



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 28, 2019 – 03:05 PM EDT

PDB ID : 1CB7
Title : GLUTAMATE MUTASE FROM CLOSTRIDIUM COCHLEARIIUM RE-
CONSTITUTED WITH METHYL-COBALAMIN
Authors : Gruber, K.; Reitzer, R.; Kratky, C.
Deposited on : 1999-03-03
Resolution : 2.00 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 : 1.8.0 (224370), CSD as540be (2019)
Xtriage (Phenix) : 1.13
EDS : 2.4
buster-report : 1.1.7 (2018)
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac : 5.8.0158
CCP4 : 7.0 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.4

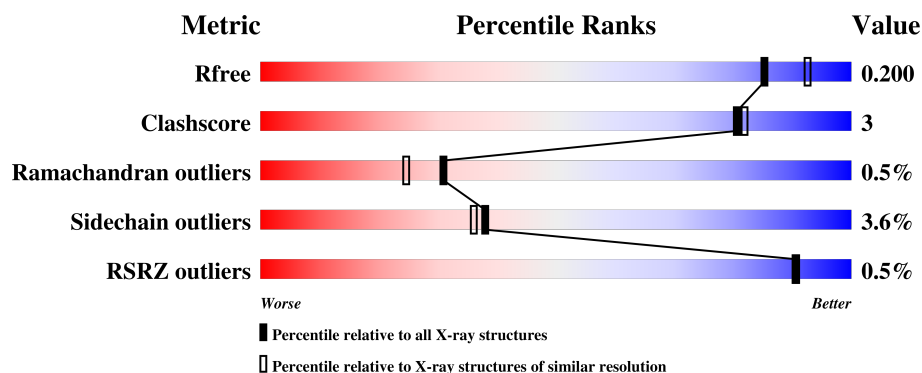
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	111664	7193 (2.00-2.00)
Clashscore	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	137	<div> <div style="width: 91%;"></div> <div style="width: 6%;"></div> <div style="width: 3%;"></div> <div style="width: 2%;"></div> </div> <div>91% 6% ..</div>
1	C	137	<div> <div style="width: 88%;"></div> <div style="width: 12%;"></div> <div style="width: 2%;"></div> </div> <div>88% 12% .</div>
2	B	483	<div> <div style="width: 90%;"></div> <div style="width: 9%;"></div> </div> <div>90% 9% .</div>
2	D	483	<div> <div style="width: 89%;"></div> <div style="width: 10%;"></div> </div> <div>89% 10% .</div>

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 10825 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 PROTEIN (GLUTAMATE MUTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	S	0	0	0
			1041	663	175	198	5			
1	C	137	Total	C	N	O	S	0	0	0
			1041	663	175	198	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	45	LEU	VAL	conflict	UNP P80078
C	45	LEU	VAL	conflict	UNP P80078
A	60	VAL	LEU	conflict	UNP P80078
C	60	VAL	LEU	conflict	UNP P80078

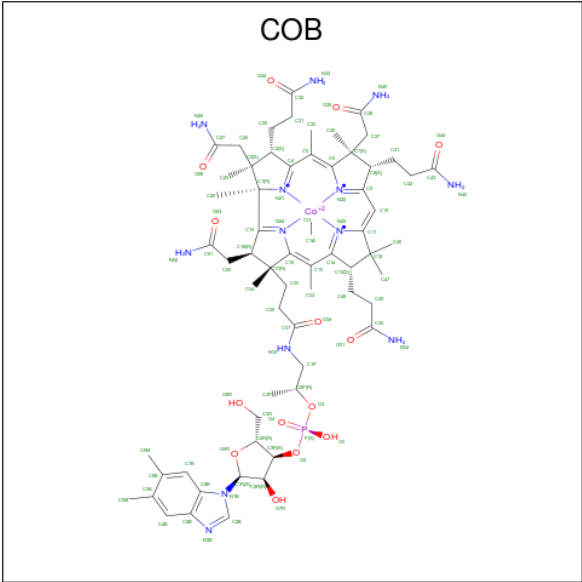
- Molecule 2 is a protein called PROTEIN (GLUTAMATE MUTASE).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	483	Total	C	N	O	S	0	0	0
			3762	2383	643	714	22			
2	D	483	Total	C	N	O	S	0	0	0
			3762	2383	643	714	22			

There are 2 discrepancies between the modelled and reference sequences:

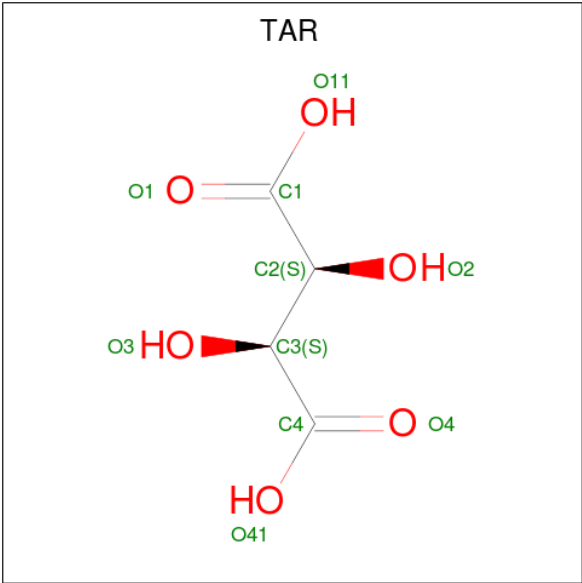
Chain	Residue	Modelled	Actual	Comment	Reference
B	130	PHE	TYR	conflict	UNP P80077
D	130	PHE	TYR	conflict	UNP P80077

- Molecule 3 is CO-METHYLCOBALAMIN (three-letter code: COB) (formula: C₆₃H₉₁CoN₁₃O₁₄P).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	Co	N	O	P	0	1
			93	64	1	13	14	1		
3	C	1	Total	C	Co	N	O	P	0	1
			93	64	1	13	14	1		

- Molecule 4 is D(-)-TARTARIC ACID (three-letter code: TAR) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			10	4	6		
4	D	1	Total	C	O	0	0
			10	4	6		

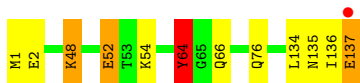
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	90	Total 90	O 90	0	0
5	B	422	Total 422	O 422	0	0
5	C	81	Total 81	O 81	0	0
5	D	420	Total 420	O 420	0	0

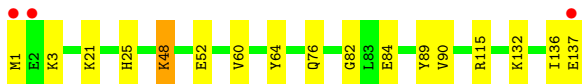
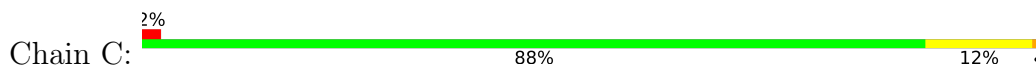
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

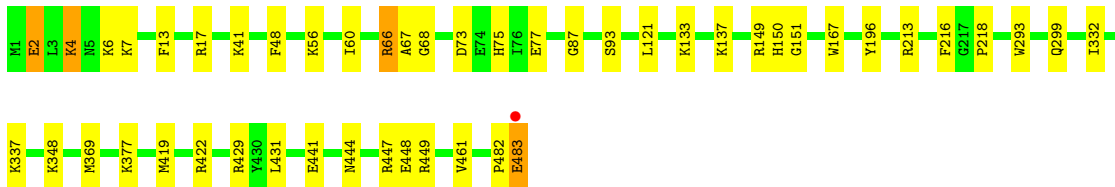
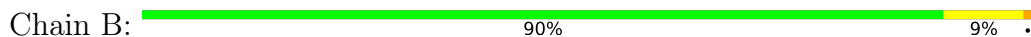
- Molecule 1: PROTEIN (GLUTAMATE MUTASE)



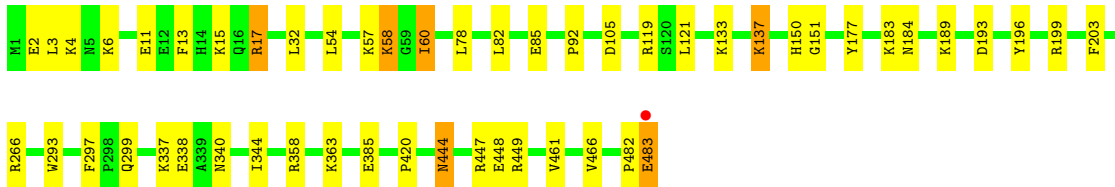
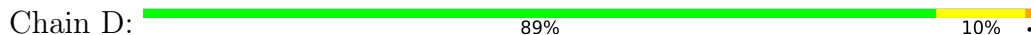
- Molecule 1: PROTEIN (GLUTAMATE MUTASE)



- Molecule 2: PROTEIN (GLUTAMATE MUTASE)



- Molecule 2: PROTEIN (GLUTAMATE MUTASE)



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	64.33Å 113.14Å 108.61Å 90.00° 95.62° 90.00°	Depositor
Resolution (Å)	25.00 – 2.00 24.94 – 2.00	Depositor EDS
% Data completeness (in resolution range)	96.1 (25.00-2.00) 92.5 (24.94-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.03 (at 1.99Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.160 , 0.218 0.157 , 0.200	Depositor DCC
R_{free} test set	10044 reflections (10.04%)	wwPDB-VP
Wilson B-factor (Å ²)	12.4	Xtriage
Anisotropy	0.699	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 75.5	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	10825	wwPDB-VP
Average B, all atoms (Å ²)	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.53% 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: COB, TAR

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	0.32	0/1058	0.93	1/1427 (0.1%)
1	C	0.33	0/1058	0.92	1/1427 (0.1%)
2	B	0.33	0/3833	0.98	9/5171 (0.2%)
2	D	0.33	0/3833	0.98	12/5171 (0.2%)
All	All	0.33	0/9782	0.97	23/13196 (0.2%)

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
2	D	0	1

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	196	TYR	CB-CG-CD1	8.80	126.28	121.00
2	B	422	ARG	NE-CZ-NH2	-8.53	116.04	120.30
2	D	447	ARG	NE-CZ-NH1	8.13	124.36	120.30
2	B	447	ARG	NE-CZ-NH1	6.87	123.74	120.30
2	D	358	ARG	NE-CZ-NH2	-6.84	116.88	120.30
2	D	196	TYR	CB-CG-CD1	6.74	125.04	121.00
1	C	89	TYR	CB-CG-CD1	6.73	125.04	121.00
1	A	64	TYR	CB-CG-CD1	6.68	125.01	121.00
2	B	66	ARG	NE-CZ-NH1	6.42	123.51	120.30
2	D	358	ARG	NE-CZ-NH1	6.14	123.37	120.30
2	B	213	ARG	NE-CZ-NH1	6.14	123.37	120.30
2	D	17	ARG	NE-CZ-NH1	6.01	123.30	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	449	ARG	CD-NE-CZ	5.95	131.93	123.60
2	B	449	ARG	CD-NE-CZ	5.85	131.79	123.60
2	D	105	ASP	CB-CG-OD1	5.82	123.53	118.30
2	D	11	GLU	C-N-CA	5.64	135.79	121.70
2	B	149	ARG	NE-CZ-NH1	5.50	123.05	120.30
2	B	429	ARG	NE-CZ-NH1	5.36	122.98	120.30
2	D	266	ARG	CD-NE-CZ	5.28	131.00	123.60
2	B	196	TYR	CG-CD1-CE1	5.23	125.49	121.30
2	D	199	ARG	NE-CZ-NH1	5.07	122.83	120.30
2	D	177	TYR	CB-CG-CD1	5.05	124.03	121.00
2	D	119	ARG	NE-CZ-NH2	-5.03	117.78	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	D	92	PRO	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1041	0	1057	7	0
1	C	1041	0	1057	8	0
2	B	3762	0	3762	20	0
2	D	3762	0	3762	18	0
3	A	93	0	0	0	0
3	C	93	0	0	0	0
4	B	10	0	4	0	0
4	D	10	0	4	0	0
5	A	90	0	0	1	0
5	B	422	0	0	8	0
5	C	81	0	0	3	0
5	D	420	0	0	4	0
All	All	10825	0	9646	53	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 3.

All (53) 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)
2:D:133:LYS:O	2:D:137:LYS:HD2	1.87	0.74
2:D:444:ASN:O	2:D:448:GLU:HG3	1.93	0.68
1:C:82:GLY:HA2	1:C:84:GLU:OE2	1.98	0.64
2:D:189:LYS:HE3	2:D:193:ASP:OD2	2.01	0.61
2:B:137:LYS:HD2	5:B:1298:HOH:O	2.00	0.60
2:B:482:PRO:O	2:B:483:GLU:HB3	2.01	0.59
2:D:461:VAL:HG22	5:D:1185:HOH:O	2.02	0.59
2:D:60:ILE:HG22	5:D:1266:HOH:O	2.04	0.57
1:C:1:MET:HG3	1:C:136:ILE:O	2.07	0.55
2:D:337:LYS:HE2	2:D:338:GLU:OE2	2.07	0.53
2:B:7:LYS:HG2	5:B:1299:HOH:O	2.08	0.53
2:B:2:GLU:OE2	2:B:4:LYS:HE3	2.09	0.52
1:C:48:LYS:HD2	5:C:843:HOH:O	2.08	0.52
2:B:369:MET:HE2	5:B:1277:HOH:O	2.08	0.52
2:B:444:ASN:O	2:B:448:GLU:HG3	2.09	0.52
1:A:48:LYS:HE2	1:A:52:GLU:OE2	2.10	0.51
2:B:73:ASP:O	2:B:77:GLU:HG3	2.11	0.50
2:D:85:GLU:HG3	5:D:1177:HOH:O	2.12	0.50
2:D:2:GLU:HG2	2:D:3:LEU:N	2.27	0.49
2:B:133:LYS:HG2	5:B:1180:HOH:O	2.13	0.47
2:D:482:PRO:O	2:D:483:GLU:HB2	2.13	0.47
1:A:1:MET:HG2	1:A:2:GLU:N	2.29	0.47
2:D:420:PRO:O	2:D:466:VAL:HG22	2.15	0.46
1:A:48:LYS:HG3	1:A:52:GLU:OE2	2.16	0.45
2:B:461:VAL:HG22	5:B:1072:HOH:O	2.15	0.45
2:D:444:ASN:ND2	5:D:1264:HOH:O	2.50	0.45
1:C:1:MET:N	5:C:862:HOH:O	2.50	0.45
2:B:377:LYS:NZ	5:B:1295:HOH:O	2.50	0.44
2:B:66:ARG:O	2:B:67:ALA:HB2	2.18	0.43
2:D:54:LEU:O	2:D:58:LYS:HG3	2.19	0.43
2:D:183:LYS:HD3	2:D:184:ASN:OD1	2.18	0.43
2:D:32:LEU:HD13	2:D:203:PHE:CE2	2.53	0.43
2:D:32:LEU:HD13	2:D:203:PHE:CZ	2.54	0.43
2:B:419:MET:SD	2:B:431:LEU:HD23	2.59	0.42
1:A:134:LEU:O	1:A:136:ILE:HG23	2.19	0.42
2:B:337:LYS:NZ	5:B:1278:HOH:O	2.50	0.42
2:B:41:LYS:HE2	5:B:1076:HOH:O	2.19	0.42
2:B:93:SER:HB2	2:B:167:TRP:CZ3	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:13:PHE:CE2	2:B:17:ARG:HD2	2.54	0.42
1:C:137:GLU:OE1	1:C:137:GLU:N	2.51	0.42
1:A:64:TYR:CE1	1:A:66:GLN:HB2	2.55	0.41
2:B:216:PHE:CD1	2:B:218:PRO:HD2	2.55	0.41
2:B:68:GLY:HA2	2:B:75:HIS:CE1	2.55	0.41
2:D:13:PHE:O	2:D:17:ARG:HG3	2.19	0.41
1:A:137:GLU:HG2	1:A:137:GLU:OXT	2.20	0.41
1:C:25:HIS:HD2	5:C:881:HOH:O	2.02	0.41
2:B:299:GLN:CD	2:B:332:ILE:HD11	2.41	0.41
2:D:340:ASN:O	2:D:344:ILE:HG13	2.21	0.41
1:C:60:VAL:O	1:C:90:VAL:HA	2.20	0.40
1:A:137:GLU:HG3	5:A:874:HOH:O	2.21	0.40
2:B:87:GLY:O	2:B:348:LYS:NZ	2.50	0.40
2:D:78:LEU:O	2:D:82:LEU:HG	2.20	0.40
1:C:115:ARG:NH2	1:C:132:LYS:HE3	2.36	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	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
1	C	135/137 (98%)	133 (98%)	2 (2%)	0	100	100
2	B	481/483 (100%)	471 (98%)	7 (2%)	3 (1%)	27	21
2	D	481/483 (100%)	470 (98%)	8 (2%)	3 (1%)	27	21
All	All	1232/1240 (99%)	1207 (98%)	19 (2%)	6 (0%)	31	25

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	150	HIS
2	B	151	GLY
2	B	293	TRP
2	D	150	HIS
2	D	151	GLY
2	D	293	TRP

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	111/111 (100%)	104 (94%)	7 (6%)	20	14
1	C	111/111 (100%)	105 (95%)	6 (5%)	24	19
2	B	396/396 (100%)	387 (98%)	9 (2%)	53	56
2	D	396/396 (100%)	382 (96%)	14 (4%)	39	37
All	All	1014/1014 (100%)	978 (96%)	36 (4%)	38	36

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	LYS
1	A	52	GLU
1	A	54	LYS
1	A	64	TYR
1	A	76	GLN
1	A	135	ASN
1	A	137	GLU
2	B	2	GLU
2	B	4	LYS
2	B	6	LYS
2	B	48	PHE
2	B	56	LYS
2	B	60	ILE
2	B	121	LEU
2	B	441	GLU
2	B	483	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	3	LYS
1	C	21	LYS
1	C	48	LYS
1	C	52	GLU
1	C	64	TYR
1	C	76	GLN
2	D	4	LYS
2	D	6	LYS
2	D	15	LYS
2	D	57	LYS
2	D	58	LYS
2	D	60	ILE
2	D	121	LEU
2	D	137	LYS
2	D	297	PHE
2	D	299	GLN
2	D	363	LYS
2	D	385	GLU
2	D	444	ASN
2	D	483	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	76	GLN
1	A	135	ASN
2	B	5	ASN
2	B	23	GLN
2	B	207	GLN
2	D	5	ASN
2	D	23	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
3	COB	A	800[A]	-	79,102,102	0.89	3 (3%)	92,170,170	1.31	14 (15%)
3	COB	A	800[B]	-	79,102,102	0.89	3 (3%)	92,170,170	1.31	14 (15%)
4	TAR	B	900	-	3,9,9	0.54	0	6,12,12	1.21	1 (16%)
3	COB	C	800[A]	-	79,102,102	0.91	5 (6%)	92,170,170	1.39	14 (15%)
3	COB	C	800[B]	-	79,102,102	0.91	5 (6%)	92,170,170	1.39	14 (15%)
4	TAR	D	900	-	3,9,9	0.63	0	6,12,12	1.43	1 (16%)

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	COB	A	800[A]	-	-	10/51/231/231	0/3/11/11
3	COB	A	800[B]	-	-	10/51/231/231	0/3/11/11
4	TAR	B	900	-	-	2/4/12/12	-
3	COB	C	800[A]	-	-	11/51/231/231	0/3/11/11
3	COB	C	800[B]	-	-	11/51/231/231	0/3/11/11
4	TAR	D	900	-	-	3/4/12/12	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800[B]	COB	C1-C19	2.78	1.54	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	800[A]	COB	C1-C19	2.78	1.54	1.51
3	C	800[A]	COB	C2-C3	-2.55	1.54	1.58
3	C	800[B]	COB	C2-C3	-2.55	1.54	1.58
3	C	800[A]	COB	C1-C19	2.51	1.54	1.51
3	C	800[B]	COB	C1-C19	2.51	1.54	1.51
3	A	800[B]	COB	C2-C3	-2.46	1.54	1.58
3	A	800[A]	COB	C2-C3	-2.46	1.54	1.58
3	C	800[A]	COB	C11-C10	-2.14	1.37	1.40
3	C	800[B]	COB	C11-C10	-2.14	1.37	1.40
3	C	800[A]	COB	O7R-C2R	-2.05	1.38	1.43
3	C	800[B]	COB	O7R-C2R	-2.05	1.38	1.43
3	A	800[B]	COB	C4B-C9B	-2.01	1.38	1.41
3	A	800[A]	COB	C4B-C9B	-2.01	1.38	1.41
3	C	800[A]	COB	C4B-C9B	-2.00	1.38	1.41
3	C	800[B]	COB	C4B-C9B	-2.00	1.38	1.41

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	800[A]	COB	C4R-O6R-C1R	-3.76	105.91	109.83
3	C	800[B]	COB	C4R-O6R-C1R	-3.76	105.91	109.83
3	A	800[B]	COB	C4R-O6R-C1R	-3.63	106.04	109.83
3	A	800[A]	COB	C4R-O6R-C1R	-3.63	106.04	109.83
3	C	800[A]	COB	C55-C17-C16	3.60	121.91	109.92
3	C	800[B]	COB	C55-C17-C16	3.60	121.91	109.92
3	A	800[B]	COB	C55-C17-C16	3.41	121.30	109.92
3	A	800[A]	COB	C55-C17-C16	3.41	121.30	109.92
3	C	800[A]	COB	C2-C3-C4	3.37	105.20	101.67
3	C	800[B]	COB	C2-C3-C4	3.37	105.20	101.67
3	A	800[B]	COB	C2-C3-C4	3.34	105.17	101.67
3	A	800[A]	COB	C2-C3-C4	3.34	105.17	101.67
3	C	800[A]	COB	C1-C19-N24	-3.04	107.19	114.53
3	C	800[B]	COB	C1-C19-N24	-3.04	107.19	114.53
3	A	800[B]	COB	C1-C19-N24	-3.00	107.29	114.53
3	A	800[A]	COB	C1-C19-N24	-3.00	107.29	114.53
3	A	800[B]	COB	C5M-C5B-C6B	2.83	126.66	120.72
3	A	800[A]	COB	C5M-C5B-C6B	2.83	126.66	120.72
3	A	800[B]	COB	C5M-C5B-C4B	-2.70	113.81	120.34
3	A	800[A]	COB	C5M-C5B-C4B	-2.70	113.81	120.34
3	C	800[A]	COB	C5M-C5B-C4B	-2.63	113.98	120.34
3	C	800[B]	COB	C5M-C5B-C4B	-2.63	113.98	120.34
3	C	800[A]	COB	C5M-C5B-C6B	2.60	126.18	120.72

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	800[B]	COB	C5M-C5B-C6B	2.60	126.18	120.72
3	C	800[A]	COB	C55-C17-C18	-2.55	105.92	111.11
3	C	800[B]	COB	C55-C17-C18	-2.55	105.92	111.11
4	D	900	TAR	C4-C3-C2	-2.53	107.66	113.11
3	C	800[A]	COB	C30-C31-C32	2.52	120.96	112.61
3	C	800[B]	COB	C30-C31-C32	2.52	120.96	112.61
3	C	800[A]	COB	C16-C15-C14	-2.51	120.24	124.23
3	C	800[B]	COB	C16-C15-C14	-2.51	120.24	124.23
3	A	800[B]	COB	C30-C31-C32	2.38	120.52	112.61
3	A	800[A]	COB	C30-C31-C32	2.38	120.52	112.61
4	B	900	TAR	O2-C2-C1	2.38	116.83	111.10
3	C	800[A]	COB	C6M-C6B-C7B	-2.37	114.60	120.34
3	C	800[B]	COB	C6M-C6B-C7B	-2.37	114.60	120.34
3	C	800[A]	COB	C6M-C6B-C5B	2.30	125.54	120.72
3	C	800[B]	COB	C6M-C6B-C5B	2.30	125.54	120.72
3	C	800[A]	COB	C4B-C9B-C8B	-2.27	118.77	121.10
3	C	800[B]	COB	C4B-C9B-C8B	-2.27	118.77	121.10
3	C	800[A]	COB	C13-C14-C15	-2.20	123.69	131.68
3	C	800[B]	COB	C13-C14-C15	-2.20	123.69	131.68
3	A	800[B]	COB	C16-C15-C14	-2.20	120.74	124.23
3	A	800[A]	COB	C16-C15-C14	-2.20	120.74	124.23
3	A	800[B]	COB	C13-C14-C15	-2.18	123.76	131.68
3	A	800[A]	COB	C13-C14-C15	-2.18	123.76	131.68
3	A	800[B]	COB	C6M-C6B-C7B	-2.18	115.06	120.34
3	A	800[A]	COB	C6M-C6B-C7B	-2.18	115.06	120.34
3	A	800[B]	COB	C55-C17-C18	-2.13	106.78	111.11
3	A	800[A]	COB	C55-C17-C18	-2.13	106.78	111.11
3	A	800[B]	COB	C18-C19-N24	-2.13	104.71	109.55
3	A	800[A]	COB	C18-C19-N24	-2.13	104.71	109.55
3	C	800[A]	COB	C18-C19-N24	-2.09	104.80	109.55
3	C	800[B]	COB	C18-C19-N24	-2.09	104.80	109.55
3	A	800[B]	COB	C6M-C6B-C5B	2.06	125.03	120.72
3	A	800[A]	COB	C6M-C6B-C5B	2.06	125.03	120.72
3	A	800[B]	COB	C36-C7-C8	-2.02	108.51	112.07
3	A	800[A]	COB	C36-C7-C8	-2.02	108.51	112.07

There are no chirality outliers.

All (47) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	800[A]	COB	C4-C3-C30-C31
3	C	800[A]	COB	C1P-C2P-O3-P

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	800[A]	COB	C3P-C2P-O3-P
3	C	800[B]	COB	C4-C3-C30-C31
3	C	800[B]	COB	C1P-C2P-O3-P
3	C	800[B]	COB	C3P-C2P-O3-P
4	D	900	TAR	C1-C2-C3-C4
4	B	900	TAR	C1-C2-C3-C4
3	A	800[B]	COB	C1P-C2P-O3-P
3	A	800[B]	COB	C3P-C2P-O3-P
3	A	800[A]	COB	C1P-C2P-O3-P
3	A	800[A]	COB	C3P-C2P-O3-P
3	C	800[A]	COB	C2P-O3-P-O2
3	C	800[B]	COB	C2P-O3-P-O2
3	A	800[B]	COB	C2P-O3-P-O2
3	A	800[A]	COB	C2P-O3-P-O2
3	A	800[B]	COB	C4-C3-C30-C31
3	A	800[A]	COB	C4-C3-C30-C31
3	C	800[A]	COB	C18-C60-C61-O63
3	C	800[A]	COB	C18-C60-C61-N62
3	C	800[B]	COB	C18-C60-C61-O63
3	C	800[B]	COB	C18-C60-C61-N62
3	A	800[B]	COB	C18-C60-C61-O63
3	A	800[B]	COB	C18-C60-C61-N62
3	A	800[A]	COB	C18-C60-C61-O63
3	A	800[A]	COB	C18-C60-C61-N62
3	C	800[A]	COB	C30-C31-C32-N33
3	C	800[B]	COB	C30-C31-C32-N33
3	A	800[B]	COB	C30-C31-C32-N33
3	A	800[A]	COB	C30-C31-C32-N33
3	C	800[A]	COB	C2P-O3-P-O5
3	C	800[B]	COB	C2P-O3-P-O5
3	A	800[B]	COB	C55-C56-C57-O58
3	A	800[A]	COB	C55-C56-C57-O58
3	C	800[A]	COB	C30-C31-C32-O34
3	C	800[B]	COB	C30-C31-C32-O34
3	A	800[B]	COB	C30-C31-C32-O34
3	A	800[A]	COB	C30-C31-C32-O34
4	D	900	TAR	C1-C2-C3-O3
4	B	900	TAR	C1-C2-C3-O3
3	C	800[A]	COB	C55-C56-C57-O58
3	C	800[B]	COB	C55-C56-C57-O58
3	A	800[B]	COB	C55-C56-C57-N59
3	A	800[A]	COB	C55-C56-C57-N59

Continued on next page...

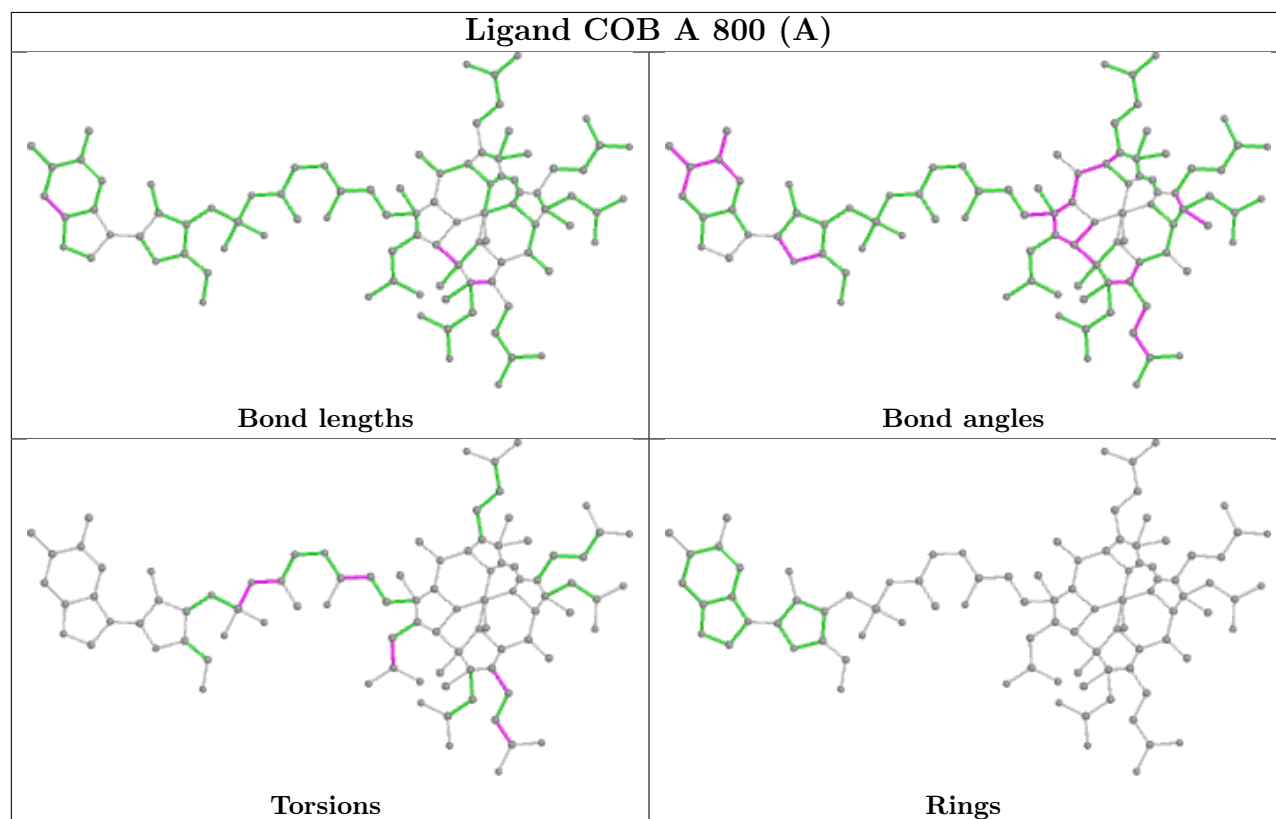
Continued from previous page...

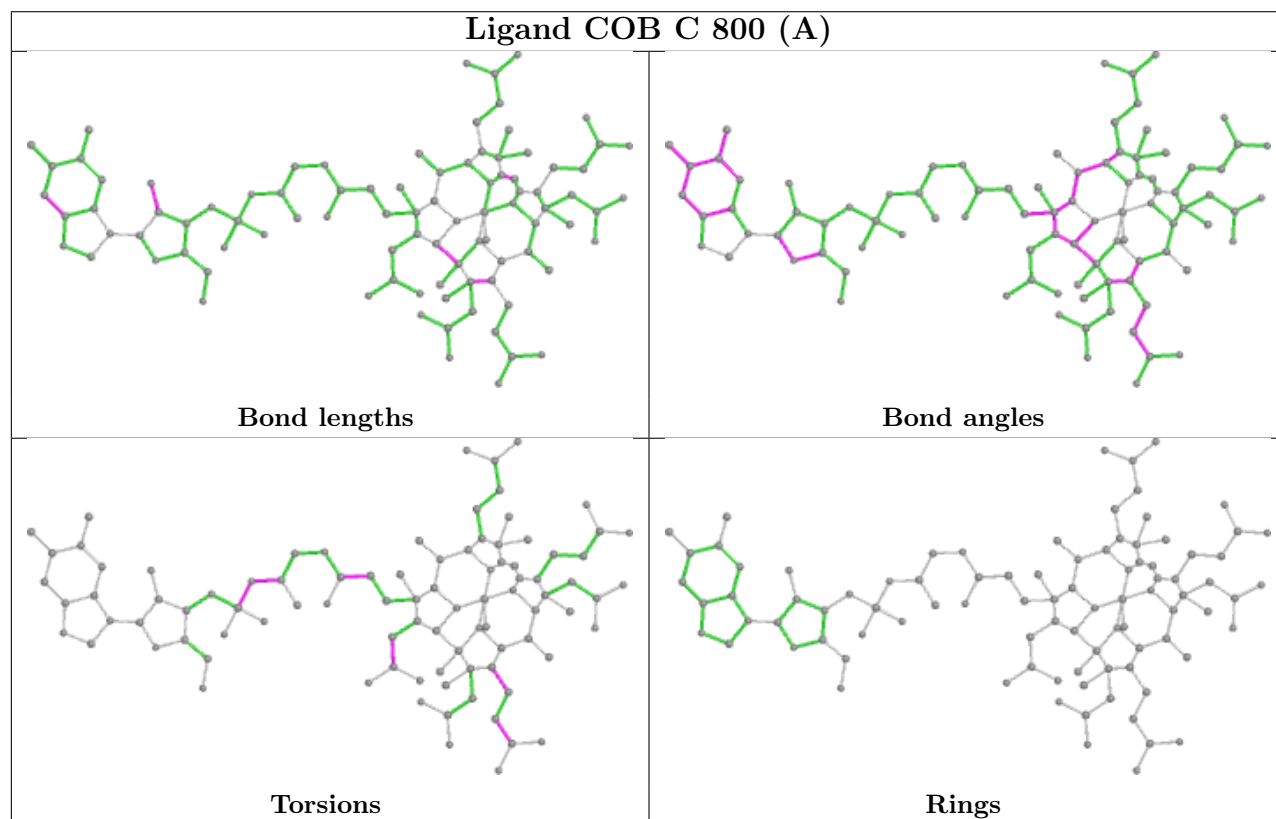
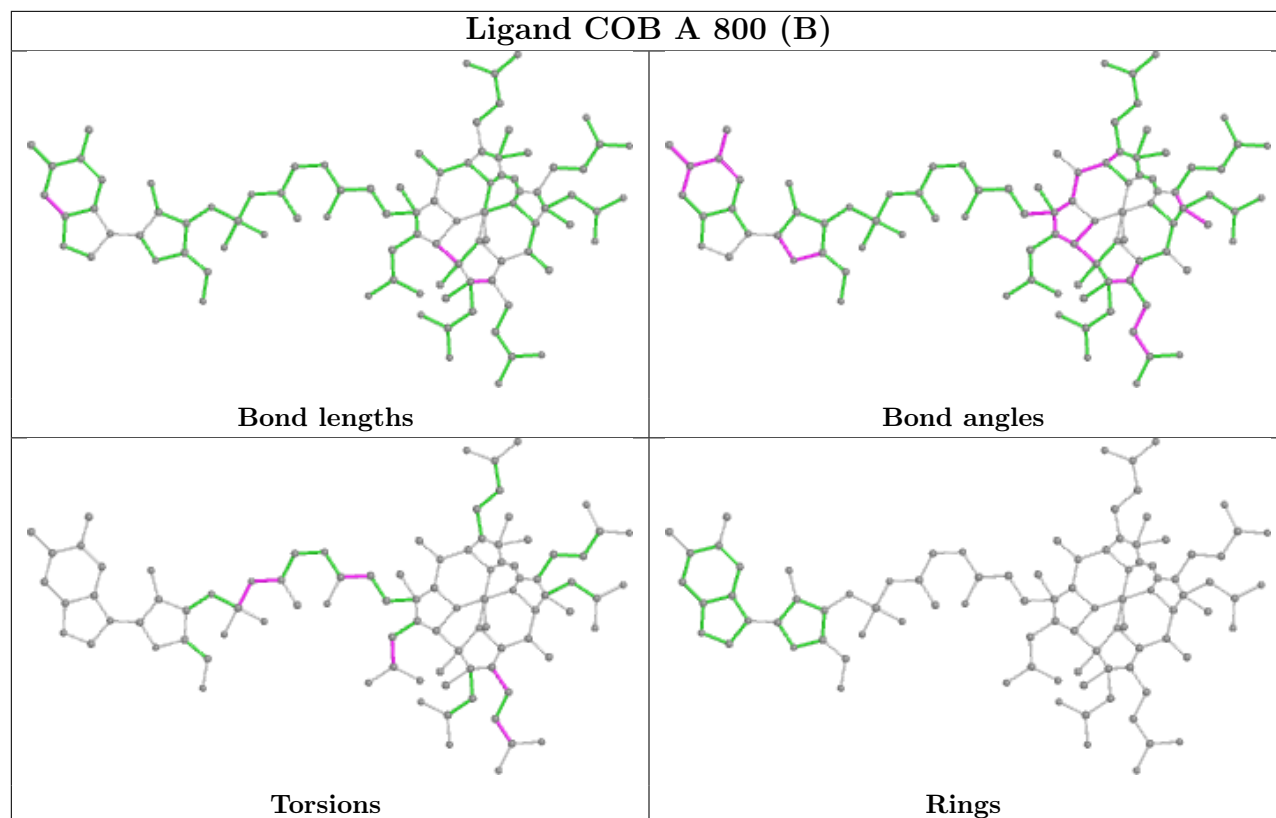
Mol	Chain	Res	Type	Atoms
3	C	800[A]	COB	C55-C56-C57-N59
3	C	800[B]	COB	C55-C56-C57-N59
4	D	900	TAR	O2-C2-C3-C4

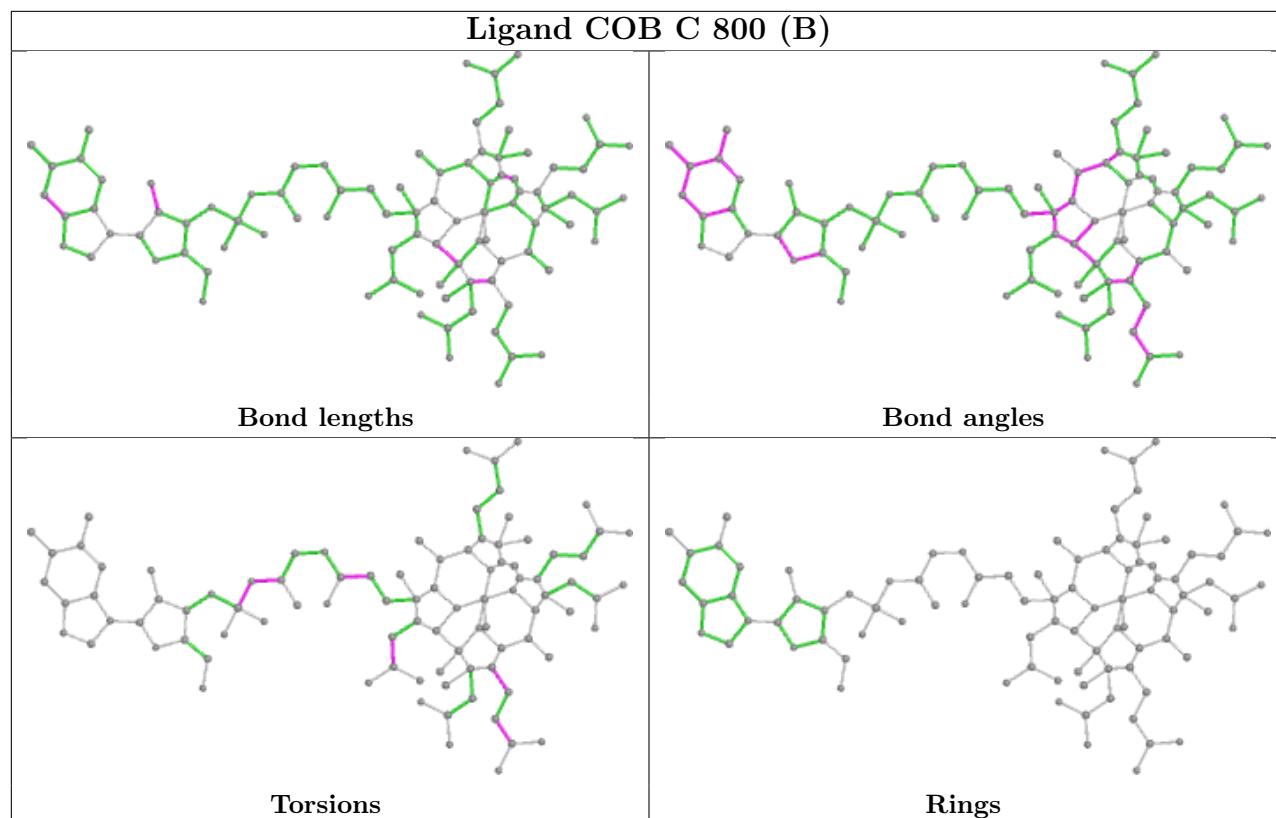
There are no ring outliers.

No monomer is involved in short contacts.

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	137/137 (100%)	-0.24	1 (0%) 87 87	12, 20, 42, 64	0
1	C	137/137 (100%)	-0.22	3 (2%) 62 60	11, 20, 43, 81	0
2	B	483/483 (100%)	-0.64	1 (0%) 94 94	9, 14, 29, 81	0
2	D	483/483 (100%)	-0.63	1 (0%) 94 94	8, 14, 31, 82	0
All	All	1240/1240 (100%)	-0.54	6 (0%) 90 90	8, 15, 33, 82	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1	MET	5.5
1	A	137	GLU	3.9
2	B	483	GLU	3.3
2	D	483	GLU	3.1
1	C	2	GLU	2.6
1	C	137	GLU	2.5

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 carbohydrates 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,

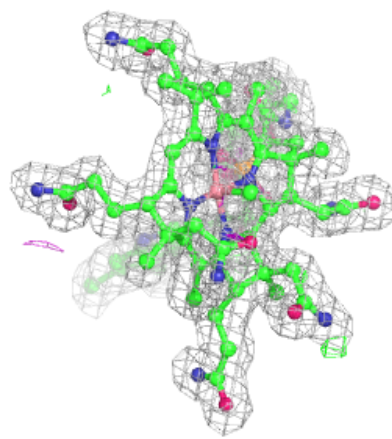
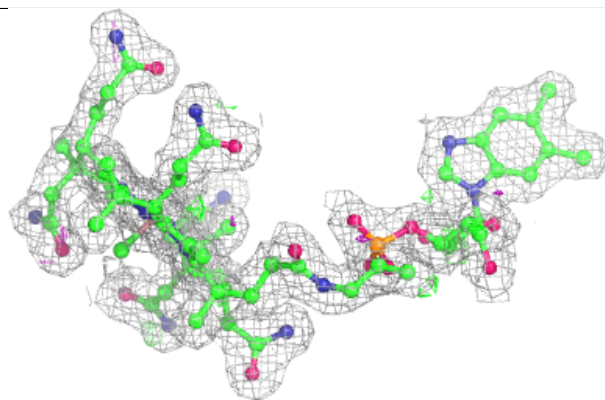
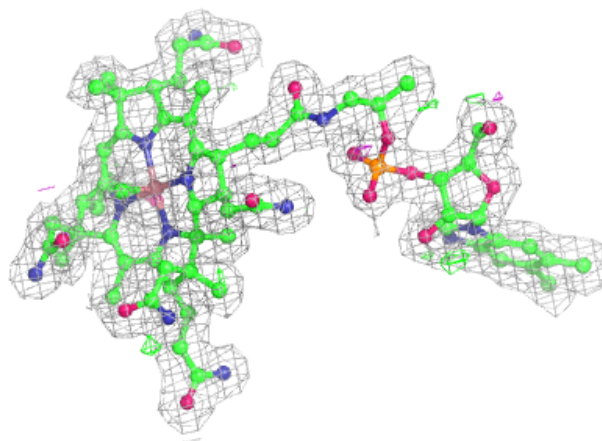
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	COB	C	800[A]	92/92	0.97	0.09	7,13,18,21	1
3	COB	C	800[B]	92/92	0.97	0.09	7,13,18,21	1
3	COB	A	800[B]	92/92	0.97	0.09	7,12,18,21	1
3	COB	A	800[A]	92/92	0.97	0.09	7,12,18,21	1
4	TAR	D	900	10/10	0.98	0.06	7,11,15,18	0
4	TAR	B	900	10/10	0.99	0.05	7,11,15,17	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.

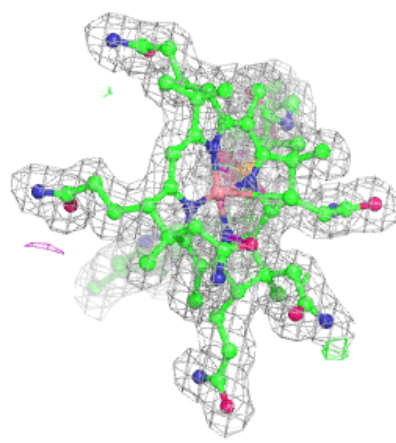
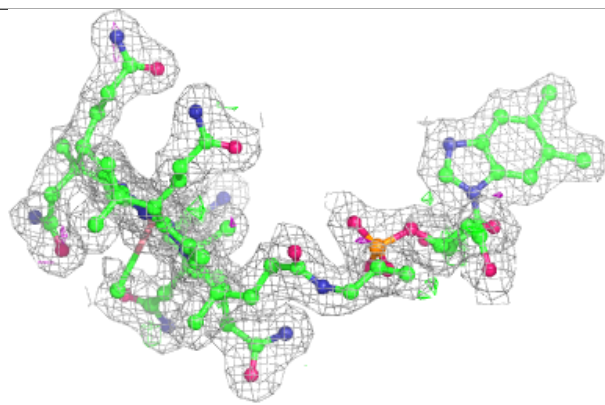
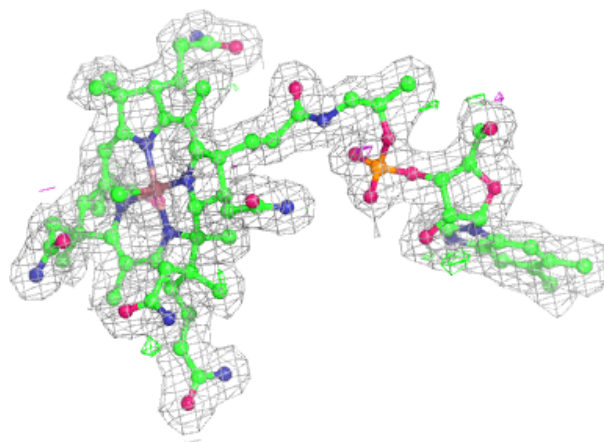
Electron density around COB C 800 (A):

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



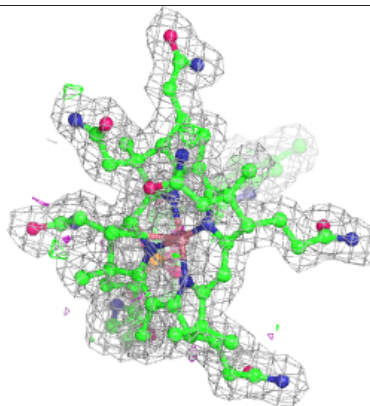
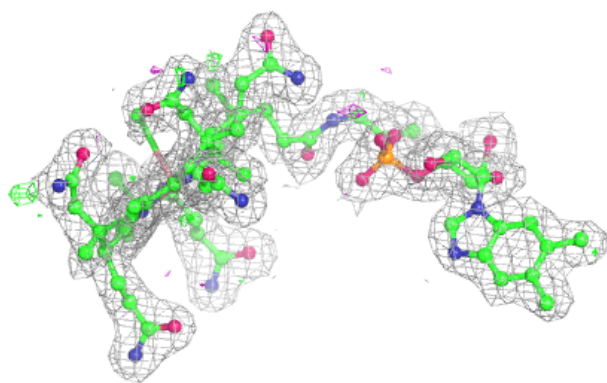
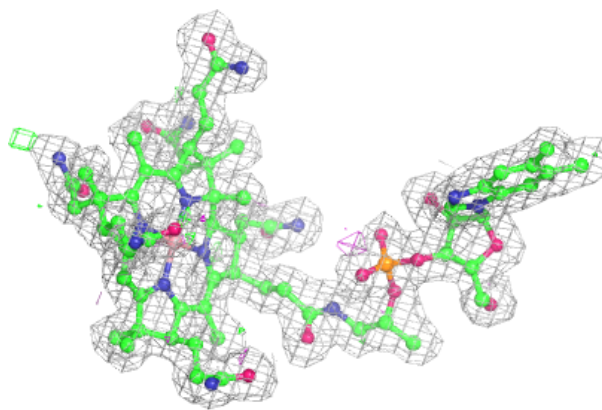
Electron density around COB C 800 (B):

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



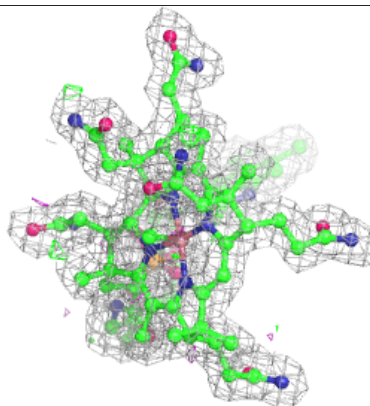
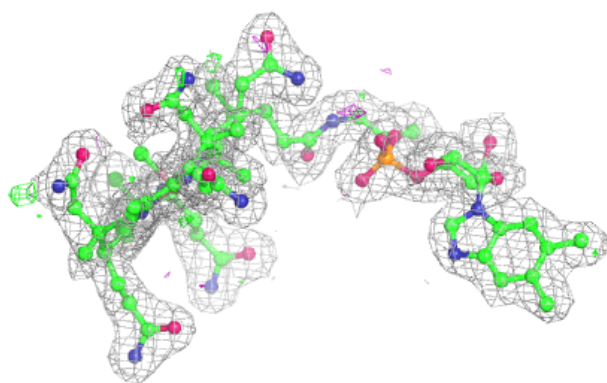
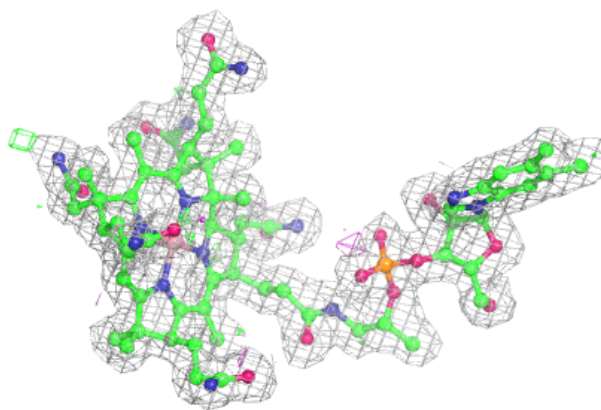
Electron density around COB A 800 (B):

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



Electron density around COB A 800 (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.