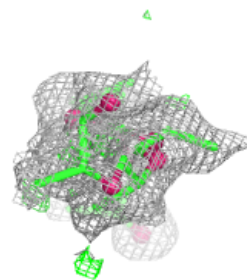
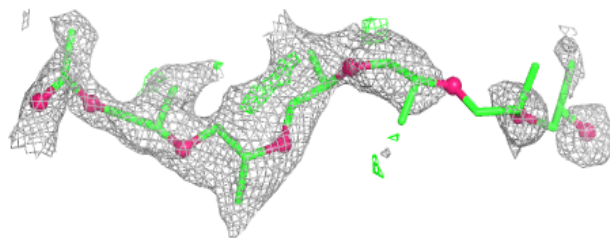
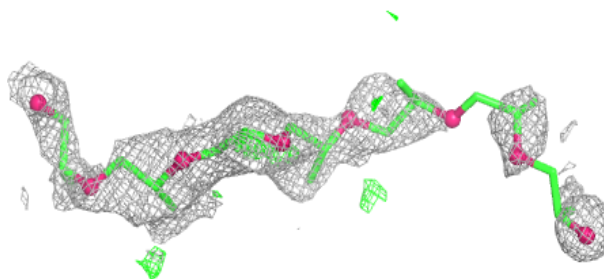
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	POG	B	504	29/29	0.78	0.16	15,29,44,50	19
4	POG	B	503	29/29	0.82	0.16	13,32,56,60	13
4	POG	A	503	29/29	0.82	0.17	12,28,46,51	14
4	POG	A	504	17/29	0.87	0.13	7,18,30,53	7
5	M7F	A	506	67/67	0.87	0.14	6,20,43,59	23
5	M7F	B	506	67/67	0.87	0.14	4,21,49,57	16
5	M7F	B	505	67/67	0.91	0.10	6,13,33,47	12
5	M7F	A	505	67/67	0.91	0.10	4,12,33,38	14
3	TRS	B	502	8/8	0.94	0.06	6,8,12,13	0
3	TRS	A	502	8/8	0.97	0.06	6,9,13,16	0
2	UDP	A	501	25/25	0.98	0.05	3,7,11,16	4
2	UDP	B	501	25/25	0.98	0.05	3,8,12,19	4

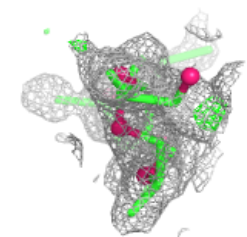
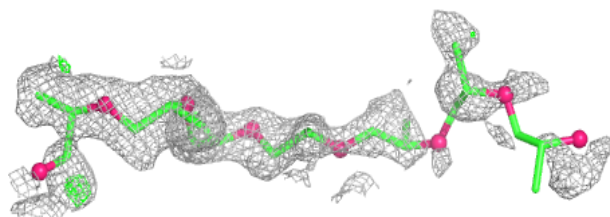
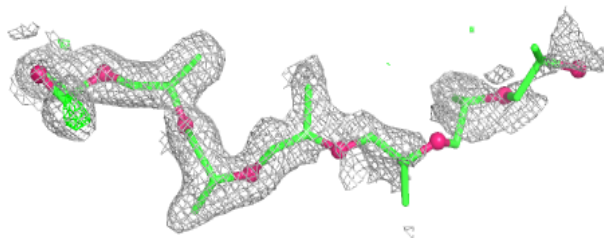
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around POG 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)

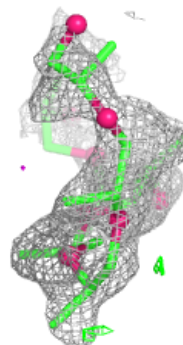
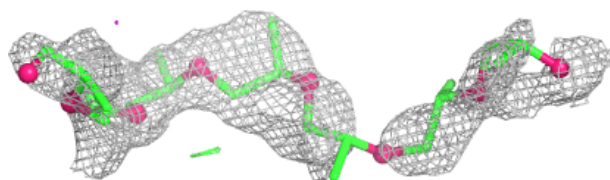
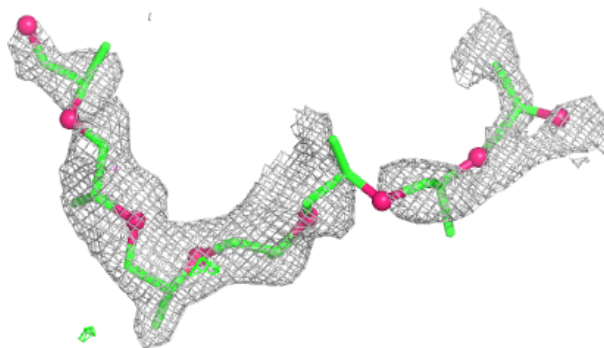
**Electron density around POG B 503:**

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

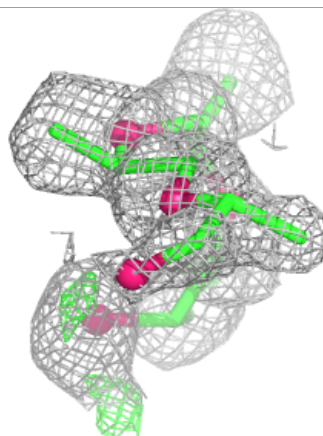
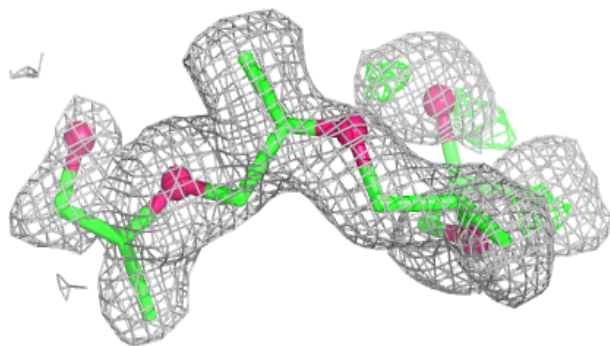
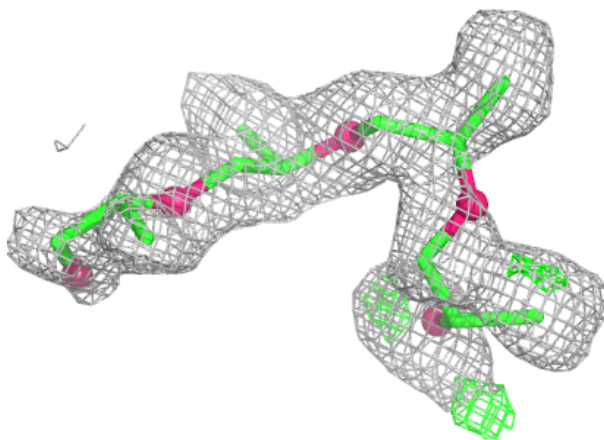


Electron density around POG A 503:

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

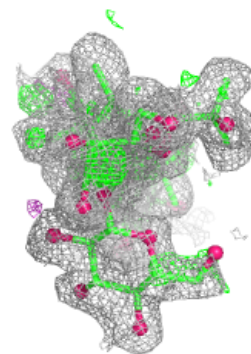
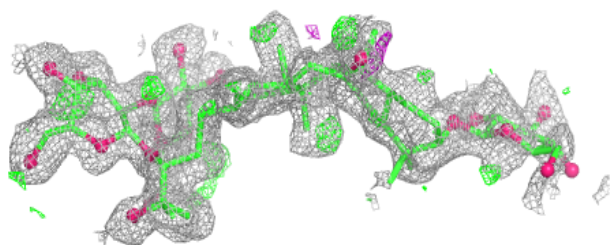
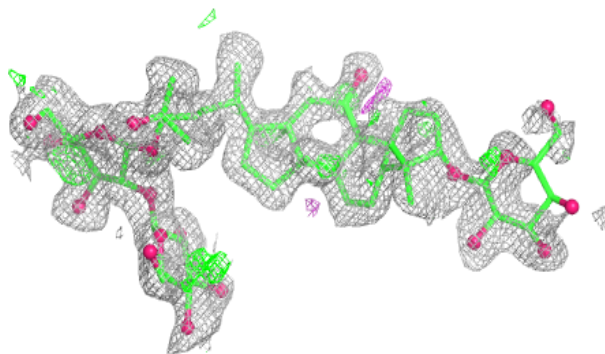
**Electron density around POG A 504:**

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

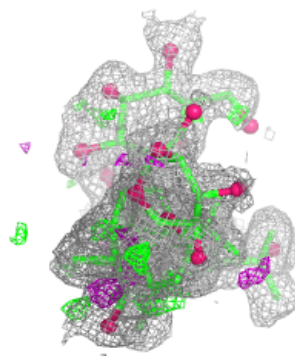
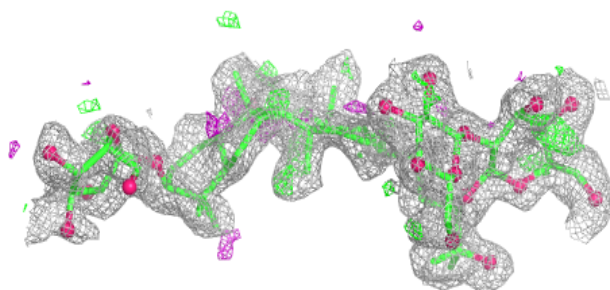
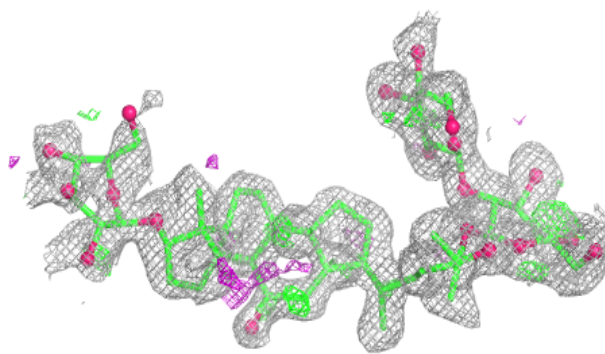


Electron density around M7F A 506:

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

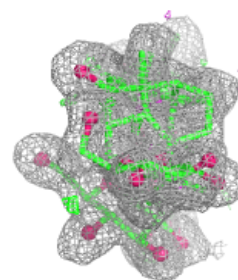
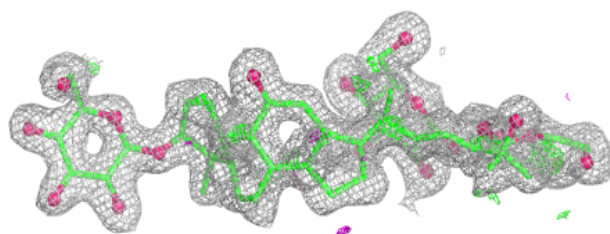
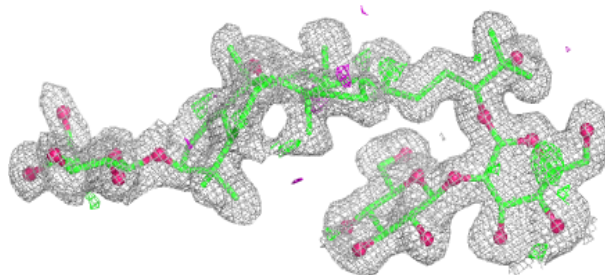
**Electron density around M7F B 506:**

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

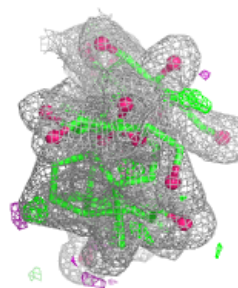
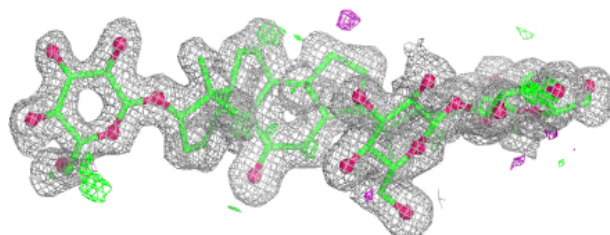
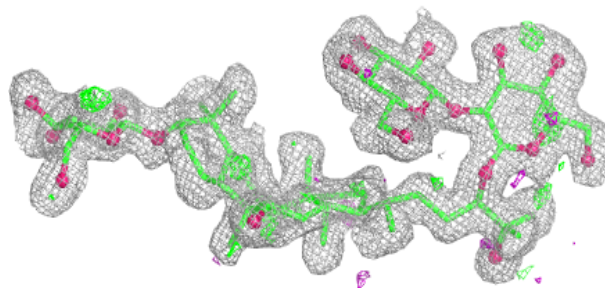


Electron density around M7F B 505:

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

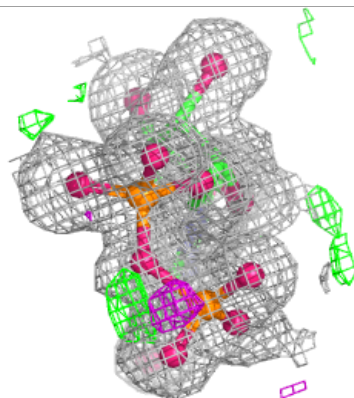
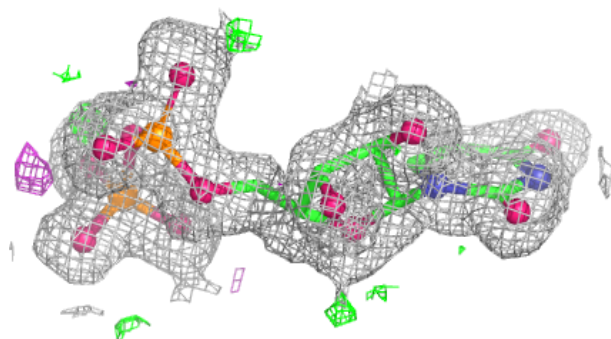
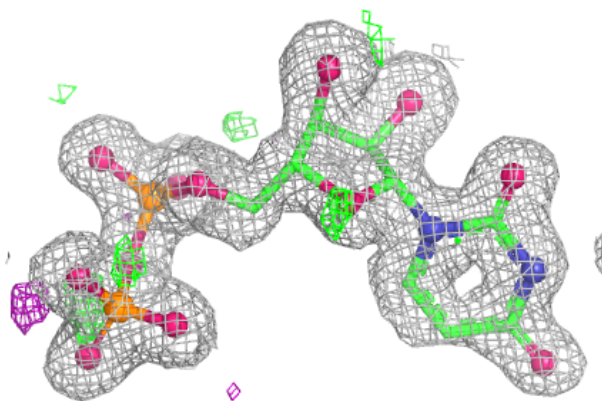
**Electron density around M7F A 505:**

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

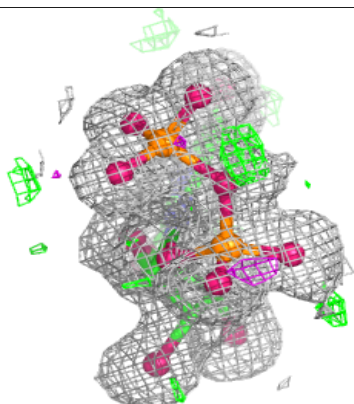
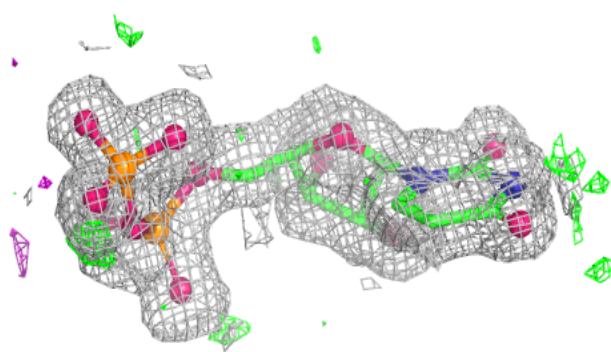
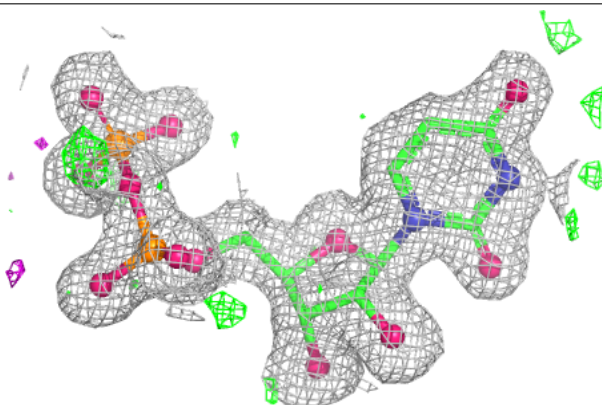


Electron density around UDP A 501:

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

**Electron density around UDP 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)



6.5 Other polymers ⓘ

There are no such residues in this entry.