



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:31 AM GMT

PDB ID : 2DEB
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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

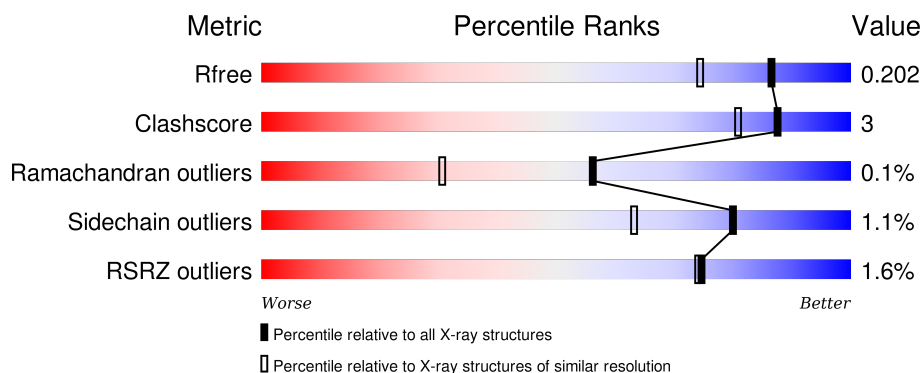
1 Overall quality at a glance ⓘ

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}	91344	2475 (1.60-1.60)
Clashscore	102246	2732 (1.60-1.60)
Ramachandran outliers	100387	2654 (1.60-1.60)
Sidechain outliers	100360	2653 (1.60-1.60)
RSRZ outliers	91569	2479 (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 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	653	<div> <div>2%</div> <div>91%</div> <div>• • •</div> </div>
1	B	653	<div> <div>%</div> <div>90%</div> <div>6% •</div> </div>

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	BOG	B	1736	-	-	-	X
3	COA	A	2350	-	-	-	X
3	COA	B	2360	-	-	-	X
4	PLM	A	2351	-	-	-	X
4	PLM	B	1600	-	-	-	X

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
1	A	627	Total	C	N	O	S	Se	0	10	0
			5031	3198	872	939	10	12			
1	B	626	Total	C	N	O	S	Se	0	15	0
			5037	3205	871	939	10	12			

There are 66 discrepancies between the modelled and reference sequences:

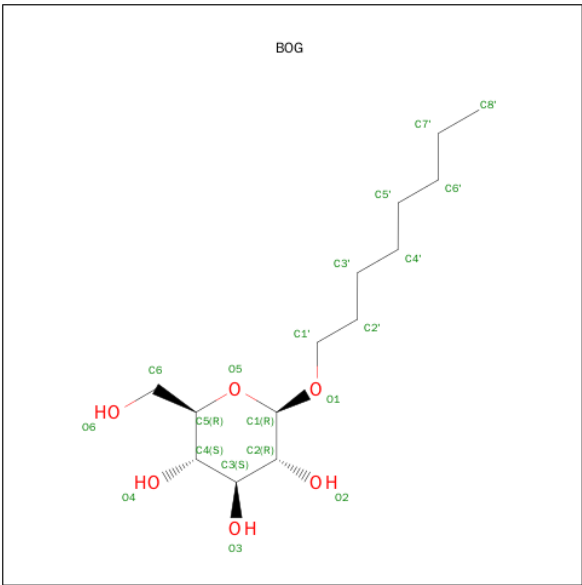
Chain	Residue	Modelled	Actual	Comment	Reference
A	6	MET	-	EXPRESSION TAG	UNP P18886
A	7	GLY	-	EXPRESSION TAG	UNP P18886
A	8	SER	-	EXPRESSION TAG	UNP P18886
A	9	SER	-	EXPRESSION TAG	UNP P18886
A	10	HIS	-	EXPRESSION TAG	UNP P18886
A	11	HIS	-	EXPRESSION TAG	UNP P18886
A	12	HIS	-	EXPRESSION TAG	UNP P18886
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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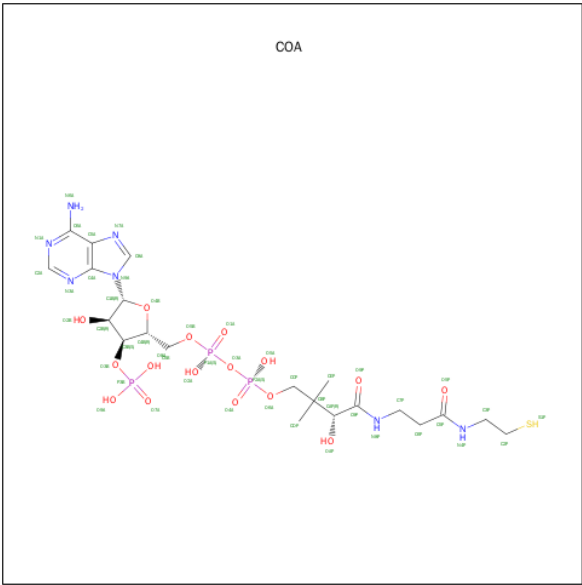
Chain	Residue	Modelled	Actual	Comment	Reference
A	214	MSE	MET	MODIFIED RESIDUE	UNP P18886
A	332	MSE	MET	MODIFIED RESIDUE	UNP P18886
A	342	MSE	MET	MODIFIED RESIDUE	UNP P18886
A	473	MSE	MET	MODIFIED RESIDUE	UNP P18886
A	531	MSE	MET	MODIFIED RESIDUE	UNP P18886
A	532	MSE	MET	MODIFIED RESIDUE	UNP P18886
A	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 SUGAR (B-OCTYLGLUCOSIDE) (three-letter code: BOG) (formula: C₁₄H₂₈O₆).



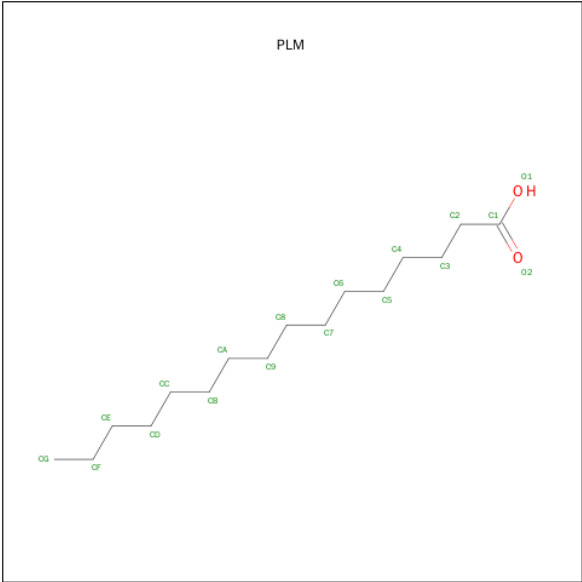
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	C	O	0	0
			20	14	6		

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



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

- Molecule 4 is PALMITIC ACID (three-letter code: PLM) (formula: C₁₆H₃₂O₂).



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

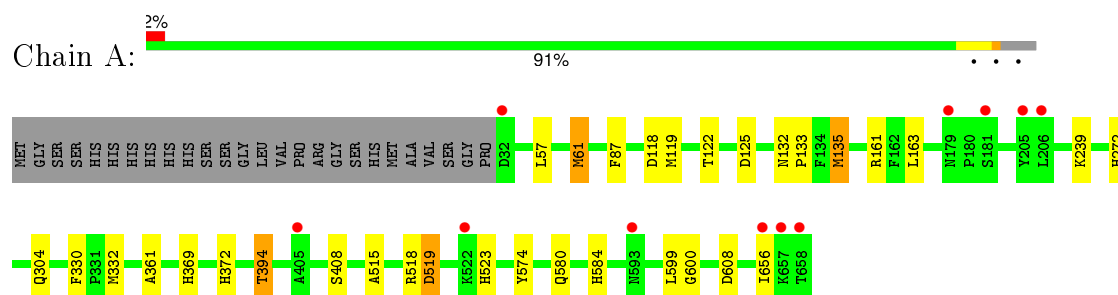
- Molecule 5 is water.

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

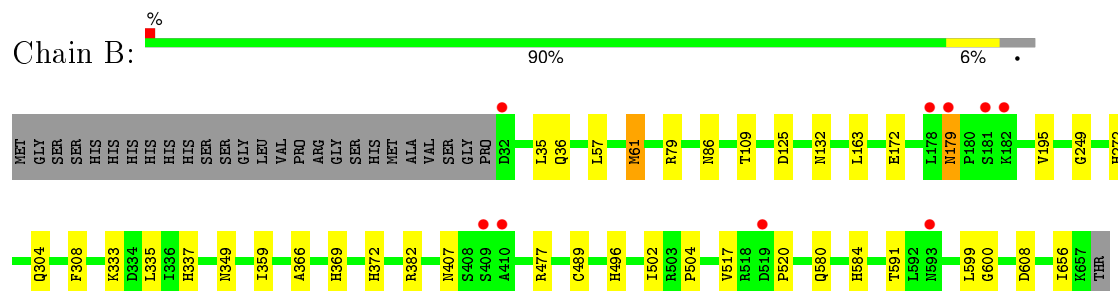
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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

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 22.62 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.8 (23.00-1.60) 99.8 (22.62-1.60)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.29 (at 1.60Å)	Xtriage
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 (5.29%)	DCC
Wilson B-factor (Å ²)	15.6	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 60.3	EDS
Estimated twinning fraction	0.035 for -k,-h,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	1 of 188485 reflections (0.001%)	Xtriage
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

Xtriage'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.*

¹ Intensities estimated from amplitudes.

² Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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, PLM, BOG

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	0.50	2/5189 (0.0%)	0.60	2/7015 (0.0%)
1	B	0.44	1/5217 (0.0%)	0.62	1/7056 (0.0%)
All	All	0.47	3/10406 (0.0%)	0.61	3/14071 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	135	MSE	SE-CE	-17.50	0.92	1.95
1	B	489	CYS	CB-SG	-5.33	1.73	1.81
1	A	119	MSE	SE-CE	-5.05	1.65	1.95

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	61	MSE	CG-SE-CE	-9.64	77.68	98.90
1	A	161[A]	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	A	161[B]	ARG	NE-CZ-NH1	5.25	122.93	120.30

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	5031	0	4925	24	0
1	B	5037	0	4924	28	0
2	B	20	0	28	1	0
3	A	31	0	11	0	0
3	B	27	0	11	0	0
4	A	16	0	31	4	0
4	B	16	0	31	3	0
5	A	650	0	0	7	0
5	B	714	0	0	6	0
All	All	11542	0	9961	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)
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	4: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	4: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	4: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:A:600:GLY:H	4:A:2351:PLM:C8	2.27	0.47
1:B:600:GLY:H	4:B:1600:PLM:CD	2.27	0.46
1:B:580:GLN:NE2	5:B:2843:HOH:O	2.49	0.45
1:B:359:ILE:O	1:B:366:ALA:HA	2.17	0.45
1:B:195:VAL:HG21	2:B:1736:BOG:H8'3	1.98	0.45
1:B:600:GLY:H	4:B:1600:PLM:HD1	1.80	0.45
1:B:79:ARG:HD2	5:B:2934:HOH:O	2.15	0.45
1:A:330:PHE:CE1	1:A:332:MSE:HE1	2.53	0.43
1:B:163:LEU:HD23	1:B:163:LEU:C	2.38	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:163:LEU:C	1:A:163:LEU:HD23	2.41	0.41
4:A:2351:PLM:HB2	4:A:2351:PLM:H82	1.95	0.41
1:A:304:GLN:NE2	5:A:2853:HOH:O	2.54	0.41
1:A:332:MSE:HE3	1:A:361:ALA:CB	2.50	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

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	635/653 (97%)	626 (99%)	8 (1%)	1 (0%)	52	28
1	B	639/653 (98%)	627 (98%)	12 (2%)	0	100	100
All	All	1274/1306 (98%)	1253 (98%)	20 (2%)	1 (0%)	56	31

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	133	PRO

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	554/553 (100%)	547 (99%)	7 (1%)	76	56
1	B	558/553 (101%)	552 (99%)	6 (1%)	80	63
All	All	1112/1106 (100%)	1099 (99%)	13 (1%)	80	60

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	61	MSE
1	A	125	ASP
1	A	135	MSE
1	A	372	HIS
1	A	394[A]	THR
1	A	394[B]	THR
1	A	519	ASP
1	B	35	LEU
1	B	125	ASP
1	B	179	ASN
1	B	335	LEU
1	B	372	HIS
1	B	407	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) 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	523	HIS
1	A	584	HIS
1	A	617	HIS
1	B	36	GLN
1	B	102	GLN
1	B	130	ASN
1	B	138	ASN
1	B	177	HIS
1	B	179	ASN
1	B	272	HIS
1	B	304	GLN
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	584	HIS

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

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$
3	COA	A	2350	-	26,33,50	1.21	2 (7%)	33,52,75	2.04	2 (6%)
4	PLM	A	2351	-	15,15,17	0.27	0	14,14,17	0.77	0
4	PLM	B	1600	-	15,15,17	0.19	0	14,14,17	0.68	0
2	BOG	B	1736	-	20,20,20	0.50	0	25,25,25	0.62	0
3	COA	B	2360	-	24,29,50	1.14	2 (8%)	28,45,75	2.45	3 (10%)

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	A	2350	-	-	0/17/37/64	0/3/3/3
4	PLM	A	2351	-	-	0/13/13/15	0/0/0/0
4	PLM	B	1600	-	-	0/13/13/15	0/0/0/0
2	BOG	B	1736	-	-	0/11/31/31	0/1/1/1
3	COA	B	2360	-	-	0/11/31/64	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2360	COA	C2A-N1A	2.44	1.38	1.33
3	A	2350	COA	C2A-N1A	2.78	1.39	1.33
3	B	2360	COA	C2A-N3A	3.49	1.38	1.32
3	A	2350	COA	C2A-N3A	4.17	1.39	1.32

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2360	COA	N3A-C2A-N1A	-12.12	119.61	128.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2350	COA	N3A-C2A-N1A	-10.59	120.78	128.89
3	A	2350	COA	P1A-O3A-P2A	-3.09	122.32	132.67
3	B	2360	COA	C1B-N9A-C4A	-2.08	123.80	126.94
3	B	2360	COA	O2A-P1A-O5B	2.07	112.52	106.56

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 8 short contacts:

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

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%)	-0.14	11 (1%) 71 70	10, 17, 33, 57	0
1	B	614/653 (94%)	-0.24	9 (1%) 76 75	11, 15, 30, 51	0
All	All	1229/1306 (94%)	-0.19	20 (1%) 74 74	10, 16, 32, 57	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	658	THR	4.6
1	A	206	LEU	4.5
1	B	179	ASN	4.5
1	B	181	SER	4.4
1	B	410	ALA	4.0
1	A	656	ILE	3.9
1	B	32	ASP	3.7
1	A	179	ASN	3.6
1	A	205	TYR	3.3
1	B	182	LYS	3.3
1	B	519	ASP	2.9
1	B	178	LEU	2.7
1	A	405	ALA	2.6
1	B	409	SER	2.6
1	A	593	ASN	2.5
1	A	181	SER	2.3
1	A	32	ASP	2.2
1	B	593[A]	ASN	2.2
1	A	657	LYS	2.1
1	A	522	LYS	2.1

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(\AA^2)	Q<0.9
2	BOG	B	1736	20/20	0.74	0.33	39.13	30,57,66,76	0
3	COA	A	2350	31/48	0.87	0.23	5.34	15,28,78,80	0
4	PLM	A	2351	16/18	0.89	0.17	5.11	9,21,37,39	0
3	COA	B	2360	27/48	0.86	0.19	3.96	18,27,63,64	0
4	PLM	B	1600	16/18	0.91	0.15	3.41	10,19,41,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.