



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 02:57 AM UTC

PDB ID : 5OGE / pdb_00005oge
Title : Crystal structure of a nucleotide sugar transporter
Authors : Newstead, S.; Parker, J.L.
Deposited on : 2017-07-12
Resolution : 3.22 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

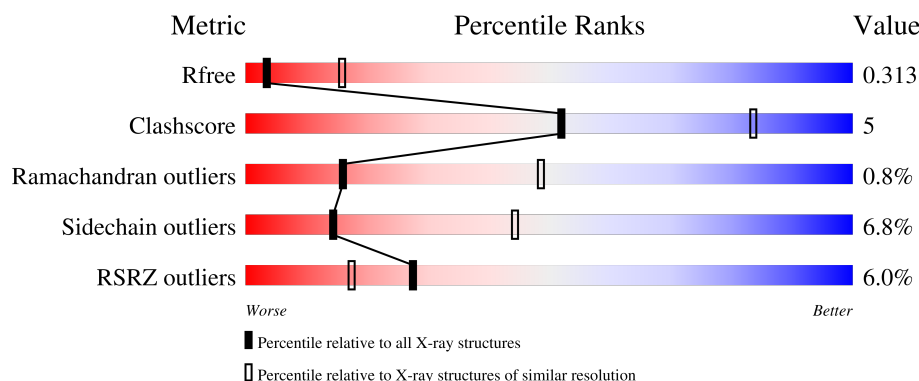
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.22 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	1768 (3.24-3.20)
Clashscore	190562	1879 (3.24-3.20)
Ramachandran outliers	187476	1844 (3.24-3.20)
Sidechain outliers	187428	1843 (3.24-3.20)
RSRZ outliers	180081	1768 (3.24-3.20)

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	337	5% 73% 14% • 11%
1	B	337	5% 71% 17% • 11%
1	C	337	4% 74% 15% • 10%
1	D	337	5% 74% 15% • 10%
1	E	337	6% 73% 17% 10%

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Mol	Chain	Length	Quality of chain
1	F	337	6% 74% 16% 9%
1	G	337	5% 75% 15% 9%
1	H	337	6% 70% 18% 11%

2 Entry composition

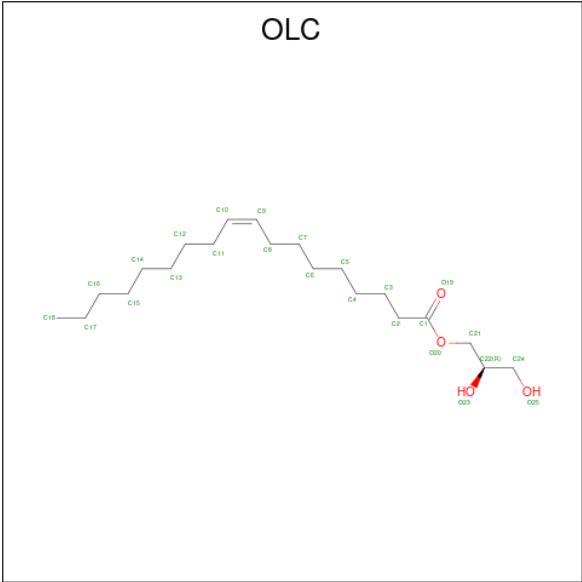
There are 2 unique types of molecules in this entry. The entry contains 19617 atoms, of which 480 are hydrogens and 0 are deuteriums.

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 GDP-mannose transporter 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	299	Total	C	N	O	S	0	0	0
			2334	1545	361	411	17			
1	B	299	Total	C	N	O	S	0	0	0
			2337	1547	362	411	17			
1	C	302	Total	C	N	O	S	0	0	0
			2355	1558	365	415	17			
1	D	303	Total	C	N	O	S	0	0	0
			2360	1561	366	416	17			
1	E	304	Total	C	N	O	S	0	0	0
			2365	1564	367	417	17			
1	F	305	Total	C	N	O	S	0	0	0
			2369	1566	368	418	17			
1	G	306	Total	C	N	O	S	0	0	0
			2386	1578	372	419	17			
1	H	299	Total	C	N	O	S	0	0	0
			2331	1541	362	411	17			

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



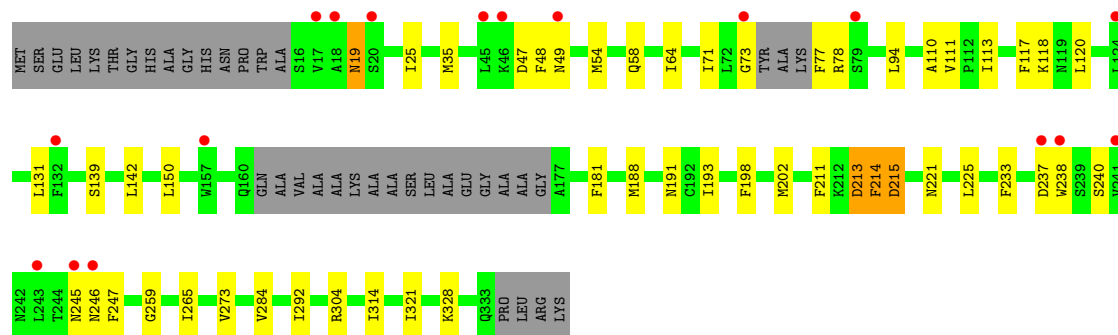
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			65	21	40	4		
2	A	1	Total	C	H	O	0	0
			65	21	40	4		
2	A	1	Total	C	H	O	0	0
			65	21	40	4		
2	A	1	Total	C	H	O	0	0
			65	21	40	4		
2	B	1	Total	C	H	O	0	0
			65	21	40	4		
2	B	1	Total	C	H	O	0	0
			65	21	40	4		
2	D	1	Total	C	H	O	0	0
			65	21	40	4		
2	D	1	Total	C	H	O	0	0
			65	21	40	4		
2	D	1	Total	C	H	O	0	0
			65	21	40	4		
2	D	1	Total	C	H	O	0	0
			65	21	40	4		
2	D	1	Total	C	H	O	0	0
			65	21	40	4		
2	E	1	Total	C	H	O	0	0
			65	21	40	4		

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.

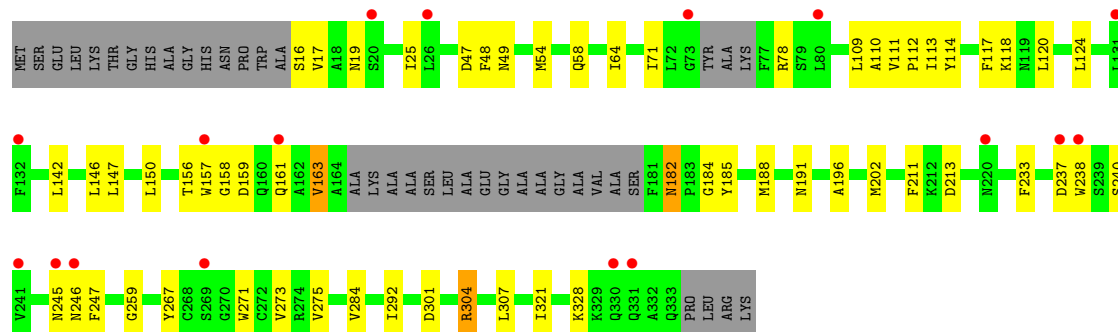
• Molecule 1: GDP-mannose transporter 1

Chain A: 



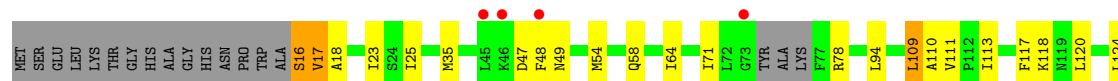
• Molecule 1: GDP-mannose transporter 1

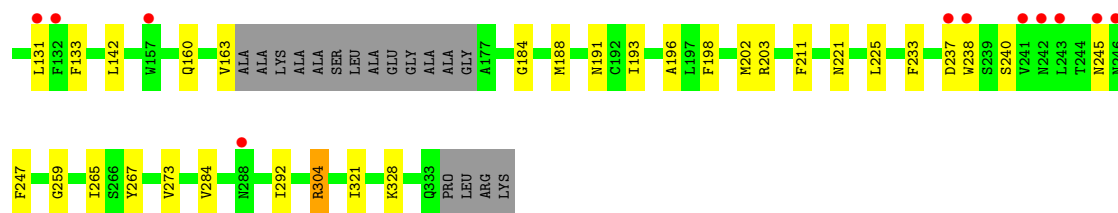
Chain B: 



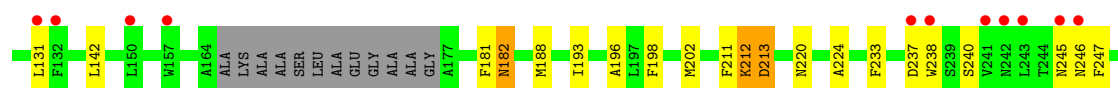
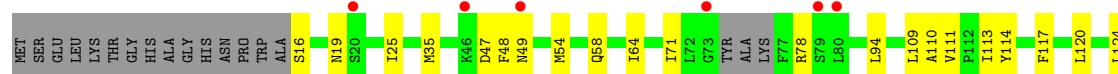
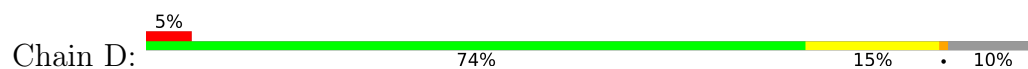
• Molecule 1: GDP-mannose transporter 1

Chain C: 

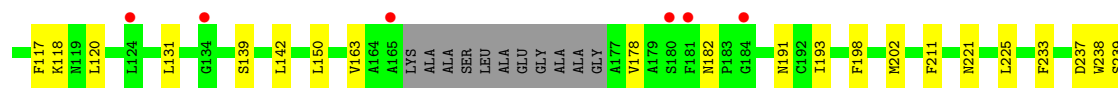
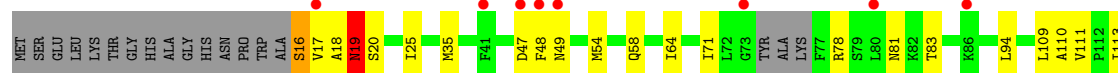




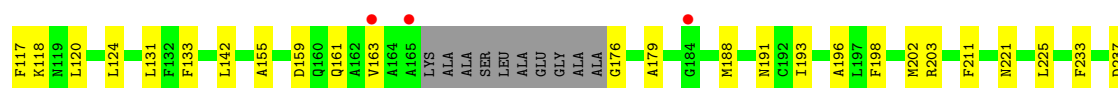
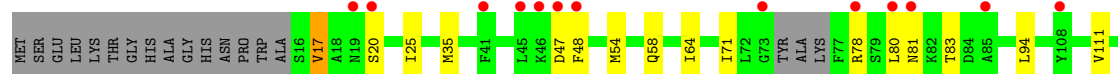
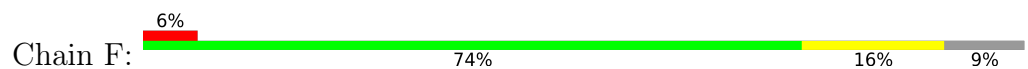
• Molecule 1: GDP-mannose transporter 1



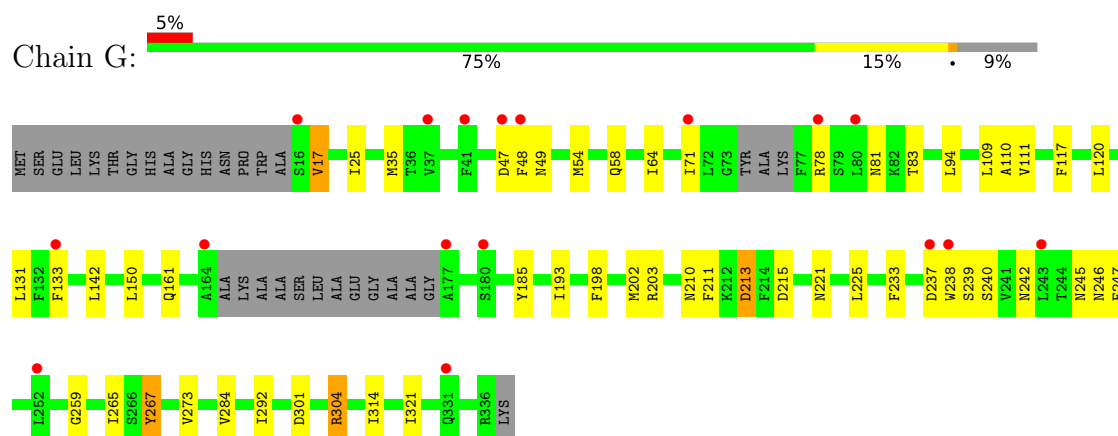
• Molecule 1: GDP-mannose transporter 1



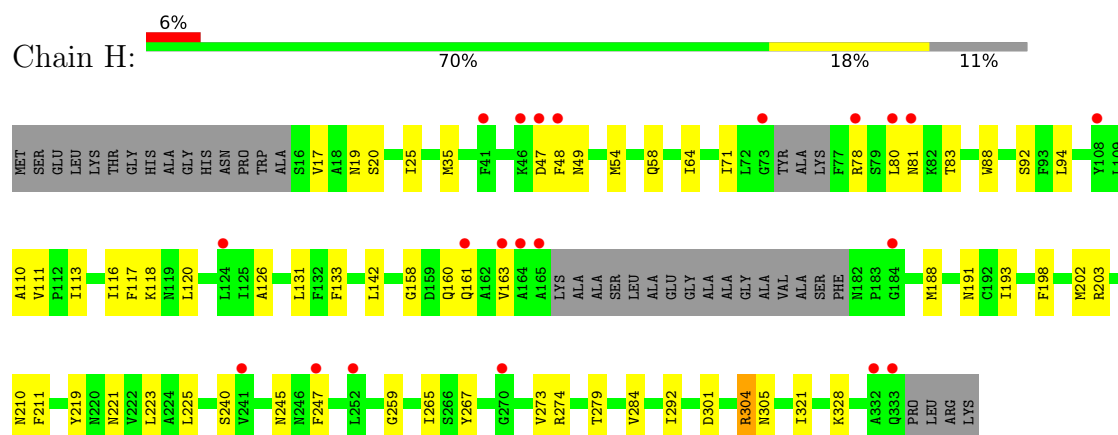
• Molecule 1: GDP-mannose transporter 1



- Molecule 1: GDP-mannose transporter 1



- Molecule 1: GDP-mannose transporter 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	45.57Å 102.91Å 181.41Å 89.92° 90.12° 90.06°	Depositor
Resolution (Å)	45.35 – 3.22 45.35 – 3.22	Depositor EDS
% Data completeness (in resolution range)	90.3 (45.35-3.22) 90.3 (45.35-3.22)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.49 (at 3.25Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.280 , 0.306 0.294 , 0.313	Depositor DCC
R_{free} test set	2328 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	87.2	Xtriage
Anisotropy	0.519	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 61.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.378 for h,-k,-l 0.368 for -h,k,-l 0.357 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	19617	wwPDB-VP
Average B, all atoms (Å ²)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.43% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: OLC

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.78	0/2384	1.44	6/3235 (0.2%)
1	B	0.79	0/2387	1.42	5/3239 (0.2%)
1	C	0.78	0/2405	1.42	5/3264 (0.2%)
1	D	0.79	0/2410	1.43	10/3271 (0.3%)
1	E	0.79	0/2415	1.41	7/3278 (0.2%)
1	F	0.80	0/2419	1.43	6/3283 (0.2%)
1	G	0.79	0/2437	1.43	5/3308 (0.2%)
1	H	0.79	0/2380	1.42	6/3230 (0.2%)
All	All	0.79	0/19237	1.42	50/26108 (0.2%)

There are no bond length outliers.

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	18	ALA	N-CA-C	-7.45	102.59	112.72
1	A	215	ASP	CA-CB-CG	6.92	119.52	112.60
1	E	19	ASN	N-CA-C	-6.74	102.35	110.44
1	D	212	LYS	CA-C-N	6.24	133.45	121.54
1	D	212	LYS	C-N-CA	6.24	133.45	121.54
1	D	182	ASN	CA-CB-CG	5.85	118.45	112.60
1	G	111	VAL	N-CA-CB	5.64	114.30	110.52
1	D	111	VAL	N-CA-CB	5.59	114.27	110.52
1	H	111	VAL	N-CA-CB	5.54	114.23	110.52
1	A	47	ASP	CA-C-N	5.51	128.54	120.71
1	A	47	ASP	C-N-CA	5.51	128.54	120.71
1	B	111	VAL	N-CA-CB	5.43	114.16	110.52
1	D	47	ASP	CA-C-N	5.37	128.34	120.71
1	D	47	ASP	C-N-CA	5.37	128.34	120.71
1	F	111	VAL	N-CA-CB	5.35	114.10	110.52
1	H	20	SER	N-CA-C	5.33	116.62	108.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	47	ASP	CA-C-N	5.29	128.23	120.71
1	B	47	ASP	C-N-CA	5.29	128.23	120.71
1	C	47	ASP	CA-C-N	5.26	128.18	120.71
1	C	47	ASP	C-N-CA	5.26	128.18	120.71
1	D	267	TYR	CA-C-N	5.25	127.74	120.29
1	D	267	TYR	C-N-CA	5.25	127.74	120.29
1	E	111	VAL	N-CA-CB	5.24	114.03	110.52
1	F	47	ASP	CA-C-N	5.23	128.13	120.71
1	F	47	ASP	C-N-CA	5.23	128.13	120.71
1	A	111	VAL	N-CA-CB	5.22	114.02	110.52
1	H	267	TYR	CA-C-N	5.21	127.68	120.29
1	H	267	TYR	C-N-CA	5.21	127.68	120.29
1	G	47	ASP	CA-C-N	5.20	128.10	120.71
1	G	47	ASP	C-N-CA	5.20	128.10	120.71
1	H	47	ASP	CA-C-N	5.20	128.09	120.71
1	H	47	ASP	C-N-CA	5.20	128.09	120.71
1	A	213	ASP	CA-C-N	5.17	131.42	121.54
1	A	213	ASP	C-N-CA	5.17	131.42	121.54
1	C	111	VAL	N-CA-CB	5.17	113.99	110.52
1	D	181	PHE	CA-C-N	5.17	127.40	120.58
1	D	181	PHE	C-N-CA	5.17	127.40	120.58
1	E	47	ASP	CA-C-N	5.17	128.05	120.71
1	E	47	ASP	C-N-CA	5.17	128.05	120.71
1	E	267	TYR	CA-C-N	5.14	127.58	120.29
1	E	267	TYR	C-N-CA	5.14	127.58	120.29
1	G	267	TYR	CA-C-N	5.13	127.58	120.29
1	G	267	TYR	C-N-CA	5.13	127.58	120.29
1	F	20	SER	N-CA-C	5.13	116.31	108.42
1	C	267	TYR	CA-C-N	5.08	127.50	120.29
1	C	267	TYR	C-N-CA	5.08	127.50	120.29
1	B	267	TYR	CA-C-N	5.06	127.47	120.29
1	B	267	TYR	C-N-CA	5.06	127.47	120.29
1	F	267	TYR	CA-C-N	5.05	127.46	120.29
1	F	267	TYR	C-N-CA	5.05	127.46	120.29

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2334	0	2410	22	0
1	B	2337	0	2413	39	0
1	C	2355	0	2432	20	0
1	D	2360	0	2437	22	0
1	E	2365	0	2442	23	0
1	F	2369	0	2445	24	0
1	G	2386	0	2468	28	0
1	H	2331	0	2409	28	0
2	A	100	160	160	0	0
2	B	50	80	80	0	0
2	D	125	200	200	0	0
2	E	25	40	40	0	0
All	All	19137	480	19936	200	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 5.

All (200) 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:E:150:LEU:HD22	1:E:314:ILE:HG21	1.41	1.02
1:G:150:LEU:HD22	1:G:314:ILE:HG21	1.44	1.00
1:D:49:ASN:ND2	1:D:246:ASN:HD21	1.61	0.99
1:A:150:LEU:HD22	1:A:314:ILE:HG21	1.48	0.96
1:B:112:PRO:HB2	1:B:156:THR:OG1	1.72	0.89
1:G:110:ALA:CB	1:G:161:GLN:HG2	2.05	0.85
1:G:110:ALA:HB1	1:G:161:GLN:HG2	1.61	0.82
1:E:150:LEU:CD2	1:E:314:ILE:HG21	2.10	0.82
1:D:114:TYR:HD1	1:D:188:MET:HE1	1.43	0.81
1:B:124:LEU:HD11	1:B:196:ALA:HB2	1.61	0.81
1:B:157:TRP:CD1	1:B:307:LEU:HD22	2.16	0.81
1:G:150:LEU:CD2	1:G:314:ILE:HG21	2.12	0.79
1:A:150:LEU:CD2	1:A:314:ILE:HG21	2.12	0.78
1:D:49:ASN:ND2	1:D:246:ASN:ND2	2.31	0.77
1:B:157:TRP:HD1	1:B:307:LEU:HD22	1.49	0.77
1:E:150:LEU:CD2	1:E:314:ILE:HD13	2.14	0.77
1:D:49:ASN:HD21	1:D:246:ASN:HD21	1.30	0.76
1:G:150:LEU:CD2	1:G:314:ILE:HD13	2.15	0.76
1:B:114:TYR:HD1	1:B:188:MET:HE1	1.49	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:LEU:CD2	1:A:314:ILE:HD13	2.16	0.75
1:B:124:LEU:CD1	1:B:196:ALA:HB2	2.17	0.75
1:E:202:MET:HE3	1:E:273:VAL:HG21	1.69	0.74
1:B:146:LEU:O	1:B:150:LEU:HG	1.87	0.74
1:H:19:ASN:ND2	1:H:274:ARG:NH2	2.36	0.73
1:D:114:TYR:CD1	1:D:188:MET:HE1	2.24	0.72
1:H:202:MET:HE3	1:H:273:VAL:HG21	1.72	0.71
1:D:109:LEU:HD12	1:D:188:MET:HE2	1.72	0.70
1:F:17:VAL:HG12	1:F:17:VAL:O	1.91	0.69
1:B:114:TYR:CD1	1:B:188:MET:HE1	2.28	0.68
1:G:110:ALA:HB2	1:G:161:GLN:HG2	1.76	0.67
1:E:150:LEU:HD22	1:E:314:ILE:CG2	2.22	0.67
1:G:17:VAL:HG12	1:G:17:VAL:O	1.95	0.66
1:B:49:ASN:HD21	1:B:246:ASN:HD21	1.43	0.65
1:F:124:LEU:HD11	1:F:196:ALA:HB2	1.79	0.64
1:A:202:MET:HE3	1:A:273:VAL:HG21	1.79	0.64
1:D:124:LEU:HD11	1:D:196:ALA:HB2	1.78	0.63
1:C:124:LEU:HD11	1:C:196:ALA:HB2	1.79	0.63
1:G:150:LEU:HD22	1:G:314:ILE:CG2	2.25	0.63
1:E:150:LEU:HD21	1:E:314:ILE:HD13	1.79	0.63
1:H:161:GLN:HG3	1:H:163:VAL:HG13	1.81	0.63
1:D:202:MET:HE3	1:D:273:VAL:HG21	1.80	0.62
1:G:150:LEU:HD21	1:G:314:ILE:HD13	1.80	0.62
1:G:202:MET:HE3	1:G:273:VAL:HG21	1.81	0.61
1:H:17:VAL:HG23	1:H:17:VAL:O	2.00	0.61
1:A:150:LEU:HD22	1:A:314:ILE:CG2	2.27	0.61
1:H:160:GLN:O	1:H:160:GLN:HG2	2.00	0.60
1:F:202:MET:HE3	1:F:273:VAL:HG21	1.82	0.60
1:A:150:LEU:HD21	1:A:314:ILE:HD13	1.82	0.60
1:B:202:MET:HE3	1:B:273:VAL:HG21	1.84	0.60
1:C:202:MET:HE3	1:C:273:VAL:HG21	1.84	0.60
1:B:158:GLY:O	1:B:159:ASP:OD1	2.20	0.59
1:C:118:LYS:HE2	1:C:191:ASN:HD21	1.67	0.59
1:A:19:ASN:ND2	1:A:213:ASP:OD2	2.37	0.57
1:B:147:LEU:HA	1:B:150:LEU:HD12	1.86	0.57
1:C:124:LEU:CD1	1:C:196:ALA:HB2	2.36	0.56
1:F:124:LEU:CD1	1:F:196:ALA:HB2	2.36	0.56
1:D:124:LEU:CD1	1:D:196:ALA:HB2	2.36	0.56
1:H:126:ALA:HA	1:H:279:THR:HG21	1.86	0.56
1:B:124:LEU:CD1	1:B:196:ALA:CB	2.82	0.56
1:B:304:ARG:HH22	1:G:304:ARG:HH12	1.54	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:49:ASN:HD22	1:D:246:ASN:ND2	2.02	0.55
1:B:17:VAL:O	1:B:17:VAL:HG13	2.07	0.55
1:A:233:PHE:HA	1:A:238:TRP:HE1	1.72	0.55
1:B:49:ASN:ND2	1:B:246:ASN:HD21	2.05	0.55
1:F:163:VAL:HG22	1:F:163:VAL:O	2.07	0.54
1:F:233:PHE:HA	1:F:238:TRP:HE1	1.72	0.54
1:B:233:PHE:HA	1:B:238:TRP:HE1	1.73	0.54
1:B:118:LYS:HE2	1:B:191:ASN:HD21	1.74	0.53
1:C:233:PHE:HA	1:C:238:TRP:HE1	1.73	0.53
1:E:233:PHE:HA	1:E:238:TRP:HE1	1.73	0.53
1:D:233:PHE:HA	1:D:238:TRP:HE1	1.74	0.53
1:B:304:ARG:HH12	1:G:304:ARG:HH22	1.57	0.53
1:C:304:ARG:HH22	1:H:304:ARG:HH12	1.57	0.53
1:G:233:PHE:HA	1:G:238:TRP:HE1	1.73	0.53
1:B:19:ASN:O	1:B:275:VAL:HG11	2.09	0.52
1:H:221:ASN:O	1:H:225:LEU:HG	2.10	0.52
1:D:49:ASN:HD22	1:D:246:ASN:HD21	1.52	0.51
1:E:118:LYS:HE2	1:E:191:ASN:HD21	1.75	0.51
1:A:118:LYS:HE2	1:A:191:ASN:HD21	1.76	0.50
1:C:304:ARG:HH12	1:H:304:ARG:HH22	1.60	0.50
1:F:117:PHE:HB2	1:F:188:MET:HE2	1.94	0.50
1:A:49:ASN:ND2	1:A:246:ASN:OD1	2.45	0.49
1:B:109:LEU:HG	1:B:184:GLY:HA3	1.94	0.49
1:B:112:PRO:HB2	1:B:156:THR:CB	2.41	0.49
1:C:18:ALA:HB1	1:C:23:ILE:HD13	1.95	0.49
1:F:17:VAL:O	1:F:17:VAL:CG1	2.58	0.49
1:F:163:VAL:O	1:F:163:VAL:HG13	2.13	0.48
1:H:58:GLN:HG2	1:H:259:GLY:HA2	1.96	0.48
1:H:88:TRP:CD1	1:H:219:TYR:HB3	2.48	0.48
1:B:49:ASN:ND2	1:B:246:ASN:ND2	2.61	0.48
1:F:161:GLN:O	1:F:161:GLN:HG2	2.14	0.48
1:G:58:GLN:HG2	1:G:259:GLY:HA2	1.96	0.48
1:E:58:GLN:HG2	1:E:259:GLY:HA2	1.95	0.48
1:B:17:VAL:O	1:B:17:VAL:HG22	2.14	0.47
1:B:19:ASN:OD1	1:B:213:ASP:OD2	2.32	0.47
1:F:58:GLN:HG2	1:F:259:GLY:HA2	1.96	0.47
1:G:17:VAL:O	1:G:17:VAL:CG1	2.61	0.47
1:B:58:GLN:HG2	1:B:259:GLY:HA2	1.97	0.47
1:C:58:GLN:HG2	1:C:259:GLY:HA2	1.97	0.47
1:D:117:PHE:HA	1:D:120:LEU:HD12	1.97	0.47
1:E:35:MET:CE	1:E:265:ILE:HD13	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:58:GLN:HG2	1:D:259:GLY:HA2	1.97	0.47
1:G:239:SER:HB2	1:G:242:ASN:HD22	1.79	0.47
1:D:19:ASN:HA	1:D:271:TRP:HZ2	1.79	0.47
1:F:155:ALA:O	1:F:159:ASP:HB2	2.15	0.47
1:D:109:LEU:CD1	1:D:188:MET:HE2	2.44	0.47
1:E:25:ILE:HG12	1:E:284:VAL:HG21	1.97	0.47
1:F:118:LYS:HE2	1:F:191:ASN:HD21	1.79	0.46
1:G:25:ILE:HG12	1:G:284:VAL:HG21	1.97	0.46
1:G:94:LEU:HB3	1:G:198:PHE:HB2	1.97	0.46
1:A:117:PHE:HA	1:A:120:LEU:HD12	1.97	0.46
1:H:126:ALA:HA	1:H:279:THR:CG2	2.45	0.46
1:B:112:PRO:HG2	1:B:156:THR:HG23	1.98	0.46
1:B:158:GLY:C	1:B:159:ASP:OD1	2.58	0.46
1:F:239:SER:HB2	1:F:242:ASN:HD22	1.79	0.46
1:A:58:GLN:HG2	1:A:259:GLY:HA2	1.98	0.46
1:E:239:SER:HB2	1:E:242:ASN:HD22	1.79	0.46
1:F:117:PHE:HA	1:F:120:LEU:HD12	1.98	0.46
1:C:117:PHE:HA	1:C:120:LEU:HD12	1.98	0.46
1:H:25:ILE:HG12	1:H:284:VAL:HG21	1.98	0.46
1:H:117:PHE:HA	1:H:120:LEU:HD12	1.98	0.46
1:B:117:PHE:HA	1:B:120:LEU:HD12	1.98	0.46
1:E:117:PHE:HA	1:E:120:LEU:HD12	1.98	0.46
1:G:117:PHE:HA	1:G:120:LEU:HD12	1.98	0.46
1:F:133:PHE:CZ	1:F:203:ARG:HG3	2.51	0.45
1:H:94:LEU:HB3	1:H:198:PHE:HB2	1.98	0.45
1:G:213:ASP:HB2	1:G:267:TYR:CE1	2.51	0.45
1:F:35:MET:CE	1:F:265:ILE:HD13	2.47	0.45
1:C:35:MET:CE	1:C:265:ILE:HD13	2.46	0.45
1:C:133:PHE:CZ	1:C:203:ARG:HG3	2.52	0.45
1:E:35:MET:HE1	1:E:265:ILE:HD13	1.99	0.45
1:H:35:MET:CE	1:H:265:ILE:HD13	2.45	0.45
1:B:19:ASN:OD1	1:B:271:TRP:NE1	2.49	0.45
1:F:25:ILE:HG12	1:F:284:VAL:HG21	1.98	0.45
1:A:117:PHE:HB2	1:A:188:MET:HE2	1.99	0.45
1:E:17:VAL:C	1:E:19:ASN:H	2.25	0.45
1:B:109:LEU:HD12	1:B:188:MET:HE2	1.99	0.44
1:E:94:LEU:HB3	1:E:198:PHE:HB2	1.99	0.44
1:A:213:ASP:O	1:A:214:PHE:HB2	2.18	0.44
1:C:117:PHE:HB2	1:C:188:MET:HE2	2.00	0.44
1:D:35:MET:CE	1:D:265:ILE:HD13	2.47	0.44
1:F:94:LEU:HB3	1:F:198:PHE:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:109:LEU:HD21	1:G:185:TYR:CD1	2.52	0.44
1:G:110:ALA:HB1	1:G:161:GLN:CG	2.42	0.44
1:H:158:GLY:O	1:H:305:ASN:ND2	2.50	0.44
1:H:19:ASN:ND2	1:H:274:ARG:HH21	2.14	0.44
1:A:35:MET:SD	1:A:265:ILE:HG21	2.58	0.44
1:B:182:ASN:HA	1:B:185:TYR:HD2	1.83	0.44
1:A:73:GLY:HA3	1:A:77:PHE:HE1	1.82	0.43
1:D:25:ILE:HG12	1:D:284:VAL:HG21	2.00	0.43
1:G:35:MET:SD	1:G:265:ILE:HG21	2.58	0.43
1:B:25:ILE:HG12	1:B:284:VAL:HG21	2.00	0.43
1:B:157:TRP:O	1:B:157:TRP:CD2	2.71	0.43
1:C:109:LEU:HD13	1:C:184:GLY:HA3	1.99	0.43
1:H:160:GLN:N	1:H:160:GLN:OE1	2.51	0.43
1:A:49:ASN:HB2	1:A:247:PHE:HZ	1.84	0.43
1:G:133:PHE:CZ	1:G:203:ARG:HG3	2.53	0.43
1:C:16:SER:HB2	1:C:17:VAL:H	1.60	0.43
1:H:133:PHE:CZ	1:H:203:ARG:HG3	2.54	0.43
1:C:25:ILE:HG12	1:C:284:VAL:HG21	2.01	0.43
1:G:81:ASN:HD22	1:G:83:THR:H	1.67	0.43
1:A:94:LEU:HB3	1:A:198:PHE:HB2	2.01	0.42
1:A:110:ALA:HB3	1:A:113:ILE:HD12	2.01	0.42
1:C:94:LEU:HB3	1:C:198:PHE:HB2	2.01	0.42
1:D:94:LEU:HB3	1:D:198:PHE:HB2	2.01	0.42
1:A:25:ILE:HG12	1:A:284:VAL:HG21	2.01	0.42
1:C:49:ASN:HB2	1:C:247:PHE:HZ	1.84	0.42
1:D:110:ALA:HB3	1:D:113:ILE:HD12	2.01	0.42
1:D:49:ASN:HB2	1:D:247:PHE:HZ	1.85	0.42
1:F:221:ASN:O	1:F:225:LEU:HG	2.19	0.42
1:H:81:ASN:HD22	1:H:83:THR:H	1.68	0.42
1:B:110:ALA:HB3	1:B:113:ILE:HD12	2.01	0.42
1:E:16:SER:HB3	1:E:19:ASN:ND2	2.34	0.42
1:E:163:VAL:O	1:E:163:VAL:HG12	2.19	0.42
1:A:139:SER:HB2	1:E:139:SER:HB2	2.01	0.41
1:E:81:ASN:HD22	1:E:83:THR:H	1.68	0.41
1:B:49:ASN:HB2	1:B:247:PHE:HZ	1.85	0.41
1:H:113:ILE:HA	1:H:116:ILE:HD12	2.01	0.41
1:A:221:ASN:O	1:A:225:LEU:HG	2.21	0.41
1:B:163:VAL:O	1:B:163:VAL:HG13	2.20	0.41
1:B:163:VAL:O	1:B:163:VAL:HG22	2.20	0.41
1:D:220:ASN:O	1:D:224:ALA:HB2	2.21	0.41
1:F:35:MET:HE1	1:F:265:ILE:HD13	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:221:ASN:O	1:G:225:LEU:HG	2.21	0.41
1:H:49:ASN:HB2	1:H:247:PHE:HZ	1.86	0.41
1:H:35:MET:HE1	1:H:265:ILE:HD13	2.02	0.41
1:H:118:LYS:HE2	1:H:191:ASN:HD21	1.86	0.41
1:H:117:PHE:HB2	1:H:188:MET:HE2	2.03	0.41
1:E:221:ASN:O	1:E:225:LEU:HG	2.20	0.41
1:G:49:ASN:HB2	1:G:247:PHE:HZ	1.86	0.41
1:H:110:ALA:HB3	1:H:113:ILE:HD12	2.02	0.41
1:E:49:ASN:HB2	1:E:247:PHE:HZ	1.86	0.41
1:F:161:GLN:OE1	1:F:161:GLN:N	2.50	0.41
1:C:221:ASN:O	1:C:225:LEU:HG	2.21	0.40
1:E:110:ALA:HB3	1:E:113:ILE:HD12	2.02	0.40
1:F:81:ASN:HD22	1:F:83:THR:H	1.69	0.40
1:F:176:GLY:HA3	1:F:179:ALA:HB3	2.03	0.40
1:H:219:TYR:O	1:H:223:LEU:HB2	2.21	0.40
1:C:110:ALA:HB3	1:C:113:ILE:HD12	2.03	0.40
1:B:304:ARG:HH22	1:G:304:ARG:HH22	1.68	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	293/337 (87%)	275 (94%)	15 (5%)	3 (1%)	12	44
1	B	293/337 (87%)	273 (93%)	18 (6%)	2 (1%)	18	52
1	C	296/337 (88%)	278 (94%)	16 (5%)	2 (1%)	18	52
1	D	297/337 (88%)	274 (92%)	20 (7%)	3 (1%)	12	44
1	E	298/337 (88%)	278 (93%)	18 (6%)	2 (1%)	18	52
1	F	299/337 (89%)	280 (94%)	17 (6%)	2 (1%)	18	52
1	G	300/337 (89%)	279 (93%)	18 (6%)	3 (1%)	12	44

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	H	293/337 (87%)	272 (93%)	19 (6%)	2 (1%)	18	52
All	All	2369/2696 (88%)	2209 (93%)	141 (6%)	19 (1%)	16	48

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	240	SER
1	B	240	SER
1	C	240	SER
1	D	213	ASP
1	D	240	SER
1	E	240	SER
1	F	240	SER
1	G	240	SER
1	H	240	SER
1	A	214	PHE
1	E	182	ASN
1	G	210	ASN
1	A	181	PHE
1	B	161	GLN
1	C	17	VAL
1	F	17	VAL
1	D	212	LYS
1	H	210	ASN
1	G	17	VAL

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	266/289 (92%)	249 (94%)	17 (6%)	16	46
1	B	266/289 (92%)	249 (94%)	17 (6%)	16	46
1	C	268/289 (93%)	249 (93%)	19 (7%)	13	43
1	D	268/289 (93%)	249 (93%)	19 (7%)	13	43

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	268/289 (93%)	247 (92%)	21 (8%)	11	39
1	F	268/289 (93%)	251 (94%)	17 (6%)	16	46
1	G	271/289 (94%)	253 (93%)	18 (7%)	15	45
1	H	265/289 (92%)	248 (94%)	17 (6%)	16	46
All	All	2140/2312 (93%)	1995 (93%)	145 (7%)	14	44

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ASN
1	A	48	PHE
1	A	54	MET
1	A	64	ILE
1	A	71	ILE
1	A	78	ARG
1	A	131	LEU
1	A	142	LEU
1	A	193	ILE
1	A	211	PHE
1	A	215	ASP
1	A	237	ASP
1	A	245	ASN
1	A	292	ILE
1	A	304	ARG
1	A	321	ILE
1	A	328	LYS
1	B	16	SER
1	B	48	PHE
1	B	54	MET
1	B	64	ILE
1	B	71	ILE
1	B	78	ARG
1	B	142	LEU
1	B	163	VAL
1	B	182	ASN
1	B	211	PHE
1	B	237	ASP
1	B	245	ASN
1	B	292	ILE
1	B	301	ASP
1	B	304	ARG

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Mol	Chain	Res	Type
1	B	321	ILE
1	B	328	LYS
1	C	16	SER
1	C	48	PHE
1	C	54	MET
1	C	64	ILE
1	C	71	ILE
1	C	78	ARG
1	C	109	LEU
1	C	131	LEU
1	C	142	LEU
1	C	160	GLN
1	C	163	VAL
1	C	193	ILE
1	C	211	PHE
1	C	237	ASP
1	C	245	ASN
1	C	292	ILE
1	C	304	ARG
1	C	321	ILE
1	C	328	LYS
1	D	16	SER
1	D	48	PHE
1	D	54	MET
1	D	64	ILE
1	D	71	ILE
1	D	78	ARG
1	D	131	LEU
1	D	142	LEU
1	D	182	ASN
1	D	193	ILE
1	D	211	PHE
1	D	213	ASP
1	D	237	ASP
1	D	245	ASN
1	D	292	ILE
1	D	301	ASP
1	D	304	ARG
1	D	321	ILE
1	D	328	LYS
1	E	16	SER
1	E	19	ASN

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Mol	Chain	Res	Type
1	E	20	SER
1	E	48	PHE
1	E	54	MET
1	E	64	ILE
1	E	71	ILE
1	E	78	ARG
1	E	109	LEU
1	E	131	LEU
1	E	142	LEU
1	E	178	VAL
1	E	193	ILE
1	E	211	PHE
1	E	237	ASP
1	E	245	ASN
1	E	292	ILE
1	E	301	ASP
1	E	304	ARG
1	E	321	ILE
1	E	328	LYS
1	F	48	PHE
1	F	54	MET
1	F	64	ILE
1	F	71	ILE
1	F	78	ARG
1	F	80	LEU
1	F	131	LEU
1	F	142	LEU
1	F	193	ILE
1	F	211	PHE
1	F	237	ASP
1	F	245	ASN
1	F	292	ILE
1	F	301	ASP
1	F	304	ARG
1	F	321	ILE
1	F	328	LYS
1	G	48	PHE
1	G	54	MET
1	G	64	ILE
1	G	71	ILE
1	G	78	ARG
1	G	131	LEU

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Mol	Chain	Res	Type
1	G	142	LEU
1	G	193	ILE
1	G	211	PHE
1	G	213	ASP
1	G	215	ASP
1	G	237	ASP
1	G	245	ASN
1	G	246	ASN
1	G	292	ILE
1	G	301	ASP
1	G	304	ARG
1	G	321	ILE
1	H	48	PHE
1	H	54	MET
1	H	64	ILE
1	H	71	ILE
1	H	78	ARG
1	H	80	LEU
1	H	92	SER
1	H	131	LEU
1	H	142	LEU
1	H	193	ILE
1	H	211	PHE
1	H	245	ASN
1	H	292	ILE
1	H	301	ASP
1	H	304	ARG
1	H	321	ILE
1	H	328	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	49	ASN
1	A	51	ASN
1	A	107	GLN
1	A	119	ASN
1	A	191	ASN
1	A	246	ASN
1	A	331	GLN
1	B	49	ASN
1	B	51	ASN

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Mol	Chain	Res	Type
1	B	58	GLN
1	B	81	ASN
1	B	107	GLN
1	B	119	ASN
1	B	191	ASN
1	B	246	ASN
1	C	51	ASN
1	C	58	GLN
1	C	107	GLN
1	C	119	ASN
1	C	191	ASN
1	C	210	ASN
1	D	49	ASN
1	D	51	ASN
1	D	58	GLN
1	D	107	GLN
1	D	119	ASN
1	D	191	ASN
1	D	331	GLN
1	E	49	ASN
1	E	51	ASN
1	E	58	GLN
1	E	81	ASN
1	E	107	GLN
1	E	119	ASN
1	E	191	ASN
1	E	242	ASN
1	E	331	GLN
1	F	49	ASN
1	F	51	ASN
1	F	58	GLN
1	F	81	ASN
1	F	107	GLN
1	F	119	ASN
1	F	182	ASN
1	F	191	ASN
1	F	242	ASN
1	F	331	GLN
1	G	51	ASN
1	G	58	GLN
1	G	81	ASN
1	G	107	GLN

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Mol	Chain	Res	Type
1	G	119	ASN
1	G	182	ASN
1	G	242	ASN
1	H	51	ASN
1	H	58	GLN
1	H	81	ASN
1	H	107	GLN
1	H	119	ASN
1	H	161	GLN
1	H	191	ASN
1	H	331	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	OLC	A	401	-	24,24,24	0.77	0	25,25,25	0.70	0
2	OLC	E	401	-	24,24,24	0.77	0	25,25,25	0.72	0
2	OLC	A	404	-	24,24,24	0.72	0	25,25,25	0.78	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	OLC	D	405	-	24,24,24	0.84	0	25,25,25	0.59	0
2	OLC	B	401	-	24,24,24	0.70	0	25,25,25	0.72	0
2	OLC	A	402	-	24,24,24	0.78	0	25,25,25	0.72	0
2	OLC	B	402	-	24,24,24	0.82	0	25,25,25	0.66	0
2	OLC	A	403	-	24,24,24	0.87	2 (8%)	25,25,25	0.65	0
2	OLC	D	404	-	24,24,24	0.74	0	25,25,25	0.62	0
2	OLC	D	403	-	24,24,24	0.76	0	25,25,25	0.95	2 (8%)
2	OLC	D	402	-	24,24,24	0.75	0	25,25,25	0.66	0
2	OLC	D	401	-	24,24,24	0.77	0	25,25,25	0.66	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	OLC	A	401	-	-	7/24/24/24	-
2	OLC	E	401	-	-	4/24/24/24	-
2	OLC	A	404	-	-	2/24/24/24	-
2	OLC	D	405	-	-	11/24/24/24	-
2	OLC	B	401	-	-	7/24/24/24	-
2	OLC	A	402	-	-	6/24/24/24	-
2	OLC	B	402	-	-	7/24/24/24	-
2	OLC	A	403	-	-	8/24/24/24	-
2	OLC	D	404	-	-	5/24/24/24	-
2	OLC	D	403	-	-	7/24/24/24	-
2	OLC	D	402	-	-	5/24/24/24	-
2	OLC	D	401	-	-	6/24/24/24	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	403	OLC	O20-C1	2.17	1.39	1.33
2	A	403	OLC	C21-C22	2.14	1.58	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	403	OLC	O20-C1-O19	-2.63	117.04	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	403	OLC	C21-O20-C1	2.05	124.60	117.12

There are no chirality outliers.

All (75) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	403	OLC	C2-C1-O20-C21
2	D	403	OLC	O19-C1-O20-C21
2	D	405	OLC	O23-C22-C24-O25
2	D	401	OLC	O20-C21-C22-O23
2	B	401	OLC	C21-C22-C24-O25
2	D	405	OLC	C21-C22-C24-O25
2	A	401	OLC	C2-C3-C4-C5
2	B	401	OLC	C3-C4-C5-C6
2	A	403	OLC	C1-C2-C3-C4
2	A	401	OLC	C14-C15-C16-C17
2	D	404	OLC	C5-C6-C7-C8
2	D	404	OLC	C4-C5-C6-C7
2	A	402	OLC	C3-C4-C5-C6
2	D	405	OLC	C14-C15-C16-C17
2	D	405	OLC	C11-C12-C13-C14
2	D	403	OLC	C14-C15-C16-C17
2	B	402	OLC	C5-C6-C7-C8
2	D	402	OLC	C4-C5-C6-C7
2	A	401	OLC	C4-C5-C6-C7
2	A	404	OLC	C5-C6-C7-C8
2	B	402	OLC	C4-C5-C6-C7
2	B	402	OLC	C12-C13-C14-C15
2	A	403	OLC	C6-C7-C8-C9
2	D	405	OLC	C6-C7-C8-C9
2	D	401	OLC	C2-C3-C4-C5
2	A	403	OLC	C3-C4-C5-C6
2	A	402	OLC	C10-C11-C12-C13
2	D	401	OLC	O20-C21-C22-C24
2	D	402	OLC	C5-C6-C7-C8
2	D	401	OLC	C13-C14-C15-C16
2	A	402	OLC	C5-C6-C7-C8
2	D	405	OLC	C12-C13-C14-C15
2	D	404	OLC	C3-C4-C5-C6
2	A	401	OLC	C10-C11-C12-C13
2	D	404	OLC	C14-C15-C16-C17
2	D	405	OLC	C3-C4-C5-C6

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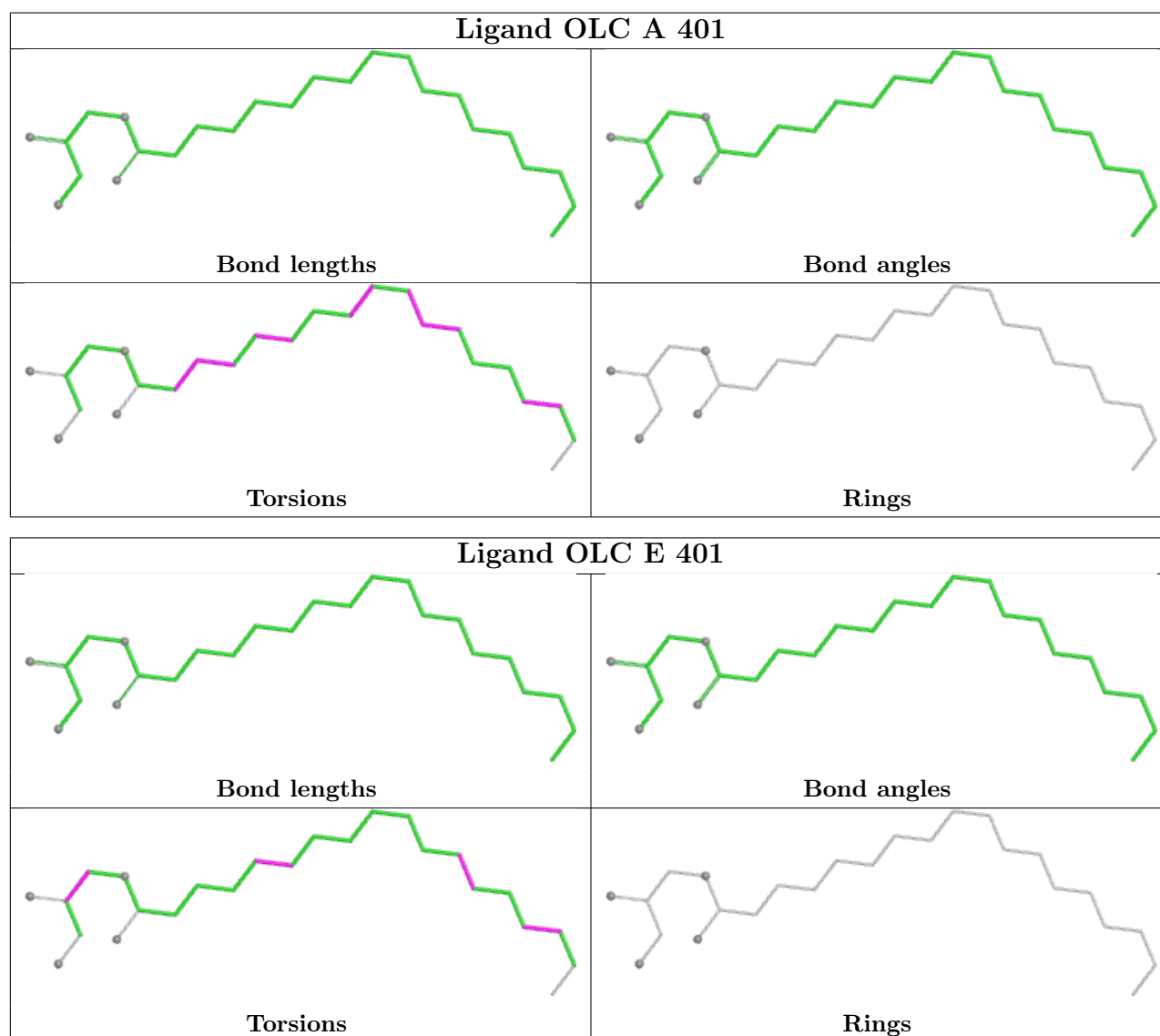
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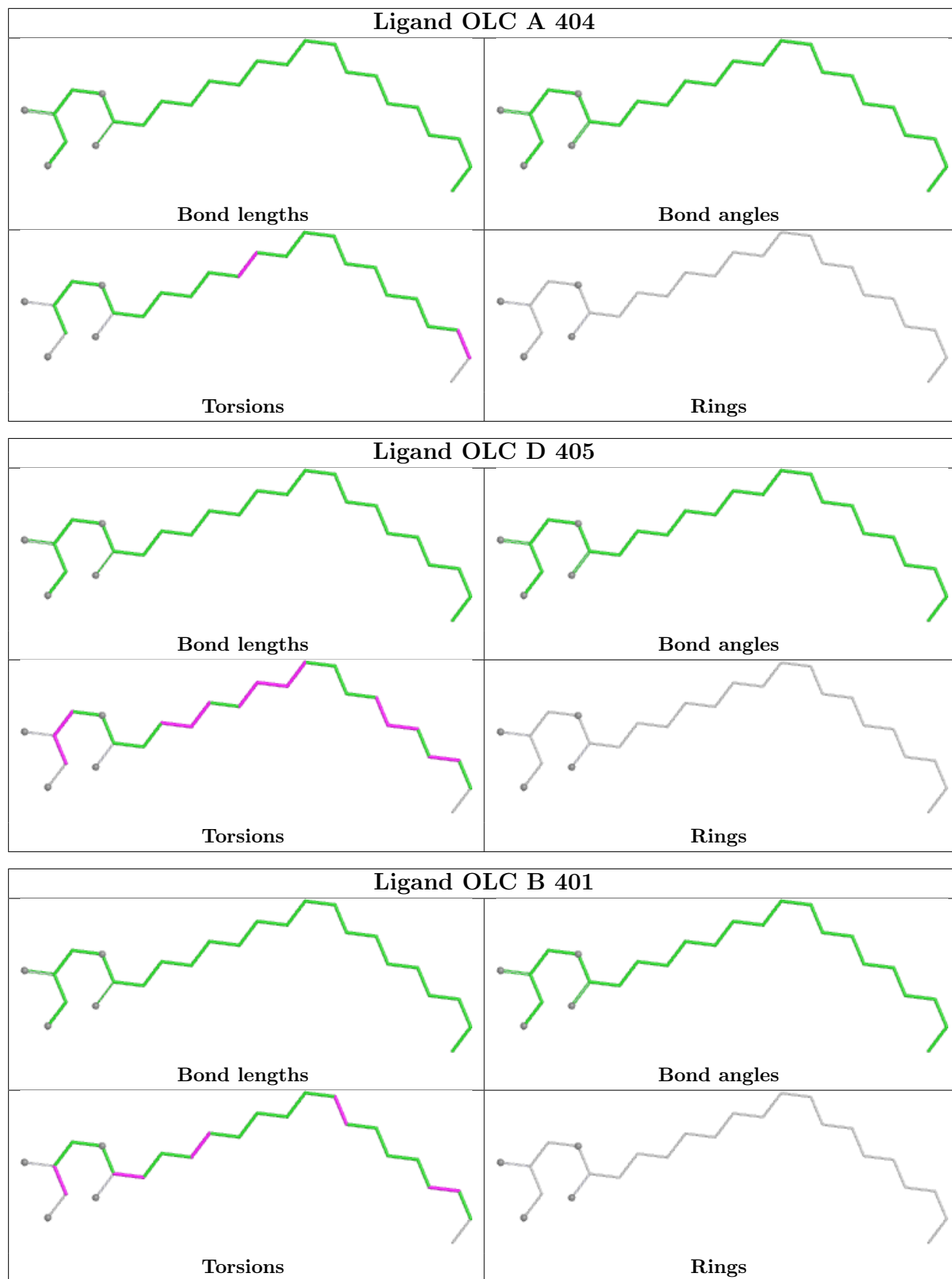
Mol	Chain	Res	Type	Atoms
2	B	402	OLC	C9-C10-C11-C12
2	B	401	OLC	C14-C15-C16-C17
2	A	403	OLC	C2-C3-C4-C5
2	B	402	OLC	C3-C4-C5-C6
2	A	403	OLC	C9-C10-C11-C12
2	D	405	OLC	C5-C6-C7-C8
2	A	402	OLC	O20-C21-C22-O23
2	A	403	OLC	C4-C5-C6-C7
2	D	405	OLC	O20-C21-C22-C24
2	D	403	OLC	C10-C11-C12-C13
2	A	401	OLC	C7-C8-C9-C10
2	D	405	OLC	C2-C3-C4-C5
2	D	403	OLC	C3-C4-C5-C6
2	B	401	OLC	C9-C10-C11-C12
2	D	401	OLC	C9-C10-C11-C12
2	D	402	OLC	C15-C16-C17-C18
2	E	401	OLC	C11-C12-C13-C14
2	E	401	OLC	O20-C21-C22-O23
2	A	402	OLC	C7-C8-C9-C10
2	B	402	OLC	C7-C8-C9-C10
2	D	401	OLC	C7-C8-C9-C10
2	B	401	OLC	O20-C1-C2-C3
2	D	405	OLC	C7-C8-C9-C10
2	A	402	OLC	C9-C10-C11-C12
2	D	403	OLC	C9-C10-C11-C12
2	D	402	OLC	O20-C1-C2-C3
2	A	404	OLC	C15-C16-C17-C18
2	B	401	OLC	O23-C22-C24-O25
2	A	401	OLC	C9-C10-C11-C12
2	A	403	OLC	O20-C1-C2-C3
2	A	403	OLC	C12-C13-C14-C15
2	D	403	OLC	C5-C6-C7-C8
2	E	401	OLC	C14-C15-C16-C17
2	E	401	OLC	C4-C5-C6-C7
2	B	401	OLC	O19-C1-C2-C3
2	B	402	OLC	O23-C22-C24-O25
2	A	401	OLC	C1-C2-C3-C4
2	D	402	OLC	O19-C1-C2-C3
2	D	404	OLC	C11-C12-C13-C14

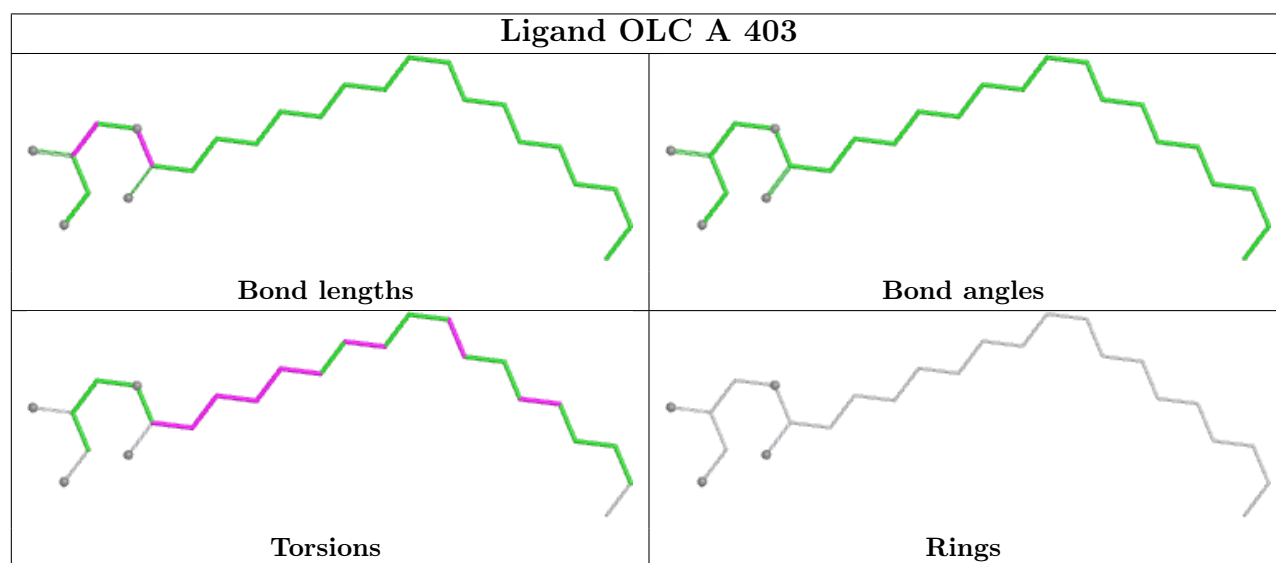
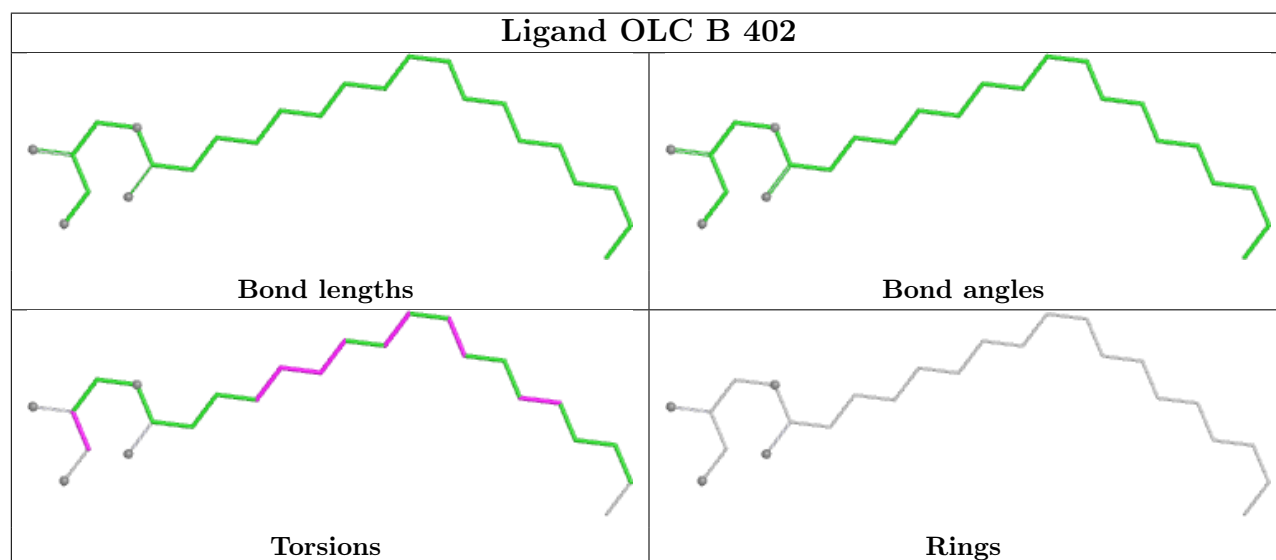
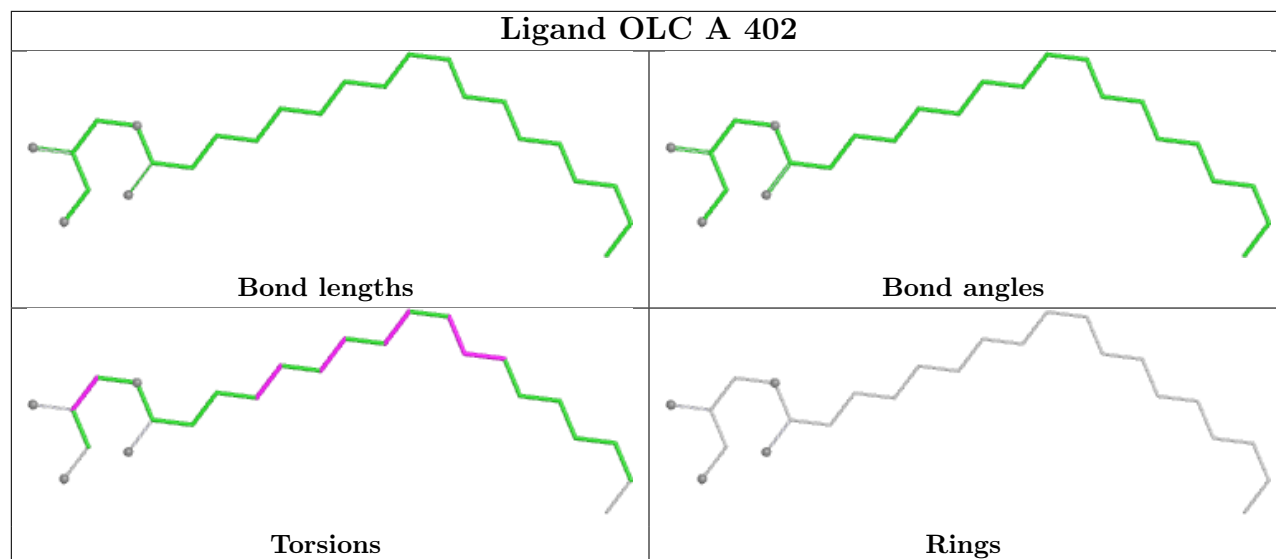
There are no ring outliers.

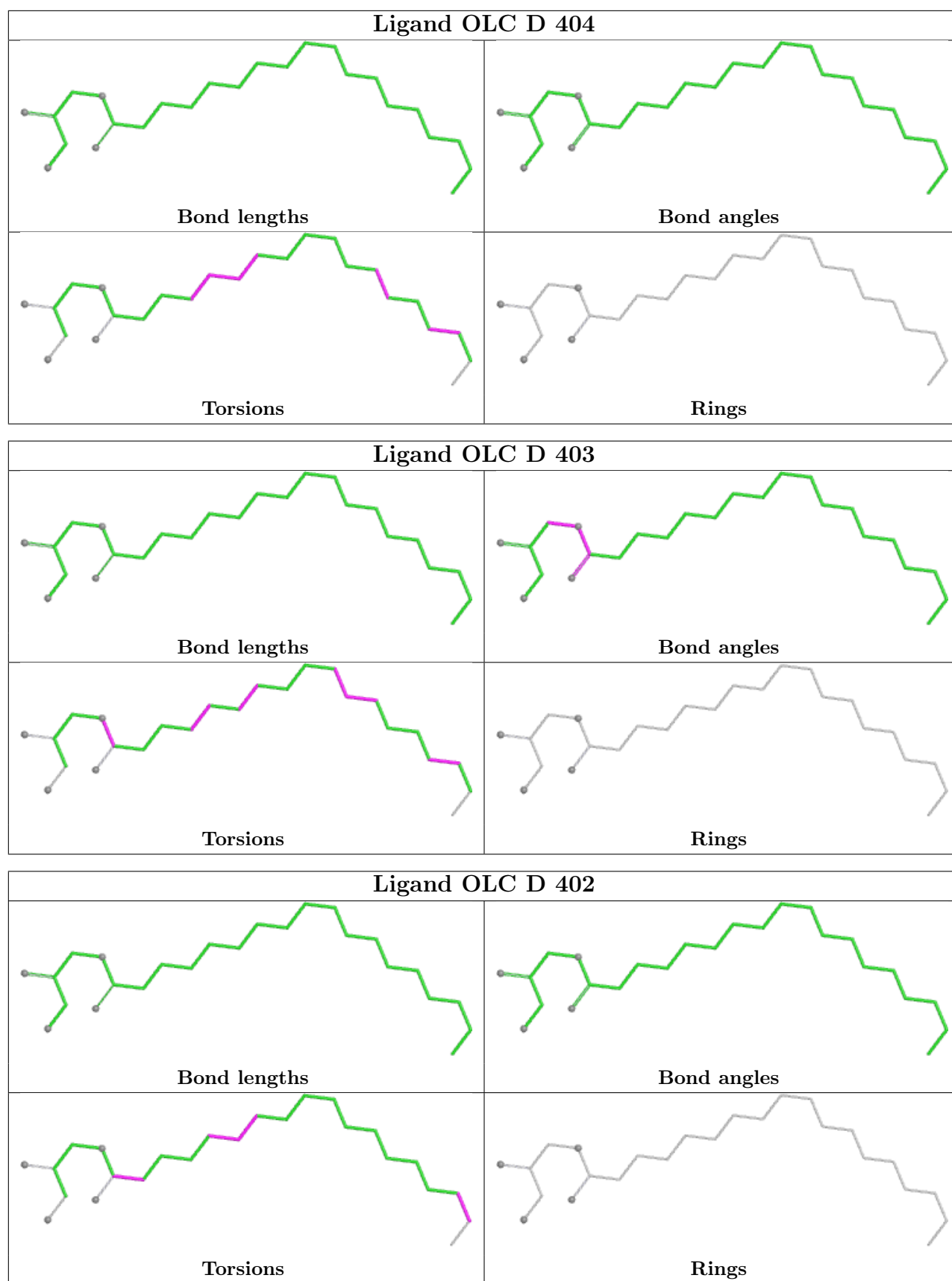
No monomer is involved in short contacts.

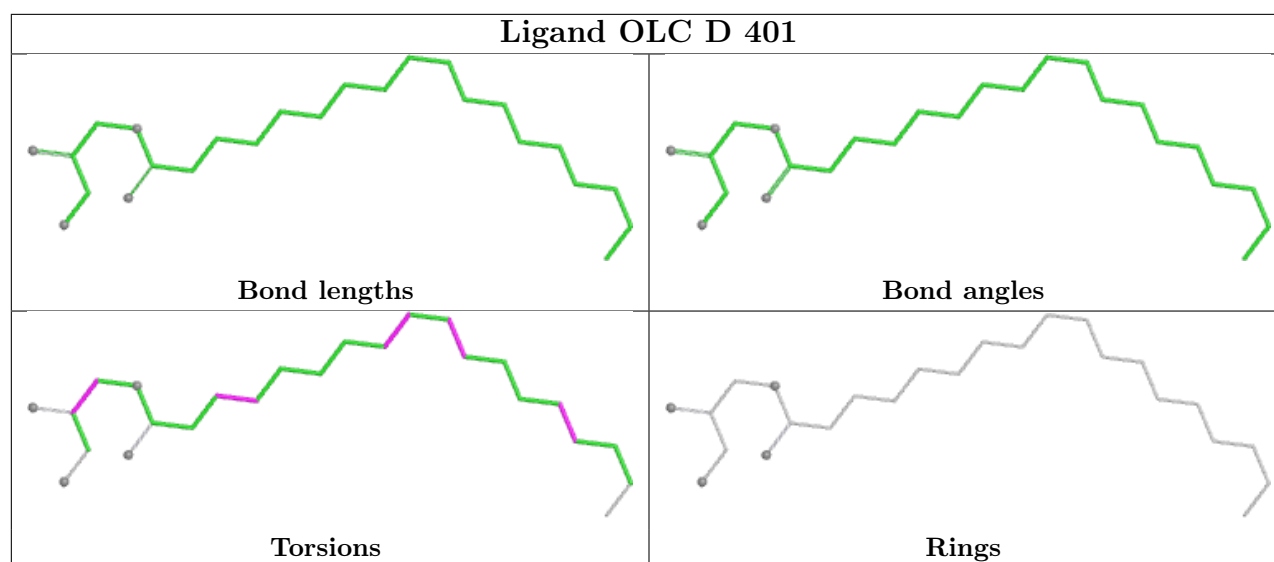
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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	299/337 (88%)	0.58	17 (5%)	29	19	67, 90, 139, 170	0
1	B	299/337 (88%)	0.57	17 (5%)	29	19	30, 89, 124, 167	0
1	C	302/337 (89%)	0.58	15 (4%)	34	22	30, 90, 131, 169	0
1	D	303/337 (89%)	0.58	17 (5%)	30	19	70, 90, 130, 153	0
1	E	304/337 (90%)	0.65	21 (6%)	23	15	67, 91, 158, 177	0
1	F	305/337 (90%)	0.65	20 (6%)	24	15	66, 91, 156, 172	0
1	G	306/337 (90%)	0.63	17 (5%)	30	19	62, 89, 158, 174	0
1	H	299/337 (88%)	0.64	21 (7%)	22	14	66, 89, 156, 175	0
All	All	2417/2696 (89%)	0.61	145 (5%)	27	17	30, 90, 147, 177	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	246	ASN	7.4
1	A	246	ASN	7.4
1	B	246	ASN	6.8
1	C	246	ASN	6.8
1	H	47	ASP	6.3
1	D	245	ASN	5.7
1	C	245	ASN	5.5
1	E	48	PHE	5.4
1	E	47	ASP	5.1
1	E	332	ALA	5.1
1	F	48	PHE	5.0
1	B	245	ASN	4.8
1	D	241	VAL	4.8
1	G	47	ASP	4.5
1	H	48	PHE	4.5
1	A	124	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	237	ASP	4.4
1	H	332	ALA	4.3
1	G	48	PHE	4.2
1	F	47	ASP	4.0
1	B	241	VAL	3.7
1	F	332	ALA	3.7
1	B	73	GLY	3.4
1	B	237	ASP	3.4
1	D	132	PHE	3.3
1	F	241	VAL	3.3
1	G	252	LEU	3.2
1	C	237	ASP	3.2
1	C	241	VAL	3.2
1	A	157	TRP	3.2
1	H	333	GLN	3.2
1	C	238	TRP	3.2
1	E	165	ALA	3.2
1	A	237	ASP	3.1
1	C	131	LEU	3.1
1	G	180	SER	3.0
1	B	20	SER	3.0
1	A	238	TRP	3.0
1	F	165	ALA	3.0
1	D	131	LEU	2.9
1	B	238	TRP	2.9
1	C	132	PHE	2.9
1	H	124	LEU	2.9
1	D	73	GLY	2.8
1	H	73	GLY	2.8
1	G	331	GLN	2.8
1	G	78	ARG	2.8
1	D	238	TRP	2.8
1	B	161	GLN	2.8
1	A	20	SER	2.8
1	A	18	ALA	2.7
1	B	330	GLN	2.7
1	A	243	LEU	2.7
1	A	245	ASN	2.7
1	D	80	LEU	2.7
1	D	49	ASN	2.7
1	E	252	LEU	2.7
1	F	331	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	F	85	ALA	2.7
1	A	241	VAL	2.7
1	E	275	VAL	2.7
1	A	132	PHE	2.6
1	A	73	GLY	2.6
1	H	252	LEU	2.6
1	G	177	ALA	2.6
1	D	79	SER	2.6
1	C	73	GLY	2.6
1	H	46	LYS	2.6
1	H	41	PHE	2.6
1	B	131	LEU	2.6
1	B	132	PHE	2.5
1	F	73	GLY	2.5
1	A	46	LYS	2.5
1	G	37	VAL	2.5
1	B	80	LEU	2.5
1	B	331	GLN	2.5
1	F	45	LEU	2.5
1	C	243	LEU	2.5
1	F	184	GLY	2.5
1	F	20	SER	2.5
1	E	17	VAL	2.5
1	E	181	PHE	2.5
1	D	46	LYS	2.5
1	E	333	GLN	2.5
1	G	41	PHE	2.4
1	G	164	ALA	2.4
1	D	243	LEU	2.4
1	G	80	LEU	2.4
1	C	242	ASN	2.4
1	F	333	GLN	2.4
1	C	48	PHE	2.4
1	C	157	TRP	2.4
1	E	184	GLY	2.4
1	F	163	VAL	2.4
1	G	238	TRP	2.4
1	A	45	LEU	2.3
1	E	80	LEU	2.3
1	C	46	LYS	2.3
1	B	220	ASN	2.3
1	C	288	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
1	G	133	PHE	2.3
1	H	161	GLN	2.3
1	B	157	TRP	2.3
1	D	20	SER	2.3
1	H	80	LEU	2.3
1	E	180	SER	2.3
1	F	80	LEU	2.3
1	F	108	TYR	2.3
1	D	242	ASN	2.3
1	E	288	ASN	2.3
1	F	81	ASN	2.3
1	F	41	PHE	2.2
1	H	78	ARG	2.2
1	G	237	ASP	2.2
1	E	331	GLN	2.2
1	A	49	ASN	2.2
1	E	41	PHE	2.2
1	H	247	PHE	2.2
1	F	78	ARG	2.2
1	H	108	TYR	2.2
1	H	241	VAL	2.2
1	A	79	SER	2.2
1	G	243	LEU	2.2
1	H	270	GLY	2.2
1	D	150	LEU	2.2
1	A	17	VAL	2.1
1	C	45	LEU	2.1
1	G	71	ILE	2.1
1	E	134	GLY	2.1
1	H	184	GLY	2.1
1	H	81	ASN	2.1
1	D	157	TRP	2.1
1	H	163	VAL	2.1
1	B	269	SER	2.1
1	B	26	LEU	2.1
1	E	73	GLY	2.1
1	E	86	LYS	2.0
1	E	241	VAL	2.0
1	G	16	SER	2.0
1	H	165	ALA	2.0
1	E	49	ASN	2.0
1	F	19	ASN	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	164	ALA	2.0
1	F	46	LYS	2.0
1	E	124	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

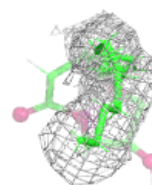
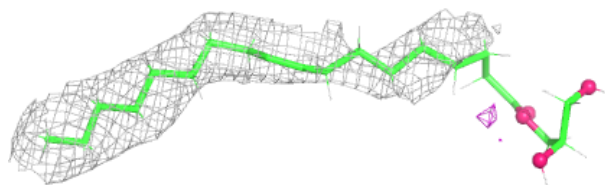
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	OLC	A	403	25/25	0.55	0.16	66,109,141,143	0
2	OLC	D	402	25/25	0.58	0.14	138,143,149,150	0
2	OLC	D	403	25/25	0.59	0.13	140,151,158,159	0
2	OLC	B	402	25/25	0.62	0.15	116,127,132,133	0
2	OLC	B	401	25/25	0.65	0.17	84,101,126,127	0
2	OLC	A	401	25/25	0.65	0.16	147,156,161,163	0
2	OLC	A	404	25/25	0.66	0.15	94,115,149,151	0
2	OLC	D	404	25/25	0.67	0.15	157,162,167,169	0
2	OLC	D	405	25/25	0.72	0.19	87,101,120,122	0
2	OLC	A	402	25/25	0.76	0.15	99,107,133,134	0
2	OLC	E	401	25/25	0.77	0.16	79,85,108,111	0
2	OLC	D	401	25/25	0.78	0.15	99,113,132,134	0

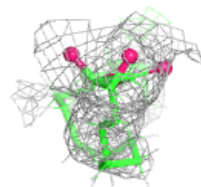
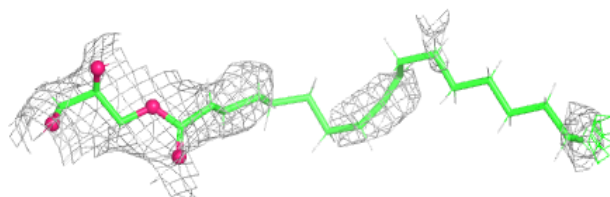
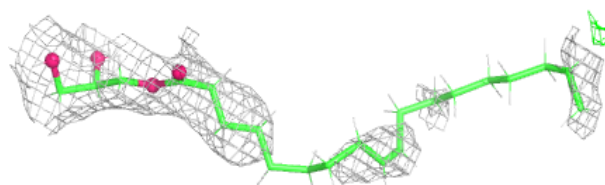
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around OLC A 403:

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

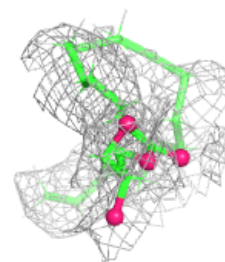
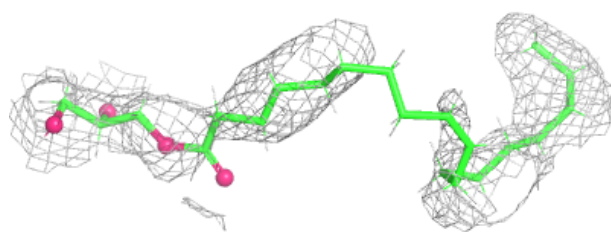
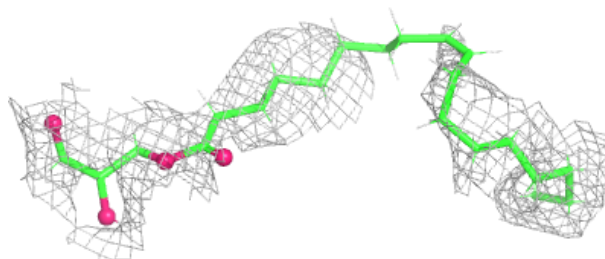
**Electron density around OLC D 402:**

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

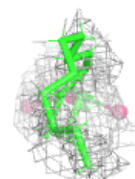
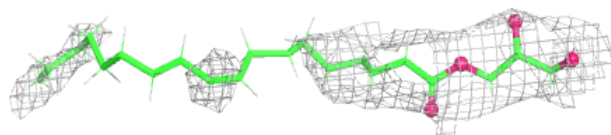
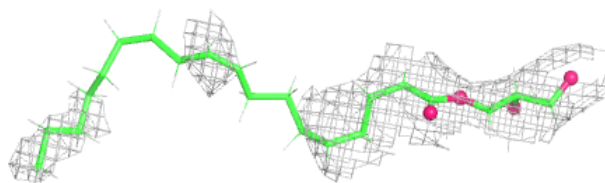


Electron density around OLC D 403:

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

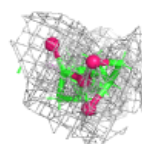
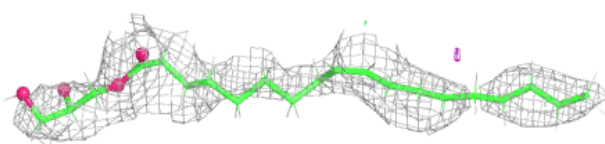
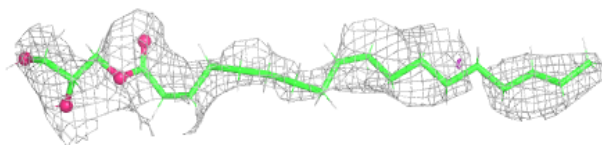
**Electron density around OLC B 402:**

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

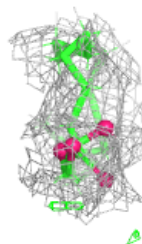
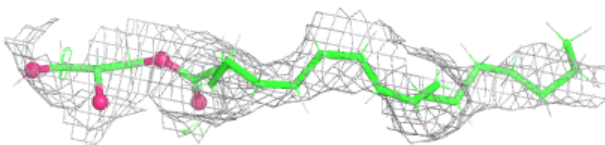


Electron density around OLC B 401:

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

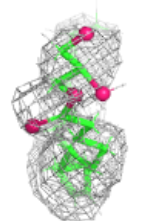
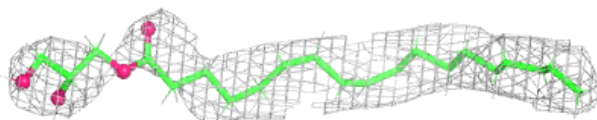
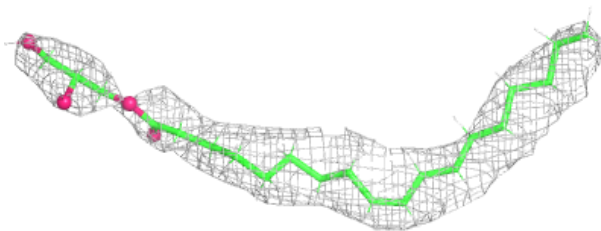
**Electron density around OLC A 401:**

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

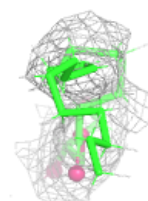
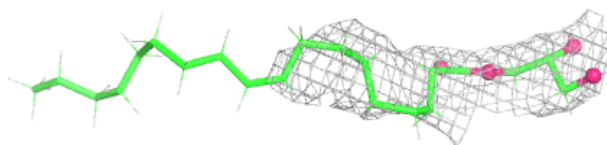


Electron density around OLC A 404:

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

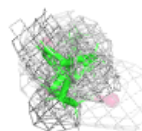
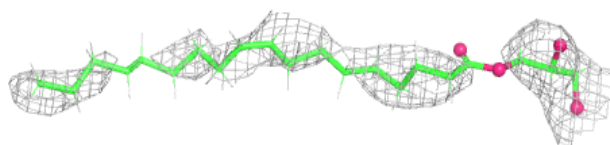
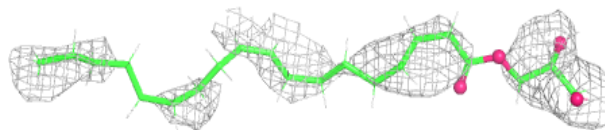
**Electron density around OLC D 404:**

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

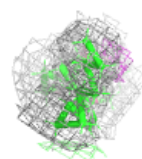
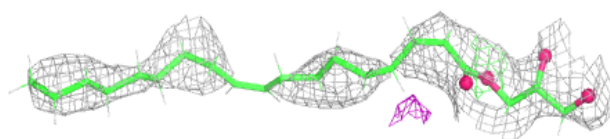
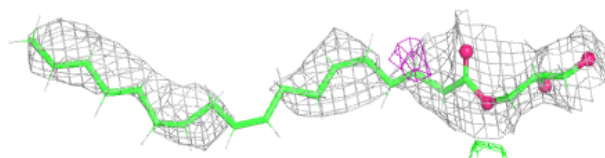


Electron density around OLC D 405:

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

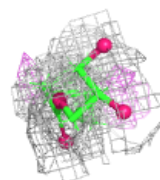
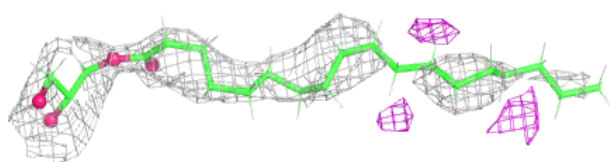
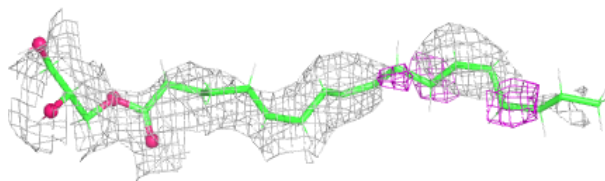
**Electron density around OLC A 402:**

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

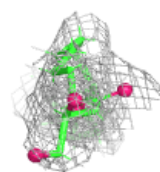
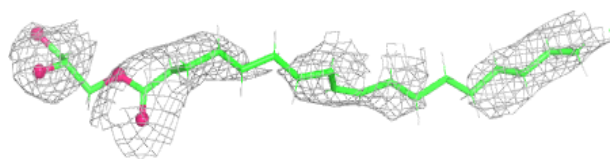
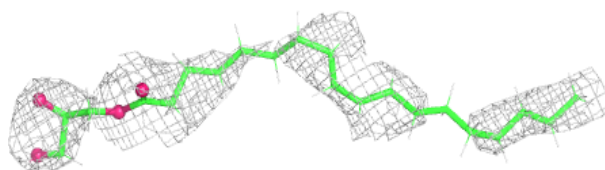


Electron density around OLC E 401:

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

**Electron density around OLC D 401:**

$2mF_o-DF_c$ (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.