



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:16 PM UTC

PDB ID : 8E62 / pdb_00008e62
Title : STRUCTURE OF Pcryo_0615 from Psychrobacter cryohalolentis, an N-acetyltransferase required to produce Diacetamido-2,3-dideoxy-D-glucuronic acid
Authors : Hofmeister, D.L.; Bockhaus, N.J.; Seltzner, C.A.; Thoden, J.B.; Holden, H.M.
Deposited on : 2022-08-22
Resolution : 1.80 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

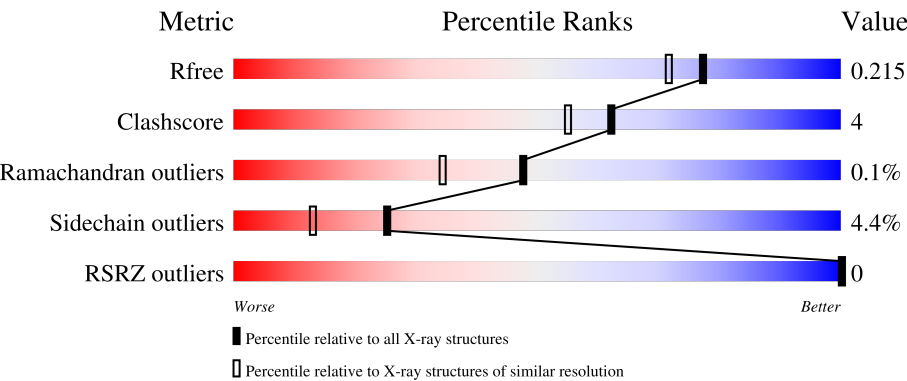
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

1 Overall quality at a glance i

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

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R _{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	189	88%6% . .
1	B	189	81%12% . 5%
1	C	189	83%13% . .
1	D	189	85%5% . 9%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	E	189	85% 11%
1	F	189	87% 9%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9286 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 UDP-N-acetylglucosamine acyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	2	0
			1380	878	232	258	12			
1	B	179	Total	C	N	O	S	0	3	0
			1366	869	229	254	14			
1	C	183	Total	C	N	O	S	0	4	0
			1409	896	241	260	12			
1	D	172	Total	C	N	O	S	0	2	0
			1308	833	219	244	12			
1	E	183	Total	C	N	O	S	0	4	0
			1400	892	236	260	12			
1	F	183	Total	C	N	O	S	0	1	0
			1382	877	233	260	12			

There are 18 discrepancies between the modelled and reference sequences:

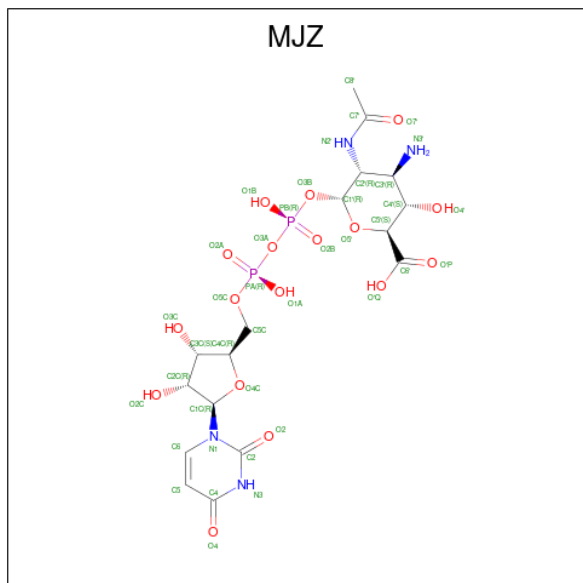
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q1QD55
A	-1	GLY	-	expression tag	UNP Q1QD55
A	0	HIS	-	expression tag	UNP Q1QD55
B	-2	GLY	-	expression tag	UNP Q1QD55
B	-1	GLY	-	expression tag	UNP Q1QD55
B	0	HIS	-	expression tag	UNP Q1QD55
C	-2	GLY	-	expression tag	UNP Q1QD55
C	-1	GLY	-	expression tag	UNP Q1QD55
C	0	HIS	-	expression tag	UNP Q1QD55
D	-2	GLY	-	expression tag	UNP Q1QD55
D	-1	GLY	-	expression tag	UNP Q1QD55
D	0	HIS	-	expression tag	UNP Q1QD55
E	-2	GLY	-	expression tag	UNP Q1QD55
E	-1	GLY	-	expression tag	UNP Q1QD55
E	0	HIS	-	expression tag	UNP Q1QD55
F	-2	GLY	-	expression tag	UNP Q1QD55
F	-1	GLY	-	expression tag	UNP Q1QD55

Continued on next page...

Continued from previous page...

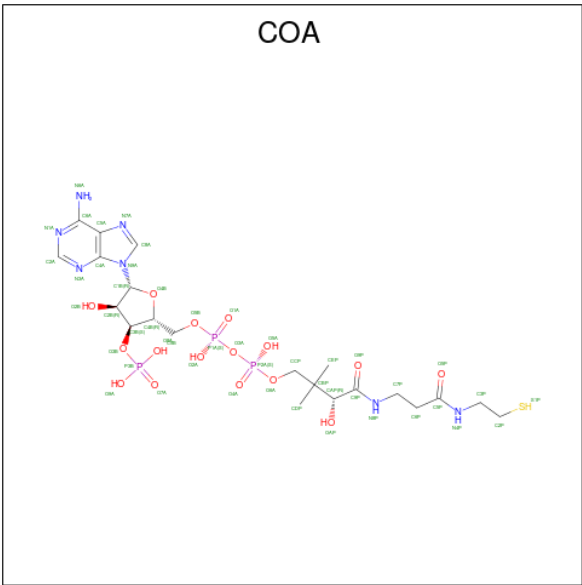
Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	expression tag	UNP Q1QD55

- Molecule 2 is (2S,3S,4R,5R,6R)-5-(acetylamino)-4-amino-6-{[(R)-{[(R)-{(2R,3S,4R,5R)-5-(2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)-3,4-dihydroxytetrahydrofuran-2-yl]methoxy}(hydroxy)phosphoryl]oxy}(hydroxy)phosphoryl]oxy}-3-hydroxytetrahydro-2H-pyran-2-carboxylic acid (CCD ID: MJZ) (formula: C₁₇H₂₆N₄O₁₇P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			40	17	4	17	2		
2	B	1	Total	C	N	O	P	0	0
			40	17	4	17	2		
2	F	1	Total	C	N	O	P	0	0
			40	17	4	17	2		

- Molecule 3 is COENZYME A (CCD ID: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	B	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	E	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	E	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		
3	F	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Na	0	0
			1	1		
4	D	1	Total	Na	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	125	Total	O	0	0
			125	125		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	90	Total 90	O 90	0	0
5	C	99	Total 99	O 99	0	0
5	D	103	Total 103	O 103	0	0
5	E	102	Total 102	O 102	0	0
5	F	112	Total 112	O 112	0	0

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: UDP-N-acetylglucosamine acyltransferase

Chain A: 



- Molecule 1: UDP-N-acetylglucosamine acyltransferase

Chain B: 



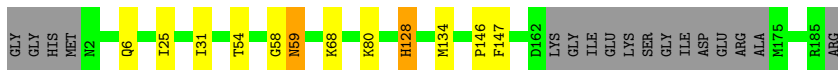
- Molecule 1: UDP-N-acetylglucosamine acyltransferase

Chain C: 



- Molecule 1: UDP-N-acetylglucosamine acyltransferase

Chain D: 



- Molecule 1: UDP-N-acetylglucosamine acyltransferase

Chain E: 



- Molecule 1: UDP-N-acetylglucosamine acyltransferase

Chain F: 

GLY	GLY	HIS	MET	ASN	ASN	N4	Q43	N59	G65	K63	M79	S97	M116	H128	K141	F147	K163	G164	I165	I170	A174	E180	F181	F182	N183	A184	R185	R186
-----	-----	-----	-----	-----	-----	----	-----	-----	-----	-----	-----	-----	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------	------

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.11Å 79.77Å 96.62Å 90.00° 114.28° 90.00°	Depositor
Resolution (Å)	48.15 – 1.80 48.15 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.0 (48.15-1.80) 98.1 (48.15-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.29 (at 1.81Å)	Xtriage
Refinement program	REFMAC 5.8.0253	Depositor
R, R_{free}	0.166 , 0.208 0.176 , 0.215	Depositor DCC
R_{free} test set	5027 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.086	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 28.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.166 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	9286	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.15% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COA, MJZ, NA

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	0/1414	1.22	2/1918 (0.1%)
1	B	1.01	0/1402	1.25	2/1902 (0.1%)
1	C	1.03	0/1449	1.24	3/1962 (0.2%)
1	D	0.97	0/1341	1.21	1/1822 (0.1%)
1	E	1.00	0/1440	1.25	2/1952 (0.1%)
1	F	1.02	0/1413	1.20	0/1917
All	All	1.01	0/8459	1.23	10/11473 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	33	TYR	CB-CA-C	5.50	119.69	109.51
1	A	59	ASN	CA-CB-CG	-5.38	107.22	112.60
1	C	34	PRO	N-CA-C	5.33	115.59	110.47
1	E	33	TYR	CB-CA-C	5.32	119.07	109.45
1	B	33	TYR	CB-CA-C	5.28	119.01	109.45
1	D	54	THR	CA-CB-OG1	-5.20	101.80	109.60
1	E	178	ILE	N-CA-C	-5.14	105.52	110.72
1	C	178	ILE	N-CA-C	-5.12	105.39	110.62
1	B	21	ASP	CA-CB-CG	5.07	117.67	112.60
1	C	33	TYR	CB-CA-C	5.02	118.54	109.45

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1380	0	1381	10	0
1	B	1366	0	1365	17	0
1	C	1409	0	1424	12	0
1	D	1308	0	1301	8	0
1	E	1400	0	1412	17	0
1	F	1382	0	1374	10	0
2	A	40	0	23	0	0
2	B	40	0	23	2	0
2	F	40	0	23	0	0
3	A	96	0	64	1	0
3	B	48	0	32	2	0
3	E	96	0	64	2	0
3	F	48	0	32	1	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	125	0	0	1	0
5	B	90	0	0	1	0
5	C	99	0	0	0	0
5	D	103	0	0	2	0
5	E	102	0	0	1	0
5	F	112	0	0	0	0
All	All	9286	0	8518	71	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 4.

All (71) 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:D:59:ASN:OD1	5:D:301:HOH:O	2.01	0.77
1:A:185:ARG:O	5:A:301:HOH:O	2.03	0.76
1:E:179:GLN:HE21	1:E:179:GLN:HA	1.59	0.68
1:A:170:ILE:HG12	1:A:174:ALA:HB3	1.79	0.65
1:B:59:ASN:HD21	1:C:59[A]:ASN:HD21	1.44	0.64
1:F:128:HIS:H	1:F:128:HIS:CD2	2.18	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:142:LEU:HD23	1:E:144:ILE:HD11	1.81	0.61
1:A:128:HIS:H	1:A:128:HIS:CD2	2.17	0.61
1:E:19:ILE:HD13	1:E:25[A]:ILE:CD1	2.31	0.60
1:A:72:ILE:HD12	1:A:90:ILE:HD12	1.82	0.60
3:E:201:COA:H21	5:E:356:HOH:O	2.01	0.60
1:B:128:HIS:CD2	1:B:128:HIS:H	2.19	0.59
1:C:72:ILE:CD1	1:C:90:ILE:HD12	2.33	0.59
1:B:72:ILE:HD12	1:B:90:ILE:HD12	1.86	0.58
1:D:128:HIS:H	1:D:128:HIS:CD2	2.23	0.57
1:D:134:MET:HE1	1:E:121:HIS:HB2	1.87	0.56
1:B:99:HIS:NE2	1:C:99:HIS:HD2	2.04	0.56
1:B:65:GLY:HA3	1:B:68:LYS:O	2.07	0.54
1:D:25[B]:ILE:HD13	1:D:31:ILE:HD12	1.88	0.54
3:A:203:COA:O2A	1:B:141:LYS:HE2	2.09	0.53
3:B:202:COA:H2A	1:C:153:ASN:OD1	2.09	0.52
1:B:131:MET:HE2	3:B:202:COA:H141	1.91	0.52
1:B:38:LYS:HG3	2:B:201:MJZ:H8'	1.92	0.51
1:B:156:LYS:HE3	5:B:308:HOH:O	2.10	0.51
1:E:72:ILE:HD12	1:E:90:ILE:HD12	1.92	0.51
1:E:19:ILE:HD13	1:E:25[A]:ILE:HD12	1.93	0.51
1:E:165:ILE:O	1:E:168:SER:OG	2.24	0.51
1:B:99:HIS:CD2	1:C:99:HIS:HD2	2.29	0.50
1:E:72:ILE:CD1	1:E:90:ILE:HD12	2.41	0.50
1:B:170:ILE:H	1:B:170:ILE:HD13	1.77	0.49
1:E:153:ASN:OD1	3:E:201:COA:H2A	2.13	0.49
1:C:35:PRO:HB3	1:C:86:HIS:HB3	1.95	0.48
1:E:147:PHE:HB3	1:E:165:ILE:HD11	1.96	0.48
1:C:25:ILE:CD1	1:C:56:ILE:HD12	2.44	0.47
1:C:179:GLN:HA	1:C:179:GLN:HE21	1.79	0.47
1:F:170:ILE:HG12	1:F:174:ALA:HB3	1.97	0.47
1:E:19:ILE:HD13	1:E:25[A]:ILE:HD11	1.95	0.47
1:C:72:ILE:HD12	1:C:90:ILE:HD12	1.96	0.47
1:F:116:MET:HG3	3:F:201:COA:H31	1.97	0.47
1:A:128:HIS:H	1:A:128:HIS:HD2	1.63	0.46
1:A:170:ILE:HG12	1:A:174:ALA:CB	2.46	0.46
1:C:142:LEU:HD23	1:C:144:ILE:HD11	1.98	0.46
1:E:142:LEU:CD2	1:E:144:ILE:HD11	2.44	0.46
1:C:65:GLY:HA3	1:C:68:LYS:O	2.16	0.46
1:E:25[B]:ILE:CD1	1:E:56:ILE:HD12	2.46	0.46
1:A:65:GLY:HA3	1:A:68:LYS:O	2.16	0.45
1:E:7:ILE:N	1:E:7:ILE:HD13	2.33	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:146:PRO:HB2	1:D:147:PHE:CD2	2.53	0.44
1:E:6:GLN:C	1:E:7:ILE:HD13	2.43	0.44
1:F:182:PHE:C	1:F:184:ALA:H	2.25	0.44
1:F:65:GLY:HA3	1:F:68:LYS:O	2.18	0.43
1:A:72:ILE:CD1	1:A:90:ILE:HD12	2.48	0.43
1:D:25[B]:ILE:HD13	1:D:31:ILE:CD1	2.48	0.43
1:A:128:HIS:CD2	1:A:128:HIS:N	2.86	0.42
1:F:170:ILE:CG1	1:F:174:ALA:HB3	2.50	0.42
1:E:179:GLN:HA	1:E:179:GLN:NE2	2.31	0.42
1:B:161:ASN:O	1:B:162:ASP:C	2.63	0.42
1:B:147:PHE:O	1:B:161:ASN:N	2.47	0.42
1:A:142:LEU:HD23	1:A:144:ILE:HD11	2.00	0.42
1:D:58:GLY:O	1:D:80:LYS:HA	2.20	0.42
1:B:8:HIS:CG	1:B:9:PRO:HD2	2.55	0.42
1:B:1[B]:MET:HE3	1:B:1[B]:MET:HB2	1.75	0.41
1:E:13:ILE:HD13	1:E:19:ILE:HD11	2.01	0.41
1:F:128:HIS:CD2	1:F:128:HIS:N	2.87	0.41
1:C:121:HIS:CE1	1:C:122:GLN:HG2	2.56	0.41
1:D:68:LYS:NZ	5:D:304:HOH:O	2.43	0.41
1:B:58:GLY:O	1:B:80:LYS:HA	2.21	0.41
1:B:86:HIS:NE2	2:B:201:MJZ:N3'	2.69	0.41
1:F:128:HIS:H	1:F:128:HIS:HD2	1.66	0.41
1:F:147:PHE:HB3	1:F:165:ILE:HD11	2.03	0.41
1:F:79:MET:HE3	1:F:97:SER:HA	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	182/189 (96%)	180 (99%)	2 (1%)	0	100 100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	177/189 (94%)	171 (97%)	5 (3%)	1 (1%)	21	11
1	C	185/189 (98%)	183 (99%)	2 (1%)	0	100	100
1	D	170/189 (90%)	166 (98%)	4 (2%)	0	100	100
1	E	185/189 (98%)	181 (98%)	4 (2%)	0	100	100
1	F	182/189 (96%)	177 (97%)	5 (3%)	0	100	100
All	All	1081/1134 (95%)	1058 (98%)	22 (2%)	1 (0%)	48	34

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2	ASN

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	150/155 (97%)	142 (95%)	8 (5%)	20	9
1	B	149/155 (96%)	145 (97%)	4 (3%)	39	27
1	C	154/155 (99%)	144 (94%)	10 (6%)	15	5
1	D	144/155 (93%)	141 (98%)	3 (2%)	47	36
1	E	153/155 (99%)	145 (95%)	8 (5%)	21	9
1	F	150/155 (97%)	143 (95%)	7 (5%)	23	11
All	All	900/930 (97%)	860 (96%)	40 (4%)	25	13

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	ASN
1	A	22	ASP
1	A	59	ASN
1	A	68	LYS
1	A	128	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	163	LYS
1	A	170	ILE
1	A	173	ARG
1	B	59	ASN
1	B	128	HIS
1	B	170	ILE
1	B	180	GLU
1	C	6	GLN
1	C	15	GLU
1	C	59[A]	ASN
1	C	59[B]	ASN
1	C	163	LYS
1	C	165	ILE
1	C	170	ILE
1	C	172	GLU
1	C	179	GLN
1	C	186	ARG
1	D	6	GLN
1	D	59	ASN
1	D	128	HIS
1	E	6	GLN
1	E	7	ILE
1	E	163	LYS
1	E	166	GLU
1	E	167	LYS
1	E	171	ASP
1	E	172	GLU
1	E	179	GLN
1	F	4	ASN
1	F	43	GLN
1	F	59	ASN
1	F	128	HIS
1	F	141	LYS
1	F	163	LYS
1	F	180	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	59	ASN
1	A	128	HIS
1	B	74	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	128	HIS
1	B	183	ASN
1	C	43	GLN
1	C	93	ASN
1	C	99	HIS
1	C	179	GLN
1	D	74	ASN
1	D	93	ASN
1	D	128	HIS
1	E	179	GLN
1	F	6	GLN
1	F	74	ASN
1	F	93	ASN
1	F	128	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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
3	COA	E	202	-	47,50,50	0.65	1 (2%)	69,75,75	0.82	2 (2%)
2	MJZ	A	201	-	41,42,42	0.69	1 (2%)	58,64,64	0.68	0
3	COA	A	202	-	47,50,50	0.65	1 (2%)	69,75,75	0.78	2 (2%)
3	COA	B	202	-	47,50,50	0.61	0	69,75,75	0.79	1 (1%)
2	MJZ	B	201	-	41,42,42	0.75	1 (2%)	58,64,64	0.59	0
2	MJZ	F	202	-	41,42,42	0.63	1 (2%)	58,64,64	0.72	0
3	COA	F	201	-	47,50,50	0.59	0	69,75,75	0.74	0
3	COA	A	203	-	47,50,50	0.64	1 (2%)	69,75,75	0.75	1 (1%)
3	COA	E	201	-	47,50,50	0.62	0	69,75,75	0.80	1 (1%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COA	E	202	-	-	4/48/64/64	0/3/3/3
2	MJZ	A	201	-	-	4/28/65/65	0/3/3/3
3	COA	A	202	-	-	5/48/64/64	0/3/3/3
3	COA	B	202	-	-	10/48/64/64	0/3/3/3
2	MJZ	B	201	-	-	3/28/65/65	0/3/3/3
2	MJZ	F	202	-	-	4/28/65/65	0/3/3/3
3	COA	F	201	-	-	9/48/64/64	0/3/3/3
3	COA	A	203	-	-	5/48/64/64	0/3/3/3
3	COA	E	201	-	-	13/48/64/64	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	202	COA	P3B-O3B	3.25	1.65	1.59
2	B	201	MJZ	O'Q-C6'	-3.10	1.20	1.30
3	E	202	COA	P3B-O3B	2.59	1.64	1.59
2	A	201	MJZ	O'Q-C6'	-2.55	1.22	1.30
2	F	202	MJZ	O'Q-C6'	-2.54	1.22	1.30
3	A	203	COA	P3B-O3B	2.12	1.63	1.59

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	201	COA	P3B-O3B-C3B	-3.32	114.56	123.43
3	B	202	COA	P3B-O3B-C3B	-3.14	115.06	123.43
3	A	202	COA	P3B-O3B-C3B	-2.75	116.08	123.43
3	E	202	COA	O5A-P2A-O4A	2.62	124.64	112.44
3	A	202	COA	O5A-P2A-O4A	2.37	123.48	112.44
3	A	203	COA	P3B-O3B-C3B	-2.30	117.28	123.43
3	E	202	COA	O3B-P3B-O7A	-2.09	101.87	109.33

There are no chirality outliers.

All (57) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	203	COA	S1P-C2P-C3P-N4P
3	B	202	COA	C5B-O5B-P1A-O1A
3	B	202	COA	C5B-O5B-P1A-O2A
3	B	202	COA	C5B-O5B-P1A-O3A
3	E	201	COA	C5B-O5B-P1A-O1A
3	E	201	COA	C5B-O5B-P1A-O2A
3	E	201	COA	S1P-C2P-C3P-N4P
3	F	201	COA	OAP-CAP-CBP-CCP
3	F	201	COA	OAP-CAP-CBP-CDP
3	B	202	COA	C3B-C4B-C5B-O5B
3	B	202	COA	O4B-C4B-C5B-O5B
3	E	201	COA	C3B-C4B-C5B-O5B
3	E	201	COA	O4B-C4B-C5B-O5B
2	F	202	MJZ	C2C-C1C-N1-C6
3	F	201	COA	OAP-CAP-CBP-CEP
3	A	202	COA	P1A-O3A-P2A-O4A
3	E	202	COA	P1A-O3A-P2A-O4A
3	E	202	COA	C3B-O3B-P3B-O8A
2	A	201	MJZ	C2C-C1C-N1-C6
3	A	202	COA	P1A-O3A-P2A-O5A
3	A	203	COA	P1A-O3A-P2A-O5A
3	E	202	COA	P1A-O3A-P2A-O5A
3	E	201	COA	CEP-CBP-CCP-O6A
3	F	201	COA	C3B-O3B-P3B-O7A
3	F	201	COA	S1P-C2P-C3P-N4P
2	F	202	MJZ	O4C-C1C-N1-C6
3	E	201	COA	C5B-O5B-P1A-O3A
2	A	201	MJZ	O4C-C1C-N1-C6
3	E	201	COA	C5P-C6P-C7P-N8P
3	A	203	COA	P1A-O3A-P2A-O4A
3	B	202	COA	P2A-O3A-P1A-O2A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	E	201	COA	P1A-O3A-P2A-O5A
3	F	201	COA	P1A-O3A-P2A-O5A
2	B	201	MJZ	C2C-C1C-N1-C6
3	E	201	COA	O5P-C5P-N4P-C3P
3	A	202	COA	C3B-O3B-P3B-O8A
3	A	202	COA	C3B-O3B-P3B-O7A
3	E	201	COA	C3B-O3B-P3B-O7A
2	F	202	MJZ	O4C-C1C-N1-C2
2	B	201	MJZ	O4C-C1C-N1-C6
2	A	201	MJZ	O4C-C1C-N1-C2
2	F	202	MJZ	C2C-C1C-N1-C2
3	F	201	COA	C9P-CAP-CBP-CDP
3	B	202	COA	P1A-O3A-P2A-O4A
3	E	201	COA	P1A-O3A-P2A-O4A
3	F	201	COA	P1A-O3A-P2A-O4A
3	A	203	COA	CEP-CBP-CCP-O6A
3	B	202	COA	C5P-C6P-C7P-N8P
3	B	202	COA	C3B-O3B-P3B-O7A
3	E	202	COA	C3B-O3B-P3B-O7A
2	A	201	MJZ	C2C-C1C-N1-C2
3	A	202	COA	N8P-C9P-CAP-OAP
3	A	203	COA	N8P-C9P-CAP-OAP
3	B	202	COA	N8P-C9P-CAP-OAP
3	E	201	COA	N8P-C9P-CAP-OAP
3	F	201	COA	N8P-C9P-CAP-OAP
2	B	201	MJZ	O4C-C1C-N1-C2

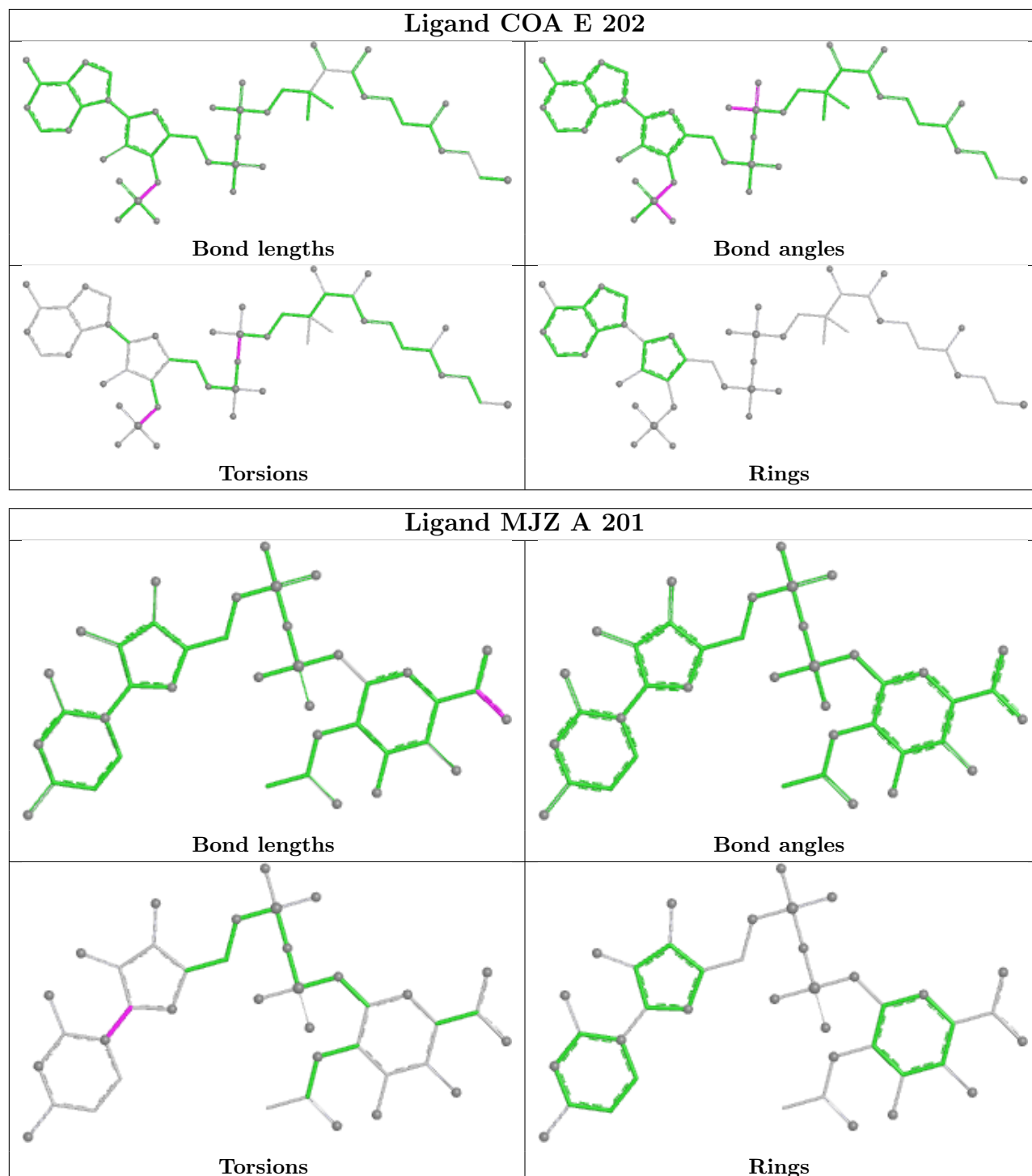
There are no ring outliers.

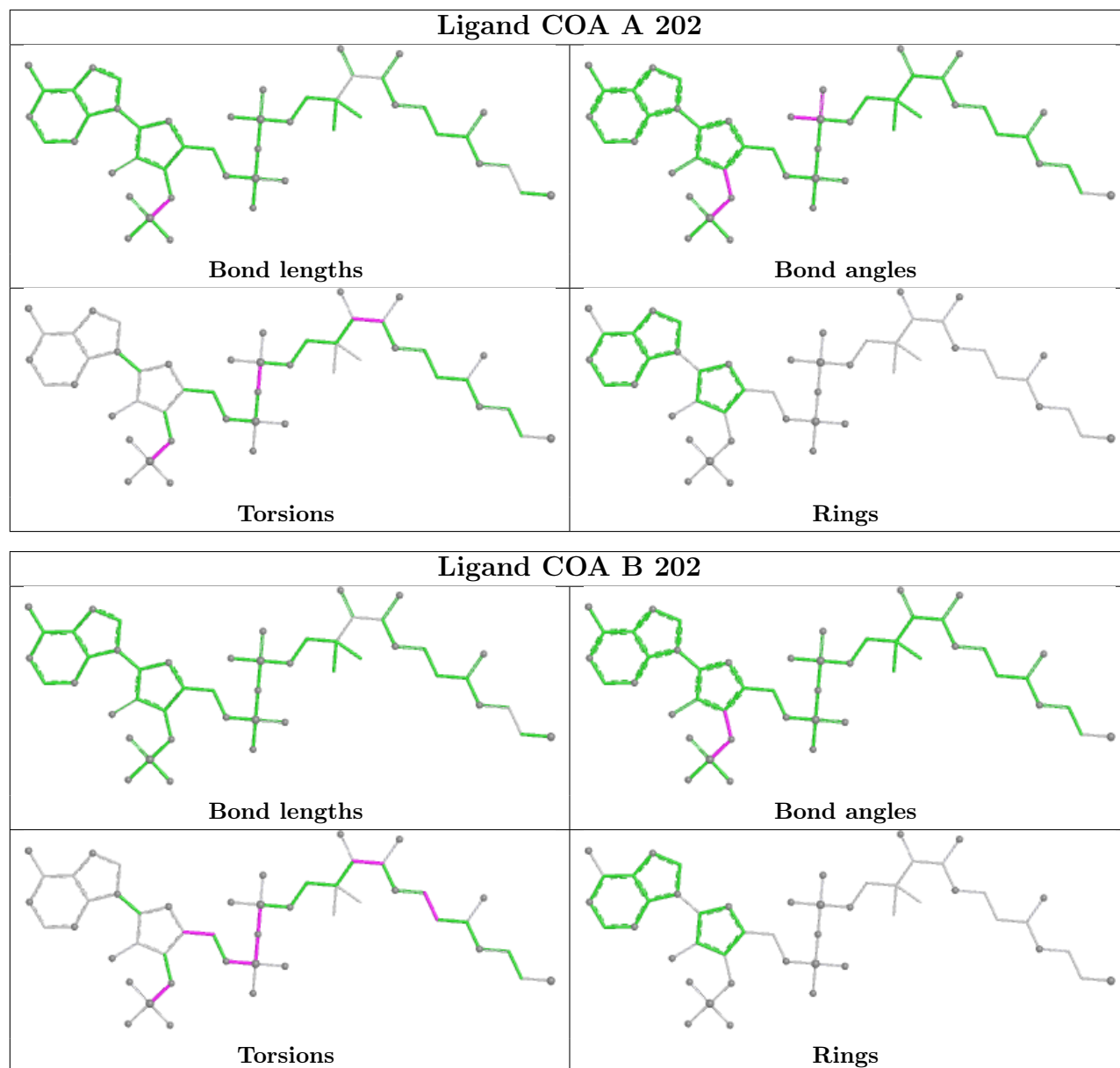
5 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	202	COA	2	0
2	B	201	MJZ	2	0
3	F	201	COA	1	0
3	A	203	COA	1	0
3	E	201	COA	2	0

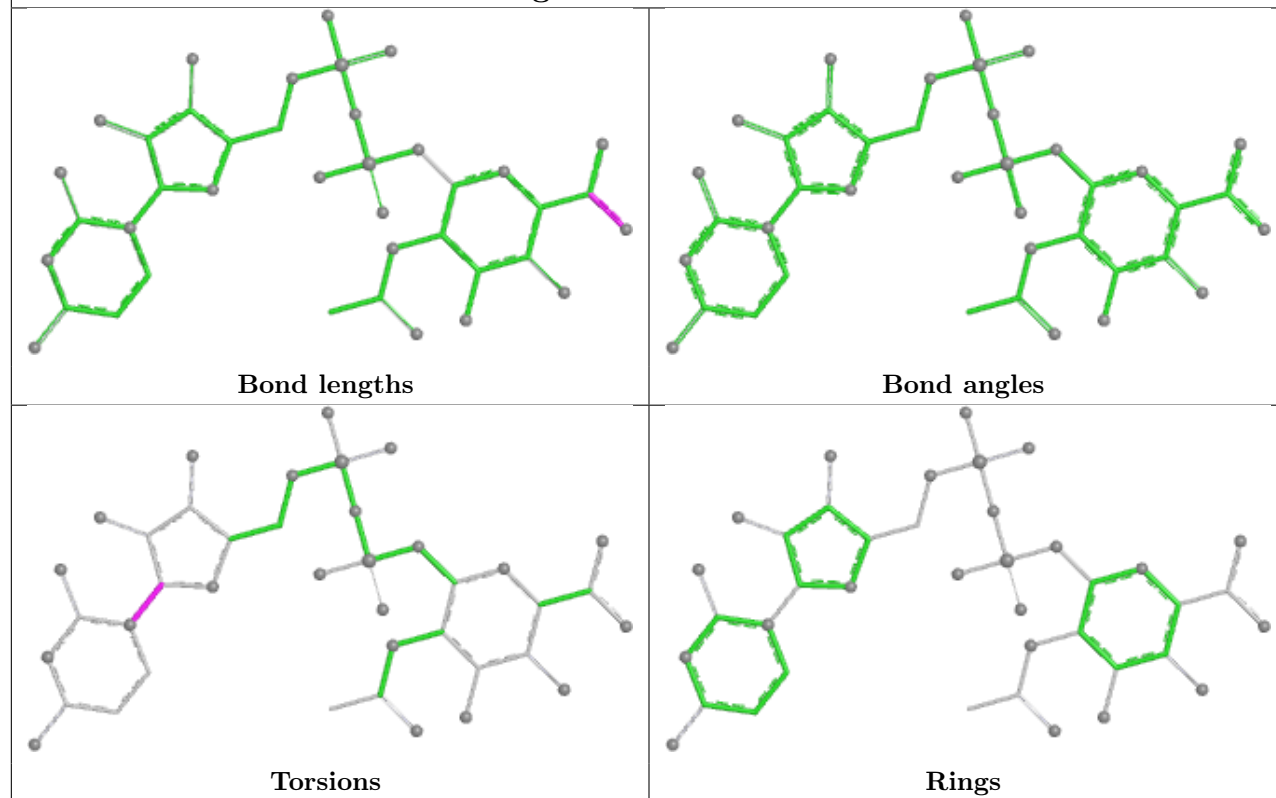
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

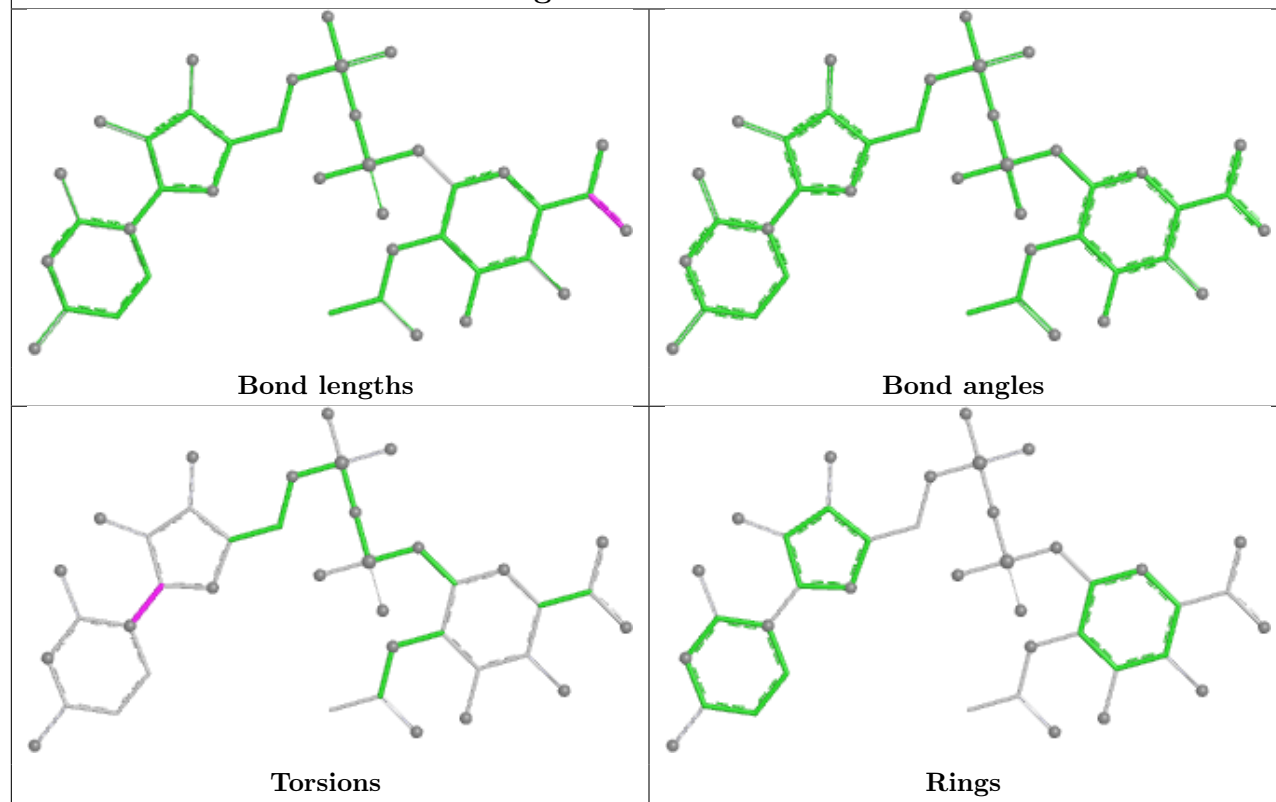


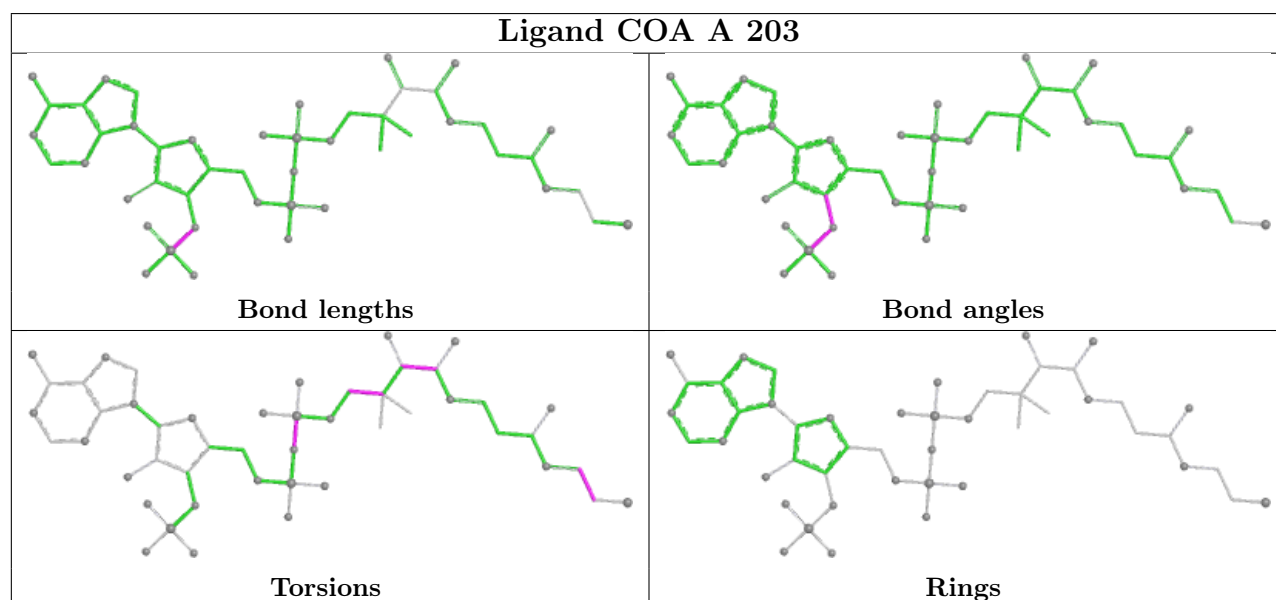
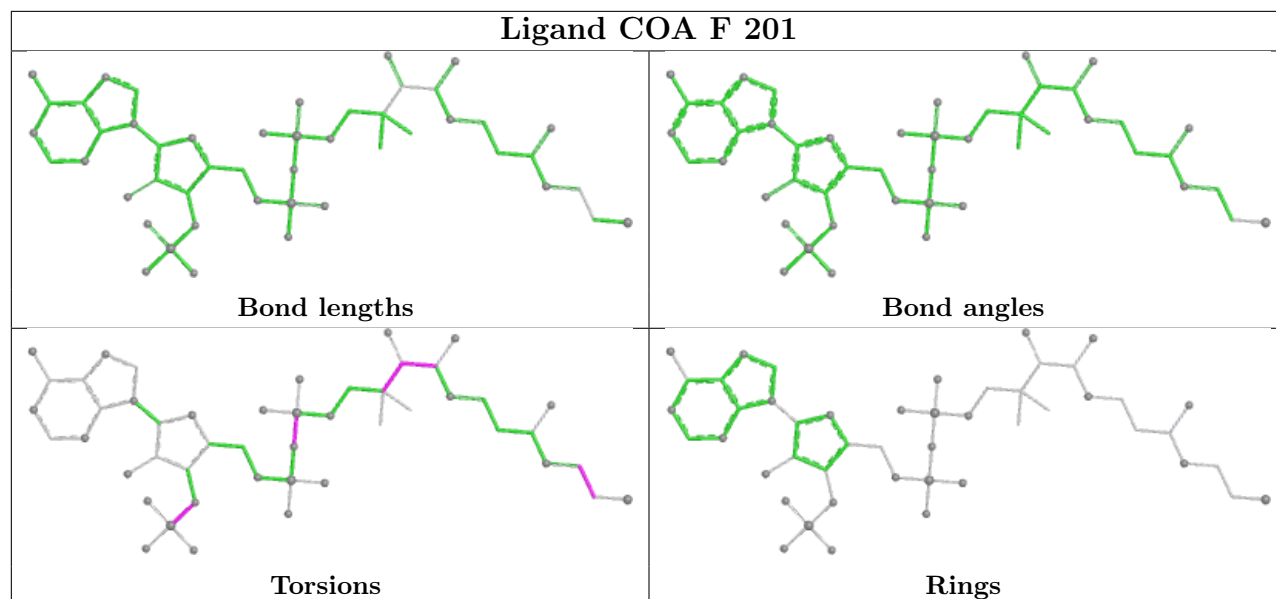


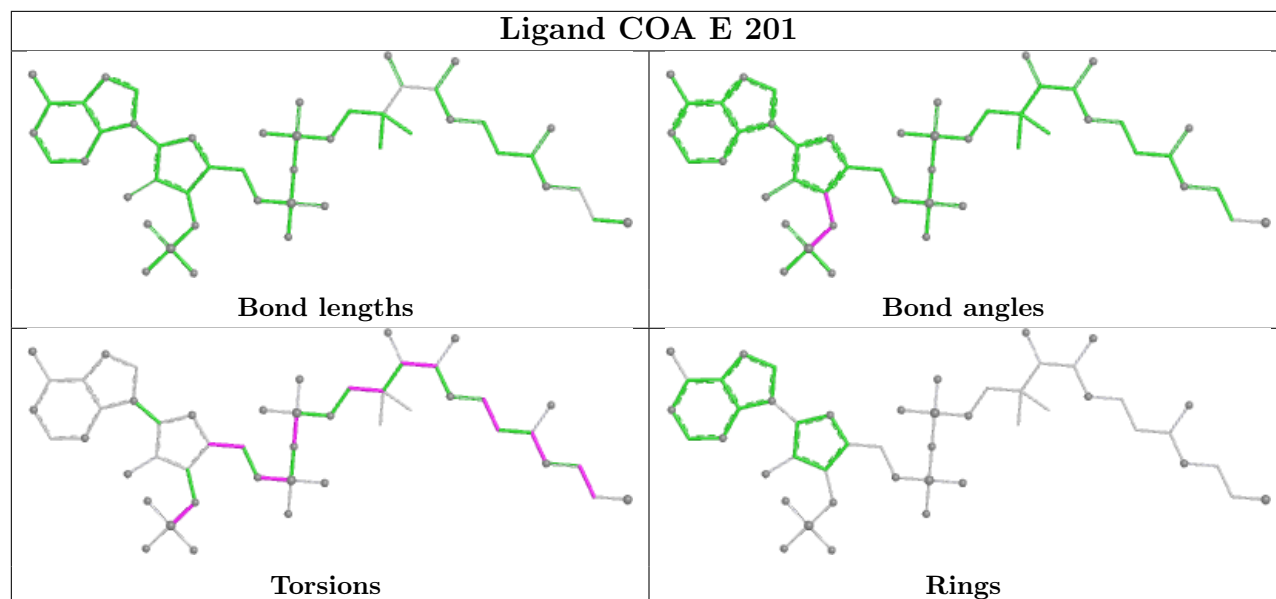
Ligand MJZ B 201



Ligand MJZ F 202







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	182/189 (96%)	-1.36	0 100 100	6, 17, 43, 67	2 (1%)
1	B	179/189 (94%)	-1.25	0 100 100	7, 19, 66, 95	3 (1%)
1	C	183/189 (96%)	-1.30	0 100 100	7, 18, 49, 76	4 (2%)
1	D	172/189 (91%)	-1.31	0 100 100	8, 18, 55, 70	2 (1%)
1	E	183/189 (96%)	-1.30	0 100 100	9, 18, 49, 80	4 (2%)
1	F	183/189 (96%)	-1.35	0 100 100	10, 16, 40, 72	1 (0%)
All	All	1082/1134 (95%)	-1.31	0 100 100	6, 18, 52, 95	16 (1%)

There are no RSRZ outliers to report.

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MJZ	B	201	40/40	0.97	0.07	26,34,39,43	40

Continued on next page...

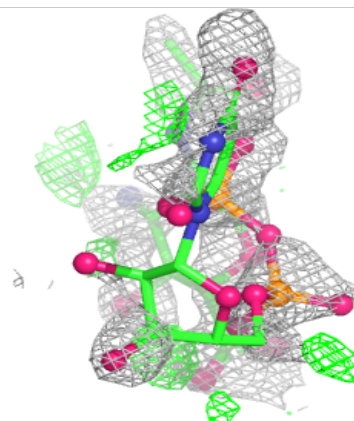
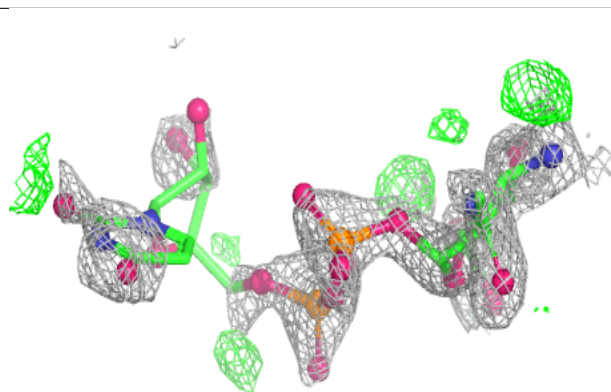
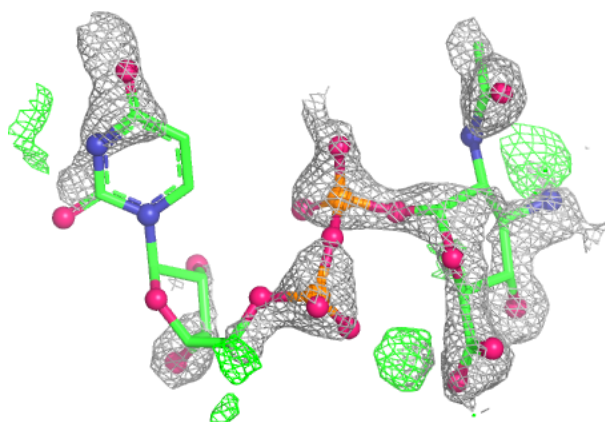
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MJZ	A	201	40/40	0.98	0.04	32,40,46,47	0
2	MJZ	F	202	40/40	0.98	0.04	24,32,36,37	0
3	COA	B	202	48/48	0.98	0.06	25,61,84,89	0
3	COA	A	203	48/48	0.99	0.04	21,34,55,58	0
3	COA	A	202	48/48	0.99	0.03	17,24,35,44	0
3	COA	E	201	48/48	0.99	0.04	26,51,72,79	0
3	COA	E	202	48/48	0.99	0.03	16,22,34,41	0
3	COA	F	201	48/48	0.99	0.04	20,32,46,50	0
4	NA	B	203	1/1	0.99	0.06	20,20,20,20	0
4	NA	D	201	1/1	0.99	0.04	22,22,22,22	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.

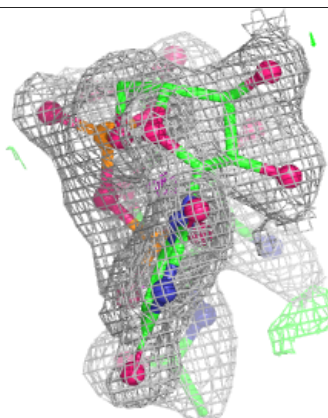
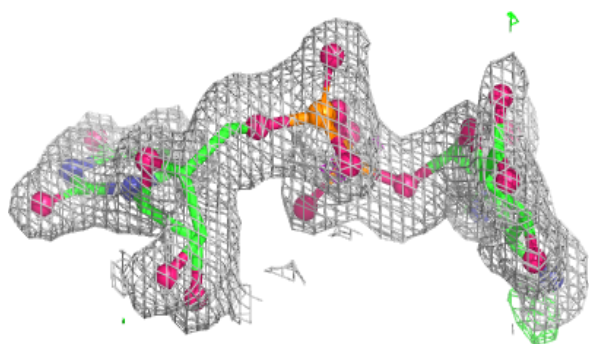
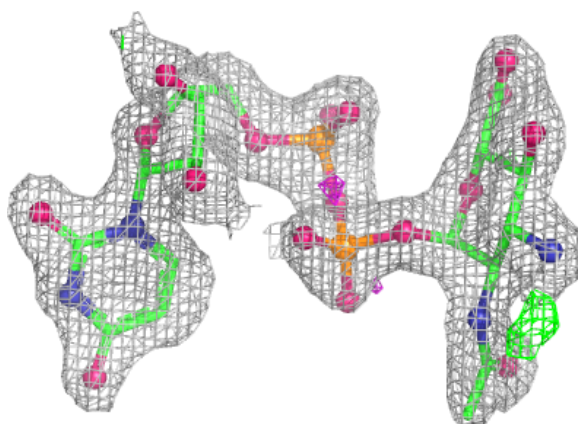
Electron density around MJZ B 201:

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

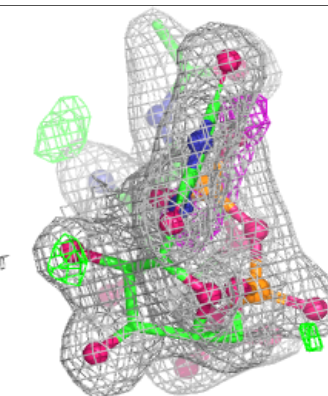
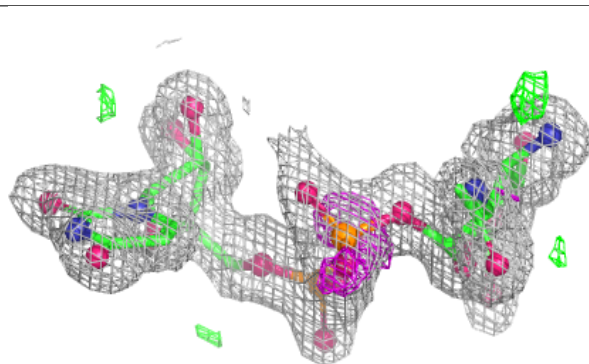
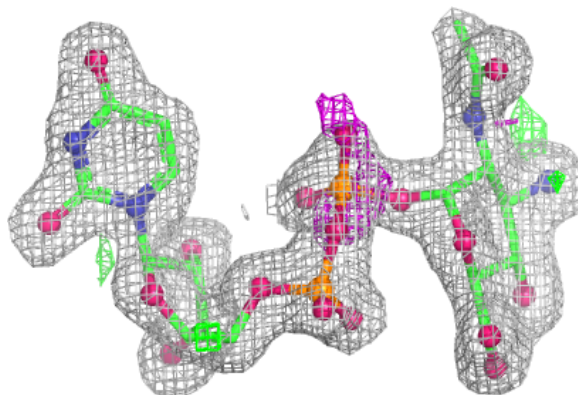


Electron density around MJZ A 201:

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

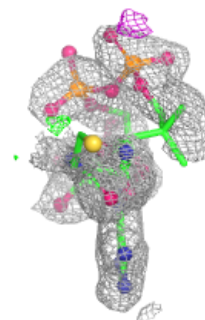
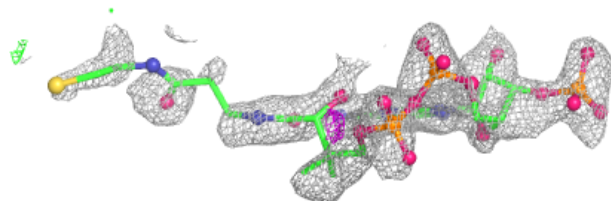
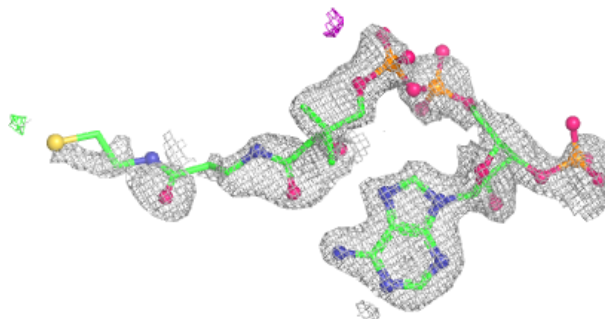
**Electron density around MJZ F 202:**

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

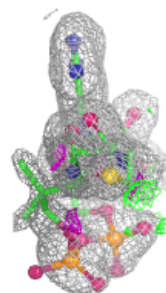
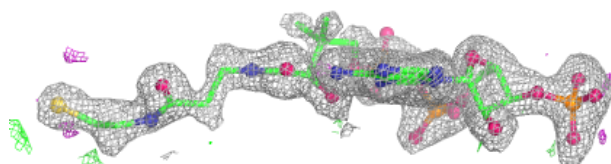
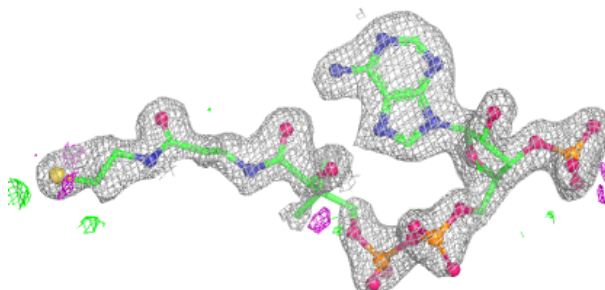


Electron density around COA B 202:

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

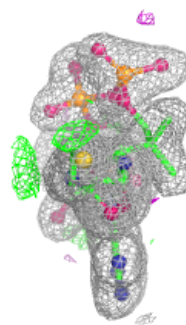
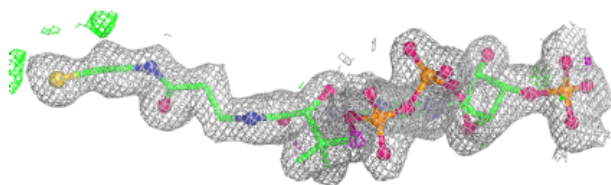
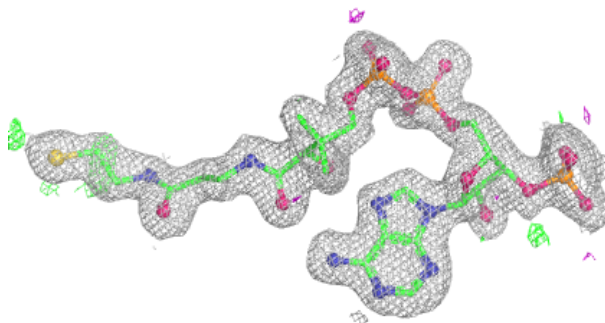
**Electron density around COA A 203:**

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

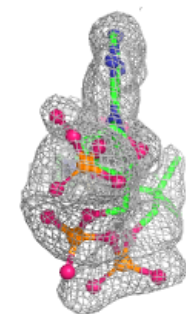
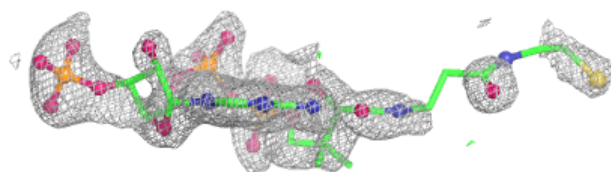
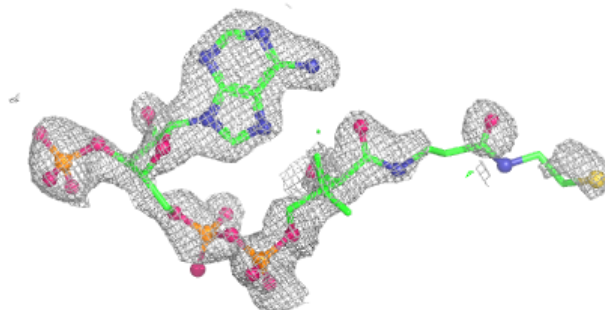


Electron density around COA A 202:

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

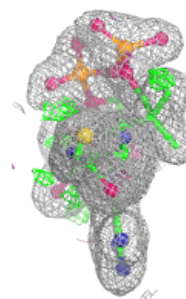
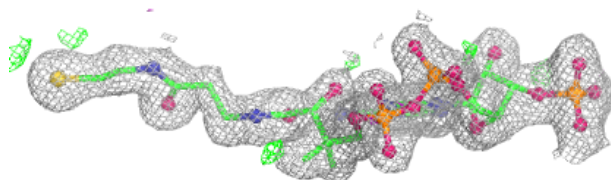
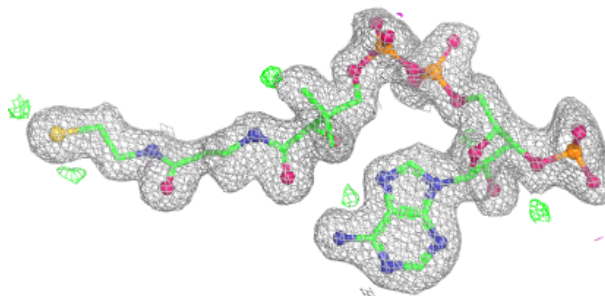
**Electron density around COA E 201:**

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

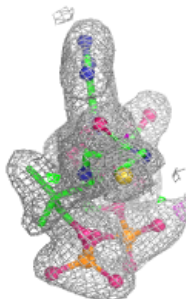
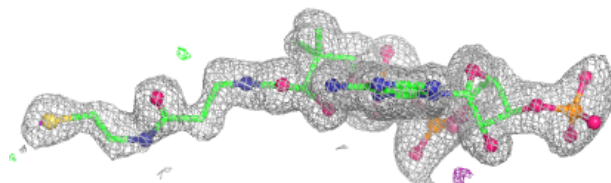
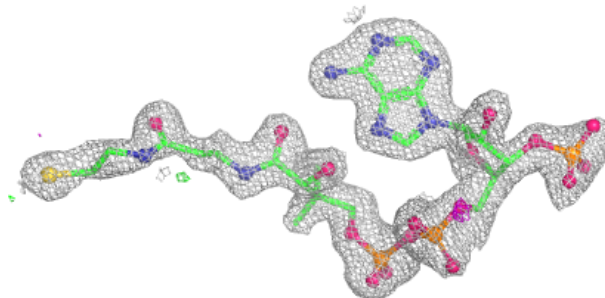


Electron density around COA E 202:

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

**Electron density around COA F 201:**

$2mF_o-DF_c$ (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.