



Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 07:32 pm BST

PDB ID : 6EE1
Title : Crystal structure of Mycobacterium tuberculosis ICL2 in complex with acetyl-CoA
Authors : Bashiri, G.; Bhusal, R.; Leung, I.
Deposited on : 2018-08-12
Resolution : 2.36 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 : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

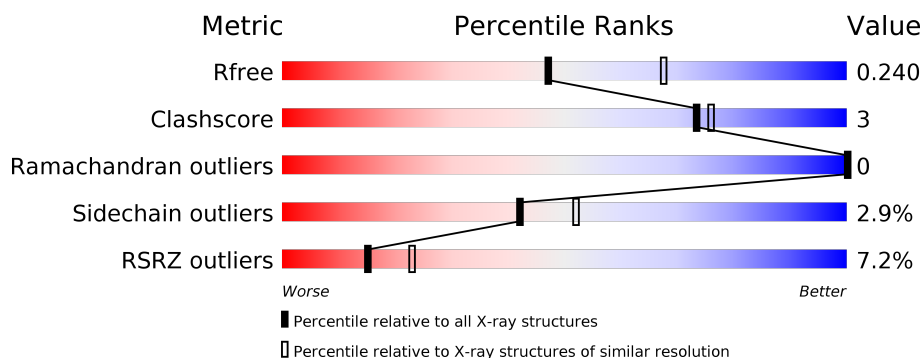
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.36 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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 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	786	<div> <div>6%</div> <div> <div></div> <div>86%</div> <div>5%</div> <div>9%</div> </div> </div>
1	B	786	<div> <div>9%</div> <div> <div></div> <div>83%</div> <div>9%</div> <div>7%</div> </div> </div>
1	C	786	<div> <div>6%</div> <div> <div></div> <div>84%</div> <div>7%</div> <div>8%</div> </div> </div>
1	D	786	<div> <div>6%</div> <div> <div></div> <div>85%</div> <div>7%</div> <div>7%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 23629 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 Isocitrate lyase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	719	Total	C	N	O	S	0	0	0
			5663	3581	1013	1050	19			
1	B	729	Total	C	N	O	S	0	0	0
			5747	3633	1028	1067	19			
1	C	722	Total	C	N	O	S	0	0	0
			5690	3596	1017	1057	20			
1	D	730	Total	C	N	O	S	0	0	0
			5753	3635	1029	1070	19			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	initiating methionine	UNP Q8VJU4
A	-18	GLY	-	expression tag	UNP Q8VJU4
A	-17	SER	-	expression tag	UNP Q8VJU4
A	-16	SER	-	expression tag	UNP Q8VJU4
A	-15	HIS	-	expression tag	UNP Q8VJU4
A	-14	HIS	-	expression tag	UNP Q8VJU4
A	-13	HIS	-	expression tag	UNP Q8VJU4
A	-12	HIS	-	expression tag	UNP Q8VJU4
A	-11	HIS	-	expression tag	UNP Q8VJU4
A	-10	HIS	-	expression tag	UNP Q8VJU4
A	-9	SER	-	expression tag	UNP Q8VJU4
A	-8	SER	-	expression tag	UNP Q8VJU4
A	-7	GLY	-	expression tag	UNP Q8VJU4
A	-6	LEU	-	expression tag	UNP Q8VJU4
A	-5	VAL	-	expression tag	UNP Q8VJU4
A	-4	PRO	-	expression tag	UNP Q8VJU4
A	-3	ARG	-	expression tag	UNP Q8VJU4
A	-2	GLY	-	expression tag	UNP Q8VJU4
A	-1	SER	-	expression tag	UNP Q8VJU4
A	0	HIS	-	expression tag	UNP Q8VJU4
B	-19	MET	-	initiating methionine	UNP Q8VJU4

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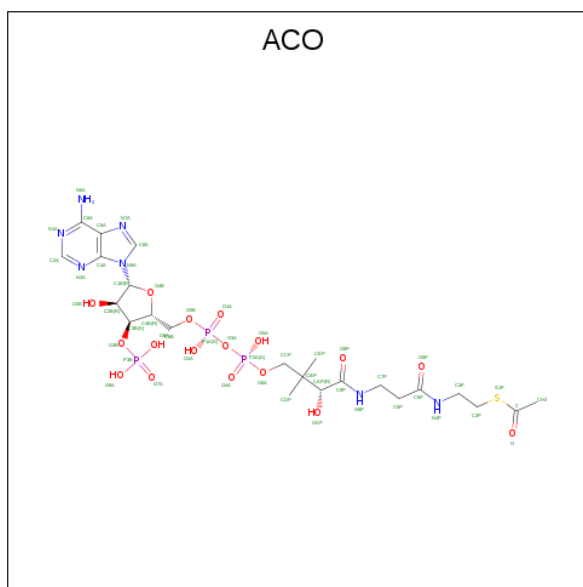
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q8VJU4
B	-17	SER	-	expression tag	UNP Q8VJU4
B	-16	SER	-	expression tag	UNP Q8VJU4
B	-15	HIS	-	expression tag	UNP Q8VJU4
B	-14	HIS	-	expression tag	UNP Q8VJU4
B	-13	HIS	-	expression tag	UNP Q8VJU4
B	-12	HIS	-	expression tag	UNP Q8VJU4
B	-11	HIS	-	expression tag	UNP Q8VJU4
B	-10	HIS	-	expression tag	UNP Q8VJU4
B	-9	SER	-	expression tag	UNP Q8VJU4
B	-8	SER	-	expression tag	UNP Q8VJU4
B	-7	GLY	-	expression tag	UNP Q8VJU4
B	-6	LEU	-	expression tag	UNP Q8VJU4
B	-5	VAL	-	expression tag	UNP Q8VJU4
B	-4	PRO	-	expression tag	UNP Q8VJU4
B	-3	ARG	-	expression tag	UNP Q8VJU4
B	-2	GLY	-	expression tag	UNP Q8VJU4
B	-1	SER	-	expression tag	UNP Q8VJU4
B	0	HIS	-	expression tag	UNP Q8VJU4
C	-19	MET	-	initiating methionine	UNP Q8VJU4
C	-18	GLY	-	expression tag	UNP Q8VJU4
C	-17	SER	-	expression tag	UNP Q8VJU4
C	-16	SER	-	expression tag	UNP Q8VJU4
C	-15	HIS	-	expression tag	UNP Q8VJU4
C	-14	HIS	-	expression tag	UNP Q8VJU4
C	-13	HIS	-	expression tag	UNP Q8VJU4
C	-12	HIS	-	expression tag	UNP Q8VJU4
C	-11	HIS	-	expression tag	UNP Q8VJU4
C	-10	HIS	-	expression tag	UNP Q8VJU4
C	-9	SER	-	expression tag	UNP Q8VJU4
C	-8	SER	-	expression tag	UNP Q8VJU4
C	-7	GLY	-	expression tag	UNP Q8VJU4
C	-6	LEU	-	expression tag	UNP Q8VJU4
C	-5	VAL	-	expression tag	UNP Q8VJU4
C	-4	PRO	-	expression tag	UNP Q8VJU4
C	-3	ARG	-	expression tag	UNP Q8VJU4
C	-2	GLY	-	expression tag	UNP Q8VJU4
C	-1	SER	-	expression tag	UNP Q8VJU4
C	0	HIS	-	expression tag	UNP Q8VJU4
D	-19	MET	-	initiating methionine	UNP Q8VJU4
D	-18	GLY	-	expression tag	UNP Q8VJU4
D	-17	SER	-	expression tag	UNP Q8VJU4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP Q8VJU4
D	-15	HIS	-	expression tag	UNP Q8VJU4
D	-14	HIS	-	expression tag	UNP Q8VJU4
D	-13	HIS	-	expression tag	UNP Q8VJU4
D	-12	HIS	-	expression tag	UNP Q8VJU4
D	-11	HIS	-	expression tag	UNP Q8VJU4
D	-10	HIS	-	expression tag	UNP Q8VJU4
D	-9	SER	-	expression tag	UNP Q8VJU4
D	-8	SER	-	expression tag	UNP Q8VJU4
D	-7	GLY	-	expression tag	UNP Q8VJU4
D	-6	LEU	-	expression tag	UNP Q8VJU4
D	-5	VAL	-	expression tag	UNP Q8VJU4
D	-4	PRO	-	expression tag	UNP Q8VJU4
D	-3	ARG	-	expression tag	UNP Q8VJU4
D	-2	GLY	-	expression tag	UNP Q8VJU4
D	-1	SER	-	expression tag	UNP Q8VJU4
D	0	HIS	-	expression tag	UNP Q8VJU4

- Molecule 2 is ACETYL COENZYME *A (three-letter code: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	B	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	D	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	161	Total	O	0	0
			161	161		
4	B	129	Total	O	0	0
			129	129		
4	C	152	Total	O	0	0
			152	152		
4	D	126	Total	O	0	0
			126	126		

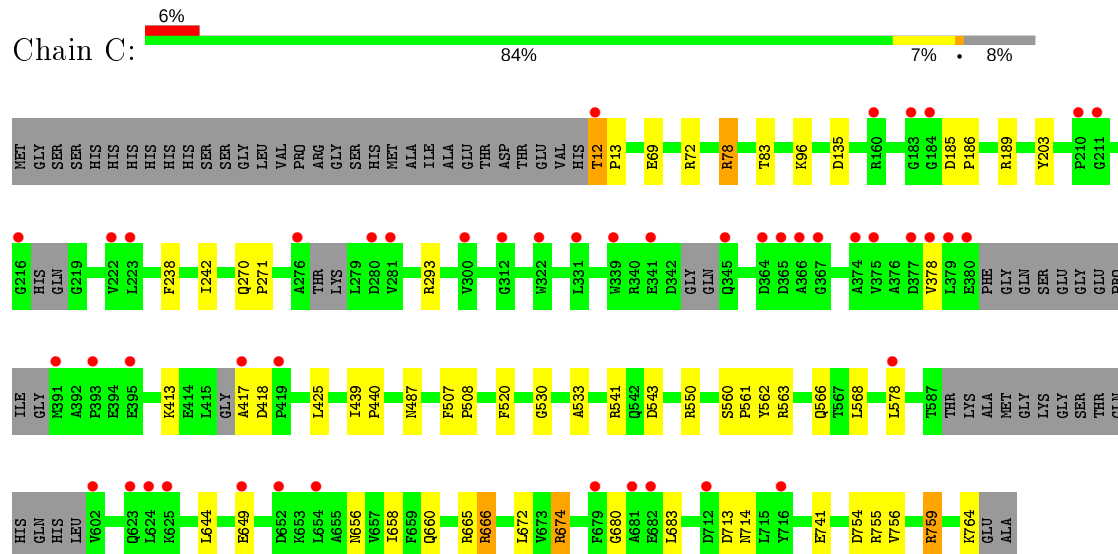
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 ($\text{RSRZ} > 2$). 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.

Chain A:

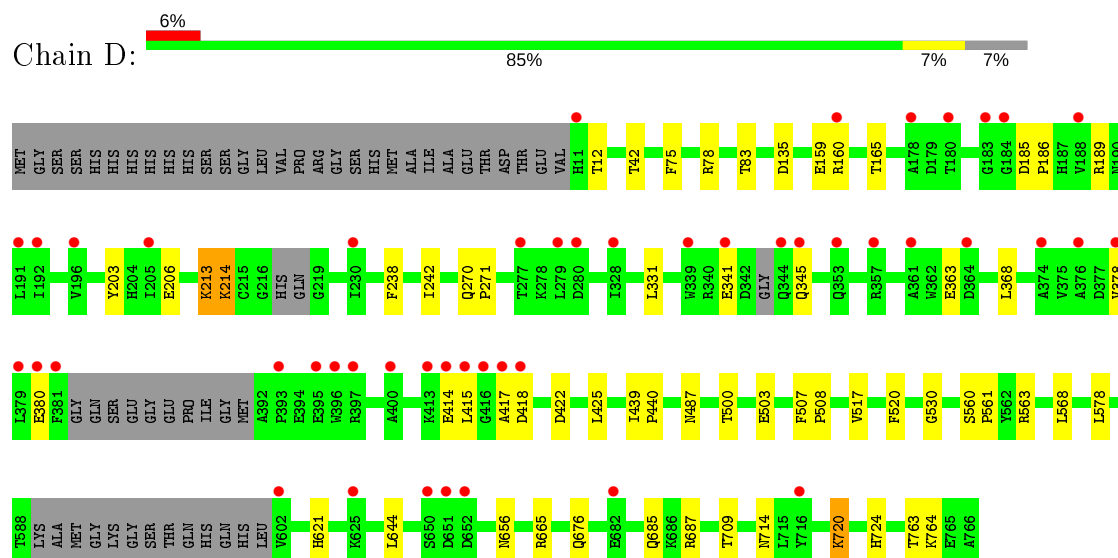
6% 86% 5% 9%

[illegible]

- Molecule 1: Isocitrate lyase 2



- Molecule 1: Isocitrate lyase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	105.47Å 169.97Å 106.42Å 90.00° 95.26° 90.00°	Depositor
Resolution (Å)	48.92 – 2.36 48.87 – 2.36	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.92-2.36) 100.0 (48.87-2.36)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.37Å)	Xtriage
Refinement program	REFMAC 5.8.0230	Depositor
R, R_{free}	0.198 , 0.232 0.208 , 0.240	Depositor DCC
R_{free} test set	7570 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	51.0	Xtriage
Anisotropy	0.081	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.074 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	23629	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.56% 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: MG, ACO

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	0.33	0/5782	0.51	0/7824
1	B	0.36	0/5870	0.53	0/7946
1	C	0.37	0/5810	0.52	0/7863
1	D	0.34	0/5877	0.52	0/7957
All	All	0.35	0/23339	0.52	0/31590

There are no bond length outliers.

There are no bond angle outliers.

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	5663	0	5585	23	0
1	B	5747	0	5662	58	0
1	C	5690	0	5605	47	0
1	D	5753	0	5663	31	0
2	A	51	0	34	2	0
2	B	51	0	34	4	0
2	C	51	0	34	2	0
2	D	51	0	34	6	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	161	0	0	1	0
4	B	129	0	0	3	0
4	C	152	0	0	3	0
4	D	126	0	0	0	0
All	All	23629	0	22651	149	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 (149) 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:B:621:HIS:CD2	1:B:763:THR:HG22	1.63	1.31
1:C:754:ASP:OD1	1:C:756:VAL:HG23	1.50	1.09
1:B:621:HIS:CD2	1:B:763:THR:CG2	2.57	0.84
1:C:754:ASP:CG	1:C:756:VAL:HG23	1.98	0.83
1:C:12:THR:HG22	1:C:13:PRO:HD2	1.66	0.77
1:C:665:ARG:NH1	1:C:665:ARG:HG2	2.02	0.74
1:B:375:VAL:HB	1:B:396:TRP:CH2	2.23	0.72
1:B:621:HIS:NE2	1:B:763:THR:HG22	2.05	0.72
1:C:665:ARG:HH11	1:C:665:ARG:HG2	1.56	0.71
1:B:372:GLY:HA2	1:B:396:TRP:CH2	2.26	0.71
1:B:414:GLU:O	1:B:415:LEU:HD22	1.92	0.70
1:B:709:THR:O	1:D:665:ARG:NH1	2.26	0.68
1:B:372:GLY:O	1:B:396:TRP:HZ3	1.76	0.67
1:B:660:GLN:OE1	1:B:674:ARG:NH2	2.26	0.67
1:A:185:ASP:OD2	1:A:189:ARG:NH1	2.28	0.67
1:B:662:ILE:HD12	1:B:672:LEU:HB2	1.78	0.66
1:D:621:HIS:CD2	1:D:763:THR:HG22	2.31	0.66
1:D:185:ASP:OD2	1:D:189:ARG:NH1	2.27	0.65
1:D:720:LYS:HD3	2:D:801:ACO:H1B	1.78	0.65
1:C:185:ASP:OD2	1:C:189:ARG:NH1	2.27	0.65
1:C:759:ARG:HH11	1:C:759:ARG:CG	2.10	0.63
1:B:658:ILE:HG13	1:B:675:ASP:HB3	1.80	0.63
1:B:372:GLY:O	1:B:396:TRP:CZ3	2.52	0.62
1:C:666:ARG:HH21	1:C:666:ARG:CG	2.13	0.62
1:B:676:GLN:HG2	2:B:801:ACO:HH32	1.81	0.61
1:C:759:ARG:HH11	1:C:759:ARG:HG3	1.65	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:GLY:O	1:B:324:GLU:HG2	2.01	0.61
1:A:422:ASP:OD2	1:A:425:LEU:HD23	2.02	0.60
1:B:662:ILE:HD13	1:B:672:LEU:HD12	1.84	0.60
1:C:754:ASP:CG	1:C:756:VAL:CG2	2.71	0.59
1:C:660:GLN:NE2	4:C:902:HOH:O	2.35	0.59
1:D:206:GLU:OE2	1:D:213:LYS:HE3	2.04	0.57
1:B:422:ASP:OD2	1:B:425:LEU:HD23	2.05	0.57
1:D:422:ASP:OD2	1:D:425:LEU:HD23	2.05	0.56
1:B:415:LEU:CD2	1:B:415:LEU:C	2.73	0.56
1:C:666:ARG:HG2	1:C:666:ARG:NH2	2.22	0.55
1:C:560:SER:O	1:C:563:ARG:HB2	2.07	0.55
1:A:561:PRO:HB2	1:A:568:LEU:HD13	1.88	0.54
1:B:676:GLN:HG2	2:B:801:ACO:CH3	2.36	0.54
1:D:676:GLN:HE21	2:D:801:ACO:HH33	1.73	0.54
1:D:724:HIS:NE2	2:D:801:ACO:O8A	2.30	0.53
1:D:560:SER:O	1:D:563:ARG:HB2	2.08	0.53
1:B:560:SER:O	1:B:563:ARG:HB2	2.07	0.53
1:B:621:HIS:HD2	1:B:763:THR:HG22	1.58	0.53
1:C:756:VAL:HG13	1:C:759:ARG:HH22	1.72	0.53
1:B:676:GLN:HE21	2:B:801:ACO:HH33	1.73	0.53
1:C:665:ARG:CG	1:C:665:ARG:HH11	2.20	0.53
1:A:560:SER:O	1:A:563:ARG:HB2	2.09	0.52
1:B:665:ARG:NH1	1:D:709:THR:O	2.37	0.52
1:D:561:PRO:HB2	1:D:568:LEU:HD13	1.91	0.52
1:C:759:ARG:NH1	1:C:759:ARG:CB	2.73	0.51
1:A:185:ASP:N	1:A:186:PRO:HD2	2.26	0.51
1:B:185:ASP:N	1:B:186:PRO:HD2	2.25	0.51
1:C:666:ARG:HH21	1:C:666:ARG:CB	2.23	0.51
1:B:378:VAL:HG11	1:B:417:ALA:HB1	1.93	0.51
1:A:215:CYS:O	1:A:215:CYS:SG	2.69	0.51
1:D:185:ASP:N	1:D:186:PRO:HD2	2.26	0.51
1:C:185:ASP:N	1:C:186:PRO:HD2	2.26	0.50
1:C:756:VAL:HG13	1:C:759:ARG:NH2	2.26	0.50
1:D:500:THR:HG23	1:D:503:GLU:H	1.77	0.50
1:B:415:LEU:HD22	1:B:415:LEU:C	2.32	0.49
1:C:759:ARG:NH1	1:C:759:ARG:CG	2.73	0.48
1:C:666:ARG:NH2	1:C:666:ARG:CG	2.73	0.48
1:D:378:VAL:HG11	1:D:417:ALA:HB1	1.96	0.48
1:C:666:ARG:HH21	1:C:666:ARG:HG2	1.77	0.48
1:C:714:ASN:ND2	2:C:801:ACO:C	2.76	0.48
1:C:96:LYS:NZ	4:C:906:HOH:O	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:676:GLN:HG2	2:D:801:ACO:CH3	2.44	0.47
1:B:662:ILE:CD1	1:B:672:LEU:HD12	2.44	0.47
1:A:238:PHE:CE2	1:A:242:ILE:HD11	2.49	0.47
1:B:238:PHE:CE2	1:B:242:ILE:HD11	2.49	0.47
1:A:550:ARG:NH1	4:A:903:HOH:O	2.37	0.47
1:B:709:THR:HG22	1:D:665:ARG:HH12	1.79	0.47
1:A:676:GLN:HG2	2:A:801:ACO:HH33	1.95	0.47
1:B:561:PRO:HB2	1:B:568:LEU:HD13	1.96	0.47
1:D:676:GLN:HG2	2:D:801:ACO:HH32	1.97	0.47
1:D:685:GLN:HG2	2:D:801:ACO:O2B	2.14	0.47
1:B:363:GLU:HG3	1:B:368:LEU:HD22	1.97	0.47
1:D:238:PHE:CE2	1:D:242:ILE:HD11	2.50	0.47
1:C:238:PHE:CE2	1:C:242:ILE:HD11	2.50	0.46
1:A:302:GLU:HG3	1:D:42:THR:HG21	1.98	0.46
1:B:327:GLY:HA2	4:B:920:HOH:O	2.15	0.46
1:B:372:GLY:HA2	1:B:396:TRP:CZ3	2.51	0.46
1:B:683:LEU:HD12	1:B:683:LEU:N	2.30	0.46
1:C:561:PRO:HB2	1:C:568:LEU:HD13	1.96	0.46
1:B:662:ILE:CD1	1:B:672:LEU:CD1	2.94	0.46
1:C:541:ARG:HH11	1:C:541:ARG:HG2	1.81	0.46
1:B:372:GLY:HA2	1:B:396:TRP:HH2	1.74	0.45
1:C:683:LEU:HD12	1:C:683:LEU:N	2.30	0.45
1:B:358:PHE:C	1:B:358:PHE:CD1	2.87	0.45
1:A:562:TYR:CZ	1:C:530:GLY:HA3	2.51	0.45
1:B:221:LYS:HE2	1:B:254:ASP:OD2	2.17	0.45
1:D:687:ARG:HE	1:D:764:LYS:HD3	1.81	0.45
1:B:83:THR:O	1:B:520:PHE:HA	2.17	0.45
1:C:666:ARG:HH21	1:C:666:ARG:HB2	1.82	0.44
1:D:214:LYS:HE3	1:D:214:LYS:HB3	1.79	0.44
1:A:363:GLU:HG2	1:A:368:LEU:HD12	1.99	0.44
1:B:345:GLN:HG3	1:B:346:SER:N	2.33	0.44
1:D:439:ILE:N	1:D:440:PRO:CD	2.81	0.44
1:B:465:LEU:HD13	1:B:507:PHE:CE2	2.53	0.44
1:B:78:ARG:HD2	1:B:78:ARG:HA	1.53	0.44
1:C:83:THR:O	1:C:520:PHE:HA	2.17	0.44
1:B:358:PHE:CD1	1:B:358:PHE:O	2.70	0.44
1:A:83:THR:O	1:A:520:PHE:HA	2.18	0.44
1:A:578:LEU:HD23	1:B:185:ASP:OD2	2.18	0.44
1:A:78:ARG:HA	1:A:78:ARG:HD3	1.76	0.44
1:D:78:ARG:HD3	1:D:78:ARG:HA	1.77	0.43
1:B:439:ILE:N	1:B:440:PRO:CD	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:562:TYR:CZ	1:D:530:GLY:HA3	2.53	0.43
1:A:439:ILE:N	1:A:440:PRO:CD	2.81	0.43
1:D:83:THR:O	1:D:520:PHE:HA	2.17	0.43
1:A:185:ASP:OD2	1:B:578:LEU:HD23	2.19	0.43
1:C:541:ARG:NH1	1:C:541:ARG:HG2	2.34	0.43
1:C:658:ILE:HG22	1:C:674:ARG:HD2	2.00	0.43
1:C:680:GLY:HA3	1:C:683:LEU:HD13	2.01	0.43
1:D:270:GLN:N	1:D:271:PRO:CD	2.81	0.43
1:A:270:GLN:N	1:A:271:PRO:CD	2.82	0.43
1:C:270:GLN:N	1:C:271:PRO:CD	2.82	0.43
1:A:416:GLY:O	1:A:418:ASP:N	2.52	0.42
1:B:415:LEU:HD23	1:B:415:LEU:O	2.19	0.42
1:B:644:LEU:O	1:B:656:ASN:HA	2.19	0.42
1:C:759:ARG:HB2	1:C:759:ARG:NH1	2.34	0.42
1:B:746:ARG:NH1	1:B:749:GLU:OE2	2.50	0.42
1:C:439:ILE:N	1:C:440:PRO:CD	2.82	0.42
1:D:363:GLU:HG2	1:D:368:LEU:HD12	2.01	0.42
1:B:270:GLN:N	1:B:271:PRO:CD	2.82	0.42
1:A:507:PHE:HB3	1:A:508:PRO:HD3	2.02	0.42
1:A:676:GLN:HG2	2:A:801:ACO:CH3	2.49	0.42
1:B:550:ARG:HD3	4:B:965:HOH:O	2.18	0.42
1:B:713:ASP:OD1	2:B:801:ACO:N6A	2.53	0.42
1:C:78:ARG:HA	1:C:78:ARG:HD2	1.29	0.42
1:B:375:VAL:HB	1:B:396:TRP:CZ2	2.54	0.42
1:B:75:PHE:HB2	1:B:517:VAL:HG11	2.01	0.42
1:C:378:VAL:HG11	1:C:417:ALA:HB1	2.02	0.42
1:D:644:LEU:O	1:D:656:ASN:HA	2.20	0.42
1:C:755:ARG:O	1:C:759:ARG:HB2	2.20	0.41
1:B:465:LEU:HD22	4:B:973:HOH:O	2.19	0.41
1:C:507:PHE:HB3	1:C:508:PRO:HD3	2.02	0.41
1:B:507:PHE:HB3	1:B:508:PRO:HD3	2.02	0.41
1:A:530:GLY:HA3	1:C:562:TYR:CZ	2.55	0.41
1:C:713:ASP:HB3	2:C:801:ACO:H143	2.01	0.41
1:B:206:GLU:OE2	1:B:213:LYS:HD2	2.21	0.41
1:C:543:ASP:OD2	1:C:550:ARG:NH2	2.53	0.41
1:A:91:GLN:HG2	1:C:533:ALA:HB2	2.03	0.41
1:C:644:LEU:O	1:C:656:ASN:HA	2.20	0.40
1:B:650:SER:O	1:B:651:ASP:HB2	2.22	0.40
1:C:674:ARG:HD3	4:C:994:HOH:O	2.21	0.40
1:D:507:PHE:HB3	1:D:508:PRO:HD3	2.02	0.40
1:D:75:PHE:HB2	1:D:517:VAL:HG11	2.03	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	703/786 (89%)	694 (99%)	9 (1%)	0	100	100
1	B	717/786 (91%)	705 (98%)	12 (2%)	0	100	100
1	C	708/786 (90%)	695 (98%)	13 (2%)	0	100	100
1	D	720/786 (92%)	706 (98%)	14 (2%)	0	100	100
All	All	2848/3144 (91%)	2800 (98%)	48 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	579/632 (92%)	569 (98%)	10 (2%)	60	72
1	B	588/632 (93%)	569 (97%)	19 (3%)	39	47
1	C	582/632 (92%)	562 (97%)	20 (3%)	37	46
1	D	588/632 (93%)	569 (97%)	19 (3%)	39	47
All	All	2337/2528 (92%)	2269 (97%)	68 (3%)	42	52

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	135	ASP
1	A	160	ARG
1	A	203	TYR
1	A	215	CYS
1	A	341	GLU
1	A	415	LEU
1	A	487	ASN
1	A	624	LEU
1	A	715	LEU
1	B	12	THR
1	B	78	ARG
1	B	135	ASP
1	B	203	TYR
1	B	213	LYS
1	B	353	GLN
1	B	358	PHE
1	B	363	GLU
1	B	415	LEU
1	B	461	LYS
1	B	465	LEU
1	B	487	ASN
1	B	658	ILE
1	B	663	GLN
1	B	668	ARG
1	B	703	GLN
1	B	714	ASN
1	B	759	ARG
1	B	762	ILE
1	C	12	THR
1	C	69	GLU
1	C	72	ARG
1	C	78	ARG
1	C	135	ASP
1	C	203	TYR
1	C	293	ARG
1	C	413	LYS
1	C	418	ASP
1	C	425	LEU
1	C	487	ASN
1	C	566	GLN
1	C	578	LEU
1	C	649	GLU

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Mol	Chain	Res	Type
1	C	666	ARG
1	C	672	LEU
1	C	674	ARG
1	C	741	GLU
1	C	759	ARG
1	C	764	LYS
1	D	12	THR
1	D	135	ASP
1	D	159	GLU
1	D	160	ARG
1	D	165	THR
1	D	203	TYR
1	D	213	LYS
1	D	214	LYS
1	D	331	LEU
1	D	341	GLU
1	D	345	GLN
1	D	380	GLU
1	D	414	GLU
1	D	415	LEU
1	D	418	ASP
1	D	487	ASN
1	D	578	LEU
1	D	714	ASN
1	D	720	LYS

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	706	HIS
1	A	714	ASN
1	A	731	ASN
1	B	663	GLN
1	C	566	GLN
1	C	706	HIS
1	C	714	ASN

5.3.3 RNA ⓘ

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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$
2	ACO	D	801	-	45,53,53	0.80	1 (2%)	56,79,79	1.07	4 (7%)
2	ACO	C	801	-	45,53,53	0.87	2 (4%)	56,79,79	1.09	5 (8%)
2	ACO	B	801	-	45,53,53	0.76	1 (2%)	56,79,79	1.28	7 (12%)
2	ACO	A	801	-	45,53,53	0.80	1 (2%)	56,79,79	1.17	7 (12%)

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	ACO	D	801	-	-	7/47/67/67	0/3/3/3
2	ACO	C	801	-	-	9/47/67/67	0/3/3/3
2	ACO	B	801	-	-	10/47/67/67	0/3/3/3
2	ACO	A	801	-	-	9/47/67/67	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	ACO	C5A-C4A	2.59	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	ACO	C5A-C4A	2.59	1.47	1.40
2	A	801	ACO	C5A-C4A	2.38	1.47	1.40
2	D	801	ACO	C5A-C4A	2.32	1.47	1.40
2	C	801	ACO	C2A-N3A	2.03	1.35	1.32

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	ACO	N3A-C2A-N1A	-4.13	122.22	128.68
2	B	801	ACO	N3A-C2A-N1A	-4.03	122.38	128.68
2	A	801	ACO	N3A-C2A-N1A	-3.65	122.97	128.68
2	C	801	ACO	N3A-C2A-N1A	-3.62	123.02	128.68
2	B	801	ACO	P2A-O3A-P1A	-2.88	122.94	132.83
2	C	801	ACO	CEP-CBP-CAP	2.63	113.39	108.82
2	A	801	ACO	P2A-O3A-P1A	-2.59	123.94	132.83
2	B	801	ACO	O6A-CCP-CBP	-2.56	106.43	110.55
2	B	801	ACO	C2A-N1A-C6A	2.48	122.99	118.75
2	B	801	ACO	O9A-P3B-O8A	2.38	116.73	107.64
2	A	801	ACO	C2P-C3P-N4P	2.34	117.33	112.42
2	A	801	ACO	C4A-C5A-N7A	-2.33	106.97	109.40
2	A	801	ACO	C2A-N1A-C6A	2.26	122.62	118.75
2	C	801	ACO	C4A-C5A-N7A	-2.24	107.06	109.40
2	B	801	ACO	C1B-N9A-C4A	-2.20	122.78	126.64
2	C	801	ACO	P2A-O3A-P1A	-2.18	125.34	132.83
2	D	801	ACO	C2A-N1A-C6A	2.16	122.45	118.75
2	B	801	ACO	CEP-CBP-CAP	2.14	112.54	108.82
2	D	801	ACO	P2A-O3A-P1A	-2.11	125.58	132.83
2	D	801	ACO	N6A-C6A-N1A	2.10	122.93	118.57
2	A	801	ACO	C1B-N9A-C4A	-2.08	123.00	126.64
2	A	801	ACO	C3P-N4P-C5P	2.07	126.68	122.84
2	C	801	ACO	C2A-N1A-C6A	2.04	122.24	118.75

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	801	ACO	C3B-O3B-P3B-O9A
2	B	801	ACO	C5B-O5B-P1A-O3A
2	B	801	ACO	O-C-S1P-C2P
2	B	801	ACO	CH3-C-S1P-C2P
2	C	801	ACO	C5B-O5B-P1A-O1A
2	C	801	ACO	N8P-C9P-CAP-OAP

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Mol	Chain	Res	Type	Atoms
2	A	801	ACO	C5B-O5B-P1A-O2A
2	A	801	ACO	C5B-O5B-P1A-O3A
2	A	801	ACO	S1P-C2P-C3P-N4P
2	A	801	ACO	O-C-S1P-C2P
2	A	801	ACO	CH3-C-S1P-C2P
2	D	801	ACO	C5B-O5B-P1A-O3A
2	D	801	ACO	O-C-S1P-C2P
2	D	801	ACO	CH3-C-S1P-C2P
2	B	801	ACO	C2B-C3B-O3B-P3B
2	B	801	ACO	C4B-C3B-O3B-P3B
2	A	801	ACO	C5P-C6P-C7P-N8P
2	C	801	ACO	O9P-C9P-CAP-OAP
2	A	801	ACO	C2P-C3P-N4P-C5P
2	B	801	ACO	CCP-O6A-P2A-O3A
2	C	801	ACO	C5B-O5B-P1A-O3A
2	B	801	ACO	P2A-O3A-P1A-O1A
2	B	801	ACO	C5B-O5B-P1A-O1A
2	D	801	ACO	C5B-O5B-P1A-O1A
2	C	801	ACO	O4B-C4B-C5B-O5B
2	C	801	ACO	C2B-C3B-O3B-P3B
2	C	801	ACO	C4B-C3B-O3B-P3B
2	C	801	ACO	C3B-C4B-C5B-O5B
2	A	801	ACO	C3B-O3B-P3B-O7A
2	B	801	ACO	C3B-O3B-P3B-O8A
2	C	801	ACO	C3B-O3B-P3B-O8A
2	D	801	ACO	C3B-O3B-P3B-O8A
2	A	801	ACO	P2A-O3A-P1A-O2A
2	D	801	ACO	C4B-C3B-O3B-P3B
2	D	801	ACO	C2B-C3B-O3B-P3B

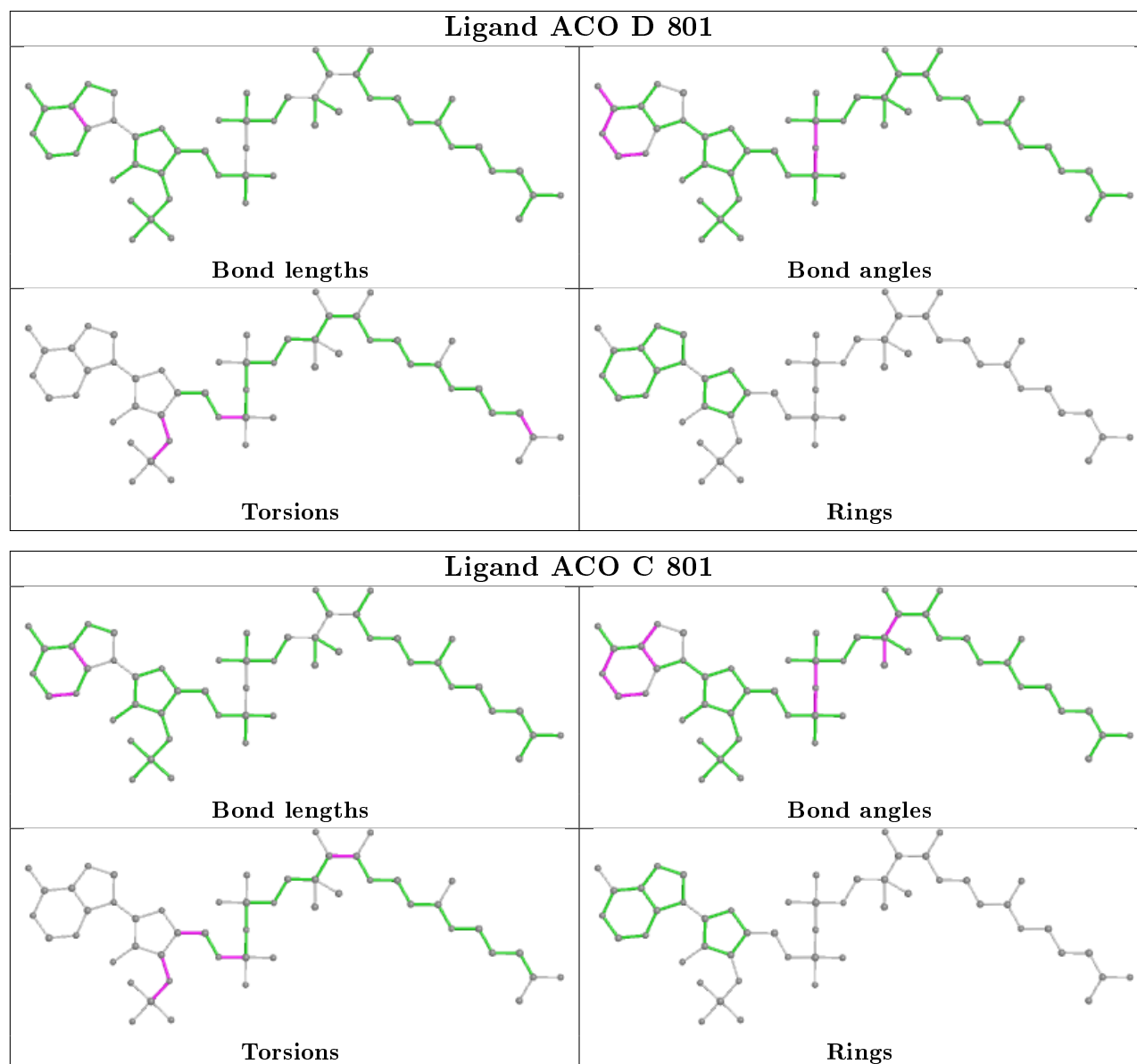
There are no ring outliers.

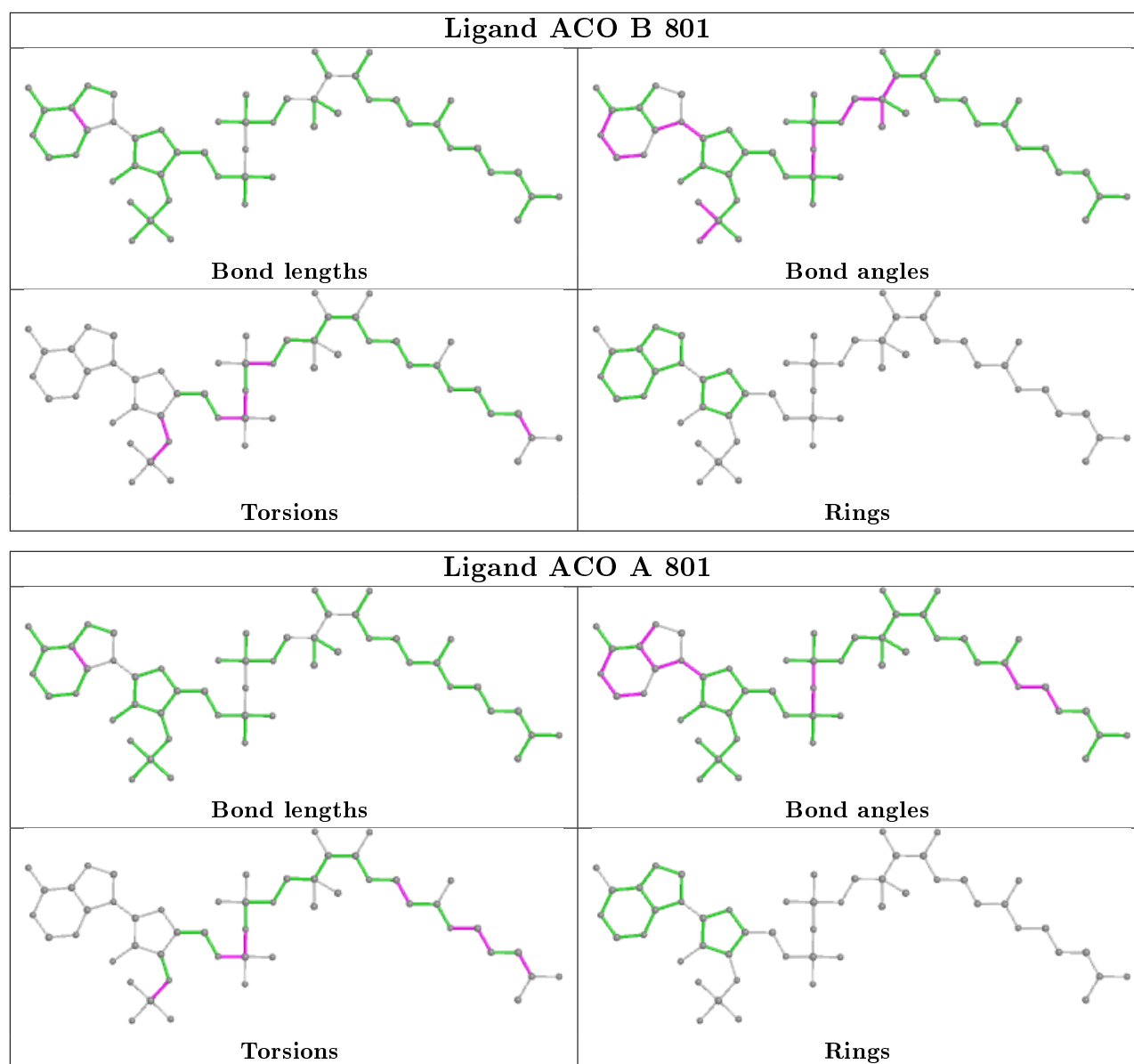
4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801	ACO	6	0
2	C	801	ACO	2	0
2	B	801	ACO	4	0
2	A	801	ACO	2	0

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

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	719/786 (91%)	0.39	46 (6%) 19 28	35, 59, 98, 134	0
1	B	729/786 (92%)	0.47	67 (9%) 9 14	37, 62, 104, 137	0
1	C	722/786 (91%)	0.37	47 (6%) 18 27	37, 60, 100, 130	0
1	D	730/786 (92%)	0.42	48 (6%) 18 26	41, 61, 104, 133	0
All	All	2900/3144 (92%)	0.41	208 (7%) 15 23	35, 61, 102, 137	0

All (208) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	280	ASP	7.7
1	C	417	ALA	6.4
1	D	160	ARG	5.5
1	B	601	LEU	5.4
1	D	279	LEU	5.4
1	A	392	ALA	5.3
1	D	379	LEU	5.3
1	D	381	PHE	5.3
1	D	625	LYS	5.1
1	B	396	TRP	4.9
1	C	366	ALA	4.7
1	B	342	ASP	4.7
1	C	379	LEU	4.7
1	D	417	ALA	4.6
1	C	345	GLN	4.5
1	B	415	LEU	4.3
1	D	341	GLU	4.3
1	C	216	GLY	4.3
1	B	381	PHE	4.2
1	C	625	LYS	4.2
1	A	322	TRP	4.1

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Mol	Chain	Res	Type	RSRZ
1	D	183	GLY	4.1
1	B	160	ARG	4.0
1	A	379	LEU	4.0
1	D	415	LEU	4.0
1	D	361	ALA	4.0
1	A	327	GLY	4.0
1	D	400	ALA	4.0
1	C	649	GLU	3.9
1	C	679	PHE	3.8
1	D	378	VAL	3.8
1	B	380	GLU	3.8
1	B	649	GLU	3.7
1	A	323	LEU	3.7
1	B	219	GLY	3.7
1	D	393	PRO	3.7
1	D	344	GLN	3.6
1	D	416	GLY	3.6
1	B	348	ASP	3.6
1	C	339	TRP	3.5
1	C	341	GLU	3.5
1	B	413	LYS	3.5
1	B	183	GLY	3.5
1	A	393	PRO	3.5
1	D	396	TRP	3.4
1	B	164	ALA	3.4
1	B	339	TRP	3.4
1	A	682	GLU	3.4
1	A	353	GLN	3.4
1	A	394	GLU	3.4
1	D	395	GLU	3.4
1	A	378	VAL	3.4
1	B	328	ILE	3.4
1	B	378	VAL	3.3
1	D	280	ASP	3.3
1	C	365	ASP	3.3
1	C	393	PRO	3.3
1	C	12	THR	3.3
1	A	623	GLN	3.3
1	A	762	ILE	3.2
1	A	279	LEU	3.2
1	B	364	ASP	3.2
1	C	391	MET	3.2

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Mol	Chain	Res	Type	RSRZ
1	B	280	ASP	3.2
1	A	654	LEU	3.2
1	B	349	GLY	3.1
1	C	623	GLN	3.1
1	B	210	PRO	3.1
1	B	279	LEU	3.0
1	A	376	ALA	3.0
1	B	395	GLU	3.0
1	B	298	LEU	3.0
1	B	350	ILE	3.0
1	B	400	ALA	3.0
1	B	299	GLY	3.0
1	A	627	LYS	3.0
1	B	376	ALA	3.0
1	D	374	ALA	3.0
1	C	682	GLU	2.9
1	C	367	GLY	2.9
1	B	344	GLN	2.9
1	A	280	ASP	2.9
1	B	417	ALA	2.9
1	D	376	ALA	2.9
1	A	649	GLU	2.9
1	B	588	THR	2.9
1	B	340	ARG	2.9
1	A	220	GLY	2.9
1	C	375	VAL	2.9
1	B	353	GLN	2.9
1	B	338	ALA	2.9
1	D	205	ILE	2.8
1	D	353	GLN	2.8
1	B	345	GLN	2.8
1	B	216	GLY	2.8
1	D	651	ASP	2.8
1	D	339	TRP	2.8
1	C	378	VAL	2.8
1	A	753	PRO	2.8
1	B	625	LYS	2.8
1	D	413	LYS	2.8
1	A	319	ALA	2.7
1	D	191	LEU	2.7
1	A	732	GLN	2.7
1	D	716	TYR	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	374	ALA	2.7
1	B	410	ALA	2.7
1	B	379	LEU	2.7
1	A	216	GLY	2.6
1	A	380	GLU	2.6
1	B	322	TRP	2.6
1	A	681	ALA	2.6
1	C	210	PRO	2.6
1	B	412	ALA	2.6
1	D	414	GLU	2.6
1	C	276	ALA	2.6
1	D	364	ASP	2.6
1	A	400	ALA	2.6
1	B	341	GLU	2.6
1	B	161	GLN	2.5
1	A	395	GLU	2.5
1	C	312	GLY	2.5
1	B	211	GLY	2.5
1	B	327	GLY	2.5
1	C	211	GLY	2.5
1	A	331	LEU	2.5
1	C	602	VAL	2.5
1	B	326	GLN	2.5
1	B	393	PRO	2.5
1	D	188	VAL	2.4
1	C	395	GLU	2.4
1	D	652	ASP	2.4
1	B	666	ARG	2.4
1	A	622	TYR	2.4
1	D	397	ARG	2.4
1	A	354	VAL	2.4
1	C	183	GLY	2.4
1	B	158	SER	2.4
1	D	11	HIS	2.4
1	A	329	PHE	2.4
1	C	652	ASP	2.4
1	B	346	SER	2.4
1	A	328	ILE	2.4
1	C	716	TYR	2.4
1	D	230	ILE	2.4
1	B	420	PRO	2.4
1	C	160	ARG	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	205	ILE	2.3
1	B	159	GLU	2.3
1	C	654	LEU	2.3
1	A	357	ARG	2.3
1	B	77	ALA	2.3
1	B	357	ARG	2.3
1	D	184	GLY	2.3
1	C	681	ALA	2.3
1	D	277	THR	2.3
1	A	16	GLN	2.3
1	A	680	GLY	2.3
1	C	322	TRP	2.3
1	C	377	ASP	2.3
1	C	712	ASP	2.3
1	D	196	VAL	2.3
1	C	624	LEU	2.2
1	B	498	GLY	2.2
1	A	339	TRP	2.2
1	C	380	GLU	2.2
1	B	184	GLY	2.2
1	B	347	ILE	2.2
1	A	415	LEU	2.2
1	B	499	MET	2.2
1	D	418	ASP	2.2
1	B	182	HIS	2.2
1	A	326	GLN	2.2
1	C	300	VAL	2.2
1	B	382	GLY	2.2
1	C	184	GLY	2.2
1	B	394	GLU	2.2
1	A	160	ARG	2.2
1	D	682	GLU	2.2
1	D	345	GLN	2.2
1	C	364	ASP	2.1
1	A	211	GLY	2.1
1	D	357	ARG	2.1
1	B	180	THR	2.1
1	B	261	ILE	2.1
1	B	325	ARG	2.1
1	B	225	PRO	2.1
1	D	192	ILE	2.1
1	C	281	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	419	PRO	2.1
1	A	413	LYS	2.1
1	D	180	THR	2.1
1	B	222	VAL	2.1
1	A	650	SER	2.1
1	C	331	LEU	2.1
1	A	183	GLY	2.1
1	D	602	VAL	2.1
1	C	223	LEU	2.0
1	B	178	ALA	2.0
1	D	650	SER	2.0
1	A	222	VAL	2.0
1	C	222	VAL	2.0
1	C	578	LEU	2.0
1	A	210	PRO	2.0
1	A	182	HIS	2.0
1	D	328	ILE	2.0
1	D	380	GLU	2.0
1	D	178	ALA	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 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.

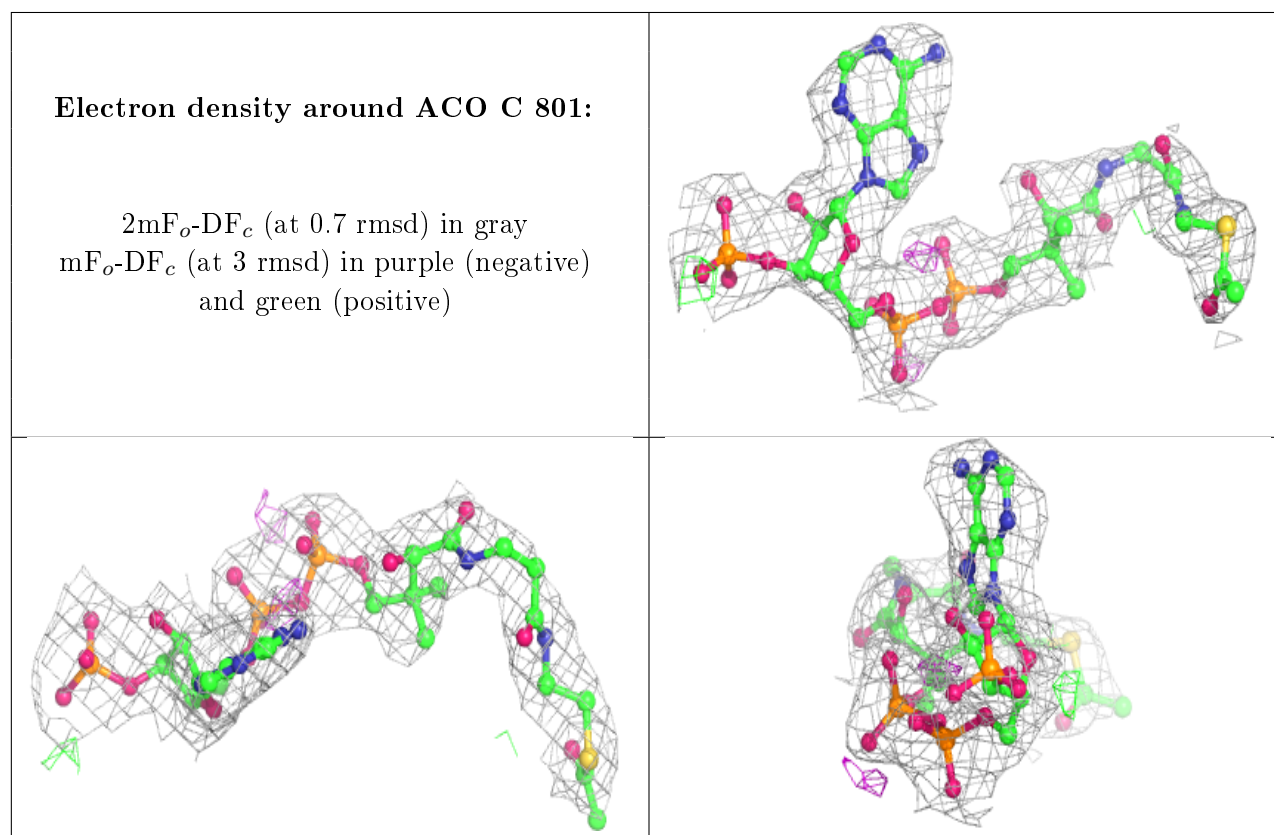
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ACO	C	801	51/51	0.92	0.17	81,95,107,117	0
3	MG	B	802	1/1	0.95	0.20	30,30,30,30	0
2	ACO	D	801	51/51	0.95	0.13	60,71,86,89	0
2	ACO	A	801	51/51	0.96	0.12	65,75,89,93	0

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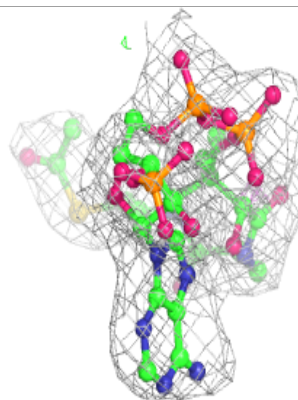
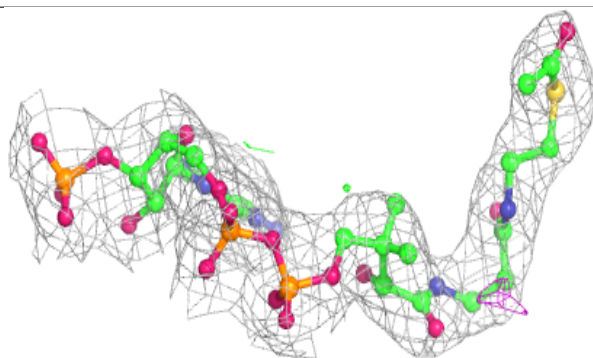
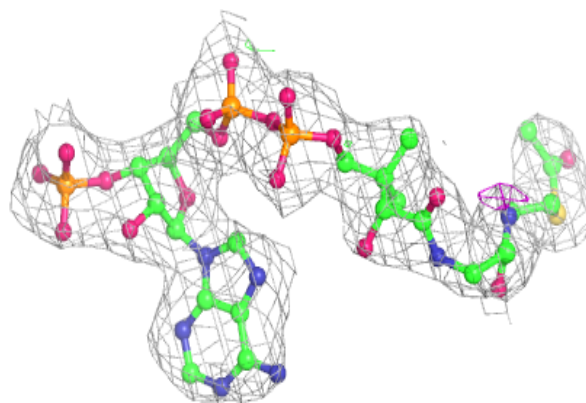
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	C	802	1/1	0.96	0.18	30,30,30,30	0
2	ACO	B	801	51/51	0.96	0.12	56,69,77,79	0
3	MG	D	802	1/1	0.97	0.15	30,30,30,30	0
3	MG	A	802	1/1	0.99	0.10	30,30,30,30	0

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.

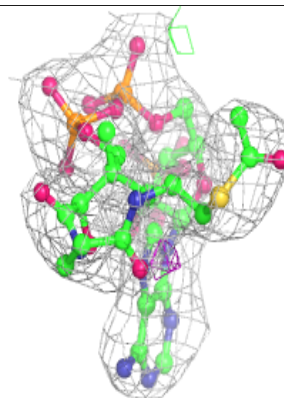
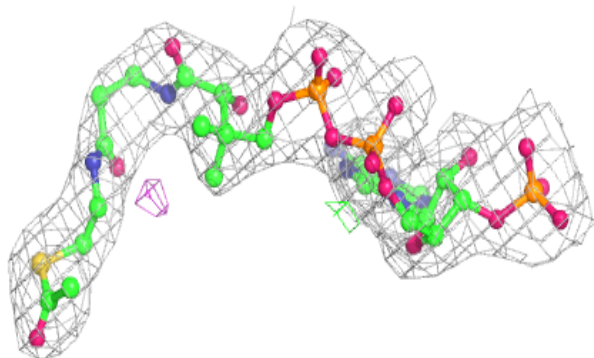
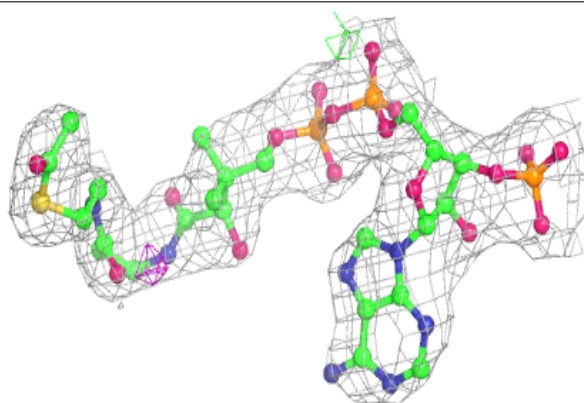


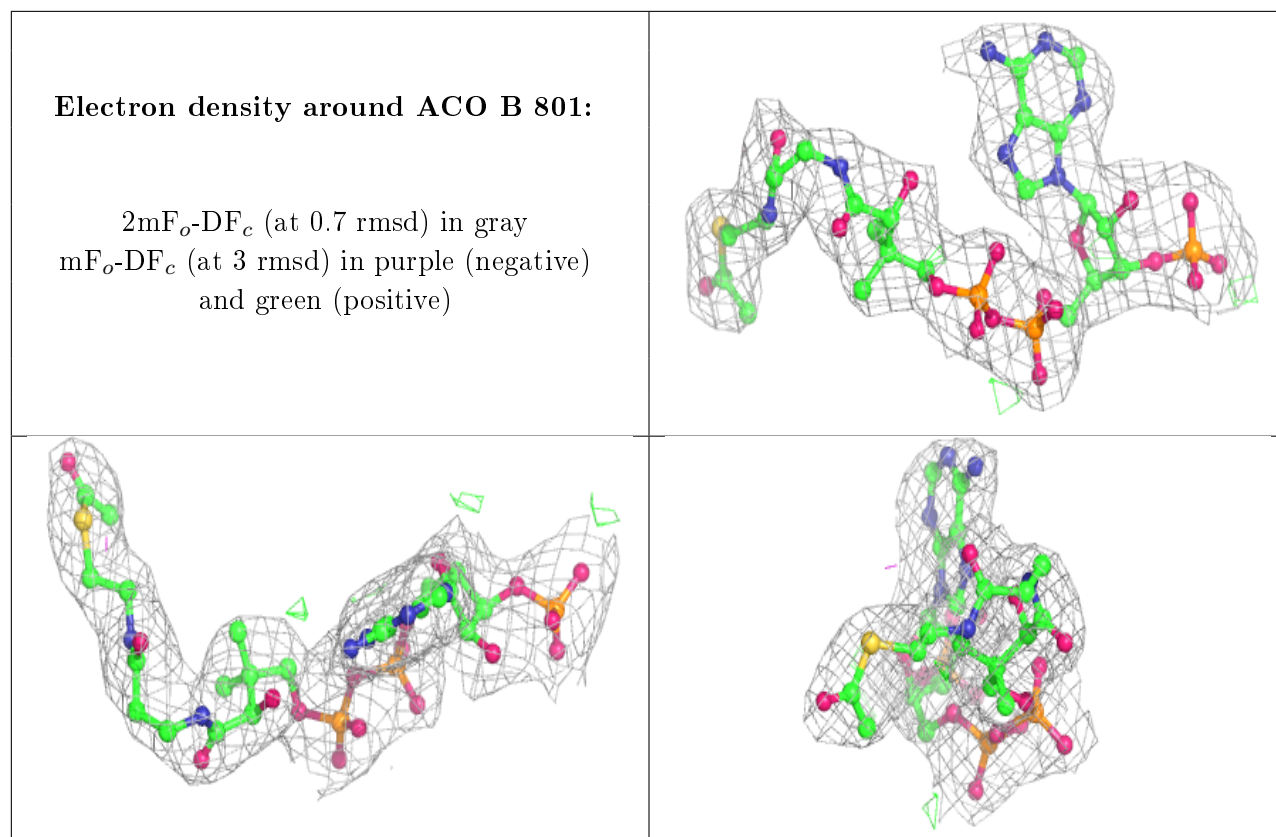
Electron density around ACO D 801:

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

**Electron density around ACO A 801:**

$2mF_o-DF_c$ (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.