



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:36 PM UTC

PDB ID : 2DEB / pdb_00002deb
Title : Crystal structure of rat carnitine palmitoyltransferase 2 in space group C2221
Authors : Rufer, A.C.; Thoma, R.; Benz, J.; Stihle, M.; Gsell, B.; De Roo, E.; Banner, D.W.; Mueller, F.; Chomienne, O.; Hennig, M.
Deposited on : 2006-02-10
Resolution : 1.60 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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

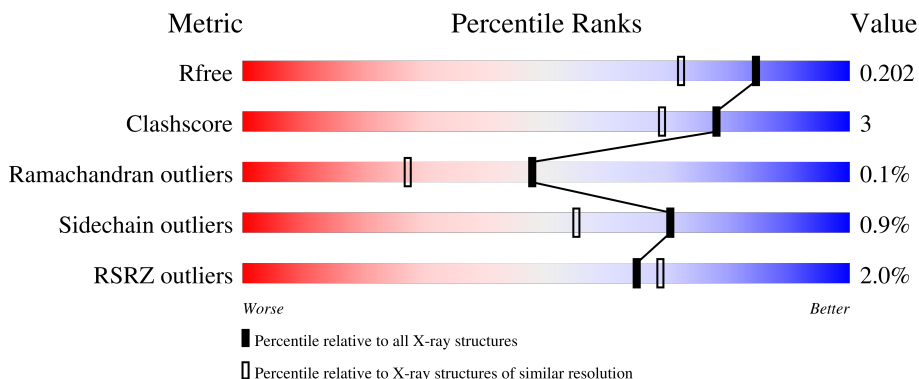
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

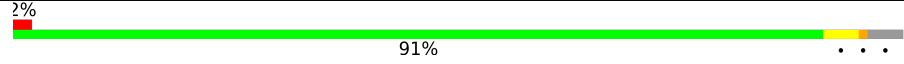
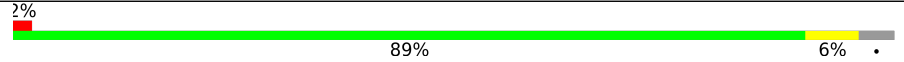
The reported resolution of this entry is 1.60 Å.

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	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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	653	
1	B	653	

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 11542 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 Carnitine O-palmitoyltransferase II, mitochondrial.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	627	5031	3198	872	939	10	12	0	10	0
1	B	626	5037	3205	871	939	10	12	0	15	0

There are 66 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	6	MET	-	expression tag	UNP P18886
A	7	GLY	-	expression tag	UNP P18886
A	8	SER	-	expression tag	UNP P18886
A	9	SER	-	expression tag	UNP P18886
A	10	HIS	-	expression tag	UNP P18886
A	11	HIS	-	expression tag	UNP P18886
A	12	HIS	-	expression tag	UNP P18886
A	13	HIS	-	expression tag	UNP P18886
A	14	HIS	-	expression tag	UNP P18886
A	15	HIS	-	expression tag	UNP P18886
A	16	SER	-	expression tag	UNP P18886
A	17	SER	-	expression tag	UNP P18886
A	18	GLY	-	expression tag	UNP P18886
A	19	LEU	-	expression tag	UNP P18886
A	20	VAL	-	expression tag	UNP P18886
A	21	PRO	-	expression tag	UNP P18886
A	22	ARG	-	expression tag	UNP P18886
A	23	GLY	-	expression tag	UNP P18886
A	24	SER	-	expression tag	UNP P18886
A	25	HIS	-	expression tag	UNP P18886
A	26	MET	-	expression tag	UNP P18886
A	43	MSE	MET	modified residue	UNP P18886
A	61	MSE	MET	modified residue	UNP P18886
A	119	MSE	MET	modified residue	UNP P18886
A	135	MSE	MET	modified residue	UNP P18886

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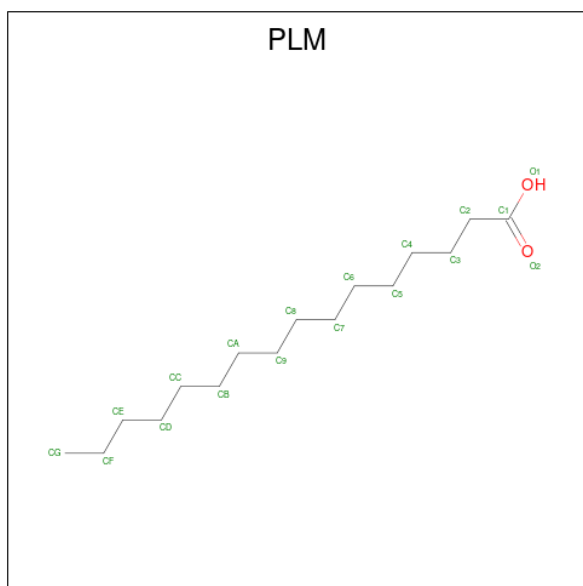
Chain	Residue	Modelled	Actual	Comment	Reference
A	214	MSE	MET	modified residue	UNP P18886
A	332	MSE	MET	modified residue	UNP P18886
A	342	MSE	MET	modified residue	UNP P18886
A	473	MSE	MET	modified residue	UNP P18886
A	531	MSE	MET	modified residue	UNP P18886
A	532	MSE	MET	modified residue	UNP P18886
A	548	MSE	MET	modified residue	UNP P18886
A	582	MSE	MET	modified residue	UNP P18886
B	6	MET	-	expression tag	UNP P18886
B	7	GLY	-	expression tag	UNP P18886
B	8	SER	-	expression tag	UNP P18886
B	9	SER	-	expression tag	UNP P18886
B	10	HIS	-	expression tag	UNP P18886
B	11	HIS	-	expression tag	UNP P18886
B	12	HIS	-	expression tag	UNP P18886
B	13	HIS	-	expression tag	UNP P18886
B	14	HIS	-	expression tag	UNP P18886
B	15	HIS	-	expression tag	UNP P18886
B	16	SER	-	expression tag	UNP P18886
B	17	SER	-	expression tag	UNP P18886
B	18	GLY	-	expression tag	UNP P18886
B	19	LEU	-	expression tag	UNP P18886
B	20	VAL	-	expression tag	UNP P18886
B	21	PRO	-	expression tag	UNP P18886
B	22	ARG	-	expression tag	UNP P18886
B	23	GLY	-	expression tag	UNP P18886
B	24	SER	-	expression tag	UNP P18886
B	25	HIS	-	expression tag	UNP P18886
B	26	MET	-	expression tag	UNP P18886
B	43	MSE	MET	modified residue	UNP P18886
B	61	MSE	MET	modified residue	UNP P18886
B	119	MSE	MET	modified residue	UNP P18886
B	135	MSE	MET	modified residue	UNP P18886
B	214	MSE	MET	modified residue	UNP P18886
B	332	MSE	MET	modified residue	UNP P18886
B	342	MSE	MET	modified residue	UNP P18886
B	473	MSE	MET	modified residue	UNP P18886
B	531	MSE	MET	modified residue	UNP P18886
B	532	MSE	MET	modified residue	UNP P18886
B	548	MSE	MET	modified residue	UNP P18886
B	582	MSE	MET	modified residue	UNP P18886

- Molecule 2 is COENZYME A (CCD ID: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



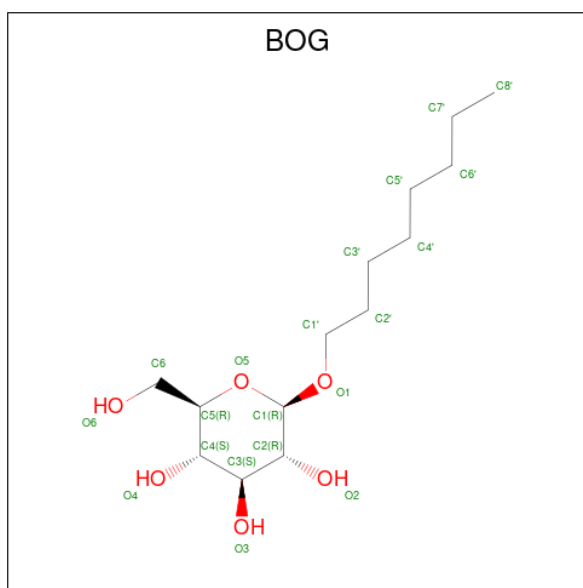
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	31	10	5	13	3	0	0
2	B	1	27	10	5	10	2	0	0

- Molecule 3 is PALMITIC ACID (CCD ID: PLM) (formula: $C_{16}H_{32}O_2$).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	C		
3	A	1	16	16	0	0
3	B	1	16	16	0	0

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



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

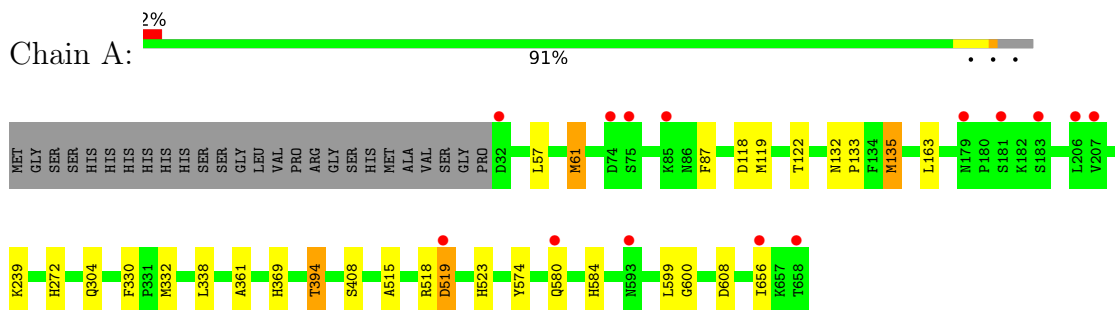
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	650	Total	O	0	0
			650	650		
5	B	714	Total	O	0	0
			714	714		

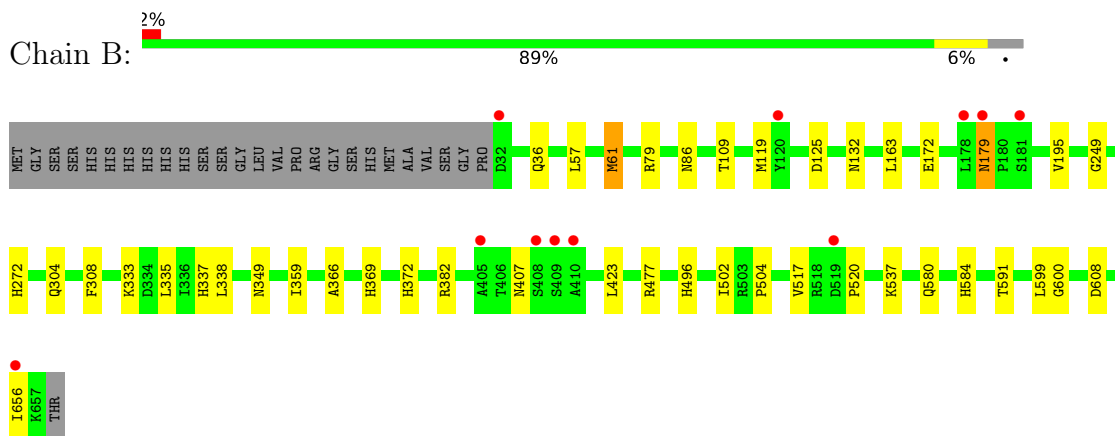
3 Residue-property plots [i](#)

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: Carnitine O-palmitoyltransferase II, mitochondrial



- Molecule 1: Carnitine O-palmitoyltransferase II, mitochondrial



4 Data and refinement statistics i

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	95.18Å 97.29Å 310.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	23.00 – 1.60 23.00 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (23.00-1.60) 99.7 (23.00-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.29 (at 1.60Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.165 , 0.194 0.175 , 0.202	Depositor DCC
R_{free} test set	9462 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	15.6	Xtrriage
Anisotropy	0.107	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.035 for -k,-h,-l	Xtrriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	11542	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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: BOG, PLM, COA

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	0.74	2/5189 (0.0%)	0.72	0/7015
1	B	0.59	2/5217 (0.0%)	0.73	1/7056 (0.0%)
All	All	0.67	4/10406 (0.0%)	0.73	1/14071 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	135	MSE	SE-CE	-34.41	0.92	1.95
1	A	119	MSE	SE-CE	-9.93	1.65	1.95
1	B	119	MSE	SE-CE	-7.95	1.71	1.95
1	B	61	MSE	SE-CE	-5.76	1.78	1.95

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	MSE	CG-SE-CE	-9.65	77.68	98.92

There are no chirality outliers.

There are no planarity outliers.

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	5031	0	4925	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5037	0	4924	30	0
2	A	31	0	11	0	0
2	B	27	0	11	0	0
3	A	16	0	31	4	0
3	B	16	0	31	3	0
4	B	20	0	28	1	0
5	A	650	0	0	7	0
5	B	714	0	0	7	0
All	All	11542	0	9961	56	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 (56) 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:518:ARG:CZ	5:A:2544:HOH:O	2.16	0.92
1:B:36:GLN:HE21	1:B:172:GLU:H	1.29	0.80
1:A:132:ASN:HD22	1:A:369:HIS:HE1	1.33	0.76
1:A:574:TYR:O	1:A:580:GLN:NE2	2.18	0.74
1:B:333:LYS:H	1:B:337:HIS:HD2	1.37	0.73
1:A:518:ARG:NE	5:A:2544:HOH:O	2.18	0.72
1:B:57:LEU:O	1:B:61:MSE:HG2	1.88	0.72
1:B:132:ASN:HD22	1:B:369:HIS:HE1	1.35	0.72
1:B:36:GLN:NE2	1:B:172:GLU:H	1.94	0.65
1:A:57:LEU:HD11	1:A:61:MSE:HE1	1.81	0.63
1:A:599:LEU:HA	3:A:2351:PLM:H81	1.83	0.61
1:A:656:ILE:HG23	5:A:2903:HOH:O	2.02	0.60
1:A:600:GLY:H	3:A:2351:PLM:H82	1.67	0.59
1:A:272:HIS:HD2	1:A:408:SER:OG	1.86	0.59
1:A:132:ASN:HD22	1:A:369:HIS:CE1	2.17	0.59
1:B:109:THR:OG1	1:B:496:HIS:HD2	1.87	0.58
1:B:599:LEU:HA	3:B:1600:PLM:HD2	1.86	0.58
1:B:132:ASN:HD22	1:B:369:HIS:CE1	2.21	0.57
1:B:520:PRO:HB2	1:B:656:ILE:HG21	1.87	0.56
1:A:584:HIS:HE1	1:A:608:ASP:OD1	1.92	0.51
1:A:515:ALA:HA	1:A:519:ASP:OD2	2.11	0.51
1:B:36:GLN:HE22	1:B:382:ARG:HH21	1.59	0.51
1:B:272:HIS:HD2	5:B:2481:HOH:O	1.94	0.50
1:A:118:ASP:O	1:A:122[B]:THR:HG22	2.12	0.49
1:A:57:LEU:HG	1:A:61:MSE:HE2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:394[A]:THR:HG22	5:A:2559:HOH:O	2.12	0.49
1:B:304:GLN:HG3	1:B:308:PHE:CZ	2.48	0.48
1:B:477[B]:ARG:NH1	1:B:517:VAL:HG22	2.26	0.48
1:B:179:ASN:ND2	5:B:2759:HOH:O	2.46	0.48
1:B:584:HIS:HE1	1:B:608:ASP:OD1	1.96	0.48
1:B:502:ILE:O	1:B:504:PRO:HD3	2.14	0.47
1:B:333:LYS:H	1:B:337:HIS:CD2	2.23	0.47
1:B:163:LEU:C	1:B:163:LEU:HD23	2.38	0.47
1:A:600:GLY:H	3:A:2351:PLM:C8	2.27	0.47
1:B:600:GLY:H	3:B:1600:PLM:CD	2.27	0.46
1:A:163:LEU:C	1:A:163:LEU:HD23	2.41	0.46
1:B:580:GLN:NE2	5:B:2843:HOH:O	2.49	0.45
1:B:195:VAL:HG21	4:B:1736:BOG:H8'3	1.98	0.45
1:B:359:ILE:O	1:B:366:ALA:HA	2.17	0.45
1:B:79:ARG:HD2	5:B:2934:HOH:O	2.15	0.45
1:B:600:GLY:H	3:B:1600:PLM:HD1	1.80	0.45
1:A:330:PHE:CE1	1:A:332:MSE:HE1	2.53	0.43
1:B:591:THR:HG22	5:B:3025:HOH:O	2.19	0.43
1:A:523:HIS:HD2	5:A:2869:HOH:O	2.01	0.43
1:A:239:LYS:NZ	5:A:2878:HOH:O	2.52	0.42
1:A:61:MSE:CE	1:A:87:PHE:HD2	2.33	0.42
1:B:520:PRO:CB	1:B:656:ILE:HG21	2.49	0.42
1:B:249:GLY:H	1:B:349:ASN:ND2	2.17	0.41
1:A:304:GLN:NE2	5:A:2853:HOH:O	2.54	0.41
3:A:2351:PLM:H82	3:A:2351:PLM:HB2	1.95	0.41
1:B:338:LEU:HD23	1:B:338:LEU:C	2.46	0.41
1:A:332:MSE:HE3	1:A:361:ALA:CB	2.50	0.41
1:A:338:LEU:HD23	1:A:338:LEU:C	2.46	0.41
1:B:86[B]:ASN:ND2	5:B:2928:HOH:O	2.43	0.41
1:A:57:LEU:CD1	1:A:61:MSE:HE1	2.49	0.40
1:B:537:LYS:NZ	5:B:2971:HOH:O	2.54	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	635/653 (97%)	626 (99%)	8 (1%)	1 (0%)	43	24
1	B	639/653 (98%)	627 (98%)	12 (2%)	0	100	100
All	All	1274/1306 (98%)	1253 (98%)	20 (2%)	1 (0%)	48	27

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	PRO

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	554/553 (100%)	549 (99%)	5 (1%)	70	55
1	B	558/553 (101%)	552 (99%)	6 (1%)	65	46
All	All	1112/1106 (100%)	1101 (99%)	11 (1%)	70	50

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	MSE
1	A	135	MSE
1	A	394[A]	THR
1	A	394[B]	THR
1	A	519	ASP
1	B	125	ASP
1	B	179	ASN
1	B	335	LEU
1	B	372	HIS
1	B	407	ASN
1	B	423	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	130	ASN
1	A	138	ASN
1	A	272	HIS
1	A	304	GLN
1	A	349	ASN
1	A	369	HIS
1	A	472	GLN
1	A	523	HIS
1	A	583	ASN
1	A	584	HIS
1	B	36	GLN
1	B	102	GLN
1	B	105	GLN
1	B	130	ASN
1	B	138	ASN
1	B	177	HIS
1	B	179	ASN
1	B	222	ASN
1	B	262	ASN
1	B	272	HIS
1	B	337	HIS
1	B	349	ASN
1	B	369	HIS
1	B	400	GLN
1	B	496	HIS
1	B	539	HIS
1	B	580	GLN
1	B	583	ASN
1	B	584	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](#)

5 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	COA	B	2360	-	29,29,50	1.07	2 (6%)	44,45,75	1.66	8 (18%)
3	PLM	A	2351	-	15,15,17	0.28	0	14,14,17	0.78	0
2	COA	A	2350	-	32,33,50	1.19	4 (12%)	50,52,75	1.45	8 (16%)
4	BOG	B	1736	-	20,20,20	0.52	0	25,25,25	0.63	0
3	PLM	B	1600	-	15,15,17	0.20	0	14,14,17	0.69	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	COA	B	2360	-	-	3/15/31/64	0/3/3/3
3	PLM	A	2351	-	-	6/13/13/15	-
2	COA	A	2350	-	-	1/21/37/64	0/3/3/3
4	BOG	B	1736	-	-	6/11/31/31	0/1/1/1
3	PLM	B	1600	-	-	4/13/13/15	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2350	COA	C2A-N3A	3.17	1.39	1.33
2	A	2350	COA	C2A-N1A	2.95	1.39	1.33
2	B	2360	COA	C2A-N1A	2.59	1.38	1.33
2	B	2360	COA	C2A-N3A	2.49	1.38	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2350	COA	P1A-O3A	2.10	1.61	1.59
2	A	2350	COA	C8A-N7A	2.07	1.35	1.31

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2360	COA	N3A-C2A-N1A	-5.93	119.61	128.58
2	A	2350	COA	N3A-C2A-N1A	-5.15	120.78	128.58
2	A	2350	COA	C5A-C4A-N3A	-3.89	121.36	126.72
2	B	2360	COA	C5A-C4A-N3A	-3.69	121.63	126.72
2	B	2360	COA	N9A-C8A-N7A	-3.62	108.80	113.94
2	A	2350	COA	N9A-C8A-N7A	-3.28	109.28	113.94
2	B	2360	COA	C2A-N3A-C4A	3.17	119.58	111.83
2	A	2350	COA	C5A-N7A-C8A	2.91	108.03	103.45
2	A	2350	COA	C2A-N3A-C4A	2.86	118.82	111.83
2	B	2360	COA	C5A-N7A-C8A	2.84	107.91	103.45
2	B	2360	COA	N3A-C4A-N9A	2.75	131.84	127.17
2	A	2350	COA	N3A-C4A-N9A	2.72	131.80	127.17
2	B	2360	COA	C4A-N9A-C8A	2.47	108.33	105.74
2	B	2360	COA	O2A-P1A-O5B	2.24	112.52	106.67
2	A	2350	COA	C6A-C5A-C4A	2.12	120.07	117.18
2	A	2350	COA	C4A-C5A-N7A	-2.04	108.24	110.58

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	2360	COA	C5B-O5B-P1A-O1A
2	B	2360	COA	C5B-O5B-P1A-O2A
2	B	2360	COA	C5B-O5B-P1A-O3A
4	B	1736	BOG	O5-C1-O1-C1'
4	B	1736	BOG	C2-C1-O1-C1'
3	A	2351	PLM	C2-C3-C4-C5
4	B	1736	BOG	C2'-C1'-O1-C1
3	A	2351	PLM	CA-CB-CC-CD
3	A	2351	PLM	CB-CC-CD-CE
4	B	1736	BOG	O1-C1'-C2'-C3'
3	B	1600	PLM	C1-C2-C3-C4
4	B	1736	BOG	C5'-C6'-C7'-C8'
3	B	1600	PLM	C3-C4-C5-C6
3	B	1600	PLM	CD-CE-CF-CG
3	A	2351	PLM	C1-C2-C3-C4

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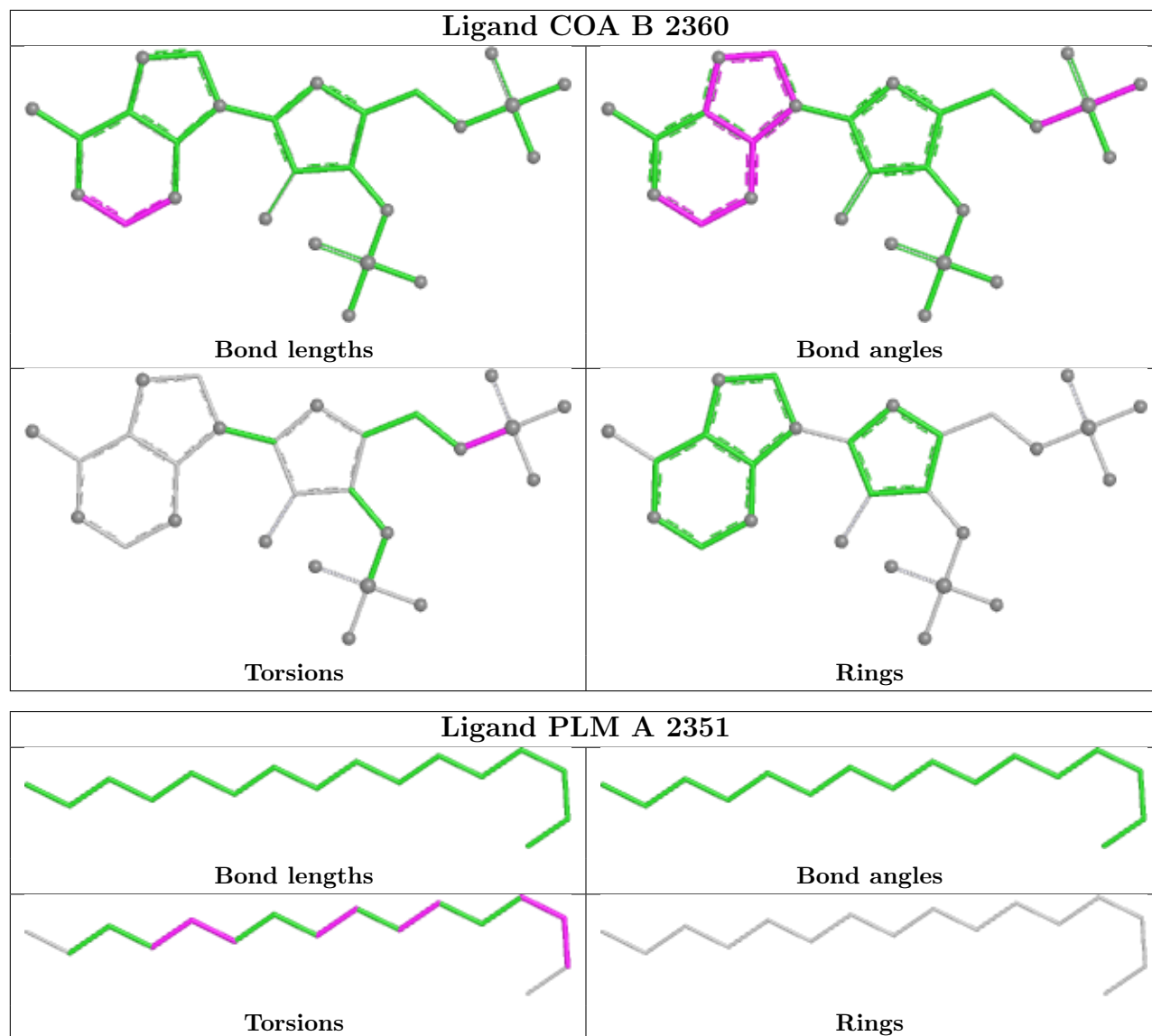
Mol	Chain	Res	Type	Atoms
3	A	2351	PLM	C5-C6-C7-C8
2	A	2350	COA	P1A-O3A-P2A-O5A
4	B	1736	BOG	C4'-C5'-C6'-C7'
3	A	2351	PLM	C7-C8-C9-CA
3	B	1600	PLM	CB-CC-CD-CE

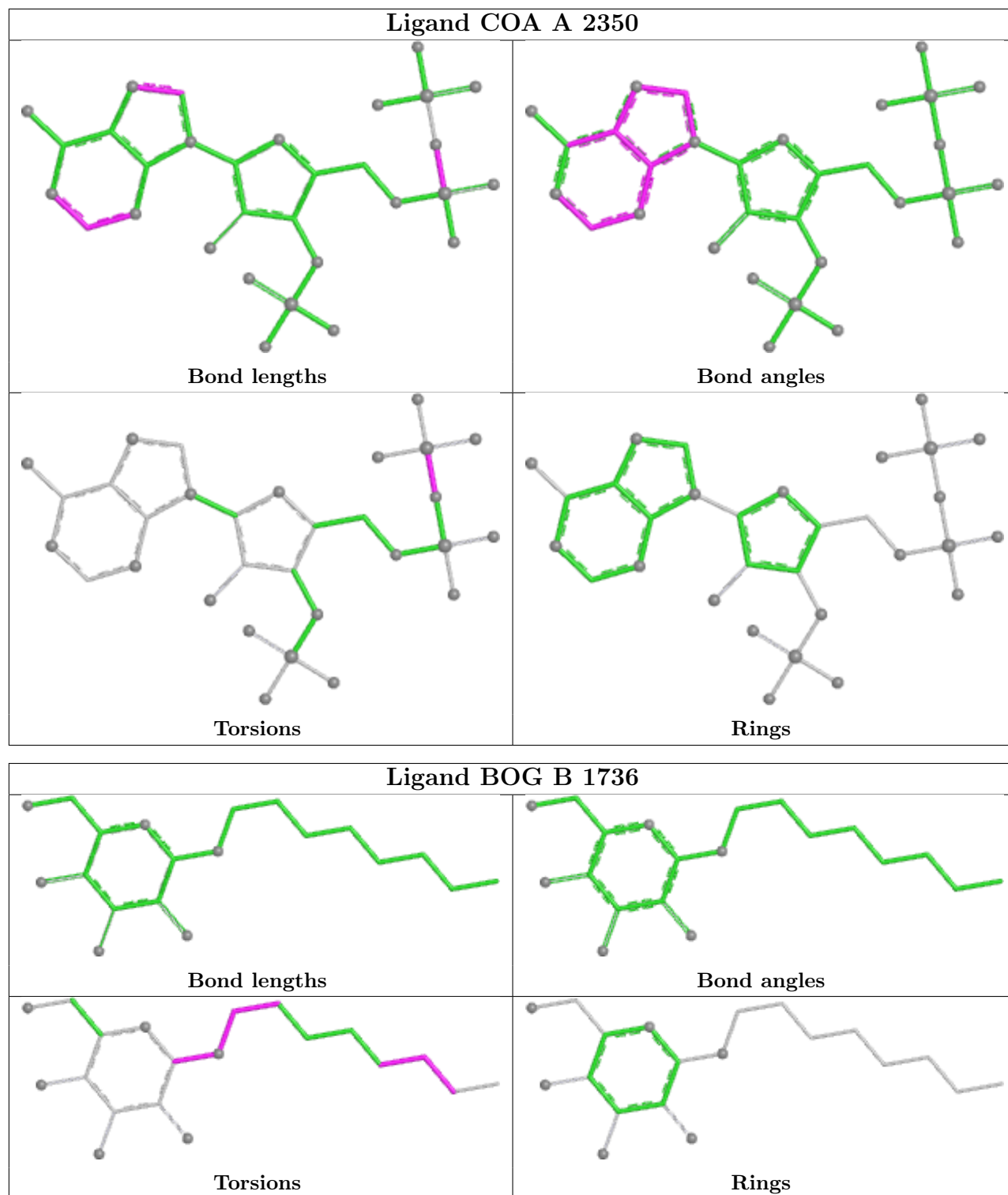
There are no ring outliers.

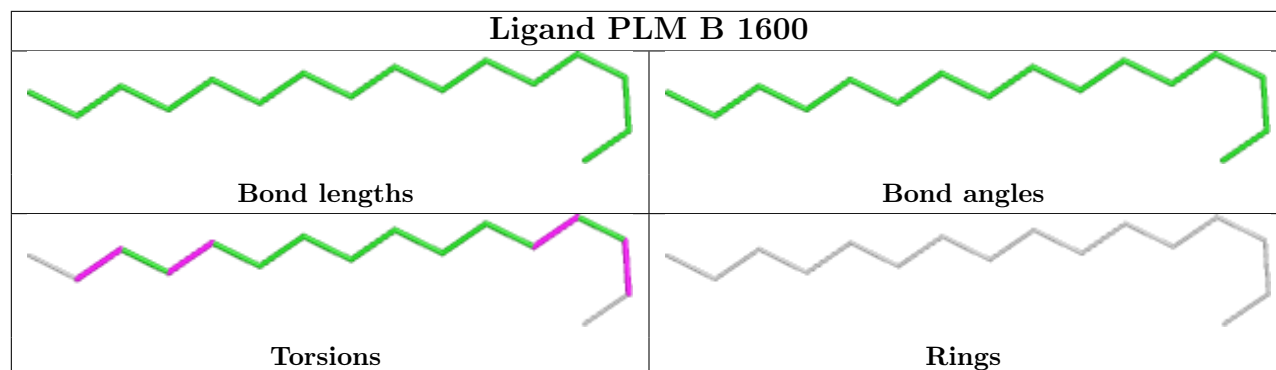
3 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	2351	PLM	4	0
4	B	1736	BOG	1	0
3	B	1600	PLM	3	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	615/653 (94%)	0.01	14 (2%) 61 64	9, 17, 33, 57	10 (1%)
1	B	614/653 (94%)	-0.13	11 (1%) 67 71	10, 15, 30, 51	15 (2%)
All	All	1229/1306 (94%)	-0.06	25 (2%) 65 69	9, 16, 32, 57	25 (2%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	658	THR	5.7
1	A	656	ILE	5.0
1	B	179	ASN	4.0
1	B	519	ASP	4.0
1	B	409	SER	3.9
1	B	408	SER	3.9
1	B	181	SER	3.1
1	A	206	LEU	3.0
1	B	178	LEU	2.8
1	B	120	TYR	2.7
1	A	179	ASN	2.7
1	B	405	ALA	2.7
1	A	181	SER	2.6
1	A	580	GLN	2.4
1	B	656	ILE	2.3
1	A	183	SER	2.2
1	B	410	ALA	2.2
1	A	32	ASP	2.1
1	A	207	VAL	2.1
1	A	593	ASN	2.0
1	A	74	ASP	2.0
1	A	519	ASP	2.0
1	B	32	ASP	2.0
1	A	75	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	85	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

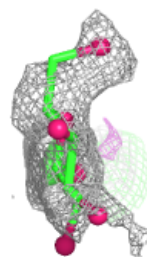
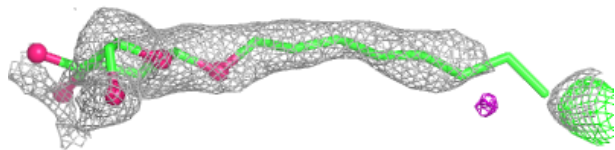
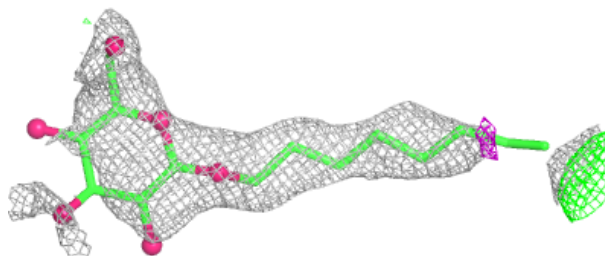
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	BOG	B	1736	20/20	0.69	0.14	30,57,66,76	0
2	COA	A	2350	31/48	0.83	0.13	15,28,78,80	0
2	COA	B	2360	27/48	0.86	0.11	18,27,63,64	0
3	PLM	B	1600	16/18	0.90	0.12	10,19,41,41	0
3	PLM	A	2351	16/18	0.90	0.13	9,21,37,39	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.

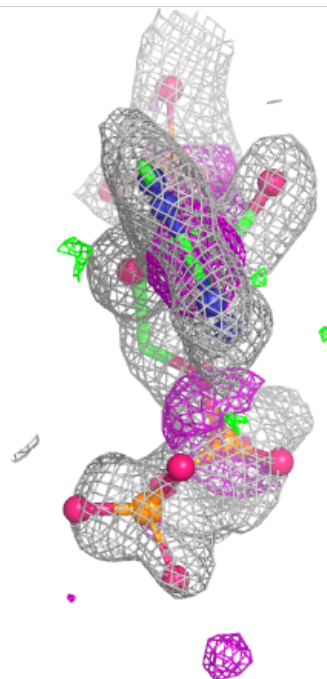
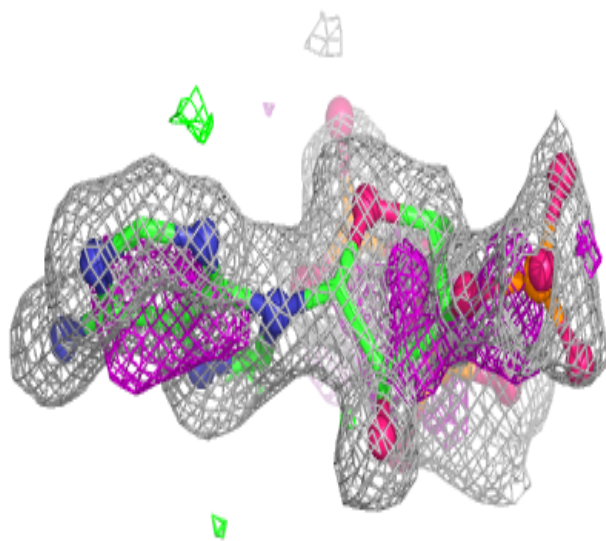
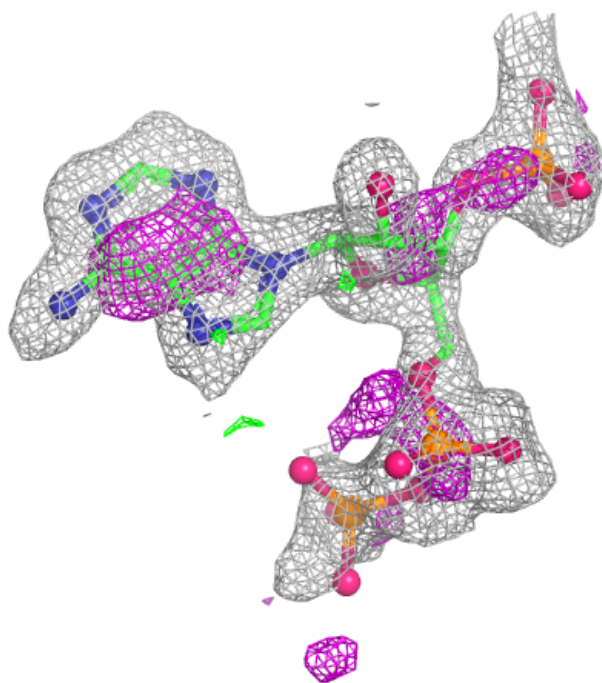
Electron density around BOG B 1736:

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



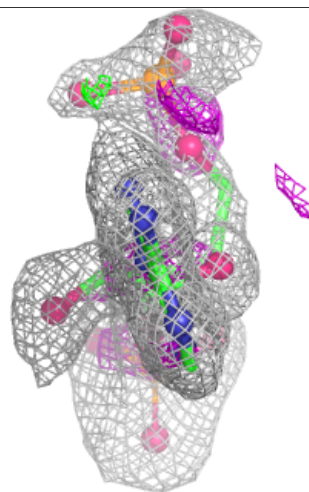
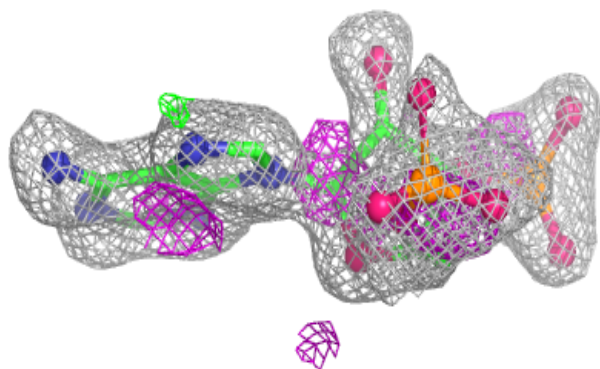
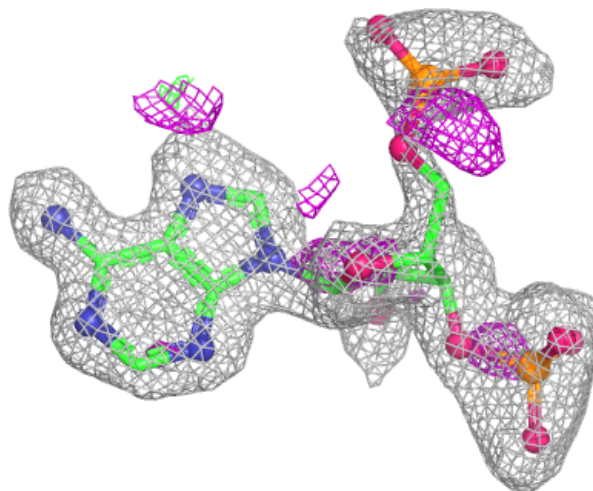
Electron density around COA A 2350:

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



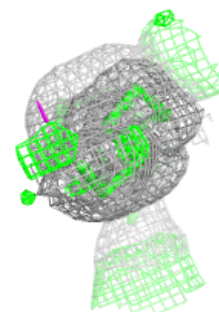
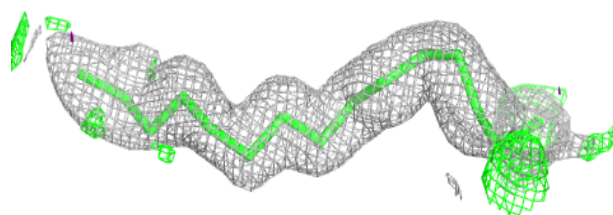
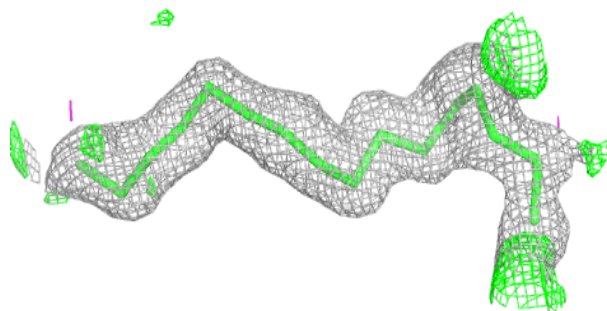
Electron density around COA B 2360:

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

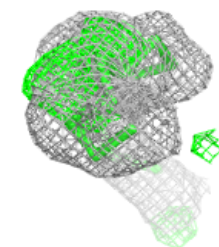
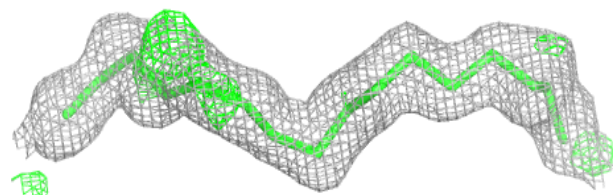
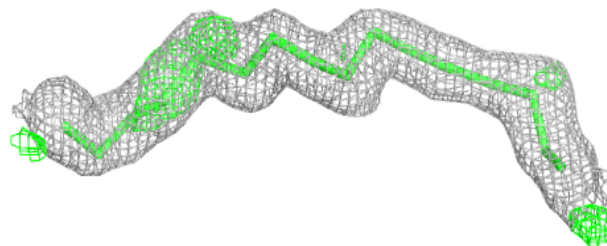


Electron density around PLM B 1600:

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

**Electron density around PLM A 2351:**

$2mF_o-DF_c$ (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.