W O R L D W I D E
wwPDB
P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Sep 30, 2021 – 10:33 AM EDT

PDB ID	:	3ODU
Title	:	The 2.5 A structure of the CXCR4 chemokine receptor in complex with small molecule antagonist IT1t
Authors	:	Wu, B.; Mol, C.D.; Han, G.W.; Katritch, V.; Chien, E.Y.T.; Liu, W.; Chere-zov, V.; Stevens, R.C.; Accelerated Technologies Center for Gene to 3D Structure (ATCG3D); GPCR Network (GPCR)
Deposited on	:	2010-08-11
Resolution	:	2.50 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

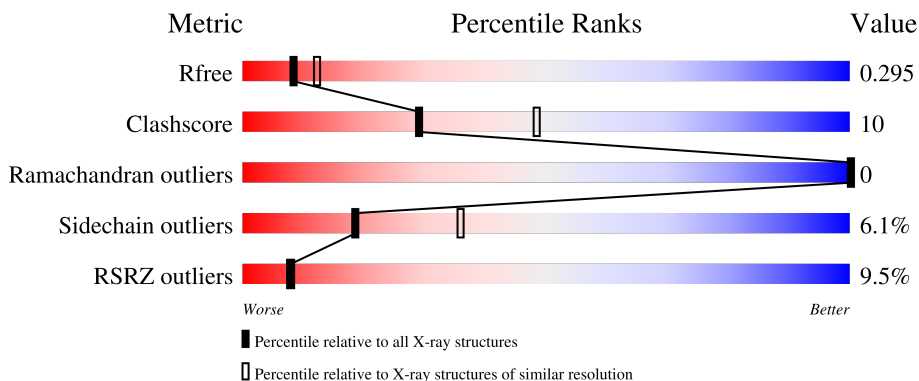|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
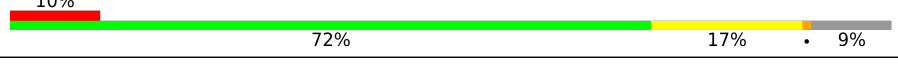*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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	Percentile Ranks	Value
Rfree		0.295
Clashscore		10
Ramachandran outliers		0
Sidechain outliers		6.1%
RSRZ outliers		9.5%

Worse Better

▮ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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	502	8% 70% 21% • 7%
1	B	502	10% 72% 17% • 9%

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 7805 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 C-X-C chemokine receptor type 4, Lysozyme Chimera.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total 3759	C 2464	N 630	O 649	S 16	0	4	0
1	B	456	Total 3661	C 2396	N 616	O 633	S 16	0	2	0

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	ASP	-	expression tag	UNP P61073
A	-8	TYR	-	expression tag	UNP P61073
A	-7	LYS	-	expression tag	UNP P61073
A	-6	ASP	-	expression tag	UNP P61073
A	-5	ASP	-	expression tag	UNP P61073
A	-4	ASP	-	expression tag	UNP P61073
A	-3	ASP	-	expression tag	UNP P61073
A	-2	ALA	-	expression tag	UNP P61073
A	-1	GLY	-	expression tag	UNP P61073
A	0	ALA	-	expression tag	UNP P61073
A	1	PRO	-	expression tag	UNP P61073
A	125	TRP	LEU	engineered mutation	UNP P61073
A	900	GLY	-	linker	UNP P61073
A	901	SER	-	linker	UNP P61073
A	1200	GLY	-	linker	UNP P61073
A	1201	SER	-	linker	UNP P61073
A	1054	THR	CYS	engineered mutation	UNP P00720
A	1097	ALA	CYS	engineered mutation	UNP P00720
A	320	GLY	-	expression tag	UNP P61073
A	321	ARG	-	expression tag	UNP P61073
A	322	PRO	-	expression tag	UNP P61073
A	323	LEU	-	expression tag	UNP P61073
A	324	GLU	-	expression tag	UNP P61073
A	325	VAL	-	expression tag	UNP P61073
A	326	LEU	-	expression tag	UNP P61073

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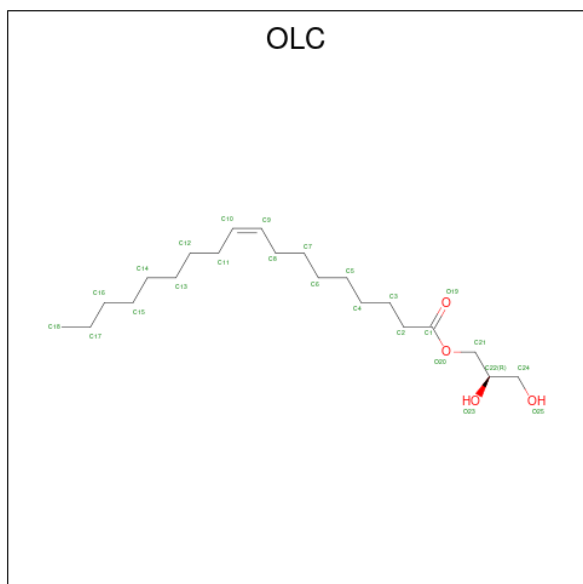
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Chain	Residue	Modelled	Actual	Comment	Reference
A	327	PHE	-	expression tag	UNP P61073
A	328	GLN	-	expression tag	UNP P61073
B	-9	ASP	-	expression tag	UNP P61073
B	-8	TYR	-	expression tag	UNP P61073
B	-7	LYS	-	expression tag	UNP P61073
B	-6	ASP	-	expression tag	UNP P61073
B	-5	ASP	-	expression tag	UNP P61073
B	-4	ASP	-	expression tag	UNP P61073
B	-3	ASP	-	expression tag	UNP P61073
B	-2	ALA	-	expression tag	UNP P61073
B	-1	GLY	-	expression tag	UNP P61073
B	0	ALA	-	expression tag	UNP P61073
B	1	PRO	-	expression tag	UNP P61073
B	125	TRP	LEU	engineered mutation	UNP P61073
B	900	GLY	-	linker	UNP P61073
B	901	SER	-	linker	UNP P61073
B	1200	GLY	-	linker	UNP P61073
B	1201	SER	-	linker	UNP P61073
B	1054	THR	CYS	engineered mutation	UNP P00720
B	1097	ALA	CYS	engineered mutation	UNP P00720
B	320	GLY	-	expression tag	UNP P61073
B	321	ARG	-	expression tag	UNP P61073
B	322	PRO	-	expression tag	UNP P61073
B	323	LEU	-	expression tag	UNP P61073
B	324	GLU	-	expression tag	UNP P61073
B	325	VAL	-	expression tag	UNP P61073
B	326	LEU	-	expression tag	UNP P61073
B	327	PHE	-	expression tag	UNP P61073
B	328	GLN	-	expression tag	UNP P61073

- Molecule 2 is (6,6-dimethyl-5,6-dihydroimidazo[2,1-b][1,3]thiazol-3-yl)methyl N,N'-dicycloh exylimidothiocarbamate (three-letter code: ITD) (formula: $C_{21}H_{34}N_4S_2$).

ITD
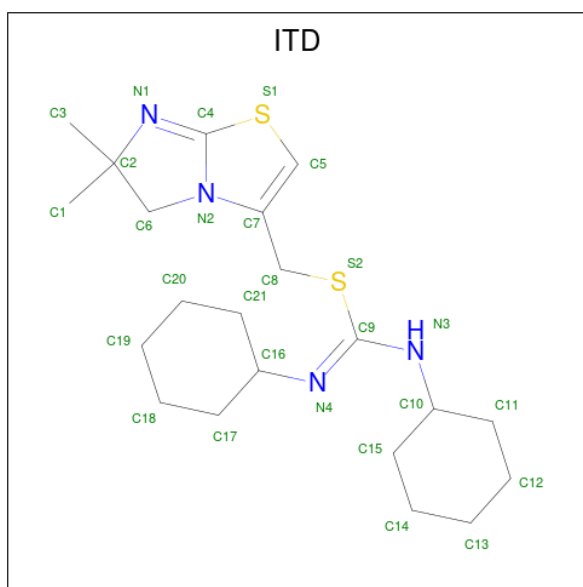
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 27	C 21	N 4	S 2	0	0
2	B	1	Total 27	C 21	N 4	S 2	0	0

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

OLC

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 18	C 14	O 4	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			22	18	4		
3	A	1	Total	C	O	0	0
			16	12	4		
3	B	1	Total	C	O	0	0
			15	11	4		
3	B	1	Total	C	O	0	0
			22	18	4		

- Molecule 4 is OLEIC ACID (three-letter code: OLA) (formula: $C_{18}H_{34}O_2$).
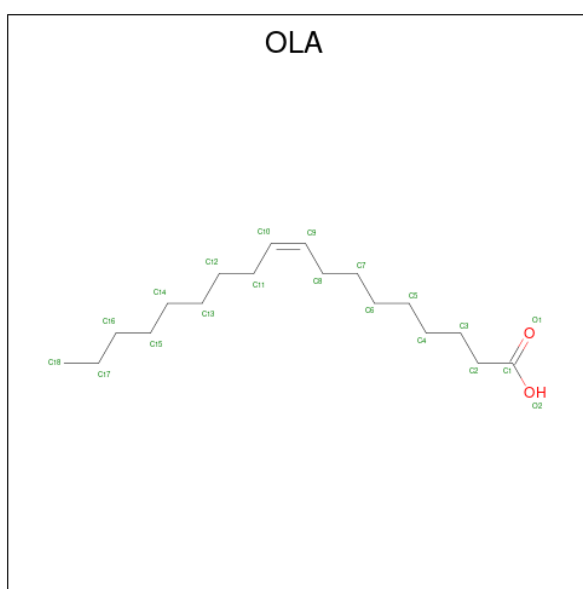
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			10	8	2		
4	B	1	Total	C	O	0	0
			20	18	2		
4	B	1	Total	C	O	0	0
			20	18	2		
4	B	1	Total	C	O	0	0
			20	18	2		
4	B	1	Total	C	O	0	0
			12	10	2		
4	B	1	Total	C	O	0	0
			13	11	2		

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	73	Total 73	O 73	0	0
5	B	69	Total 70	O 70	0	1

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
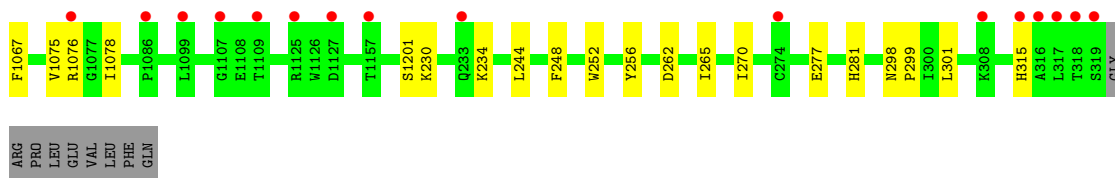
- Molecule 1: C-X-C chemokine receptor type 4, Lysozyme Chimera
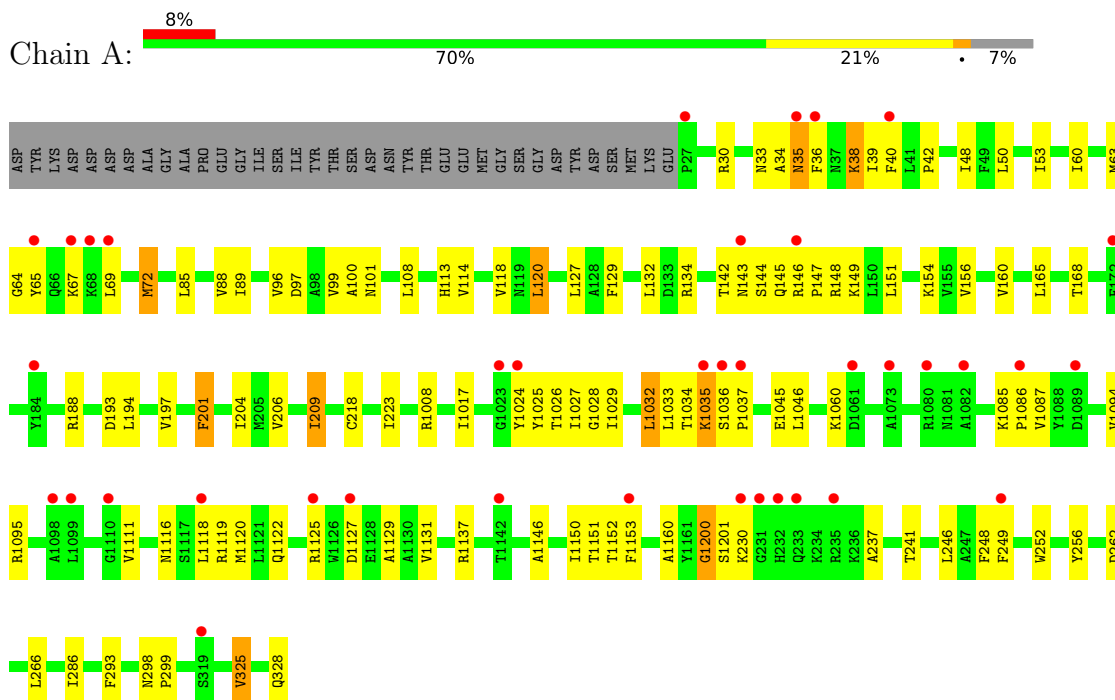
- Molecule 1: C-X-C chemokine receptor type 4, Lysozyme Chimera
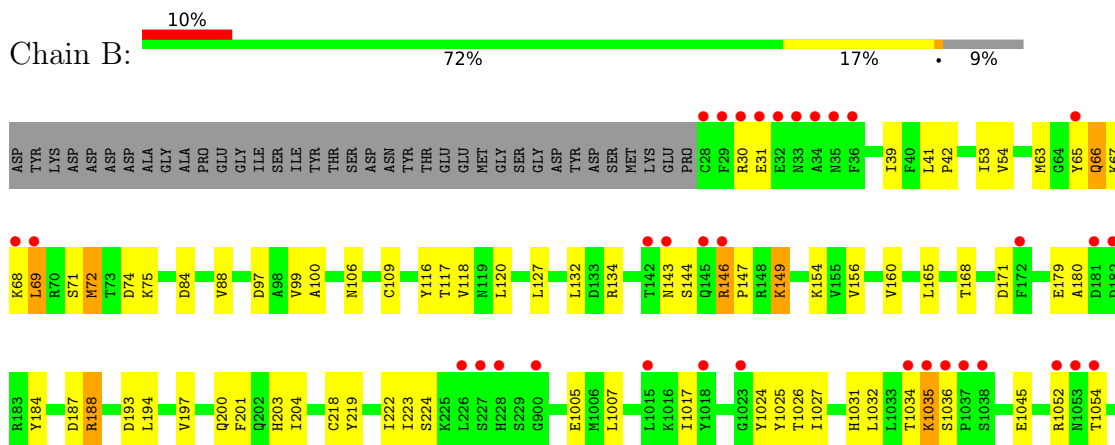
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	64.54Å 83.69Å 120.00Å 90.00° 102.17° 90.00°	Depositor
Resolution (Å)	19.98 – 2.50 19.90 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.98-2.50) 95.7 (19.90-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.00 (at 2.50Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.237 , 0.282 0.244 , 0.295	Depositor DCC
R_{free} test set	2079 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	37.1	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 66.3	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	7805	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.15% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: OLA, OLC, ITD

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	0.77	1/3863 (0.0%)	0.71	1/5242 (0.0%)
1	B	0.66	1/3758 (0.0%)	0.77	7/5102 (0.1%)
All	All	0.72	2/7621 (0.0%)	0.74	8/10344 (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	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	206	VAL	CB-CG2	-5.97	1.40	1.52
1	B	184	TYR	CD2-CE2	-5.64	1.30	1.39

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	65	TYR	CB-CA-C	13.41	137.23	110.40
1	B	63	MET	CB-CA-C	11.22	132.84	110.40
1	A	1200	GLY	N-CA-C	8.84	135.19	113.10
1	B	65	TYR	N-CA-CB	-7.81	96.54	110.60
1	B	100	ALA	N-CA-CB	-6.76	100.63	110.10
1	B	230	LYS	N-CA-C	-5.72	95.56	111.00
1	B	68	LYS	N-CA-C	5.43	125.67	111.00
1	B	66	GLN	N-CA-C	5.38	125.52	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1200	GLY	Peptide
1	A	1201	SER	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	3759	0	3838	95	0
1	B	3661	0	3726	59	0
2	A	27	0	34	3	0
2	B	27	0	34	3	0
3	A	56	0	75	9	0
3	B	37	0	50	1	0
4	A	10	0	12	1	0
4	B	85	0	130	8	0
5	A	73	0	0	2	0
5	B	70	0	0	0	0
All	All	7805	0	7899	150	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 (150) 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:35:ASN:ND2	1:A:36:PHE:H	1.62	0.95
1:A:197:VAL:HG21	1:B:194:LEU:HD22	1.50	0.94
1:B:144:SER:O	1:B:147:PRO:HD2	1.68	0.93
1:A:35:ASN:HD22	1:A:36:PHE:H	1.15	0.92
1:A:34:ALA:HA	1:A:38:LYS:HG2	1.59	0.84
1:A:142:THR:HG23	1:A:143:ASN:OD1	1.80	0.80
1:B:42:PRO:HG3	1:B:99:VAL:HG12	1.62	0.80
1:A:194:LEU:HD22	1:B:197:VAL:HG21	1.63	0.80
1:A:35:ASN:ND2	1:A:36:PHE:N	2.30	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:35:ASN:O	1:A:39:ILE:HD12	1.83	0.77
1:A:1087:VAL:HG22	1:A:1122:GLN:HB2	1.67	0.77
1:A:34:ALA:HA	1:A:38:LYS:CG	2.16	0.76
1:A:35:ASN:HD22	1:A:36:PHE:N	1.84	0.76
1:A:97:ASP:HA	1:A:101:ASN:O	1.86	0.74
1:A:193:ASP:OD2	1:B:194:LEU:HD21	1.88	0.72
1:A:1027:ILE:HG13	1:A:1028:GLY:N	2.03	0.72
1:B:144:SER:C	1:B:147:PRO:HD2	2.10	0.71
1:A:142:THR:HG23	1:A:143:ASN:N	2.05	0.71
1:B:132:LEU:HD23	1:B:218:CYS:SG	2.32	0.69
1:B:1075:VAL:HA	1:B:1078:ILE:HD12	1.75	0.69
1:A:237:ALA:O	1:A:241:THR:HG23	1.94	0.67
1:A:146:ARG:HB3	1:A:147:PRO:HD3	1.79	0.65
1:A:34:ALA:HB1	1:A:38:LYS:HG3	1.79	0.65
1:A:1127:ASP:O	1:A:1131:VAL:HG23	1.97	0.64
1:A:48:ILE:HD11	1:A:293:PHE:CD2	2.35	0.61
1:B:146:ARG:N	1:B:147:PRO:CD	2.62	0.61
1:A:33:ASN:OD1	1:A:35:ASN:ND2	2.33	0.60
1:A:35:ASN:HD22	1:A:35:ASN:N	2.00	0.60
1:A:63:MET:HA	1:A:67:LYS:HG2	1.85	0.59
1:A:1116:ASN:OD1	1:A:1119:ARG:NH1	2.35	0.59
1:A:63:MET:HA	1:A:67:LYS:CG	2.33	0.59
1:A:65:TYR:CD1	1:A:65:TYR:N	2.69	0.59
1:A:256:TYR:CD1	3:A:1604:OLC:H4	2.38	0.59
1:B:200:GLN:HE21	1:B:204:ILE:HG13	1.67	0.59
1:B:187:ASP:OD2	1:B:188:ARG:N	2.36	0.58
1:B:42:PRO:HG3	1:B:99:VAL:CG1	2.33	0.58
1:B:244:LEU:HD13	1:B:301:LEU:HD12	1.87	0.57
1:A:33:ASN:OD1	1:A:34:ALA:N	2.38	0.57
1:A:204:ILE:HG12	3:A:1604:OLC:H5	1.86	0.56
1:A:1029:ILE:HG22	1:A:1029:ILE:O	2.04	0.56
1:A:142:THR:CG2	1:A:143:ASN:N	2.68	0.56
1:A:201:PHE:CE2	3:A:1603:OLC:H12	2.40	0.55
1:B:39:ILE:HG23	4:B:1605:OLA:H162	1.88	0.55
1:A:204:ILE:HG12	3:A:1604:OLC:H3A	1.88	0.55
1:B:72:MET:HE2	1:B:149:LYS:HA	1.88	0.55
1:A:53[A]:ILE:HD13	1:A:85:LEU:HD12	1.88	0.55
1:B:146:ARG:N	1:B:147:PRO:HD3	2.22	0.55
1:B:203[B]:HIS:CE1	4:B:1609:OLA:H41	2.42	0.55
1:B:1034:THR:HG21	1:B:1045:GLU:OE2	2.07	0.55
1:B:165:LEU:HD11	4:B:1607:OLA:H132	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:ALA:CB	1:A:38:LYS:HG3	2.38	0.54
1:B:204:ILE:HG12	4:B:1609:OLA:H61	1.90	0.54
1:B:256:TYR:CD2	4:B:1609:OLA:H72	2.43	0.54
1:B:71:SER:HB3	1:B:74:ASP:OD1	2.08	0.54
1:B:53:ILE:HD12	1:B:54:VAL:N	2.23	0.53
1:A:42:PRO:HG3	1:A:99:VAL:CG1	2.38	0.53
1:A:108:LEU:HD11	3:A:1600:OLC:H2A	1.91	0.53
1:A:34:ALA:O	1:A:35:ASN:C	2.46	0.53
1:A:144:SER:O	1:A:147:PRO:HD2	2.08	0.53
1:A:1017:ILE:HD11	1:A:1046:LEU:HD22	1.90	0.53
1:A:120:LEU:HD13	3:A:1604:OLC:H21	1.91	0.52
1:A:1024:TYR:CE2	1:A:1035:LYS:HD2	2.45	0.52
1:B:106:ASN:O	1:B:109:CYS:HB3	2.09	0.52
1:A:1094:VAL:HG12	1:A:1152:THR:CG2	2.38	0.52
1:A:1027:ILE:HG13	1:A:1028:GLY:H	1.73	0.52
1:B:1025:TYR:O	1:B:1032:LEU:HD12	2.10	0.52
1:A:1146:ALA:O	1:A:1150:ILE:HD12	2.10	0.51
1:B:118:VAL:HG23	1:B:168:THR:HG21	1.92	0.51
1:A:42:PRO:HG3	1:A:99:VAL:HG12	1.92	0.51
1:A:1120:MET:HB3	1:A:1129:ALA:HB2	1.92	0.51
1:B:265:ILE:HD13	1:B:277:GLU:HG2	1.92	0.51
1:A:144:SER:HB2	1:A:148:ARG:HD2	1.93	0.51
1:A:34:ALA:CA	1:A:38:LYS:CG	2.89	0.50
1:A:53[A]:ILE:CD1	1:A:88:VAL:HG12	2.41	0.50
1:A:97:ASP:OD1	2:A:1500:ITD:H16	2.12	0.50
1:B:219:TYR:HD1	1:B:222:ILE:HD12	1.76	0.50
1:A:142:THR:CG2	1:A:143:ASN:H	2.24	0.49
1:A:194:LEU:HD22	1:B:197:VAL:CG2	2.39	0.49
1:A:298:ASN:HB3	1:A:299:PRO:HD3	1.94	0.49
1:A:252:TRP:HB3	1:A:256:TYR:CZ	2.48	0.49
1:A:156:VAL:O	1:A:160:VAL:HB	2.13	0.49
1:B:252:TRP:HB3	1:B:256:TYR:CZ	2.48	0.49
1:A:266:LEU:HD12	3:A:1603:OLC:H5	1.93	0.49
1:A:34:ALA:CA	1:A:38:LYS:HG3	2.43	0.49
1:A:1095:ARG:NH1	1:A:1153:PHE:O	2.46	0.49
1:B:223:ILE:HD12	1:B:224:SER:N	2.28	0.48
1:B:120:LEU:HD13	1:B:203[B]:HIS:NE2	2.28	0.48
1:A:142:THR:HG23	1:A:143:ASN:H	1.74	0.48
1:A:96:VAL:HA	1:A:99:VAL:HG22	1.96	0.48
1:A:194:LEU:HD23	1:B:194:LEU:HD23	1.96	0.47
1:B:200:GLN:HG2	4:B:1606:OLA:H32	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:ILE:HD12	1:A:85:LEU:HD22	1.95	0.47
1:B:1201:SER:HB3	1:B:234:LYS:NZ	2.29	0.47
1:A:72:MET:CE	1:A:149:LYS:HA	2.45	0.47
1:B:116:TYR:CE2	2:B:1500:ITD:H3B	2.50	0.47
1:A:63:MET:O	1:A:64:GLY:C	2.54	0.46
1:B:1017:ILE:HG13	1:B:1027:ILE:HD12	1.98	0.46
1:B:72:MET:HE3	1:B:75:LYS:HD3	1.98	0.46
1:A:1033:LEU:O	1:A:1034:THR:CG2	2.64	0.46
1:B:1024:TYR:HB3	1:B:1032:LEU:HD11	1.98	0.46
1:A:100:ALA:HB2	4:A:1610:OLA:H21	1.98	0.46
1:A:36:PHE:CZ	1:A:40:PHE:CD2	3.04	0.46
1:A:132:LEU:HD23	1:A:218:CYS:SG	2.56	0.46
1:B:223:ILE:HD12	1:B:223:ILE:C	2.36	0.45
1:B:270:ILE:HG22	3:B:1602:OLC:H3A	1.98	0.45
1:A:114:VAL:O	1:A:118:VAL:HG23	2.17	0.45
1:B:156:VAL:O	1:B:160:VAL:HB	2.17	0.45
1:A:146:ARG:CB	1:A:147:PRO:HD3	2.46	0.45
1:A:1025:TYR:O	1:A:1032:LEU:HD23	2.16	0.45
1:B:127:LEU:HD11	1:B:248:PHE:CG	2.52	0.45
1:A:50:LEU:O	1:A:53[B]:ILE:HG22	2.17	0.45
1:A:1111:VAL:O	1:A:1118:LEU:HD11	2.18	0.44
1:A:72:MET:HE1	1:A:149:LYS:HA	1.99	0.44
1:B:179:GLU:O	1:B:180:ALA:HB2	2.16	0.44
1:A:1085:LYS:HB3	1:A:1086:PRO:HD3	2.00	0.43
1:A:1151:THR:HG21	1:A:1160:ALA:HB2	2.00	0.43
1:B:1035:LYS:H	1:B:1035:LYS:HG2	1.50	0.43
1:A:48:ILE:HD11	1:A:293:PHE:CG	2.53	0.43
1:B:97:ASP:OD1	2:B:1500:ITD:H15	2.18	0.43
1:A:65:TYR:N	1:A:65:TYR:HD1	2.15	0.43
1:A:113:HIS:O	1:A:114:VAL:C	2.55	0.43
1:A:209:ILE:O	1:A:209:ILE:HG22	2.18	0.43
1:B:69:LEU:HD13	1:B:69:LEU:HA	1.74	0.43
1:B:84:ASP:O	1:B:88:VAL:HB	2.19	0.43
1:A:201:PHE:CE2	3:A:1603:OLC:H14	2.54	0.43
1:A:1017:ILE:HD11	1:A:1046:LEU:CD2	2.49	0.43
3:A:1600:OLC:H21A	5:A:1704:HOH:O	2.17	0.43
1:B:42:PRO:HB2	4:B:1605:OLA:H121	2.01	0.42
1:A:48:ILE:CD1	1:A:293:PHE:CD2	3.03	0.42
1:A:127:LEU:HD11	1:A:248:PHE:CG	2.54	0.42
1:A:246:LEU:O	1:A:249[B]:PHE:HD2	2.03	0.42
1:A:35:ASN:ND2	1:A:35:ASN:N	2.66	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53[A]:ILE:HD11	1:A:89:ILE:HG13	2.01	0.41
1:A:129:PHE:CE2	1:A:151:LEU:HD22	2.55	0.41
1:A:197:VAL:CG2	1:B:194:LEU:HD22	2.34	0.41
1:B:1007:LEU:HD13	1:B:1067:PHE:CE1	2.55	0.41
1:B:97:ASP:OD1	2:B:1500:ITD:H16	2.21	0.41
1:A:118:VAL:HG23	1:A:168:THR:HG21	2.03	0.41
1:A:1120:MET:CB	1:A:1129:ALA:HB2	2.51	0.41
1:B:41:LEU:N	1:B:42:PRO:HD2	2.36	0.41
1:B:117:THR:HB	1:B:168:THR:HG22	2.02	0.41
1:B:120:LEU:HD22	4:B:1609:OLA:H21	2.03	0.41
1:A:97:ASP:OD1	2:A:1500:ITD:H15	2.21	0.41
2:A:1500:ITD:H6A	5:A:1720:HOH:O	2.21	0.41
1:B:1052:ARG:HH21	1:B:1054:THR:HG22	1.86	0.40
1:A:142:THR:CG2	1:A:143:ASN:OD1	2.59	0.40
1:A:325:VAL:HA	1:A:328:GLN:HG3	2.02	0.40
1:B:262:ASP:OD2	1:B:281:HIS:NE2	2.51	0.40
1:B:298:ASN:HB3	1:B:299:PRO:HD3	2.03	0.40
1:B:1026:THR:HA	1:B:1031:HIS:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	468/502 (93%)	451 (96%)	17 (4%)	0	100	100
1	B	456/502 (91%)	440 (96%)	16 (4%)	0	100	100
All	All	924/1004 (92%)	891 (96%)	33 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	406/432 (94%)	378 (93%)	28 (7%)	15	30
1	B	393/432 (91%)	373 (95%)	20 (5%)	24	45
All	All	799/864 (92%)	751 (94%)	48 (6%)	18	37

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ARG
1	A	35	ASN
1	A	38	LYS
1	A	69	LEU
1	A	72	MET
1	A	120	LEU
1	A	134	ARG
1	A	145	GLN
1	A	154	LYS
1	A	165	LEU
1	A	188	ARG
1	A	201	PHE
1	A	209	ILE
1	A	223	ILE
1	A	1008	ARG
1	A	1026	THR
1	A	1032	LEU
1	A	1035	LYS
1	A	1036	SER
1	A	1037	PRO
1	A	1045	GLU
1	A	1060	LYS
1	A	1125	ARG
1	A	1137	ARG
1	A	230	LYS
1	A	262	ASP
1	A	286	ILE

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Mol	Chain	Res	Type
1	A	325	VAL
1	B	30	ARG
1	B	31	GLU
1	B	66	GLN
1	B	67	LYS
1	B	69	LEU
1	B	72	MET
1	B	134	ARG
1	B	143	ASN
1	B	146	ARG
1	B	149	LYS
1	B	154	LYS
1	B	171	ASP
1	B	188	ARG
1	B	193	ASP
1	B	201	PHE
1	B	1005	GLU
1	B	1035	LYS
1	B	1036	SER
1	B	1076	ARG
1	B	315	HIS

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

Mol	Chain	Res	Type
1	A	35	ASN
1	B	37	ASN
1	B	143	ASN
1	B	200	GLN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\#|Z| > 2$
4	OLA	B	1606	-	16,19,19	0.25	0	15,19,19	0.55	0
3	OLC	A	1600	-	17,17,24	0.54	0	18,18,25	0.72	0
3	OLC	B	1601	-	14,14,24	0.55	0	15,15,25	0.65	0
4	OLA	A	1610	-	6,9,19	0.27	0	5,9,19	0.54	0
3	OLC	B	1602	-	21,21,24	0.45	0	22,22,25	0.54	0
3	OLC	A	1603	-	21,21,24	0.49	0	22,22,25	0.58	0
2	ITD	A	1500	-	24,30,30	1.85	6 (25%)	27,42,42	2.07	9 (33%)
4	OLA	B	1605	-	16,19,19	0.27	0	15,19,19	0.55	0
2	ITD	B	1500	-	24,30,30	1.90	6 (25%)	27,42,42	1.96	8 (29%)
4	OLA	B	1608	-	8,11,19	0.35	0	7,11,19	0.78	0
3	OLC	A	1604	-	15,15,24	0.52	0	16,16,25	0.76	0
4	OLA	B	1607	-	16,19,19	0.25	0	15,19,19	0.53	0
4	OLA	B	1609	-	9,12,19	0.35	0	8,12,19	0.56	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	OLA	B	1606	-	-	12/15/17/17	-
3	OLC	A	1600	-	-	6/17/17/24	-
3	OLC	B	1601	-	-	9/14/14/24	-
4	OLA	A	1610	-	-	3/5/7/17	-
3	OLC	B	1602	-	-	9/21/21/24	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	OLC	A	1603	-	-	11/21/21/24	-
2	ITD	A	1500	-	-	2/11/39/39	0/4/4/4
4	OLA	B	1605	-	-	9/15/17/17	-
2	ITD	B	1500	-	-	3/11/39/39	0/4/4/4
4	OLA	B	1608	-	-	6/7/9/17	-
3	OLC	A	1604	-	-	3/15/15/24	-
4	OLA	B	1607	-	-	7/15/17/17	-
4	OLA	B	1609	-	-	7/8/10/17	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1500	ITD	C9-S2	-6.30	1.67	1.75
2	A	1500	ITD	C9-S2	-6.19	1.67	1.75
2	A	1500	ITD	C9-N4	3.84	1.34	1.26
2	B	1500	ITD	C9-N4	3.75	1.34	1.26
2	B	1500	ITD	C2-N1	-3.18	1.46	1.49
2	B	1500	ITD	C5-S1	3.15	1.75	1.70
2	A	1500	ITD	C5-S1	2.90	1.74	1.70
2	A	1500	ITD	C2-N1	-2.86	1.46	1.49
2	A	1500	ITD	C4-N1	2.17	1.34	1.31
2	A	1500	ITD	C8-S2	-2.16	1.77	1.82
2	B	1500	ITD	C4-N1	2.10	1.34	1.31
2	B	1500	ITD	C8-S2	-2.06	1.77	1.82

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	ITD	C17-C16-N4	5.54	117.45	109.32
2	B	1500	ITD	C17-C16-N4	4.83	116.41	109.32
2	A	1500	ITD	C8-S2-C9	3.90	108.26	100.12
2	B	1500	ITD	C16-N4-C9	3.79	127.84	121.07
2	B	1500	ITD	C6-C2-N1	3.68	106.40	102.90
2	A	1500	ITD	C15-C10-N3	3.66	118.13	110.56
2	A	1500	ITD	C16-N4-C9	3.39	127.11	121.07
2	B	1500	ITD	C10-N3-C9	3.33	130.54	124.65
2	B	1500	ITD	C8-S2-C9	3.13	106.67	100.12
2	A	1500	ITD	C6-C2-N1	3.07	105.82	102.90
2	A	1500	ITD	C10-N3-C9	3.01	129.97	124.65
2	A	1500	ITD	C21-C16-N4	2.61	113.15	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1500	ITD	C15-C10-N3	2.34	115.40	110.56
2	B	1500	ITD	C21-C16-N4	2.28	112.66	109.32
2	A	1500	ITD	C7-C8-S2	-2.19	107.99	112.70
2	A	1500	ITD	C11-C10-N3	2.07	114.86	110.56
2	B	1500	ITD	C3-C2-C6	-2.01	109.07	112.08

There are no chirality outliers.

All (87) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1500	ITD	C17-C16-N4-C9
2	B	1500	ITD	C15-C10-N3-C9
2	B	1500	ITD	C17-C16-N4-C9
3	A	1600	OLC	O20-C21-C22-C24
3	A	1603	OLC	C21-C22-C24-O25
4	A	1610	OLA	C1-C2-C3-C4
4	B	1605	OLA	C1-C2-C3-C4
4	B	1607	OLA	C1-C2-C3-C4
4	B	1608	OLA	C1-C2-C3-C4
4	B	1609	OLA	C1-C2-C3-C4
3	A	1603	OLC	C2-C1-O20-C21
3	A	1603	OLC	O19-C1-O20-C21
3	A	1600	OLC	O20-C21-C22-O23
2	A	1500	ITD	C15-C10-N3-C9
3	B	1602	OLC	C1-C2-C3-C4
3	B	1602	OLC	C2-C1-O20-C21
3	A	1603	OLC	C11-C12-C13-C14
4	B	1609	OLA	C4-C5-C6-C7
3	B	1601	OLC	C3-C4-C5-C6
4	B	1606	OLA	C14-C15-C16-C17
3	A	1600	OLC	C5-C6-C7-C8
4	B	1606	OLA	C5-C6-C7-C8
4	B	1605	OLA	C2-C3-C4-C5
3	B	1601	OLC	O20-C21-C22-O23
3	A	1603	OLC	C1-C2-C3-C4
3	B	1601	OLC	C1-C2-C3-C4
3	A	1600	OLC	C4-C5-C6-C7
4	A	1610	OLA	C3-C4-C5-C6
3	B	1602	OLC	O19-C1-O20-C21
4	B	1607	OLA	C14-C15-C16-C17
4	B	1607	OLA	C2-C3-C4-C5
3	A	1600	OLC	C2-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
3	A	1600	OLC	C1-C2-C3-C4
4	B	1606	OLA	C10-C11-C12-C13
3	A	1603	OLC	C10-C11-C12-C13
3	B	1602	OLC	C6-C7-C8-C9
4	B	1607	OLA	C6-C7-C8-C9
4	B	1607	OLA	C10-C11-C12-C13
4	B	1608	OLA	C6-C7-C8-C9
3	A	1603	OLC	O23-C22-C24-O25
4	B	1606	OLA	C3-C4-C5-C6
4	B	1609	OLA	C6-C7-C8-C9
3	B	1601	OLC	C2-C1-O20-C21
3	A	1603	OLC	C5-C6-C7-C8
4	B	1605	OLA	C13-C14-C15-C16
4	B	1605	OLA	C4-C5-C6-C7
3	B	1601	OLC	O19-C1-O20-C21
3	A	1603	OLC	C12-C13-C14-C15
3	B	1601	OLC	C4-C5-C6-C7
3	B	1601	OLC	C5-C6-C7-C8
4	B	1606	OLA	C4-C5-C6-C7
3	B	1601	OLC	C2-C3-C4-C5
4	B	1605	OLA	C12-C13-C14-C15
4	B	1609	OLA	C2-C3-C4-C5
3	A	1604	OLC	C1-C2-C3-C4
3	B	1602	OLC	C4-C5-C6-C7
4	B	1606	OLA	C11-C12-C13-C14
4	B	1605	OLA	C5-C6-C7-C8
4	B	1608	OLA	C2-C3-C4-C5
4	B	1605	OLA	C10-C11-C12-C13
4	B	1606	OLA	C1-C2-C3-C4
3	A	1603	OLC	C4-C5-C6-C7
4	A	1610	OLA	C4-C5-C6-C7
4	B	1609	OLA	C5-C6-C7-C8
4	B	1608	OLA	C3-C4-C5-C6
3	B	1602	OLC	C11-C12-C13-C14
3	A	1604	OLC	C3-C4-C5-C6
4	B	1606	OLA	C15-C16-C17-C18
4	B	1605	OLA	C3-C4-C5-C6
4	B	1606	OLA	C2-C3-C4-C5
4	B	1607	OLA	C4-C5-C6-C7
4	B	1608	OLA	C7-C8-C9-C10
3	A	1603	OLC	C2-C3-C4-C5
4	B	1609	OLA	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
4	B	1608	OLA	C5-C6-C7-C8
3	B	1602	OLC	C21-C22-C24-O25
4	B	1607	OLA	C5-C6-C7-C8
3	A	1604	OLC	C6-C7-C8-C9
2	B	1500	ITD	N3-C9-S2-C8
4	B	1609	OLA	C7-C8-C9-C10
4	B	1606	OLA	C13-C14-C15-C16
4	B	1605	OLA	C7-C8-C9-C10
4	B	1606	OLA	C9-C10-C11-C12
3	B	1602	OLC	C7-C8-C9-C10
4	B	1606	OLA	C7-C8-C9-C10
3	B	1602	OLC	O20-C1-C2-C3
3	B	1601	OLC	O23-C22-C24-O25

There are no ring outliers.

11 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1606	OLA	1	0
3	A	1600	OLC	2	0
4	A	1610	OLA	1	0
3	B	1602	OLC	1	0
3	A	1603	OLC	3	0
2	A	1500	ITD	3	0
4	B	1605	OLA	2	0
2	B	1500	ITD	3	0
3	A	1604	OLC	4	0
4	B	1607	OLA	1	0
4	B	1609	OLA	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 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 OLA B 1606

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC A 1600

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC B 1601

Bond lengths

Bond angles

Torsions

Rings

Ligand OLA A 1610

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC B 1602

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC A 1603

Bond lengths

Bond angles

Torsions

Rings

Ligand ITD A 1500

Bond lengths

Bond angles

Torsions

Rings

Ligand OLA B 1605

Bond lengths

Bond angles

Torsions

Rings

Ligand ITD B 1500

Bond lengths

Bond angles

Torsions

Rings

Ligand OLA B 1608

Bond lengths

Bond angles

Torsions

Rings

Ligand OLC A 1604

Bond lengths

Bond angles

Torsions

Rings

Ligand OLA B 1607

Bond lengths

Bond angles

Torsions

Rings

Ligand OLA B 1609

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	466/502 (92%)	0.47	38 (8%)	11	11	19, 41, 69, 87	0
1	B	456/502 (90%)	0.60	50 (10%)	5	5	21, 41, 80, 112	0
All	All	922/1004 (91%)	0.54	88 (9%)	8	8	19, 41, 74, 112	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	317	LEU	7.5
1	B	28	CYS	6.4
1	B	316	ALA	6.4
1	A	35	ASN	5.8
1	B	1037	PRO	5.6
1	B	1034	THR	5.5
1	B	1035	LYS	5.4
1	B	35	ASN	4.9
1	B	1053	ASN	4.9
1	B	65	TYR	4.6
1	B	36	PHE	4.6
1	B	1076	ARG	4.4
1	A	36	PHE	4.3
1	B	228	HIS	4.2
1	B	315	HIS	4.1
1	B	29	PHE	4.1
1	A	69	LEU	3.9
1	A	1037	PRO	3.8
1	A	1110	GLY	3.8
1	B	318	THR	3.7
1	A	67	LYS	3.6
1	A	68	LYS	3.6
1	B	1036	SER	3.5
1	B	1038	SER	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	235	ARG	3.5
1	B	33	ASN	3.5
1	A	1127	ASP	3.4
1	B	142	THR	3.4
1	B	319	SER	3.4
1	A	1153	PHE	3.3
1	A	1080	ARG	3.3
1	B	182	ASP	3.3
1	B	32	GLU	3.2
1	B	143	ASN	3.2
1	A	172	PHE	3.2
1	B	274	CYS	3.2
1	A	40	PHE	3.2
1	B	1054	THR	3.1
1	B	233	GLN	3.1
1	B	181	ASP	3.1
1	B	145	GLN	3.1
1	B	227	SER	3.0
1	A	1024	TYR	3.0
1	B	226	LEU	3.0
1	B	1127	ASP	3.0
1	B	1099	LEU	2.9
1	A	1099	LEU	2.9
1	B	69	LEU	2.9
1	A	27	PRO	2.8
1	A	230	LYS	2.8
1	B	308	LYS	2.7
1	B	1107	GLY	2.6
1	A	143	ASN	2.6
1	B	31	GLU	2.6
1	A	1098	ALA	2.6
1	B	146	ARG	2.6
1	B	1157	THR	2.6
1	B	30	ARG	2.6
1	A	1142	THR	2.5
1	A	65	TYR	2.5
1	B	900	GLY	2.5
1	B	1052	ARG	2.5
1	A	233	GLN	2.5
1	A	1118	LEU	2.5
1	A	1035	LYS	2.4
1	A	232	HIS	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	249[A]	PHE	2.4
1	A	231	GLY	2.4
1	B	68	LYS	2.4
1	A	319	SER	2.4
1	B	1015	LEU	2.4
1	A	1086	PRO	2.3
1	B	1125	ARG	2.3
1	B	1023	GLY	2.3
1	B	1086	PRO	2.3
1	A	1073	ALA	2.3
1	B	34	ALA	2.3
1	B	1018	TYR	2.3
1	A	1036	SER	2.2
1	B	172	PHE	2.2
1	A	146	ARG	2.2
1	A	1125	ARG	2.2
1	A	184	TYR	2.1
1	A	1089	ASP	2.1
1	A	1061	ASP	2.0
1	A	1082	ALA	2.0
1	B	1109	THR	2.0
1	A	1023	GLY	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides 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(Å^2)	Q<0.9
4	OLA	B	1605	20/20	0.79	0.23	32,48,83,150	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	OLA	B	1606	20/20	0.79	0.23	30,54,125,154	0
4	OLA	A	1610	10/20	0.80	0.31	23,39,73,117	0
3	OLC	B	1602	22/25	0.81	0.27	29,52,104,134	0
3	OLC	A	1604	16/25	0.81	0.24	26,43,97,150	0
4	OLA	B	1609	13/20	0.82	0.27	22,36,70,105	0
3	OLC	A	1600	18/25	0.84	0.18	43,58,112,115	0
3	OLC	A	1603	22/25	0.84	0.22	23,46,79,134	0
4	OLA	B	1607	20/20	0.85	0.23	34,54,124,155	0
4	OLA	B	1608	12/20	0.89	0.14	27,49,72,76	0
3	OLC	B	1601	15/25	0.92	0.20	17,34,71,103	0
2	ITD	B	1500	27/27	0.92	0.18	15,35,59,114	0
2	ITD	A	1500	27/27	0.94	0.21	15,40,115,153	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.
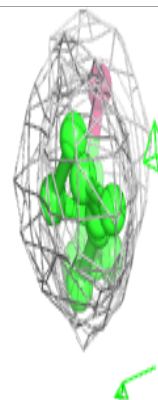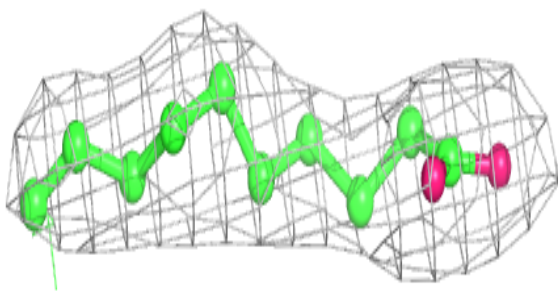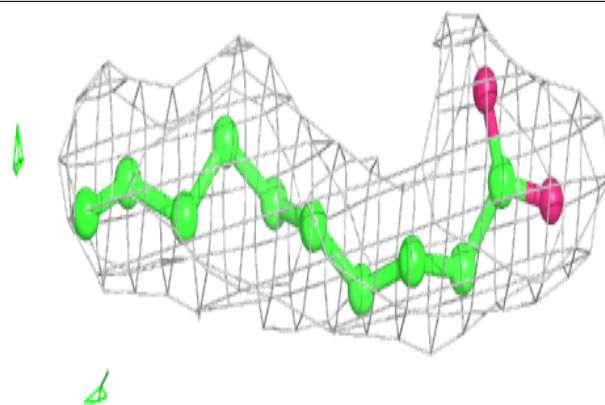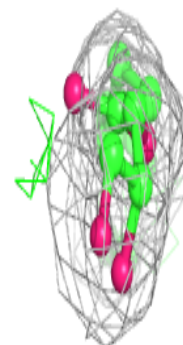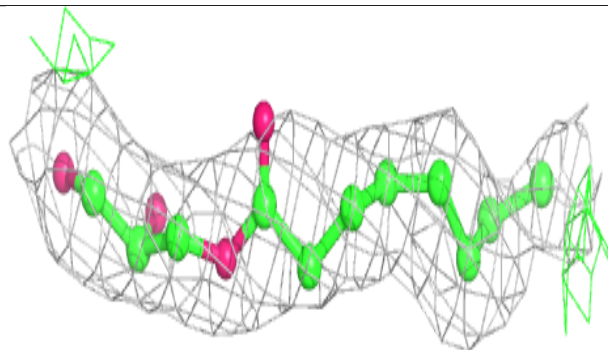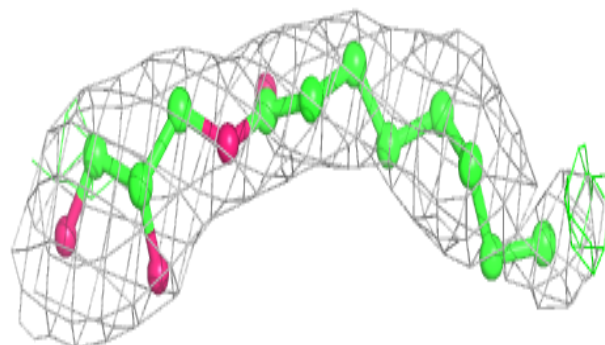

Electron density around OLA B 1605:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)
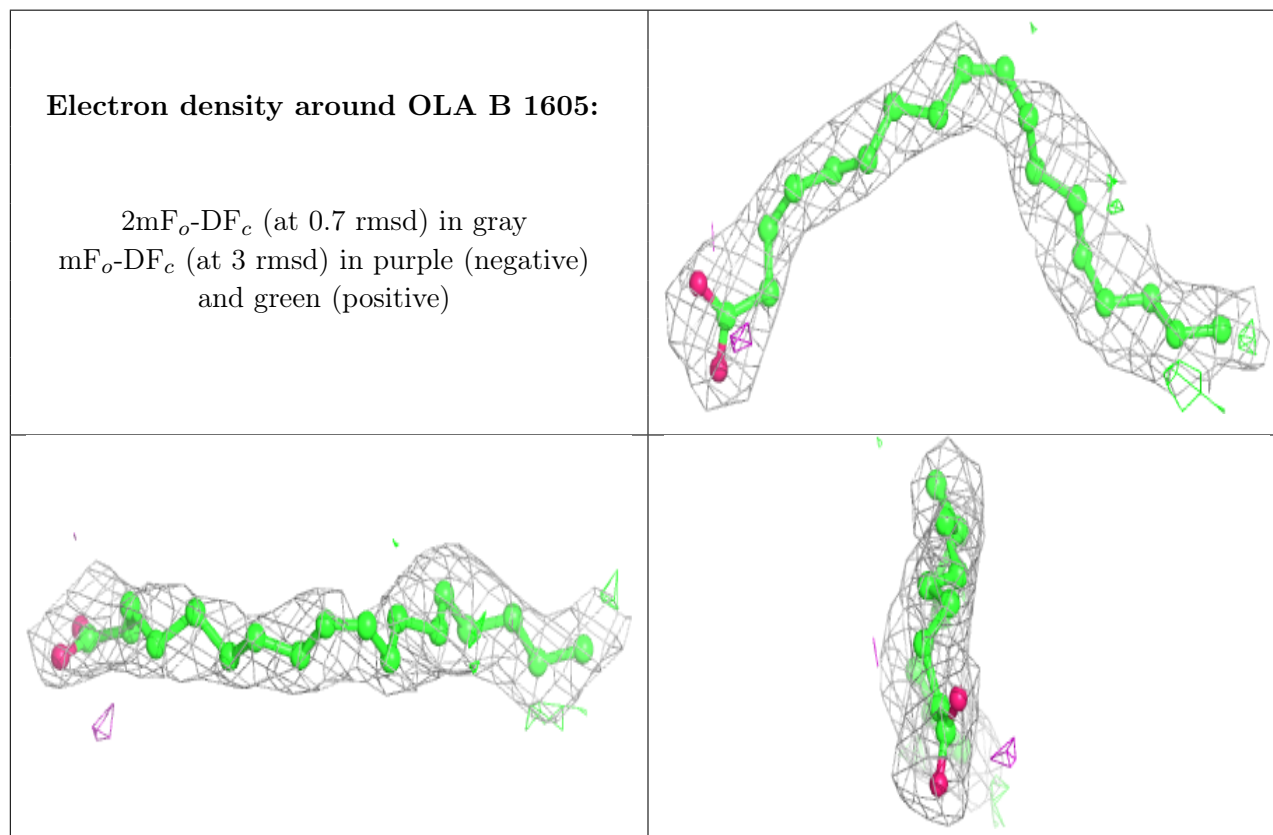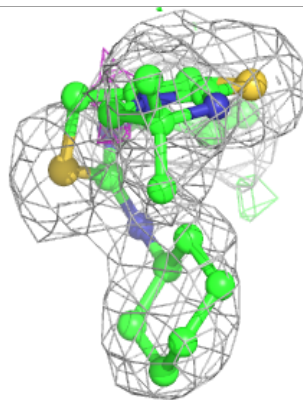
Electron density around OLA B 1606:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
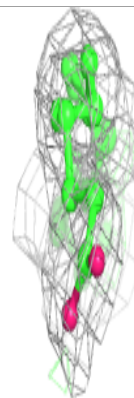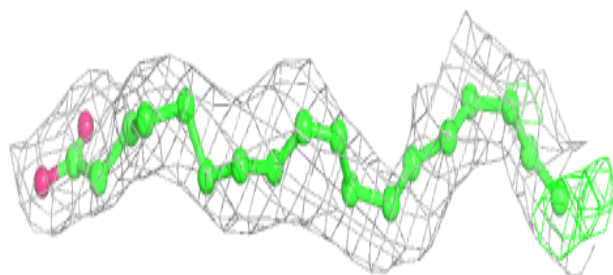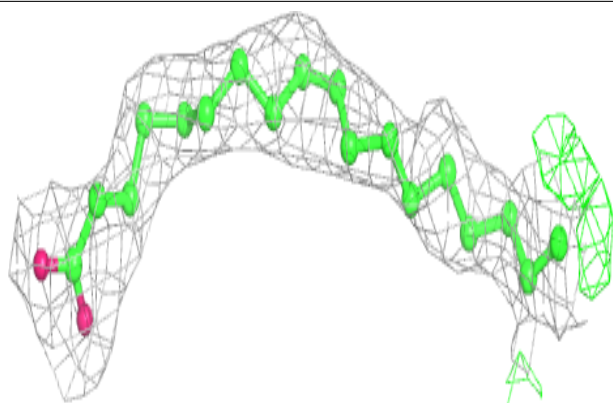
Electron density around OLA A 1610:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
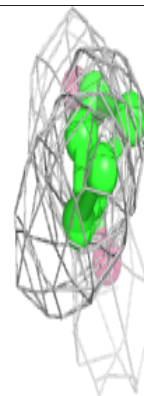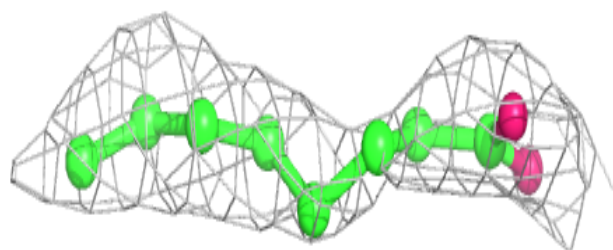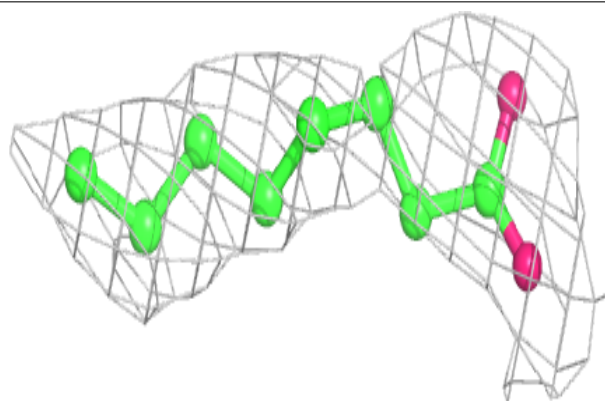
Electron density around OLC B 1602:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
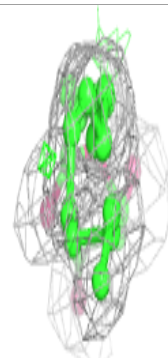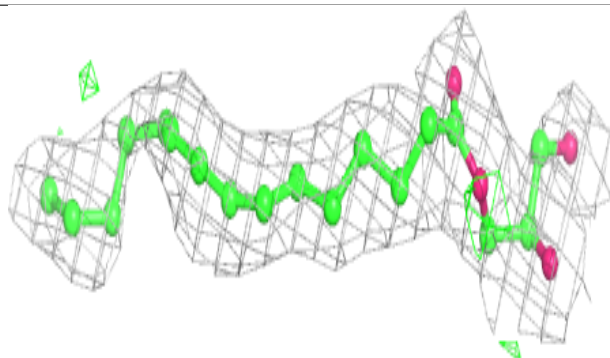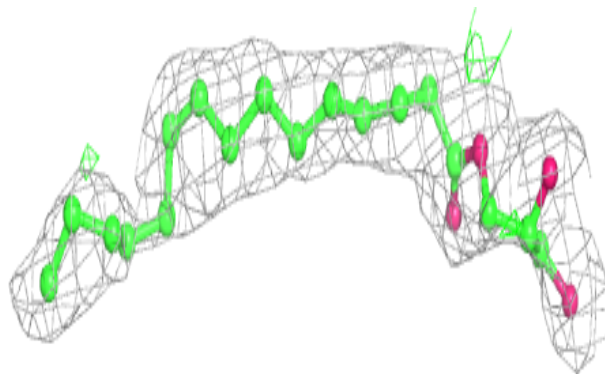
Electron density around OLC A 1604:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
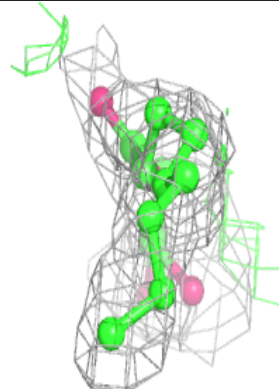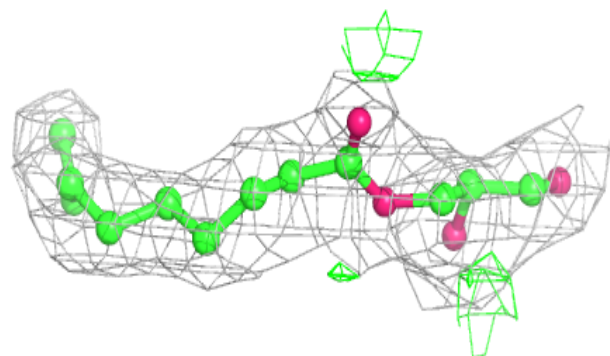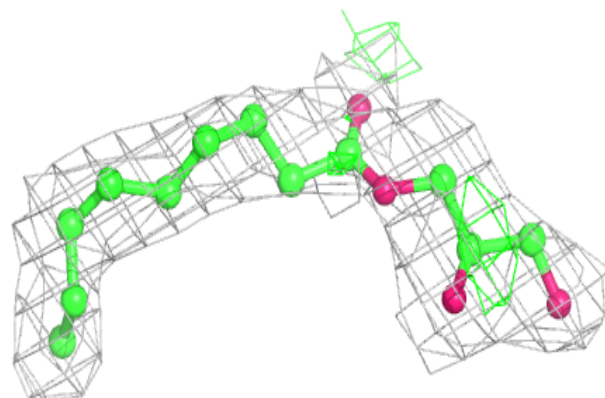
Electron density around OLA B 1609:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
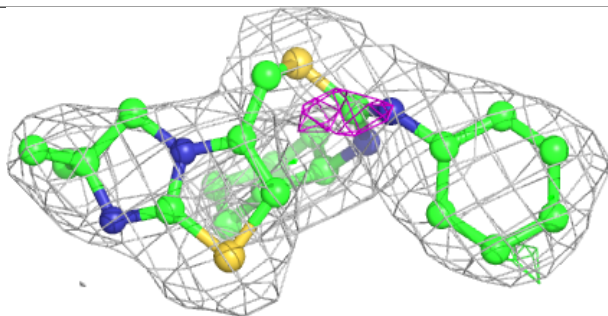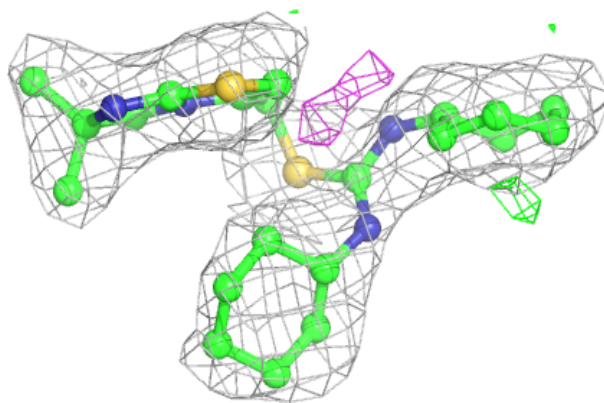and green (positive)
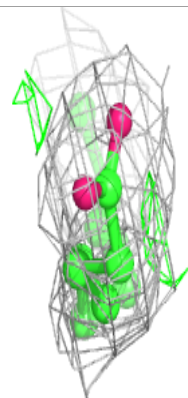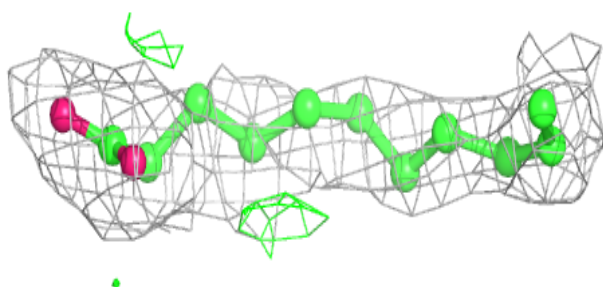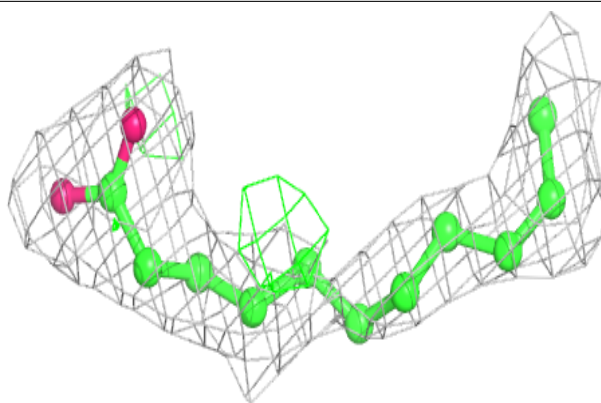
Electron density around OLC A 1600:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
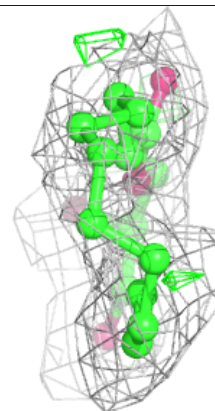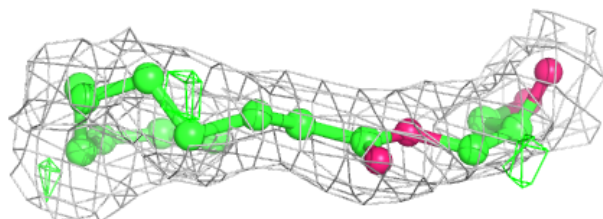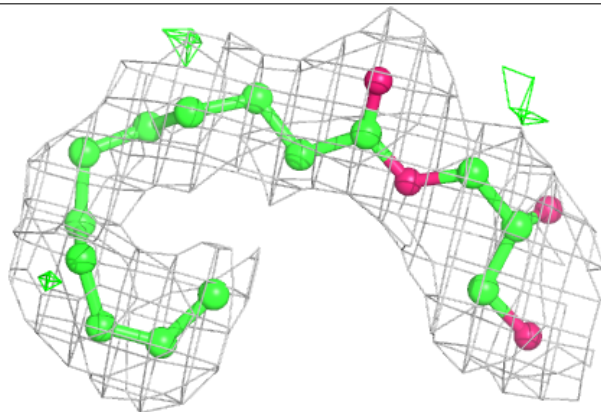
Electron density around OLC A 1603:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
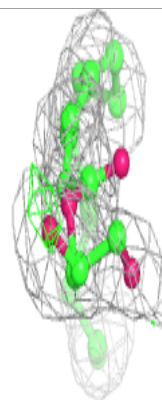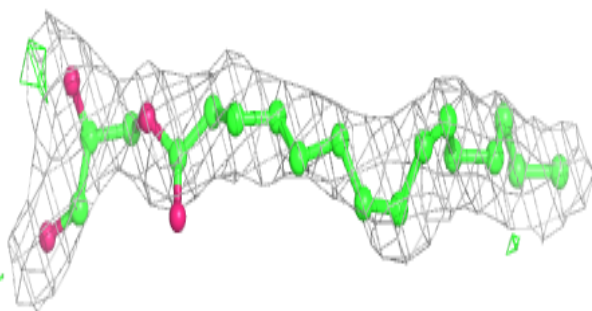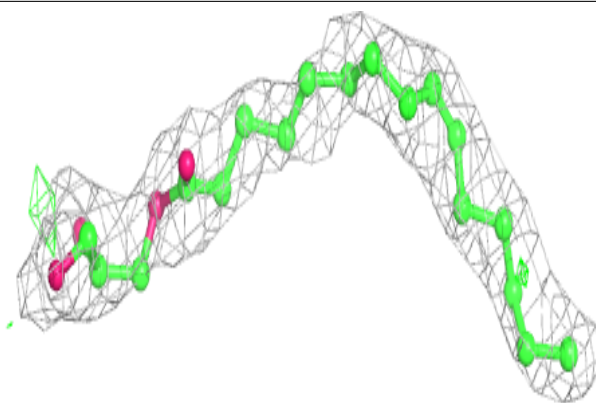
Electron density around OLA B 1607:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
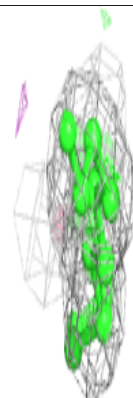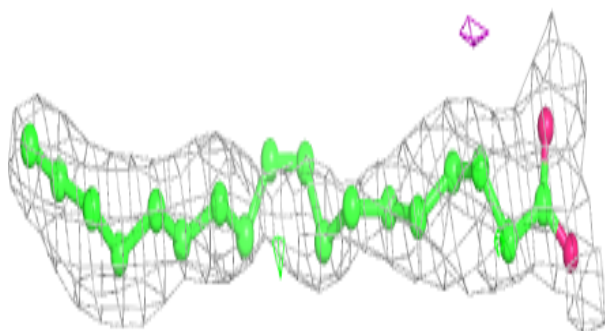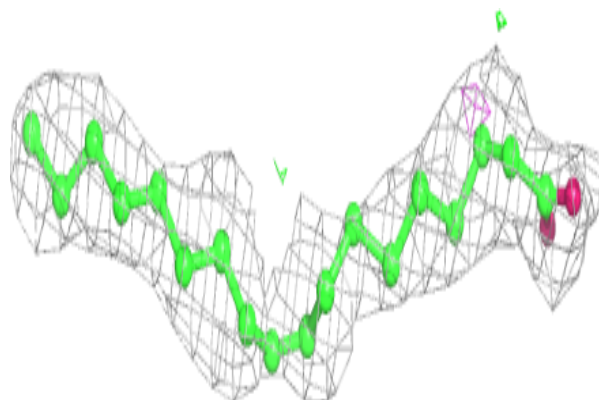
Electron density around OLA B 1608:

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 1601:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
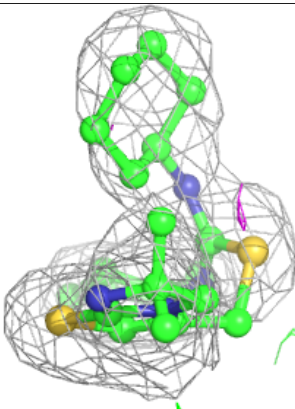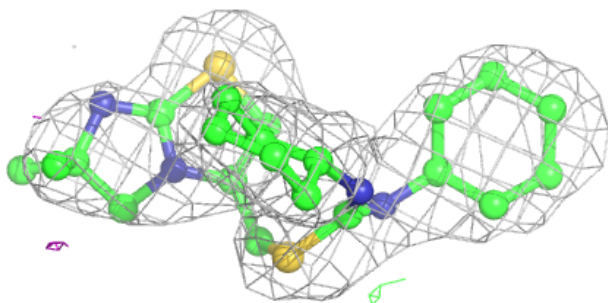mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
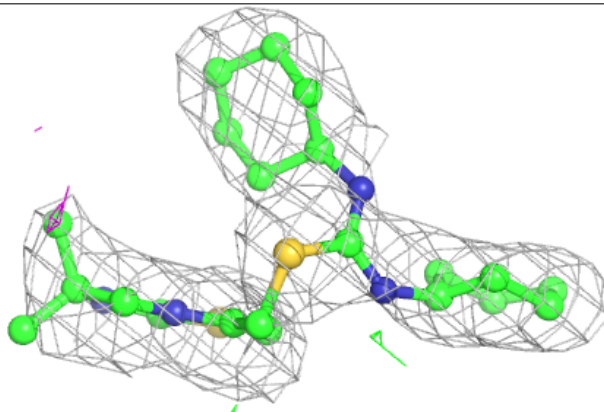and green (positive)

Electron density around ITD B 1500:

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

Electron density around ITD A 1500:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.