



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2023 – 01:37 PM JST

PDB ID : 5AZP
Title : Crystal structure of a membrane protein from *Pseudomonas aeruginosa*
Authors : Yonehara, R.; Yamashita, E.; Nakagawa, A.
Deposited on : 2015-10-21
Resolution : 1.69 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 : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.36
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.36

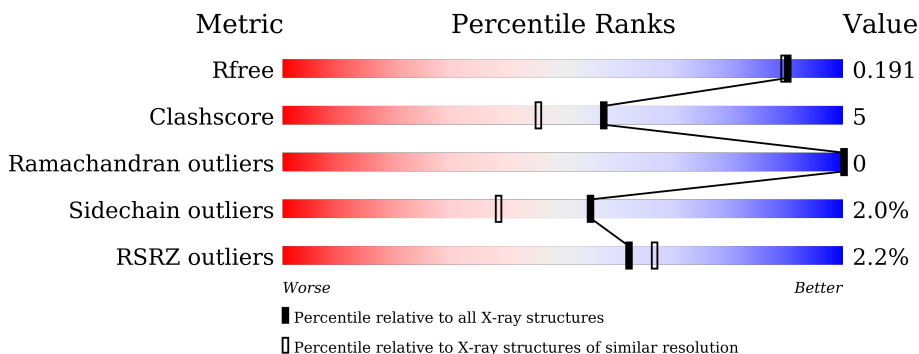
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.69 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	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	455	 2% 85% 12% ..
1	B	455	 2% 86% 10% ..
1	C	455	 2% 88% 9% ..

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
5	GOL	B	505	-	-	X	-
6	FMT	C	511	-	-	X	-
8	ACT	B	515	-	-	X	-
8	ACT	B	516	-	-	X	-
8	ACT	C	519	-	-	X	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 13057 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 Multidrug efflux outer membrane protein OprN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	446	3584	2216	672	695	1	0	30	0
1	B	450	3620	2244	673	702	1	0	30	0
1	C	444	3589	2229	666	693	1	0	34	0

There are 24 discrepancies between the modelled and reference sequences:

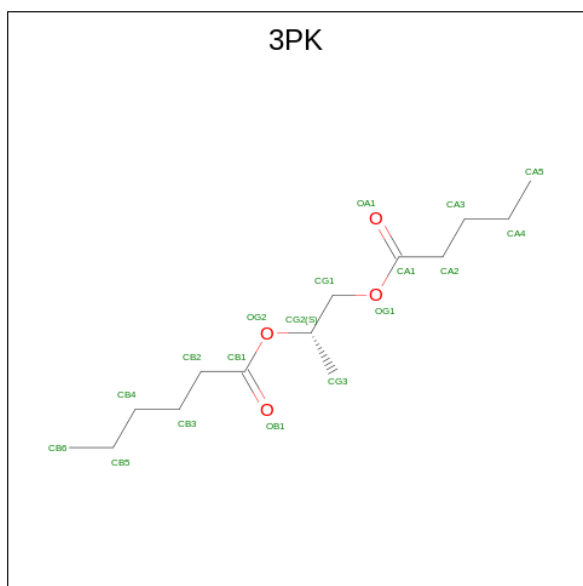
Chain	Residue	Modelled	Actual	Comment	Reference
A	448	GLY	-	expression tag	UNP Q9I0Y7
A	449	SER	-	expression tag	UNP Q9I0Y7
A	450	HIS	-	expression tag	UNP Q9I0Y7
A	451	HIS	-	expression tag	UNP Q9I0Y7
A	452	HIS	-	expression tag	UNP Q9I0Y7
A	453	HIS	-	expression tag	UNP Q9I0Y7
A	454	HIS	-	expression tag	UNP Q9I0Y7
A	455	HIS	-	expression tag	UNP Q9I0Y7
B	448	GLY	-	expression tag	UNP Q9I0Y7
B	449	SER	-	expression tag	UNP Q9I0Y7
B	450	HIS	-	expression tag	UNP Q9I0Y7
B	451	HIS	-	expression tag	UNP Q9I0Y7
B	452	HIS	-	expression tag	UNP Q9I0Y7
B	453	HIS	-	expression tag	UNP Q9I0Y7
B	454	HIS	-	expression tag	UNP Q9I0Y7
B	455	HIS	-	expression tag	UNP Q9I0Y7
C	448	GLY	-	expression tag	UNP Q9I0Y7
C	449	SER	-	expression tag	UNP Q9I0Y7
C	450	HIS	-	expression tag	UNP Q9I0Y7
C	451	HIS	-	expression tag	UNP Q9I0Y7
C	452	HIS	-	expression tag	UNP Q9I0Y7
C	453	HIS	-	expression tag	UNP Q9I0Y7
C	454	HIS	-	expression tag	UNP Q9I0Y7

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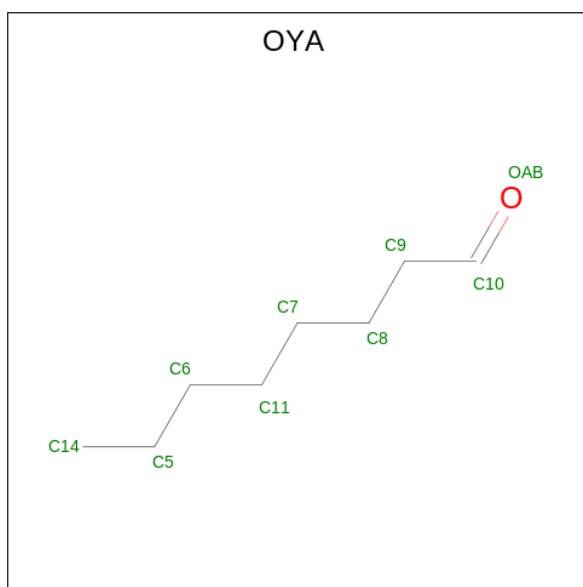
Chain	Residue	Modelled	Actual	Comment	Reference
C	455	HIS	-	expression tag	UNP Q9I0Y7

- Molecule 2 is (2S)-1-(pentanoyloxy)propan-2-yl hexanoate (three-letter code: 3PK) (formula: $C_{14}H_{26}O_4$).



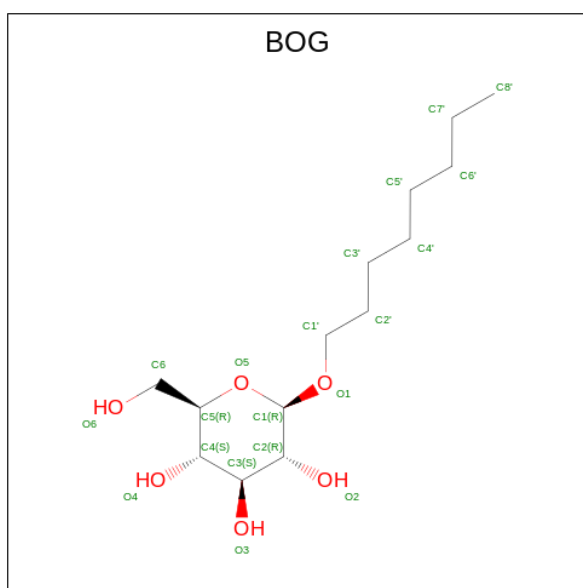
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			18	14	4		
2	C	1	Total	C	O	0	0
			18	14	4		

- Molecule 3 is OCTANAL (three-letter code: OYA) (formula: $C_8H_{16}O$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			9	8	1		
3	C	1	Total	C	O	0	0
			9	8	1		

- Molecule 4 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



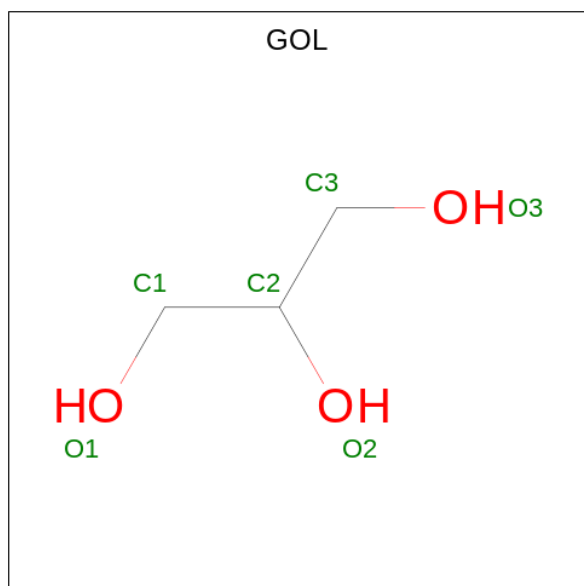
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		
4	A	1	Total	C	O	0	0
			20	14	6		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			20	14	6		
4	B	1	Total	C	O	0	0
			20	14	6		
4	C	1	Total	C	O	0	0
			20	14	6		
4	C	1	Total	C	O	0	0
			20	14	6		
4	C	1	Total	C	O	0	0
			20	14	6		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



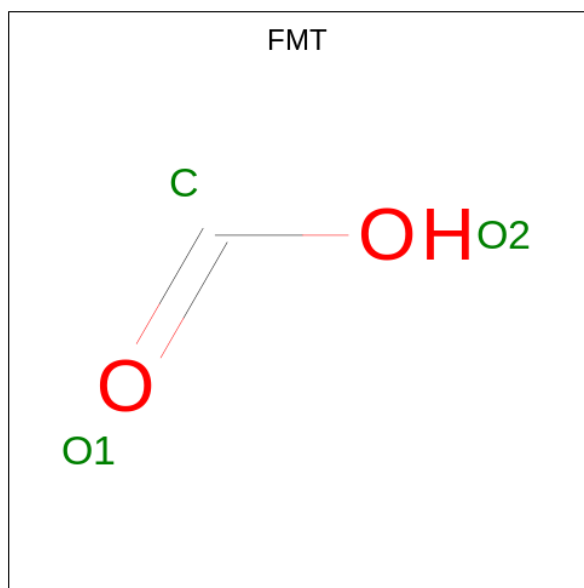
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	A	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	B	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		
5	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 6 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			3	1	2		
6	A	1	Total	C	O	0	0
			3	1	2		
6	A	1	Total	C	O	0	0
			3	1	2		
6	A	1	Total	C	O	0	0
			3	1	2		

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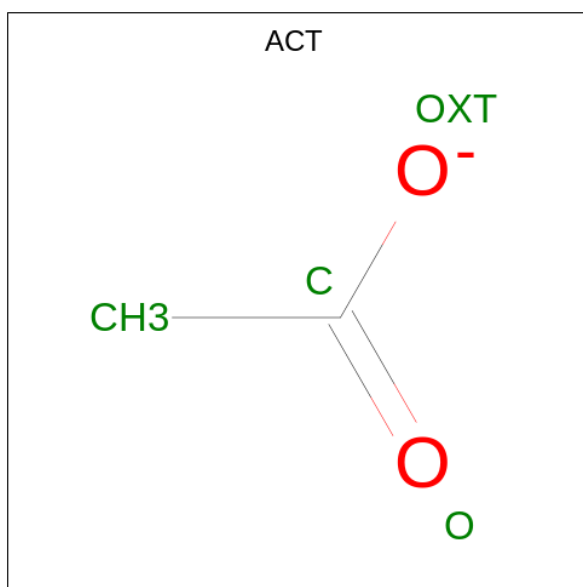
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 3 1 2	0	0
6	A	1	Total C O 3 1 2	0	0
6	B	1	Total C O 3 1 2	0	0
6	B	1	Total C O 3 1 2	0	0
6	B	1	Total C O 3 1 2	0	0
6	B	1	Total C O 3 1 2	0	0
6	B	1	Total C O 3 1 2	0	0
6	B	1	Total C O 3 1 2	0	0
6	B	1	Total C O 3 1 2	0	0
6	B	1	Total C O 3 1 2	0	0
6	C	1	Total C O 3 1 2	0	0
6	C	1	Total C O 3 1 2	0	0
6	C	1	Total C O 3 1 2	0	0
6	C	1	Total C O 3 1 2	0	0
6	C	1	Total C O 3 1 2	0	0

- Molecule 7 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total Na 1 1	0	0
7	B	1	Total Na 1 1	0	0
7	C	1	Total Na 1 1	0	0

- Molecule 8 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total C O 4 2 2	0	0
8	A	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	B	1	Total C O 4 2 2	0	0
8	C	1	Total C O 4 2 2	0	0
8	C	1	Total C O 4 2 2	0	0
8	C	1	Total C O 4 2 2	0	0
8	C	1	Total C O 4 2 2	0	0

- Molecule 9 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	660	Total O 660 660	0	0
9	B	627	Total O 627 627	0	0
9	C	598	Total O 598 598	0	0

4 Data and refinement statistics

Property	Value	Source
Space group	I 4	Depositor
Cell constants a, b, c, α , β , γ	257.51Å 257.51Å 81.83Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.69 39.92 – 1.69	Depositor EDS
% Data completeness (in resolution range)	99.4 (50.00-1.69) 99.4 (39.92-1.69)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.94 (at 1.69Å)	Xtrriage
Refinement program	REFMAC 5.8.0131	Depositor
R, R_{free}	0.160 , 0.180 0.173 , 0.191	Depositor DCC
R_{free} test set	15033 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtrriage
Anisotropy	0.026	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 58.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.010 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13057	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: 3PK, GOL, NA, FMT, BOG, ACT, OYA

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	1.01	5/3720 (0.1%)	1.12	36/5030 (0.7%)
1	B	1.07	7/3760 (0.2%)	1.30	36/5084 (0.7%)
1	C	1.02	7/3739 (0.2%)	1.12	29/5056 (0.6%)
All	All	1.03	19/11219 (0.2%)	1.19	101/15170 (0.7%)

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

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

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	399	GLU	CD-OE1	7.28	1.33	1.25
1	B	399	GLU	CB-CG	-6.68	1.39	1.52
1	A	31	GLU	CD-OE1	6.64	1.32	1.25
1	A	235	GLU	CD-OE2	6.39	1.32	1.25
1	B	152	GLU	CD-OE1	6.31	1.32	1.25
1	C	48	GLU	CD-OE2	6.29	1.32	1.25
1	B	413	GLU	CD-OE2	5.94	1.32	1.25
1	B	235	GLU	CD-OE1	5.76	1.31	1.25
1	A	425	GLU	CD-OE2	5.73	1.31	1.25
1	A	361	GLU	CD-OE1	5.51	1.31	1.25
1	C	413	GLU	CD-OE2	5.50	1.31	1.25
1	C	411	GLU	CG-CD	5.43	1.60	1.51
1	C	119	ASP	N-CA	5.39	1.57	1.46
1	C	274[A]	ARG	CZ-NH1	-5.32	1.26	1.33
1	C	274[B]	ARG	CZ-NH1	-5.32	1.26	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1	CYS	CA-CB	5.23	1.65	1.53
1	B	399	GLU	CD-OE2	-5.10	1.20	1.25
1	C	235	GLU	CD-OE1	5.06	1.31	1.25
1	B	1	CYS	CA-CB	5.00	1.65	1.53

All (101) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	65[A]	ARG	NE-CZ-NH1	-21.97	109.31	120.30
1	B	65[B]	ARG	NE-CZ-NH1	-21.97	109.31	120.30
1	B	65[A]	ARG	NE-CZ-NH2	19.70	130.15	120.30
1	B	65[B]	ARG	NE-CZ-NH2	19.70	130.15	120.30
1	C	123[A]	ARG	NE-CZ-NH2	-12.92	113.84	120.30
1	C	123[B]	ARG	NE-CZ-NH2	-12.92	113.84	120.30
1	B	381	ARG	NE-CZ-NH1	12.88	126.74	120.30
1	B	412	ARG	NE-CZ-NH1	-11.71	114.44	120.30
1	B	123[A]	ARG	NE-CZ-NH1	11.51	126.06	120.30
1	B	123[B]	ARG	NE-CZ-NH1	11.51	126.06	120.30
1	B	412	ARG	NE-CZ-NH2	11.07	125.84	120.30
1	A	269[A]	ARG	NE-CZ-NH2	-10.71	114.94	120.30
1	A	269[B]	ARG	NE-CZ-NH2	-10.71	114.94	120.30
1	B	381	ARG	NE-CZ-NH2	-10.68	114.96	120.30
1	C	63	ARG	NE-CZ-NH1	10.35	125.47	120.30
1	B	123[A]	ARG	NE-CZ-NH2	-10.01	115.30	120.30
1	B	123[B]	ARG	NE-CZ-NH2	-10.01	115.30	120.30
1	B	264	ARG	NE-CZ-NH1	9.87	125.24	120.30
1	C	63	ARG	CB-CG-CD	8.98	134.95	111.60
1	A	372	ARG	NE-CZ-NH2	-8.75	115.92	120.30
1	C	233	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	B	70[A]	LEU	CB-CG-CD1	8.64	125.70	111.00
1	B	70[B]	LEU	CB-CG-CD1	8.64	125.70	111.00
1	A	123[A]	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	A	123[B]	ARG	NE-CZ-NH2	-8.53	116.03	120.30
1	B	264	ARG	NE-CZ-NH2	-8.43	116.08	120.30
1	C	334	ARG	NE-CZ-NH2	-8.39	116.11	120.30
1	C	123[A]	ARG	NE-CZ-NH1	8.33	124.46	120.30
1	C	123[B]	ARG	NE-CZ-NH1	8.33	124.46	120.30
1	C	63	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	C	412	ARG	NE-CZ-NH2	7.85	124.22	120.30
1	A	141	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	A	123[A]	ARG	NE-CZ-NH1	7.77	124.18	120.30
1	A	123[B]	ARG	NE-CZ-NH1	7.77	124.18	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	GLU	OE1-CD-OE2	7.71	132.55	123.30
1	C	381	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	B	188	ARG	NE-CZ-NH1	7.59	124.09	120.30
1	A	240	ASP	CB-CG-OD1	7.55	125.10	118.30
1	A	233	ARG	NE-CZ-NH2	-7.45	116.57	120.30
1	A	120	LEU	CB-CG-CD1	7.41	123.60	111.00
1	A	55	ARG	NE-CZ-NH2	-7.27	116.66	120.30
1	A	396	ARG	NE-CZ-NH2	7.25	123.92	120.30
1	A	329	ASP	CB-CG-OD2	-7.24	111.79	118.30
1	C	305	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	B	55	ARG	NE-CZ-NH1	7.03	123.82	120.30
1	A	188	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	B	399	GLU	CB-CA-C	-6.85	96.69	110.40
1	A	403	ASP	CB-CG-OD1	6.67	124.30	118.30
1	A	152	GLU	OE1-CD-OE2	6.66	131.30	123.30
1	A	269[A]	ARG	CG-CD-NE	-6.66	97.82	111.80
1	A	269[B]	ARG	CG-CD-NE	-6.66	97.82	111.80
1	B	233	ARG	NE-CZ-NH2	-6.61	117.00	120.30
1	A	396	ARG	NE-CZ-NH1	-6.57	117.02	120.30
1	C	269	ARG	NE-CZ-NH2	6.56	123.58	120.30
1	A	237	LEU	CA-CB-CG	6.55	130.37	115.30
1	A	125	ARG	NE-CZ-NH1	-6.51	117.05	120.30
1	C	152	GLU	OE1-CD-OE2	6.49	131.09	123.30
1	A	265	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	C	412	ARG	NE-CZ-NH1	-6.40	117.10	120.30
1	C	330	LEU	CB-CG-CD2	6.39	121.86	111.00
1	C	381	ARG	NE-CZ-NH2	-6.32	117.14	120.30
1	A	265	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	A	29	ARG	CG-CD-NE	-6.10	98.99	111.80
1	B	399	GLU	CG-CD-OE2	-6.08	106.15	118.30
1	A	264	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	C	264	ARG	NE-CZ-NH1	5.99	123.30	120.30
1	B	181	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	B	398	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	412	ARG	NE-CZ-NH2	5.83	123.22	120.30
1	C	233	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	C	240	ASP	CB-CG-OD1	5.68	123.41	118.30
1	C	264	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	372	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	B	188	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	B	245	ASP	CB-CG-OD1	5.55	123.30	118.30
1	B	336[A]	ARG	NE-CZ-NH2	-5.55	117.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	336[B]	ARG	NE-CZ-NH2	-5.55	117.53	120.30
1	C	72	ASP	CB-CG-OD1	5.49	123.24	118.30
1	A	225	ARG	NE-CZ-NH2	5.47	123.04	120.30
1	C	120	LEU	CB-CG-CD1	5.46	120.29	111.00
1	B	233	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	C	8	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	269[A]	ARG	NE-CZ-NH1	-5.35	117.63	120.30
1	B	269[B]	ARG	NE-CZ-NH1	-5.35	117.63	120.30
1	A	197	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	329	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	C	58	ARG	CG-CD-NE	5.32	122.98	111.80
1	C	334	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	428	LEU	CA-CB-CG	5.29	127.46	115.30
1	A	55	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	A	398	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	B	403	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	B	403	ASP	CB-CG-OD1	5.14	122.93	118.30
1	C	68[A]	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	C	68[B]	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	B	437	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	29	ARG	NE-CZ-NH1	-5.05	117.78	120.30
1	A	428	LEU	CB-CG-CD2	5.03	119.55	111.00
1	A	107	ARG	CG-CD-NE	-5.01	101.27	111.80
1	C	336	ARG	NE-CZ-NH2	5.01	122.81	120.30
1	B	265	ARG	NE-CZ-NH1	5.00	122.80	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	399	GLU	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3584	0	3636	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3620	0	3677	53	0
1	C	3589	0	3662	26	0
2	A	18	0	25	0	0
2	C	18	0	25	0	0
3	A	9	0	15	0	0
3	C	9	0	15	0	0
4	A	60	0	84	0	0
4	B	20	0	28	0	0
4	C	80	0	112	1	0
5	A	24	0	32	3	0
5	B	24	0	32	10	0
5	C	24	0	32	3	0
6	A	18	0	8	0	0
6	B	21	0	8	1	0
6	C	15	0	6	3	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	8	0	6	1	0
8	B	12	0	9	7	0
8	C	16	0	12	3	0
9	A	660	0	0	6	4
9	B	627	0	0	16	3
9	C	598	0	0	10	0
All	All	13057	0	11424	111	4

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 (111) 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:181[A]:ARG:NH2	1:A:185:GLU:OE1	1.87	1.05
1:B:29[A]:ARG:NH1	9:B:601:HOH:O	2.03	0.91
1:B:37[B]:GLN:HE22	1:B:254:PRO:HG2	1.36	0.90
1:B:37[B]:GLN:HE22	1:B:254:PRO:CG	1.85	0.89
1:B:57[A]:LEU:HD12	1:B:142[A]:LEU:CD1	2.04	0.87
1:B:57[A]:LEU:CD1	1:B:142[A]:LEU:CD1	2.54	0.86
5:A:509:GOL:H2	9:A:606:HOH:O	1.76	0.84
1:B:412:ARG:HD3	5:B:505:GOL:H12	1.65	0.79
1:A:224:HIS:NE2	9:A:601:HOH:O	2.18	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37[A]:GLN:HE22	1:C:254:PRO:HG2	1.50	0.75
1:B:57[A]:LEU:CD1	1:B:142[A]:LEU:HD11	2.17	0.73
1:B:399:GLU:OE2	5:B:504:GOL:O3	2.05	0.72
1:B:57[A]:LEU:CD1	1:B:142[A]:LEU:HD12	2.20	0.72
1:B:331:GLY:O	8:B:515:ACT:H3	1.91	0.70
1:B:204:ARG:HA	5:B:505:GOL:H31	1.73	0.70
1:A:63[B]:ARG:NE	9:A:602:HOH:O	2.21	0.69
1:B:57[A]:LEU:HD11	1:B:142[A]:LEU:CD1	2.21	0.69
1:B:65[A]:ARG:NH1	1:C:345:ASP:OD2	2.24	0.69
1:B:57[A]:LEU:HD11	1:B:142[A]:LEU:HD11	1.74	0.69
1:A:37[A]:GLN:HE22	1:A:254:PRO:HG2	1.58	0.68
1:C:182[B]:GLN:NE2	9:C:601:HOH:O	2.27	0.68
1:A:233:ARG:HE	8:A:517:ACT:H3	1.58	0.68
1:B:412:ARG:CD	5:B:505:GOL:H12	2.25	0.67
1:B:61[B]:PHE:CE2	9:B:897:HOH:O	2.47	0.66
1:B:338:ARG:HH12	8:B:515:ACT:H1	1.59	0.66
1:C:37[A]:GLN:HE22	1:C:254:PRO:CG	2.08	0.65
1:B:269[A]:ARG:HG3	9:B:617:HOH:O	1.94	0.65
1:B:37[B]:GLN:NE2	1:B:254:PRO:HG2	2.12	0.64
1:C:354:GLN:HG2	9:C:637:HOH:O	1.98	0.63
1:B:61[B]:PHE:HZ	9:B:610:HOH:O	1.80	0.63
1:C:61[B]:PHE:CD2	1:C:65:ARG:NH1	2.67	0.63
1:A:37[A]:GLN:HE22	1:A:254:PRO:CG	2.12	0.63
1:B:441:GLY:HA3	9:B:630:HOH:O	1.98	0.63
1:A:96:PRO:HG2	1:B:107:ARG:HG3	1.81	0.62
1:B:95:GLN:NE2	1:B:105:SER:OG	2.33	0.62
1:B:412:ARG:HD3	5:B:505:GOL:C1	2.29	0.61
1:B:7:TYR:HA	8:B:516:ACT:H2	1.83	0.60
1:B:57[A]:LEU:HD12	1:B:142[A]:LEU:HD12	1.80	0.59
1:C:37[B]:GLN:HE22	1:C:254:PRO:HD2	1.68	0.59
1:C:37[B]:GLN:HG3	1:C:249:ILE:CD1	2.33	0.59
1:B:295:LEU:HD11	1:B:319:VAL:CG1	2.33	0.58
1:A:353:GLN:HE21	5:C:508:GOL:H31	1.67	0.58
1:A:353:GLN:HE21	5:C:508:GOL:C3	2.16	0.58
1:B:392:GLN:HG3	9:B:606:HOH:O	2.02	0.58
1:A:221[B]:ARG:NH1	9:A:604:HOH:O	2.37	0.58
8:B:516:ACT:H3	9:B:813:HOH:O	2.03	0.57
1:C:55:ARG:HH22	6:C:511:FMT:C	2.19	0.56
1:A:37[B]:GLN:HG3	1:A:249:ILE:CD1	2.35	0.56
1:B:441:GLY:HA3	9:B:862:HOH:O	2.07	0.55
1:A:37[A]:GLN:HE22	1:A:254:PRO:CD	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29[B]:ARG:HG2	1:B:30:PHE:H	1.72	0.55
1:B:354:GLN:HG2	9:B:653:HOH:O	2.06	0.55
1:A:2[A]:THR:OG1	1:A:125:ARG:NH1	2.40	0.54
1:B:61[B]:PHE:CZ	9:B:897:HOH:O	2.59	0.54
1:A:37[A]:GLN:NE2	1:A:254:PRO:HG2	2.22	0.54
1:B:204:ARG:HD2	5:B:505:GOL:H2	1.88	0.54
1:A:61[B]:PHE:CE1	1:A:142:LEU:HD21	2.43	0.54
1:B:142[B]:LEU:HD11	1:B:146:GLN:NE2	2.24	0.53
1:B:1:CYS:N	9:B:602:HOH:O	2.15	0.52
1:B:118:LEU:HB3	1:B:120:LEU:HD13	1.91	0.51
1:C:182[B]:GLN:HG2	9:C:601:HOH:O	2.11	0.51
1:B:37[A]:GLN:HG3	1:B:249:ILE:HD13	1.93	0.50
1:C:57[B]:LEU:HD23	1:C:145[B]:LEU:HD13	1.92	0.50
8:C:519:ACT:H1	9:C:994:HOH:O	2.11	0.50
1:C:274[A]:ARG:NH2	9:C:607:HOH:O	2.37	0.50
1:C:146[A]:GLN:NE2	9:C:613:HOH:O	2.47	0.48
1:A:288:ASP:O	5:A:509:GOL:H31	2.13	0.48
5:B:505:GOL:O3	1:C:413:GLU:OE1	2.25	0.48
1:B:204:ARG:NH2	5:B:505:GOL:O1	2.47	0.48
8:C:518:ACT:H2	9:C:855:HOH:O	2.13	0.48
1:B:8:ARG:H	8:B:516:ACT:H2	1.79	0.47
1:B:220:GLU:OE1	1:B:223[B]:ARG:NH2	2.47	0.47
1:B:175[B]:GLU:HG2	9:B:629:HOH:O	2.13	0.47
1:A:61[B]:PHE:CD1	1:A:142:LEU:HD21	2.50	0.47
1:B:325:TRP:HA	5:B:502:GOL:H32	1.96	0.47
1:C:37[B]:GLN:HG3	1:C:249:ILE:HD13	1.96	0.47
5:A:508:GOL:H12	9:C:708:HOH:O	2.14	0.47
1:A:357:LEU:HD11	5:C:508:GOL:H31	1.97	0.46
1:C:286:THR:HG21	4:C:505:BOG:H1	1.98	0.46
5:B:502:GOL:H2	9:B:609:HOH:O	2.16	0.45
1:C:57[B]:LEU:HD11	1:C:149:LEU:HD23	1.98	0.45
1:A:2[B]:THR:HG22	9:A:864:HOH:O	2.15	0.45
1:C:37[B]:GLN:HE22	1:C:254:PRO:CD	2.29	0.45
1:B:29[B]:ARG:HG2	1:B:30:PHE:N	2.32	0.44
1:C:178:LYS:HA	1:C:205[A]:LEU:HD11	1.99	0.44
1:A:223[A]:ARG:HG3	1:A:241:LEU:HD12	1.99	0.43
1:A:392:GLN:NE2	9:A:607:HOH:O	2.43	0.43
1:C:428:LEU:C	1:C:428:LEU:HD13	2.38	0.43
6:C:514:FMT:C	9:C:636:HOH:O	2.65	0.43
1:B:441:GLY:CA	9:B:630:HOH:O	2.64	0.43
1:B:347:ALA:HB1	9:B:624:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123[B]:ARG:NH1	1:B:284:VAL:O	2.52	0.42
1:C:231:GLY:O	6:C:511:FMT:C	2.68	0.42
1:A:204[B]:ARG:HE	1:A:204[B]:ARG:HB2	1.30	0.42
1:A:382:GLN:OE1	1:A:413:GLU:OE2	2.37	0.42
1:B:57[A]:LEU:HD11	1:B:142[A]:LEU:HD12	1.93	0.42
1:C:37[A]:GLN:NE2	1:C:254:PRO:HG2	2.25	0.42
1:B:139:GLU:OE2	6:B:507:FMT:C	2.68	0.42
8:C:519:ACT:H2	9:C:1010:HOH:O	2.19	0.41
1:B:275:LEU:N	9:B:624:HOH:O	2.53	0.41
1:B:338:ARG:HH22	8:B:515:ACT:H1	1.85	0.41
1:C:57[B]:LEU:HD23	1:C:145[B]:LEU:CD1	2.51	0.41
1:A:63[B]:ARG:HA	1:A:63[B]:ARG:HD3	1.90	0.41
1:C:37[A]:GLN:HE22	1:C:254:PRO:CD	2.33	0.41
1:B:185[B]:GLU:HG3	1:B:188:ARG:NH2	2.36	0.41
1:C:37[B]:GLN:CG	1:C:249:ILE:CD1	2.98	0.41
1:C:428:LEU:HD13	1:C:428:LEU:O	2.21	0.41
1:B:8:ARG:H	8:B:516:ACT:CH3	2.33	0.40

All (4) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1055:HOH:O	9:B:1089:HOH:O[8_445]	1.74	0.46
9:A:672:HOH:O	9:B:1089:HOH:O[8_445]	2.01	0.19
9:A:922:HOH:O	9:A:1078:HOH:O[8_445]	2.07	0.13
9:A:1055:HOH:O	9:B:844:HOH:O[8_445]	2.16	0.04

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	474/455 (104%)	468 (99%)	6 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	479/455 (105%)	472 (98%)	7 (2%)	0	100	100
1	C	476/455 (105%)	467 (98%)	9 (2%)	0	100	100
All	All	1429/1365 (105%)	1407 (98%)	22 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	376/353 (106%)	368 (98%)	8 (2%)	53	36
1	B	379/353 (107%)	368 (97%)	11 (3%)	42	23
1	C	378/353 (107%)	373 (99%)	5 (1%)	69	56
All	All	1133/1059 (107%)	1109 (98%)	24 (2%)	55	36

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LYS
1	A	71	ARG
1	A	89	ASP
1	A	105	SER
1	A	120	LEU
1	A	251	LYS
1	A	322	SER
1	A	428	LEU
1	B	29[A]	ARG
1	B	29[B]	ARG
1	B	37[A]	GLN
1	B	37[B]	GLN
1	B	70[A]	LEU
1	B	70[B]	LEU
1	B	71	ARG
1	B	105	SER

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Mol	Chain	Res	Type
1	B	120	LEU
1	B	238	THR
1	B	251	LYS
1	C	16	LYS
1	C	31	GLU
1	C	71	ARG
1	C	120	LEU
1	C	330	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	45	GLN
1	A	308	GLN
1	A	353	GLN
1	A	354	GLN
1	A	382	GLN
1	B	45	GLN
1	B	76	ASN
1	B	95	GLN
1	B	159	GLN
1	B	176	ASN
1	B	182	GLN
1	C	159	GLN
1	C	176	ASN
1	C	391	GLN
1	C	392	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 54 ligands modelled in this entry, 3 are monoatomic - leaving 51 for Mogul analysis.

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
8	ACT	B	515	-	3,3,3	1.51	1 (33%)	3,3,3	0.56	0
8	ACT	A	518	-	3,3,3	0.72	0	3,3,3	0.89	0
6	FMT	B	510	-	2,2,2	0.72	0	1,1,1	0.71	0
6	FMT	B	512	-	2,2,2	0.93	0	1,1,1	0.61	0
5	GOL	B	505	-	5,5,5	0.10	0	5,5,5	1.18	0
8	ACT	C	520	-	3,3,3	0.74	0	3,3,3	0.84	0
4	BOG	C	504	-	20,20,20	0.54	0	25,25,25	0.90	2 (8%)
8	ACT	C	518	-	3,3,3	0.99	0	3,3,3	0.93	0
4	BOG	A	503	-	20,20,20	0.51	0	25,25,25	0.83	1 (4%)
3	OYA	A	502	1	8,8,8	0.72	0	7,7,7	0.69	0
6	FMT	A	510	-	2,2,2	2.26	1 (50%)	1,1,1	0.48	0
6	FMT	B	509	-	2,2,2	1.02	0	1,1,1	0.52	0
4	BOG	A	504	-	20,20,20	0.84	1 (5%)	25,25,25	1.47	4 (16%)
5	GOL	C	507	-	5,5,5	0.35	0	5,5,5	0.45	0
5	GOL	C	509	-	5,5,5	0.39	0	5,5,5	0.50	0
6	FMT	B	511	-	2,2,2	0.70	0	1,1,1	0.74	0
4	BOG	B	501	-	20,20,20	0.56	0	25,25,25	0.78	0
6	FMT	C	514	-	2,2,2	0.96	0	1,1,1	0.42	0
6	FMT	B	507	-	2,2,2	1.38	0	1,1,1	0.38	0
5	GOL	B	503	-	5,5,5	0.41	0	5,5,5	0.22	0
6	FMT	C	513	-	2,2,2	0.93	0	1,1,1	0.40	0
5	GOL	B	502	-	5,5,5	0.38	0	5,5,5	1.20	0
5	GOL	C	508	-	5,5,5	0.45	0	5,5,5	1.13	0
8	ACT	C	519	-	3,3,3	0.76	0	3,3,3	1.08	0
8	ACT	C	517	-	3,3,3	0.64	0	3,3,3	1.55	1 (33%)
5	GOL	A	507	-	5,5,5	0.70	0	5,5,5	1.47	1 (20%)
5	GOL	A	509	-	5,5,5	0.44	0	5,5,5	0.61	0
8	ACT	B	516	-	3,3,3	0.76	0	3,3,3	0.41	0
6	FMT	C	512	-	2,2,2	1.12	0	1,1,1	0.36	0
4	BOG	C	503	-	20,20,20	0.75	1 (5%)	25,25,25	1.51	4 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	B	504	-	5,5,5	0.36	0	5,5,5	0.82	0
6	FMT	A	513	-	2,2,2	0.80	0	1,1,1	0.55	0
3	OYA	C	502	1	8,8,8	0.73	0	7,7,7	0.37	0
4	BOG	C	505	-	20,20,20	1.84	3 (15%)	25,25,25	2.47	11 (44%)
5	GOL	A	508	-	5,5,5	0.20	0	5,5,5	1.03	0
6	FMT	A	514	7	2,2,2	0.71	0	1,1,1	0.67	0
6	FMT	B	508	-	2,2,2	1.21	0	1,1,1	0.30	0
6	FMT	A	512	-	2,2,2	0.81	0	1,1,1	0.55	0
8	ACT	A	517	-	3,3,3	0.86	0	3,3,3	0.39	0
6	FMT	A	515	-	2,2,2	0.99	0	1,1,1	0.49	0
6	FMT	C	511	-	2,2,2	1.18	0	1,1,1	0.24	0
8	ACT	B	514	-	3,3,3	1.12	0	3,3,3	0.80	0
2	3PK	C	501	1	17,17,17	0.55	0	19,19,19	0.81	1 (5%)
4	BOG	A	505	-	20,20,20	0.75	1 (5%)	25,25,25	1.31	2 (8%)
5	GOL	C	510	-	5,5,5	0.44	0	5,5,5	0.26	0
4	BOG	C	506	-	20,20,20	0.49	0	25,25,25	1.39	5 (20%)
6	FMT	A	511	-	2,2,2	1.26	0	1,1,1	0.28	0
6	FMT	C	515	-	2,2,2	0.71	0	1,1,1	0.72	0
5	GOL	A	506	-	5,5,5	0.44	0	5,5,5	0.44	0
2	3PK	A	501	1	17,17,17	0.58	0	19,19,19	0.36	0
6	FMT	B	506	-	2,2,2	0.91	0	1,1,1	0.58	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
5	GOL	B	505	-	-	3/4/4/4	-
4	BOG	C	504	-	-	3/11/31/31	0/1/1/1
4	BOG	A	503	-	-	8/11/31/31	0/1/1/1
3	OYA	A	502	1	-	2/5/6/6	-
4	BOG	A	504	-	-	5/11/31/31	0/1/1/1
5	GOL	C	507	-	-	0/4/4/4	-
5	GOL	C	509	-	-	2/4/4/4	-
4	BOG	B	501	-	-	1/11/31/31	0/1/1/1
5	GOL	B	503	-	-	2/4/4/4	-
5	GOL	B	502	-	-	2/4/4/4	-
5	GOL	C	508	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GOL	A	507	-	-	2/4/4/4	-
5	GOL	A	509	-	-	2/4/4/4	-
4	BOG	C	503	-	-	7/11/31/31	0/1/1/1
5	GOL	B	504	-	-	4/4/4/4	-
3	OYA	C	502	1	-	3/5/6/6	-
4	BOG	C	505	-	-	8/11/31/31	0/1/1/1
5	GOL	A	508	-	-	4/4/4/4	-
2	3PK	C	501	1	-	8/18/18/18	-
4	BOG	A	505	-	-	5/11/31/31	0/1/1/1
5	GOL	C	510	-	-	2/4/4/4	-
4	BOG	C	506	-	-	3/11/31/31	0/1/1/1
5	GOL	A	506	-	-	2/4/4/4	-
2	3PK	A	501	1	-	6/18/18/18	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	505	BOG	O1-C1	4.97	1.48	1.40
4	C	505	BOG	O5-C1	4.27	1.52	1.41
4	C	505	BOG	O5-C5	4.09	1.54	1.44
4	A	504	BOG	O1-C1	2.79	1.45	1.40
4	C	503	BOG	O1-C1	2.74	1.44	1.40
6	A	510	FMT	O2-C	2.65	1.42	1.28
4	A	505	BOG	O1-C1	2.29	1.44	1.40
8	B	515	ACT	O-C	2.28	1.32	1.22

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	505	BOG	O5-C1-O1	5.87	123.88	109.97
4	C	505	BOG	C4-C3-C2	-4.94	102.19	110.82
4	A	505	BOG	O1-C1-C2	3.88	114.36	108.30
4	C	503	BOG	C1'-O1-C1	3.86	120.23	113.84
4	A	504	BOG	C3-C4-C5	3.80	117.02	110.24
4	C	503	BOG	O5-C5-C4	3.66	116.33	109.69
4	C	505	BOG	C6-C5-C4	-3.60	104.58	113.00
4	C	503	BOG	C1-O5-C5	3.54	120.63	113.69
4	C	505	BOG	O5-C5-C6	3.49	115.11	106.44
4	A	504	BOG	C4-C3-C2	3.33	116.64	110.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	504	BOG	C1-C2-C3	3.28	116.83	110.00
4	C	506	BOG	C1-O5-C5	3.09	119.76	113.69
4	C	505	BOG	O5-C5-C4	3.06	115.25	109.69
4	C	505	BOG	C1-C2-C3	-3.05	103.64	110.00
4	C	506	BOG	O5-C5-C4	3.00	115.15	109.69
4	C	505	BOG	O1-C1'-C2'	2.90	119.74	109.56
2	C	501	3PK	CG2-OG2-CB1	2.82	121.50	117.88
4	C	503	BOG	C3-C4-C5	2.64	114.96	110.24
4	C	505	BOG	O4-C4-C5	2.64	115.85	109.30
4	A	505	BOG	C1'-O1-C1	-2.63	109.48	113.84
4	C	505	BOG	O6-C6-C5	2.62	120.30	111.29
4	A	504	BOG	O5-C5-C6	2.53	112.72	106.44
4	C	505	BOG	C1'-O1-C1	2.52	118.03	113.84
4	C	506	BOG	C1'-O1-C1	-2.45	109.78	113.84
4	C	504	BOG	O5-C5-C6	2.42	112.46	106.44
4	C	506	BOG	O5-C5-C6	-2.24	100.86	106.44
5	A	507	GOL	C3-C2-C1	-2.18	103.23	111.70
8	C	517	ACT	O-C-CH3	-2.18	113.86	122.33
4	A	503	BOG	C1'-O1-C1	2.17	117.44	113.84
4	C	506	BOG	O5-C1-O1	-2.14	104.90	109.97
4	C	504	BOG	C1'-O1-C1	-2.14	110.29	113.84
4	C	505	BOG	O2-C2-C1	2.07	115.06	110.05

There are no chirality outliers.

All (86) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	3PK	OG1-CG1-CG2-OG2
2	C	501	3PK	CG3-CG2-OG2-CB1
4	A	504	BOG	C2-C1-O1-C1'
4	A	504	BOG	O5-C1-O1-C1'
4	C	503	BOG	O5-C1-O1-C1'
4	C	505	BOG	C2-C1-O1-C1'
4	C	505	BOG	O5-C1-O1-C1'
5	A	506	GOL	O1-C1-C2-C3
5	A	508	GOL	O1-C1-C2-C3
5	A	508	GOL	C1-C2-C3-O3
5	B	504	GOL	O1-C1-C2-C3
5	B	505	GOL	O1-C1-C2-C3
5	C	508	GOL	O1-C1-C2-C3
5	C	510	GOL	O1-C1-C2-O2
5	C	510	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	C	503	BOG	O5-C5-C6-O6
2	C	501	3PK	OB1-CB1-OG2-CG2
4	A	504	BOG	O5-C5-C6-O6
2	C	501	3PK	CB2-CB1-OG2-CG2
4	A	503	BOG	C4-C5-C6-O6
4	C	503	BOG	C4-C5-C6-O6
5	A	508	GOL	O1-C1-C2-O2
4	A	503	BOG	O5-C5-C6-O6
4	A	504	BOG	C4-C5-C6-O6
2	C	501	3PK	CA2-CA1-OG1-CG1
2	C	501	3PK	CB1-CB2-CB3-CB4
4	C	503	BOG	O1-C1'-C2'-C3'
4	C	503	BOG	C2-C1-O1-C1'
3	A	502	OYA	C7-C11-C6-C5
2	C	501	3PK	OA1-CA1-OG1-CG1
4	A	504	BOG	C4'-C5'-C6'-C7'
5	A	509	GOL	O1-C1-C2-C3
5	B	502	GOL	O1-C1-C2-C3
5	B	503	GOL	O1-C1-C2-C3
5	B	504	GOL	C1-C2-C3-O3
5	C	509	GOL	O1-C1-C2-C3
4	A	503	BOG	C4'-C5'-C6'-C7'
4	A	503	BOG	C2'-C1'-O1-C1
5	A	506	GOL	O1-C1-C2-O2
5	A	508	GOL	O2-C2-C3-O3
5	A	509	GOL	O1-C1-C2-O2
5	B	505	GOL	O1-C1-C2-O2
5	C	508	GOL	O1-C1-C2-O2
2	A	501	3PK	OB1-CB1-OG2-CG2
2	A	501	3PK	CA1-CA2-CA3-CA4
4	C	505	BOG	C2'-C3'-C4'-C5'
4	A	503	BOG	O1-C1'-C2'-C3'
4	C	506	BOG	C3'-C4'-C5'-C6'
2	A	501	3PK	CB2-CB1-OG2-CG2
4	A	505	BOG	C2'-C3'-C4'-C5'
4	A	505	BOG	C3'-C4'-C5'-C6'
4	C	506	BOG	O5-C5-C6-O6
4	C	505	BOG	O5-C5-C6-O6
4	C	505	BOG	C3'-C4'-C5'-C6'
4	C	503	BOG	C4'-C5'-C6'-C7'
5	A	507	GOL	O1-C1-C2-O2
5	B	504	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	A	501	3PK	CA2-CA3-CA4-CA5
4	B	501	BOG	C5'-C6'-C7'-C8'
2	A	501	3PK	OG1-CG1-CG2-CG3
5	B	505	GOL	O2-C2-C3-O3
3	A	502	OYA	C6-C11-C7-C8
4	C	505	BOG	C4'-C5'-C6'-C7'
4	A	503	BOG	C2'-C3'-C4'-C5'
4	C	505	BOG	O1-C1'-C2'-C3'
3	C	502	OYA	C11-C7-C8-C9
5	A	507	GOL	O1-C1-C2-C3
4	C	504	BOG	O1-C1'-C2'-C3'
4	C	504	BOG	C3'-C4'-C5'-C6'
4	C	506	BOG	C2'-C3'-C4'-C5'
3	C	502	OYA	C7-C8-C9-C10
4	A	505	BOG	C1'-C2'-C3'-C4'
5	B	504	GOL	O1-C1-C2-O2
4	A	503	BOG	C5'-C6'-C7'-C8'
3	C	502	OYA	C6-C11-C7-C8
4	C	505	BOG	C1'-C2'-C3'-C4'
4	A	505	BOG	C4-C5-C6-O6
2	C	501	3PK	CB3-CB4-CB5-CB6
5	B	502	GOL	O1-C1-C2-O2
5	B	503	GOL	O1-C1-C2-O2
4	C	504	BOG	O5-C5-C6-O6
4	C	503	BOG	C1'-C2'-C3'-C4'
4	A	503	BOG	C1'-C2'-C3'-C4'
5	C	509	GOL	O1-C1-C2-O2
4	A	505	BOG	O5-C5-C6-O6
2	C	501	3PK	OB1-CB1-CB2-CB3

There are no ring outliers.

15 monomers are involved in 32 short contacts:

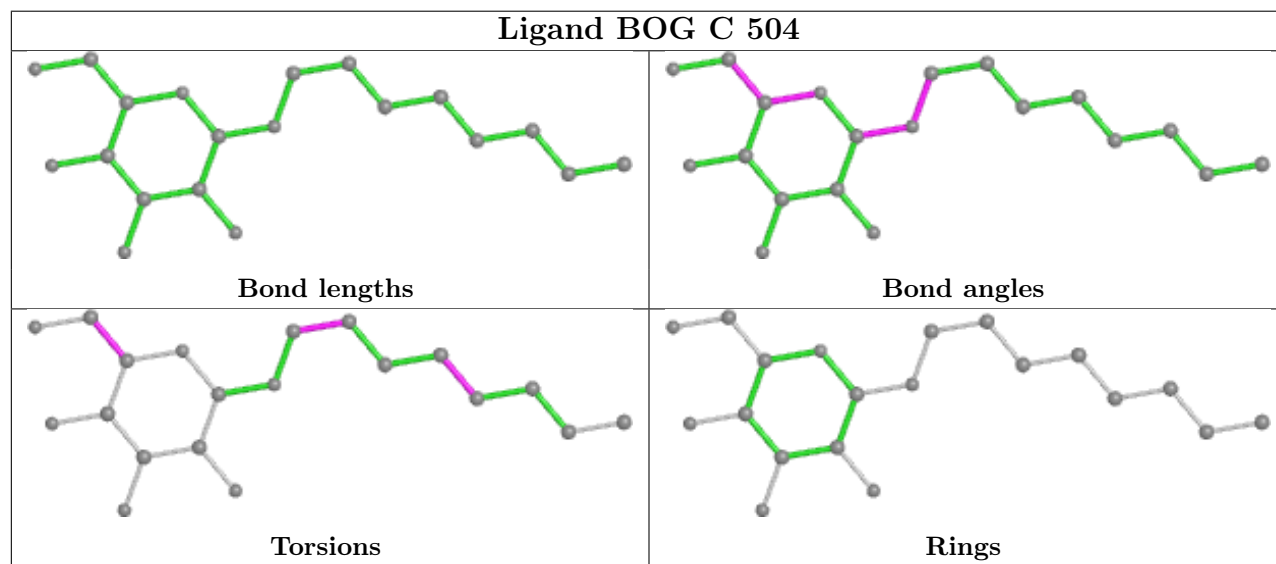
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	B	515	ACT	3	0
5	B	505	GOL	7	0
8	C	518	ACT	1	0
6	C	514	FMT	1	0
6	B	507	FMT	1	0
5	B	502	GOL	2	0
5	C	508	GOL	3	0
8	C	519	ACT	2	0

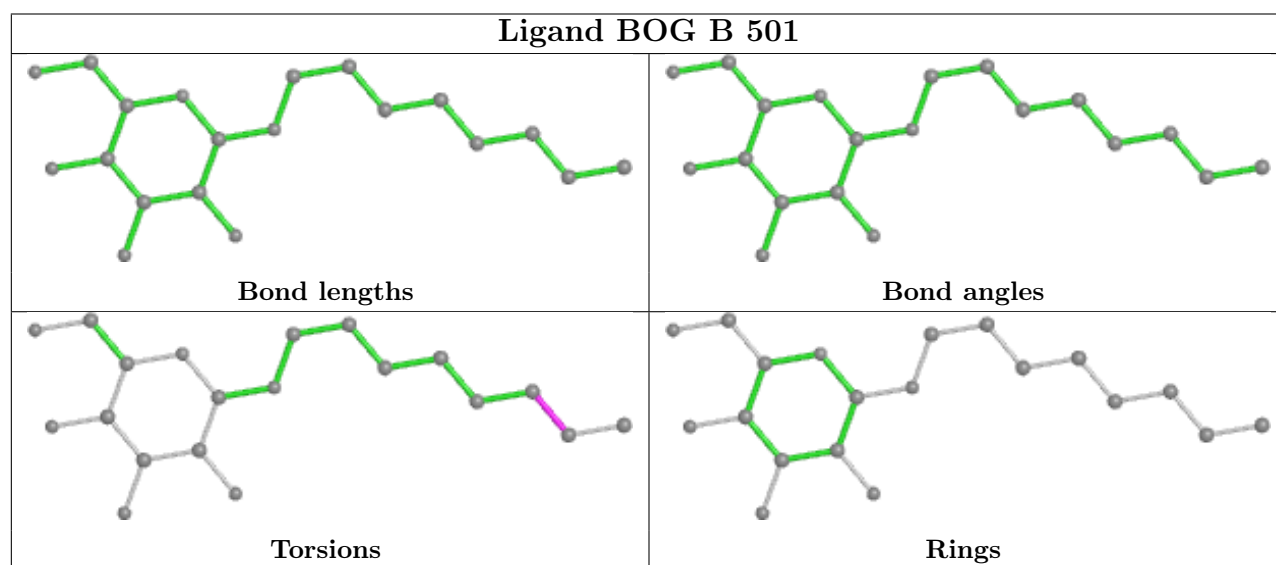
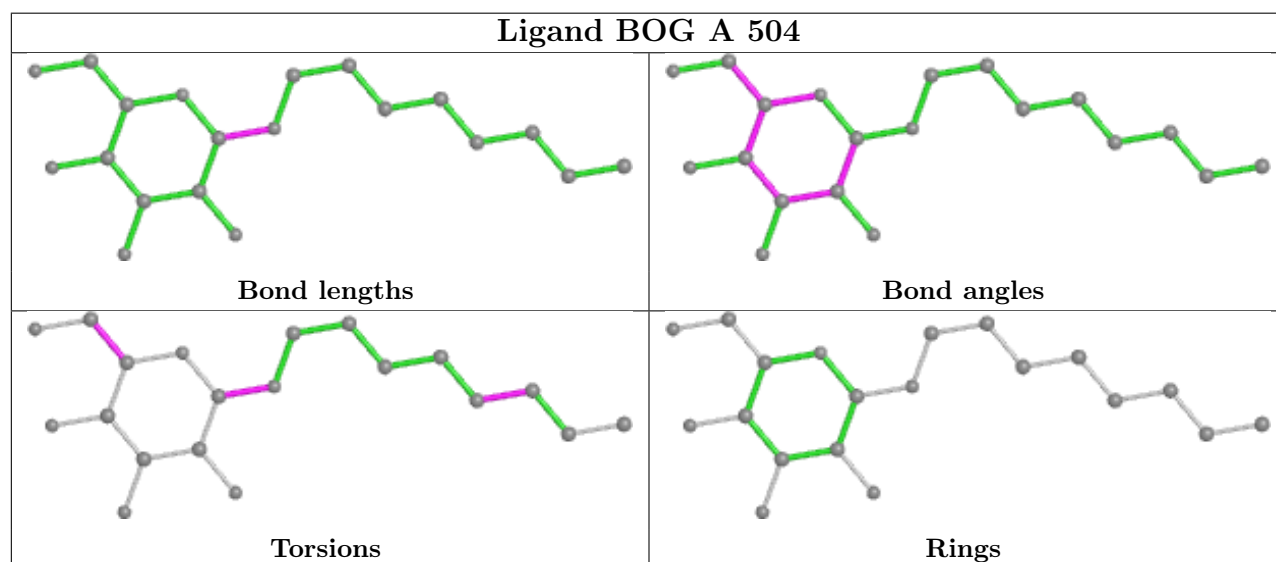
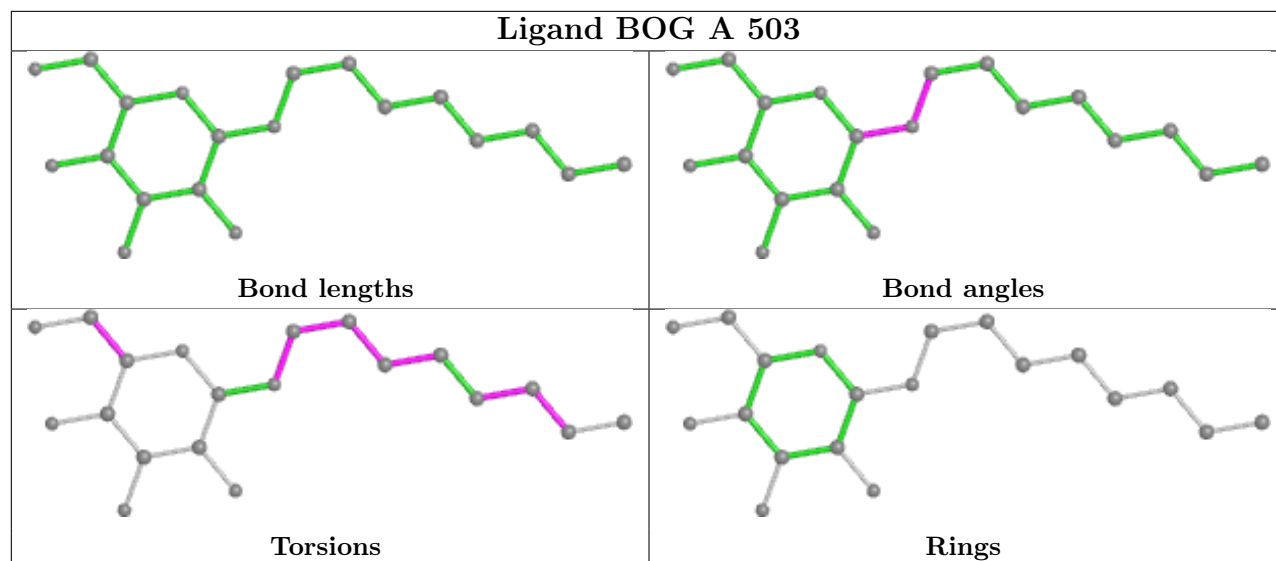
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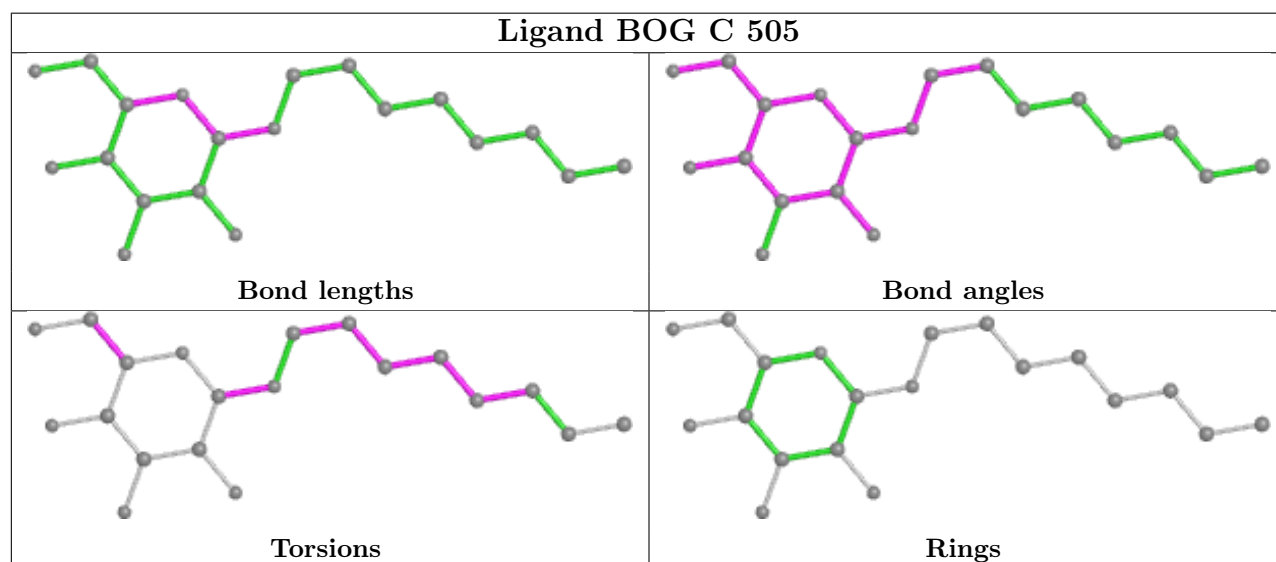
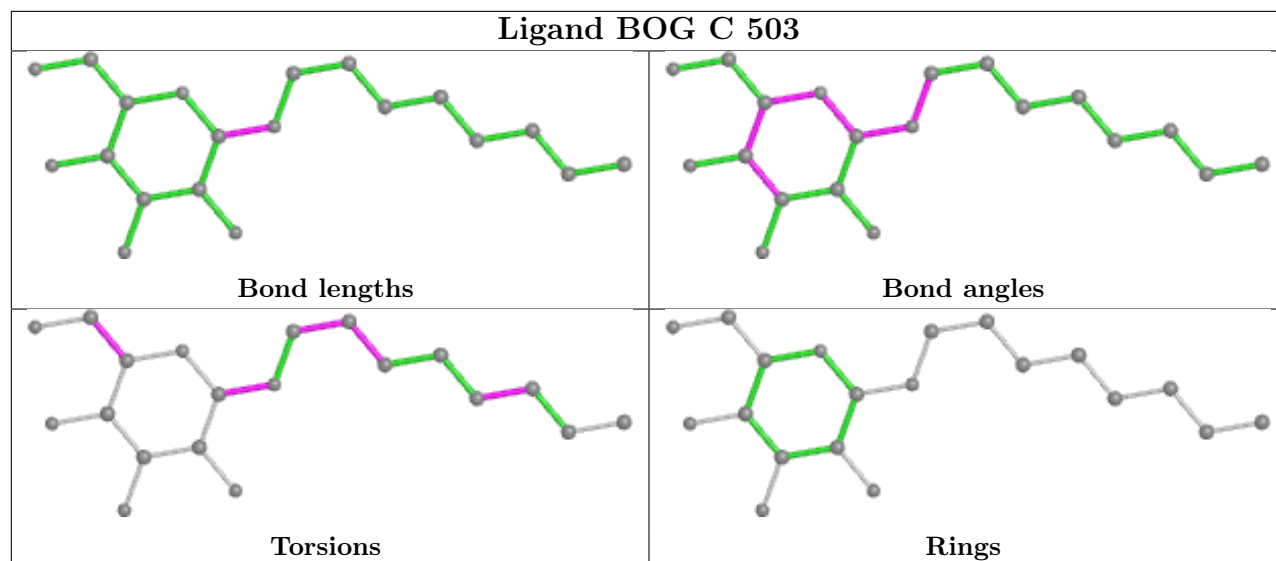
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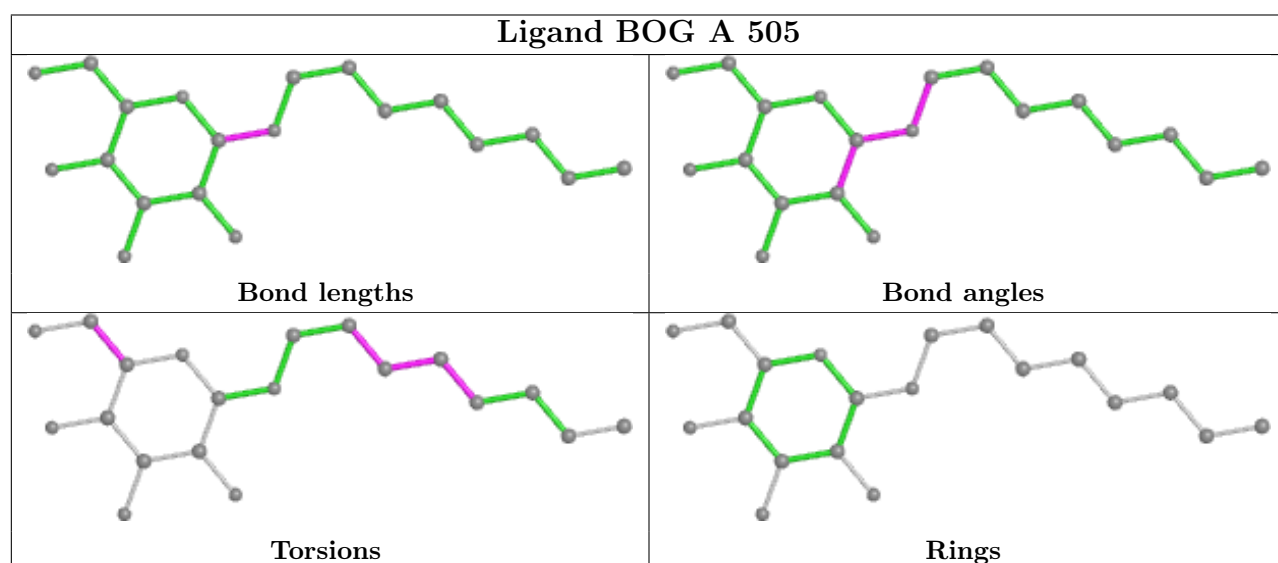
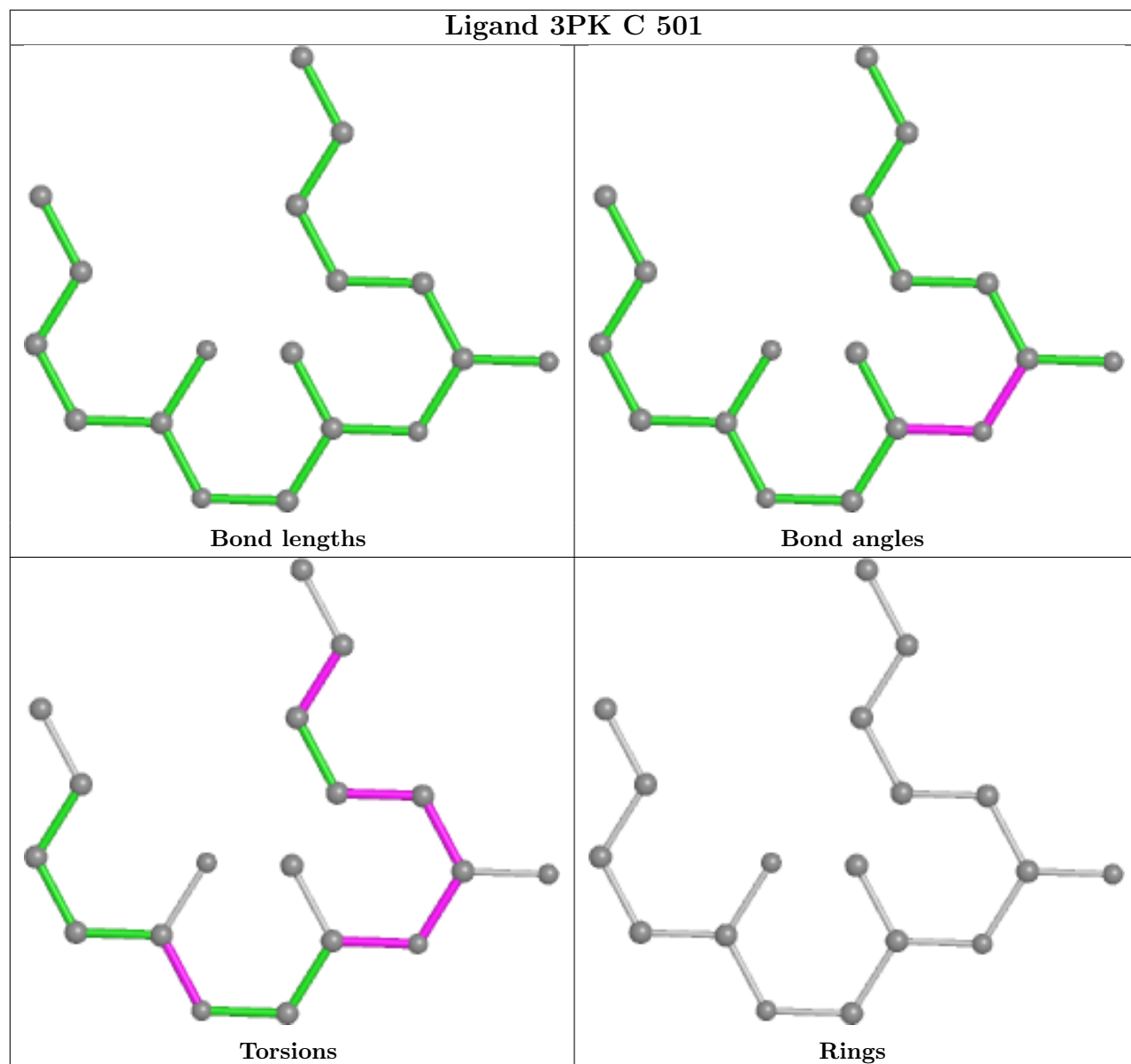
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	509	GOL	2	0
8	B	516	ACT	4	0
5	B	504	GOL	1	0
4	C	505	BOG	1	0
5	A	508	GOL	1	0
8	A	517	ACT	1	0
6	C	511	FMT	2	0

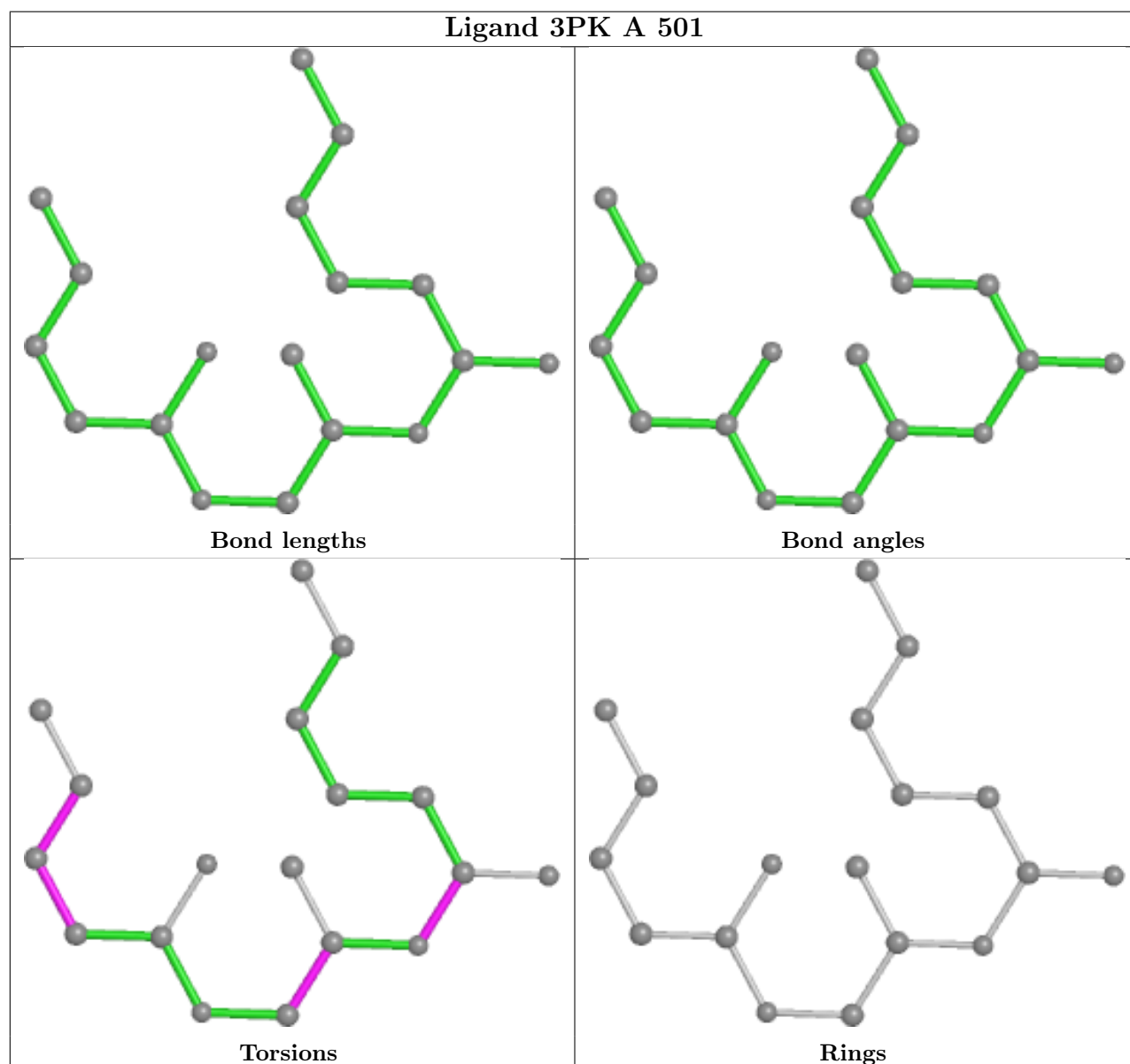
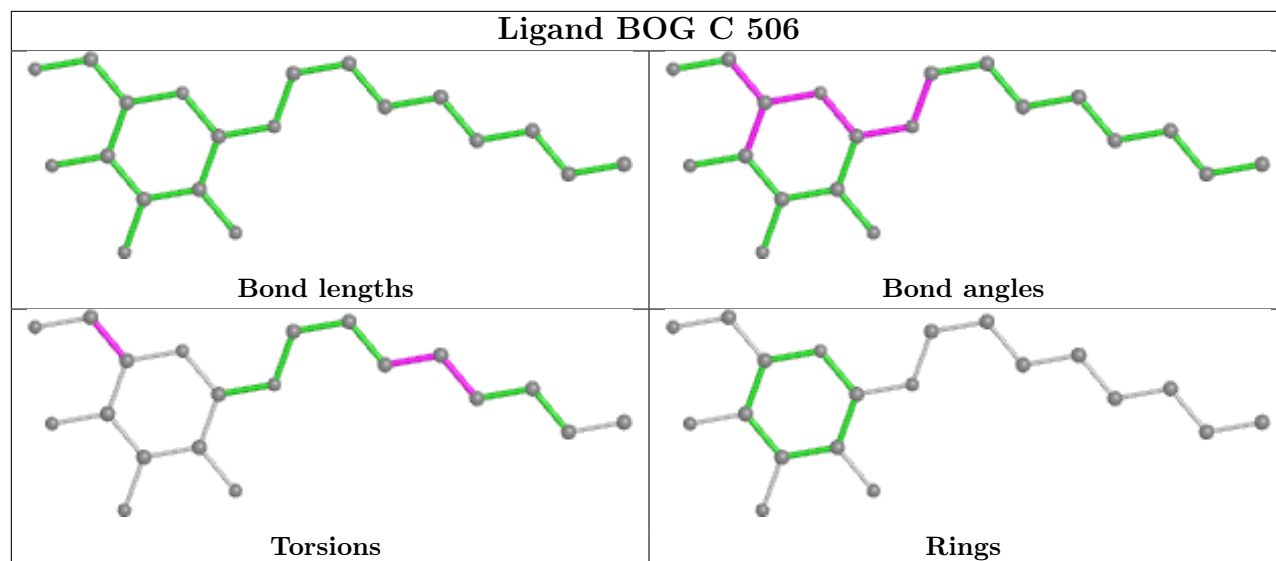
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

6.1 Protein, DNA and RNA chains [i](#)

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	446/455 (98%)	-0.26	11 (2%) 57 61	13, 22, 44, 62	0
1	B	450/455 (98%)	-0.31	11 (2%) 59 63	14, 21, 42, 53	0
1	C	444/455 (97%)	-0.37	7 (1%) 72 76	14, 21, 42, 64	0
All	All	1340/1365 (98%)	-0.32	29 (2%) 62 66	13, 21, 43, 64	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	97	GLY	3.8
1	A	402[A]	THR	3.7
1	C	98	VAL	3.6
1	B	238	THR	3.2
1	B	23	LYS	3.2
1	B	97	GLY	3.2
1	B	18	ASP	3.2
1	C	99	THR	3.1
1	C	21	ALA	3.0
1	A	401	THR	2.8
1	A	97	GLY	2.8
1	B	98	VAL	2.8
1	B	250	THR	2.7
1	A	305	ARG	2.7
1	C	11	ASP	2.6
1	A	400	GLY	2.5
1	B	1	CYS	2.5
1	A	22	SER	2.5
1	A	21	ALA	2.4
1	A	23	LYS	2.3
1	A	61[A]	PHE	2.3
1	B	61[A]	PHE	2.3
1	A	18	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	95	GLN	2.2
1	B	21	ALA	2.2
1	B	105	SER	2.1
1	B	99	THR	2.1
1	C	23	LYS	2.0
1	A	101	ASP	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
8	ACT	B	515	4/4	0.45	0.26	31,41,46,47	0
6	FMT	C	514	3/3	0.55	0.23	50,50,59,60	0
5	GOL	B	503	6/6	0.57	0.21	64,71,73,77	0
8	ACT	B	516	4/4	0.57	0.22	30,46,52,55	0
8	ACT	C	519	4/4	0.57	0.28	55,58,62,64	0
2	3PK	A	501	18/18	0.58	0.20	54,66,68,69	0
4	BOG	A	504	20/20	0.59	0.35	57,80,89,94	0
6	FMT	C	511	3/3	0.62	0.26	45,45,47,49	0
6	FMT	B	512	3/3	0.64	0.17	53,53,57,61	0
4	BOG	C	506	20/20	0.67	0.21	50,65,76,84	0
6	FMT	A	515	3/3	0.68	0.16	48,48,53,59	0
4	BOG	A	505	20/20	0.69	0.23	43,56,64,66	0
2	3PK	C	501	18/18	0.69	0.16	42,56,62,68	0
8	ACT	C	520	4/4	0.71	0.15	52,59,63,66	0
5	GOL	A	507	6/6	0.73	0.16	40,52,55,59	0
5	GOL	C	509	6/6	0.74	0.18	55,60,61,61	0
4	BOG	C	505	20/20	0.75	0.24	38,52,60,62	0

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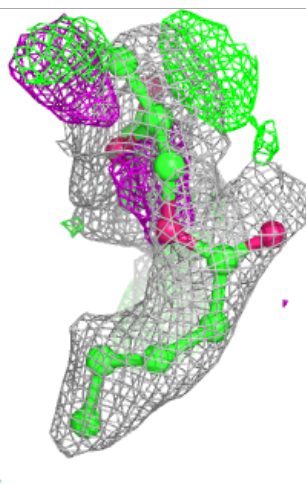
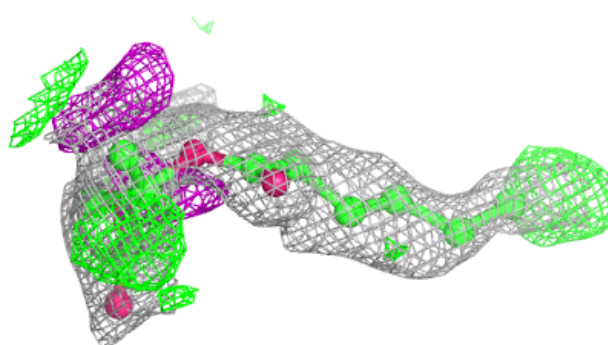
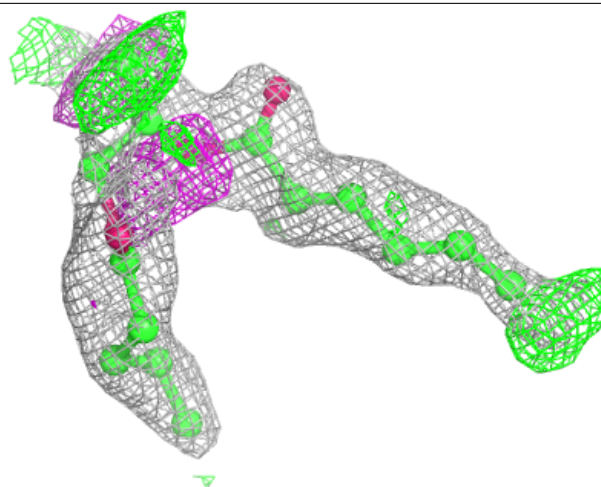
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
8	ACT	A	518	4/4	0.75	0.28	67,68,70,71	0
3	OYA	A	502	9/9	0.78	0.15	49,54,62,62	0
5	GOL	C	510	6/6	0.78	0.27	58,61,63,63	0
6	FMT	A	512	3/3	0.78	0.21	48,48,61,66	0
4	BOG	C	503	20/20	0.80	0.18	55,65,82,82	0
5	GOL	B	505	6/6	0.80	0.30	41,48,50,59	0
4	BOG	C	504	20/20	0.81	0.21	40,49,62,64	0
6	FMT	A	511	3/3	0.81	0.28	41,41,42,52	0
6	FMT	B	506	3/3	0.82	0.15	40,40,54,56	0
6	FMT	A	510	3/3	0.82	0.22	24,24,33,39	0
4	BOG	B	501	20/20	0.82	0.19	46,53,63,66	0
3	OYA	C	502	9/9	0.83	0.19	39,57,70,70	0
6	FMT	B	507	3/3	0.83	0.24	34,34,47,48	0
6	FMT	B	509	3/3	0.84	0.16	44,44,54,55	0
8	ACT	B	514	4/4	0.84	0.13	38,38,39,45	0
6	FMT	C	513	3/3	0.85	0.13	37,37,45,50	0
5	GOL	C	508	6/6	0.85	0.17	41,46,52,52	0
6	FMT	B	510	3/3	0.86	0.10	71,71,78,80	0
4	BOG	A	503	20/20	0.87	0.17	41,52,72,75	0
8	ACT	C	517	4/4	0.87	0.15	34,43,47,48	0
5	GOL	A	509	6/6	0.88	0.22	34,50,57,59	0
5	GOL	C	507	6/6	0.88	0.12	44,45,47,48	0
5	GOL	B	504	6/6	0.89	0.11	44,45,48,53	0
5	GOL	B	502	6/6	0.89	0.28	36,49,53,55	0
8	ACT	A	517	4/4	0.89	0.10	34,35,39,45	0
5	GOL	A	508	6/6	0.89	0.34	40,47,49,49	0
6	FMT	B	508	3/3	0.89	0.20	36,36,41,50	0
6	FMT	C	512	3/3	0.90	0.10	30,30,42,48	0
8	ACT	C	518	4/4	0.91	0.11	37,39,40,44	0
5	GOL	A	506	6/6	0.92	0.17	25,36,47,55	0
6	FMT	C	515	3/3	0.93	0.08	56,56,56,60	0
6	FMT	A	514	3/3	0.94	0.26	49,49,49,54	0
6	FMT	A	513	3/3	0.94	0.14	33,33,40,47	0
7	NA	A	516	1/1	0.97	0.08	32,32,32,32	0
6	FMT	B	511	3/3	0.97	0.29	46,46,52,52	0
7	NA	C	516	1/1	0.98	0.06	30,30,30,30	0
7	NA	B	513	1/1	0.99	0.10	27,27,27,27	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.

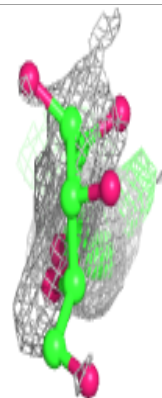
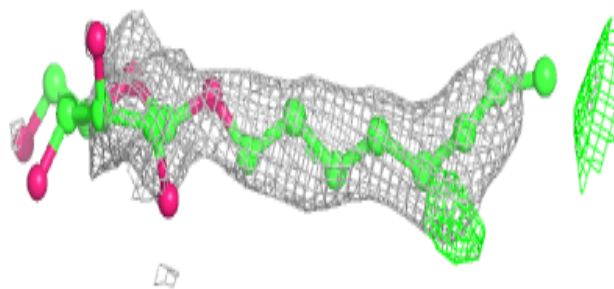
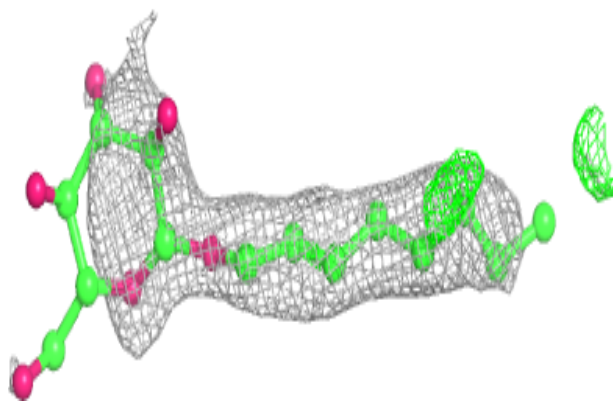
Electron density around 3PK A 501:

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

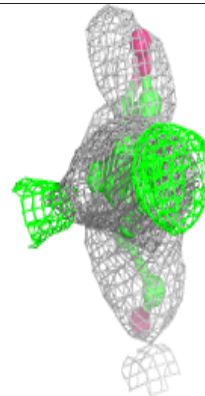
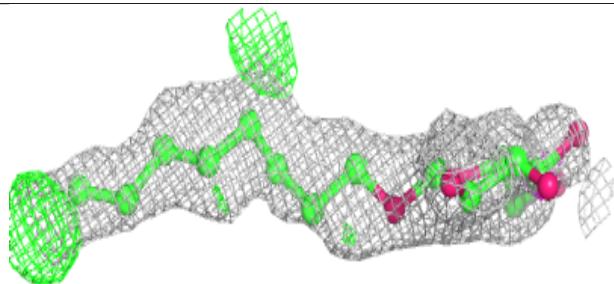
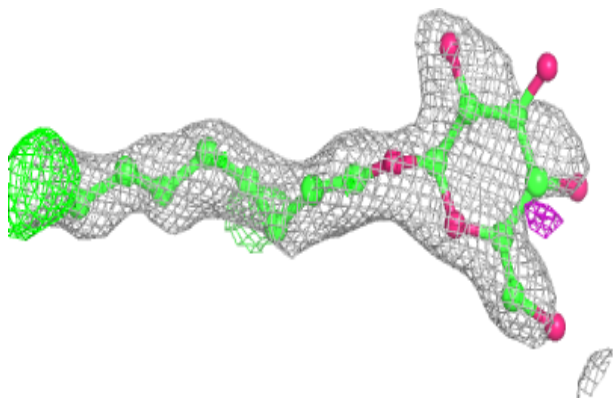


Electron density around BOG A 504:

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

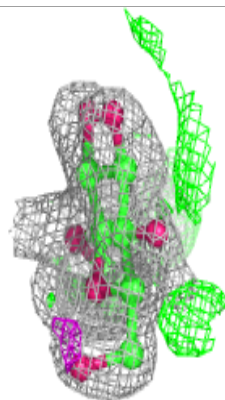
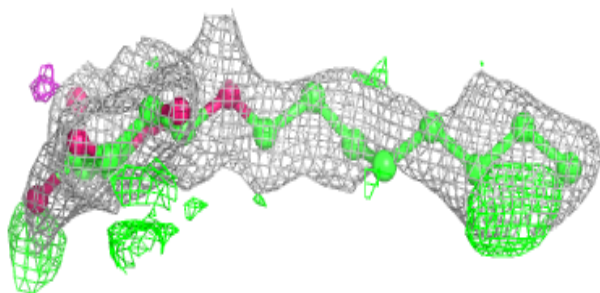
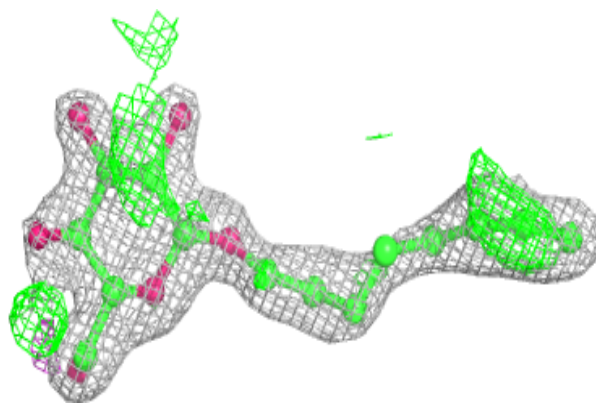
**Electron density around BOG C 506:**

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



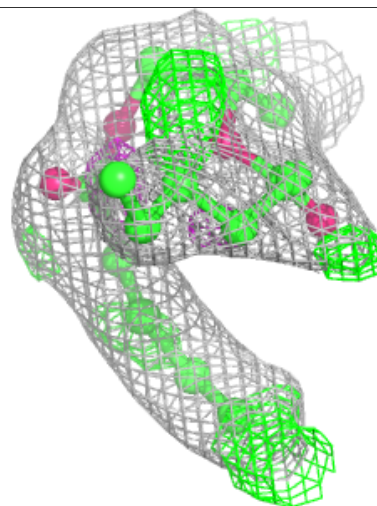
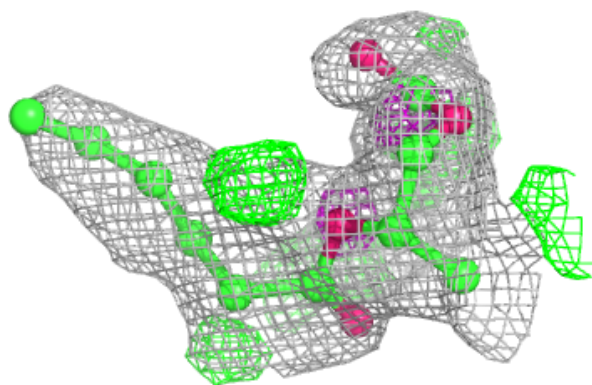
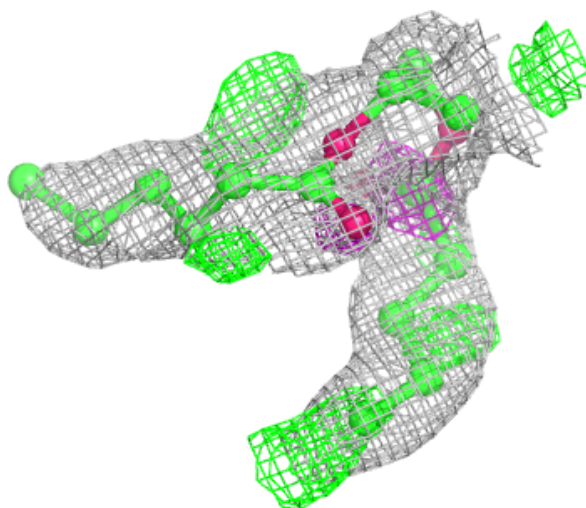
Electron density around BOG A 505:

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



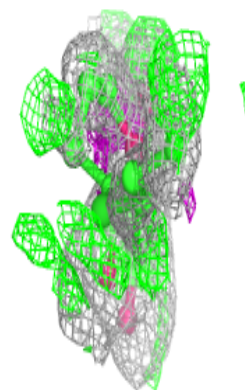
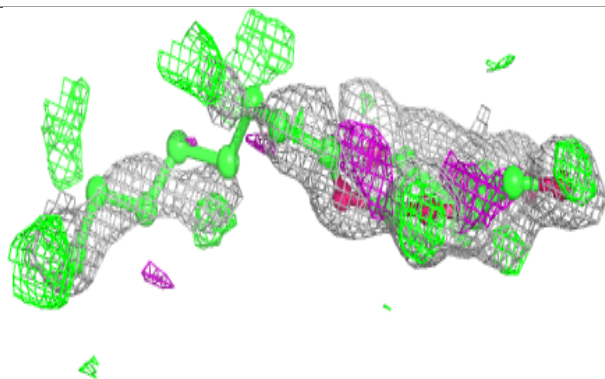
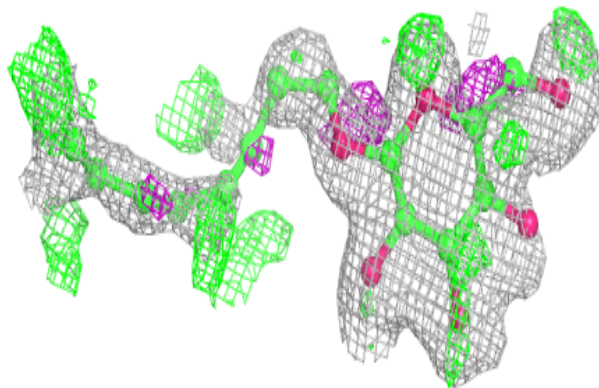
Electron density around 3PK C 501:

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

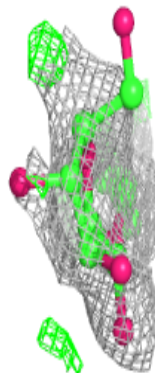
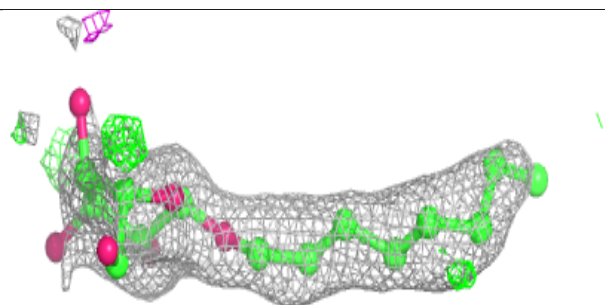
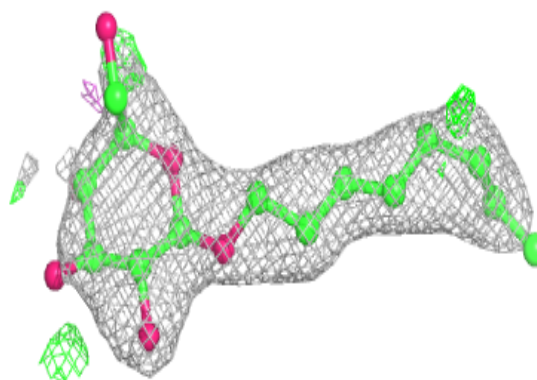


Electron density around BOG C 505:

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

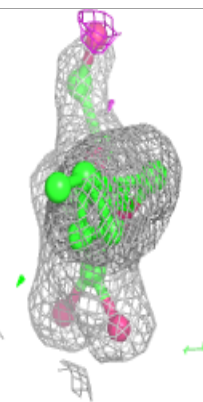
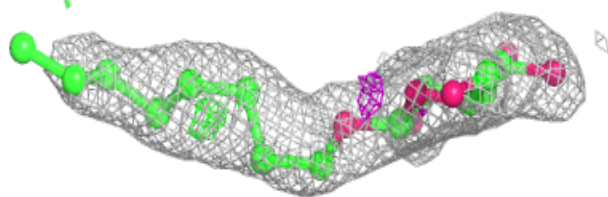
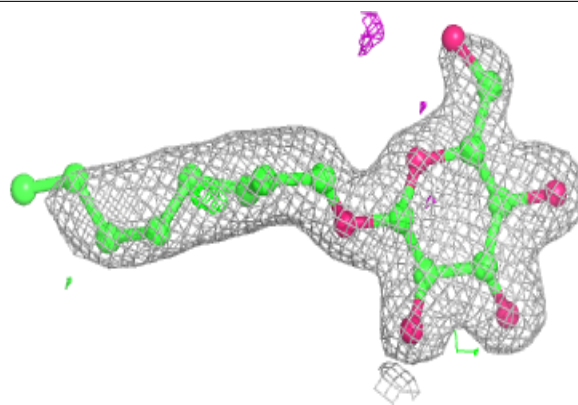
**Electron density around BOG C 503:**

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

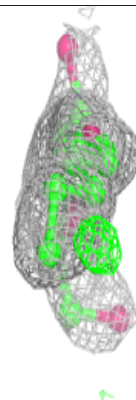
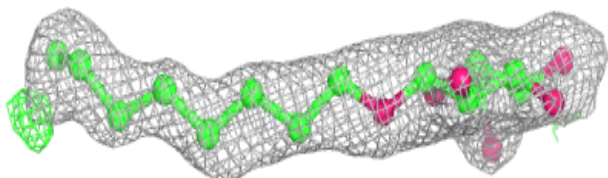
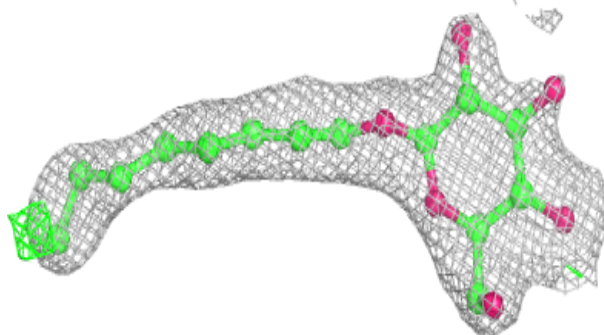


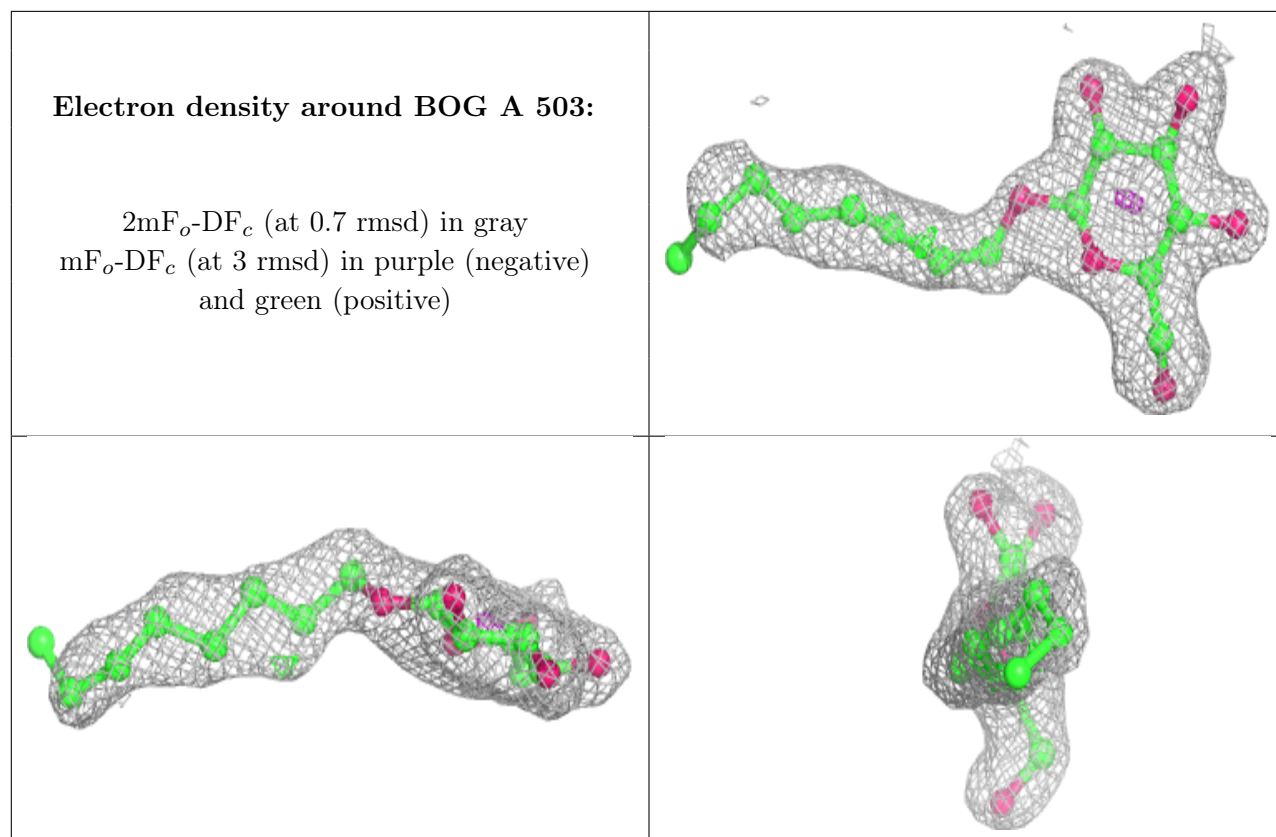
Electron density around BOG C 504:

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

**Electron density around BOG B 501:**

$2mF_o-DF_c$ (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.