Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:46 AM UTC

PDB ID	:	6TPN / pdb_00006tpn
Title	:	Crystal structure of the Orexin-2 receptor in complex with HTL6641 at 2.61 A resolution
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Deposited on	:	2019-12-13
Resolution	:	2.61 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:

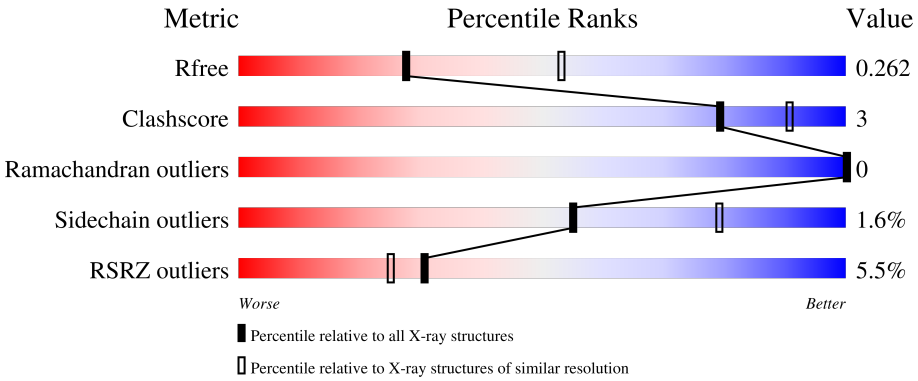
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)

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 2.61 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	564	5% 83% 7% 10%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 4269 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 Orexin receptor type 2,GlgA glycogen synthase,Orexin receptor type 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	510	4100	2691	677	702	30	0	0	0

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-10	GLN	-	expression tag	UNP O43614
A	-9	ASP	-	expression tag	UNP O43614
A	-8	LEU	-	expression tag	UNP O43614
A	-7	ASP	-	expression tag	UNP O43614
A	-6	TYR	-	expression tag	UNP O43614
A	-5	LYS	-	expression tag	UNP O43614
A	-4	ASP	-	expression tag	UNP O43614
A	-3	ASP	-	expression tag	UNP O43614
A	-2	ASP	-	expression tag	UNP O43614
A	-1	ASP	-	expression tag	UNP O43614
A	0	LYS	-	expression tag	UNP O43614
A	14	ASP	ASN	engineered mutation	UNP O43614
A	22	ASP	ASN	engineered mutation	UNP O43614
A	28	LEU	PHE	engineered mutation	UNP O43614
A	30	ASP	ASN	engineered mutation	UNP O43614
A	54	ALA	GLU	engineered mutation	UNP O43614
A	91	LEU	TYR	engineered mutation	UNP O43614
A	100	ALA	ASP	engineered mutation	UNP O43614
A	142	ALA	VAL	engineered mutation	UNP O43614
A	170	LEU	ARG	engineered mutation	UNP O43614
A	202	ASP	ASN	engineered mutation	UNP O43614
A	206	ALA	LEU	engineered mutation	UNP O43614
A	219	ALA	TYR	engineered mutation	UNP O43614
A	233	ALA	MET	engineered mutation	UNP O43614
A	242	LEU	ALA	engineered mutation	UNP O43614
A	308	VAL	ILE	engineered mutation	UNP O43614

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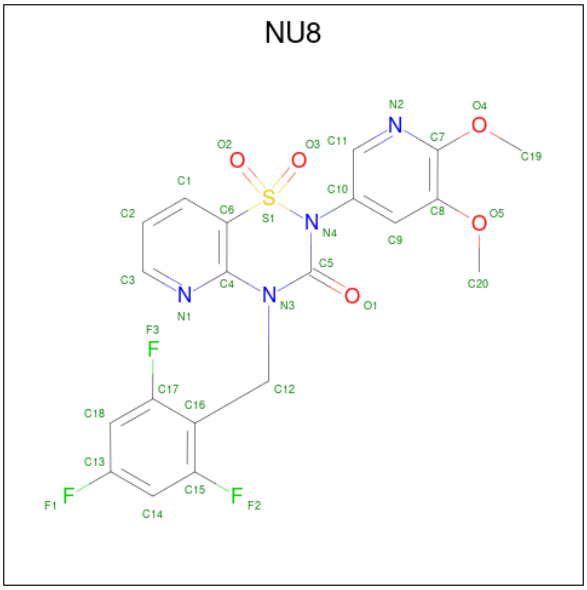
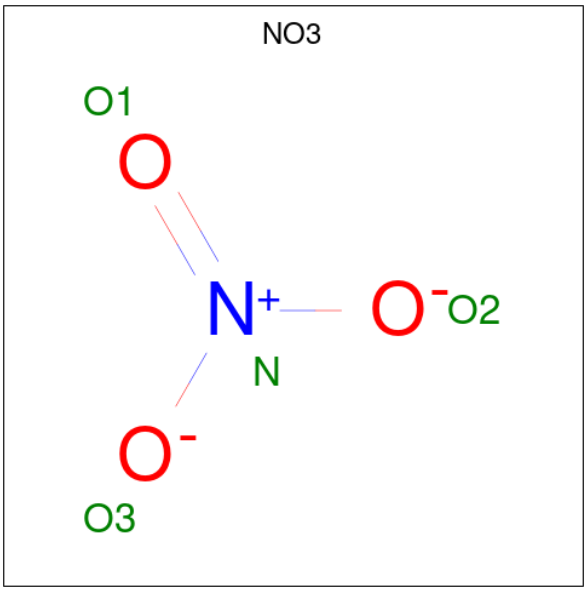
Chain	Residue	Modelled	Actual	Comment	Reference
A	310	VAL	LEU	engineered mutation	UNP O43614
A	318	ALA	LEU	engineered mutation	UNP O43614
A	347	ALA	THR	engineered mutation	UNP O43614
A	381	TRP	CYS	engineered mutation	UNP O43614
A	382	TRP	CYS	engineered mutation	UNP O43614
A	383	TRP	CYS	engineered mutation	UNP O43614
A	389	HIS	-	expression tag	UNP O43614
A	390	HIS	-	expression tag	UNP O43614
A	391	HIS	-	expression tag	UNP O43614
A	392	HIS	-	expression tag	UNP O43614
A	393	HIS	-	expression tag	UNP O43614
A	394	HIS	-	expression tag	UNP O43614
A	395	HIS	-	expression tag	UNP O43614
A	396	HIS	-	expression tag	UNP O43614

- Molecule 2 is 2-(5,6-dimethoxypyridin-3-yl)-1,1-bis(oxidanylidene)-4-[[2,4,6-tris(fluoranyl)phenyl]methyl]pyrido[2,3-e][1,2,4]thiadiazin-3-one (CCD ID: NU8) (formula: $C_{20}H_{15}F_3N_4O_5S$) (labeled as "Ligand of Interest" by depositor).



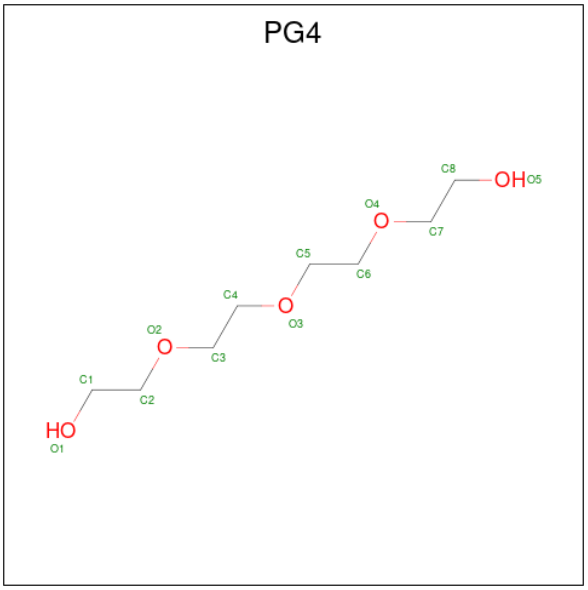
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	S	0	0
			33	20	3	4	5	1		

- Molecule 3 is NITRATE ION (CCD ID: NO3) (formula: NO_3).



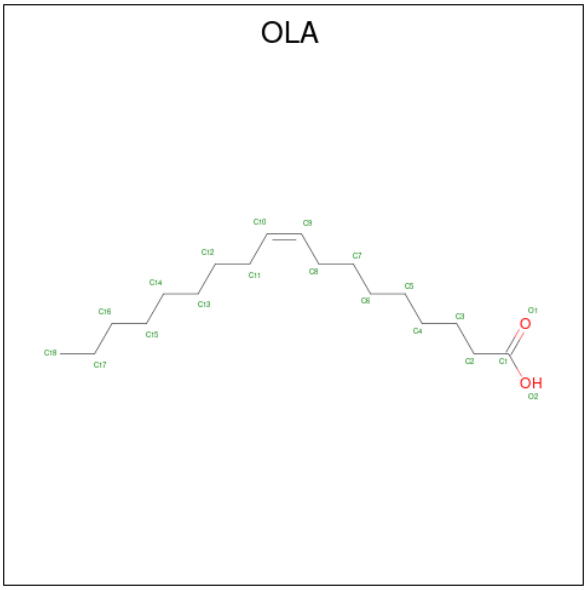
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total N O 4 1 3	0	0
3	A	1	Total N O 4 1 3	0	0

- Molecule 4 is TETRAETHYLENE GLYCOL (CCD ID: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 13 8 5	0	0
4	A	1	Total C O 13 8 5	0	0

- Molecule 5 is OLEIC ACID (CCD ID: OLA) (formula: $C_{18}H_{34}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 13 11 2	0	0
5	A	1	Total C O 10 8 2	0	0
5	A	1	Total C O 20 18 2	0	0
5	A	1	Total C O 13 11 2	0	0

- Molecule 6 is water.

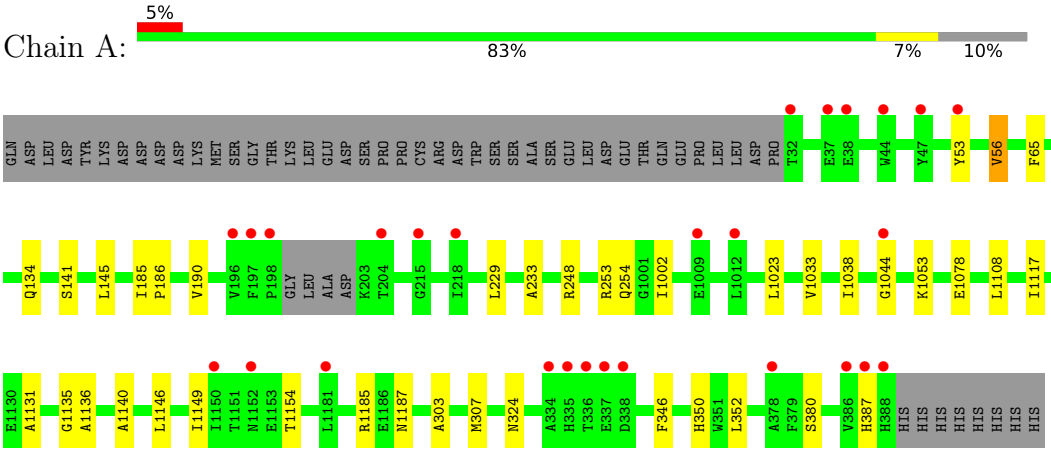
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	46	Total O 46 46	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Orexin receptor type 2,GlgA glycogen synthase,Orexin receptor type 2

Chain A:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	90.94Å 173.95Å 78.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.48 – 2.61 41.48 – 2.61	Depositor EDS
% Data completeness (in resolution range)	60.5 (41.48-2.61) 80.2 (41.48-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	-0.04 (at 1.98Å)	Xtriage
Refinement program	PHENIX 1.13_2998	Depositor
R, R_{free}	0.214 , 0.251 (Not available) , 0.262	Depositor DCC
R_{free} test set	2145 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	8.6	Xtriage
Anisotropy	0.488	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 47.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	4269	wwPDB-VP
Average B, all atoms (Å^2)	56.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.42% 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: NO3, YCM, OLA, NU8, PG4

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	0/4192	0.45	0/5681

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	4100	0	4176	23	0
2	A	33	0	0	1	0
3	A	8	0	0	0	0
4	A	26	0	36	0	0
5	A	56	0	77	0	0
6	A	46	0	0	2	0
All	All	4269	0	4289	23	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 3.

All (23) 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:1078:GLU:HG3	6:A:1320:HOH:O	1.85	0.76
1:A:380:SER:CB	1:A:387:HIS:ND1	2.70	0.55
1:A:380:SER:HB2	1:A:387:HIS:ND1	2.22	0.55
1:A:134:GLN:O	1:A:134:GLN:HG2	2.07	0.53
1:A:346:PHE:O	1:A:350:HIS:HD2	1.91	0.52
1:A:1140:ALA:HB1	1:A:1146:LEU:HD13	1.92	0.52
1:A:248:ARG:HH21	1:A:253:ARG:HE	1.58	0.50
1:A:380:SER:CB	1:A:387:HIS:CE1	2.96	0.49
1:A:1135:GLY:O	1:A:1185:ARG:HD2	2.14	0.47
1:A:1023:LEU:HD21	1:A:1108:LEU:HD23	1.96	0.47
1:A:1044:GLY:O	1:A:1120:TYR:HB2	2.15	0.46
1:A:303:ALA:HB1	1:A:307:MET:HE3	1.97	0.46
1:A:324:ASN:ND2	2:A:1201:NU8:N1	2.62	0.46
1:A:229:LEU:HA	1:A:233:ALA:HB3	1.97	0.45
1:A:1154:THR:HG22	1:A:1187:ASN:HB3	1.98	0.45
1:A:65:PHE:HD2	1:A:108:LEU:HD22	1.80	0.45
1:A:141:SER:O	1:A:145:LEU:HD12	2.17	0.45
1:A:185:ILE:N	1:A:186:PRO:HD2	2.34	0.43
1:A:1053:LYS:NZ	6:A:1303:HOH:O	2.52	0.42
1:A:53:TYR:O	1:A:56:VAL:HG12	2.20	0.42
1:A:1131:ALA:HB1	1:A:1136:ALA:HB3	2.01	0.42
1:A:1129:LEU:HG	1:A:1149:ILE:HD13	2.01	0.42
1:A:352:LEU:HD12	1:A:352:LEU:HA	1.90	0.42

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	505/564 (90%)	491 (97%)	14 (3%)	0	100 100

There are no Ramachandran outliers to report.

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	441/491 (90%)	434 (98%)	7 (2%)	55 79

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

Mol	Chain	Res	Type
1	A	56	VAL
1	A	190	VAL
1	A	254	GLN
1	A	1002	ILE
1	A	1033	VAL
1	A	1038	ILE
1	A	1117	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	ASN
1	A	254	GLN
1	A	295	GLN
1	A	324	ASN
1	A	350	HIS
1	A	388	HIS

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	$\#\|Z\| > 2$
1	YCM	A	1004	1	7,9,10	1.13	0	5,10,12	0.52	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
1	YCM	A	1004	1	-	0/6/8/10	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

9 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	$\#\|Z\|>2$
2	NU8	A	1201	-	35,36,36	1.57	5 (14%)	42,54,54	2.75	19 (45%)
5	OLA	A	1209	-	12,12,19	0.62	0	12,12,19	1.01	0
5	OLA	A	1207	-	9,9,19	0.68	0	9,9,19	1.09	1 (11%)
5	OLA	A	1208	-	19,19,19	0.48	0	19,19,19	0.87	1 (5%)
3	NO3	A	1203	-	1,3,3	0.55	0	0,3,3	-	-
3	NO3	A	1202	-	1,3,3	0.71	0	0,3,3	-	-
5	OLA	A	1206	-	12,12,19	0.62	0	12,12,19	0.95	0
4	PG4	A	1204	-	12,12,12	0.46	0	11,11,11	0.35	0
4	PG4	A	1205	-	12,12,12	0.46	0	11,11,11	0.31	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	NU8	A	1201	-	-	1/12/36/36	0/3/4/4
5	OLA	A	1209	-	-	4/10/10/17	-
5	OLA	A	1206	-	-	8/10/10/17	-
5	OLA	A	1208	-	-	10/17/17/17	-
4	PG4	A	1204	-	-	3/10/10/10	-
4	PG4	A	1205	-	-	0/10/10/10	-
5	OLA	A	1207	-	-	5/7/7/17	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1201	NU8	C10-N4	-5.00	1.39	1.45
2	A	1201	NU8	C5-N3	-3.36	1.33	1.37
2	A	1201	NU8	O4-C7	2.94	1.39	1.35
2	A	1201	NU8	C7-N2	2.31	1.37	1.32
2	A	1201	NU8	C6-S1	-2.17	1.72	1.75

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	NU8	C19-O4-C7	8.11	124.78	117.20
2	A	1201	NU8	C14-C15-C16	-6.76	119.42	124.45
2	A	1201	NU8	O3-S1-N4	-5.52	102.69	107.97
2	A	1201	NU8	O4-C7-N2	-4.99	114.47	120.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1201	NU8	O4-C7-C8	4.43	124.21	116.80
2	A	1201	NU8	C15-C14-C13	3.85	120.77	116.67
2	A	1201	NU8	C18-C13-C14	-3.41	119.36	123.50
2	A	1201	NU8	F1-C13-C14	3.23	122.87	118.28
2	A	1201	NU8	O3-S1-O2	3.21	122.61	118.53
2	A	1201	NU8	C17-C18-C13	3.04	119.91	116.67
2	A	1201	NU8	C18-C17-C16	-3.02	122.21	124.45
2	A	1201	NU8	C17-C16-C15	2.81	118.33	114.54
2	A	1201	NU8	C4-N3-C5	2.56	124.54	122.23
2	A	1201	NU8	F2-C15-C16	2.53	120.80	117.64
2	A	1201	NU8	C12-N3-C5	2.52	118.29	116.75
2	A	1201	NU8	C11-C10-N4	2.48	122.19	119.50
5	A	1207	OLA	C3-C2-C1	-2.26	108.61	114.51
5	A	1208	OLA	C3-C2-C1	-2.21	108.73	114.51
2	A	1201	NU8	O5-C8-C9	-2.18	120.32	124.08
2	A	1201	NU8	C8-C7-N2	-2.17	121.32	123.57
2	A	1201	NU8	C12-C16-C17	-2.06	117.90	122.50

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1201	NU8	C16-C12-N3-C5
5	A	1209	OLA	C1-C2-C3-C4
5	A	1206	OLA	C2-C3-C4-C5
5	A	1207	OLA	C4-C5-C6-C7
5	A	1208	OLA	C3-C4-C5-C6
5	A	1206	OLA	C6-C7-C8-C9
5	A	1208	OLA	C6-C7-C8-C9
5	A	1209	OLA	C4-C5-C6-C7
5	A	1206	OLA	C4-C5-C6-C7
5	A	1208	OLA	C10-C11-C12-C13
5	A	1206	OLA	C5-C6-C7-C8
5	A	1208	OLA	C12-C13-C14-C15
5	A	1208	OLA	C2-C3-C4-C5
5	A	1208	OLA	C14-C15-C16-C17
5	A	1209	OLA	C5-C6-C7-C8
5	A	1207	OLA	C1-C2-C3-C4
4	A	1204	PG4	C6-C5-O3-C4
5	A	1208	OLA	C7-C8-C9-C10
5	A	1207	OLA	C5-C6-C7-C8
5	A	1206	OLA	O2-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	A	1204	PG4	O2-C3-C4-O3
5	A	1206	OLA	O1-C1-C2-C3
5	A	1208	OLA	O1-C1-C2-C3
5	A	1208	OLA	O2-C1-C2-C3
5	A	1208	OLA	C4-C5-C6-C7
5	A	1207	OLA	O2-C1-C2-C3
5	A	1207	OLA	O1-C1-C2-C3
4	A	1204	PG4	C4-C3-O2-C2
5	A	1206	OLA	C7-C8-C9-C10
5	A	1206	OLA	C1-C2-C3-C4
5	A	1209	OLA	C6-C7-C8-C9

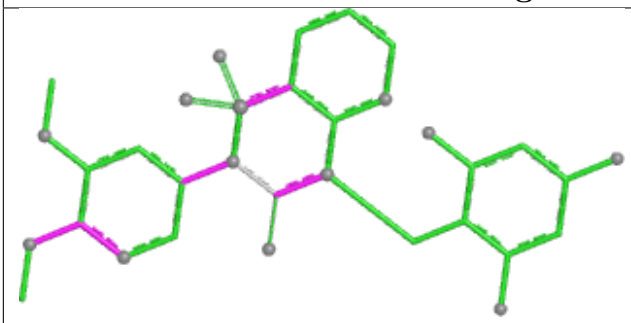
There are no ring outliers.

1 monomer is involved in 1 short contact:

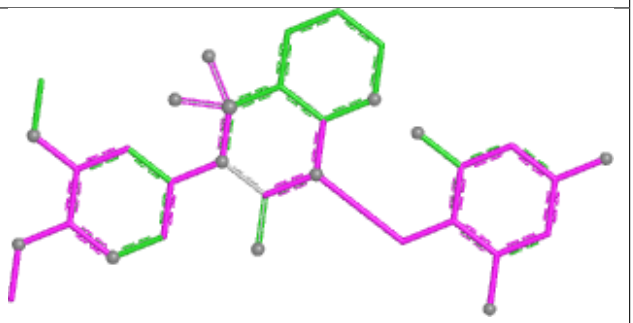
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1201	NU8	1	0

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 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.

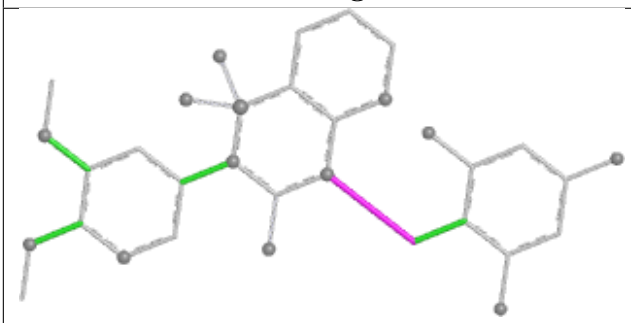
Ligand NU8 A 1201



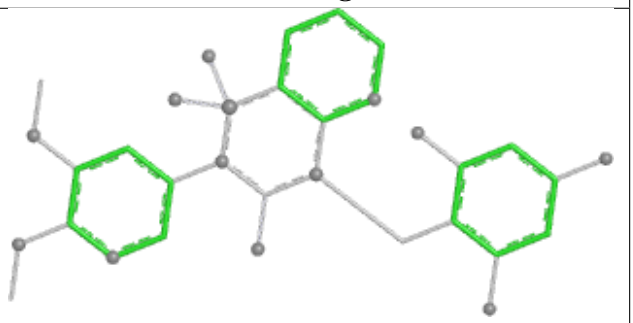
Bond lengths



Bond angles

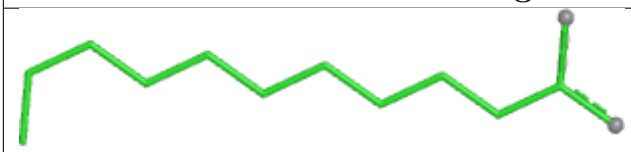


Torsions

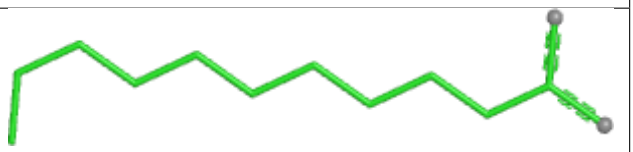


Rings

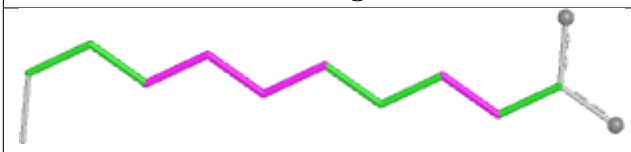
Ligand OLA A 1209



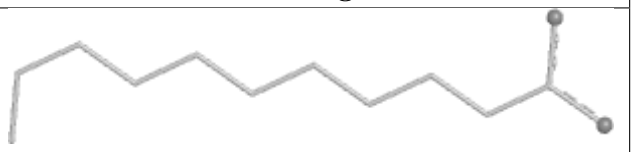
Bond lengths



Bond angles

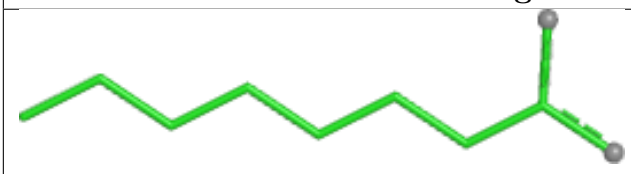


Torsions

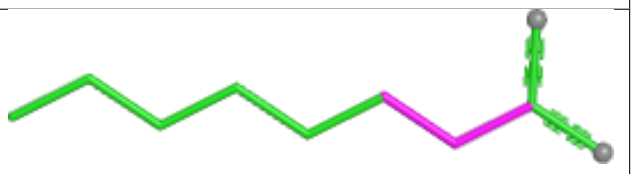


Rings

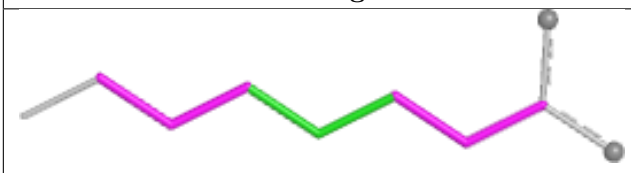
Ligand OLA A 1207



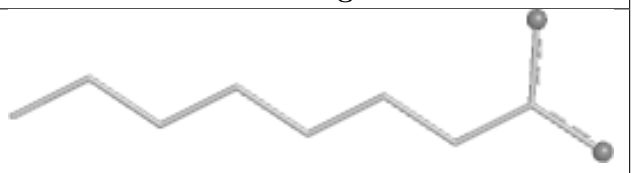
Bond lengths



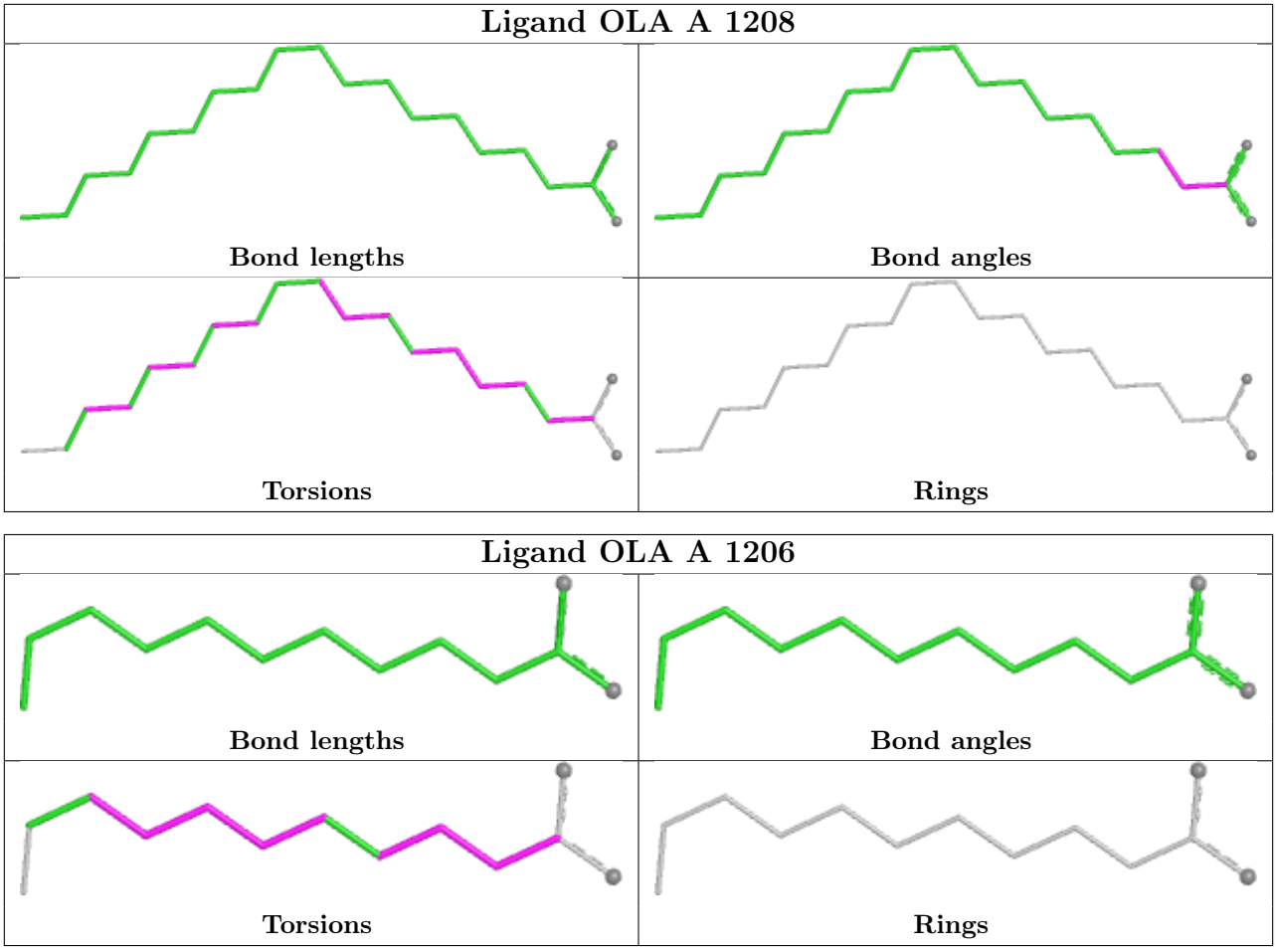
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	509/564 (90%)	0.43	28 (5%) 30 25	28, 49, 98, 179	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	197	PHE	4.3
1	A	388	HIS	3.5
1	A	1044	GLY	3.4
1	A	338	ASP	3.4
1	A	386	VAL	3.4
1	A	1012	LEU	3.1
1	A	1152	ASN	3.1
1	A	198	PRO	3.0
1	A	1009	GLU	3.0
1	A	387	HIS	2.8
1	A	337	GLU	2.8
1	A	334	ALA	2.7
1	A	32	THR	2.7
1	A	378	ALA	2.7
1	A	37	GLU	2.4
1	A	204	THR	2.4
1	A	1181	LEU	2.3
1	A	53	TYR	2.3
1	A	336	THR	2.3
1	A	1150	ILE	2.3
1	A	335	HIS	2.3
1	A	47	TYR	2.2
1	A	44	TRP	2.2
1	A	38	GLU	2.2
1	A	80	TRP	2.1
1	A	218	ILE	2.1
1	A	196	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	215	GLY	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
1	YCM	A	1004	10/11	0.86	0.11	51,57,75,75	0

6.3 Carbohydrates (i)

There are no oligosaccharides in this entry.

6.4 Ligands (i)

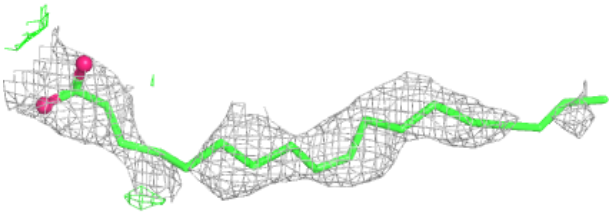
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

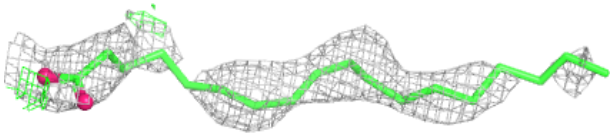
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NO3	A	1202	4/4	0.64	0.17	92,92,92,92	0
3	NO3	A	1203	4/4	0.64	0.14	99,99,99,100	0
5	OLA	A	1208	20/20	0.70	0.16	44,54,74,74	0
2	NU8	A	1201	33/33	0.72	0.18	61,72,78,79	5
5	OLA	A	1209	13/20	0.73	0.16	68,69,74,75	0
5	OLA	A	1206	13/20	0.75	0.17	59,61,69,70	0
4	PG4	A	1205	13/13	0.76	0.18	53,64,70,71	0
5	OLA	A	1207	10/20	0.81	0.16	64,65,68,69	0
4	PG4	A	1204	13/13	0.86	0.17	71,73,77,78	0

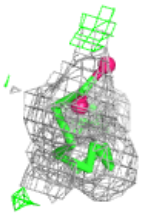
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA A 1208:

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

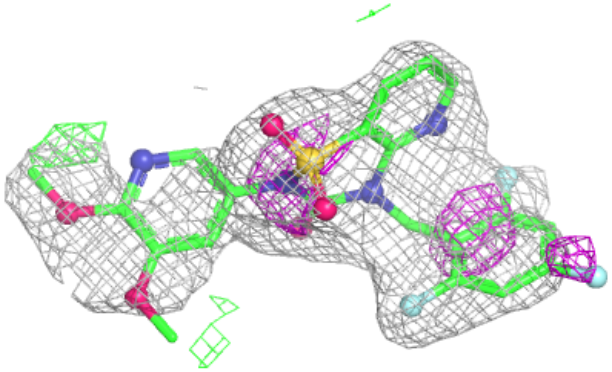


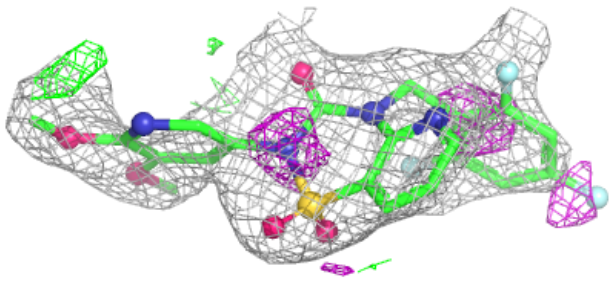


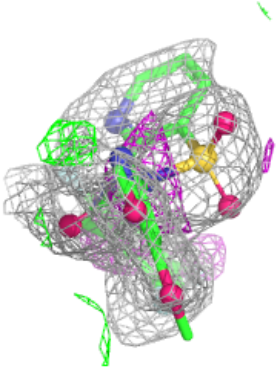


Electron density around NU8 A 1201:

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







Electron density around OLA A 1209:

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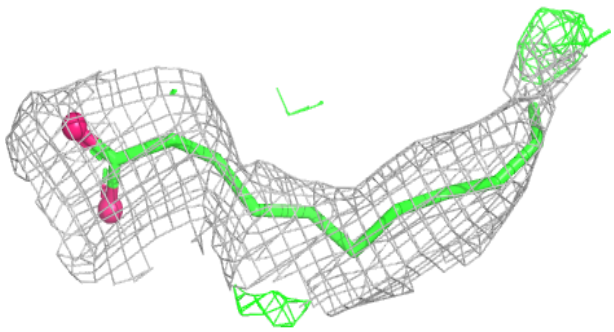
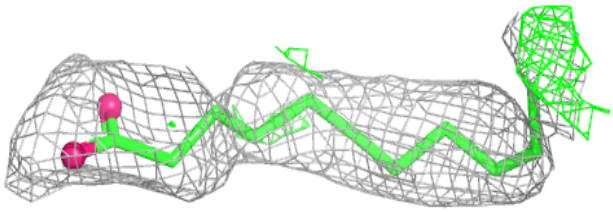
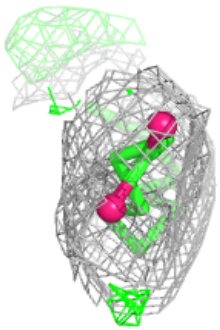
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

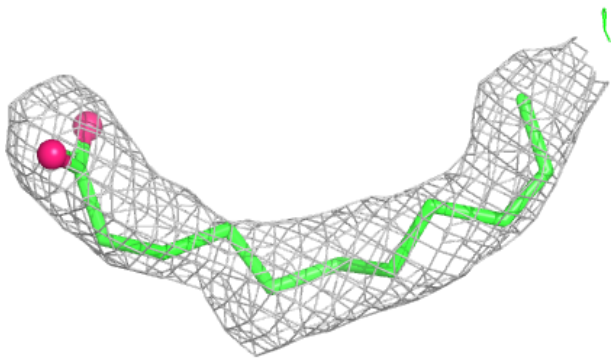


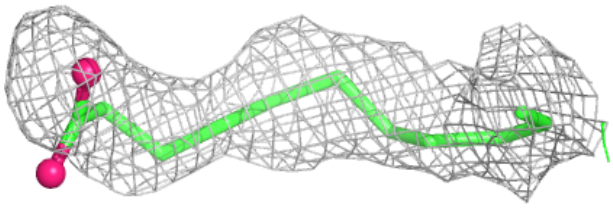


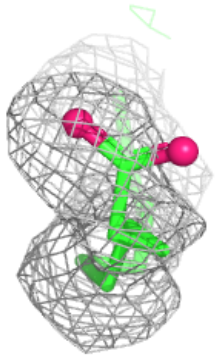


Electron density around OLA A 1206:

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







Electron density around OLA A 1207:

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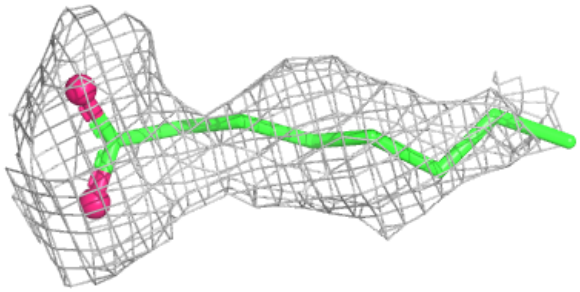
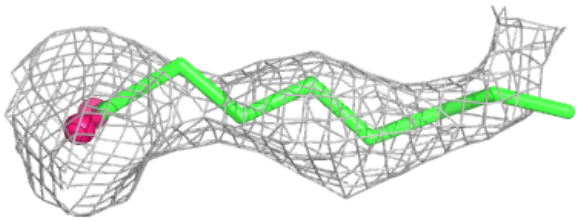
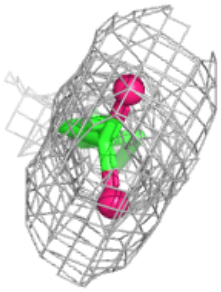
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)







6.5 Other polymers

There are no such residues in this entry.