



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 03:00 PM UTC

PDB ID : 3ODU / pdb_00003odu
Title : The 2.5 Å 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.; Cherezov, 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)

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](#) ①) 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

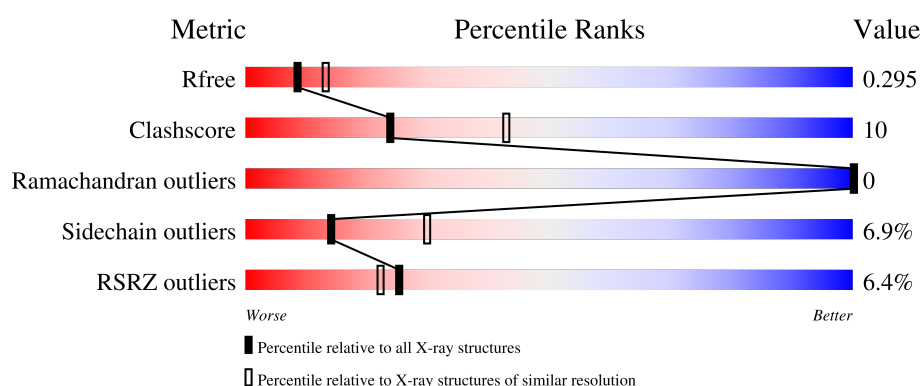
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (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 $\leq 5\%$. 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	502	5% 67% 22% • 7%
1	B	502	7% 69% 20% • 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	C	N	O	S	0	4	0
			3759	2464	630	649	16			
1	B	456	Total	C	N	O	S	0	2	0
			3661	2396	616	633	16			

There are 54 discrepancies between the modelled and reference sequences:

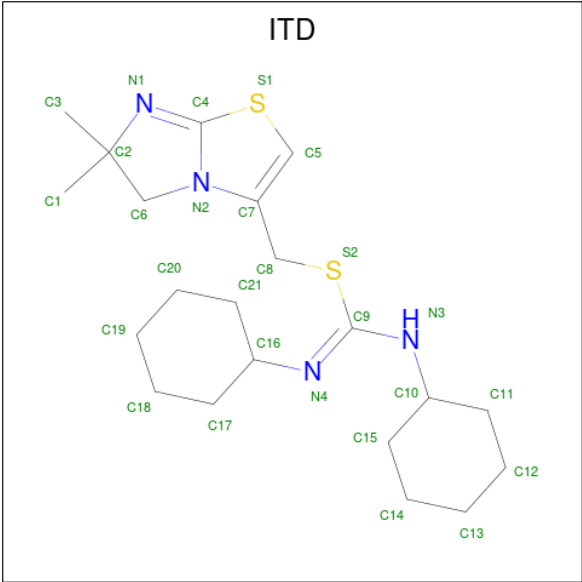
Chain	Residue	Modelled	Actual	Comment	Reference
A	-9	ASP	-	expression tag	UNP P61073
A	-8	TYR	-	expression tag	UNP P61073
A	-7	LYS	-	expression tag	UNP P61073
A	-6	ASP	-	expression tag	UNP P61073
A	-5	ASP	-	expression tag	UNP P61073
A	-4	ASP	-	expression tag	UNP P61073
A	-3	ASP	-	expression tag	UNP P61073
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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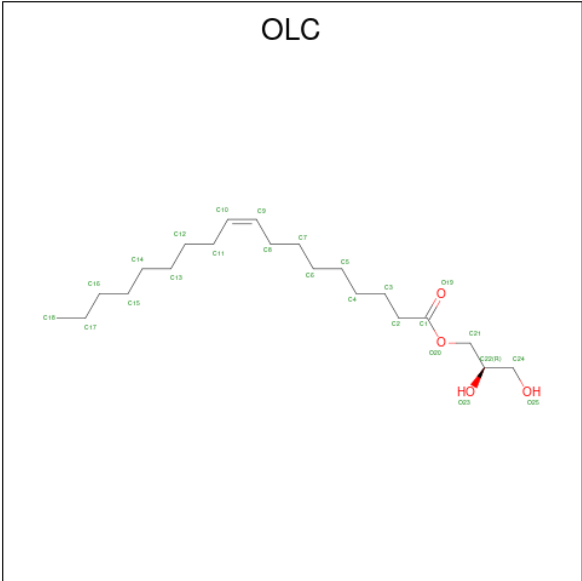
Chain	Residue	Modelled	Actual	Comment	Reference
A	327	PHE	-	expression tag	UNP P61073
A	328	GLN	-	expression tag	UNP P61073
B	-9	ASP	-	expression tag	UNP P61073
B	-8	TYR	-	expression tag	UNP P61073
B	-7	LYS	-	expression tag	UNP P61073
B	-6	ASP	-	expression tag	UNP P61073
B	-5	ASP	-	expression tag	UNP 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'-dicyclohexylimidothiocarbamate (CCD ID: ITD) (formula: C₂₁H₃₄N₄S₂).



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

- Molecule 3 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (CCD ID: OLC) (formula: C₂₁H₄₀O₄).



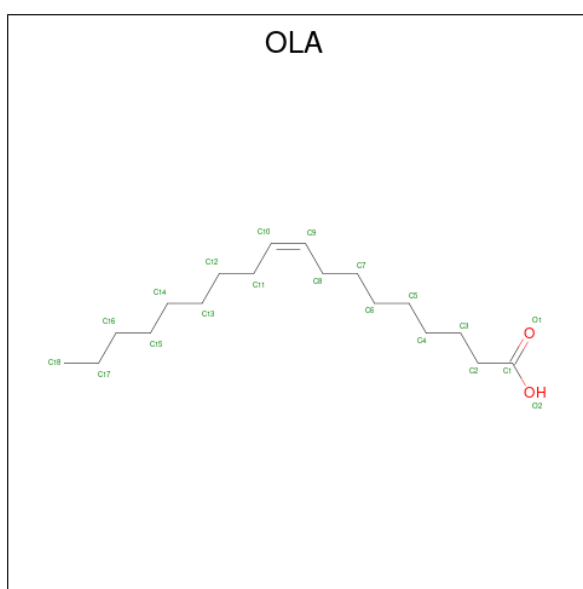
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			18	14	4		

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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 (CCD ID: 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		

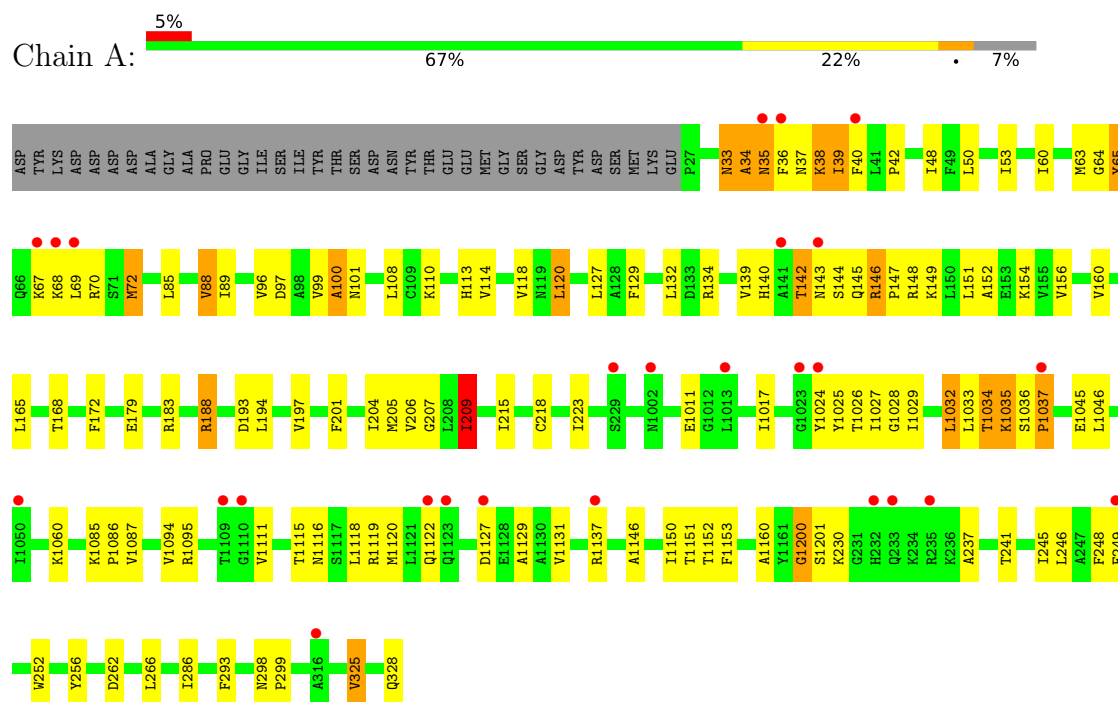
- Molecule 5 is water.

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

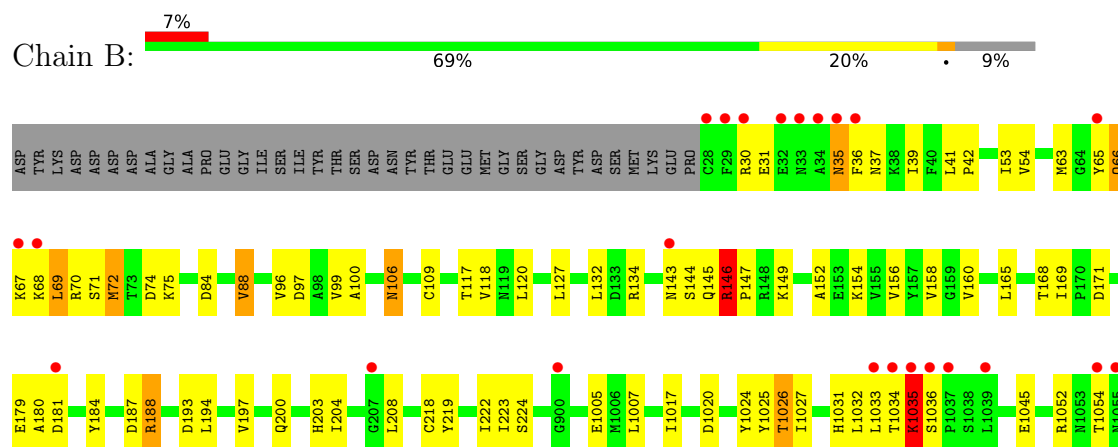
3 Residue-property plots [i](#)

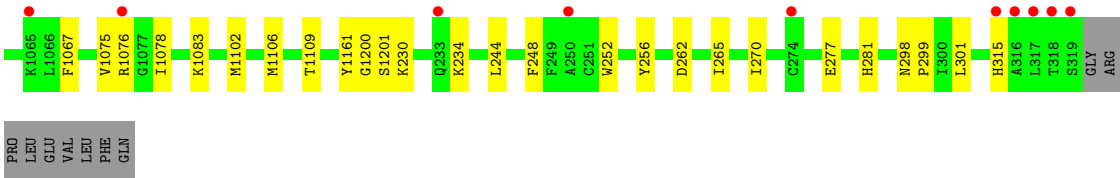
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 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

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 19.98 – 2.50	Depositor EDS
% Data completeness (in resolution range)	(Not available) (19.98-2.50) 95.4 (19.98-2.50)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 , 66.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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.*

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: 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	0.99	10/3863 (0.3%)	1.04	21/5242 (0.4%)
1	B	0.89	4/3758 (0.1%)	1.13	24/5102 (0.5%)
All	All	0.94	14/7621 (0.2%)	1.08	45/10344 (0.4%)

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 (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	39	ILE	CA-CB	-6.60	1.46	1.54
1	A	34	ALA	CA-C	-6.48	1.46	1.52
1	A	209	ILE	C-O	-6.21	1.16	1.24
1	B	37	ASN	C-O	-5.88	1.16	1.24
1	A	207	GLY	C-O	-5.56	1.17	1.23
1	A	39	ILE	C-O	-5.53	1.18	1.23
1	A	205	MET	C-O	-5.42	1.17	1.24
1	B	1161	TYR	C-O	-5.38	1.17	1.23
1	B	146	ARG	C-O	-5.32	1.19	1.24
1	A	146	ARG	C-O	-5.31	1.19	1.24
1	A	215	ILE	CA-CB	5.26	1.60	1.54
1	A	139	VAL	C-O	-5.16	1.18	1.24
1	A	188	ARG	C-O	-5.13	1.17	1.24
1	B	184	TYR	C-O	-5.03	1.18	1.24

All (45) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65	TYR	CB-CA-C	13.47	137.23	110.42
1	B	68	LYS	N-CA-C	13.45	125.67	111.14
1	B	66	GLN	N-CA-C	13.32	125.52	111.14
1	B	230	LYS	N-CA-C	-12.04	95.56	110.61
1	B	63	MET	CB-CA-C	11.66	132.84	111.03
1	A	1200	GLY	N-CA-C	9.29	135.19	113.18
1	B	1035	LYS	N-CA-C	8.72	123.34	112.87
1	A	37	ASN	N-CA-C	8.27	121.41	111.82
1	B	65	TYR	N-CA-CB	-8.26	96.54	110.49
1	A	1115	THR	N-CA-C	8.05	119.69	111.07
1	B	36	PHE	N-CA-C	7.97	123.59	113.55
1	A	139	VAL	N-CA-C	7.84	118.64	110.72
1	B	208	LEU	N-CA-C	7.04	122.77	114.04
1	A	142	THR	N-CA-C	-6.94	103.64	111.07
1	A	209	ILE	CB-CA-C	-6.90	101.92	111.65
1	B	208	LEU	N-CA-CB	-6.79	100.76	110.81
1	B	70	ARG	N-CA-C	6.72	119.90	109.07
1	A	68	LYS	CA-C-N	-6.55	113.81	123.11
1	A	68	LYS	C-N-CA	-6.55	113.81	123.11
1	B	35	ASN	CA-C-N	-6.51	111.20	122.79
1	B	35	ASN	C-N-CA	-6.51	111.20	122.79
1	B	1033	LEU	N-CA-C	-6.47	99.69	109.79
1	A	65	TYR	N-CA-C	6.44	120.95	112.13
1	B	1200	GLY	CA-C-N	-6.39	110.12	121.81
1	B	1200	GLY	C-N-CA	-6.39	110.12	121.81
1	B	100	ALA	N-CA-C	6.15	120.36	112.12
1	B	68	LYS	CA-C-N	-6.06	114.36	122.42
1	B	68	LYS	C-N-CA	-6.06	114.36	122.42
1	A	1037	PRO	N-CA-C	5.99	121.85	113.53
1	A	140	HIS	CB-CA-C	-5.96	103.09	111.85
1	A	33	ASN	CA-C-N	-5.91	112.74	122.79
1	A	33	ASN	C-N-CA	-5.91	112.74	122.79
1	A	206	VAL	CA-C-N	5.80	126.38	120.00
1	A	206	VAL	C-N-CA	5.80	126.38	120.00
1	A	245	ILE	N-CA-C	5.58	115.78	110.42
1	A	100	ALA	N-CA-C	5.48	122.47	110.80
1	B	70	ARG	CA-C-N	5.37	129.37	120.94
1	B	70	ARG	C-N-CA	5.37	129.37	120.94
1	B	96	VAL	CB-CA-C	-5.29	105.08	112.02
1	A	39	ILE	CB-CA-C	-5.26	106.25	111.30
1	A	1034	THR	N-CA-CB	5.24	119.52	111.56
1	A	183	ARG	N-CA-C	5.17	116.15	108.60
1	B	181	ASP	N-CA-CB	-5.17	104.23	111.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	100	ALA	N-CA-CB	-5.16	100.63	110.63
1	A	1115	THR	CB-CA-C	-5.04	102.97	110.88

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 ⓘ

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	99	0
1	B	3661	0	3726	62	0
2	A	27	0	34	3	0
2	B	27	0	34	2	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	157	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 (157) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:144:SER:C	1:B:147:PRO:HD2	2.10	0.76
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: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:B:72:MET:HE2	1:B:152:ALA:HB3	1.81	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:72:MET:HE3	1:B:75:LYS:HD3	1.85	0.58
1:B:42:PRO:HG3	1:B:99:VAL:CG1	2.33	0.58
1:A:34:ALA:O	1:A:35:ASN:C	2.46	0.57
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:ILE:HG23	4:B:1605:OLA:H162	1.88	0.55
1:A:1029:ILE:HG22	1:A:1029:ILE:O	2.04	0.55
1:A:204:ILE:HG12	3:A:1604:OLC:H3A	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
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: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:63:MET:O	1:A:64:GLY:C	2.54	0.51
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:B:223:ILE:C	1:B:223:ILE:HD12	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:72:MET:HE3	1:A:152:ALA:HB3	1.95	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
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:72:MET:HE3	1:B:75:LYS:CD	2.44	0.47
1:A:113:HIS:O	1:A:114:VAL:C	2.55	0.47
1:B:1017:ILE:HG13	1:B:1027:ILE:HD12	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: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:B:1102:MET:HE3	1:B:1106:MET:HE1	2.00	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:110:LYS:NZ	1:A:172:PHE:O	2.43	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
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:64:GLY:C	1:A:65:TYR:CD1	2.98	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:B:1020:ASP:OD1	1:B:1020:ASP:C	2.63	0.41
1:A:97:ASP:OD1	2:A:1500:ITD:H15	2.21	0.41
1:A:1033:LEU:C	1:A:1034:THR:HG23	2.46	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:A:33:ASN:OD1	1:A:33:ASN:C	2.65	0.40
1:B:298:ASN:HB3	1:B:299:PRO:HD3	2.03	0.40
1:B:145:GLN:O	1:B:146:ARG:C	2.58	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%)	14	30
1	B	393/432 (91%)	366 (93%)	27 (7%)	14	30
All	All	799/864 (92%)	744 (93%)	55 (7%)	14	30

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	38	LYS
1	A	69	LEU
1	A	70	ARG
1	A	72	MET
1	A	88	VAL
1	A	120	LEU
1	A	134	ARG
1	A	145	GLN
1	A	154	LYS
1	A	165	LEU
1	A	179	GLU
1	A	188	ARG
1	A	209	ILE
1	A	223	ILE

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Mol	Chain	Res	Type
1	A	1011	GLU
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	1137	ARG
1	A	230	LYS
1	A	262	ASP
1	A	286	ILE
1	A	325	VAL
1	B	30	ARG
1	B	31	GLU
1	B	35	ASN
1	B	66	GLN
1	B	67	LYS
1	B	69	LEU
1	B	72	MET
1	B	88	VAL
1	B	106	ASN
1	B	134	ARG
1	B	143	ASN
1	B	146	ARG
1	B	149	LYS
1	B	154	LYS
1	B	158	VAL
1	B	169	ILE
1	B	171	ASP
1	B	188	ARG
1	B	193	ASP
1	B	1005	GLU
1	B	1026	THR
1	B	1035	LYS
1	B	1036	SER
1	B	1076	ARG
1	B	1083	LYS
1	B	1109	THR
1	B	315	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	37	ASN
1	A	203	HIS
1	A	294	HIS
1	B	37	ASN
1	B	200	GLN
1	B	1055	ASN
1	B	1132	ASN
1	B	232	HIS
1	B	272	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 oligosaccharides 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	$\# Z > 2$
3	OLC	B	1601	-	14,14,24	0.55	0	15,15,25	0.66	0
3	OLC	B	1602	-	21,21,24	0.45	0	22,22,25	0.55	0
2	ITD	A	1500	-	28,30,30	2.46	6 (21%)	30,42,42	2.13	10 (33%)
3	OLC	A	1600	-	17,17,24	0.54	0	18,18,25	0.73	0
4	OLA	B	1607	-	19,19,19	0.52	0	19,19,19	0.79	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	OLA	B	1608	-	11,11,19	0.66	0	11,11,19	1.15	1 (9%)
4	OLA	B	1606	-	19,19,19	0.51	0	19,19,19	0.82	0
2	ITD	B	1500	-	28,30,30	2.47	6 (21%)	30,42,42	2.04	10 (33%)
3	OLC	A	1603	-	21,21,24	0.49	0	22,22,25	0.58	0
4	OLA	B	1609	-	12,12,19	0.70	0	12,12,19	0.94	0
4	OLA	B	1605	-	19,19,19	0.51	0	19,19,19	0.90	1 (5%)
3	OLC	A	1604	-	15,15,24	0.52	0	16,16,25	0.77	0
4	OLA	A	1610	-	9,9,19	0.69	0	9,9,19	1.13	1 (11%)

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	OLC	B	1601	-	-	9/14/14/24	-
3	OLC	B	1602	-	-	8/21/21/24	-
2	ITD	A	1500	-	-	4/12/39/39	0/4/4/4
3	OLC	A	1600	-	-	6/17/17/24	-
4	OLA	B	1607	-	-	7/17/17/17	-
4	OLA	B	1608	-	-	8/9/9/17	-
4	OLA	B	1606	-	-	12/17/17/17	-
2	ITD	B	1500	-	-	4/12/39/39	0/4/4/4
3	OLC	A	1603	-	-	11/21/21/24	-
4	OLA	B	1609	-	-	9/10/10/17	-
4	OLA	B	1605	-	-	11/17/17/17	-
3	OLC	A	1604	-	-	3/15/15/24	-
4	OLA	A	1610	-	-	6/7/7/17	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	ITD	C4-N1	7.30	1.34	1.28
2	B	1500	ITD	C4-N1	7.19	1.34	1.28
2	B	1500	ITD	C5-C7	6.67	1.42	1.34
2	A	1500	ITD	C5-C7	6.63	1.42	1.34
2	B	1500	ITD	C9-S2	-6.05	1.67	1.75
2	A	1500	ITD	C9-S2	-5.94	1.67	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1500	ITD	C4-N2	-3.85	1.31	1.38
2	B	1500	ITD	C4-N2	-3.67	1.31	1.38
2	B	1500	ITD	C2-N1	-3.32	1.46	1.49
2	A	1500	ITD	C2-N1	-2.99	1.46	1.49
2	A	1500	ITD	C8-S2	-2.33	1.77	1.80
2	B	1500	ITD	C8-S2	-2.17	1.77	1.80

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1500	ITD	C17-C16-N4	5.24	117.45	109.34
2	B	1500	ITD	C17-C16-N4	4.57	116.41	109.34
2	B	1500	ITD	C6-C2-N1	4.38	106.40	102.83
2	A	1500	ITD	C15-C10-N3	3.78	118.13	110.57
2	A	1500	ITD	N2-C4-N1	-3.71	111.73	116.95
2	A	1500	ITD	S1-C4-N2	3.70	114.78	109.31
2	A	1500	ITD	C6-C2-N1	3.66	105.82	102.83
2	B	1500	ITD	N2-C4-N1	-3.63	111.83	116.95
2	B	1500	ITD	S1-C4-N2	3.62	114.66	109.31
2	B	1500	ITD	C10-N3-C9	3.45	130.54	124.48
2	A	1500	ITD	C8-S2-C9	3.29	108.26	100.98
2	A	1500	ITD	C10-N3-C9	3.13	129.97	124.48
2	A	1500	ITD	C7-C5-S1	-2.97	108.94	113.11
2	B	1500	ITD	C7-C5-S1	-2.75	109.26	113.11
2	B	1500	ITD	C8-S2-C9	2.57	106.67	100.98
2	A	1500	ITD	C21-C16-N4	2.46	113.15	109.34
2	B	1500	ITD	C15-C10-N3	2.41	115.40	110.57
4	B	1605	OLA	O2-C1-C2	2.29	121.23	114.00
4	A	1610	OLA	O2-C1-C2	2.21	120.97	114.00
2	B	1500	ITD	C3-C2-C6	-2.20	109.07	112.09
2	B	1500	ITD	C21-C16-N4	2.15	112.66	109.34
2	A	1500	ITD	C11-C10-N3	2.14	114.86	110.57
4	B	1608	OLA	O2-C1-C2	2.10	120.62	114.00

There are no chirality outliers.

All (98) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1500	ITD	S2-C9-N4-C16
2	A	1500	ITD	C17-C16-N4-C9
2	B	1500	ITD	C15-C10-N3-C9
2	B	1500	ITD	S2-C9-N4-C16

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

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Mol	Chain	Res	Type	Atoms
4	B	1605	OLA	C13-C14-C15-C16
3	A	1603	OLC	C5-C6-C7-C8
3	A	1603	OLC	C12-C13-C14-C15
4	B	1605	OLA	C4-C5-C6-C7
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
4	B	1605	OLA	C10-C11-C12-C13
4	B	1606	OLA	C11-C12-C13-C14
3	B	1602	OLC	C4-C5-C6-C7
4	B	1605	OLA	C5-C6-C7-C8
3	A	1604	OLC	C1-C2-C3-C4
4	B	1608	OLA	C2-C3-C4-C5
3	A	1603	OLC	C4-C5-C6-C7
4	A	1610	OLA	C4-C5-C6-C7
4	B	1608	OLA	C3-C4-C5-C6
4	B	1609	OLA	C5-C6-C7-C8
2	A	1500	ITD	N3-C9-S2-C8
2	B	1500	ITD	N3-C9-S2-C8
3	B	1602	OLC	C11-C12-C13-C14
4	B	1606	OLA	C1-C2-C3-C4
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	1609	OLA	O2-C1-C2-C3
4	B	1609	OLA	O1-C1-C2-C3
3	A	1603	OLC	C2-C3-C4-C5
4	B	1608	OLA	C7-C8-C9-C10
4	B	1608	OLA	C5-C6-C7-C8
4	B	1609	OLA	C3-C4-C5-C6
4	B	1607	OLA	C5-C6-C7-C8
3	A	1604	OLC	C6-C7-C8-C9
4	B	1605	OLA	C7-C8-C9-C10
4	B	1609	OLA	C7-C8-C9-C10
4	B	1606	OLA	C9-C10-C11-C12
3	B	1601	OLC	O23-C22-C24-O25
4	B	1606	OLA	C13-C14-C15-C16

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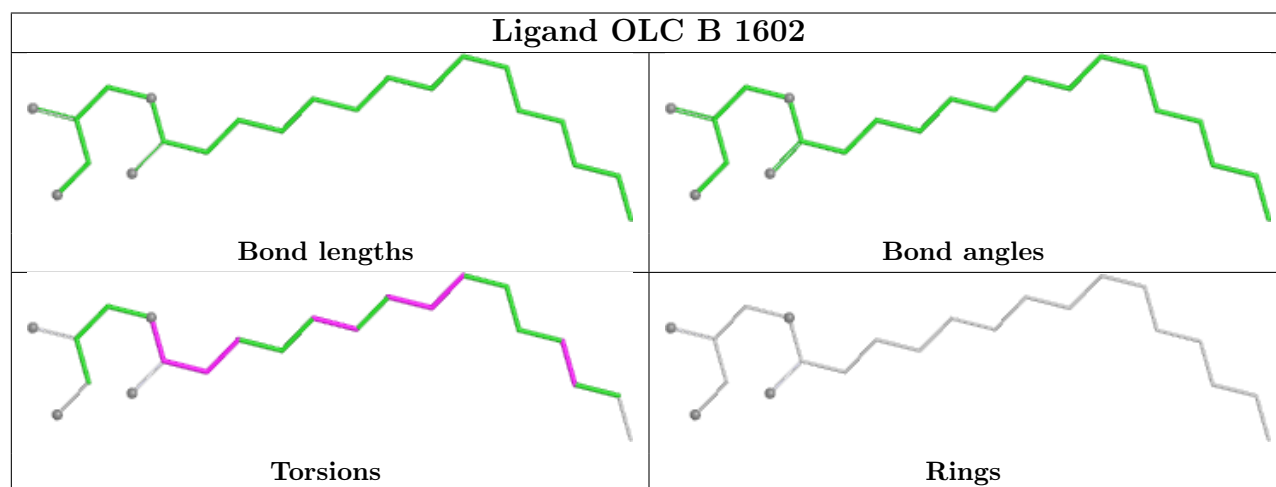
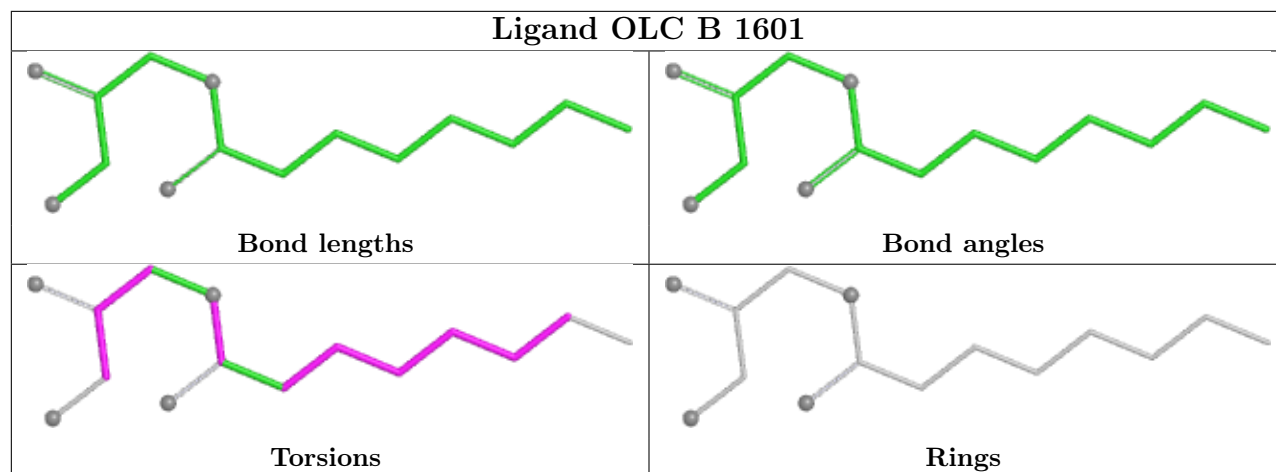
Mol	Chain	Res	Type	Atoms
3	B	1602	OLC	C7-C8-C9-C10
4	B	1606	OLA	C7-C8-C9-C10
4	B	1608	OLA	O1-C1-C2-C3
4	B	1605	OLA	O1-C1-C2-C3
4	B	1608	OLA	O2-C1-C2-C3
3	B	1602	OLC	O20-C1-C2-C3
4	A	1610	OLA	O2-C1-C2-C3
4	A	1610	OLA	O1-C1-C2-C3
4	B	1605	OLA	O2-C1-C2-C3
4	A	1610	OLA	C5-C6-C7-C8

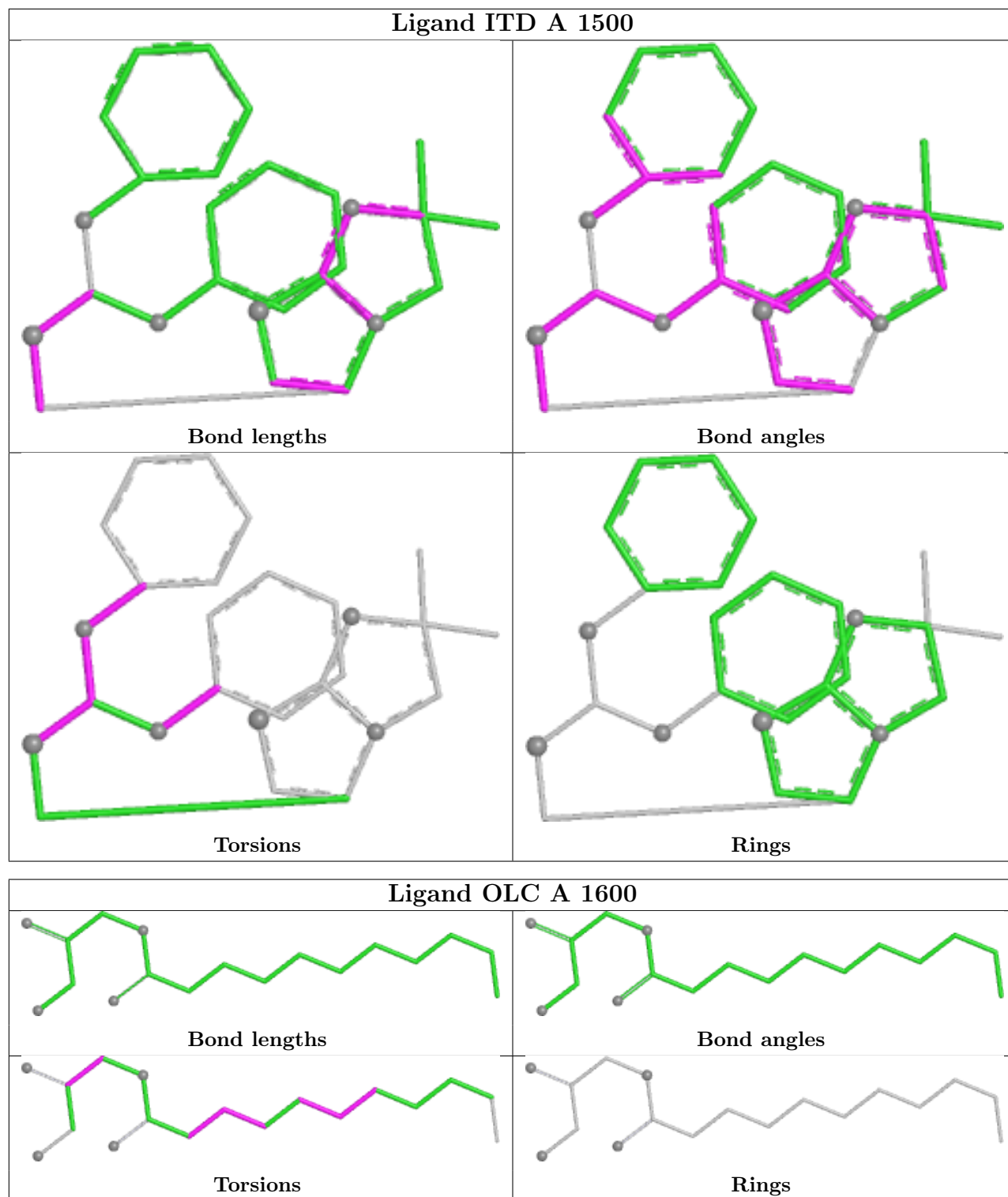
There are no ring outliers.

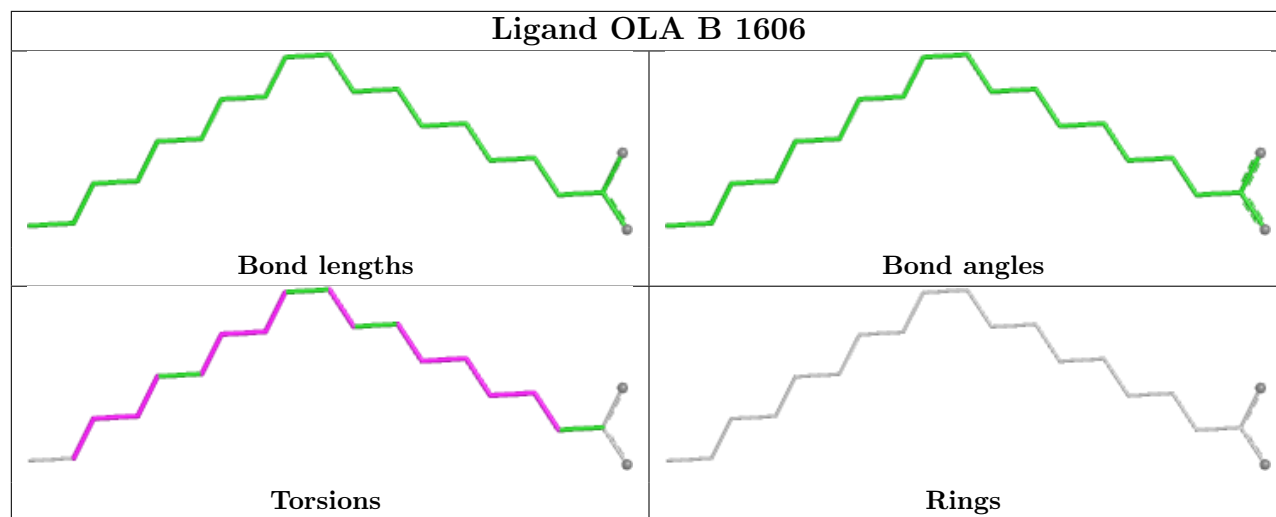
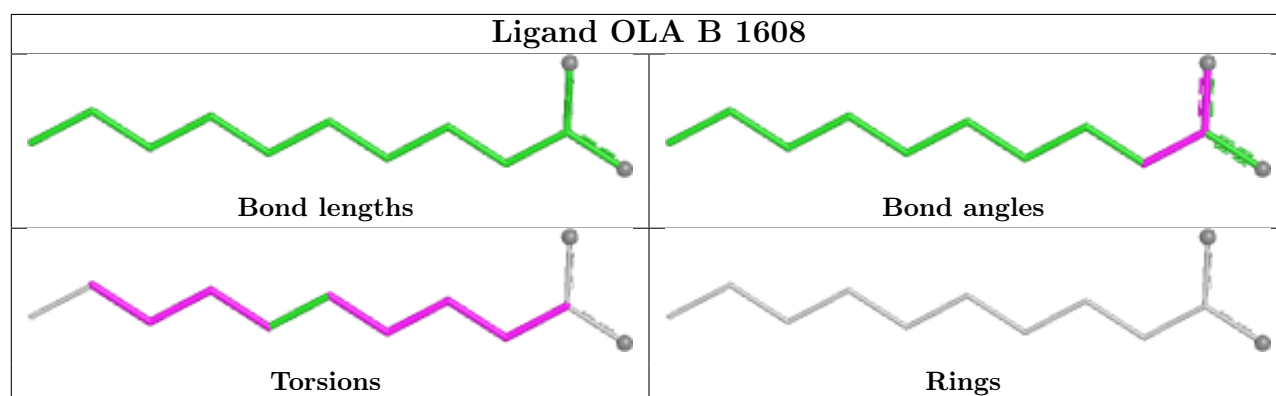
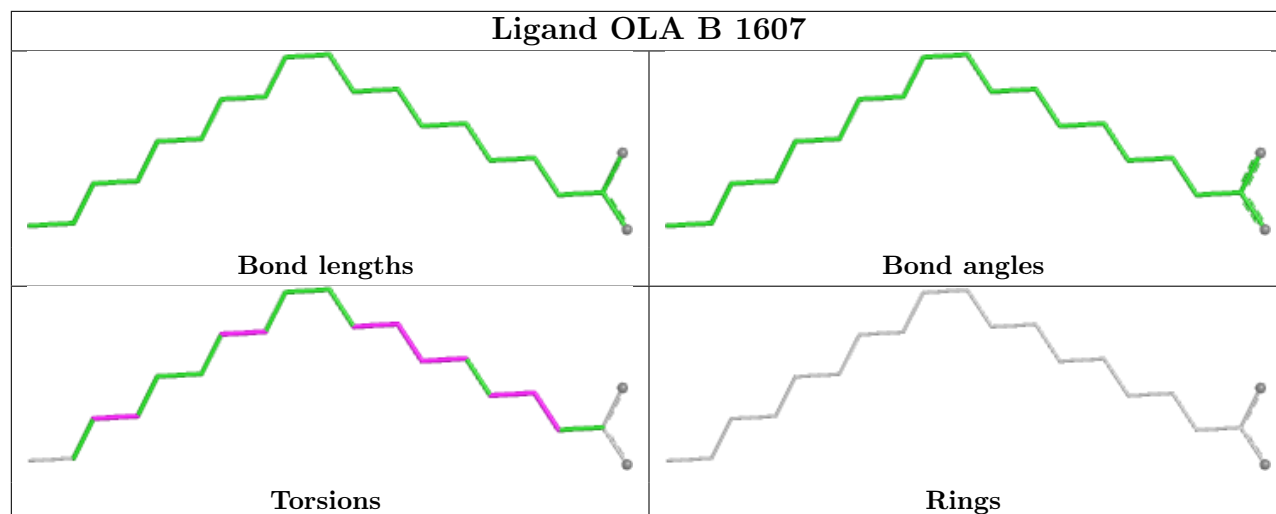
11 monomers are involved in 24 short contacts:

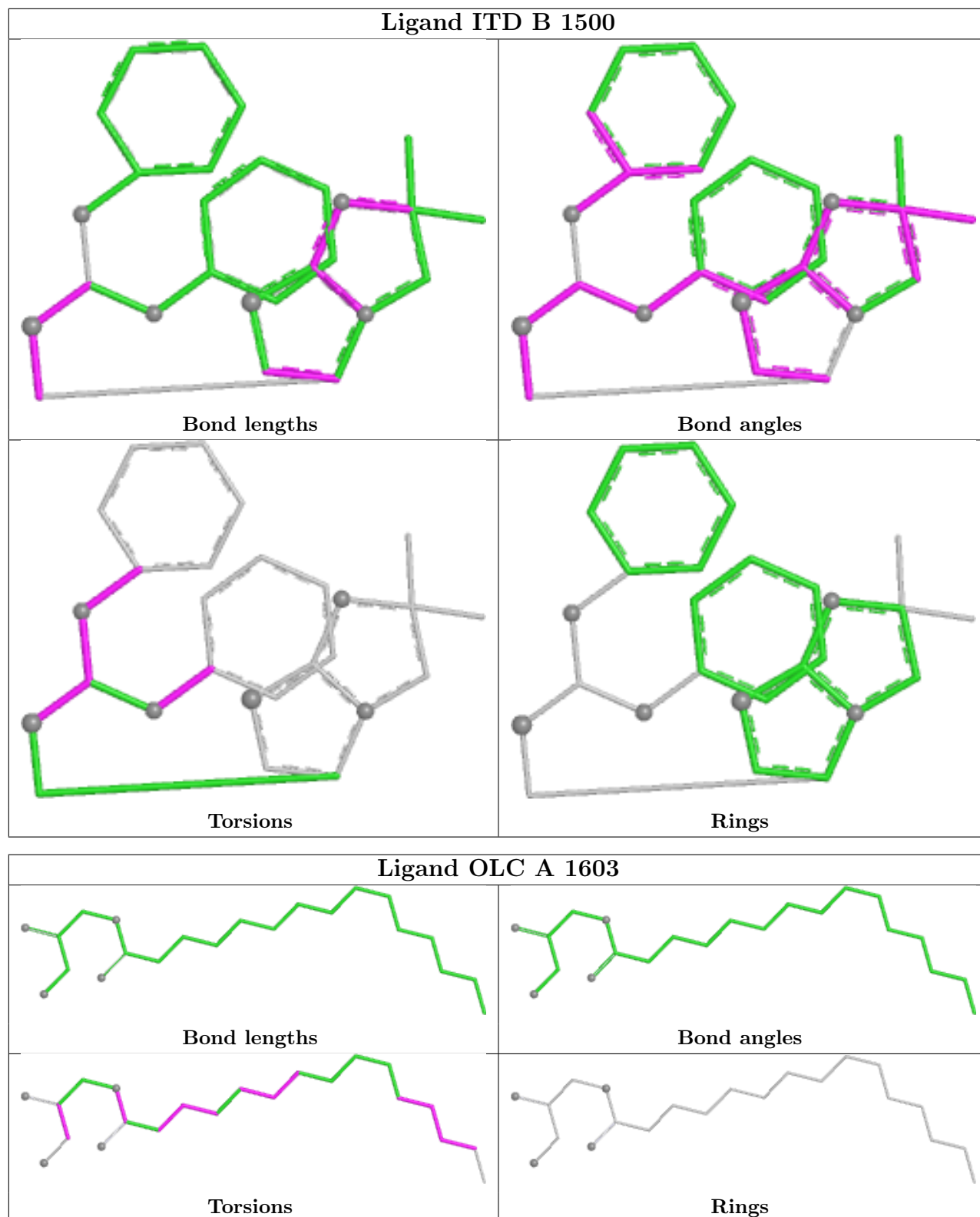
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1602	OLC	1	0
2	A	1500	ITD	3	0
3	A	1600	OLC	2	0
4	B	1607	OLA	1	0
4	B	1606	OLA	1	0
2	B	1500	ITD	2	0
3	A	1603	OLC	3	0
4	B	1609	OLA	4	0
4	B	1605	OLA	2	0
3	A	1604	OLC	4	0
4	A	1610	OLA	1	0

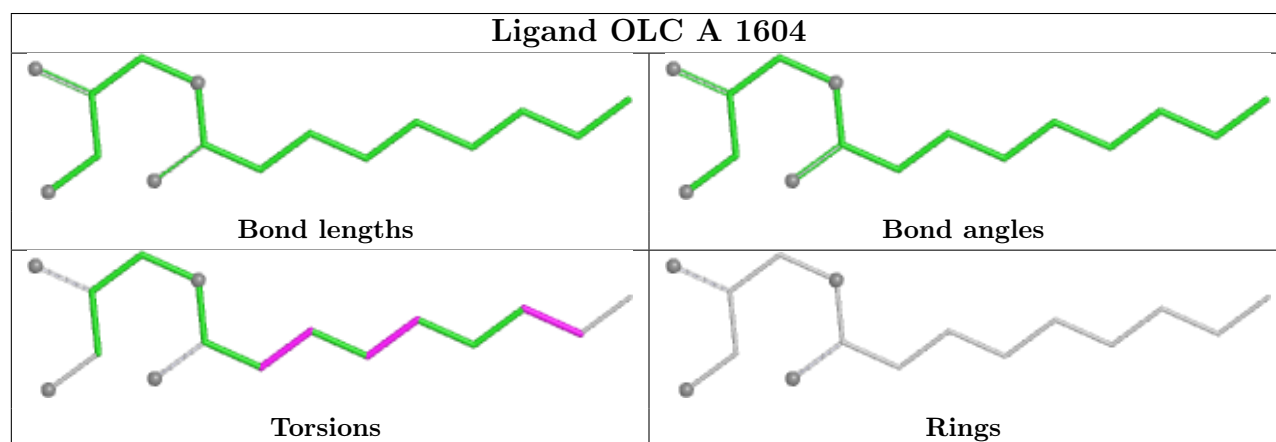
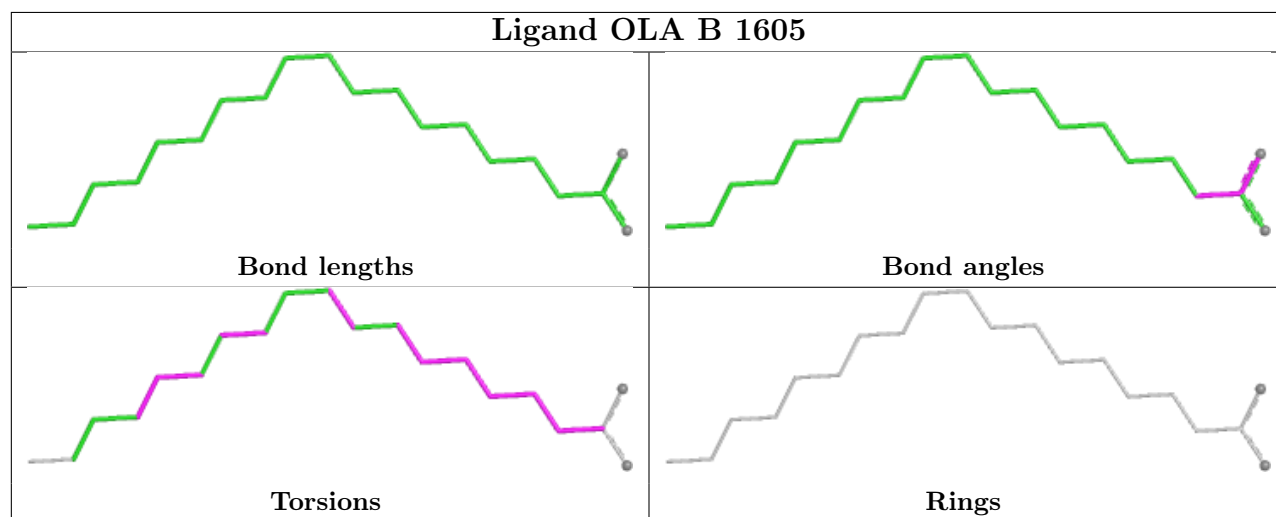
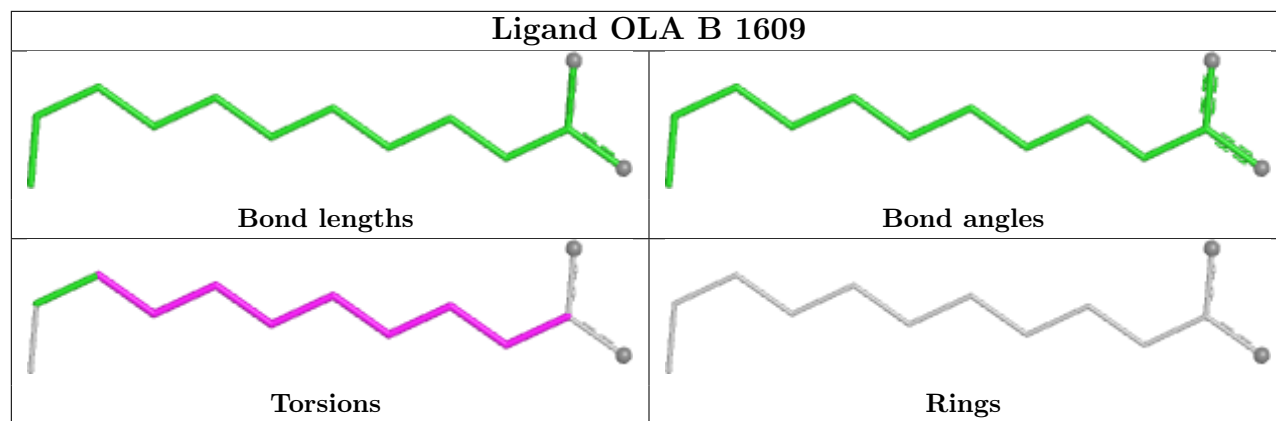
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

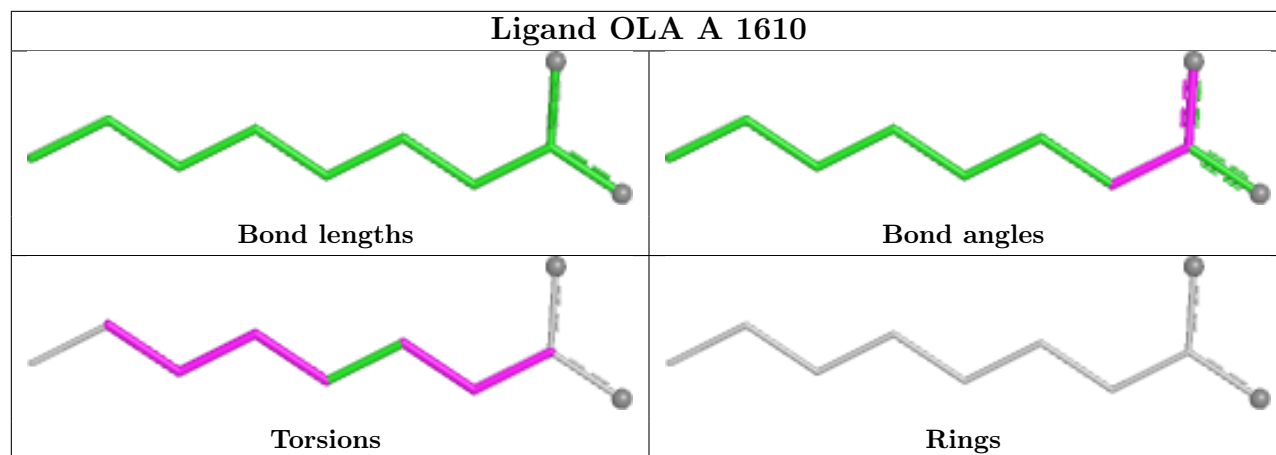












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	466/502 (92%)	0.56	26 (5%)	30 26	12, 41, 69, 87	4 (0%)
1	B	456/502 (90%)	0.57	33 (7%)	21 19	18, 41, 80, 112	2 (0%)
All	All	922/1004 (91%)	0.57	59 (6%)	25 22	12, 41, 74, 112	6 (0%)

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	316	ALA	6.3
1	B	317	LEU	5.9
1	B	65	TYR	4.6
1	B	28	CYS	4.5
1	B	1034	THR	4.2
1	A	143	ASN	4.1
1	A	1037	PRO	3.9
1	B	34	ALA	3.9
1	B	32	GLU	3.6
1	B	1037	PRO	3.5
1	B	319	SER	3.4
1	A	249[A]	PHE	3.3
1	B	35	ASN	3.1
1	A	35	ASN	3.1
1	A	67	LYS	3.0
1	A	1023	GLY	3.0
1	A	40	PHE	3.0
1	B	33	ASN	3.0
1	A	36	PHE	2.9
1	B	36	PHE	2.9
1	A	1123	GLN	2.8
1	B	68	LYS	2.8
1	B	1033	LEU	2.7
1	A	68	LYS	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1002	ASN	2.7
1	A	229	SER	2.7
1	B	30	ARG	2.7
1	B	1035	LYS	2.6
1	A	1024	TYR	2.6
1	B	233	GLN	2.5
1	B	143	ASN	2.5
1	A	235	ARG	2.4
1	A	1127	ASP	2.4
1	A	1013	LEU	2.4
1	A	1110	GLY	2.3
1	B	207	GLY	2.3
1	B	1076	ARG	2.3
1	B	67	LYS	2.3
1	A	1050	ILE	2.3
1	B	318	THR	2.2
1	B	29	PHE	2.2
1	B	1055	ASN	2.2
1	B	1054	THR	2.2
1	B	900	GLY	2.2
1	A	141	ALA	2.2
1	B	274	CYS	2.2
1	B	1036	SER	2.2
1	B	1065	LYS	2.2
1	A	316	ALA	2.1
1	A	69	LEU	2.1
1	B	315	HIS	2.1
1	A	1122	GLN	2.1
1	A	233	GLN	2.1
1	B	1039	LEU	2.1
1	B	181	ASP	2.1
1	B	250	ALA	2.1
1	A	1109	THR	2.1
1	A	232	HIS	2.0
1	A	1137	ARG	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 [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

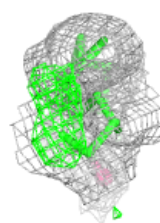
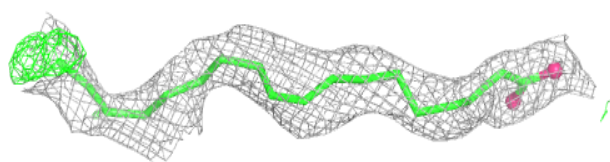
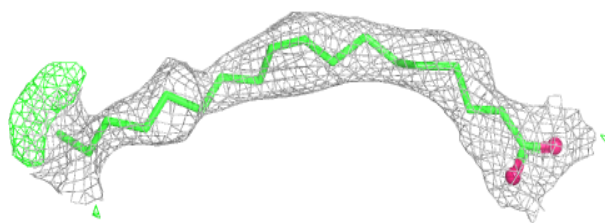
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	OLA	B	1606	20/20	0.79	0.19	30,54,125,154	0
3	OLC	A	1600	18/25	0.80	0.16	43,58,112,115	0
4	OLA	B	1609	13/20	0.83	0.18	22,36,70,105	0
4	OLA	B	1605	20/20	0.84	0.15	32,48,83,150	0
3	OLC	A	1603	22/25	0.85	0.16	23,46,79,134	0
4	OLA	B	1607	20/20	0.87	0.17	34,54,124,155	0
3	OLC	A	1604	16/25	0.88	0.15	26,43,97,150	0
3	OLC	B	1601	15/25	0.88	0.14	17,34,71,103	0
4	OLA	A	1610	10/20	0.89	0.14	23,39,73,117	0
3	OLC	B	1602	22/25	0.90	0.13	29,52,104,134	0
4	OLA	B	1608	12/20	0.90	0.14	27,49,72,76	0
2	ITD	B	1500	27/27	0.90	0.13	15,35,59,114	0
2	ITD	A	1500	27/27	0.93	0.14	15,40,115,153	0

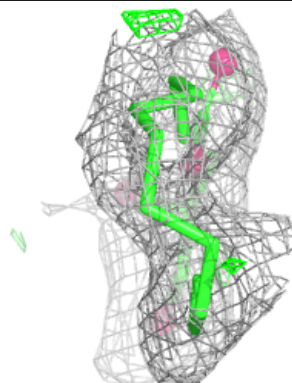
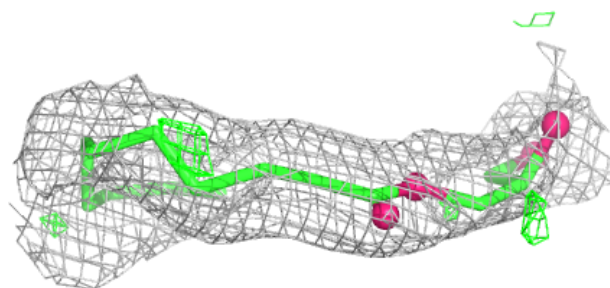
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLA B 1606:

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

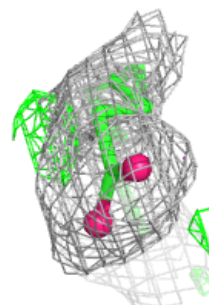
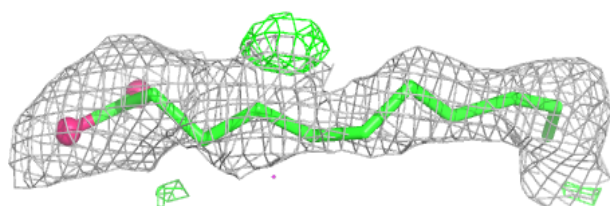
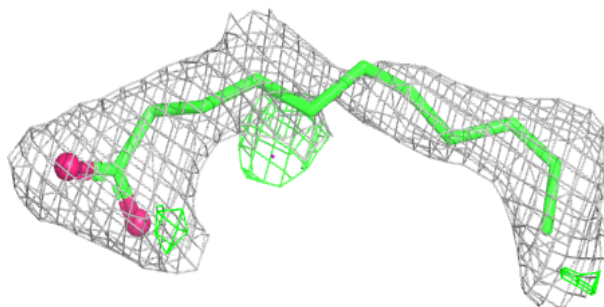
**Electron density around OLC A 1600:**

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

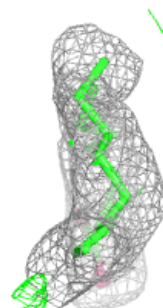
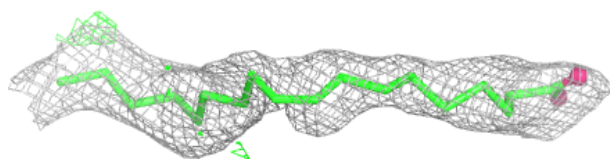
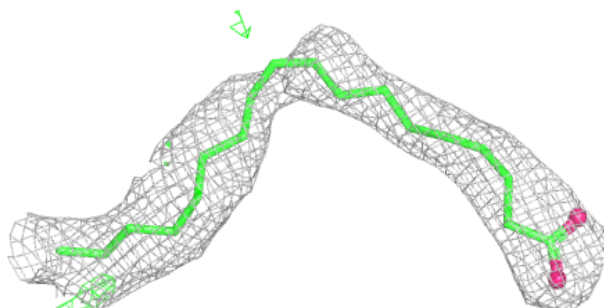


Electron density around OLA B 1609:

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

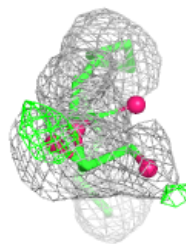
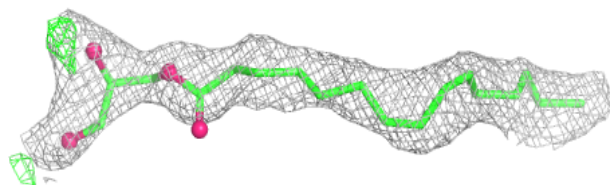
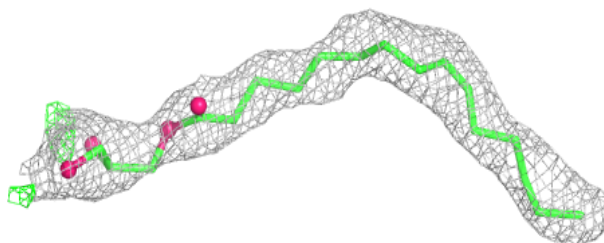
**Electron density around OLA B 1605:**

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

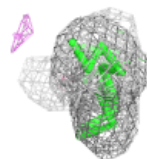
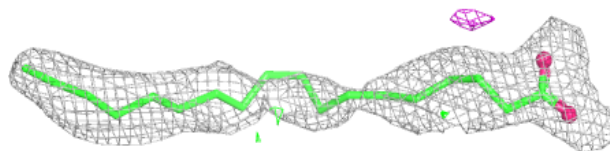
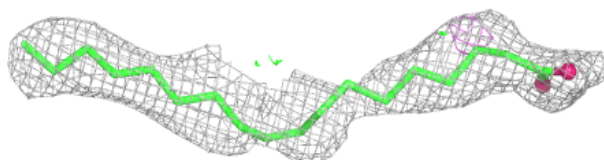


Electron density around OLC A 1603:

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

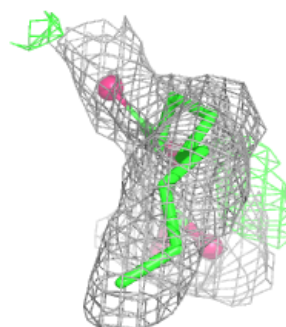
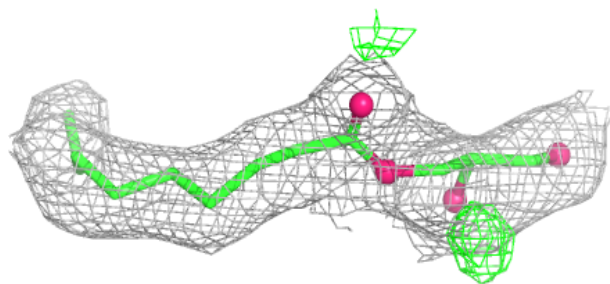
**Electron density around OLA B 1607:**

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

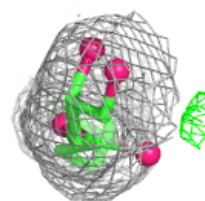
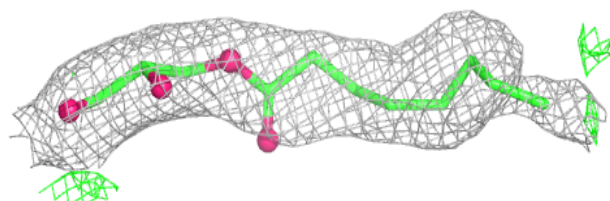
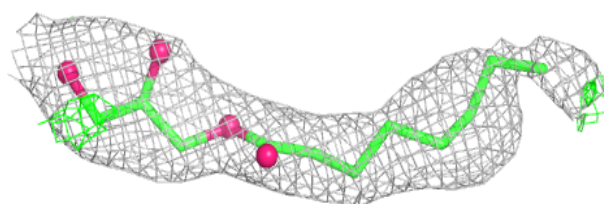


Electron density around OLC A 1604:

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

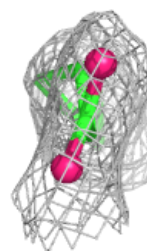
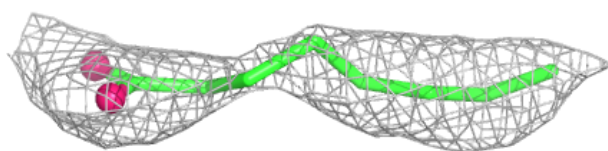
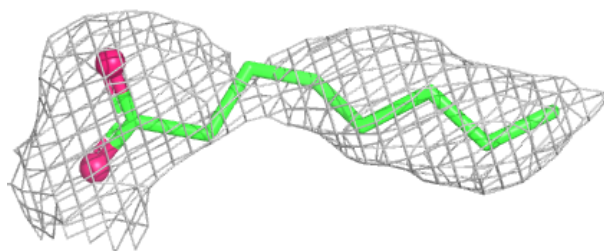
**Electron density around OLC B 1601:**

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

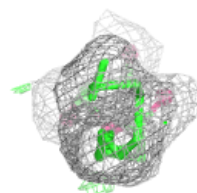
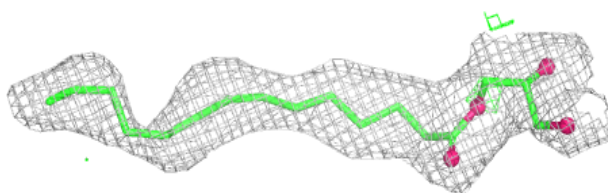
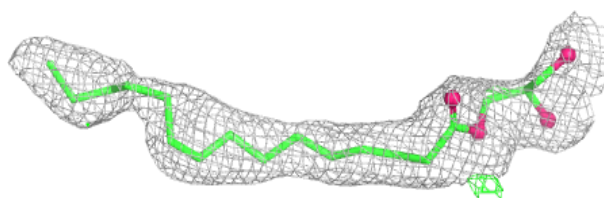


Electron density around OLA A 1610:

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

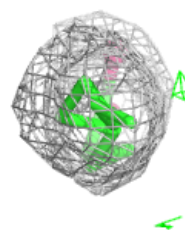
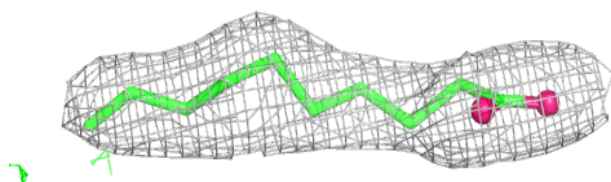
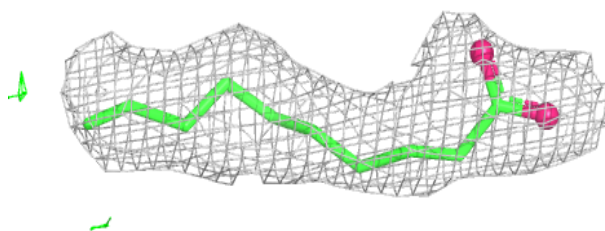
**Electron density around OLC B 1602:**

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

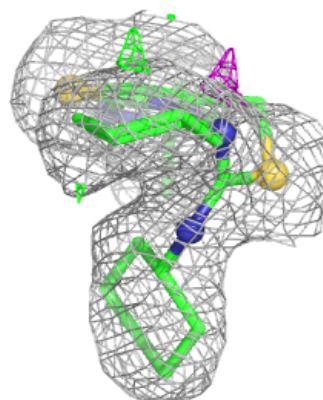
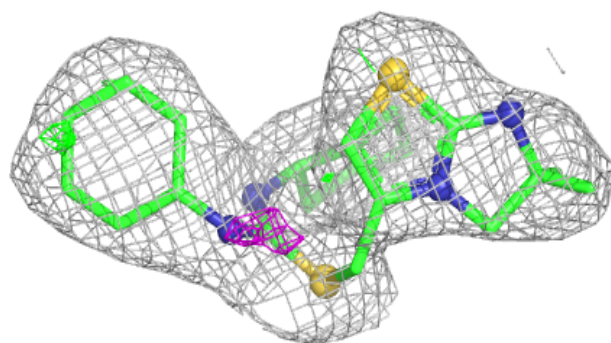
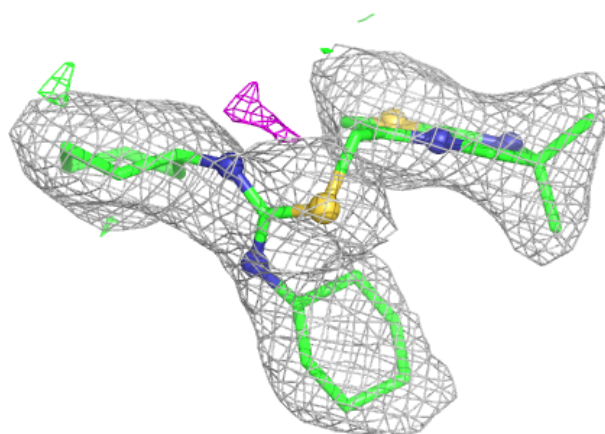


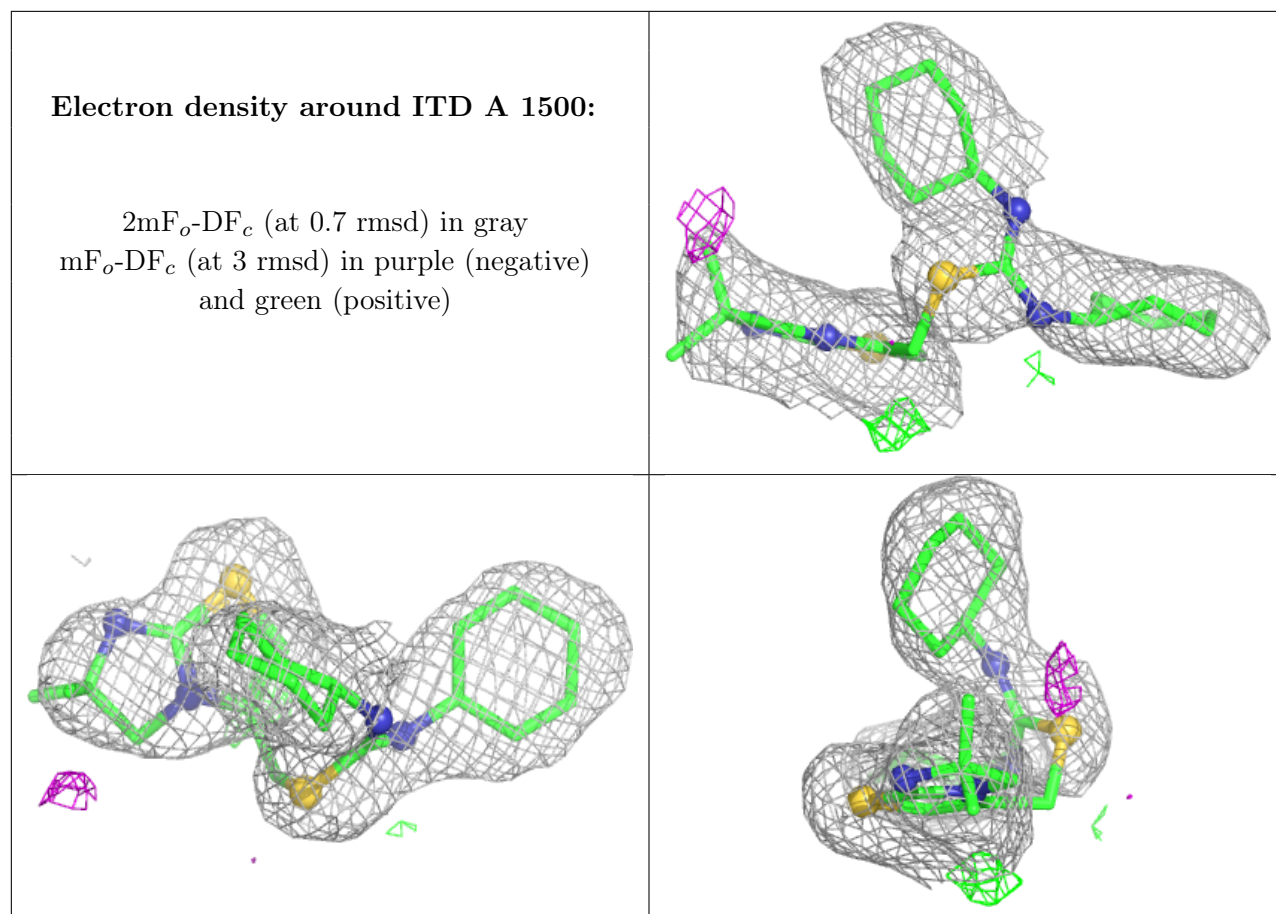
Electron density around OLA B 1608:

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

**Electron density around 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.