



Full wwPDB X-ray Structure Validation Report ⓘ

May 12, 2022 – 10:04 AM EDT

PDB ID : 7SPS
Title : Crystal structure of human glucose transporter GLUT3 bound with exofacial inhibitor SA47
Authors : Wang, N.; Jiang, X.; Yan, N.
Deposited on : 2021-11-03
Resolution : 2.30 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.28.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.28.1

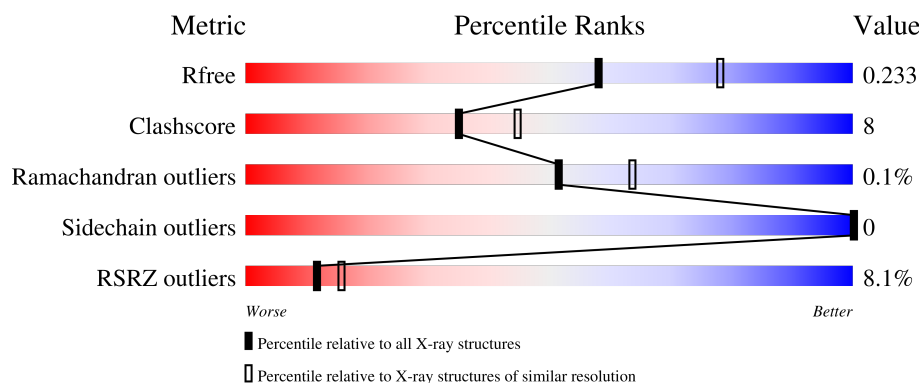
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	523	 8% 76% 13% 11%
1	B	523	 6% 77% 12% 11%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	OLC	A	503	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7607 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 Solute carrier family 2, facilitated glucose transporter member 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	468	Total	C	N	O	S	3	2	0
			3610	2373	584	633	20			
1	B	468	Total	C	N	O	S	5	2	0
			3602	2367	582	633	20			

There are 56 discrepancies between the modelled and reference sequences:

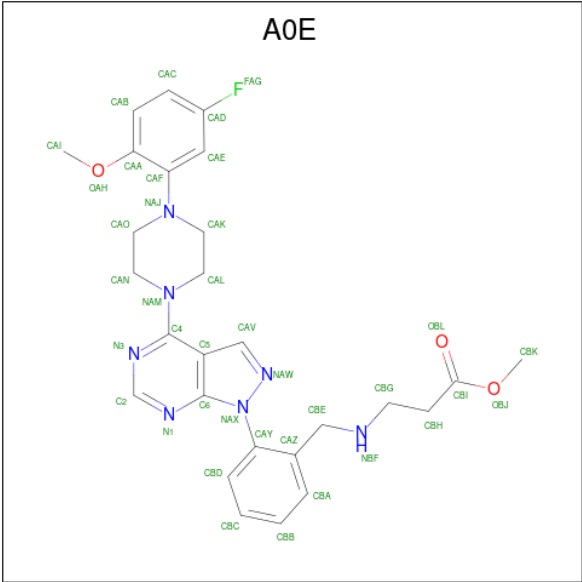
Chain	Residue	Modelled	Actual	Comment	Reference
A	-26	MET	-	expression tag	UNP P11169
A	-25	HIS	-	expression tag	UNP P11169
A	-24	HIS	-	expression tag	UNP P11169
A	-23	HIS	-	expression tag	UNP P11169
A	-22	HIS	-	expression tag	UNP P11169
A	-21	HIS	-	expression tag	UNP P11169
A	-20	HIS	-	expression tag	UNP P11169
A	-19	HIS	-	expression tag	UNP P11169
A	-18	HIS	-	expression tag	UNP P11169
A	-17	HIS	-	expression tag	UNP P11169
A	-16	HIS	-	expression tag	UNP P11169
A	-15	SER	-	expression tag	UNP P11169
A	-14	GLY	-	expression tag	UNP P11169
A	-13	ASP	-	expression tag	UNP P11169
A	-12	GLU	-	expression tag	UNP P11169
A	-11	VAL	-	expression tag	UNP P11169
A	-10	ASP	-	expression tag	UNP P11169
A	-9	ALA	-	expression tag	UNP P11169
A	-8	GLY	-	expression tag	UNP P11169
A	-7	SER	-	expression tag	UNP P11169
A	-6	GLY	-	expression tag	UNP P11169
A	-5	GLN	-	expression tag	UNP P11169
A	-4	VAL	-	expression tag	UNP P11169
A	-3	ASP	-	expression tag	UNP P11169

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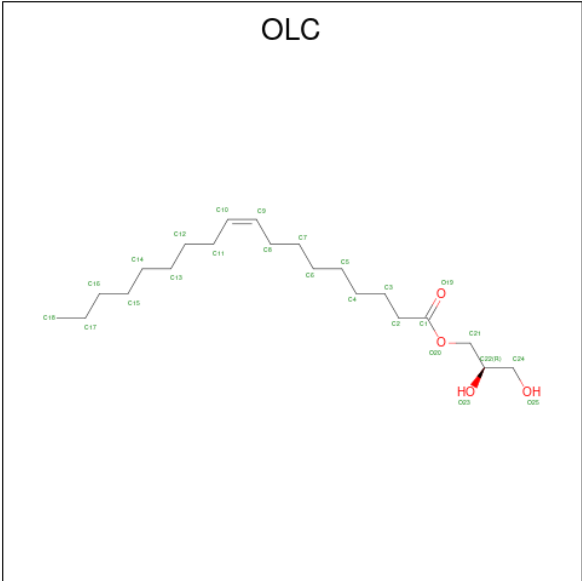
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	ALA	-	expression tag	UNP P11169
A	-1	GLY	-	expression tag	UNP P11169
A	0	THR	-	expression tag	UNP P11169
A	43	THR	ASN	engineered mutation	UNP P11169
B	-26	MET	-	expression tag	UNP P11169
B	-25	HIS	-	expression tag	UNP P11169
B	-24	HIS	-	expression tag	UNP P11169
B	-23	HIS	-	expression tag	UNP P11169
B	-22	HIS	-	expression tag	UNP P11169
B	-21	HIS	-	expression tag	UNP P11169
B	-20	HIS	-	expression tag	UNP P11169
B	-19	HIS	-	expression tag	UNP P11169
B	-18	HIS	-	expression tag	UNP P11169
B	-17	HIS	-	expression tag	UNP P11169
B	-16	HIS	-	expression tag	UNP P11169
B	-15	SER	-	expression tag	UNP P11169
B	-14	GLY	-	expression tag	UNP P11169
B	-13	ASP	-	expression tag	UNP P11169
B	-12	GLU	-	expression tag	UNP P11169
B	-11	VAL	-	expression tag	UNP P11169
B	-10	ASP	-	expression tag	UNP P11169
B	-9	ALA	-	expression tag	UNP P11169
B	-8	GLY	-	expression tag	UNP P11169
B	-7	SER	-	expression tag	UNP P11169
B	-6	GLY	-	expression tag	UNP P11169
B	-5	GLN	-	expression tag	UNP P11169
B	-4	VAL	-	expression tag	UNP P11169
B	-3	ASP	-	expression tag	UNP P11169
B	-2	ALA	-	expression tag	UNP P11169
B	-1	GLY	-	expression tag	UNP P11169
B	0	THR	-	expression tag	UNP P11169
B	43	THR	ASN	engineered mutation	UNP P11169

- Molecule 2 is methyl N-[(2-{4-[4-(5-fluoro-2-methoxyphenyl)piperazin-1-yl]-1H-pyrazol-5-yl}phenyl)methyl]-beta-alaninate (three-letter code: A0E) (formula: C₂₇H₃₀FN₇O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	1
			76	54	2	14	6		
2	B	1	Total	C	F	N	O	0	1
			76	54	2	14	6		

- Molecule 3 is (2R)-2,3-dihydroxypropyl (9Z)-octadec-9-enoate (three-letter code: OLC) (formula: C₂₁H₄₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			25	21	4		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			25	21	4		
3	B	1	Total	C	O	0	0
			25	21	4		
3	B	1	Total	C	O	0	0
			25	21	4		
3	B	1	Total	C	O	0	0
			25	21	4		

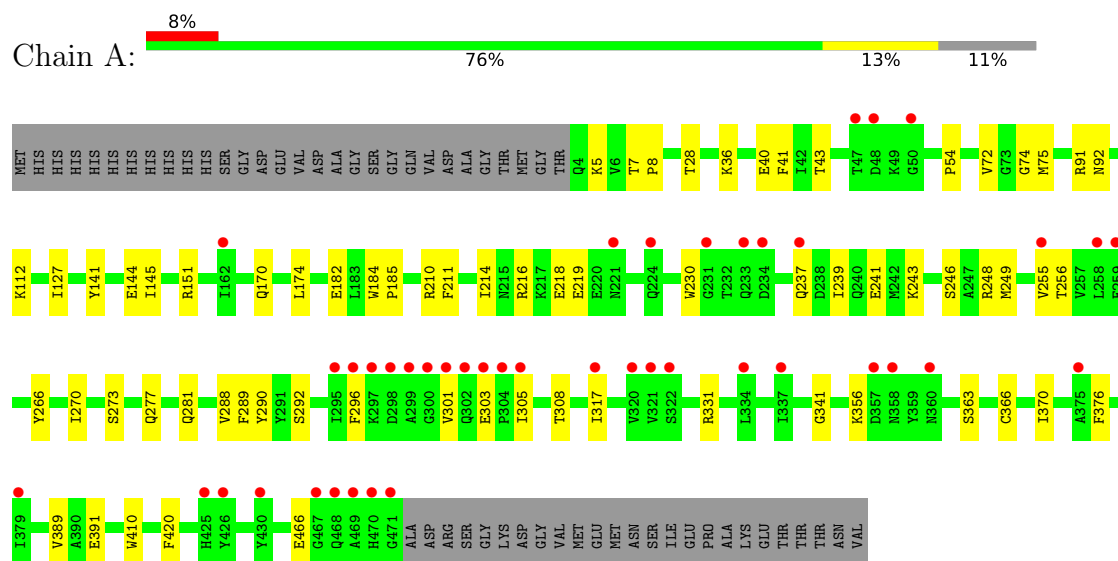
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	46	Total	O	0	0
			46	46		
4	B	72	Total	O	0	0
			72	72		

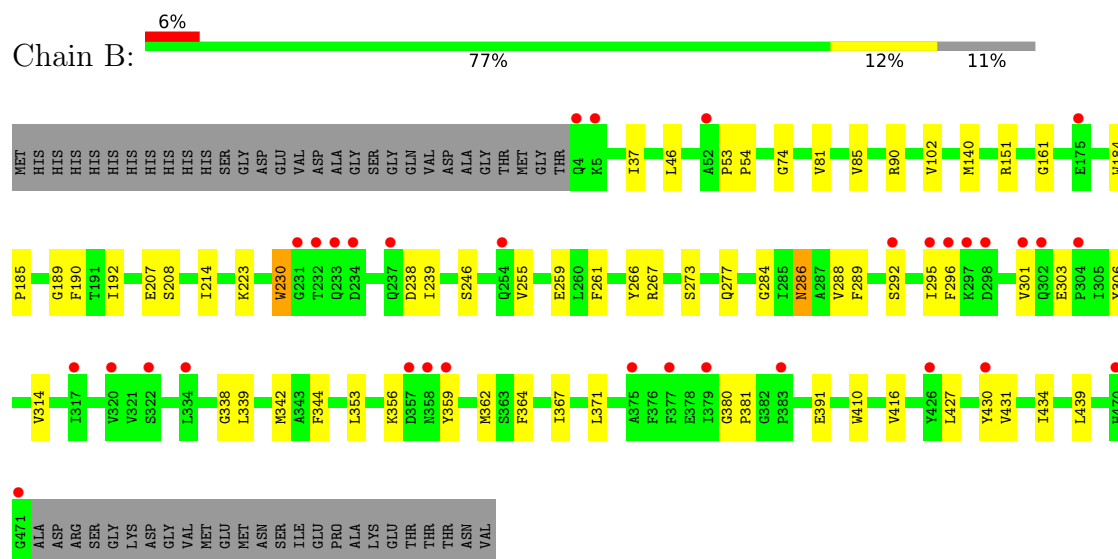
3 Residue-property plots [i](#)

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: Solute carrier family 2, facilitated glucose transporter member 3



- Molecule 1: Solute carrier family 2, facilitated glucose transporter member 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	77.59Å 121.55Å 95.87Å 90.00° 108.14° 90.00°	Depositor
Resolution (Å)	46.39 – 2.30 46.90 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.8 (46.39-2.30) 99.1 (46.90-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.10Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.212 , 0.234 0.211 , 0.233	Depositor DCC
R_{free} test set	4866 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	45.4	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 63.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7607	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 39.56 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.1155e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: A0E, 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	0.35	0/3693	0.48	0/5013
1	B	0.35	0/3685	0.46	0/5005
All	All	0.35	0/7378	0.47	0/10018

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	B	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	230[B]	TRP	Mainchain
1	B	286[B]	ASN	Mainchain

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	3610	0	3700	63	0
1	B	3602	0	3678	55	0
2	A	76	0	0	6	0
2	B	76	0	0	2	0
3	A	50	0	80	0	0
3	B	75	0	120	10	0
4	A	46	0	0	1	0
4	B	72	0	0	2	0
All	All	7607	0	7578	124	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 8.

All (124) 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:288:VAL:CG1	1:A:370:ILE:HG23	2.01	0.90
1:A:255:VAL:HG21	1:A:266:TYR:HE2	1.36	0.90
1:B:85:VAL:HG11	1:B:140:MET:SD	2.13	0.88
1:A:255:VAL:HG21	1:A:266:TYR:CE2	2.14	0.82
1:B:427:LEU:HD13	1:B:434:ILE:HD11	1.62	0.80
1:B:427:LEU:HD13	1:B:434:ILE:CD1	2.13	0.78
1:B:338:GLY:O	1:B:342:MET:HG3	1.83	0.78
1:B:85:VAL:HG12	1:B:90:ARG:NH1	2.02	0.75
1:B:190:PHE:HE1	3:B:504:OLC:H12A	1.52	0.74
1:A:301:VAL:HG12	1:A:303:GLU:H	1.52	0.74
1:B:255:VAL:HG13	1:B:259:GLU:HB2	1.73	0.70
1:B:289:PHE:HA	1:B:292:SER:OG	1.92	0.70
1:A:273:SER:O	1:A:277:GLN:HG2	1.92	0.69
1:B:339:LEU:HA	1:B:342:MET:CE	2.24	0.68
3:B:502:OLC:H5A	3:B:502:OLC:C9	2.23	0.67
1:B:284:GLY:O	1:B:288:VAL:HG23	1.96	0.65
1:B:261:PHE:O	1:B:267:ARG:NH2	2.28	0.65
1:A:255:VAL:HG12	1:A:256:THR:O	1.98	0.64
1:A:219:GLU:OE2	1:A:243:LYS:CE	2.48	0.61
1:B:190:PHE:CE1	3:B:504:OLC:H12A	2.34	0.61
1:B:339:LEU:HD23	1:B:342:MET:CE	2.31	0.60
1:B:339:LEU:HA	1:B:342:MET:HE3	1.84	0.60
1:A:366:CYS:O	1:A:370:ILE:HG13	2.02	0.60
1:A:219:GLU:OE2	1:A:243:LYS:HE2	2.02	0.60
1:A:43:THR:HG23	1:A:54:PRO:HD2	1.84	0.59
1:A:331:ARG:NH2	1:A:391:GLU:OE2	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:TYR:O	1:A:145:ILE:HG22	2.03	0.58
1:A:219:GLU:CD	1:A:243:LYS:HE2	2.23	0.58
1:A:273:SER:CB	1:A:389:VAL:HG22	2.34	0.58
1:B:359:TYR:O	1:B:362:MET:HG2	2.05	0.57
1:A:91:ARG:NH1	1:A:92:ASN:OD1	2.38	0.56
1:B:431:VAL:HA	1:B:434:ILE:HD13	1.87	0.56
1:B:161:GLY:HA2	3:B:504:OLC:H21	1.87	0.56
1:B:255:VAL:HG21	1:B:266:TYR:HE2	1.70	0.56
1:A:214:ILE:HG23	1:A:246:SER:HA	1.87	0.56
1:A:182:GLU:N	1:A:182:GLU:OE1	2.39	0.55
1:B:255:VAL:HG13	1:B:259:GLU:CB	2.36	0.55
1:A:281:GLN:HE22	2:A:501[A]:A0E:CAK	2.20	0.55
1:A:317:ILE:HG12	3:B:503:OLC:H11	1.87	0.55
3:B:502:OLC:C9	3:B:502:OLC:C5	2.85	0.54
1:B:214:ILE:HG23	1:B:246:SER:HA	1.90	0.54
1:B:184:TRP:CG	1:B:185:PRO:HD3	2.43	0.53
1:B:46:LEU:HD12	1:B:54:PRO:HG3	1.91	0.53
1:A:391:GLU:HG3	4:A:607:HOH:O	2.09	0.52
1:B:81:VAL:O	1:B:85:VAL:HG23	2.09	0.52
1:B:431:VAL:HA	1:B:434:ILE:CD1	2.40	0.52
2:A:501[A]:A0E:OBL	2:A:501[A]:A0E:NBF	2.42	0.52
1:B:296:PHE:HE1	1:B:367:ILE:HG13	1.73	0.52
1:A:292:SER:HB2	1:A:296:PHE:CE2	2.45	0.52
1:B:427:LEU:HD13	1:B:434:ILE:HD13	1.91	0.52
1:A:36:LYS:HE2	1:A:40:GLU:OE2	2.10	0.51
1:B:339:LEU:HA	1:B:342:MET:HE2	1.92	0.51
1:A:356:LYS:HE3	1:A:363:SER:OG	2.09	0.51
1:B:344:PHE:CE1	3:B:503:OLC:H12A	2.46	0.51
1:B:295:ILE:HD11	1:B:353:LEU:HD21	1.93	0.51
1:A:5:LYS:HB2	1:A:230[A]:TRP:O	2.11	0.51
1:A:317:ILE:HG23	3:B:503:OLC:H8A	1.93	0.51
1:B:342:MET:HE3	1:B:439:LEU:HD22	1.94	0.50
1:A:248:ARG:NH1	1:A:466:GLU:OE2	2.38	0.50
1:A:174:LEU:HD23	1:A:305:ILE:HG21	1.94	0.49
1:B:286[A]:ASN:HD22	1:B:416:VAL:HG21	1.78	0.49
1:B:289:PHE:HA	1:B:292:SER:CB	2.42	0.49
2:B:501[B]:A0E:NAW	2:B:501[B]:A0E:NBF	2.60	0.49
1:A:273:SER:HB3	1:A:389:VAL:CG2	2.43	0.49
1:B:286[B]:ASN:HD22	1:B:416:VAL:HG23	1.78	0.49
1:B:364:PHE:O	1:B:367:ILE:HG22	2.12	0.49
1:A:216:ARG:NH1	1:A:218:GLU:OE2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:ILE:HG12	4:B:652:HOH:O	2.12	0.49
1:B:391:GLU:HG3	4:B:628:HOH:O	2.13	0.48
1:B:189:GLY:O	1:B:192:ILE:HG12	2.13	0.48
1:A:28:THR:HG23	2:A:501[A]:A0E:FAG	2.04	0.48
1:A:237:GLN:O	1:A:241:GLU:HG3	2.14	0.48
1:A:301:VAL:C	1:A:303:GLU:H	2.16	0.47
1:A:288:VAL:HG11	1:A:370:ILE:HG23	1.90	0.47
1:A:28:THR:HG23	2:A:501[B]:A0E:FAG	2.03	0.47
1:A:74:GLY:HA3	1:A:410:TRP:CE3	2.50	0.47
1:B:296:PHE:CE1	1:B:367:ILE:HG13	2.49	0.47
1:A:28:THR:HG23	2:A:501[B]:A0E:CAD	2.45	0.47
1:A:288:VAL:HG12	1:A:370:ILE:HG23	1.92	0.46
1:B:151:ARG:NE	1:B:391:GLU:HG2	2.31	0.46
1:A:28:THR:HG23	2:A:501[A]:A0E:CAD	2.47	0.45
3:B:502:OLC:H5A	3:B:502:OLC:H9	1.96	0.45
1:A:214:ILE:HG22	1:A:249:MET:HE1	1.98	0.45
1:A:7:THR:HB	1:A:8:PRO:CD	2.48	0.44
1:B:430:TYR:O	1:B:434:ILE:HD12	2.16	0.44
1:A:273:SER:OG	1:A:389:VAL:HG22	2.17	0.44
1:B:53:PRO:HA	1:B:54:PRO:HD3	1.90	0.44
1:B:161:GLY:CA	3:B:504:OLC:H21	2.47	0.44
1:B:342:MET:HE2	1:B:381:PRO:HG2	2.00	0.44
1:B:356:LYS:HA	1:B:362:MET:HB2	1.98	0.44
1:A:270:ILE:HD12	1:A:270:ILE:HA	1.90	0.44
1:A:296:PHE:O	1:A:301:VAL:HB	2.18	0.44
1:A:288:VAL:HG13	1:A:370:ILE:HG23	1.92	0.43
1:A:184:TRP:CG	1:A:185:PRO:HD3	2.53	0.43
1:B:339:LEU:HD23	1:B:342:MET:HE1	1.99	0.43
1:A:170:GLN:NE2	1:A:308:THR:CG2	2.81	0.43
1:B:303:GLU:HB3	1:B:306:TYR:HD2	1.83	0.43
1:B:102:VAL:HA	1:B:192:ILE:HG22	2.00	0.42
1:B:273:SER:O	1:B:277:GLN:HG2	2.18	0.42
1:A:170:GLN:NE2	1:A:308:THR:HG22	2.34	0.42
1:A:273:SER:CB	1:A:389:VAL:CG2	2.98	0.42
1:A:72:VAL:HA	1:A:75:MET:HE3	2.02	0.42
1:A:127:ILE:HD12	1:A:127:ILE:HA	1.89	0.42
1:A:273:SER:HB3	1:A:389:VAL:HG21	2.01	0.42
1:B:342:MET:HE3	1:B:342:MET:HB2	1.97	0.42
1:A:7:THR:HB	1:A:8:PRO:HD2	2.02	0.42
1:A:301:VAL:C	1:A:303:GLU:N	2.73	0.42
1:B:314:VAL:HG21	1:B:371:LEU:HD22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:501[B]:A0E:NBF	2:B:501[B]:A0E:NAX	2.68	0.41
1:B:207:GLU:OE2	1:B:208:SER:N	2.52	0.41
1:A:289:PHE:HA	1:A:292:SER:HB3	2.02	0.41
1:A:72:VAL:HA	1:A:75:MET:CE	2.50	0.41
1:B:74:GLY:HA3	1:B:410:TRP:CE3	2.56	0.41
1:A:151:ARG:NE	1:A:391:GLU:HG2	2.37	0.40
1:A:239:ILE:HG22	1:A:243:LYS:HE3	2.03	0.40
1:A:341:GLY:HA3	1:A:376:PHE:CD1	2.56	0.40
1:B:223:LYS:HA	1:B:239:ILE:HD11	2.02	0.40
1:A:144:GLU:O	1:A:210:ARG:HG3	2.21	0.40
1:B:230[A]:TRP:HZ3	1:B:238:ASP:OD2	2.03	0.40
1:B:296:PHE:O	1:B:301:VAL:HG23	2.20	0.40
1:A:41:PHE:CE1	1:A:112:LYS:HA	2.56	0.40
1:A:290:TYR:CD2	1:A:420:PHE:HE2	2.38	0.40
1:A:211:PHE:CE2	1:A:216:ARG:HD2	2.56	0.40
1:A:239:ILE:O	1:A:243:LYS:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	468/523 (90%)	460 (98%)	8 (2%)	0	100	100
1	B	468/523 (90%)	458 (98%)	9 (2%)	1 (0%)	47	58
All	All	936/1046 (90%)	918 (98%)	17 (2%)	1 (0%)	51	64

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	380	GLY

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	388/431 (90%)	388 (100%)	0	100	100
1	B	386/431 (90%)	386 (100%)	0	100	100
All	All	774/862 (90%)	774 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	GLN
1	A	315	ASN
1	B	315	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 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	A0E	B	501[B]	-	40,42,42	4.13	21 (52%)	47,58,58	2.28	14 (29%)
2	A0E	B	501[A]	-	40,42,42	4.07	20 (50%)	47,58,58	2.15	14 (29%)
2	A0E	A	501[B]	-	40,42,42	4.19	19 (47%)	47,58,58	2.15	13 (27%)
3	OLC	B	502	-	24,24,24	0.81	1 (4%)	25,25,25	1.04	2 (8%)
3	OLC	B	503	-	24,24,24	0.92	1 (4%)	25,25,25	0.87	1 (4%)
3	OLC	A	503	-	24,24,24	0.92	1 (4%)	25,25,25	0.87	1 (4%)
3	OLC	A	502	-	24,24,24	0.92	1 (4%)	25,25,25	0.88	1 (4%)
3	OLC	B	504	-	24,24,24	0.93	1 (4%)	25,25,25	0.88	1 (4%)
2	A0E	A	501[A]	-	40,42,42	4.21	21 (52%)	47,58,58	2.01	12 (25%)

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	A0E	B	501[B]	-	-	12/23/33/33	0/5/5/5
2	A0E	B	501[A]	-	-	6/23/33/33	0/5/5/5
2	A0E	A	501[B]	-	-	10/23/33/33	0/5/5/5
3	OLC	B	502	-	-	7/24/24/24	-
3	OLC	B	503	-	-	10/24/24/24	-
3	OLC	A	503	-	-	9/24/24/24	-
3	OLC	A	502	-	-	7/24/24/24	-
3	OLC	B	504	-	-	10/24/24/24	-
2	A0E	A	501[A]	-	-	13/23/33/33	0/5/5/5

All (86) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501[B]	A0E	CAV-C5	10.64	1.63	1.40
2	B	501[B]	A0E	CAY-CAZ	10.64	1.56	1.40
2	A	501[B]	A0E	CAY-CAZ	10.62	1.56	1.40
2	A	501[A]	A0E	CAY-CAZ	10.61	1.56	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501[A]	A0E	CAV-C5	10.57	1.63	1.40
2	B	501[B]	A0E	CAV-C5	10.49	1.63	1.40
2	B	501[A]	A0E	CAV-C5	10.41	1.63	1.40
2	B	501[A]	A0E	CAY-CAZ	10.05	1.55	1.40
2	A	501[A]	A0E	CAC-CAD	8.57	1.53	1.37
2	A	501[B]	A0E	CAC-CAD	8.40	1.53	1.37
2	B	501[B]	A0E	CAC-CAD	8.25	1.53	1.37
2	B	501[A]	A0E	CAC-CAD	8.16	1.53	1.37
2	A	501[A]	A0E	C2-N3	7.58	1.48	1.33
2	A	501[B]	A0E	C2-N3	7.47	1.47	1.33
2	A	501[B]	A0E	CAE-CAF	7.19	1.51	1.39
2	A	501[A]	A0E	C6-N1	7.10	1.45	1.35
2	A	501[A]	A0E	CAE-CAF	7.05	1.51	1.39
2	B	501[B]	A0E	C2-N3	6.97	1.46	1.33
2	B	501[B]	A0E	CAE-CAF	6.96	1.51	1.39
2	B	501[A]	A0E	CAE-CAF	6.93	1.50	1.39
2	A	501[B]	A0E	CBC-CBD	6.93	1.53	1.38
2	A	501[A]	A0E	CBC-CBD	6.85	1.53	1.38
2	B	501[A]	A0E	C2-N3	6.83	1.46	1.33
2	A	501[B]	A0E	C6-N1	6.75	1.45	1.35
2	B	501[B]	A0E	CBC-CBD	6.52	1.52	1.38
2	B	501[A]	A0E	CBC-CBD	6.48	1.52	1.38
2	A	501[A]	A0E	CBB-CBA	6.40	1.52	1.38
2	A	501[B]	A0E	CBB-CBA	6.35	1.52	1.38
2	B	501[B]	A0E	C6-N1	6.33	1.44	1.35
2	B	501[A]	A0E	CBB-CBA	6.15	1.51	1.38
2	B	501[A]	A0E	NAW-NAX	-6.13	1.27	1.39
2	B	501[B]	A0E	CBB-CBA	6.04	1.51	1.38
2	B	501[B]	A0E	NAW-NAX	-6.03	1.27	1.39
2	B	501[A]	A0E	C6-N1	5.94	1.43	1.35
2	A	501[A]	A0E	NAW-NAX	-5.66	1.28	1.39
2	A	501[B]	A0E	NAW-NAX	-5.63	1.28	1.39
2	A	501[B]	A0E	CAB-CAA	5.47	1.51	1.39
2	A	501[A]	A0E	CAB-CAA	5.45	1.51	1.39
2	B	501[B]	A0E	CAB-CAA	5.21	1.50	1.39
2	B	501[A]	A0E	CAB-CAA	5.15	1.50	1.39
2	B	501[A]	A0E	C5-C6	-4.72	1.31	1.43
2	B	501[B]	A0E	C5-C6	-4.64	1.31	1.43
3	B	504	OLC	O20-C1	4.31	1.45	1.33
3	A	503	OLC	O20-C1	4.28	1.45	1.33
3	A	502	OLC	O20-C1	4.25	1.45	1.33
3	B	503	OLC	O20-C1	4.25	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501[A]	A0E	C5-C6	-4.12	1.33	1.43
2	A	501[B]	A0E	C5-C6	-4.09	1.33	1.43
3	B	502	OLC	O20-C1	3.57	1.43	1.33
2	B	501[A]	A0E	CAL-NAM	-3.26	1.41	1.46
2	A	501[B]	A0E	OBJ-CBI	3.22	1.43	1.33
2	A	501[A]	A0E	OBJ-CBI	3.16	1.43	1.33
2	B	501[A]	A0E	CBD-CAY	-3.13	1.33	1.39
2	B	501[B]	A0E	CAL-NAM	-3.12	1.41	1.46
2	B	501[A]	A0E	OBJ-CBI	3.08	1.42	1.33
2	B	501[B]	A0E	OBJ-CBI	3.05	1.42	1.33
2	A	501[B]	A0E	C4-C5	3.02	1.50	1.43
2	B	501[B]	A0E	CBD-CAY	-2.96	1.33	1.39
2	A	501[B]	A0E	OAH-CAA	2.95	1.41	1.37
2	A	501[A]	A0E	C4-C5	2.92	1.50	1.43
2	B	501[A]	A0E	CBA-CAZ	-2.89	1.34	1.39
2	A	501[A]	A0E	OAH-CAA	2.89	1.41	1.37
2	B	501[B]	A0E	CBA-CAZ	-2.83	1.34	1.39
2	A	501[B]	A0E	CAL-NAM	-2.72	1.42	1.46
2	A	501[B]	A0E	CBD-CAY	-2.71	1.34	1.39
2	A	501[A]	A0E	CBD-CAY	-2.64	1.34	1.39
2	B	501[B]	A0E	C4-C5	2.61	1.49	1.43
2	B	501[A]	A0E	C4-N3	-2.59	1.29	1.33
2	A	501[A]	A0E	CBA-CAZ	-2.53	1.35	1.39
2	A	501[B]	A0E	C4-NAM	2.50	1.44	1.37
2	A	501[A]	A0E	C4-NAM	2.50	1.44	1.37
2	A	501[B]	A0E	CAF-NAJ	2.49	1.46	1.41
2	A	501[B]	A0E	CBA-CAZ	-2.48	1.35	1.39
2	A	501[A]	A0E	CAL-NAM	-2.46	1.42	1.46
2	B	501[B]	A0E	C4-N3	-2.44	1.29	1.33
2	B	501[A]	A0E	C4-C5	2.35	1.48	1.43
2	A	501[A]	A0E	CAO-NAJ	-2.31	1.43	1.46
2	A	501[A]	A0E	CAF-NAJ	2.17	1.46	1.41
2	B	501[A]	A0E	CAO-NAJ	-2.16	1.43	1.46
2	B	501[B]	A0E	CAO-NAJ	-2.14	1.43	1.46
2	B	501[B]	A0E	OAH-CAA	2.11	1.40	1.37
2	B	501[B]	A0E	C4-NAM	2.09	1.43	1.37
2	B	501[B]	A0E	CAF-NAJ	2.07	1.45	1.41
2	B	501[A]	A0E	CAC-CAB	-2.06	1.35	1.38
2	A	501[A]	A0E	C2-N1	2.04	1.35	1.32
2	B	501[A]	A0E	OAH-CAA	2.03	1.40	1.37

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501[B]	A0E	N1-C2-N3	-5.67	119.82	128.68
2	A	501[A]	A0E	N1-C2-N3	-5.51	120.06	128.68
2	A	501[B]	A0E	CBA-CAZ-CAY	5.46	120.13	115.66
2	B	501[B]	A0E	N1-C2-N3	-5.40	120.24	128.68
2	B	501[A]	A0E	N1-C2-N3	-5.30	120.40	128.68
2	A	501[A]	A0E	CBA-CAZ-CAY	5.25	119.95	115.66
2	B	501[A]	A0E	CAO-NAJ-CAK	5.09	122.76	111.52
2	B	501[B]	A0E	CAO-NAJ-CAK	4.95	122.45	111.52
2	B	501[B]	A0E	CAZ-CAY-NAX	4.90	122.11	117.83
2	B	501[B]	A0E	CBD-CAY-CAZ	-4.89	119.51	122.88
2	A	501[B]	A0E	CAO-NAJ-CAK	4.86	122.25	111.52
2	B	501[A]	A0E	CBA-CAZ-CAY	4.84	119.62	115.66
2	B	501[B]	A0E	CBA-CAZ-CAY	4.64	119.45	115.66
2	A	501[A]	A0E	CBD-CAY-CAZ	-4.23	119.96	122.88
2	A	501[B]	A0E	CBD-CAY-CAZ	-4.08	120.06	122.88
2	B	501[A]	A0E	OAH-CAA-CAF	3.99	121.51	116.06
2	B	501[B]	A0E	OAH-CAA-CAF	3.97	121.47	116.06
2	B	501[A]	A0E	OAH-CAA-CAB	-3.90	117.69	124.37
2	B	501[B]	A0E	OAH-CAA-CAB	-3.87	117.74	124.37
2	A	501[A]	A0E	CAO-NAJ-CAK	3.86	120.03	111.52
2	A	501[B]	A0E	OAH-CAA-CAF	3.83	121.29	116.06
2	A	501[A]	A0E	CAN-NAM-CAL	3.81	119.92	111.52
2	A	501[B]	A0E	CAN-CAO-NAJ	3.73	117.95	110.70
2	B	501[A]	A0E	CAI-OAH-CAA	-3.68	111.98	117.53
2	B	501[B]	A0E	CAI-OAH-CAA	-3.66	112.01	117.53
2	B	501[A]	A0E	CBD-CAY-CAZ	-3.55	120.43	122.88
2	B	501[B]	A0E	CAL-CAK-NAJ	3.49	117.48	110.70
2	B	501[A]	A0E	CAL-CAK-NAJ	3.44	117.38	110.70
2	A	501[B]	A0E	OAH-CAA-CAB	-3.32	118.69	124.37
2	A	501[B]	A0E	CAL-CAK-NAJ	3.24	116.99	110.70
2	B	501[A]	A0E	CAN-NAM-CAL	3.21	118.61	111.52
2	B	501[B]	A0E	CAN-NAM-CAL	3.17	118.51	111.52
3	B	502	OLC	O20-C1-C2	3.17	121.84	111.91
2	B	501[A]	A0E	CAN-CAO-NAJ	2.92	116.38	110.70
2	B	501[A]	A0E	C5-CAV-NAW	-2.92	104.39	110.43
2	A	501[A]	A0E	OAH-CAA-CAF	2.90	120.02	116.06
2	A	501[B]	A0E	CAN-NAM-CAL	2.86	117.83	111.52
2	A	501[A]	A0E	C5-CAV-NAW	-2.83	104.57	110.43
2	B	501[B]	A0E	C5-CAV-NAW	-2.77	104.68	110.43
2	B	501[B]	A0E	CAN-CAO-NAJ	2.76	116.07	110.70
2	A	501[B]	A0E	C5-CAV-NAW	-2.76	104.72	110.43
3	B	503	OLC	O20-C1-C2	2.65	120.23	111.91
3	A	502	OLC	O20-C1-C2	2.64	120.21	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	504	OLC	O20-C1-C2	2.64	120.20	111.91
2	A	501[A]	A0E	CAZ-CAY-NAX	2.63	120.13	117.83
3	A	503	OLC	O20-C1-C2	2.62	120.13	111.91
2	A	501[A]	A0E	OAH-CAA-CAB	-2.56	119.98	124.37
2	A	501[B]	A0E	CAE-CAF-NAJ	-2.54	118.77	122.52
3	B	502	OLC	O20-C1-O19	-2.54	117.19	123.59
2	A	501[A]	A0E	CAC-CAD-CAE	-2.49	120.05	123.29
2	A	501[A]	A0E	CAI-OAH-CAA	-2.38	113.94	117.53
2	A	501[B]	A0E	CAC-CAD-CAE	-2.29	120.32	123.29
2	B	501[A]	A0E	CBG-CBH-CBI	-2.26	108.12	113.06
2	B	501[A]	A0E	CAE-CAF-NAJ	-2.25	119.19	122.52
2	B	501[B]	A0E	CAE-CAF-NAJ	-2.19	119.28	122.52
2	B	501[A]	A0E	OBJ-CBI-CBH	2.11	120.57	112.23
2	A	501[A]	A0E	CAL-CAK-NAJ	2.05	114.69	110.70
2	B	501[B]	A0E	CAC-CAD-CAE	-2.02	120.66	123.29
2	A	501[B]	A0E	CAI-OAH-CAA	-2.01	114.50	117.53

There are no chirality outliers.

All (84) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501[A]	A0E	C5-C4-NAM-CAL
2	A	501[A]	A0E	N3-C4-NAM-CAL
2	A	501[A]	A0E	CAY-CAZ-CBE-NBF
2	A	501[A]	A0E	CBH-CBI-OBJ-CBK
2	A	501[B]	A0E	C5-C4-NAM-CAL
2	A	501[B]	A0E	N3-C4-NAM-CAL
2	B	501[A]	A0E	C5-C4-NAM-CAL
2	B	501[A]	A0E	N3-C4-NAM-CAL
2	B	501[B]	A0E	C5-C4-NAM-CAL
2	B	501[B]	A0E	N3-C4-NAM-CAL
2	B	501[B]	A0E	CAY-CAZ-CBE-NBF
3	B	503	OLC	O20-C21-C22-C24
3	B	503	OLC	O20-C21-C22-O23
3	B	504	OLC	O20-C21-C22-O23
2	A	501[A]	A0E	OBL-CBI-OBJ-CBK
2	B	501[B]	A0E	CBH-CBI-OBJ-CBK
2	B	501[B]	A0E	OBL-CBI-OBJ-CBK
2	B	501[B]	A0E	CAZ-CBE-NBF-CBG
3	A	503	OLC	C2-C1-O20-C21
3	A	503	OLC	O19-C1-O20-C21
3	B	502	OLC	C3-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
2	A	501[B]	A0E	CAZ-CBE-NBF-CBG
2	A	501[B]	A0E	CBH-CBI-OBJ-CBK
2	B	501[B]	A0E	CBH-CBG-NBF-CBE
3	A	502	OLC	C1-C2-C3-C4
3	A	503	OLC	C1-C2-C3-C4
3	B	502	OLC	C1-C2-C3-C4
2	B	501[A]	A0E	NBF-CBG-CBH-CBI
2	B	501[B]	A0E	NBF-CBG-CBH-CBI
2	A	501[A]	A0E	CAF-CAA-OAH-CAI
3	B	502	OLC	C5-C6-C7-C8
3	B	504	OLC	O20-C21-C22-C24
2	A	501[A]	A0E	CAA-CAF-NAJ-CAK
2	A	501[B]	A0E	CAA-CAF-NAJ-CAK
2	B	501[A]	A0E	CAA-CAF-NAJ-CAK
2	B	501[B]	A0E	CAA-CAF-NAJ-CAK
2	A	501[A]	A0E	CAZ-CBE-NBF-CBG
3	B	503	OLC	C1-C2-C3-C4
3	A	502	OLC	C2-C3-C4-C5
3	B	504	OLC	C1-C2-C3-C4
3	A	503	OLC	C6-C7-C8-C9
3	B	502	OLC	C11-C12-C13-C14
3	A	502	OLC	C6-C7-C8-C9
3	A	502	OLC	C4-C5-C6-C7
3	A	502	OLC	C14-C15-C16-C17
3	B	503	OLC	C3-C4-C5-C6
2	A	501[A]	A0E	CAB-CAA-OAH-CAI
3	B	504	OLC	C7-C8-C9-C10
3	B	504	OLC	C12-C13-C14-C15
3	B	504	OLC	C2-C3-C4-C5
3	A	502	OLC	C15-C16-C17-C18
2	A	501[B]	A0E	CAY-CAZ-CBE-NBF
3	A	503	OLC	C3-C4-C5-C6
3	A	503	OLC	C2-C3-C4-C5
2	A	501[B]	A0E	CAE-CAF-NAJ-CAK
3	B	503	OLC	C11-C12-C13-C14
2	B	501[B]	A0E	CBA-CAZ-CBE-NBF
2	A	501[A]	A0E	CAE-CAF-NAJ-CAK
2	B	501[A]	A0E	CAA-CAF-NAJ-CAO
3	A	503	OLC	C4-C5-C6-C7
2	A	501[A]	A0E	CBA-CAZ-CBE-NBF
2	B	501[B]	A0E	CAE-CAF-NAJ-CAK
2	B	501[A]	A0E	CAE-CAF-NAJ-CAK

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Mol	Chain	Res	Type	Atoms
3	B	503	OLC	C4-C5-C6-C7
2	A	501[B]	A0E	OBL-CBI-OBJ-CBK
3	A	503	OLC	C9-C10-C11-C12
3	B	502	OLC	C14-C15-C16-C17
3	B	502	OLC	C15-C16-C17-C18
3	B	504	OLC	C15-C16-C17-C18
2	A	501[A]	A0E	CAA-CAF-NAJ-CAO
2	B	501[B]	A0E	CAA-CAF-NAJ-CAO
3	B	502	OLC	C7-C8-C9-C10
3	B	503	OLC	C7-C8-C9-C10
3	B	503	OLC	C9-C10-C11-C12
3	B	504	OLC	C3-C4-C5-C6
3	B	504	OLC	C4-C5-C6-C7
2	A	501[B]	A0E	CBG-CBH-CBI-OBL
3	B	503	OLC	O19-C1-O20-C21
3	B	503	OLC	C2-C1-O20-C21
2	A	501[A]	A0E	CBH-CBG-NBF-CBE
3	B	504	OLC	C9-C10-C11-C12
3	A	502	OLC	C9-C10-C11-C12
3	A	503	OLC	C11-C12-C13-C14
2	A	501[B]	A0E	CBG-CBH-CBI-OBJ

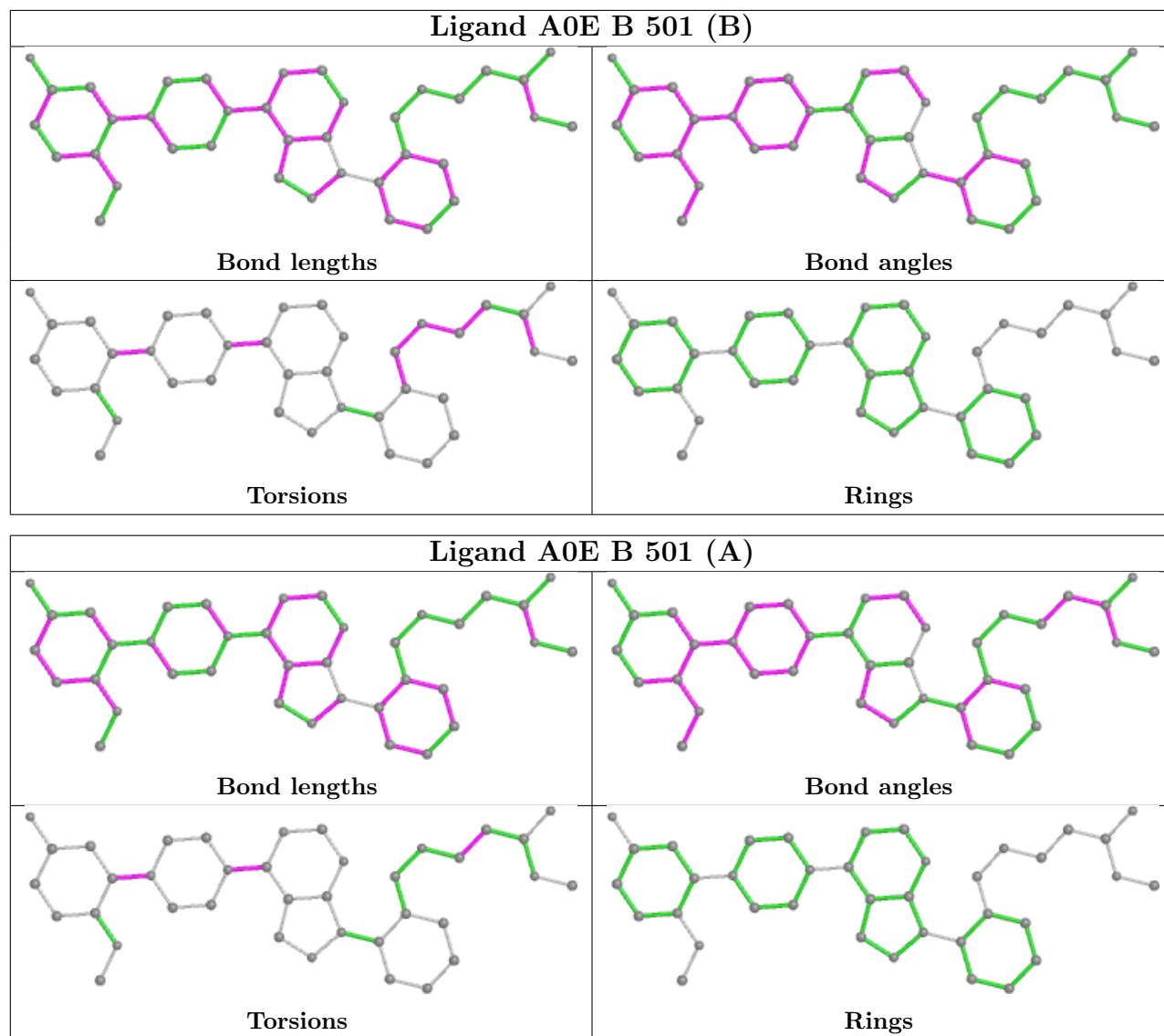
There are no ring outliers.

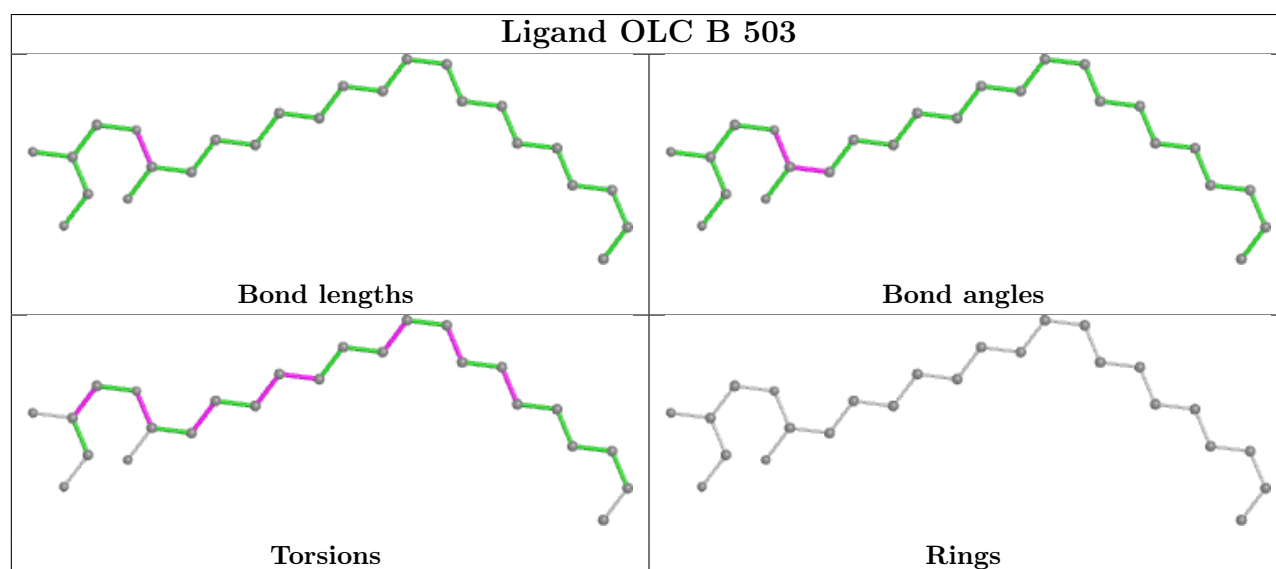
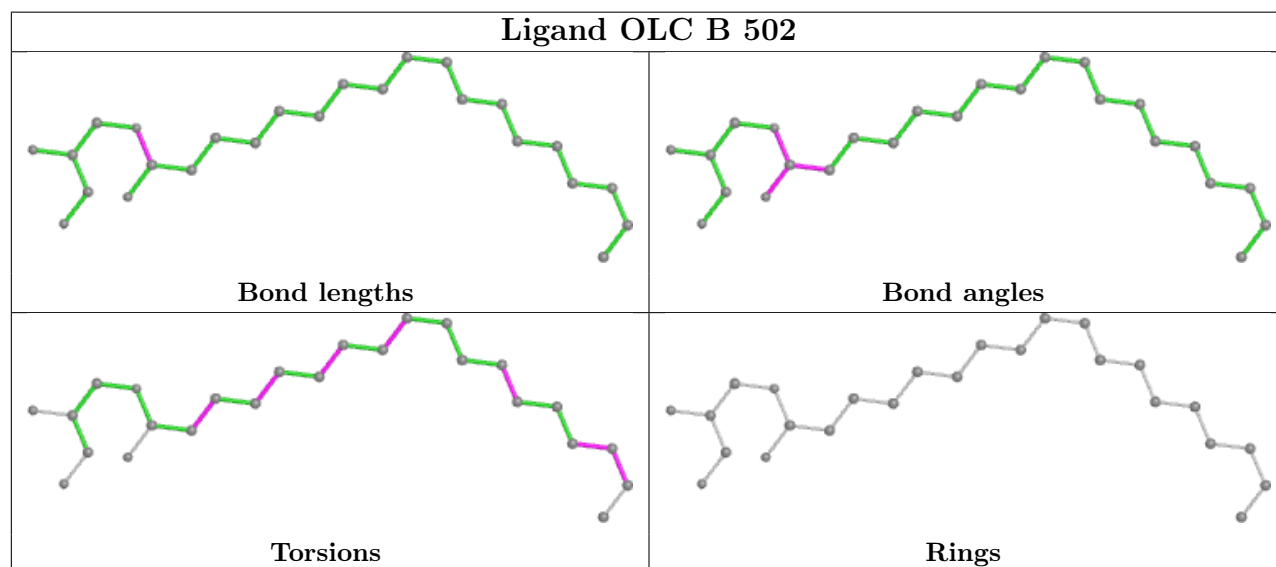
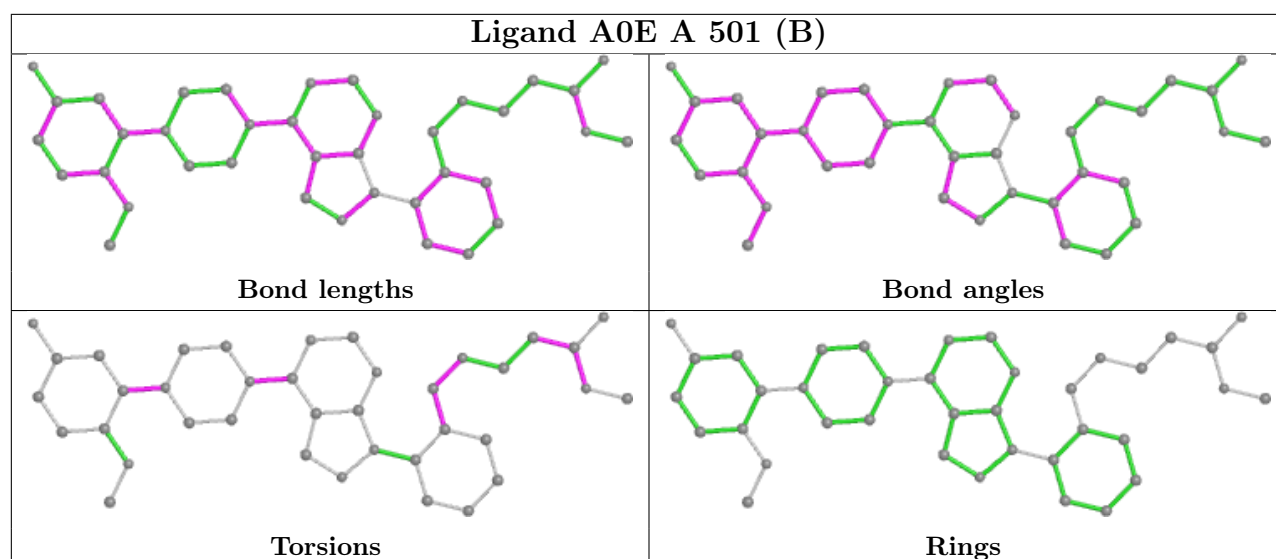
6 monomers are involved in 18 short contacts:

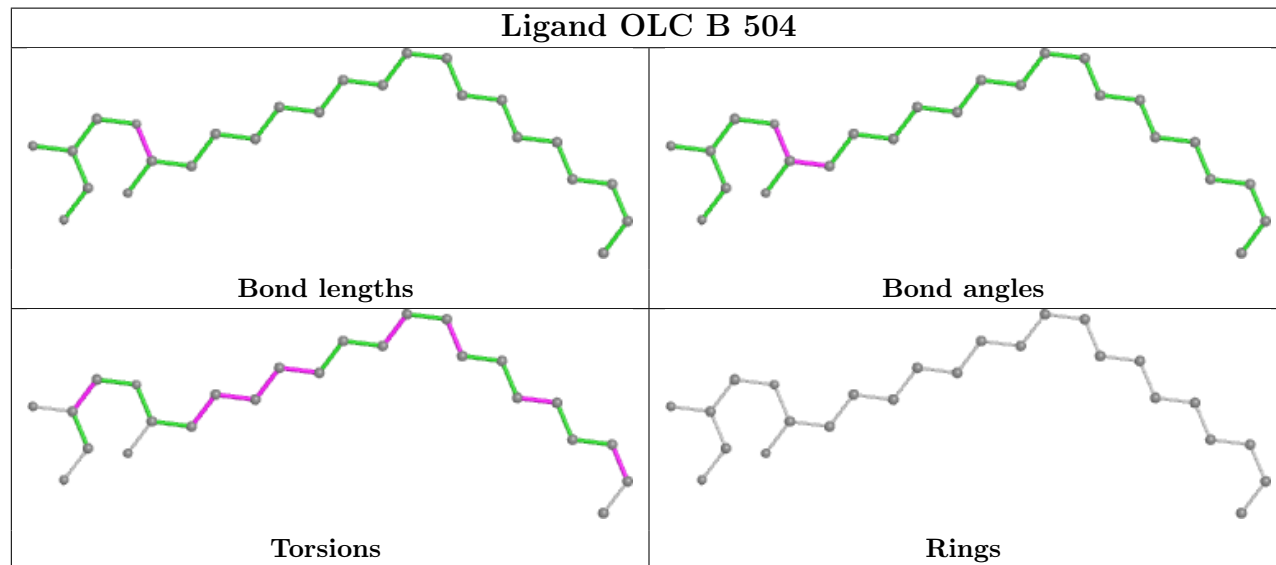
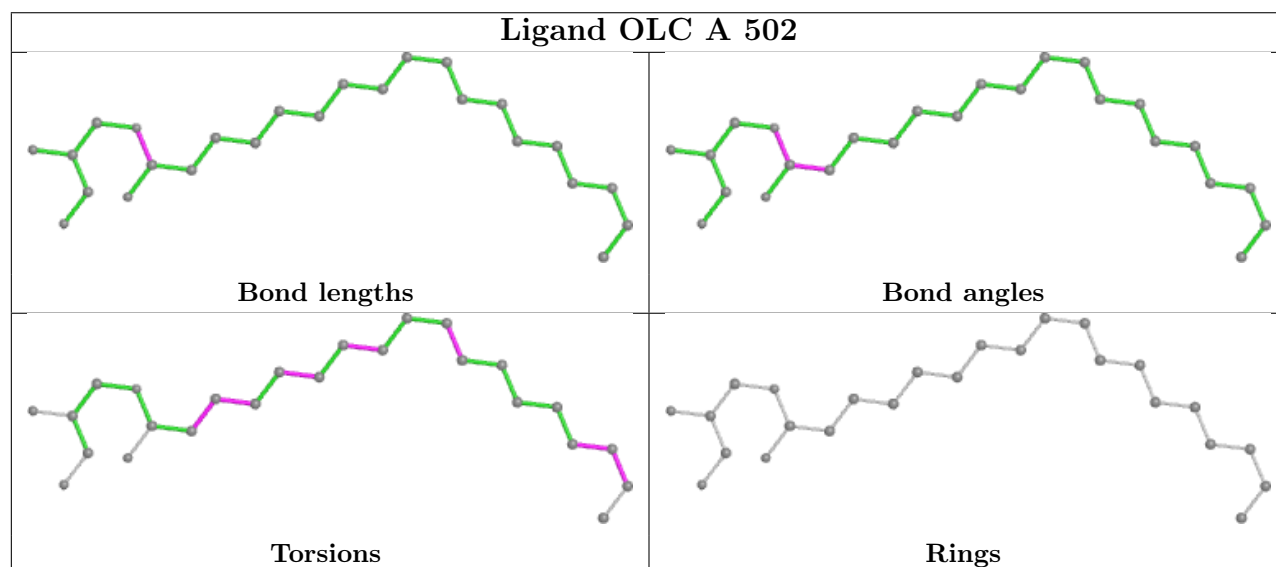
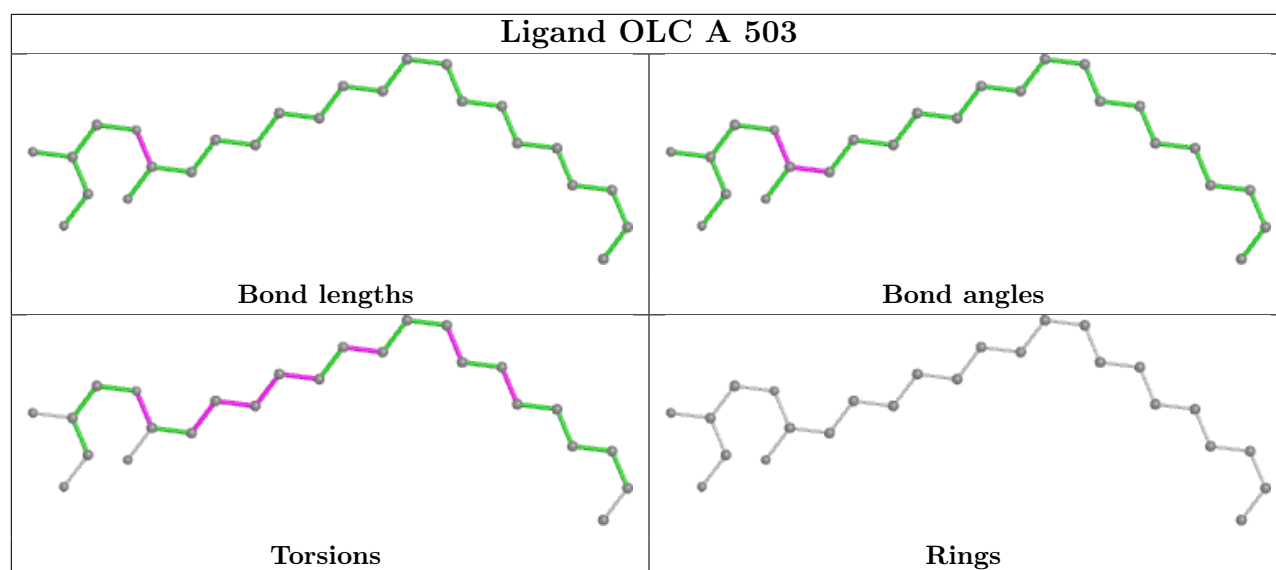
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	501[B]	A0E	2	0
2	A	501[B]	A0E	2	0
3	B	502	OLC	3	0
3	B	503	OLC	3	0
3	B	504	OLC	4	0
2	A	501[A]	A0E	4	0

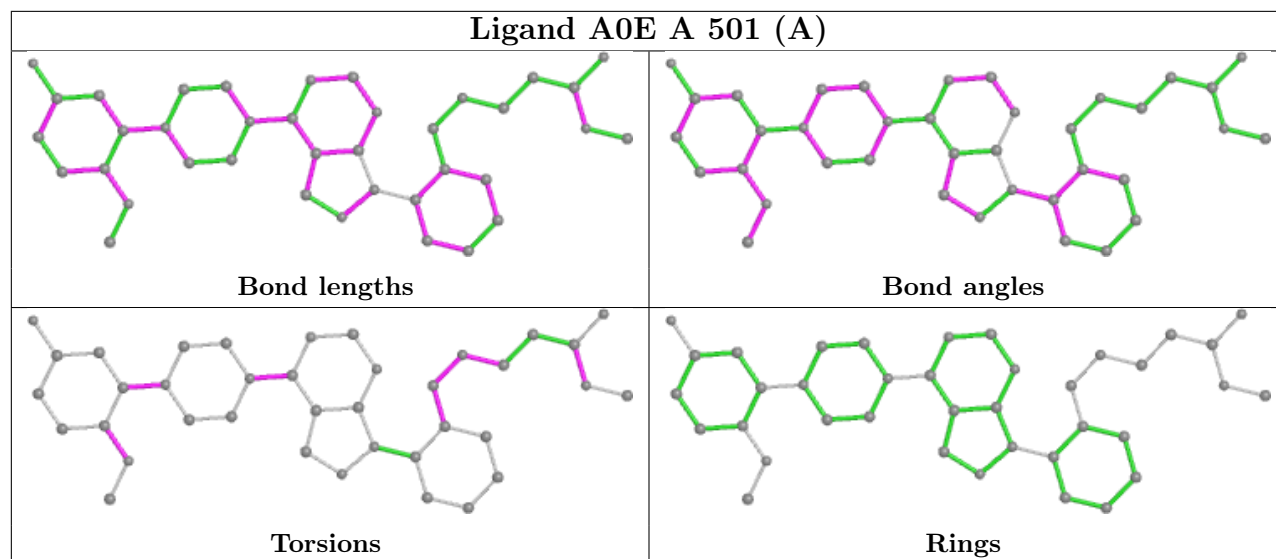
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	468/523 (89%)	0.27	43 (9%) 9 12	37, 50, 88, 141	3 (0%)
1	B	468/523 (89%)	0.13	33 (7%) 16 21	35, 48, 82, 120	4 (0%)
All	All	936/1046 (89%)	0.20	76 (8%) 12 16	35, 49, 84, 141	7 (0%)

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	301	VAL	15.1
1	A	300	GLY	9.2
1	A	299	ALA	6.3
1	A	302	GLN	5.8
1	B	358	ASN	5.7
1	A	296	PHE	5.4
1	A	471	GLY	5.2
1	B	4	GLN	5.1
1	B	302	GLN	4.7
1	A	357	ASP	4.6
1	A	470	HIS	4.6
1	A	305	ILE	4.2
1	B	5	LYS	3.9
1	B	296	PHE	3.9
1	A	358	ASN	3.8
1	A	259	GLU	3.8
1	B	426	TYR	3.7
1	B	301	VAL	3.6
1	A	48	ASP	3.4
1	A	303	GLU	3.4
1	B	357	ASP	3.3
1	A	298	ASP	3.3
1	A	50	GLY	3.3
1	A	304	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	425	HIS	3.2
1	B	359	TYR	3.1
1	A	468	GLN	3.1
1	B	379	ILE	3.0
1	A	426	TYR	3.0
1	A	233	GLN	3.0
1	B	304	PRO	3.0
1	A	375	ALA	2.9
1	A	297	LYS	2.9
1	A	469	ALA	2.8
1	A	430	TYR	2.8
1	A	237	GLN	2.8
1	B	232	THR	2.8
1	B	298	ASP	2.8
1	B	320	VAL	2.8
1	A	224	GLN	2.8
1	B	375	ALA	2.7
1	A	467	GLY	2.7
1	B	231	GLY	2.7
1	A	379	ILE	2.6
1	B	237	GLN	2.6
1	B	52	ALA	2.5
1	B	430	TYR	2.4
1	B	254	GLN	2.4
1	A	255	VAL	2.4
1	B	233	GLN	2.4
1	A	322	SER	2.4
1	B	322	SER	2.4
1	A	320	VAL	2.4
1	B	292	SER	2.4
1	A	360	ASN	2.4
1	A	295	ILE	2.4
1	A	334	LEU	2.4
1	B	317	ILE	2.3
1	A	258	LEU	2.3
1	A	162	ILE	2.3
1	B	297	LYS	2.3
1	B	470	HIS	2.3
1	B	295	ILE	2.3
1	A	234	ASP	2.2
1	B	234	ASP	2.2
1	A	221	ASN	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	334	LEU	2.2
1	A	321	VAL	2.2
1	B	175	GLU	2.2
1	A	337	ILE	2.1
1	B	471	GLY	2.1
1	A	231	GLY	2.1
1	B	377	PHE	2.1
1	B	383	PRO	2.1
1	A	317	ILE	2.0
1	A	47	THR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

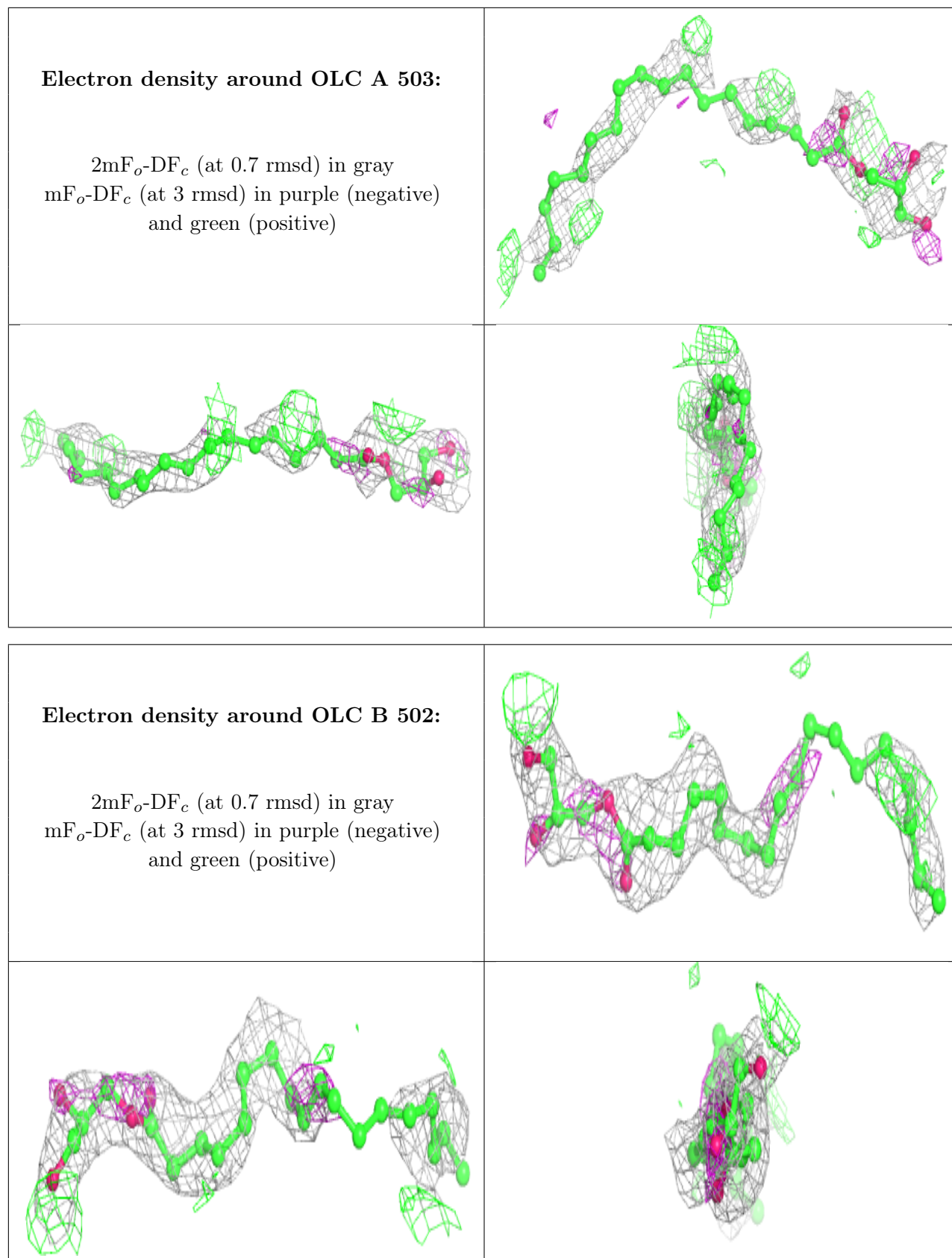
6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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
3	OLC	A	503	25/25	0.57	0.43	68,84,93,106	0
3	OLC	B	502	25/25	0.69	0.38	49,66,78,89	0
3	OLC	B	504	25/25	0.75	0.23	55,67,80,83	0
3	OLC	A	502	25/25	0.81	0.23	47,58,79,86	0
2	A0E	B	501[A]	38/38	0.83	0.30	50,57,66,76	38
2	A0E	B	501[B]	38/38	0.83	0.30	50,55,61,66	38
3	OLC	B	503	25/25	0.86	0.21	49,61,74,77	0
2	A0E	A	501[B]	38/38	0.92	0.22	43,50,61,64	38
2	A0E	A	501[A]	38/38	0.92	0.22	43,50,62,65	38

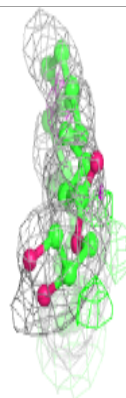
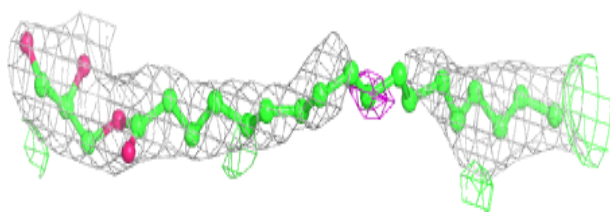
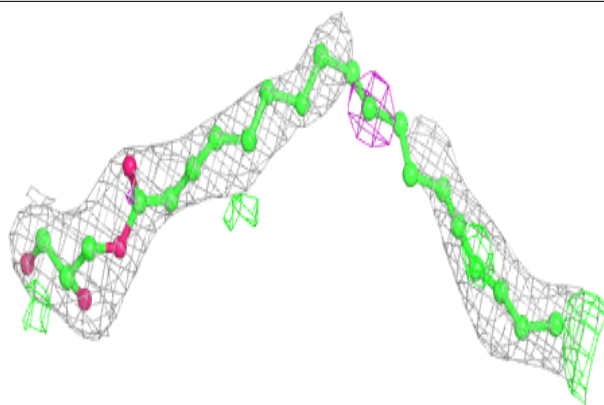
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different

orientation to approximate a three-dimensional view.

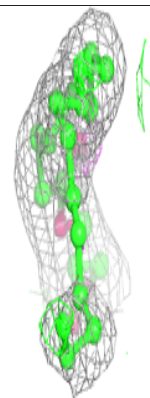
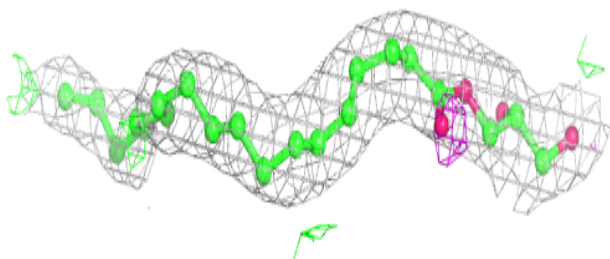
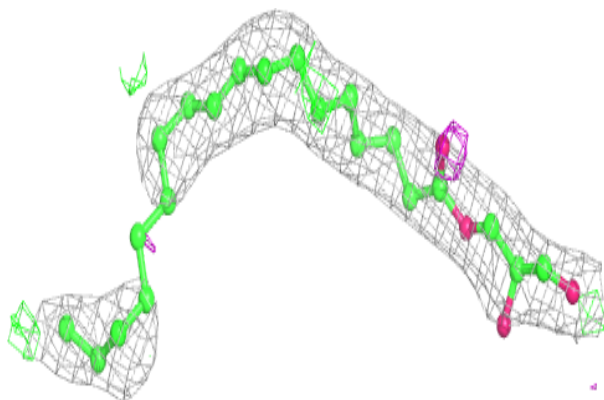


Electron density around OLC B 504:

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

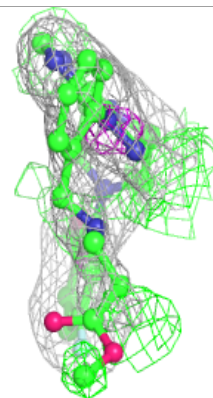
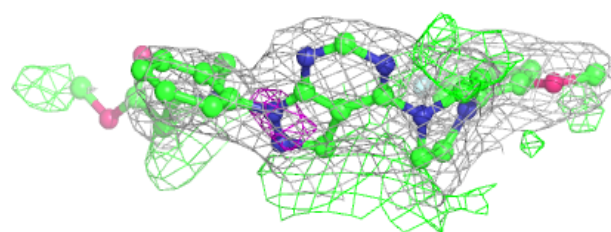
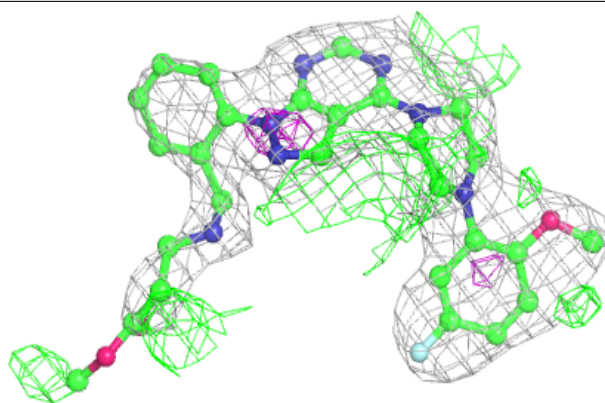
**Electron density around OLC A 502:**

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



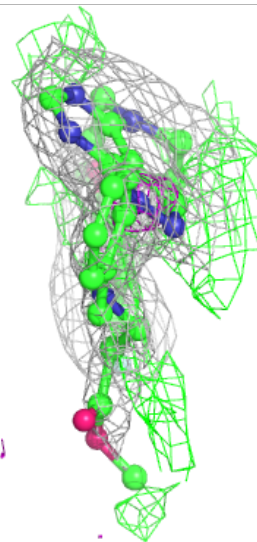
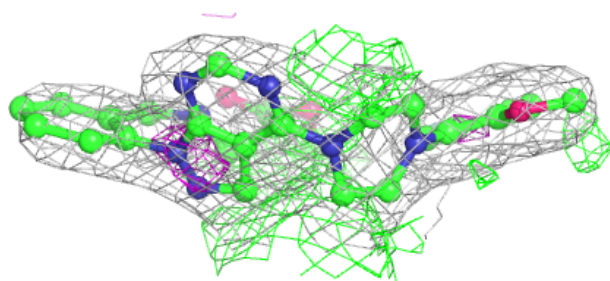
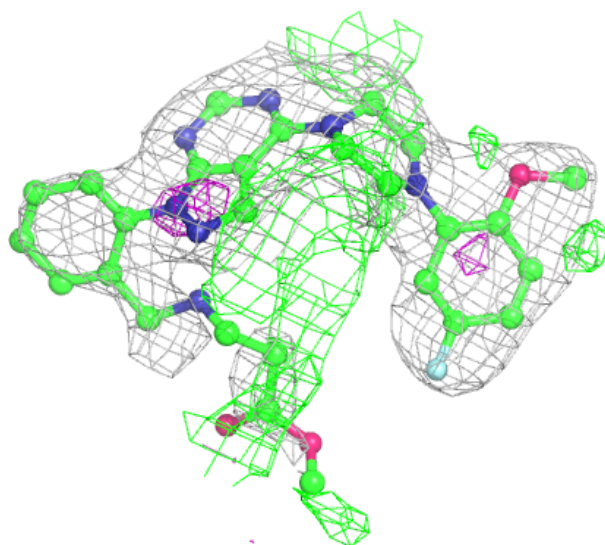
Electron density around A0E B 501 (A):

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



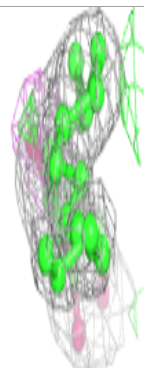
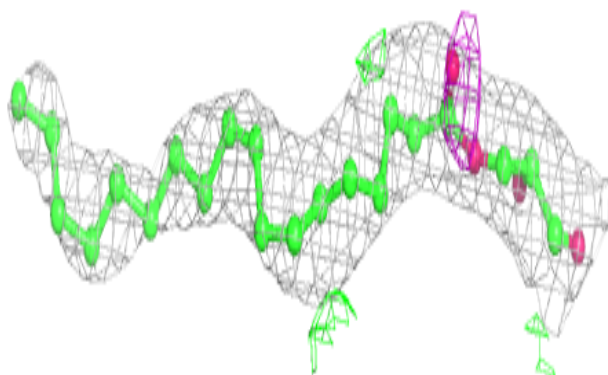
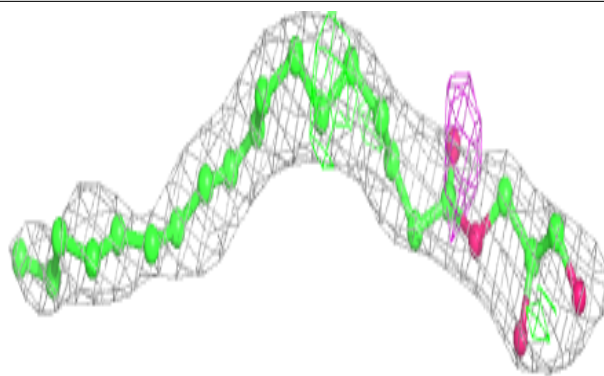
Electron density around A0E B 501 (B):

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



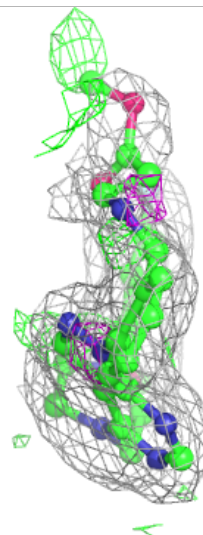
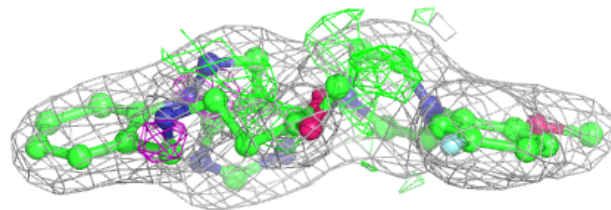
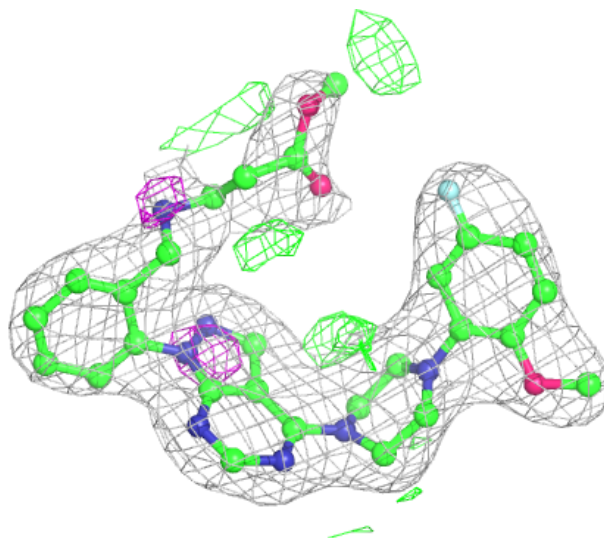
Electron density around OLC B 503:

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



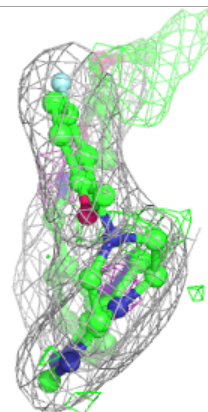
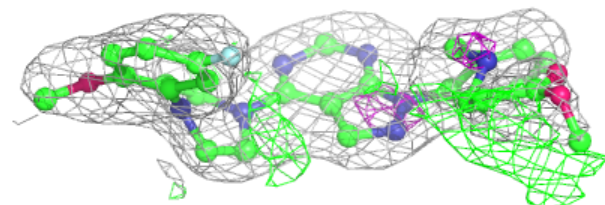
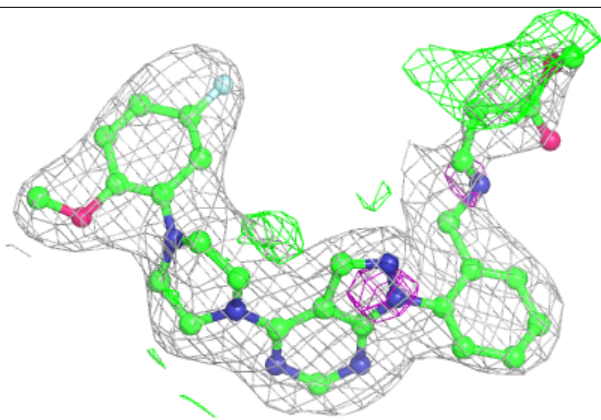
Electron density around A0E A 501 (B):

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



Electron density around A0E A 501 (A):

$2mF_o - DF_c$ (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.