



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:31 PM UTC

PDB ID : 6DO1 / pdb_00006do1
Title : Structure of nanobody-stabilized angiotensin II type 1 receptor bound to S1I8
Authors : Wingler, L.M.; McMahon, C.; Staus, D.P.; Lefkowitz, R.J.; Kruse, A.C.
Deposited on : 2018-06-08
Resolution : 2.90 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

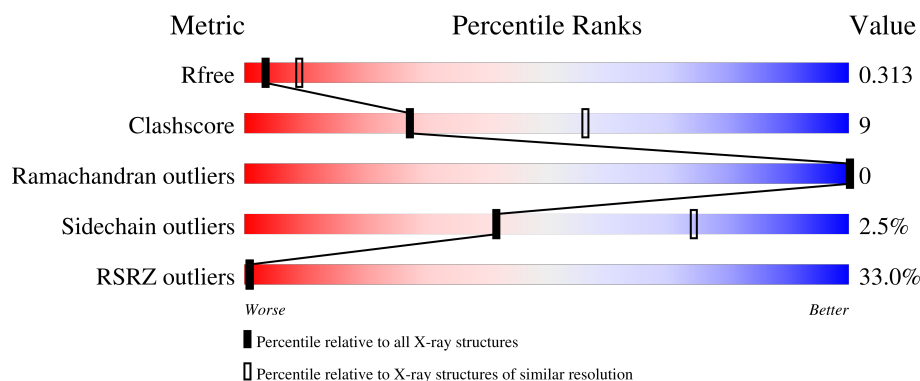
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	425	15% 53% 17% 28%
1	B	425	16% 55% 16% 28%
2	C	126	35% 81% 18%
2	D	126	38% 79% 21%
2	E	126	33% 42% 54%

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Mol	Chain	Length	Quality of chain
2	F	126	52% 45% 13% 40%
3	G	8	12% 62% 25% 12%
3	H	8	38% 50% 12%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7930 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 Type-1 angiotensin II receptor,Soluble cytochrome b562 BRIL fusion protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2411	1628	378	389	16			
1	B	304	Total	C	N	O	S	0	0	0
			2388	1614	373	385	16			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	ASP	-	expression tag	UNP P30556
A	-5	TYR	-	expression tag	UNP P30556
A	-4	LYS	-	expression tag	UNP P30556
A	-3	ASP	-	expression tag	UNP P30556
A	-2	ASP	-	expression tag	UNP P30556
A	-1	ASP	-	expression tag	UNP P30556
A	0	ASP	-	expression tag	UNP P30556
A	1	LYS	-	expression tag	UNP P30556
A	?	TRP	MET	engineered mutation	UNP P0ABE7
B	-6	ASP	-	expression tag	UNP P30556
B	-5	TYR	-	expression tag	UNP P30556
B	-4	LYS	-	expression tag	UNP P30556
B	-3	ASP	-	expression tag	UNP P30556
B	-2	ASP	-	expression tag	UNP P30556
B	-1	ASP	-	expression tag	UNP P30556
B	0	ASP	-	expression tag	UNP P30556
B	1	LYS	-	expression tag	UNP P30556
B	?	TRP	MET	engineered mutation	UNP P0ABE7

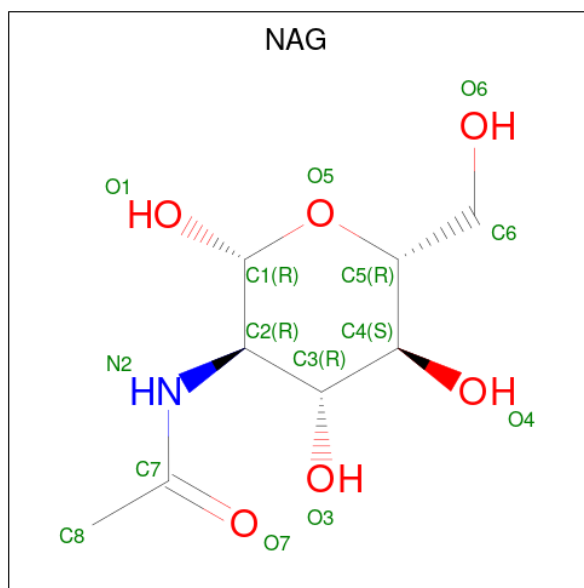
- Molecule 2 is a protein called Nanobody Nb.AT110i1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	125	Total	C	N	O	S	0	0	0
			933	583	155	191	4			
2	D	126	Total	C	N	O	S	0	0	0
			931	582	155	190	4			
2	E	58	Total	C	N	O	S	0	0	0
			411	259	63	86	3			
2	F	75	Total	C	N	O	S	0	0	0
			532	326	93	109	4			

- Molecule 3 is a protein called Angiotensin-like peptide S1I8.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	8	Total	C	N	O	0	0	0
			69	46	13	10			
3	H	8	Total	C	N	O	0	0	0
			69	46	13	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

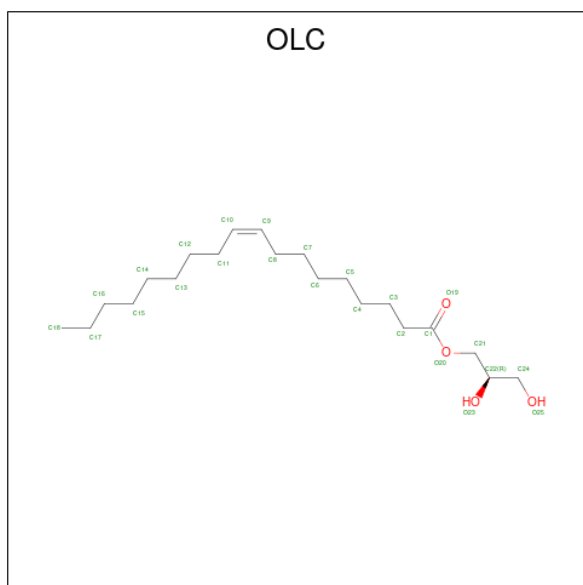


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	3	Total Cl 3 3	0	0
5	B	2	Total Cl 2 2	0	0

- Molecule 6 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: $C_{21}H_{40}O_4$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 17 13 4	0	0
6	A	1	Total C O 13 9 4	0	0
6	B	1	Total C O 19 15 4	0	0
6	B	1	Total C 14 14	0	0
6	B	1	Total C O 14 10 4	0	0

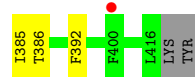
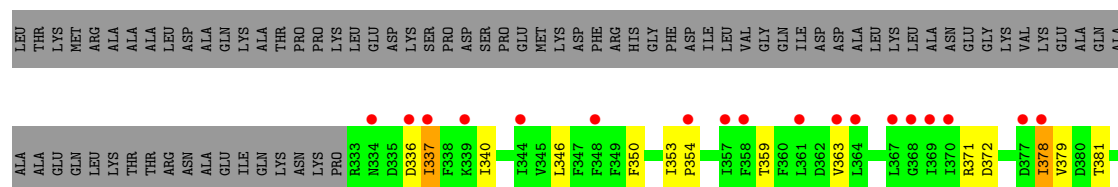
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	38	Total O 38 38	0	0
7	B	28	Total O 28 28	0	0

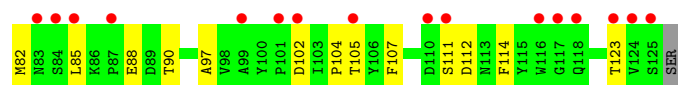
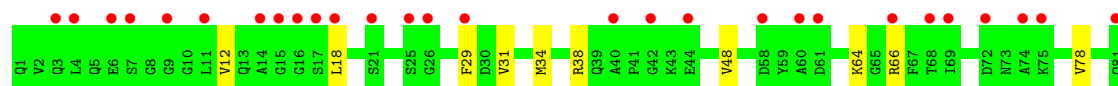
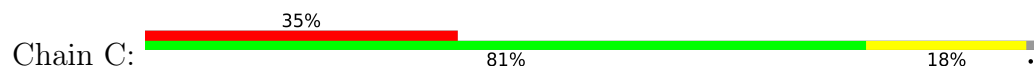
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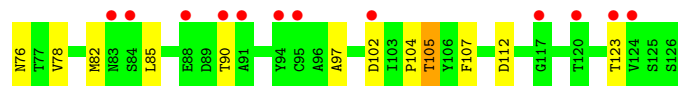
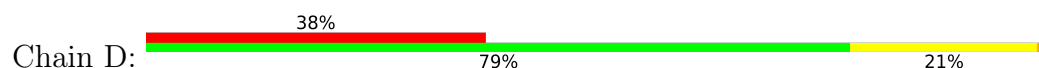
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	1	Total 1	O 1	0	0
7	D	4	Total 4	O 4	0	0
7	E	1	Total 1	O 1	0	0
7	G	3	Total 3	O 3	0	0
7	H	1	Total 1	O 1	0	0



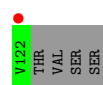
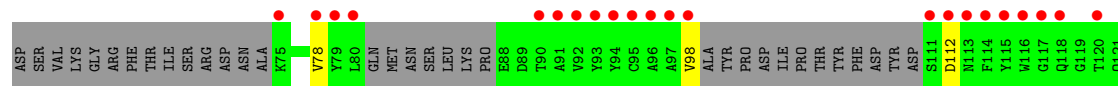
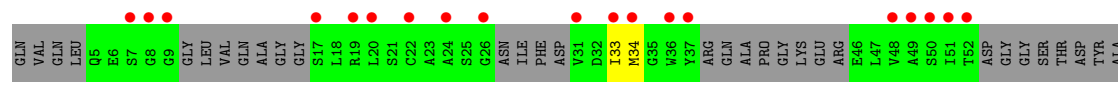
- Molecule 2: Nanobody Nb.AT110i1



- Molecule 2: Nanobody Nb.AT110i1

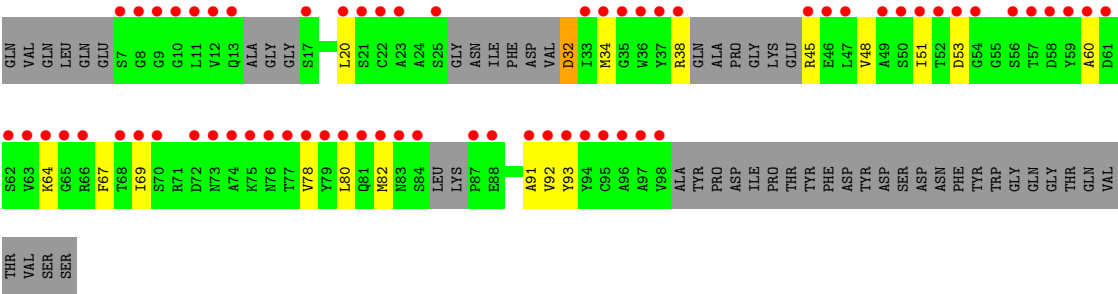


- Molecule 2: Nanobody Nb.AT110i1



- Molecule 2: Nanobody Nb.AT110i1

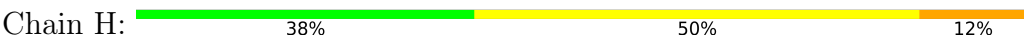




● Molecule 3: Angiotensin-like peptide S1I8



● Molecule 3: Angiotensin-like peptide S1I8



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2	Depositor
Cell constants a, b, c, α , β , γ	135.68Å 227.80Å 41.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.62 – 2.90 43.62 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.2 (43.62-2.90) 97.2 (43.62-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.22 (at 2.90Å)	Xtrriage
Refinement program	PHENIX (1.13_2998)	Depositor
R, R_{free}	0.304 , 0.359 0.309 , 0.313	Depositor DCC
R_{free} test set	1989 reflections (6.67%)	wwPDB-VP
Wilson B-factor (Å ²)	48.8	Xtrriage
Anisotropy	0.474	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 70.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	7930	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 60.80 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.4413e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NAG, OLC, CL, SAR

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	0.14	0/2476	0.37	0/3375
1	B	0.15	0/2452	0.38	0/3343
2	C	0.11	0/953	0.32	0/1300
2	D	0.12	0/951	0.33	0/1298
2	E	0.08	0/413	0.24	0/557
2	F	0.11	0/535	0.30	0/719
3	G	0.13	0/66	0.35	0/88
3	H	0.12	0/66	0.39	0/88
All	All	0.13	0/7912	0.35	0/10768

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	2411	0	2447	53	2
1	B	2388	0	2412	46	2
2	C	933	0	847	12	0
2	D	931	0	842	18	0
2	E	411	0	344	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	532	0	482	15	0
3	G	69	0	73	3	0
3	H	69	0	73	6	0
4	A	14	0	13	0	0
4	B	14	0	13	0	0
5	A	3	0	0	0	0
5	B	2	0	0	0	0
6	A	30	0	37	4	0
6	B	47	0	64	0	0
7	A	38	0	0	2	0
7	B	28	0	0	2	0
7	C	1	0	0	0	0
7	D	4	0	0	0	0
7	E	1	0	0	0	0
7	G	3	0	0	0	0
7	H	1	0	0	0	0
All	All	7930	0	7647	141	2

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 9.

All (141) 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:B:27:ILE:HD11	1:B:381:THR:HG23	1.64	0.80
1:A:333:ARG:O	1:A:334:ASN:ND2	2.18	0.76
1:A:167:ARG:NH2	3:H:6:HIS:O	2.19	0.74
2:D:64:LYS:HA	2:F:92:VAL:HG23	1.73	0.69
1:A:125:ASP:OD2	1:A:126:ARG:NH1	2.26	0.68
1:A:27:ILE:HD11	1:A:381:THR:HG23	1.76	0.67
1:B:15:GLN:NE2	1:B:173:GLU:OE1	2.29	0.66
1:B:106:ALA:HB2	1:B:164:ILE:HG12	1.79	0.65
1:A:126:ARG:NH2	2:C:112:ASP:OD1	2.30	0.64
2:F:32:ASP:OD1	2:F:32:ASP:N	2.29	0.64
2:D:90:THR:HG23	2:D:123:THR:HA	1.79	0.63
1:A:199:LYS:NZ	3:H:8:ILE:OXT	2.32	0.63
1:B:80:THR:HG21	1:B:104:ALA:HA	1.81	0.62
1:B:371:ARG:NH2	7:B:1104:HOH:O	2.32	0.62
2:D:31:VAL:HG11	2:D:97:ALA:HB1	1.80	0.62
1:B:199:LYS:NZ	3:G:8:ILE:OXT	2.34	0.61
2:D:64:LYS:O	2:D:66:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:32:ASP:N	2:F:53:ASP:OD2	2.33	0.61
2:D:30:ASP:OD1	2:D:76:ASN:ND2	2.20	0.61
1:A:362:ASP:OD1	3:H:2:ARG:NH1	2.34	0.60
2:C:90:THR:HG23	2:C:123:THR:HA	1.84	0.60
1:A:93:ARG:NH1	7:A:1104:HOH:O	2.35	0.59
1:B:386:THR:O	7:B:1101:HOH:O	2.17	0.59
1:B:167:ARG:NH2	3:G:6:HIS:O	2.36	0.59
2:D:65:GLY:H	2:F:92:VAL:HG23	1.67	0.59
1:B:125:ASP:OD2	1:B:126:ARG:NH1	2.36	0.59
2:C:31:VAL:HG11	2:C:97:ALA:HB1	1.84	0.58
1:B:21:ALA:O	1:B:23:ARG:NH2	2.35	0.58
1:A:414:GLN:NE2	7:A:1106:HOH:O	2.37	0.57
1:B:336:ASP:OD1	1:B:336:ASP:N	2.38	0.57
1:A:337:ILE:HA	1:A:340:ILE:HD12	1.87	0.56
1:A:90:MET:HG2	6:A:1006:OLC:C24	2.36	0.56
1:A:21:ALA:O	1:A:23:ARG:NH2	2.39	0.55
1:B:337:ILE:HA	1:B:340:ILE:HD12	1.88	0.55
1:A:98:ASN:HD21	1:A:102:LYS:HE3	1.71	0.55
2:E:33:ILE:HB	2:E:98:VAL:HB	1.89	0.54
1:B:378:ILE:HG13	1:B:379:VAL:N	2.21	0.54
1:B:31:ILE:HD11	1:B:385:ILE:HD13	1.90	0.54
1:B:353:ILE:HG22	1:B:354:PRO:HD3	1.90	0.54
1:B:38:ILE:HG12	1:B:392:PHE:HD1	1.72	0.54
1:B:117:PHE:HB3	1:B:152:ILE:HD12	1.89	0.54
1:A:184:TYR:HE2	3:H:4:TYR:HB2	1.74	0.53
1:A:346:LEU:HD22	1:A:350:PHE:HE2	1.72	0.53
1:A:375:ILE:HA	1:A:378:ILE:HD12	1.90	0.53
1:A:117:PHE:HB3	1:A:152:ILE:HD12	1.91	0.53
2:C:34:MET:HB2	2:C:78:VAL:HG21	1.91	0.52
2:D:65:GLY:H	2:F:92:VAL:CG2	2.22	0.52
1:A:350:PHE:HA	1:A:353:ILE:HG22	1.91	0.52
2:D:38:ARG:HH12	2:D:63:VAL:HG11	1.75	0.52
1:A:90:MET:HG2	6:A:1006:OLC:H24	1.92	0.51
1:A:364:LEU:HD13	1:A:369:ILE:HD11	1.92	0.51
1:A:199:LYS:HG2	1:A:356:GLN:HE22	1.75	0.50
1:B:112:LEU:O	1:B:116:VAL:HG23	2.12	0.50
1:A:103:ILE:HG13	1:A:104:ALA:N	2.26	0.49
1:A:167:ARG:HG2	1:A:182:PHE:CE1	2.47	0.49
1:A:199:LYS:HD2	1:A:359:THR:HG21	1.94	0.49
2:C:102:ASP:O	2:C:104:PRO:HD3	2.12	0.49
2:E:34:MET:HE2	2:E:78:VAL:HG22	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:38:ARG:HG2	2:D:48:VAL:HG22	1.95	0.49
1:A:38:ILE:HG12	1:A:392:PHE:HD1	1.78	0.49
2:D:58:ASP:CG	2:F:45:ARG:HH12	2.22	0.48
1:B:189:SER:O	1:B:192:PRO:HD3	2.14	0.48
2:D:102:ASP:O	2:D:104:PRO:HD3	2.12	0.48
1:B:98:ASN:OD1	1:B:168:ASN:ND2	2.46	0.48
1:B:102:LYS:HE2	1:B:167:ARG:O	2.13	0.48
1:B:62:VAL:HG13	1:B:145:ALA:HB2	1.95	0.48
2:C:82:MET:HB3	2:C:85:LEU:HD21	1.95	0.48
2:D:53:ASP:OD1	2:D:54:GLY:N	2.47	0.48
2:F:60:ALA:O	2:F:64:LYS:HG3	2.14	0.48
1:B:167:ARG:NH1	1:B:180:CYS:O	2.47	0.47
1:B:82:PRO:O	1:B:86:VAL:HG22	2.13	0.47
1:A:16:ASP:HB3	1:A:19:PRO:HB3	1.95	0.47
1:B:93:ARG:HG2	1:B:177:ILE:HG23	1.97	0.47
1:A:336:ASP:N	1:A:336:ASP:OD1	2.48	0.47
2:C:64:LYS:O	2:C:66:ARG:NH2	2.48	0.47
2:D:82:MET:HB3	2:D:85:LEU:HD21	1.97	0.46
1:A:112:LEU:O	1:A:116:VAL:HG23	2.14	0.46
1:B:34:LEU:O	1:B:38:ILE:HG13	2.15	0.46
1:B:98:ASN:HD21	1:B:102:LYS:HE3	1.81	0.46
1:A:163:ALA:O	1:A:167:ARG:HB2	2.16	0.46
1:B:227:ASP:O	1:B:231:ASN:N	2.49	0.46
1:A:99:TYR:O	1:A:103:ILE:HG23	2.16	0.45
1:A:394:ASN:O	1:A:397:ASN:HB2	2.17	0.45
3:H:5:ILE:HD13	3:H:5:ILE:H	1.81	0.45
1:A:39:PHE:HB2	1:A:81:LEU:HD23	1.99	0.45
1:B:167:ARG:NH1	1:B:180:CYS:SG	2.90	0.45
2:C:38:ARG:HG2	2:C:48:VAL:HG22	1.97	0.45
2:D:59:TYR:CE2	2:F:92:VAL:HG11	2.52	0.45
1:B:126:ARG:NH2	2:D:112:ASP:OD1	2.40	0.45
1:B:167:ARG:HG2	1:B:182:PHE:CE1	2.52	0.44
1:A:96:PHE:HB3	1:A:100:LEU:HD12	1.99	0.44
1:A:168:ASN:HB2	1:A:170:PHE:CZ	2.53	0.44
1:A:146:LYS:O	1:A:150:ILE:HG23	2.17	0.44
1:B:86:VAL:HG21	1:B:96:PHE:HZ	1.82	0.44
1:B:163:ALA:O	1:B:167:ARG:HB2	2.16	0.44
2:C:111:SER:OG	2:C:114:PHE:O	2.35	0.44
1:A:74:ASP:HA	1:A:111:ASN:ND2	2.33	0.44
1:A:90:MET:HG2	6:A:1006:OLC:H24A	1.98	0.44
1:B:146:LYS:O	1:B:150:ILE:HG23	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:TYR:CE2	3:H:4:TYR:HB2	2.51	0.44
1:A:206:PHE:HB2	1:A:207:PRO:HD3	2.00	0.44
1:A:116:VAL:HG13	1:A:348:PHE:HZ	1.83	0.44
1:A:353:ILE:HG23	1:A:354:PRO:HD3	2.00	0.43
1:B:16:ASP:H	1:B:174:ASN:HD21	1.65	0.43
1:A:102:LYS:HD3	1:A:167:ARG:O	2.19	0.43
2:C:88:GLU:OE1	2:C:88:GLU:N	2.48	0.43
1:A:34:LEU:O	1:A:38:ILE:HG13	2.18	0.43
1:A:403:PHE:CD2	1:A:409:LYS:HG3	2.53	0.43
1:B:74:ASP:HA	1:B:111:ASN:ND2	2.33	0.43
2:C:12:VAL:HG21	2:C:18:LEU:HG	2.00	0.43
2:F:48:VAL:HG21	2:F:93:TYR:HD2	1.84	0.43
1:B:104:ALA:O	1:B:108:VAL:HG23	2.19	0.42
1:A:60:LYS:C	1:A:142:MET:HE1	2.44	0.42
1:B:197:LEU:O	1:B:201:ILE:HG22	2.18	0.42
2:F:38:ARG:HB2	2:F:91:ALA:HB3	2.01	0.42
1:A:197:LEU:O	1:A:201:ILE:HG22	2.19	0.42
1:B:60:LYS:HE2	1:B:60:LYS:HB3	1.84	0.42
1:B:346:LEU:HD22	1:B:350:PHE:HE2	1.84	0.42
2:C:105:THR:C	2:C:107:PHE:H	2.28	0.42
1:B:57:MET:HE3	1:B:57:MET:HB2	1.93	0.42
2:F:69:ILE:HB	2:F:80:LEU:HD13	2.02	0.42
1:B:337:ILE:H	1:B:337:ILE:HG13	1.65	0.42
1:A:206:PHE:O	1:A:210:ILE:HG13	2.19	0.41
1:B:359:THR:O	1:B:363:VAL:HG23	2.20	0.41
1:A:86:VAL:CG2	1:A:90:MET:HE3	2.50	0.41
2:F:67:PHE:CE1	2:F:82:MET:HB3	2.55	0.41
3:G:5:ILE:H	3:G:5:ILE:HD13	1.84	0.41
2:D:34:MET:HB2	2:D:78:VAL:HG11	2.01	0.41
2:D:59:TYR:CZ	2:D:69:ILE:HG22	2.56	0.41
2:F:20:LEU:HD23	2:F:20:LEU:HA	1.85	0.41
1:A:219:TRP:CH2	1:A:338:PHE:HB3	2.56	0.41
1:A:106:ALA:HB2	1:A:164:ILE:HG12	2.02	0.41
1:B:53:ILE:HD12	1:B:53:ILE:HA	1.92	0.41
2:D:105:THR:C	2:D:107:PHE:H	2.27	0.41
1:A:21:ALA:HB1	1:A:377:ASP:HA	2.03	0.41
1:B:77:PHE:HB2	1:B:111:ASN:HB2	2.03	0.41
1:B:119:LEU:HD23	1:B:119:LEU:HA	1.93	0.40
2:F:34:MET:HB2	2:F:78:VAL:HG11	2.04	0.40
1:A:79:LEU:HD23	1:A:79:LEU:HA	1.83	0.40
1:A:86:VAL:HB	6:A:1006:OLC:H2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:80:LEU:HD23	2:F:82:MET:HE2	2.03	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ASP:OD2	1:B:127:TYR:OH[4_556]	2.01	0.19
1:A:127:TYR:OH	1:B:372:ASP:OD2[4_555]	2.13	0.07

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	298/425 (70%)	283 (95%)	15 (5%)	0	100	100
1	B	298/425 (70%)	284 (95%)	14 (5%)	0	100	100
2	C	123/126 (98%)	112 (91%)	11 (9%)	0	100	100
2	D	124/126 (98%)	113 (91%)	11 (9%)	0	100	100
2	E	44/126 (35%)	40 (91%)	4 (9%)	0	100	100
2	F	65/126 (52%)	62 (95%)	3 (5%)	0	100	100
3	G	6/8 (75%)	6 (100%)	0	0	100	100
3	H	6/8 (75%)	6 (100%)	0	0	100	100
All	All	964/1370 (70%)	906 (94%)	58 (6%)	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	254/373 (68%)	248 (98%)	6 (2%)	43	75
1	B	249/373 (67%)	243 (98%)	6 (2%)	43	75
2	C	94/102 (92%)	93 (99%)	1 (1%)	65	88
2	D	93/102 (91%)	91 (98%)	2 (2%)	45	77
2	E	38/102 (37%)	37 (97%)	1 (3%)	40	73
2	F	52/102 (51%)	50 (96%)	2 (4%)	29	64
3	G	7/7 (100%)	6 (86%)	1 (14%)	3	11
3	H	7/7 (100%)	6 (86%)	1 (14%)	3	11
All	All	794/1168 (68%)	774 (98%)	20 (2%)	42	74

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ILE
1	A	103	ILE
1	A	126	ARG
1	A	334	ASN
1	A	353	ILE
1	A	415	LEU
1	B	43	ILE
1	B	56	TYR
1	B	126	ARG
1	B	191	LEU
1	B	337	ILE
1	B	378	ILE
2	C	29	PHE
2	D	29	PHE
2	D	105	THR
2	E	112	ASP
2	F	32	ASP
2	F	51	ILE
3	G	5	ILE
3	H	5	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	69	ASN
1	A	98	ASN
1	A	168	ASN
1	A	355	HIS
1	A	356	GLN
1	A	394	ASN
1	A	414	GLN
1	B	98	ASN
1	B	166	HIS
1	B	168	ASN
1	B	200	ASN
2	C	27	ASN
2	C	39	GLN
2	D	13	GLN
2	D	113	ASN
2	F	76	ASN
2	F	83	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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	SAR	G	1	3	3,4,5	1.30	0	1,3,5	1.55	0
3	SAR	H	1	3	3,4,5	1.30	0	1,3,5	1.41	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
3	SAR	G	1	3	-	1/1/2/3	-
3	SAR	H	1	3	-	1/1/2/3	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	G	1	SAR	C-CA-N-CN
3	H	1	SAR	C-CA-N-CN

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](#)

Of 12 ligands modelled in this entry, 5 are monoatomic - leaving 7 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	$\# Z > 2$
4	NAG	B	1001	1	14,14,15	0.18	0	17,19,21	0.50	0
6	OLC	A	1006	-	12,12,24	1.40	1 (8%)	13,13,25	1.32	1 (7%)
6	OLC	B	1004	-	18,18,24	1.18	1 (5%)	19,19,25	6.08	4 (21%)
6	OLC	B	1006	-	13,13,24	1.22	1 (7%)	14,14,25	1.06	1 (7%)
4	NAG	A	1001	1	14,14,15	0.20	0	17,19,21	0.51	0
6	OLC	A	1005	-	16,16,24	1.14	1 (6%)	17,17,25	1.09	1 (5%)
6	OLC	B	1005	-	13,13,24	0.21	0	12,12,25	0.68	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
4	NAG	B	1001	1	-	2/6/23/26	0/1/1/1
6	OLC	A	1006	-	-	5/12/12/24	-
6	OLC	B	1004	-	-	6/18/18/24	-
6	OLC	B	1006	-	-	2/13/13/24	-
4	NAG	A	1001	1	-	0/6/23/26	0/1/1/1
6	OLC	A	1005	-	-	2/16/16/24	-
6	OLC	B	1005	-	-	6/11/11/24	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	1004	OLC	O20-C1	4.76	1.47	1.33
6	A	1006	OLC	O20-C1	4.73	1.47	1.33
6	A	1005	OLC	O20-C1	4.29	1.45	1.33
6	B	1006	OLC	O20-C1	4.18	1.45	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	1004	OLC	O20-C1-O19	-17.89	78.88	123.63
6	B	1004	OLC	O20-C1-C2	15.73	159.80	111.83
6	B	1004	OLC	O19-C1-C2	-10.95	80.94	123.78
6	A	1005	OLC	O20-C1-C2	2.90	120.69	111.83
6	A	1006	OLC	O20-C1-C2	2.80	120.36	111.83
6	B	1006	OLC	O20-C1-C2	2.68	120.02	111.83
6	B	1004	OLC	C21-O20-C1	2.49	126.20	117.12

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	1005	OLC	O20-C21-C22-O23
6	A	1006	OLC	O20-C21-C22-C24
6	B	1004	OLC	O20-C21-C22-C24
6	B	1006	OLC	C21-C22-C24-O25
6	B	1004	OLC	C2-C1-O20-C21

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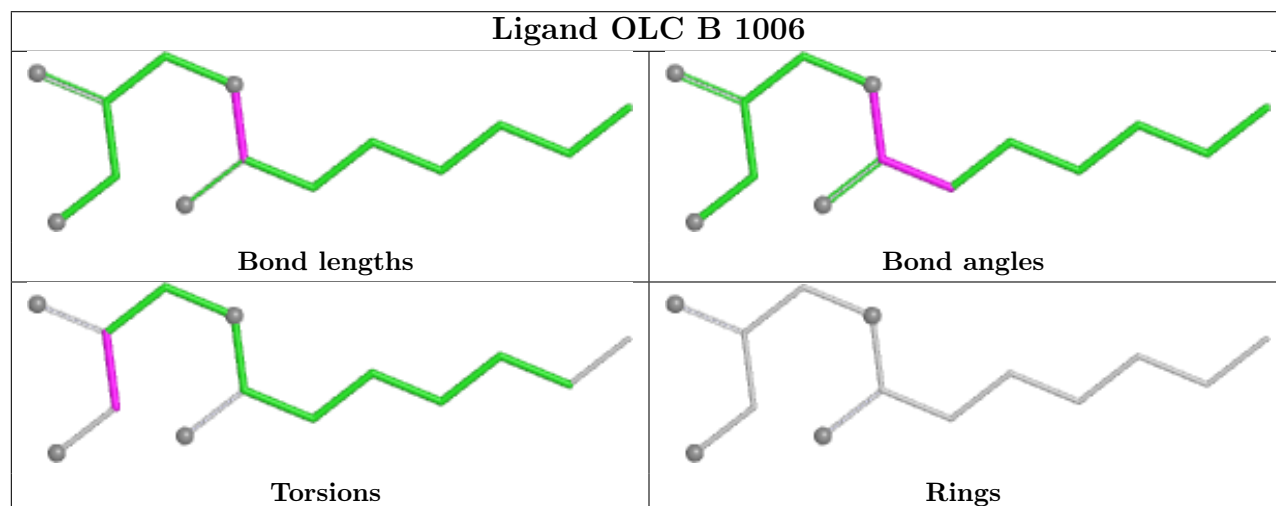
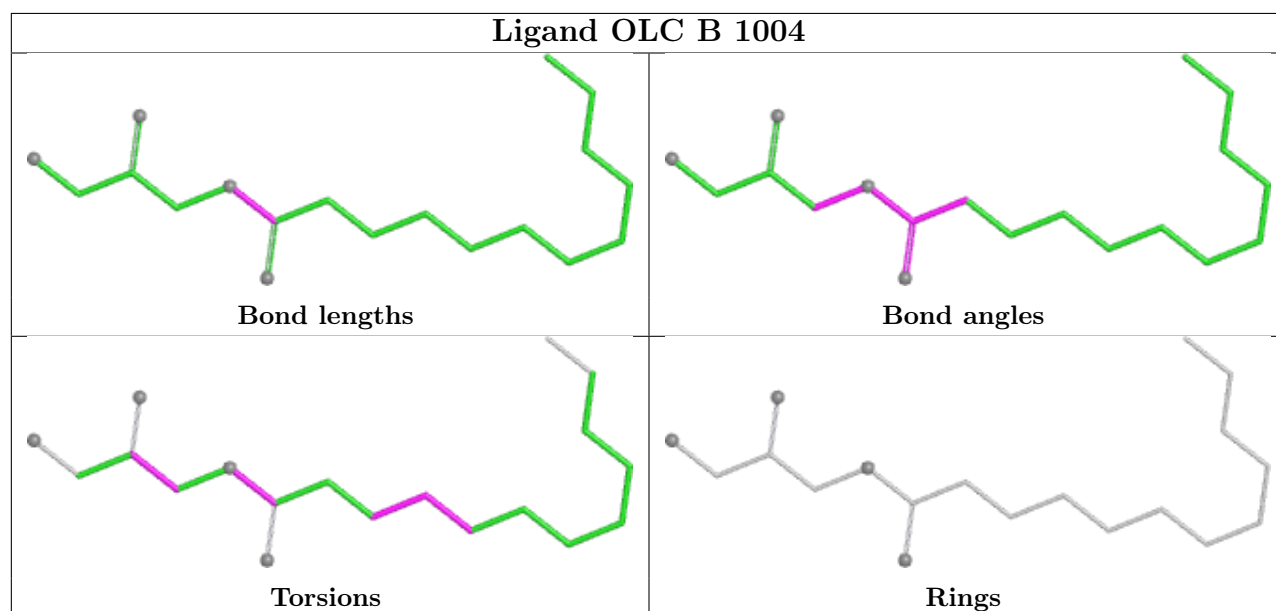
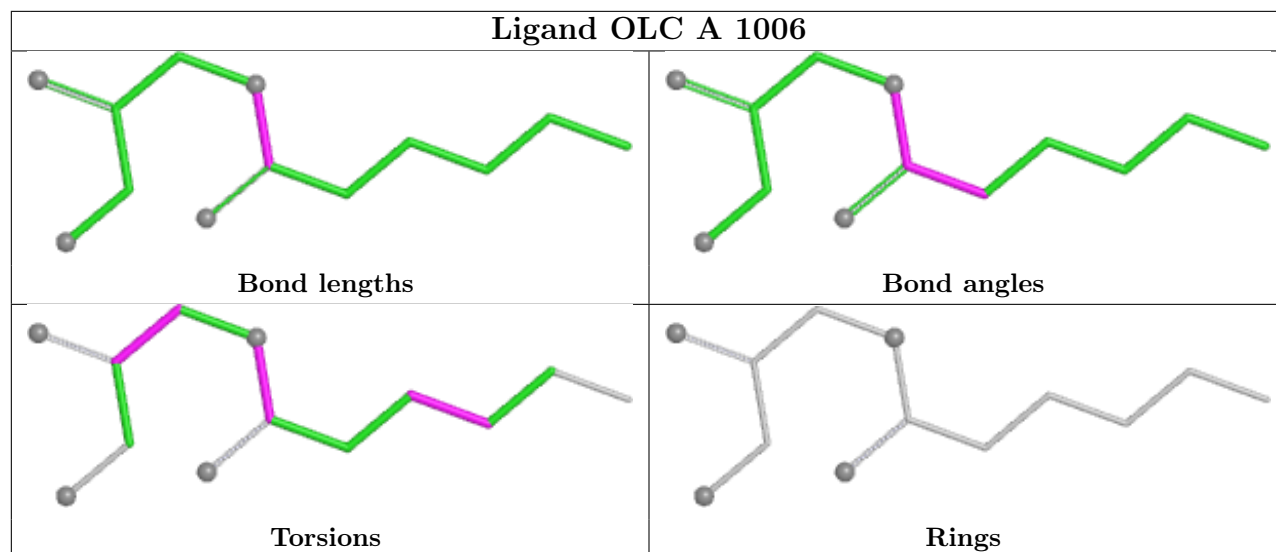
Mol	Chain	Res	Type	Atoms
6	B	1004	OLC	O19-C1-O20-C21
6	A	1006	OLC	O20-C21-C22-O23
4	B	1001	NAG	O5-C5-C6-O6
4	B	1001	NAG	C4-C5-C6-O6
6	B	1004	OLC	O20-C21-C22-O23
6	B	1005	OLC	C5-C6-C7-C8
6	A	1005	OLC	O20-C21-C22-C24
6	B	1005	OLC	C6-C7-C8-C9
6	B	1005	OLC	C4-C5-C6-C7
6	B	1004	OLC	C3-C4-C5-C6
6	B	1005	OLC	C3-C4-C5-C6
6	B	1006	OLC	O23-C22-C24-O25
6	B	1005	OLC	C11-C12-C13-C14
6	A	1006	OLC	C2-C1-O20-C21
6	B	1005	OLC	C13-C14-C15-C16
6	A	1006	OLC	O19-C1-O20-C21
6	B	1004	OLC	C2-C3-C4-C5
6	A	1006	OLC	C2-C3-C4-C5

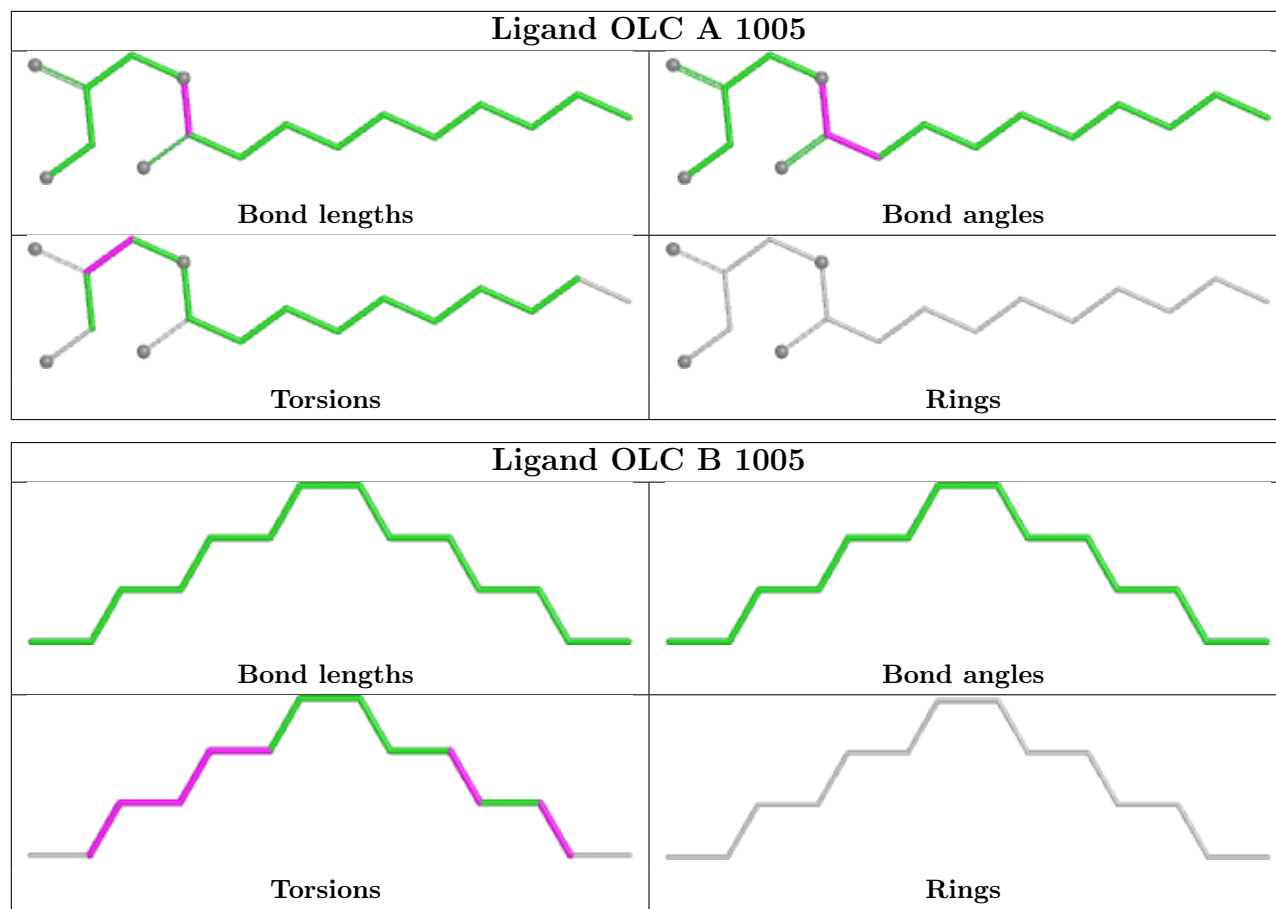
There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	1006	OLC	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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	304/425 (71%)	1.27	62 (20%) 3 2	22, 42, 72, 97	0
1	B	304/425 (71%)	1.43	70 (23%) 2 2	20, 41, 70, 84	0
2	C	125/126 (99%)	1.82	44 (35%) 1 1	43, 71, 97, 111	0
2	D	126/126 (100%)	1.97	48 (38%) 1 0	44, 75, 98, 111	0
2	E	58/126 (46%)	2.88	42 (72%) 0 0	76, 114, 136, 139	0
2	F	75/126 (59%)	3.16	65 (86%) 0 0	96, 120, 144, 155	0
3	G	7/8 (87%)	1.22	1 (14%) 6 5	27, 33, 42, 52	0
3	H	7/8 (87%)	0.11	0 100 100	24, 38, 43, 49	0
All	All	1006/1370 (73%)	1.70	332 (33%) 1 1	20, 49, 123, 155	0

All (332) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	15	GLY	6.9
2	F	10	GLY	6.8
2	F	25	SER	6.6
2	C	105	THR	6.4
2	F	93	TYR	6.4
2	F	58	ASP	6.1
1	B	185	GLU	6.1
2	D	84	SER	5.9
2	F	92	VAL	5.9
2	D	61	ASP	5.6
2	F	37	TYR	5.6
2	F	94	TYR	5.4
2	E	50	SER	5.4
2	E	95	CYS	5.3
2	C	84	SER	5.3
1	A	228	LEU	5.2

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Mol	Chain	Res	Type	RSRZ
2	F	98	VAL	5.2
2	E	97	ALA	5.1
2	C	15	GLY	5.1
2	E	7	SER	5.1
2	F	33	ILE	5.0
1	A	334	ASN	5.0
2	D	75	LYS	5.0
2	F	11	LEU	4.9
2	D	58	ASP	4.9
2	E	51	ILE	4.9
2	F	87	PRO	4.9
2	D	117	GLY	4.8
2	E	8	GLY	4.8
2	C	125	SER	4.8
2	F	97	ALA	4.7
2	D	43	LYS	4.7
2	D	66	ARG	4.6
2	F	56	SER	4.5
2	E	22	CYS	4.5
2	E	75	LYS	4.4
2	C	117	GLY	4.3
2	C	102	ASP	4.3
2	F	68	THR	4.2
2	C	29	PHE	4.1
2	E	20	LEU	4.1
1	B	369	ILE	4.0
2	F	96	ALA	4.0
2	D	123	THR	4.0
2	F	45	ARG	3.9
2	D	8	GLY	3.9
1	A	76	CYS	3.9
1	B	14	ILE	3.9
2	C	123	THR	3.9
2	C	61	ASP	3.9
2	F	83	ASN	3.9
2	E	48	VAL	3.9
2	F	57	THR	3.9
1	B	229	GLU	3.8
2	F	61	ASP	3.8
2	F	72	ASP	3.8
2	C	118	GLN	3.8
2	D	18	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	B	9	ASP	3.8
1	B	227	ASP	3.8
2	D	64	LYS	3.8
2	D	65	GLY	3.8
2	F	9	GLY	3.8
1	A	190	THR	3.8
1	B	178	THR	3.8
1	A	411	TYR	3.7
2	E	80	LEU	3.7
1	B	10	GLY	3.7
2	E	111	SER	3.7
2	F	91	ALA	3.7
2	F	84	SER	3.7
1	B	44	PHE	3.7
2	E	26	GLY	3.7
2	C	4	LEU	3.6
2	F	34	MET	3.6
1	B	370	ILE	3.6
2	E	52	THR	3.6
2	D	124	VAL	3.6
1	B	228	LEU	3.6
2	D	40	ALA	3.5
1	A	115	SER	3.5
2	E	9	GLY	3.5
1	A	231	ASN	3.5
2	E	114	PHE	3.5
2	D	16	GLY	3.5
2	D	102	ASP	3.5
2	D	44	GLU	3.5
2	E	116	TRP	3.5
2	F	79	TYR	3.4
1	B	197	LEU	3.4
2	C	85	LEU	3.4
2	E	24	ALA	3.4
2	E	98	VAL	3.4
1	B	173	GLU	3.4
1	B	192	PRO	3.4
2	C	16	GLY	3.3
1	A	177	ILE	3.3
2	D	69	ILE	3.3
1	A	191	LEU	3.3
2	F	62	SER	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	43	ILE	3.3
1	B	76	CYS	3.3
1	A	10	GLY	3.3
2	E	36	TRP	3.3
1	A	337	ILE	3.2
2	F	69	ILE	3.2
2	C	40	ALA	3.2
2	F	75	LYS	3.2
2	F	50	SER	3.1
2	C	75	LYS	3.1
2	E	94	TYR	3.1
1	B	115	SER	3.1
1	B	231	ASN	3.1
2	D	26	GLY	3.1
2	E	117	GLY	3.1
2	E	96	ALA	3.1
2	E	17	SER	3.1
1	A	14	ILE	3.1
1	A	226	TYR	3.1
2	E	19	ARG	3.1
2	F	38	ARG	3.1
2	C	81	GLN	3.0
1	B	75	LEU	3.0
2	D	68	THR	3.0
1	B	216	THR	3.0
1	B	196	GLY	3.0
1	B	334	ASN	3.0
2	E	49	ALA	3.0
2	E	79	TYR	3.0
2	C	42	GLY	3.0
1	A	192	PRO	3.0
1	B	18	CYS	2.9
1	A	225	ALA	2.9
2	C	3	GLN	2.9
2	C	44	GLU	2.9
2	F	36	TRP	2.9
1	B	230	ASP	2.9
2	D	56	SER	2.9
2	F	7	SER	2.9
2	D	54	GLY	2.9
1	A	333	ARG	2.9
2	F	21	SER	2.9

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Mol	Chain	Res	Type	RSRZ
2	E	120	THR	2.9
2	F	65	GLY	2.8
2	F	82	MET	2.8
2	F	66	ARG	2.8
2	F	77	THR	2.8
2	F	80	LEU	2.8
1	B	225	ALA	2.8
1	B	191	LEU	2.8
1	B	377	ASP	2.8
2	D	10	GLY	2.8
1	A	19	PRO	2.8
1	A	56	TYR	2.8
1	B	177	ILE	2.8
2	D	9	GLY	2.8
2	F	78	VAL	2.8
2	E	91	ALA	2.8
2	F	52	THR	2.8
2	D	45	ARG	2.7
2	F	49	ALA	2.7
1	B	337	ILE	2.7
2	F	47	LEU	2.7
1	B	213	THR	2.7
1	A	64	SER	2.7
1	A	179	VAL	2.7
2	E	31	VAL	2.7
2	E	78	VAL	2.7
2	F	12	VAL	2.7
1	B	130	ILE	2.7
2	D	4	LEU	2.7
2	F	64	LYS	2.7
1	B	107	SER	2.7
2	E	118	GLN	2.7
2	F	88	GLU	2.7
1	A	48	LEU	2.7
2	E	113	ASN	2.7
2	C	101	PRO	2.7
1	A	366	GLN	2.7
2	C	111	SER	2.7
2	D	2	VAL	2.7
1	B	357	ILE	2.7
1	A	371	ARG	2.7
1	A	367	LEU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	105	SER	2.7
1	B	153	TRP	2.6
2	C	66	ARG	2.6
2	C	58	ASP	2.6
1	B	127	TYR	2.6
1	B	368	GLY	2.6
1	B	190	THR	2.6
1	A	345	VAL	2.6
1	B	168	ASN	2.6
1	B	217	LEU	2.6
2	F	60	ALA	2.6
1	B	87	TYR	2.6
2	E	115	TYR	2.6
2	D	11	LEU	2.6
1	A	185	GLU	2.6
1	B	170	PHE	2.6
1	A	336	ASP	2.6
1	B	354	PRO	2.6
2	D	59	TYR	2.6
1	A	143	LEU	2.6
1	B	48	LEU	2.6
1	B	164	ILE	2.6
2	F	17	SER	2.5
1	B	378	ILE	2.5
1	A	15	GLN	2.5
2	D	1	GLN	2.5
2	C	99	ALA	2.5
2	D	53	ASP	2.5
2	C	69	ILE	2.5
2	F	95	CYS	2.5
1	A	17	ASP	2.5
2	F	35	GLY	2.5
1	A	153	TRP	2.5
1	A	87	TYR	2.5
1	A	397	ASN	2.5
1	B	174	ASN	2.5
1	B	81	LEU	2.5
2	C	14	ALA	2.5
2	F	20	LEU	2.4
1	B	47	SER	2.4
2	C	116	TRP	2.4
1	A	44	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	67	PHE	2.4
2	F	74	ALA	2.4
2	C	83	ASN	2.4
1	A	59	LEU	2.4
1	A	70	LEU	2.4
1	A	72	LEU	2.4
1	A	149	CYS	2.4
1	A	202	LEU	2.4
1	A	357	ILE	2.4
2	E	112	ASP	2.4
2	F	53	ASP	2.4
2	C	9	GLY	2.4
2	F	46	GLU	2.4
2	D	94	TYR	2.4
2	F	13	GLN	2.4
2	D	57	THR	2.4
2	D	90	THR	2.4
1	B	336	ASP	2.4
2	E	122	VAL	2.4
1	A	71	ALA	2.4
1	B	344	ILE	2.4
1	B	171	PHE	2.4
1	B	348	PHE	2.4
1	A	54	TYR	2.4
1	A	413	LEU	2.4
1	B	361	LEU	2.4
1	A	27	ILE	2.4
2	F	51	ILE	2.4
1	B	358	PHE	2.3
2	F	22	CYS	2.3
2	C	74	ALA	2.3
2	D	24	ALA	2.3
1	A	141	THR	2.3
1	A	148	THR	2.3
1	A	184	TYR	2.3
1	B	69	ASN	2.3
2	D	88	GLU	2.3
2	E	34	MET	2.3
1	B	123	SER	2.3
1	A	11	ILE	2.3
2	D	29	PHE	2.3
2	C	6	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	227	ASP	2.3
2	D	20	LEU	2.3
1	B	27	ILE	2.3
2	F	70	SER	2.3
1	B	56	TYR	2.3
2	E	37	TYR	2.3
2	C	124	VAL	2.3
2	D	12	VAL	2.3
2	C	26	GLY	2.3
1	A	173	GLU	2.2
2	D	27	ASN	2.2
1	A	93	ARG	2.2
2	C	87	PRO	2.2
2	F	8	GLY	2.2
1	B	400	PHE	2.2
1	A	75	LEU	2.2
2	C	11	LEU	2.2
2	D	83	ASN	2.2
1	A	13	ARG	2.2
1	B	363	VAL	2.2
2	C	60	ALA	2.2
2	F	23	ALA	2.2
1	A	372	ASP	2.2
2	C	72	ASP	2.2
2	F	63	VAL	2.2
1	A	67	LEU	2.2
1	B	364	LEU	2.2
1	A	229	GLU	2.2
1	A	151	ILE	2.1
1	A	369	ILE	2.1
2	C	68	THR	2.1
2	E	90	THR	2.1
1	B	367	LEU	2.1
2	C	18	LEU	2.1
2	D	74	ALA	2.1
2	F	81	GLN	2.1
2	F	73	ASN	2.1
2	D	120	THR	2.1
2	E	93	TYR	2.1
2	F	59	TYR	2.1
2	C	7	SER	2.1
2	E	33	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	138	LEU	2.1
1	B	182	PHE	2.1
2	C	17	SER	2.1
2	D	95	CYS	2.1
2	D	42	GLY	2.1
1	A	103	ILE	2.1
2	D	91	ALA	2.1
1	B	339	LYS	2.0
2	C	21	SER	2.0
2	C	25	SER	2.0
3	G	7	PRO	2.0
1	B	139	ARG	2.0
1	A	145	ALA	2.0
1	B	85	ALA	2.0
2	C	110	ASP	2.0
1	B	219	TRP	2.0
1	B	57	MET	2.0
2	F	76	ASN	2.0
1	A	400	PHE	2.0
1	B	110	PHE	2.0
2	F	54	GLY	2.0
2	E	92	VAL	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($\text{\AA}^2$)	Q<0.9
3	SAR	H	1	5/6	0.89	0.23	41,45,48,56	0
3	SAR	G	1	5/6	0.90	0.23	40,42,48,49	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

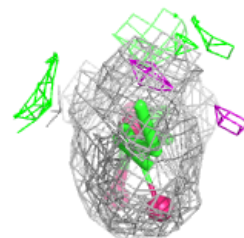
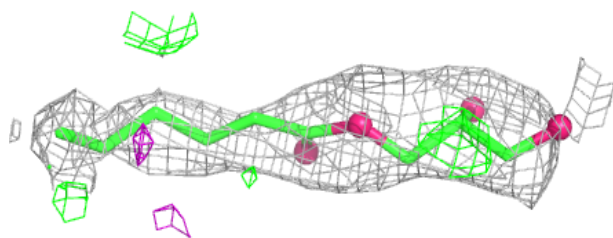
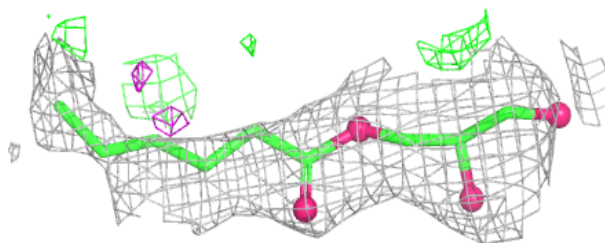
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	NAG	A	1001	14/15	0.63	0.15	65,83,111,115	0
4	NAG	B	1001	14/15	0.72	0.15	69,83,104,107	0
6	OLC	A	1006	13/25	0.74	0.19	33,49,64,81	0
6	OLC	B	1005	14/25	0.79	0.17	11,34,61,64	0
5	CL	A	1003	1/1	0.83	0.11	41,41,41,41	0
6	OLC	B	1004	19/25	0.83	0.15	28,46,60,61	0
6	OLC	A	1005	17/25	0.83	0.15	21,45,58,74	0
5	CL	A	1002	1/1	0.86	0.09	53,53,53,53	0
6	OLC	B	1006	14/25	0.87	0.14	25,47,83,93	0
5	CL	B	1003	1/1	0.92	0.11	42,42,42,42	0
5	CL	B	1002	1/1	0.92	0.16	40,40,40,40	0
5	CL	A	1004	1/1	0.99	0.07	28,28,28,28	0

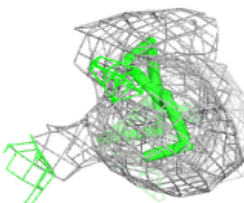
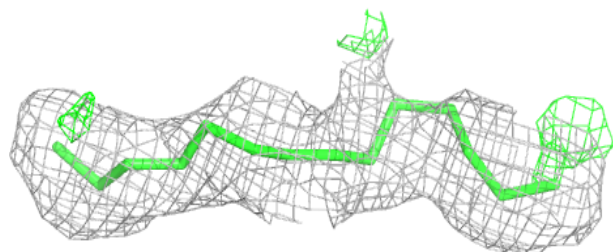
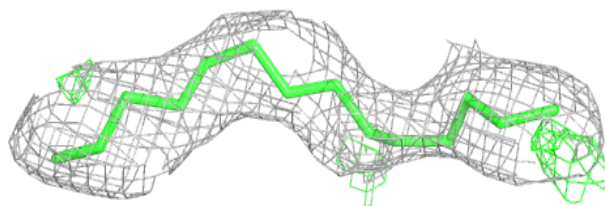
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 1006:

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

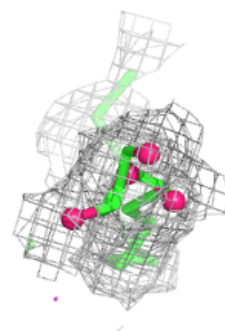
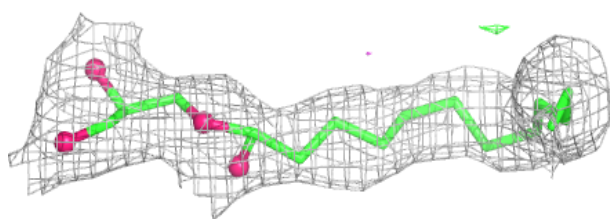
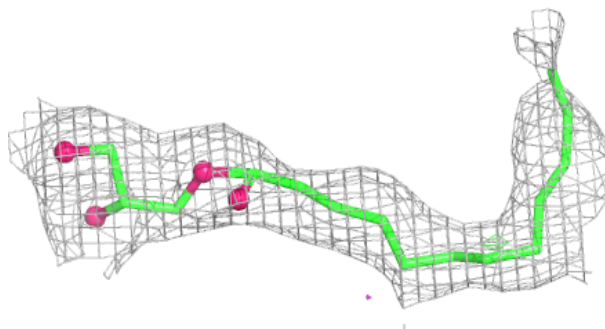
**Electron density around OLC B 1005:**

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

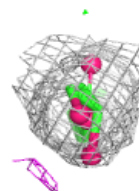
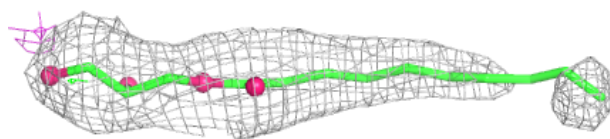
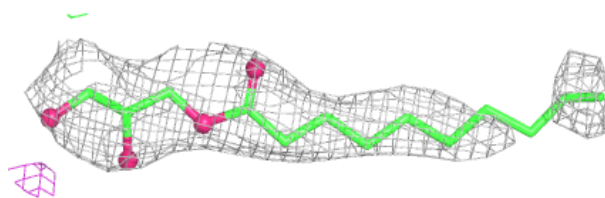


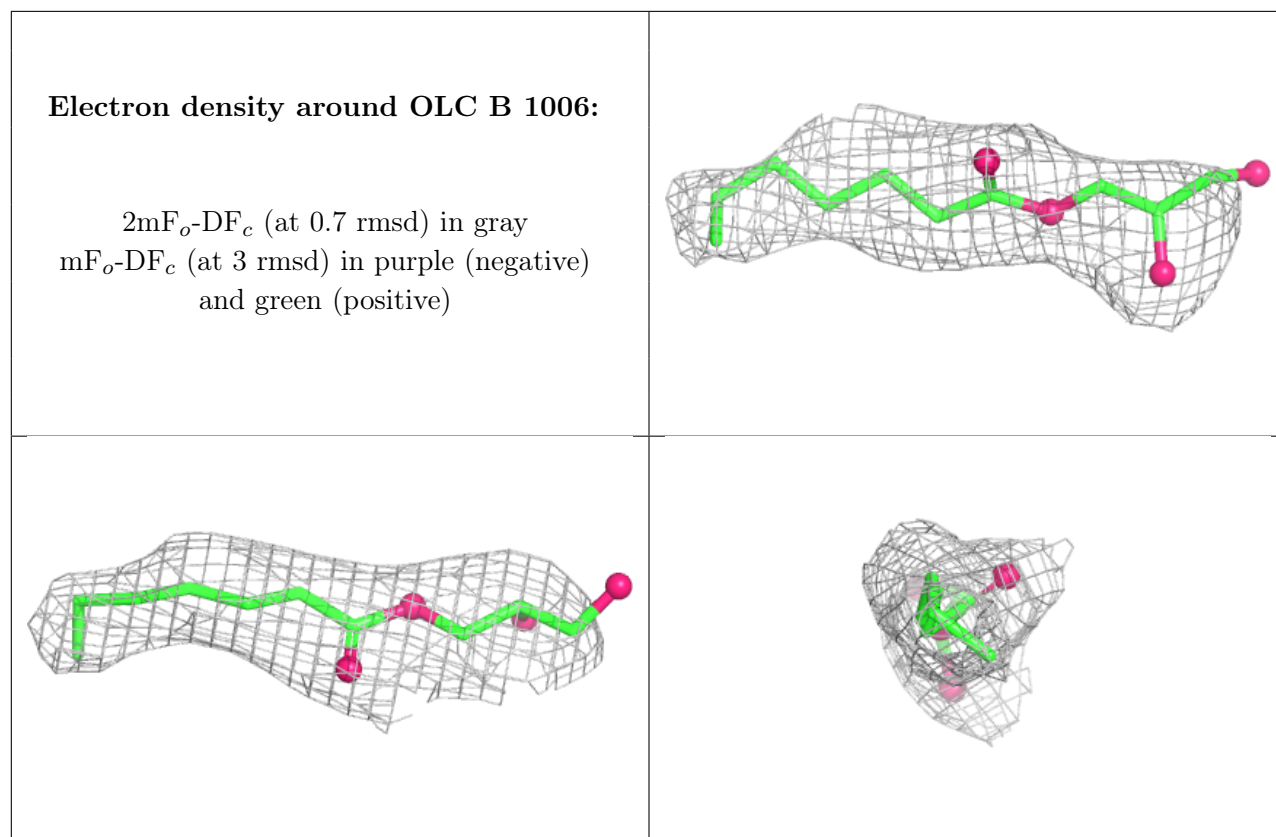
Electron density around OLC B 1004:

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

**Electron density around OLC A 1005:**

$2mF_o-DF_c$ (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.