Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 01:00 PM JST

PDB ID	:	5XAN
Title	:	Crystal structure of SecDF in I form (P212121 space group)
Authors	:	Tsukazaki, T.; Tanaka, Y.; Furukwa, A.
Deposited on	:	2017-03-14
Resolution	:	2.75 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 (i) 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 (i)) were used in the production of this report:

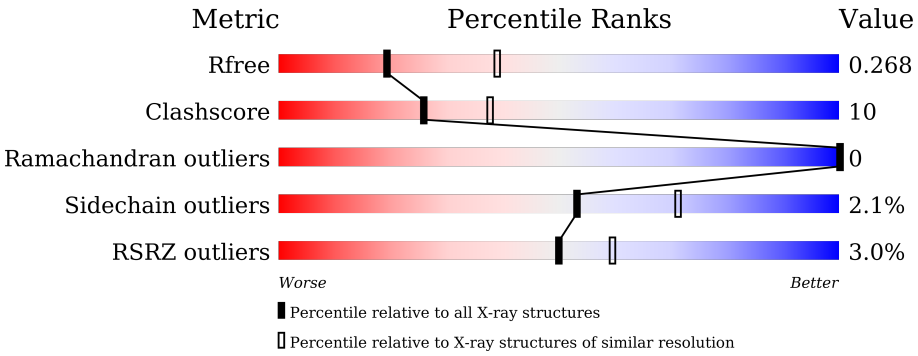
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.75 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	1235 (2.78-2.74)
Clashscore	141614	1277 (2.78-2.74)
Ramachandran outliers	138981	1257 (2.78-2.74)
Sidechain outliers	138945	1257 (2.78-2.74)
RSRZ outliers	127900	1207 (2.78-2.74)

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	750	4% 73% 23%
1	B	750	2% 78% 19%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11313 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.

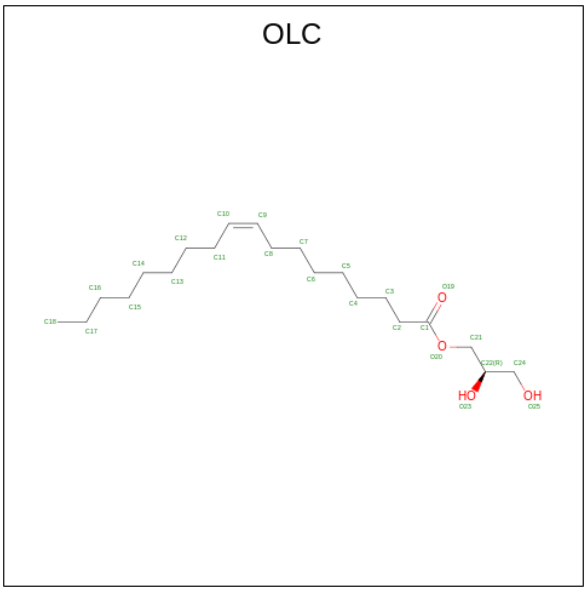
- Molecule 1 is a protein called Protein translocase subunit SecD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5495	3533	938	1010	14			
1	B	733	Total	C	N	O	S	0	0	0
			5540	3558	951	1017	14			

There are 22 discrepancies between the modelled and reference sequences:

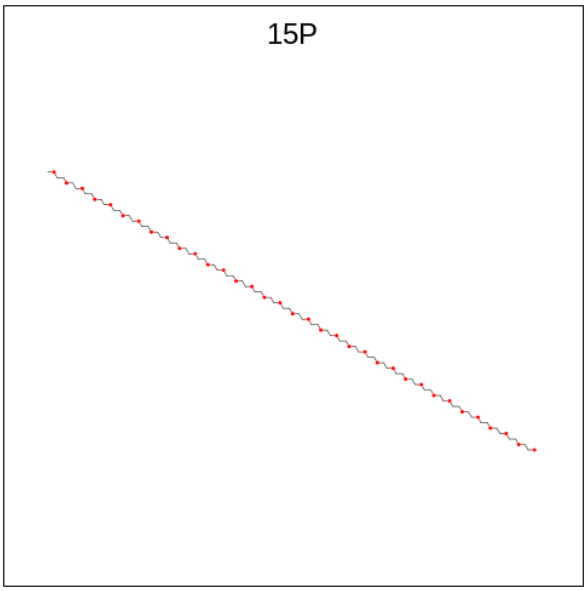
Chain	Residue	Modelled	Actual	Comment	Reference
A	27	MET	-	expression tag	UNP Q9RTE3
A	143	CYS	ILE	engineered mutation	UNP Q9RTE3
A	268	CYS	LEU	engineered mutation	UNP Q9RTE3
A	769	HIS	-	expression tag	UNP Q9RTE3
A	770	HIS	-	expression tag	UNP Q9RTE3
A	771	HIS	-	expression tag	UNP Q9RTE3
A	772	HIS	-	expression tag	UNP Q9RTE3
A	773	HIS	-	expression tag	UNP Q9RTE3
A	774	HIS	-	expression tag	UNP Q9RTE3
A	775	HIS	-	expression tag	UNP Q9RTE3
A	776	HIS	-	expression tag	UNP Q9RTE3
B	27	MET	-	expression tag	UNP Q9RTE3
B	143	CYS	ILE	engineered mutation	UNP Q9RTE3
B	268	CYS	LEU	engineered mutation	UNP Q9RTE3
B	769	HIS	-	expression tag	UNP Q9RTE3
B	770	HIS	-	expression tag	UNP Q9RTE3
B	771	HIS	-	expression tag	UNP Q9RTE3
B	772	HIS	-	expression tag	UNP Q9RTE3
B	773	HIS	-	expression tag	UNP Q9RTE3
B	774	HIS	-	expression tag	UNP Q9RTE3
B	775	HIS	-	expression tag	UNP Q9RTE3
B	776	HIS	-	expression tag	UNP Q9RTE3

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C 10 10	0	0
2	A	1	Total C 8 8	0	0
2	A	1	Total C 10 10	0	0
2	A	1	Total C 13 13	0	0
2	B	1	Total C O 21 19 2	0	0
2	B	1	Total C O 25 21 4	0	0
2	B	1	Total C 14 14	0	0
2	B	1	Total C 6 6	0	0
2	B	1	Total C 5 5	0	0

- Molecule 3 is POLYETHYLENE GLYCOL (N=34) (three-letter code: 15P) (formula: $C_{69}H_{140}O_{35}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 13 8 5	0	0
3	B	1	Total C O 12 8 4	0	0
3	B	1	Total C O 10 6 4	0	0
3	B	1	Total C O 9 6 3	0	0

- Molecule 4 is water.

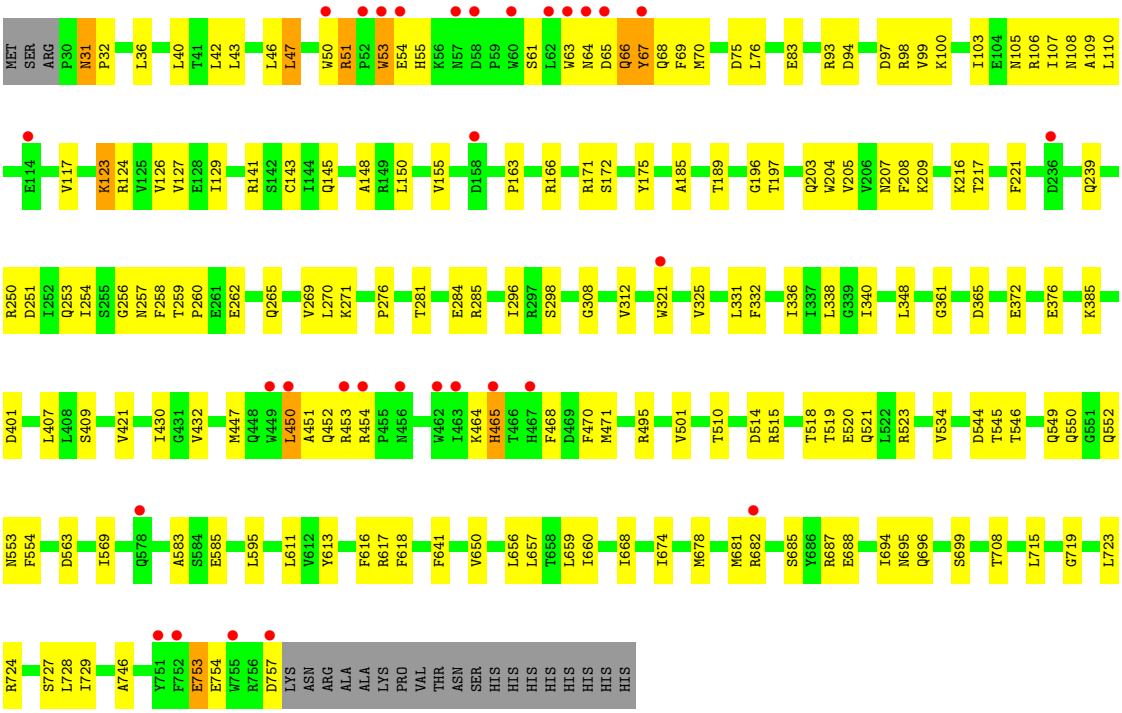
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	54	Total O 54 54	0	0
4	B	68	Total O 68 68	0	0

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.

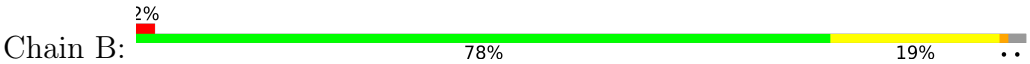
• Molecule 1: Protein translocase subunit SecD

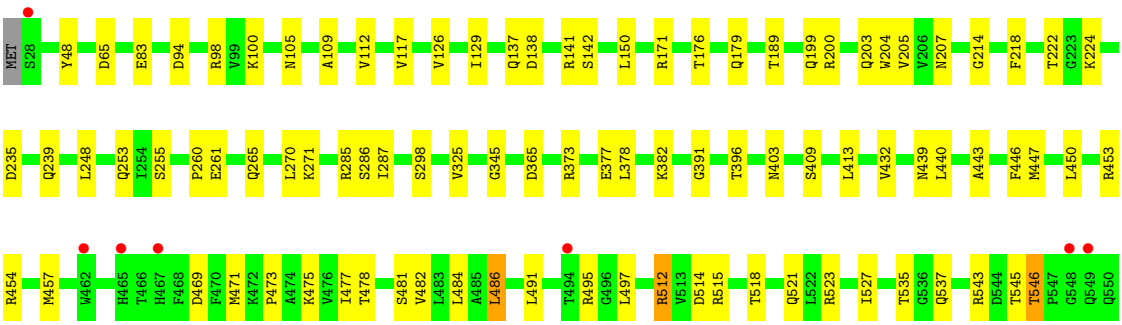
Chain A:

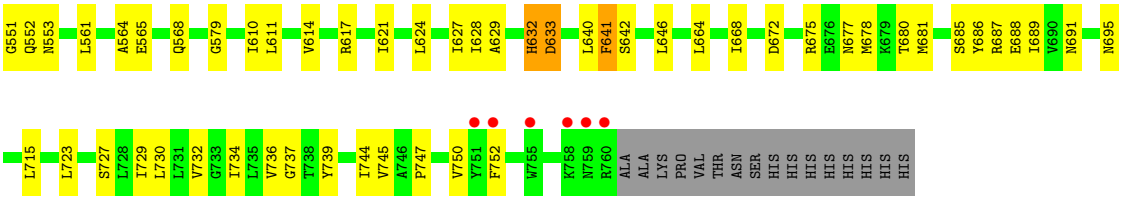


• Molecule 1: Protein translocase subunit SecD

Chain B:






G551
Q552
N553
L561
A564
E565
Q568
G579
I610
L611
V614
R617
I621
L624
I627
I628
A629
H632
D633
L640
F641
S642
L646
L664
I668
D672
R675
E676
N677
M678
K679
T680
M681
S685
Y686
R687
E688
I689
V690
N691
N695
L715
L723
S727
L728
I729
L730
L731
V732
G733
I734
L735
V736
G737
T738
Y739
I744
V745
A746
P747
V750
V751
F752
W755
K758
N759
R760
ALA
ALA
LYS
PRO
VAL
THR
ASN
SER
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4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	63.55Å 73.81Å 369.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.20 – 2.75 48.20 – 2.75	Depositor EDS
% Data completeness (in resolution range)	98.3 (48.20-2.75) 98.3 (48.20-2.75)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.63 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.212 , 0.268 0.212 , 0.268	Depositor DCC
R_{free} test set	1927 reflections (4.21%)	wwPDB-VP
Wilson B-factor (Å^2)	41.9	Xtriage
Anisotropy	0.653	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 48.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	11313	wwPDB-VP
Average B, all atoms (Å^2)	47.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.85% 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: 15P, OLC

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	0.55	3/5595 (0.1%)	0.66	5/7614 (0.1%)
1	B	0.49	0/5640	0.64	3/7673 (0.0%)
All	All	0.52	3/11235 (0.0%)	0.65	8/15287 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	67	TYR	CG-CD2	-10.46	1.25	1.39
1	A	67	TYR	CE1-CZ	-8.16	1.27	1.38
1	A	67	TYR	CG-CD1	-6.49	1.30	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	51	ARG	NE-CZ-NH2	-10.74	114.93	120.30
1	A	51	ARG	NE-CZ-NH1	10.32	125.46	120.30
1	A	450	LEU	CB-CG-CD2	-7.98	97.44	111.00
1	B	235	ASP	CB-CG-OD1	7.62	125.15	118.30
1	A	659	LEU	CA-CB-CG	6.15	129.44	115.30
1	B	484	LEU	CB-CG-CD1	-5.90	100.97	111.00
1	A	67	TYR	CA-CB-CG	5.17	123.22	113.40
1	B	546	THR	CA-CB-CG2	-5.07	105.30	112.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	66	GLN	Peptide

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	5495	0	5673	138	0
1	B	5540	0	5722	103	0
2	A	41	0	67	1	0
2	B	71	0	112	4	0
3	B	44	0	52	4	0
4	A	54	0	0	2	0
4	B	68	0	0	1	0
All	All	11313	0	11626	239	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 10.

All (239) 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:464:LYS:O	1:A:465:HIS:CD2	1.68	1.47
1:A:464:LYS:O	1:A:465:HIS:HD2	1.13	0.95
1:A:51:ARG:HH11	1:A:51:ARG:HG2	1.33	0.93
1:B:471:MET:O	1:B:475:LYS:NZ	2.02	0.92
1:A:285:ARG:NH1	1:A:585:GLU:OE1	2.05	0.89
1:A:401:ASP:OD2	1:A:617:ARG:NH1	2.06	0.88
1:B:617:ARG:NH2	1:B:672:ASP:OD2	2.10	0.85
1:A:117:VAL:HG13	1:A:127:VAL:HG12	1.59	0.83
1:B:545:THR:HG22	1:B:553:ASN:H	1.47	0.80
1:B:109:ALA:HB2	1:B:271:LYS:HE3	1.67	0.77
1:A:53:TRP:CD1	1:A:54:GLU:HG3	2.20	0.76
1:A:53:TRP:HD1	1:A:54:GLU:HG3	1.50	0.76
1:B:715:LEU:HD23	1:B:727:SER:HB2	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LEU:HD22	1:A:270:LEU:HD22	1.67	0.75
1:A:105:ASN:O	1:A:271:LYS:NZ	2.20	0.75
1:B:207:ASN:HD21	1:B:253:GLN:HE21	1.32	0.74
1:B:481:SER:HB3	1:B:632:HIS:NE2	2.03	0.73
1:A:365:ASP:OD1	4:A:901:HOH:O	2.06	0.73
1:A:321:TRP:CE3	1:A:450:LEU:HD21	2.24	0.73
1:A:715:LEU:HD23	1:A:727:SER:HB3	1.72	0.71
1:B:482:VAL:HG12	1:B:486:LEU:HD11	1.71	0.71
1:A:93:ARG:HH12	1:B:65:ASP:HB3	1.55	0.71
1:B:176:THR:H	1:B:179:GLN:HE21	1.38	0.71
1:A:66:GLN:N	1:A:66:GLN:OE1	2.22	0.71
1:A:51:ARG:NH2	1:A:68:GLN:C	2.45	0.70
1:A:464:LYS:C	1:A:465:HIS:CD2	2.64	0.69
1:A:545:THR:HG22	1:A:553:ASN:H	1.57	0.69
1:A:471:MET:HG3	1:A:687:ARG:HG3	1.75	0.69
1:A:141:ARG:NH2	1:A:284:GLU:OE2	2.27	0.68
1:A:94:ASP:HA	1:A:97:ASP:HB2	1.75	0.67
1:B:518:THR:HG23	1:B:521:GLN:H	1.59	0.67
1:B:543:ARG:NH1	1:B:552:GLN:OE1	2.28	0.67
1:A:321:TRP:HE3	1:A:450:LEU:HD21	1.57	0.67
1:B:373:ARG:NH1	1:B:377:GLU:OE1	2.27	0.67
1:A:549:GLN:NE2	1:A:550:GLN:O	2.27	0.67
1:B:222:THR:HG21	1:B:248:LEU:HB2	1.76	0.67
1:A:520:GLU:OE2	1:A:523:ARG:NH1	2.18	0.66
1:A:51:ARG:HH11	1:A:51:ARG:CG	2.07	0.66
1:A:753:GLU:OE1	1:A:753:GLU:O	2.15	0.65
1:A:259:THR:OG1	1:A:262:GLU:HG2	1.97	0.64
1:B:83:GLU:HG2	1:B:126:VAL:HG22	1.78	0.64
1:B:614:VAL:HG11	1:B:627:ILE:HD11	1.78	0.64
1:A:76:LEU:HB3	1:A:296:ILE:HD11	1.80	0.64
1:A:145:GLN:NE2	1:A:281:THR:OG1	2.31	0.64
1:A:103:ILE:HG21	1:A:127:VAL:HG11	1.79	0.63
1:B:633:ASP:OD2	1:B:737:GLY:HA2	1.99	0.63
1:B:204:TRP:CE2	1:B:260:PRO:HG3	2.34	0.63
1:B:325:VAL:HG21	1:B:447:MET:HG2	1.81	0.62
1:A:51:ARG:CZ	1:A:69:PHE:HA	2.30	0.62
1:A:332:PHE:O	1:A:336:ILE:HD12	2.00	0.61
1:A:51:ARG:HH21	1:A:68:GLN:N	1.98	0.61
1:B:691:ASN:O	1:B:695:ASN:ND2	2.33	0.61
1:B:298:SER:OG	1:B:546:THR:HG21	2.02	0.60
1:A:64:ASN:OD1	1:A:65:ASP:N	2.30	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:VAL:HG21	1:A:569:ILE:HD11	1.83	0.60
1:B:641:PHE:CE2	1:B:729:ILE:HD11	2.37	0.60
1:A:546:THR:O	1:A:549:GLN:HB2	2.02	0.60
1:A:61:SER:O	1:A:67:TYR:HE2	1.85	0.59
1:A:55:HIS:CD2	1:A:67:TYR:CE1	2.91	0.59
1:B:685:SER:O	1:B:689:ILE:HG13	2.03	0.59
1:B:515:ARG:HG3	1:B:552:GLN:HG3	1.85	0.58
1:A:42:LEU:HB2	1:A:332:PHE:HE1	1.68	0.58
1:A:141:ARG:HD2	1:A:563:ASP:OD2	2.04	0.58
1:B:478:THR:O	1:B:482:VAL:HG23	2.04	0.58
1:B:138:ASP:OD1	1:B:141:ARG:NH1	2.37	0.57
1:B:736:VAL:HA	1:B:739:TYR:CE2	2.40	0.57
1:B:248:LEU:HD11	3:B:806:15P:H371	1.87	0.57
1:A:450:LEU:HD12	1:A:450:LEU:O	2.05	0.56
1:A:63:TRP:O	1:A:64:ASN:HB2	2.05	0.56
1:A:385:LYS:HZ1	1:A:452:GLN:N	2.04	0.56
1:A:618:PHE:CZ	1:A:668:ILE:HG13	2.40	0.56
1:B:617:ARG:HH21	1:B:672:ASP:CG	2.08	0.56
1:B:482:VAL:HG12	1:B:486:LEU:CD1	2.35	0.55
1:A:208:PHE:CE1	1:A:270:LEU:HD13	2.42	0.55
1:B:687:ARG:HA	1:B:750:VAL:HG21	1.87	0.55
1:A:55:HIS:CG	1:A:67:TYR:CE1	2.95	0.55
1:B:473:PRO:O	1:B:477:ILE:HG22	2.07	0.54
1:A:47:LEU:HA	1:A:50:TRP:HB3	1.89	0.54
1:A:108:ASN:OD1	1:A:109:ALA:N	2.41	0.54
1:B:481:SER:HG	1:B:739:TYR:HE1	1.54	0.54
1:B:248:LEU:HD21	3:B:806:15P:H361	1.89	0.54
1:B:365:ASP:OD1	4:B:901:HOH:O	2.19	0.54
1:A:674:ILE:O	1:A:678:MET:HG3	2.06	0.54
1:A:514:ASP:OD1	1:A:515:ARG:HG2	2.07	0.54
1:B:285:ARG:HD2	1:B:287:ILE:HD11	1.88	0.54
1:A:549:GLN:OE1	1:A:552:GLN:HA	2.09	0.53
1:A:209:LYS:HE2	1:A:251:ASP:OD1	2.09	0.53
1:A:616:PHE:CE1	2:A:804:OLC:H10	2.44	0.53
1:A:514:ASP:OD1	1:A:515:ARG:N	2.37	0.53
1:A:208:PHE:CE2	1:A:254:ILE:HG12	2.44	0.53
1:A:171:ARG:NH2	1:A:262:GLU:OE1	2.41	0.53
1:A:518:THR:HG23	1:A:521:GLN:H	1.74	0.53
1:A:681:MET:CE	1:A:696:GLN:HE22	2.23	0.52
1:B:610:ILE:HG22	1:B:611:LEU:HD23	1.91	0.52
1:A:372:GLU:O	1:A:376:GLU:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:GLN:NE2	1:B:286:SER:OG	2.42	0.52
1:A:207:ASN:HD21	1:A:253:GLN:HE21	1.56	0.52
1:A:325:VAL:HG21	1:A:447:MET:HB3	1.92	0.52
1:A:51:ARG:NH1	1:A:69:PHE:HA	2.24	0.52
1:A:61:SER:O	1:A:67:TYR:CE2	2.63	0.52
1:A:407:LEU:HD13	1:A:432:VAL:HG11	1.92	0.51
1:A:687:ARG:NH1	1:A:754:GLU:OE1	2.41	0.51
1:A:83:GLU:HG2	1:A:126:VAL:HG22	1.92	0.51
1:A:208:PHE:HE2	1:A:254:ILE:HG12	1.76	0.51
1:A:31:ASN:HD22	1:A:32:PRO:CD	2.23	0.51
1:B:373:ARG:HG3	1:B:391:GLY:HA2	1.93	0.51
1:A:204:TRP:CZ2	1:A:260:PRO:HG3	2.46	0.51
1:A:42:LEU:HG	1:A:46:LEU:HD11	1.91	0.51
1:B:677:ASN:HB3	1:B:689:ILE:CG2	2.40	0.51
1:A:31:ASN:HD22	1:A:32:PRO:HD2	1.76	0.50
1:B:450:LEU:HB3	1:B:457:MET:HE1	1.93	0.50
1:B:686:TYR:HD2	1:B:750:VAL:HG23	1.75	0.50
1:B:523:ARG:O	1:B:527:ILE:HG13	2.11	0.50
1:A:217:THR:HG23	1:B:200:ARG:HG3	1.94	0.50
1:B:345:GLY:HA3	2:B:802:OLC:H24	1.93	0.50
1:A:715:LEU:HD11	1:A:723:LEU:HD13	1.93	0.50
1:A:208:PHE:HE1	1:A:270:LEU:HD13	1.76	0.49
1:A:43:LEU:O	1:A:47:LEU:HD22	2.12	0.49
1:B:518:THR:CG2	1:B:521:GLN:HB2	2.43	0.49
1:B:403:ASN:HB3	1:B:432:VAL:HG13	1.93	0.49
1:B:94:ASP:OD2	1:B:98:ARG:NH2	2.45	0.49
1:B:453:ARG:HD3	1:B:453:ARG:N	2.27	0.49
1:A:36:LEU:O	1:A:40:LEU:HG	2.13	0.49
1:A:685:SER:OG	1:A:688:GLU:HG3	2.13	0.49
1:A:361:GLY:HA3	1:A:708:THR:HA	1.95	0.49
1:B:497:LEU:HD23	1:B:642:SER:HB2	1.95	0.49
1:B:680:THR:HG22	1:B:681:MET:HG3	1.94	0.49
1:B:641:PHE:CE1	1:B:646:LEU:HB2	2.48	0.48
1:B:105:ASN:O	1:B:271:LYS:HD2	2.13	0.48
1:B:48:TYR:CG	2:B:802:OLC:H8A	2.48	0.48
1:B:325:VAL:HG22	1:B:446:PHE:CD2	2.47	0.48
1:B:189:THR:HG21	1:B:218:PHE:CE1	2.48	0.48
1:A:641:PHE:CE2	1:A:729:ILE:HD11	2.48	0.48
1:B:482:VAL:O	1:B:486:LEU:HD12	2.13	0.48
1:B:512:ARG:HA	1:B:552:GLN:O	2.14	0.48
1:A:123:LYS:HZ1	1:A:124:ARG:CZ	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:70:MET:HE3	1:A:348:LEU:HD22	1.96	0.47
1:A:421:VAL:HG21	1:A:650:VAL:HG12	1.96	0.47
1:A:687:ARG:NH2	1:A:754:GLU:OE2	2.48	0.47
1:A:172:SER:OG	1:A:175:TYR:O	2.32	0.47
1:A:256:GLY:O	1:A:258:PHE:N	2.47	0.47
1:A:385:LYS:HZ3	1:A:451:ALA:HB3	1.80	0.47
1:A:204:TRP:CE2	1:A:260:PRO:HG3	2.50	0.47
1:A:209:LYS:HA	1:A:250:ARG:O	2.14	0.47
1:A:271:LYS:HE3	1:A:271:LYS:HB3	1.60	0.47
1:B:545:THR:CG2	1:B:553:ASN:H	2.20	0.47
1:A:308:GLY:O	1:A:312:VAL:HG13	2.15	0.47
1:A:510:THR:HB	1:A:583:ALA:HB3	1.96	0.47
1:B:112:VAL:HG11	1:B:129:ILE:HG23	1.96	0.47
1:B:454:ARG:HB2	1:B:457:MET:HB2	1.97	0.47
1:A:203:GLN:NE2	1:A:257:ASN:HA	2.30	0.47
1:A:544:ASP:HB2	1:A:724:ARG:HH22	1.80	0.47
1:B:561:LEU:HB3	1:B:565:GLU:HG3	1.96	0.47
2:B:801:OLC:H11A	2:B:801:OLC:H8	1.70	0.47
1:B:378:LEU:HD23	1:B:382:LYS:O	2.15	0.46
1:A:55:HIS:CE1	1:A:67:TYR:CE1	3.04	0.46
1:A:98:ARG:HB3	1:A:276:PRO:HG2	1.97	0.46
1:B:621:ILE:HG21	1:B:752:PHE:CD2	2.51	0.46
1:B:564:ALA:O	1:B:568:GLN:HG3	2.16	0.46
1:A:203:GLN:OE1	1:A:204:TRP:N	2.46	0.46
1:B:261:GLU:H	1:B:261:GLU:CD	2.20	0.45
1:A:519:THR:HG22	1:A:554:PHE:HE2	1.81	0.45
1:B:171:ARG:NH2	1:B:239:GLN:OE1	2.49	0.45
1:B:512:ARG:O	1:B:579:GLY:HA2	2.16	0.45
1:B:664:LEU:O	1:B:668:ILE:HG13	2.17	0.45
1:B:189:THR:HG23	1:B:214:GLY:CA	2.46	0.45
1:A:340:ILE:HG21	1:A:430:ILE:HD12	1.99	0.45
1:B:730:LEU:O	1:B:734:ILE:HG13	2.16	0.45
1:B:518:THR:HG23	1:B:521:GLN:HB2	1.99	0.44
1:A:468:PHE:H	1:A:695:ASN:HD21	1.64	0.44
1:B:514:ASP:OD1	1:B:515:ARG:N	2.49	0.44
1:A:99:VAL:HG22	1:A:276:PRO:HD2	1.99	0.44
1:A:51:ARG:CG	1:A:51:ARG:NH1	2.72	0.44
1:A:163:PRO:HA	1:A:166:ARG:NH2	2.32	0.44
1:B:640:LEU:HD13	1:B:732:VAL:HG21	1.99	0.44
1:B:744:ILE:C	1:B:747:PRO:HD2	2.37	0.44
1:B:176:THR:N	1:B:179:GLN:HE21	2.11	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:189:THR:HG23	1:B:214:GLY:HA3	2.00	0.44
1:A:46:LEU:HD12	1:A:46:LEU:H	1.83	0.44
1:A:611:LEU:HD23	1:A:611:LEU:HA	1.85	0.44
1:A:657:LEU:HA	1:A:657:LEU:HD23	1.72	0.44
1:B:629:ALA:O	1:B:632:HIS:N	2.51	0.44
1:B:633:ASP:N	1:B:633:ASP:OD1	2.51	0.44
1:A:185:ALA:HA	1:B:199:GLN:O	2.18	0.44
1:B:142:SER:HB2	1:B:265:GLN:NE2	2.33	0.43
1:A:51:ARG:NH2	1:A:69:PHE:N	2.66	0.43
1:B:535:THR:OG1	1:B:537:GLN:HG2	2.18	0.43
1:B:629:ALA:HB2	1:B:745:VAL:HG22	1.99	0.43
1:B:715:LEU:HD11	1:B:723:LEU:HD13	1.98	0.43
1:A:155:VAL:O	4:A:902:HOH:O	2.21	0.43
1:B:205:VAL:HG12	1:B:255:SER:HB3	2.00	0.43
1:B:439:ASN:O	1:B:443:ALA:HB3	2.19	0.43
1:A:595:LEU:HD23	1:A:595:LEU:HA	1.89	0.43
1:B:481:SER:HG	1:B:739:TYR:HH	1.64	0.43
1:B:624:LEU:O	1:B:628:ILE:HG12	2.18	0.43
1:A:171:ARG:HB3	1:A:239:GLN:O	2.19	0.43
1:A:31:ASN:HD22	1:A:32:PRO:N	2.17	0.43
1:A:66:GLN:CD	1:A:67:TYR:HB3	2.39	0.43
1:A:501:VAL:HG21	1:A:585:GLU:HG2	2.00	0.43
1:A:69:PHE:HE2	1:A:338:LEU:HD13	1.85	0.42
1:A:409:SER:HB2	1:A:657:LEU:HB3	2.01	0.42
1:B:100:LYS:HG3	1:B:117:VAL:HG12	2.01	0.42
1:A:42:LEU:O	1:A:46:LEU:HD12	2.20	0.42
1:A:68:GLN:HB3	1:A:70:MET:O	2.20	0.42
1:A:106:ARG:NH2	1:A:143:CYS:O	2.52	0.42
1:B:189:THR:HG21	1:B:218:PHE:CD1	2.54	0.42
1:B:203:GLN:HE21	1:B:203:GLN:HB3	1.68	0.42
1:A:464:LYS:O	1:A:465:HIS:CG	2.53	0.42
1:A:51:ARG:NH2	1:A:68:GLN:CA	2.83	0.42
1:B:150:LEU:HD13	1:B:270:LEU:HD22	2.00	0.42
1:B:447:MET:HB3	1:B:447:MET:HE2	1.79	0.42
1:B:396:THR:HG23	1:B:440:LEU:HD13	2.02	0.42
1:A:100:LYS:NZ	1:A:117:VAL:O	2.51	0.41
1:B:48:TYR:CD2	2:B:802:OLC:H8A	2.53	0.41
1:A:107:ILE:HD12	1:A:129:ILE:HD11	2.02	0.41
1:A:468:PHE:HB2	1:A:470:PHE:CE2	2.55	0.41
1:B:515:ARG:HH21	1:B:551:GLY:H	1.67	0.41
1:A:196:GLY:O	1:A:205:VAL:N	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:613:TYR:HE2	1:A:668:ILE:HD11	1.85	0.41
1:A:694:ILE:HD11	1:A:746:ALA:HB3	2.03	0.41
1:B:675:ARG:HA	1:B:678:MET:HE2	2.01	0.41
1:B:413:LEU:HB3	3:B:808:15P:H352	2.03	0.41
1:A:69:PHE:CE2	1:A:338:LEU:HD13	2.55	0.41
1:A:189:THR:CG2	1:B:199:GLN:HB3	2.51	0.41
1:A:253:GLN:O	1:A:254:ILE:HD13	2.20	0.41
1:B:491:LEU:O	1:B:495:ARG:HB3	2.21	0.41
1:A:298:SER:HB3	1:A:719:GLY:HA2	2.02	0.41
1:A:563:ASP:N	1:A:563:ASP:OD1	2.53	0.41
1:A:753:GLU:OE1	1:A:757:ASP:OD1	2.39	0.41
1:A:148:ALA:HB1	1:A:269:VAL:HB	2.02	0.41
1:B:469:ASP:OD1	1:B:471:MET:N	2.44	0.40
1:A:197:THR:HA	1:A:204:TRP:HA	2.03	0.40
1:B:515:ARG:HA	1:B:552:GLN:HG3	2.02	0.40
3:B:807:15P:H362	3:B:807:15P:H382	1.72	0.40
1:A:110:LEU:HD13	1:A:110:LEU:HA	1.81	0.40
1:B:440:LEU:HD23	1:B:440:LEU:HA	1.87	0.40
1:A:64:ASN:HB3	1:A:66:GLN:OE1	2.22	0.40
1:A:514:ASP:CG	1:A:515:ARG:N	2.75	0.40
1:A:656:LEU:O	1:A:660:ILE:HG13	2.21	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	726/750 (97%)	705 (97%)	21 (3%)	0	100	100
1	B	731/750 (98%)	713 (98%)	18 (2%)	0	100	100
All	All	1457/1500 (97%)	1418 (97%)	39 (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	583/603 (97%)	566 (97%)	17 (3%)	42	62
1	B	588/603 (98%)	580 (99%)	8 (1%)	67	79
All	All	1171/1206 (97%)	1146 (98%)	25 (2%)	53	71

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	47	LEU
1	A	53	TRP
1	A	75	ASP
1	A	123	LYS
1	A	216	LYS
1	A	221	PHE
1	A	265	GLN
1	A	331	LEU
1	A	453	ARG
1	A	454	ARG
1	A	465	HIS
1	A	495	ARG
1	A	682	ARG
1	A	699	SER
1	A	728	LEU
1	A	753	GLU
1	B	224	LYS
1	B	409	SER
1	B	486	LEU
1	B	512	ARG
1	B	632	HIS
1	B	633	ASP
1	B	641	PHE
1	B	688	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	ASN
1	A	105	ASN
1	A	137	GLN
1	A	145	GLN
1	A	146	GLN
1	A	207	ASN
1	A	403	ASN
1	A	448	GLN
1	A	465	HIS
1	A	677	ASN
1	A	696	GLN
1	B	57	ASN
1	B	105	ASN
1	B	137	GLN
1	B	179	GLN
1	B	203	GLN
1	B	245	ASN
1	B	253	GLN
1	B	549	GLN
1	B	677	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

13 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	OLC	A	804	-	12,12,24	0.26	0	11,11,25	0.54	0
2	OLC	A	803	-	9,9,24	0.42	0	8,8,25	0.66	0
2	OLC	B	805	-	4,4,24	0.36	0	3,3,25	0.29	0
2	OLC	B	801	-	20,20,24	0.98	1 (5%)	20,20,25	0.83	0
2	OLC	B	803	-	13,13,24	0.29	0	12,12,25	0.60	0
2	OLC	B	804	-	5,5,24	0.41	0	4,4,25	0.33	0
3	15P	B	806	-	12,12,103	0.46	0	11,11,102	0.41	0
2	OLC	A	802	-	7,7,24	0.31	0	6,6,25	0.49	0
2	OLC	A	801	-	9,9,24	0.30	0	8,8,25	0.88	0
2	OLC	B	802	-	24,24,24	1.05	1 (4%)	25,25,25	0.85	1 (4%)
3	15P	B	809	-	8,8,103	0.53	0	7,7,102	0.46	0
3	15P	B	808	-	9,9,103	0.40	0	8,8,102	0.39	0
3	15P	B	807	-	11,11,103	0.49	0	10,10,102	0.45	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	OLC	A	804	-	-	3/10/10/24	-
2	OLC	A	803	-	-	1/7/7/24	-
2	OLC	B	805	-	-	0/2/2/24	-
2	OLC	B	801	-	-	3/19/19/24	-
2	OLC	B	803	-	-	2/11/11/24	-
2	OLC	B	804	-	-	2/3/3/24	-
3	15P	B	806	-	-	5/10/10/101	-
2	OLC	A	802	-	-	1/5/5/24	-
2	OLC	A	801	-	-	0/7/7/24	-
2	OLC	B	802	-	-	6/24/24/24	-
3	15P	B	809	-	-	4/6/6/101	-
3	15P	B	808	-	-	2/7/7/101	-
3	15P	B	807	-	-	2/9/9/101	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	802	OLC	O20-C1	4.75	1.47	1.33
2	B	801	OLC	O20-C1	4.17	1.46	1.33

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	802	OLC	O20-C1-C2	2.41	119.47	111.91

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	807	15P	C38-C37-O18-C36
3	B	806	15P	O16-C33-C34-O17
2	B	801	OLC	C2-C1-O20-C21
3	B	809	15P	O18-C37-C38-O19
3	B	809	15P	O17-C35-C36-O18
2	B	801	OLC	O19-C1-O20-C21
2	A	804	OLC	C6-C7-C8-C9
2	A	804	OLC	C4-C5-C6-C7
2	B	802	OLC	C10-C11-C12-C13
3	B	806	15P	O18-C37-C38-O19
2	B	802	OLC	C5-C6-C7-C8
3	B	809	15P	C33-C34-O17-C35
2	B	802	OLC	C2-C1-O20-C21
2	A	804	OLC	C5-C6-C7-C8
2	A	802	OLC	C13-C14-C15-C16
2	B	802	OLC	O19-C1-O20-C21
3	B	806	15P	C38-C37-O18-C36
3	B	809	15P	C36-C35-O17-C34
2	A	803	OLC	C13-C14-C15-C16
3	B	806	15P	C31-C32-O16-C33
3	B	808	15P	O16-C33-C34-O17
2	B	804	OLC	C11-C12-C13-C14
2	B	803	OLC	C11-C12-C13-C14
2	B	803	OLC	C7-C8-C9-C10
3	B	807	15P	C31-C32-O16-C33
3	B	808	15P	C35-C36-O18-C37
2	B	802	OLC	C12-C13-C14-C15
2	B	802	OLC	C15-C16-C17-C18
2	B	804	OLC	C12-C13-C14-C15

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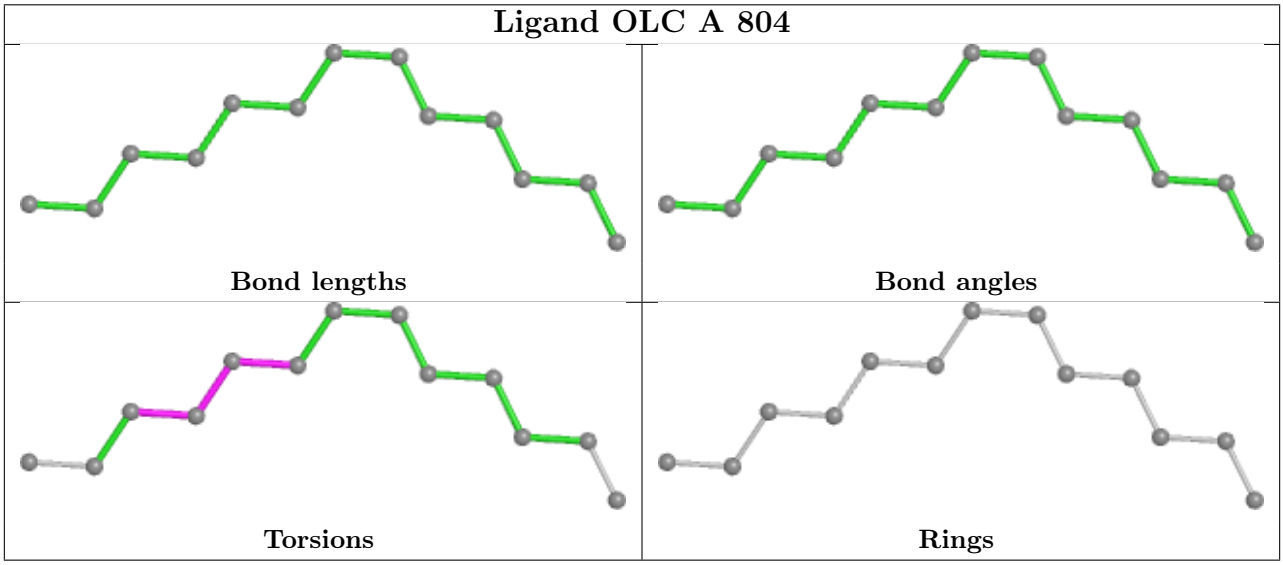
Mol	Chain	Res	Type	Atoms
2	B	801	OLC	C12-C13-C14-C15
3	B	806	15P	O17-C35-C36-O18

There are no ring outliers.

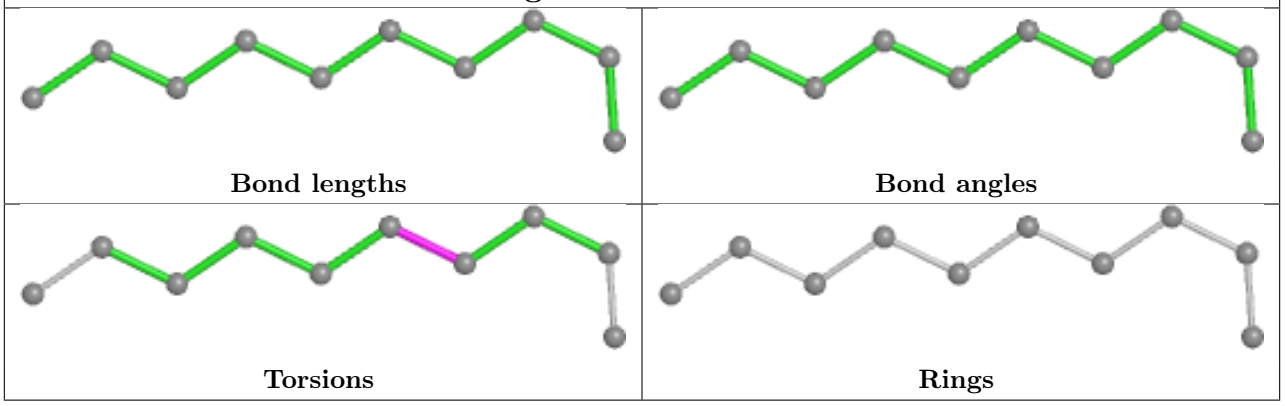
6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	804	OLC	1	0
2	B	801	OLC	1	0
3	B	806	15P	2	0
2	B	802	OLC	3	0
3	B	808	15P	1	0
3	B	807	15P	1	0

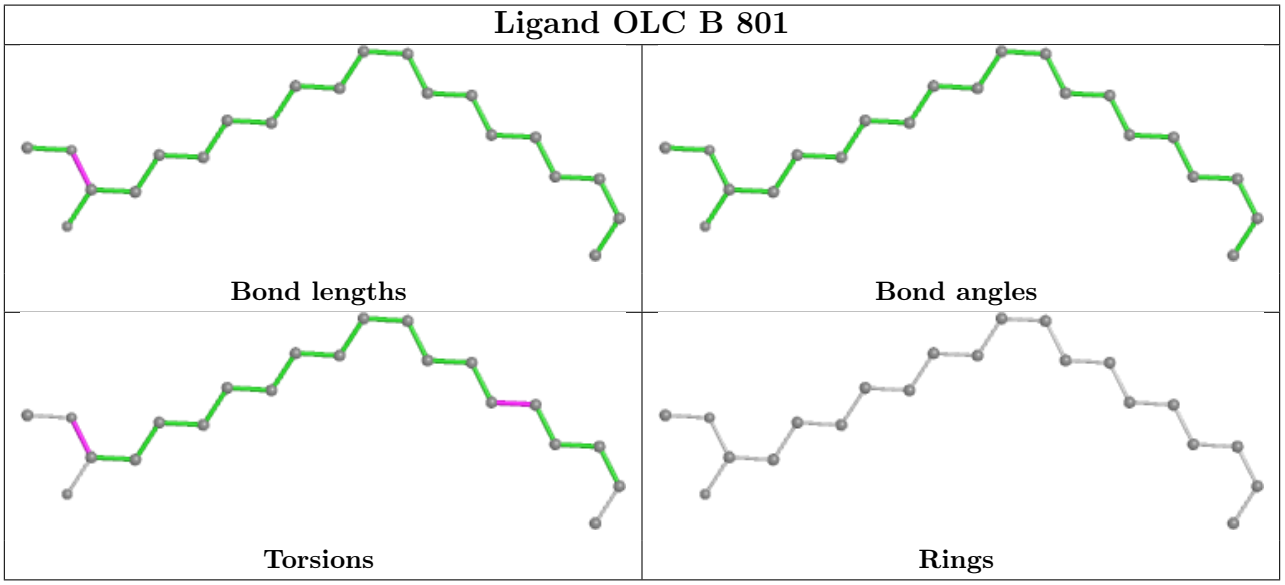
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



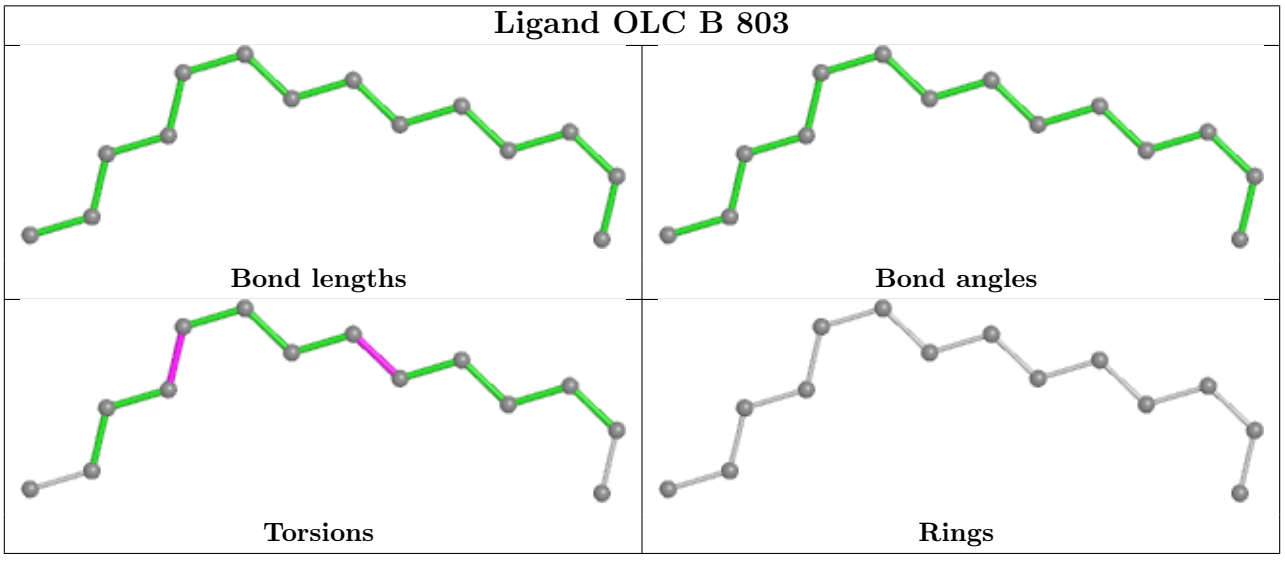
Ligand OLC A 803



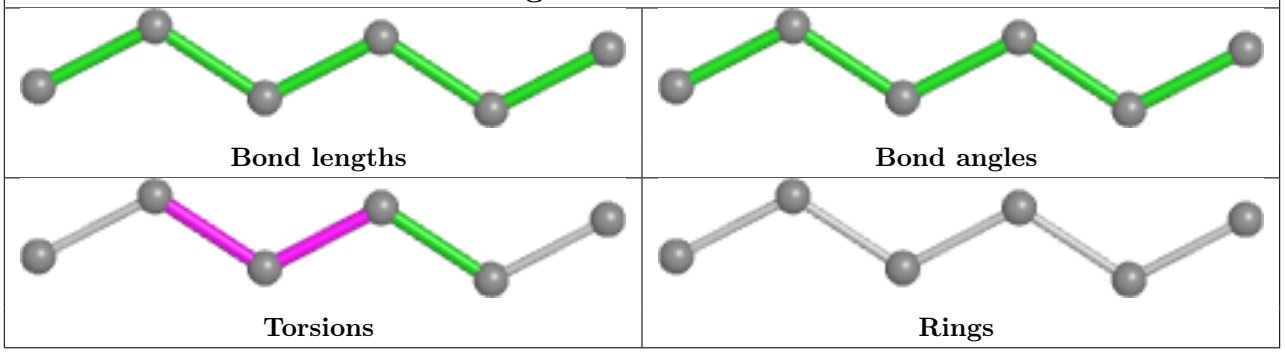
Ligand OLC B 801



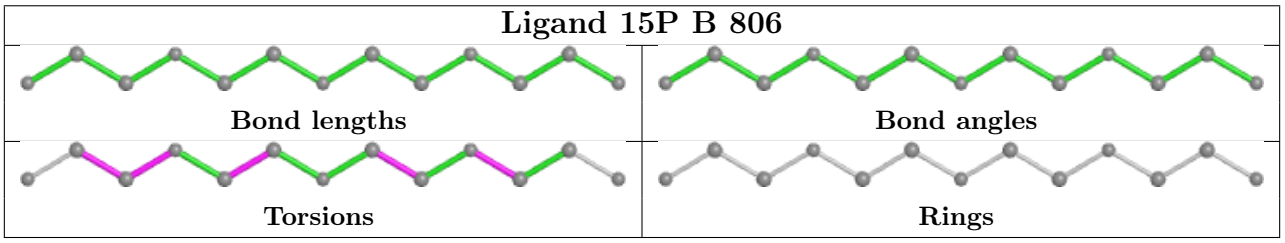
Ligand OLC B 803



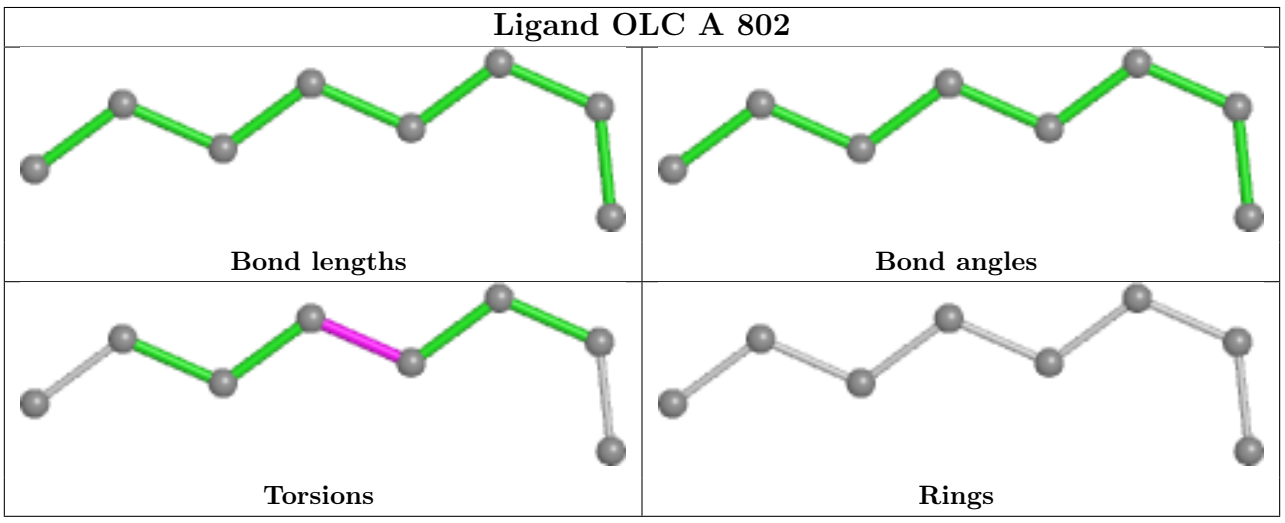
Ligand OLC B 804



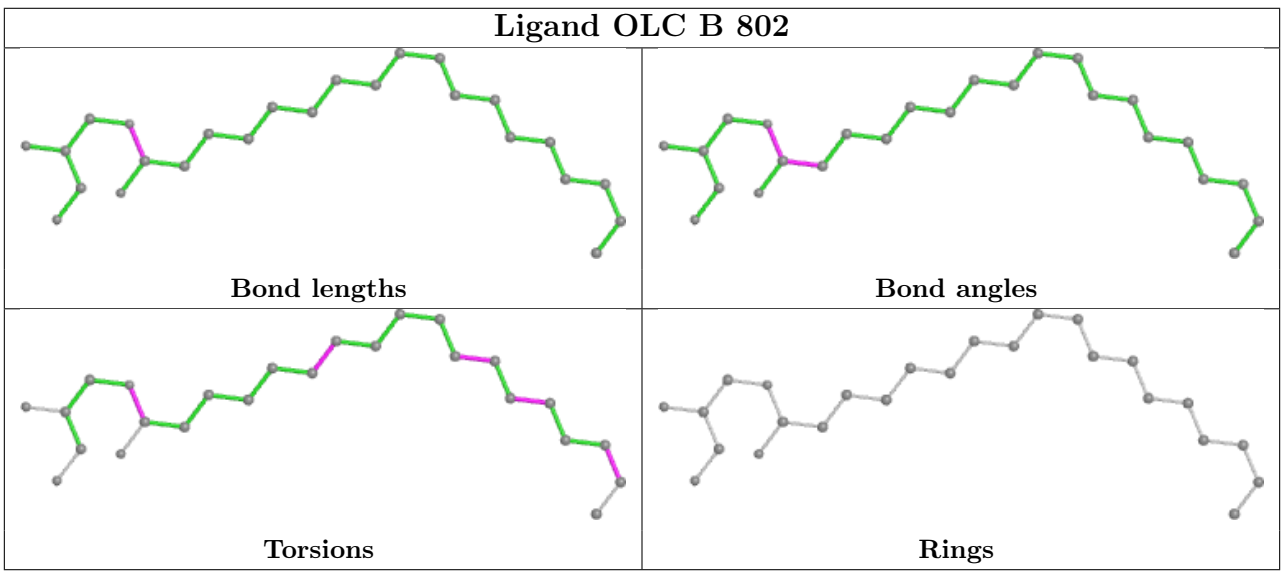
Ligand 15P B 806

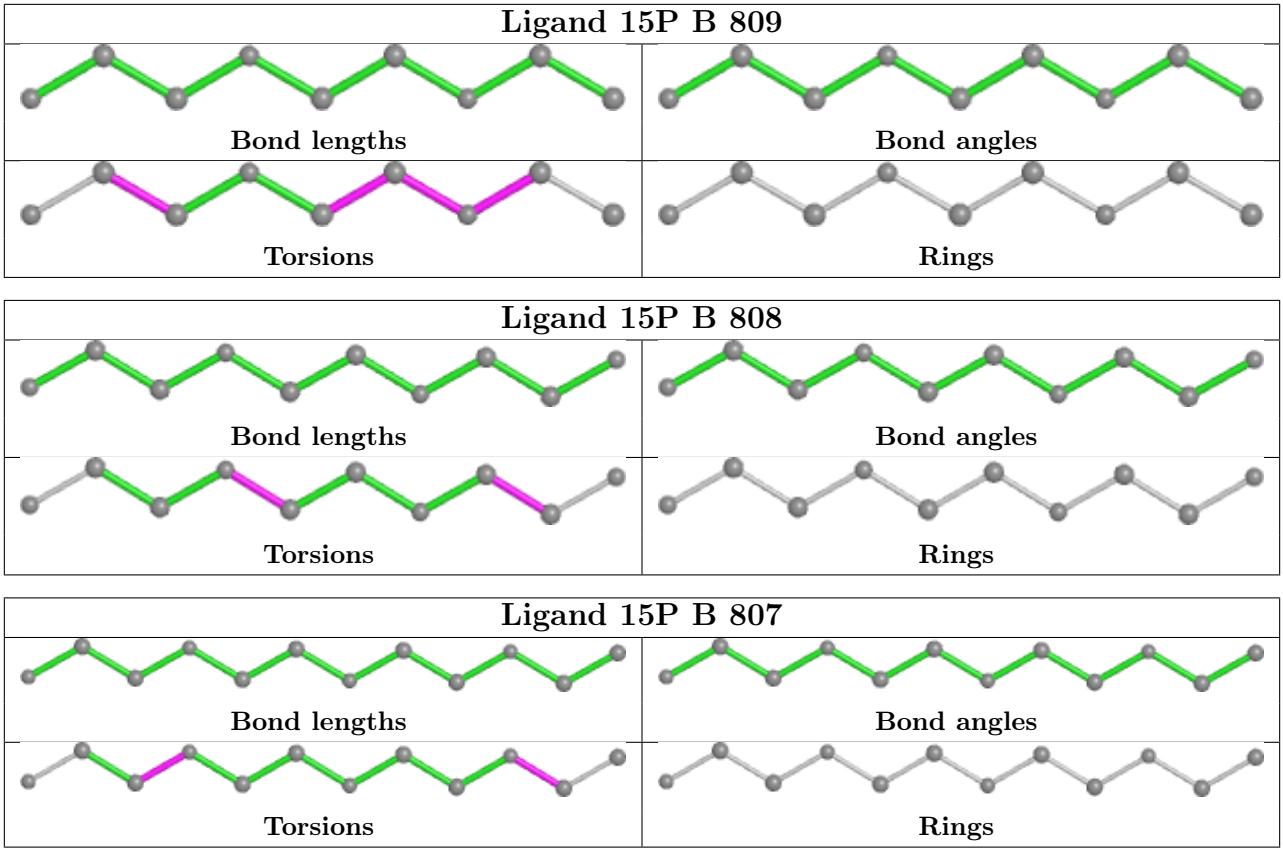


Ligand OLC A 802



Ligand OLC B 802





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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	728/750 (97%)	0.09	31 (4%)	35	42	20, 44, 97, 185	0
1	B	733/750 (97%)	-0.07	13 (1%)	68	76	22, 37, 79, 142	0
All	All	1461/1500 (97%)	0.01	44 (3%)	50	59	20, 40, 87, 185	0

All (44) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	759	ASN	5.9
1	A	64	ASN	5.8
1	A	67	TYR	5.6
1	A	50	TRP	4.6
1	B	752	PHE	4.5
1	B	751	TYR	4.4
1	B	755	TRP	4.4
1	A	465	HIS	4.3
1	A	53	TRP	4.1
1	A	453	ARG	3.7
1	A	463	ILE	3.6
1	B	465	HIS	3.4
1	A	62	LEU	3.3
1	B	28	SER	3.2
1	A	751	TYR	3.1
1	A	63	TRP	3.1
1	B	760	ARG	3.0
1	A	114	GLU	2.9
1	B	758	LYS	2.9
1	A	467	HIS	2.8
1	A	682	ARG	2.7
1	A	757	ASP	2.6
1	A	65	ASP	2.5
1	A	755	TRP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	752	PHE	2.5
1	A	52	PRO	2.5
1	A	57	ASN	2.4
1	B	548	GLY	2.4
1	B	467	HIS	2.4
1	A	454	ARG	2.3
1	B	462	TRP	2.2
1	A	60	TRP	2.2
1	A	450	LEU	2.2
1	A	578	GLN	2.2
1	A	158	ASP	2.2
1	A	449	TRP	2.2
1	A	456	ASN	2.1
1	A	58	ASP	2.1
1	B	494	THR	2.1
1	A	462	TRP	2.1
1	A	54	GLU	2.0
1	B	549	GLN	2.0
1	A	236	ASP	2.0
1	A	321	TRP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (i)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	OLC	B	805	5/25	0.85	0.26	34,34,34,34	0
2	OLC	B	802	25/25	0.86	0.23	30,38,50,50	0
2	OLC	A	804	13/25	0.88	0.18	54,54,55,55	0

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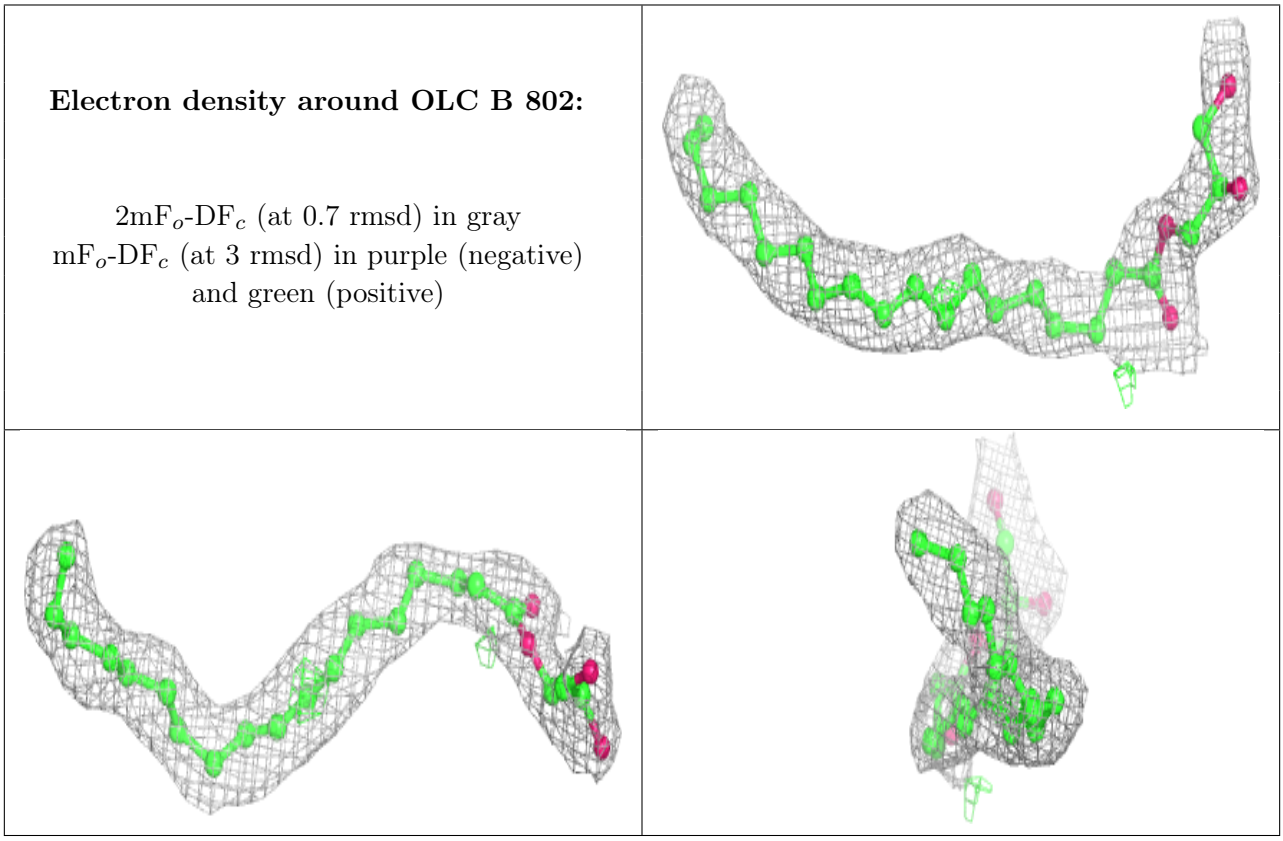
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	15P	B	806	13/104	0.88	0.18	50,51,52,52	0
3	15P	B	809	9/104	0.89	0.19	60,61,61,61	0
3	15P	B	807	12/104	0.90	0.22	58,59,60,60	0
3	15P	B	808	10/104	0.90	0.21	66,67,68,69	0
2	OLC	A	801	10/25	0.90	0.25	42,44,45,45	0
2	OLC	B	804	6/25	0.92	0.23	27,27,27,27	0
2	OLC	B	801	21/25	0.92	0.21	37,38,45,46	0
2	OLC	A	802	8/25	0.92	0.19	32,34,34,34	0
2	OLC	A	803	10/25	0.93	0.17	34,36,36,37	0
2	OLC	B	803	14/25	0.95	0.18	36,38,41,41	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.

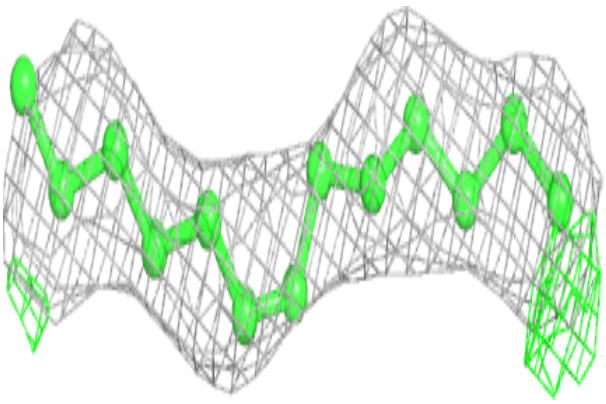
Electron density around OLC B 802:

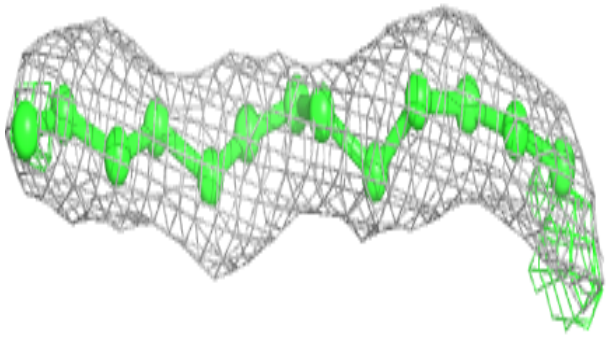
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

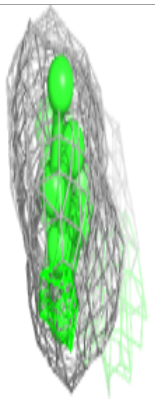


Electron density around OLC A 804:

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

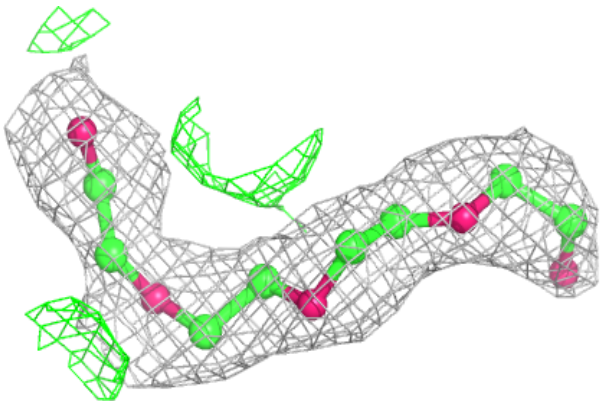


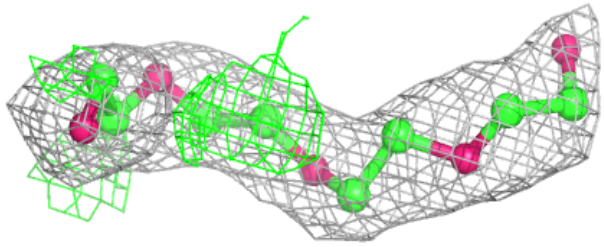


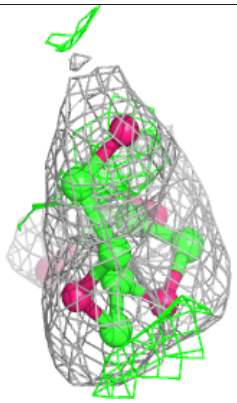


Electron density around 15P B 806:

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

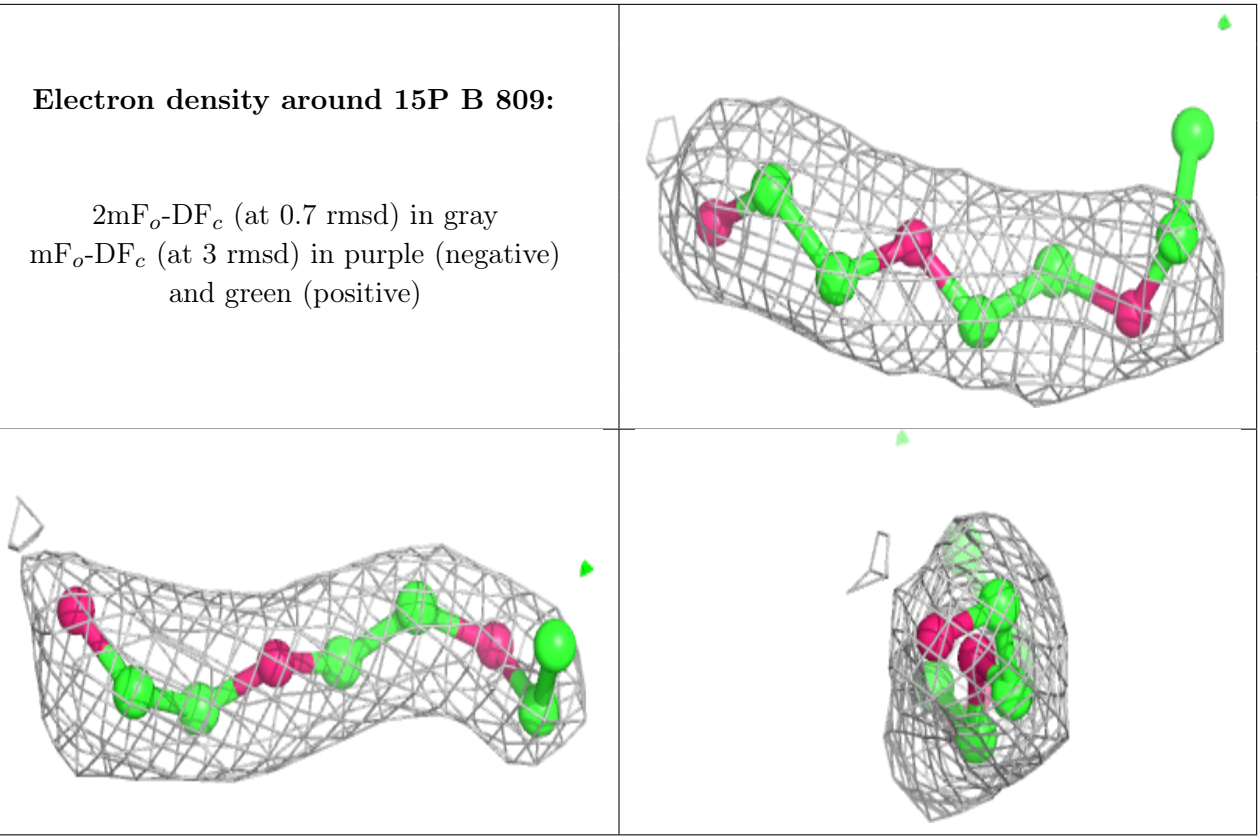






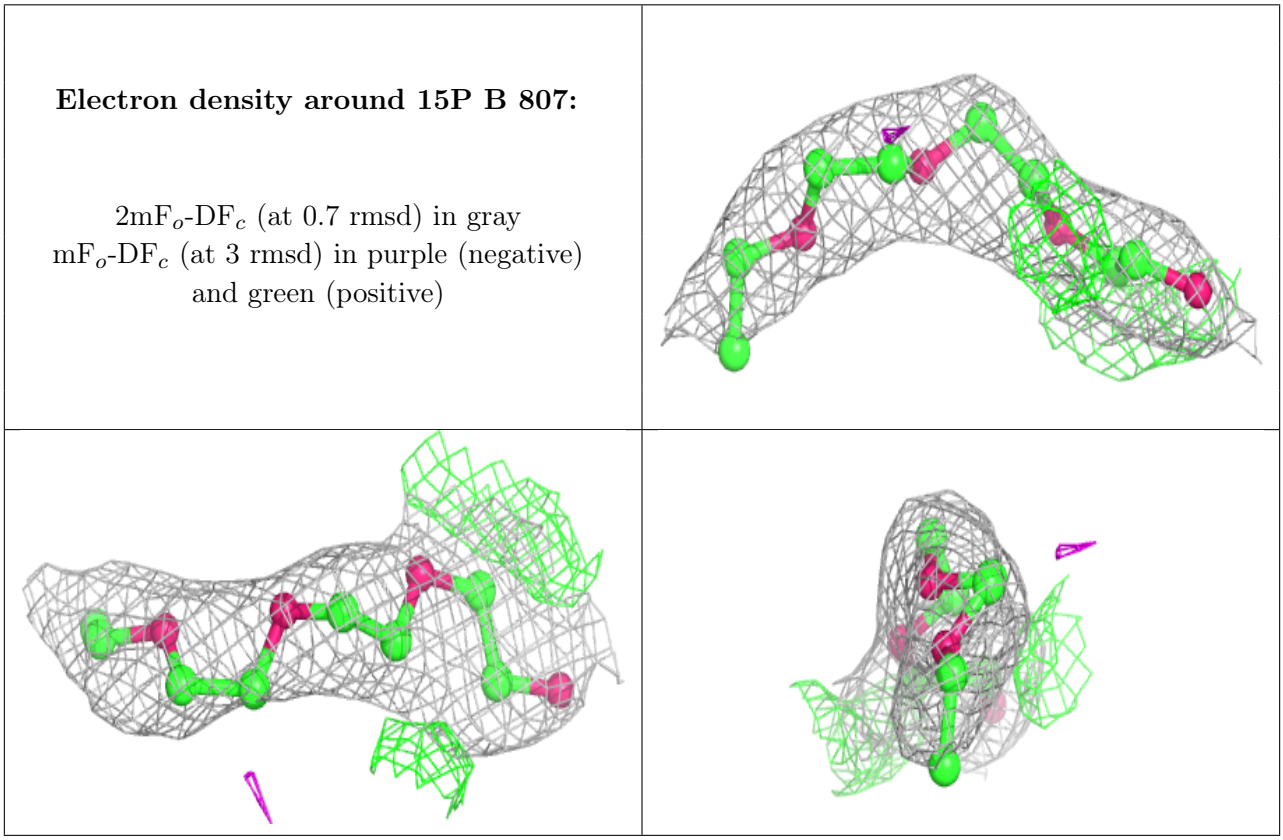
Electron density around 15P B 809:

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



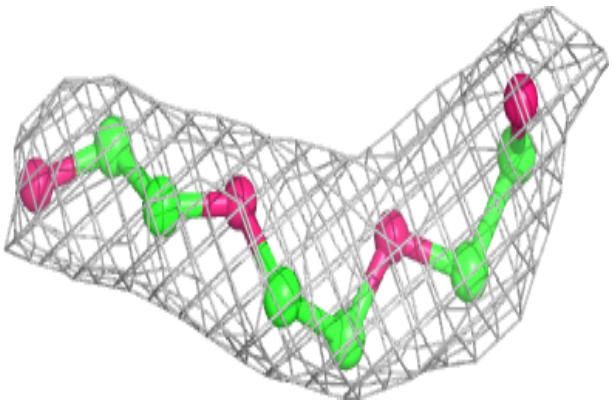
Electron density around 15P B 807:

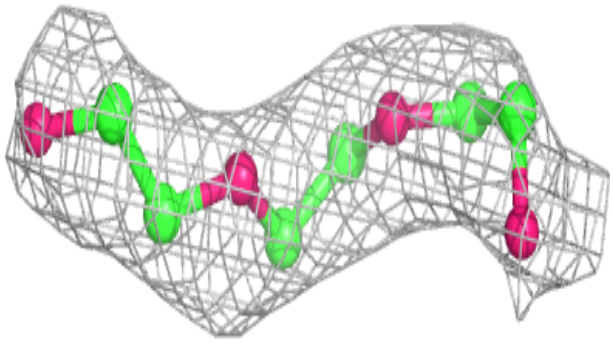
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

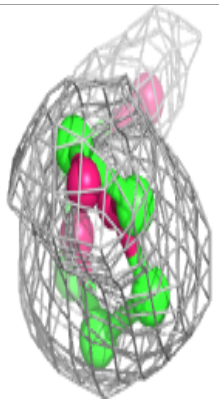


Electron density around 15P B 808:

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

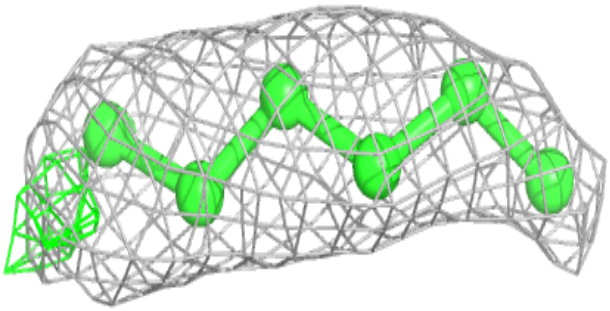


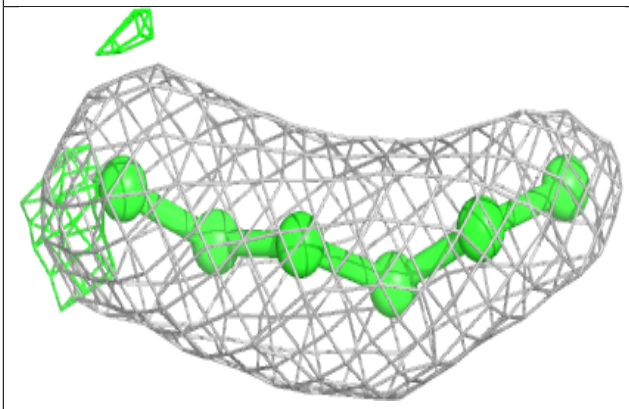


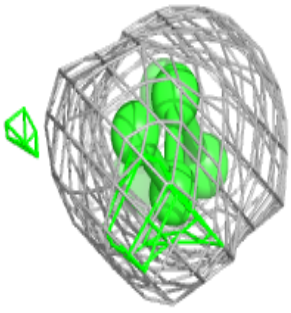


Electron density around OLC B 804:

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

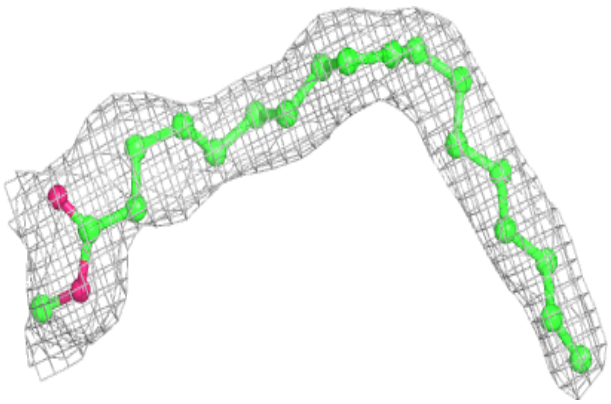


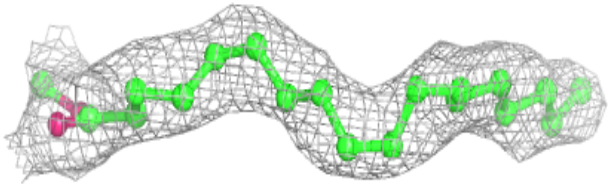


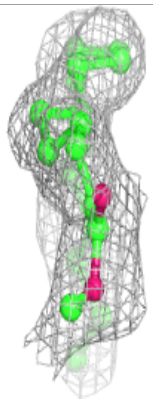


Electron density around OLC B 801:

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

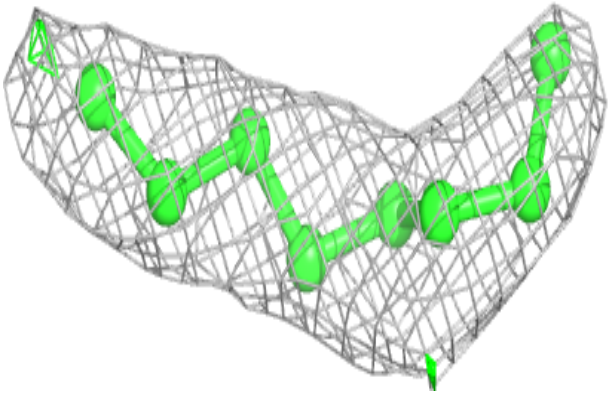


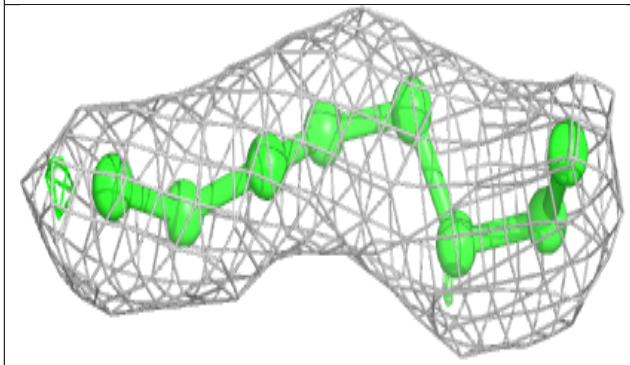


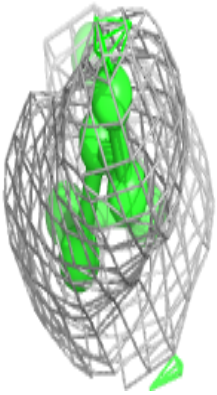


Electron density around OLC A 802:

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

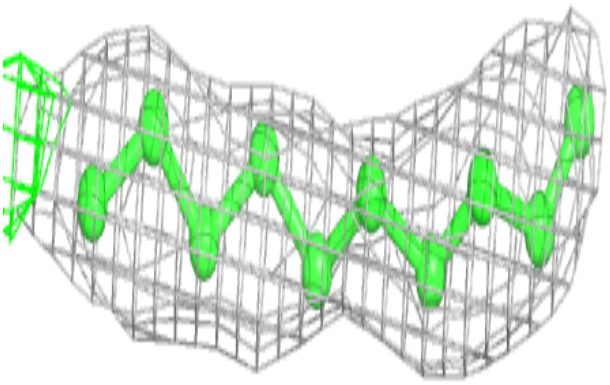


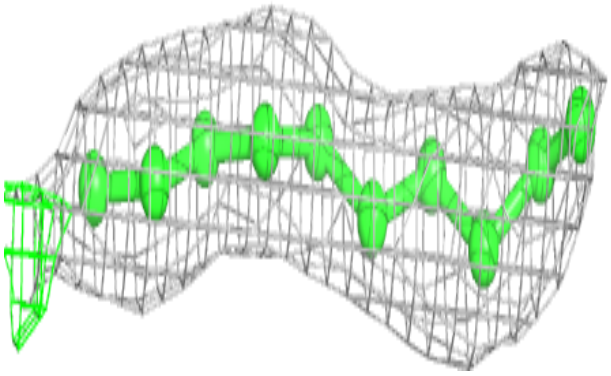


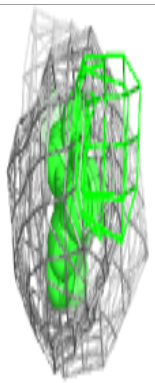


Electron density around OLC A 803:

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

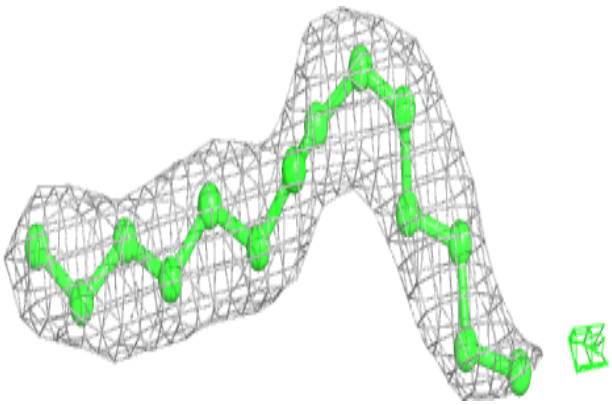


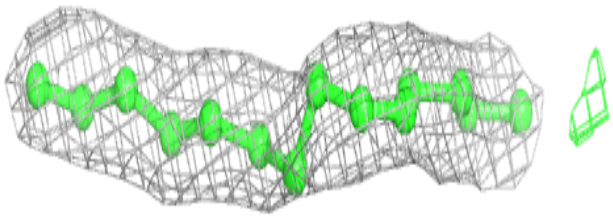


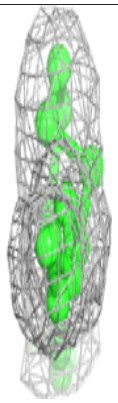


Electron density around OLC B 803:

$2mF_o$-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.