



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2021 – 10:08 AM JST

PDB ID : 7E9S
Title : Archaeal oligosaccharyltransferase AglB from *Archaeoglobus fulgidus* in complex with an inhibitory peptide and a dolichol-phosphate
Authors : Taguchi, Y.; Hirata, K.; Kohda, D.
Deposited on : 2021-03-05
Resolution : 2.70 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 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 : 2.23.1
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) : 2.23.1

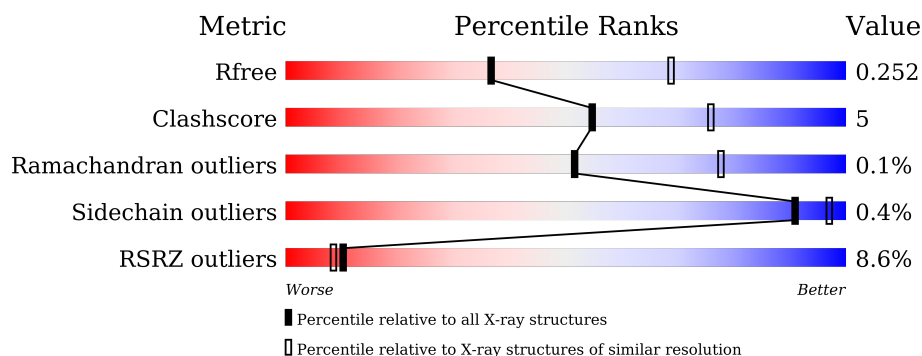
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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	875	<div> <div>8%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
2	B	10	<div> <div>40%</div> <div>70%</div> <div>20%</div> <div>10%</div> </div>

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:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	PEG	A	905	-	-	-	X
5	PEG	A	906	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7233 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 Dolichyl-phosphooligosaccharide-protein glycotransferase 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	867	Total	C	N	O	S	0	0	0
			6970	4628	1111	1214	17			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	617	CYS	GLY	engineered mutation	UNP O29867
A	869	GLU	-	expression tag	UNP O29867
A	870	LEU	-	expression tag	UNP O29867
A	871	ALA	-	expression tag	UNP O29867
A	872	LEU	-	expression tag	UNP O29867
A	873	VAL	-	expression tag	UNP O29867
A	874	PRO	-	expression tag	UNP O29867
A	875	ARG	-	expression tag	UNP O29867

- Molecule 2 is a protein called a polypeptide linked to an inhibitory N-glycosylation sequon-containing peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	9	Total	C	N	O	S	0	0	0
			62	39	10	12	1			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

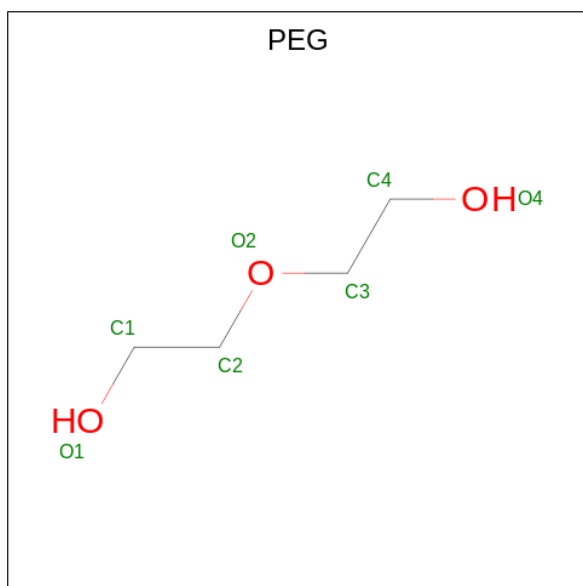
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Mn	0	0
			1	1		

- Molecule 4 is [(3S,6Z,10Z,14Z,18Z,22Z,26Z,30Z,34Z,39S,43S)-3,7,11,15,19,23,27,31,35,39,43,47-dodecamethyloctatetraconta-6,10,14,18,22,26,30,34-octaenyl] dihydrogen phosphate (three-letter code: J06) (formula: C₆₀H₁₀₇O₄P) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	O	P	0	0
			65	60	4	1		

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



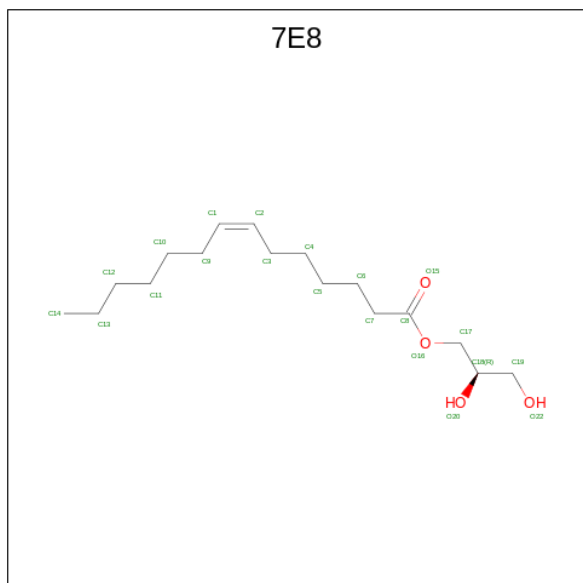
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		
5	A	1	Total	C	O	0	0
			7	4	3		

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

- Molecule 6 is (2R)-2,3-DIHYDROXYPROPYL (7Z)-TETRADEC-7-ENOATE (three-letter code: 7E8) (formula: C₁₇H₃₂O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			21	17	4		
6	A	1	Total	C	O	0	0
			21	17	4		
6	A	1	Total	C	O	0	0
			21	17	4		
6	A	1	Total	C	O	0	0
			21	17	4		

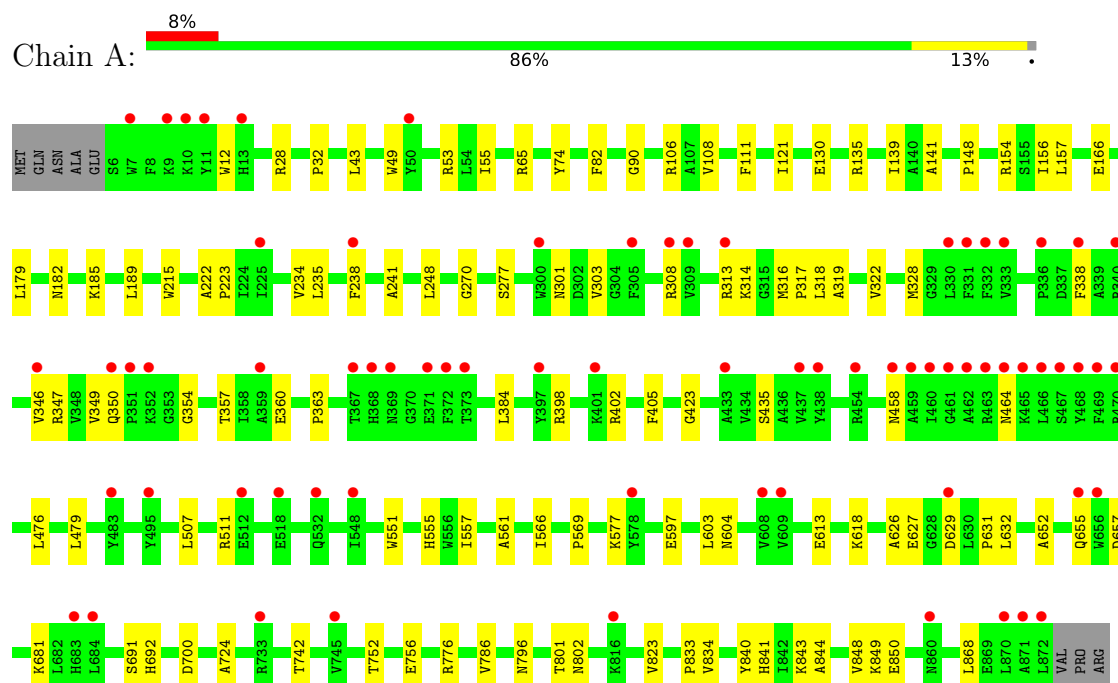
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	16	Total	O	0	0
			16	16		

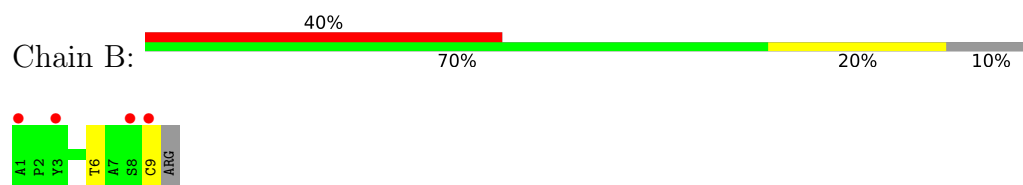
3 Residue-property plots

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: Dolichyl-phosphooligosaccharide-protein glycotransferase 3



- Molecule 2: a polypeptide linked to an inhibitory N-glycosylation sequon-containing peptide



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	345.74Å 48.69Å 63.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.84 – 2.70 24.84 – 2.70	Depositor EDS
% Data completeness (in resolution range)	99.8 (24.84-2.70) 99.9 (24.84-2.70)	Depositor EDS
R_{merge}	0.43	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 2.72Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.215 , 0.252 0.215 , 0.252	Depositor DCC
R_{free} test set	1485 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	70.2	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 67.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7233	wwPDB-VP
Average B, all atoms (Å ²)	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.24% 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: 7E8, J06, DAB, MN, PEG

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	0.26	0/7197	0.43	0/9824
2	B	0.22	0/55	0.55	0/74
All	All	0.26	0/7252	0.44	0/9898

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	6970	0	6872	74	0
2	B	62	0	60	2	0
3	A	1	0	0	0	0
4	A	65	0	0	0	0
5	A	35	0	50	3	0
6	A	84	0	128	5	0
7	A	16	0	0	0	0
All	All	7233	0	7110	75	0

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 5.

All (75) 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)
5:A:906:PEG:H42	5:A:907:PEG:H32	1.73	0.71
1:A:121:ILE:HG23	1:A:141:ALA:HB1	1.79	0.64
1:A:613:GLU:HB3	1:A:618:LYS:HD2	1.80	0.62
1:A:796:ASN:HB3	1:A:841:HIS:HB2	1.81	0.62
1:A:802:ASN:HB3	1:A:833:PRO:HB2	1.83	0.61
1:A:618:LYS:HE2	2:B:6:THR:HB	1.83	0.59
1:A:349:VAL:HG12	6:A:911:7E8:H8	1.82	0.59
1:A:629:ASP:HB3	1:A:632:LEU:HB3	1.85	0.58
1:A:652:ALA:HB1	1:A:657:ASP:HB2	1.87	0.56
1:A:597:GLU:OE1	1:A:776:ARG:NH1	2.38	0.56
1:A:65:ARG:NH2	1:A:82:PHE:O	2.39	0.56
1:A:843:LYS:HG3	1:A:848:VAL:HG22	1.87	0.56
1:A:627:GLU:HB3	1:A:632:LEU:HD23	1.88	0.56
1:A:314:LYS:HG3	1:A:318:LEU:HD23	1.87	0.55
1:A:350:GLN:HE21	1:A:363:PRO:HD3	1.71	0.55
1:A:314:LYS:O	1:A:318:LEU:HD23	2.06	0.55
1:A:566:ILE:HD12	1:A:603:LEU:HB3	1.88	0.55
1:A:32:PRO:HG3	1:A:156:ILE:HG13	1.89	0.54
1:A:314:LYS:HE3	1:A:318:LEU:HD21	1.88	0.53
1:A:346:VAL:HA	1:A:349:VAL:HG22	1.89	0.53
1:A:55:ILE:HD13	1:A:90:GLY:HA3	1.90	0.53
1:A:476:LEU:O	1:A:479:LEU:HB3	2.09	0.53
1:A:752:THR:HA	1:A:756:GLU:HB2	1.92	0.52
1:A:629:ASP:OD2	1:A:631:PRO:HG2	2.10	0.52
1:A:135:ARG:O	1:A:139:ILE:HD12	2.09	0.51
1:A:458:ASN:HD21	1:A:464:ASN:HB2	1.74	0.51
1:A:681:LYS:HE3	5:A:903:PEG:H11	1.91	0.51
1:A:700:ASP:HB2	5:A:906:PEG:H32	1.94	0.50
1:A:786:VAL:HG23	1:A:844:ALA:HB1	1.94	0.49
1:A:108:VAL:HG13	6:A:909:7E8:H111	1.95	0.49
1:A:43:LEU:HG	1:A:106:ARG:HD2	1.95	0.48
1:A:234:VAL:HG23	1:A:235:LEU:HD13	1.94	0.48
1:A:234:VAL:HA	1:A:317:PRO:HB3	1.95	0.48
1:A:166:GLU:OE2	1:A:215:TRP:CD2	2.67	0.48
1:A:319:ALA:HA	1:A:322:VAL:HG22	1.94	0.48
1:A:692:HIS:HE1	6:A:910:7E8:H122	1.79	0.47
1:A:166:GLU:OE2	1:A:215:TRP:CE2	2.68	0.47
1:A:577:LYS:HD3	1:A:626:ALA:HB1	1.97	0.47
1:A:235:LEU:HB3	1:A:238:PHE:HB3	1.97	0.47
1:A:849:LYS:HB2	1:A:868:LEU:HD21	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:GLU:HG3	1:A:179:LEU:HB2	1.96	0.47
1:A:111:PHE:HE2	6:A:909:7E8:H31C	1.80	0.46
1:A:111:PHE:CE2	6:A:909:7E8:H31C	2.50	0.46
1:A:347:ARG:HA	1:A:347:ARG:HD3	1.74	0.45
1:A:655:GLN:H	1:A:655:GLN:CD	2.20	0.45
1:A:398:ARG:HG3	1:A:402:ARG:HD3	1.99	0.45
1:A:384:LEU:O	1:A:435:SER:HB2	2.16	0.45
1:A:303:VAL:HG22	1:A:308:ARG:HH12	1.82	0.45
1:A:566:ILE:HG21	1:A:603:LEU:HD13	2.00	0.44
1:A:154:ARG:NH2	1:A:360:GLU:OE1	2.50	0.44
1:A:314:LYS:HG3	1:A:318:LEU:CD2	2.48	0.44
1:A:691:SER:HB2	1:A:823:VAL:HB	1.99	0.44
1:A:28:ARG:HA	1:A:156:ILE:HD12	2.00	0.43
1:A:840:TYR:O	1:A:850:GLU:HA	2.18	0.43
1:A:318:LEU:O	1:A:322:VAL:HG13	2.19	0.43
1:A:182:ASN:HA	1:A:185:LYS:HE2	2.01	0.42
1:A:555:HIS:CE1	1:A:569:PRO:HD2	2.54	0.42
1:A:74:TYR:HE2	1:A:604:ASN:HB3	1.83	0.42
1:A:801:THR:HA	1:A:834:VAL:HG22	2.00	0.42
1:A:458:ASN:ND2	1:A:464:ASN:HB2	2.35	0.42
1:A:222:ALA:HB3	1:A:223:PRO:HD3	2.01	0.41
1:A:241:ALA:HB2	1:A:405:PHE:HB2	2.01	0.41
1:A:301:ASN:HB2	1:A:316:MET:HG3	2.02	0.41
1:A:189:LEU:HD13	1:A:248:LEU:HD13	2.02	0.41
1:A:350:GLN:NE2	1:A:423:GLY:O	2.32	0.41
1:A:618:LYS:HG3	2:B:9:CYS:SG	2.61	0.41
1:A:270:GLY:O	1:A:277:SER:HB2	2.20	0.41
1:A:507:LEU:HD22	1:A:557:ILE:HA	2.02	0.41
1:A:32:PRO:HG2	1:A:157:LEU:HB3	2.03	0.40
1:A:724:ALA:HB1	1:A:742:THR:HG23	2.01	0.40
1:A:551:TRP:CE3	1:A:569:PRO:HA	2.57	0.40
1:A:43:LEU:O	1:A:49:TRP:NE1	2.53	0.40
1:A:511:ARG:HB2	1:A:561:ALA:HA	2.03	0.40
1:A:328:MET:O	1:A:338:PHE:HZ	2.04	0.40
1:A:354:GLY:O	1:A:357:THR:OG1	2.37	0.40

There are no symmetry-related clashes.

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	865/875 (99%)	828 (96%)	36 (4%)	1 (0%)	51	78
2	B	6/10 (60%)	4 (67%)	2 (33%)	0	100	100
All	All	871/885 (98%)	832 (96%)	38 (4%)	1 (0%)	51	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	148	PRO

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	720/728 (99%)	717 (100%)	3 (0%)	91	97
2	B	6/7 (86%)	6 (100%)	0	100	100
All	All	726/735 (99%)	723 (100%)	3 (0%)	91	97

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	TRP
1	A	53	ARG
1	A	313	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	81	HIS
1	A	368	HIS
1	A	841	HIS
1	A	859	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

1 non-standard protein/DNA/RNA residue is 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	$\# Z > 2$
2	DAB	B	4	2	5,6,7	0.85	0	1,6,8	0.41	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
2	DAB	B	4	2	-	1/4/5/7	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	4	DAB	N-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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$
6	7E8	A	909	-	20,20,20	1.30	1 (5%)	21,21,21	0.82	2 (9%)
5	PEG	A	907	-	6,6,6	1.00	0	5,5,5	0.70	0
5	PEG	A	906	-	6,6,6	0.97	0	5,5,5	0.73	0
4	J06	A	902	-	64,64,64	1.29	3 (4%)	77,78,78	1.38	13 (16%)
6	7E8	A	910	-	20,20,20	1.30	2 (10%)	21,21,21	0.87	2 (9%)
5	PEG	A	904	-	6,6,6	0.98	0	5,5,5	0.73	0
6	7E8	A	911	-	20,20,20	1.41	2 (10%)	21,21,21	0.89	2 (9%)
5	PEG	A	905	-	6,6,6	0.97	0	5,5,5	0.70	0
5	PEG	A	903	-	6,6,6	1.04	0	5,5,5	0.68	0
6	7E8	A	908	-	20,20,20	1.32	1 (5%)	21,21,21	0.87	2 (9%)

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
6	7E8	A	909	-	-	10/20/20/20	-
5	PEG	A	907	-	-	1/4/4/4	-
5	PEG	A	906	-	-	1/4/4/4	-
4	J06	A	902	-	-	22/73/73/73	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	7E8	A	910	-	-	12/20/20/20	-
5	PEG	A	904	-	-	1/4/4/4	-
6	7E8	A	911	-	-	7/20/20/20	-
5	PEG	A	905	-	-	0/4/4/4	-
5	PEG	A	903	-	-	2/4/4/4	-
6	7E8	A	908	-	-	12/20/20/20	-

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	902	J06	P62-O61	7.58	1.84	1.60
6	A	911	7E8	O16-C8	3.55	1.43	1.33
6	A	909	7E8	O16-C8	3.42	1.43	1.33
6	A	908	7E8	O16-C8	3.41	1.43	1.33
6	A	910	7E8	O16-C8	3.37	1.43	1.33
4	A	902	J06	C59-C60	2.51	1.59	1.50
4	A	902	J06	O61-C60	-2.16	1.35	1.44
6	A	911	7E8	C17-C18	2.12	1.58	1.51
6	A	910	7E8	C17-C18	2.10	1.58	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	902	J06	C35-C36-C37	2.97	122.76	112.98
4	A	902	J06	C41-C42-C44	2.86	126.91	121.12
4	A	902	J06	C15-C16-C17	2.85	120.92	113.45
4	A	902	J06	C25-C26-C27	2.84	122.31	112.98
6	A	910	7E8	O16-C8-C7	2.67	120.29	111.91
6	A	908	7E8	O16-C8-C7	2.63	120.15	111.91
6	A	911	7E8	O16-C8-C7	2.59	120.05	111.91
6	A	911	7E8	O16-C8-O15	-2.53	117.21	123.59
6	A	908	7E8	O16-C8-O15	-2.47	117.36	123.59
6	A	910	7E8	O16-C8-O15	-2.44	117.43	123.59
6	A	909	7E8	O16-C8-C7	2.39	119.40	111.91
4	A	902	J06	C30-C31-C32	2.38	120.82	112.98
4	A	902	J06	O65-P62-O61	-2.38	100.40	106.73
6	A	909	7E8	O16-C8-O15	-2.33	117.70	123.59
4	A	902	J06	C51-C52-C54	2.22	125.61	121.12
4	A	902	J06	C41-C40-C39	2.21	119.14	111.88
4	A	902	J06	O65-P62-O64	2.16	115.90	107.64
4	A	902	J06	O64-P62-O61	-2.06	101.26	106.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	902	J06	C50-C51-C52	2.05	119.72	112.98
4	A	902	J06	C46-C47-C49	2.04	125.24	121.12
4	A	902	J06	C31-C30-C29	2.00	118.47	111.88

There are no chirality outliers.

All (68) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	902	J06	C58-C57-C59-C60
6	A	908	7E8	O16-C17-C18-O20
6	A	909	7E8	O16-C17-C18-O20
6	A	910	7E8	O16-C17-C18-C19
6	A	911	7E8	O16-C17-C18-C19
6	A	911	7E8	O15-C8-O16-C17
6	A	911	7E8	C7-C8-O16-C17
6	A	910	7E8	O15-C8-O16-C17
6	A	910	7E8	C7-C8-O16-C17
6	A	908	7E8	O15-C8-O16-C17
6	A	908	7E8	C7-C8-O16-C17
4	A	902	J06	C14-C15-C16-C17
4	A	902	J06	C24-C25-C26-C27
4	A	902	J06	C55-C56-C57-C58
6	A	911	7E8	O16-C17-C18-O20
4	A	902	J06	C09-C10-C11-C12
4	A	902	J06	C49-C50-C51-C52
6	A	910	7E8	O16-C17-C18-O20
5	A	907	PEG	O1-C1-C2-O2
6	A	910	7E8	C4-C5-C6-C7
6	A	908	7E8	C3-C4-C5-C6
6	A	908	7E8	C17-C18-C19-O22
6	A	910	7E8	C9-C10-C11-C12
6	A	910	7E8	C5-C6-C7-C8
6	A	908	7E8	O20-C18-C19-O22
4	A	902	J06	C07-C09-C10-C11
6	A	908	7E8	C4-C5-C6-C7
4	A	902	J06	C55-C56-C57-C59
6	A	908	7E8	C2-C3-C4-C5
6	A	911	7E8	C2-C3-C4-C5
6	A	909	7E8	O16-C17-C18-C19
6	A	909	7E8	C2-C3-C4-C5
6	A	909	7E8	C11-C10-C9-C1
6	A	909	7E8	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
6	A	910	7E8	C11-C10-C9-C1
6	A	910	7E8	C11-C12-C13-C14
4	A	902	J06	C10-C11-C12-C14
6	A	908	7E8	O16-C17-C18-C19
6	A	908	7E8	C11-C10-C9-C1
4	A	902	J06	C29-C30-C31-C32
4	A	902	J06	C08-C07-C09-C10
4	A	902	J06	C06-C07-C09-C10
4	A	902	J06	C12-C14-C15-C16
6	A	909	7E8	C11-C12-C13-C14
4	A	902	J06	C56-C57-C59-C60
5	A	904	PEG	C1-C2-O2-C3
5	A	903	PEG	O1-C1-C2-O2
5	A	906	PEG	C4-C3-O2-C2
4	A	902	J06	C05-C06-C07-C09
5	A	903	PEG	C1-C2-O2-C3
6	A	909	7E8	C1-C2-C3-C4
6	A	908	7E8	C5-C6-C7-C8
4	A	902	J06	C13-C12-C14-C15
6	A	909	7E8	C9-C10-C11-C12
4	A	902	J06	C50-C51-C52-C53
6	A	909	7E8	C17-C18-C19-O22
4	A	902	J06	C45-C46-C47-C48
4	A	902	J06	C50-C51-C52-C54
4	A	902	J06	C10-C11-C12-C13
6	A	911	7E8	C1-C2-C3-C4
6	A	910	7E8	C2-C1-C9-C10
6	A	910	7E8	C10-C11-C12-C13
6	A	909	7E8	O20-C18-C19-O22
4	A	902	J06	C11-C12-C14-C15
6	A	908	7E8	C2-C1-C9-C10
6	A	910	7E8	C1-C2-C3-C4
4	A	902	J06	C37-C39-C40-C41
6	A	911	7E8	C2-C1-C9-C10

There are no ring outliers.

6 monomers are involved in 8 short contacts:

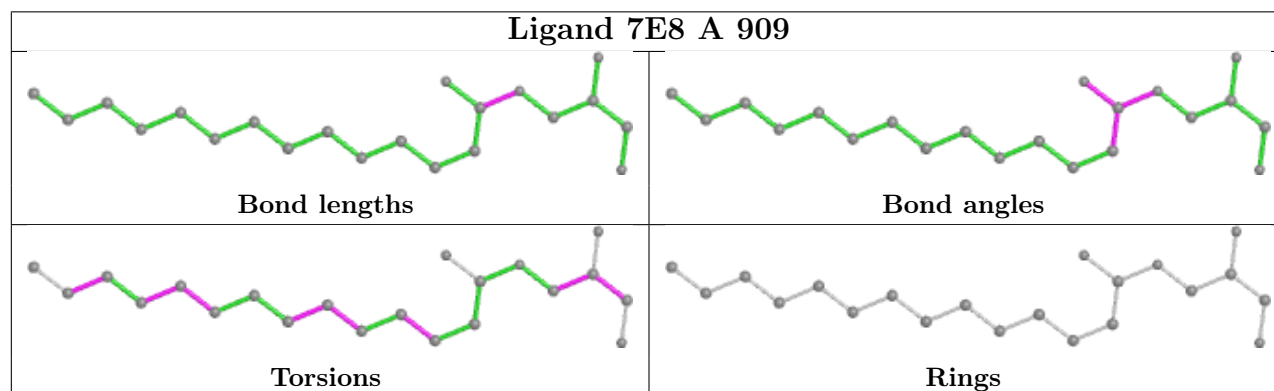
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	909	7E8	3	0
5	A	907	PEG	1	0
5	A	906	PEG	2	0

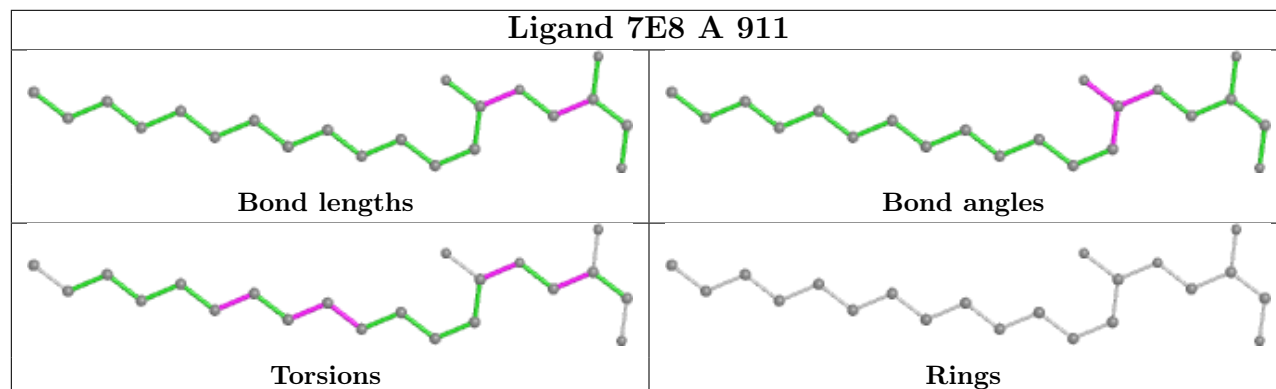
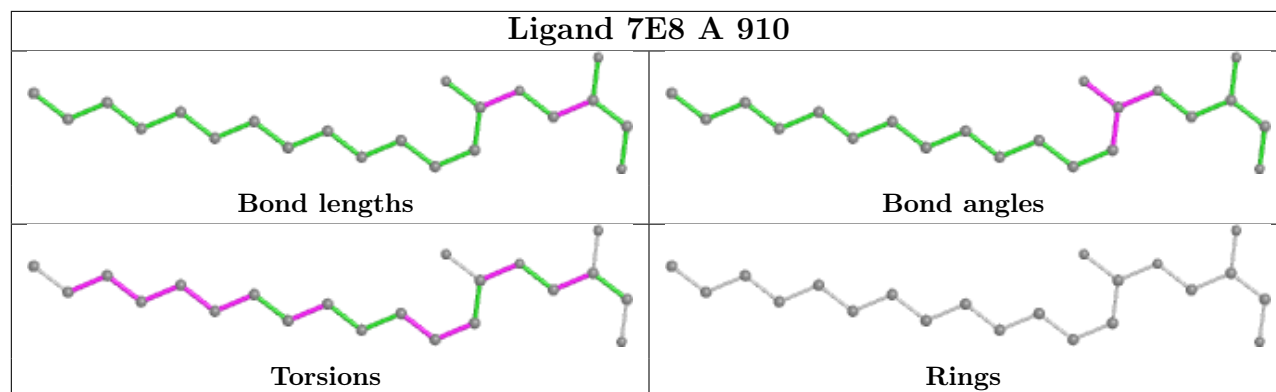
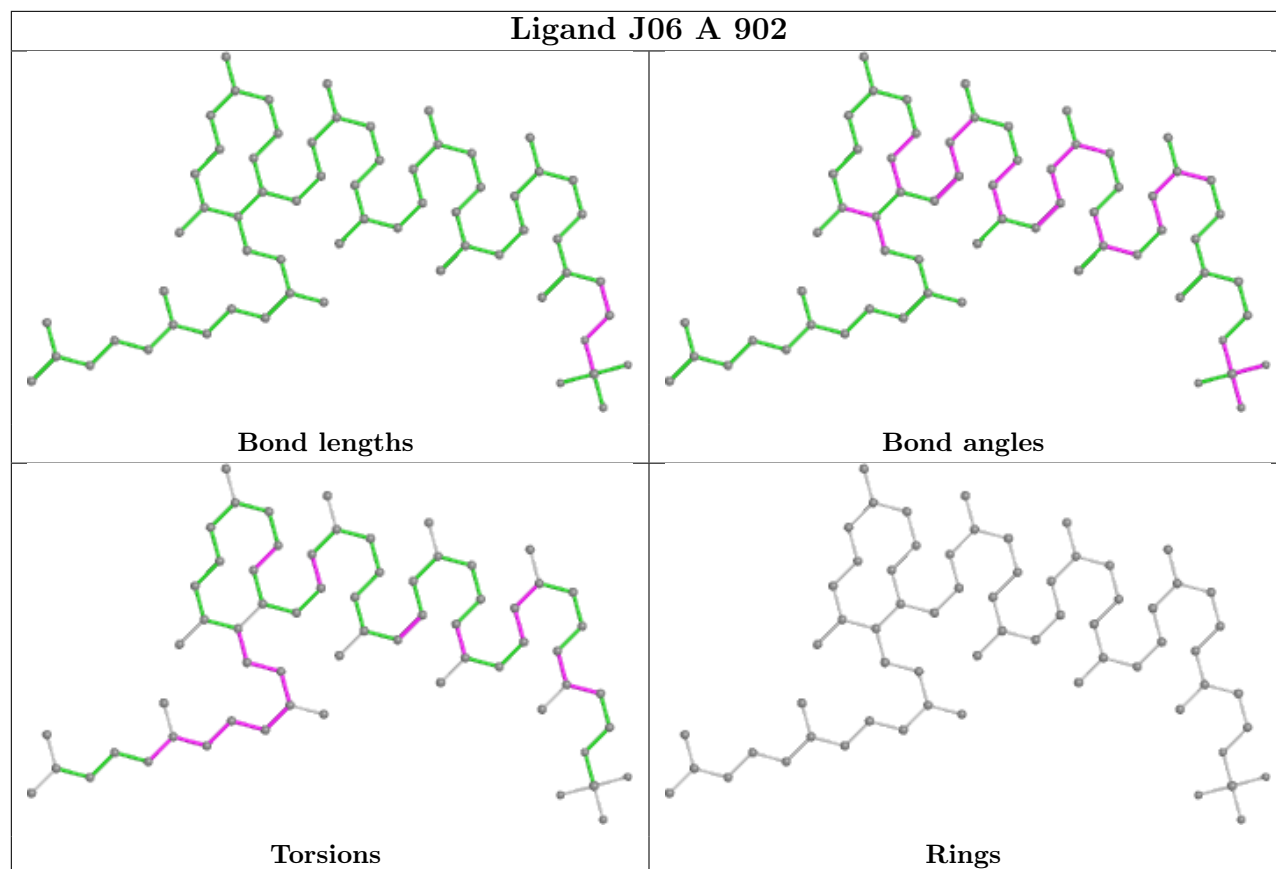
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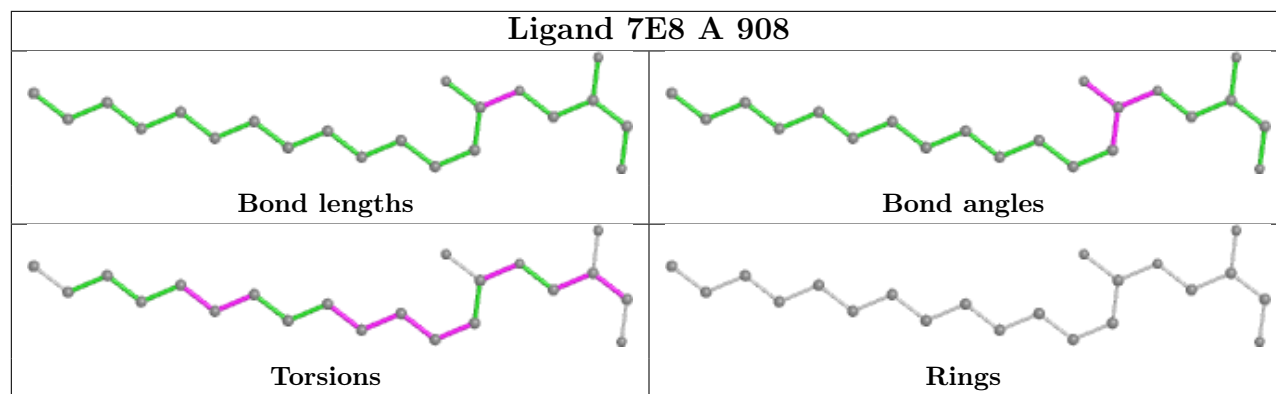
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	910	7E8	1	0
6	A	911	7E8	1	0
5	A	903	PEG	1	0

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	867/875 (99%)	0.45	71 (8%)	11 9	53, 72, 122, 159	0
2	B	8/10 (80%)	1.79	4 (50%)	0 0	86, 106, 142, 193	0
All	All	875/885 (98%)	0.46	75 (8%)	10 8	53, 72, 124, 193	0

All (75) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	461	GLY	14.3
1	A	463	ARG	7.0
1	A	238	PHE	5.4
1	A	459	ALA	5.0
1	A	656	TRP	5.0
1	A	351	PRO	4.9
1	A	332	PHE	4.8
1	A	10	LYS	4.8
1	A	465	LYS	4.7
1	A	7	TRP	4.5
1	A	433	ALA	4.4
1	A	469	PHE	4.1
2	B	9	CYS	4.0
1	A	13	HIS	3.8
1	A	305	PHE	3.8
1	A	462	ALA	3.8
1	A	369	ASN	3.8
1	A	460	ILE	3.7
1	A	308	ARG	3.6
1	A	368	HIS	3.6
1	A	350	GLN	3.6
1	A	464	ASN	3.6
1	A	870	LEU	3.5
1	A	333	VAL	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	352	LYS	3.3
1	A	372	PHE	3.3
1	A	871	ALA	3.3
1	A	371	GLU	3.3
1	A	359	ALA	3.3
1	A	483	TYR	3.1
1	A	532	GLN	3.1
1	A	437	VAL	3.0
1	A	309	VAL	3.0
1	A	733	ARG	3.0
1	A	495	TYR	3.0
1	A	313	ARG	2.9
1	A	745	VAL	2.9
1	A	458	ASN	2.8
1	A	330	LEU	2.8
2	B	1	ALA	2.8
1	A	9	LYS	2.8
1	A	683	HIS	2.8
1	A	512	GLU	2.7
1	A	438	TYR	2.6
2	B	3	TYR	2.6
1	A	466	LEU	2.6
1	A	578	TYR	2.6
2	B	8	SER	2.6
1	A	300	TRP	2.5
1	A	50	TYR	2.5
1	A	548	ILE	2.5
1	A	816	LYS	2.5
1	A	397	TYR	2.5
1	A	629	ASP	2.5
1	A	11	TYR	2.4
1	A	331	PHE	2.4
1	A	467	SER	2.4
1	A	684	LEU	2.3
1	A	609	VAL	2.3
1	A	225	ILE	2.3
1	A	401	LYS	2.2
1	A	518	GLU	2.2
1	A	340	ARG	2.2
1	A	470	ARG	2.2
1	A	860	ASN	2.2
1	A	373	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	454	ARG	2.2
1	A	338	PHE	2.2
1	A	468	TYR	2.1
1	A	336	PRO	2.1
1	A	346	VAL	2.1
1	A	655	GLN	2.1
1	A	367	THR	2.0
1	A	608	VAL	2.0
1	A	872	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
2	DAB	B	4	7/8	0.82	0.21	78,81,88,95	0

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, 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
5	PEG	A	905	7/7	0.42	0.61	104,117,124,126	0
6	7E8	A	911	21/21	0.51	0.37	85,100,114,124	0
5	PEG	A	906	7/7	0.60	0.70	77,88,101,114	0
5	PEG	A	907	7/7	0.63	0.27	87,106,113,114	0
6	7E8	A	908	21/21	0.67	0.23	78,83,100,107	0
4	J06	A	902	65/65	0.71	0.34	71,89,108,113	0
6	7E8	A	910	21/21	0.75	0.35	70,81,91,108	0
6	7E8	A	909	21/21	0.75	0.29	64,87,102,103	0

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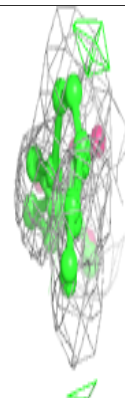
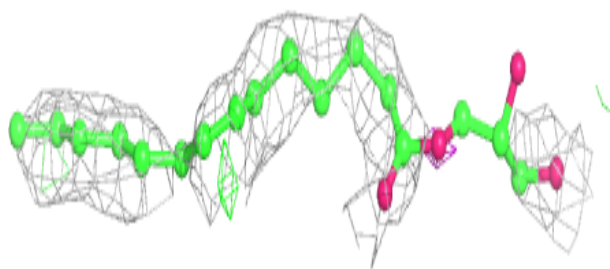
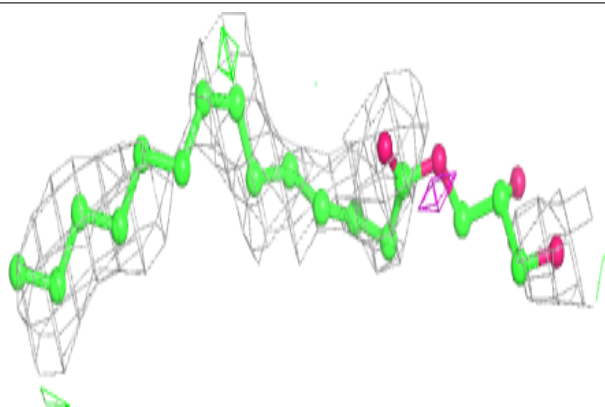
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	PEG	A	904	7/7	0.82	0.36	76,80,82,85	0
5	PEG	A	903	7/7	0.88	0.12	67,71,78,78	0
3	MN	A	901	1/1	0.99	0.18	73,73,73,73	0

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.

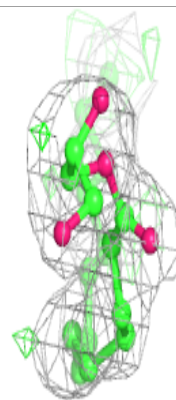
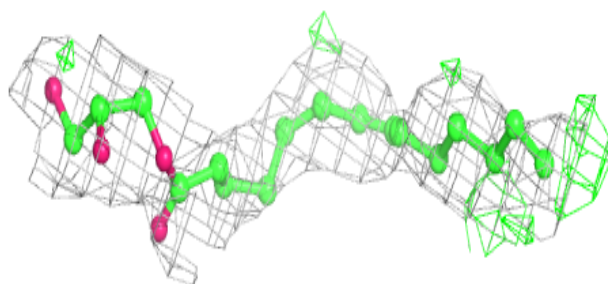
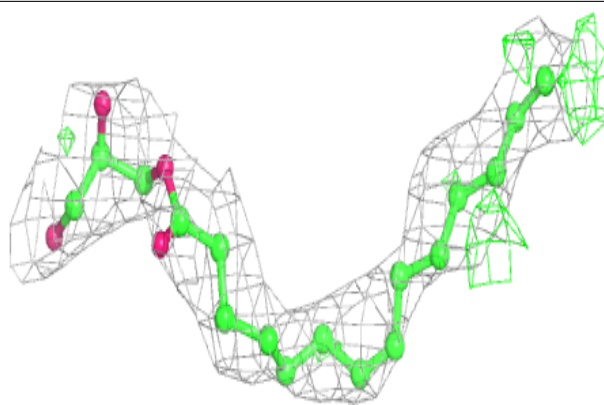
Electron density around 7E8 A 911:

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

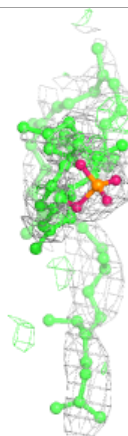
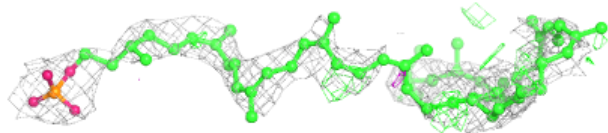
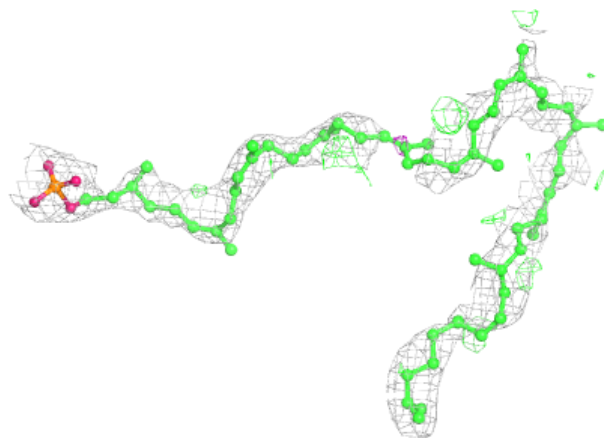


Electron density around 7E8 A 908:

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

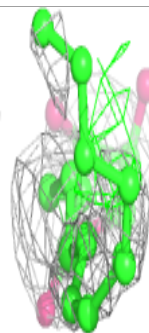
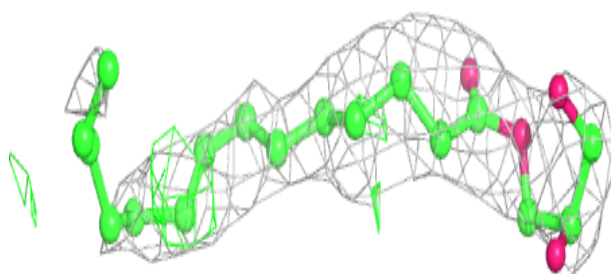
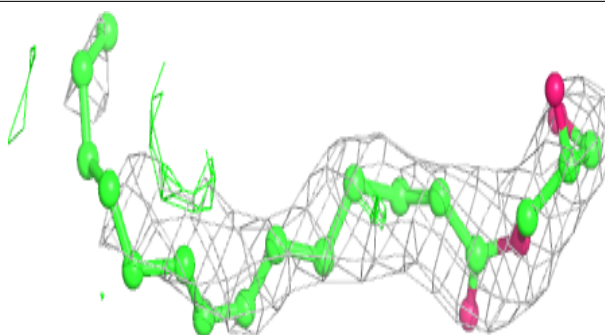
**Electron density around J06 A 902:**

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 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

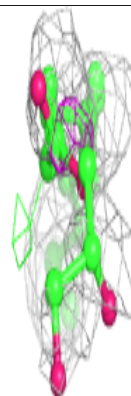
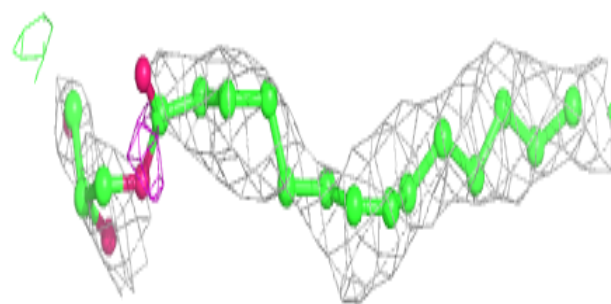
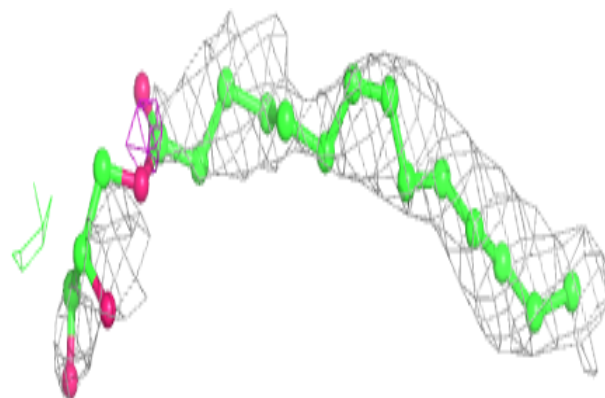


Electron density around 7E8 A 910:

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

**Electron density around 7E8 A 909:**

$2mF_o-DF_c$ (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.