



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 13, 2026 – 07:03 PM UTC

PDB ID : 6EE1 / pdb_00006ee1
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 types of validation reports are described at

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

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

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

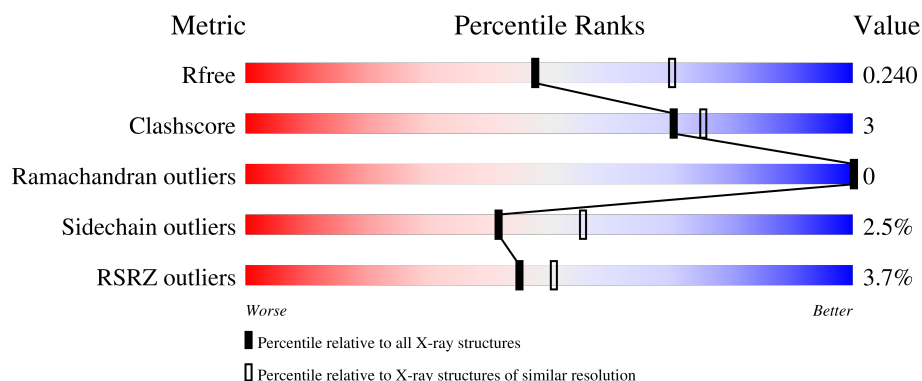
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

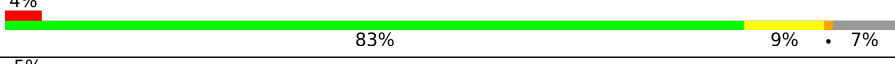
The reported resolution of this entry is 2.36 Å.

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}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (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 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	786	
1	B	786	
1	C	786	
1	D	786	

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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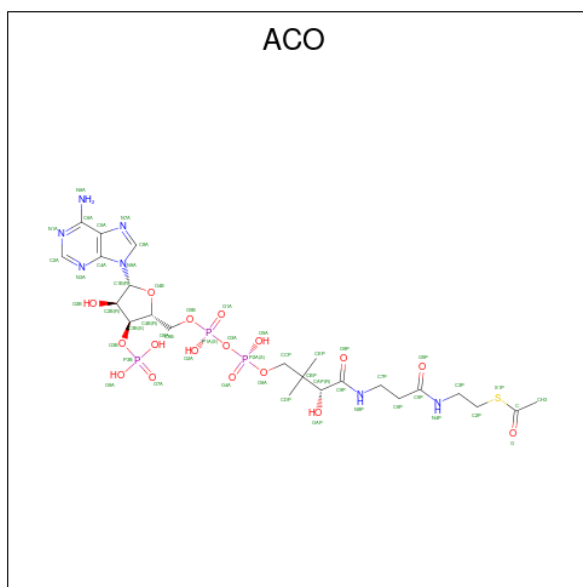
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP Q8VJU4
B	-17	SER	-	expression tag	UNP Q8VJU4
B	-16	SER	-	expression tag	UNP Q8VJU4
B	-15	HIS	-	expression tag	UNP Q8VJU4
B	-14	HIS	-	expression tag	UNP Q8VJU4
B	-13	HIS	-	expression tag	UNP Q8VJU4
B	-12	HIS	-	expression tag	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 (CCD ID: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



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 (CCD ID: MG) (formula: Mg).

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

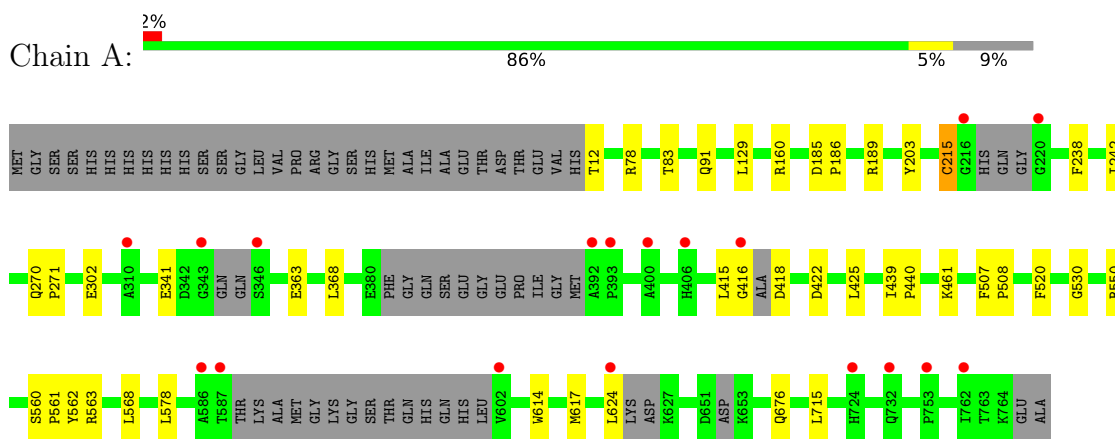
- Molecule 4 is water.

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		

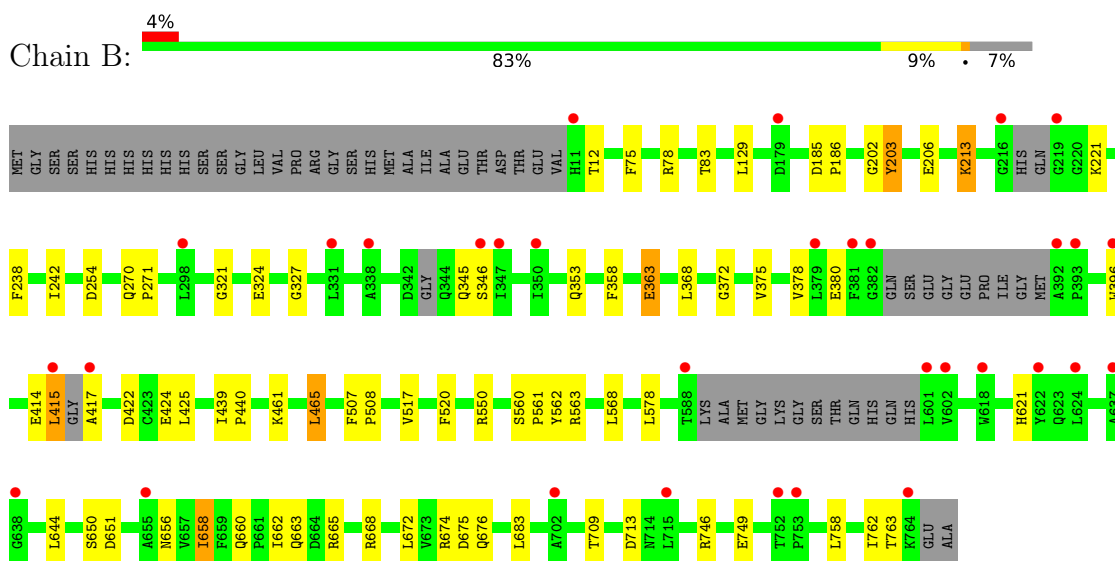
3 Residue-property plots [i](#)

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.

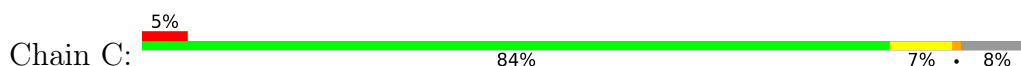
• Molecule 1: Isocitrate lyase 2

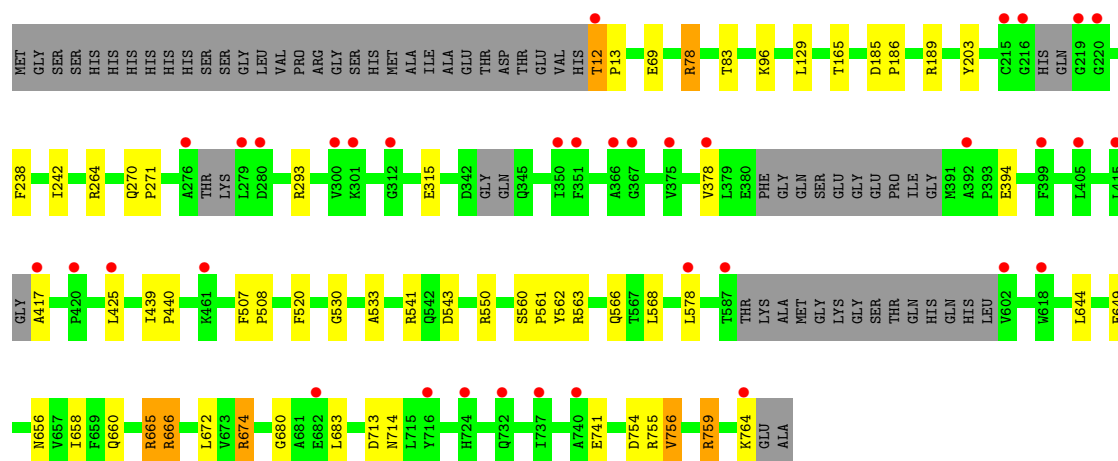


• Molecule 1: Isocitrate lyase 2

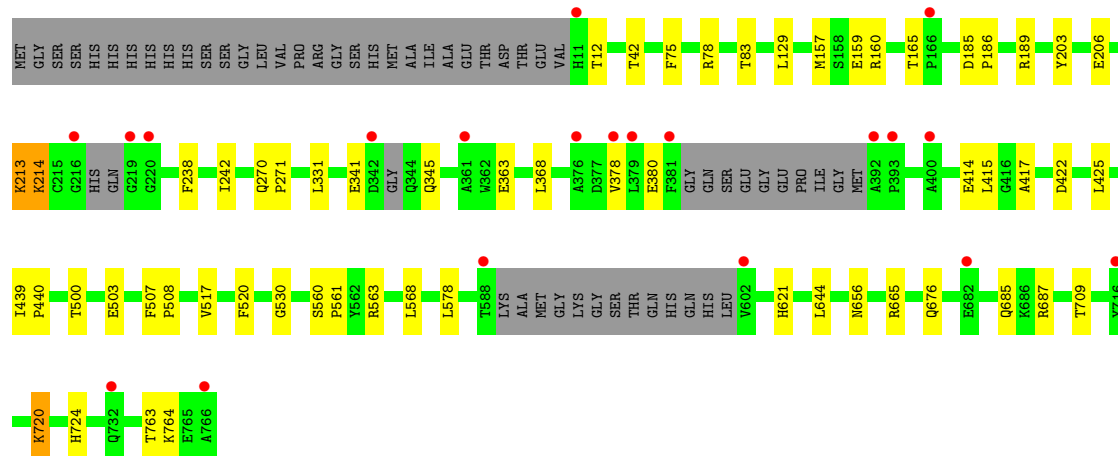
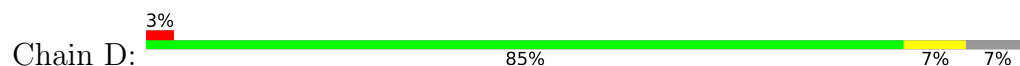


• Molecule 1: Isocitrate lyase 2





• 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 48.92 – 2.36	Depositor EDS
% Data completeness (in resolution range)	100.0 (48.92-2.36) 100.0 (48.92-2.36)	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)	0.32 , 33.8	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	0.96	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: ACO, MG

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	0.59	0/5782	0.95	0/7824
1	B	0.62	0/5870	0.97	0/7946
1	C	0.63	0/5810	0.98	0/7863
1	D	0.60	0/5877	0.97	0/7957
All	All	0.61	0/23339	0.97	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	25	0
1	B	5747	0	5662	61	0
1	C	5690	0	5605	49	0
1	D	5753	0	5663	33	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	157	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 (157) 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:C:754:ASP:CG	1:C:756:VAL:HG23	1.98	0.88
1:B:621:HIS:CD2	1:B:763:THR:CG2	2.57	0.84
1:C:12:THR:HG22	1:C:13:PRO:HD2	1.66	0.77
1:C:665:ARG:HG2	1:C:665:ARG:NH1	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:HG2	1:C:665:ARG:HH11	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:754:ASP:CG	1:C:756:VAL:CG2	2.71	0.64
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:CG	1:C:666:ARG:HH21	2.13	0.62
1:B:676:GLN:HG2	2:B:801:ACO:HH32	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:759:ARG:HH11	1:C:759:ARG:HG3	1.65	0.61
1:B:321:GLY:O	1:B:324:GLU:HG2	2.01	0.61
1:B:415:LEU:CD2	1:B:415:LEU:C	2.73	0.60
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: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:C:666:ARG:NH2	1:C:666:ARG:HG2	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:B:415:LEU:HD22	1:B:415:LEU:C	2.32	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:HH11	1:C:665:ARG:CG	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:A:614:TRP:HA	1:A:617:MET:HE2	1.92	0.51
1:C:759:ARG:CB	1:C:759:ARG:NH1	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:358:PHE:C	1:B:358:PHE:CD1	2.87	0.50
1:C:759:ARG:CG	1:C:759:ARG:NH1	2.73	0.48
1:C:666:ARG:CG	1:C:666:ARG:NH2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:N	1:C:683:LEU:HD12	2.30	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:HB3	1:D:214:LYS:HE3	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:HA	1:B:78:ARG:HD2	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:78:ARG:HD3	1:A:78:ARG:HA	1.76	0.44
1:A:578:LEU:HD23	1:B:185:ASP:OD2	2.18	0.44
1:D:78:ARG:HD3	1:D:78:ARG:HA	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:439:ILE:N	1:B:440:PRO:CD	2.81	0.43
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:HG2	1:C:541:ARG:NH1	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:NH1	1:C:759:ARG:HB2	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:D:129:LEU:C	1:D:129:LEU:HD12	2.45	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:424:GLU:CD	1:C:264:ARG:HH21	2.28	0.42
1:A:129:LEU:C	1:A:129:LEU:HD12	2.45	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:C:129:LEU:C	1:C:129:LEU:HD12	2.45	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:B:129:LEU:HD12	1:B:129:LEU:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:GLN:HG2	1:C:533:ALA:HB2	2.03	0.41
1:B:202:GLY:C	1:B:203:TYR:CG	2.99	0.41
1:D:157:MET:HB2	1:D:157:MET:HE2	1.77	0.40
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:75:PHE:HB2	1:D:517:VAL:HG11	2.03	0.40
1:D:507:PHE:HB3	1:D:508:PRO:HD3	2.02	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%)	570 (98%)	9 (2%)	55	70
1	B	588/632 (93%)	574 (98%)	14 (2%)	43	57
1	C	582/632 (92%)	562 (97%)	20 (3%)	32	43
1	D	588/632 (93%)	573 (97%)	15 (3%)	40	54
All	All	2337/2528 (92%)	2279 (98%)	58 (2%)	42	55

All (58) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	THR
1	A	160	ARG
1	A	203	TYR
1	A	215	CYS
1	A	341	GLU
1	A	415	LEU
1	A	461	LYS
1	A	624	LEU
1	A	715	LEU
1	B	12	THR
1	B	203	TYR
1	B	213	LYS
1	B	353	GLN
1	B	363	GLU
1	B	380	GLU
1	B	415	LEU
1	B	461	LYS
1	B	465	LEU
1	B	658	ILE
1	B	663	GLN
1	B	668	ARG
1	B	758	LEU
1	B	762	ILE
1	C	12	THR
1	C	69	GLU
1	C	78	ARG
1	C	165	THR
1	C	203	TYR
1	C	293	ARG
1	C	315	GLU
1	C	394	GLU
1	C	425	LEU
1	C	566	GLN

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Mol	Chain	Res	Type
1	C	578	LEU
1	C	649	GLU
1	C	665	ARG
1	C	666	ARG
1	C	672	LEU
1	C	674	ARG
1	C	741	GLU
1	C	756	VAL
1	C	759	ARG
1	C	764	LYS
1	D	12	THR
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	578	LEU
1	D	720	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	HIS
1	A	470	GLN
1	A	663	GLN
1	A	706	HIS
1	A	714	ASN
1	B	566	GLN
1	B	621	HIS
1	B	631	GLN
1	B	647	HIS
1	B	663	GLN
1	C	156	GLN
1	C	470	GLN
1	C	476	HIS

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Mol	Chain	Res	Type
1	C	621	HIS
1	C	631	GLN
1	C	647	HIS
1	C	714	ASN
1	D	57	HIS
1	D	470	GLN
1	D	621	HIS
1	D	631	GLN
1	D	647	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 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	-	51,53,53	1.17	6 (11%)	73,79,79	1.52	11 (15%)
2	ACO	A	801	-	51,53,53	1.17	7 (13%)	73,79,79	1.59	14 (19%)
2	ACO	B	801	-	51,53,53	1.14	6 (11%)	73,79,79	1.59	13 (17%)
2	ACO	C	801	-	51,53,53	1.29	6 (11%)	73,79,79	1.54	11 (15%)

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	-	-	8/51/67/67	0/3/3/3
2	ACO	A	801	-	-	8/51/67/67	0/3/3/3
2	ACO	B	801	-	-	10/51/67/67	0/3/3/3
2	ACO	C	801	-	-	9/51/67/67	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	ACO	C5A-C4A	4.88	1.47	1.39
2	C	801	ACO	C5A-C4A	4.87	1.47	1.39
2	A	801	ACO	C5A-C4A	4.57	1.47	1.39
2	D	801	ACO	C5A-C4A	4.47	1.47	1.39
2	C	801	ACO	P2A-O3A	3.50	1.63	1.59
2	C	801	ACO	P1A-O3A	2.73	1.62	1.59
2	C	801	ACO	C5A-C6A	2.65	1.48	1.41
2	B	801	ACO	C5A-C6A	2.64	1.48	1.41
2	D	801	ACO	C5A-N7A	-2.63	1.34	1.39
2	A	801	ACO	C5A-C6A	2.57	1.48	1.41
2	B	801	ACO	C8A-N7A	2.47	1.36	1.31
2	D	801	ACO	P2A-O3A	2.42	1.62	1.59
2	D	801	ACO	P1A-O3A	2.40	1.62	1.59
2	A	801	ACO	C4A-N9A	-2.35	1.32	1.37
2	D	801	ACO	C8A-N7A	2.31	1.36	1.31
2	C	801	ACO	C5A-N7A	-2.31	1.34	1.39
2	A	801	ACO	C8A-N7A	2.30	1.36	1.31
2	C	801	ACO	C8A-N7A	2.27	1.36	1.31
2	D	801	ACO	C5A-C6A	2.24	1.47	1.41
2	B	801	ACO	C4A-N9A	-2.19	1.33	1.37
2	A	801	ACO	P2A-O3A	2.19	1.61	1.59
2	A	801	ACO	C5A-N7A	-2.15	1.35	1.39
2	B	801	ACO	C5A-N7A	-2.14	1.35	1.39
2	A	801	ACO	P1A-O3A	2.11	1.61	1.59
2	B	801	ACO	P2A-O3A	2.05	1.61	1.59

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	ACO	C5A-C4A-N3A	-5.50	119.14	126.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	801	ACO	C5A-C4A-N3A	-5.32	119.39	126.72
2	A	801	ACO	C5A-C4A-N3A	-4.95	119.90	126.72
2	B	801	ACO	C5A-C4A-N3A	-4.88	119.99	126.72
2	C	801	ACO	N3A-C4A-N9A	4.76	135.26	127.17
2	D	801	ACO	N3A-C4A-N9A	4.61	135.00	127.17
2	A	801	ACO	N3A-C4A-N9A	4.34	134.54	127.17
2	D	801	ACO	N3A-C2A-N1A	-4.20	122.22	128.58
2	B	801	ACO	N3A-C4A-N9A	4.14	134.20	127.17
2	B	801	ACO	N3A-C2A-N1A	-4.09	122.38	128.58
2	A	801	ACO	C4A-N9A-C8A	3.96	109.89	105.74
2	D	801	ACO	C2A-N3A-C4A	3.83	121.19	111.83
2	D	801	ACO	O4B-C1B-N9A	3.77	115.34	108.09
2	A	801	ACO	N3A-C2A-N1A	-3.71	122.97	128.58
2	C	801	ACO	N3A-C2A-N1A	-3.67	123.02	128.58
2	C	801	ACO	C2A-N3A-C4A	3.67	120.81	111.83
2	B	801	ACO	C2A-N3A-C4A	3.67	120.80	111.83
2	A	801	ACO	C2A-N3A-C4A	3.52	120.44	111.83
2	C	801	ACO	C4A-N9A-C8A	3.23	109.13	105.74
2	B	801	ACO	O4B-C1B-N9A	3.20	114.23	108.09
2	A	801	ACO	C4A-C5A-N7A	-3.16	106.97	110.58
2	C	801	ACO	O4B-C1B-N9A	3.13	114.09	108.09
2	C	801	ACO	C4A-C5A-N7A	-3.08	107.06	110.58
2	B	801	ACO	C4A-N9A-C8A	3.03	108.92	105.74
2	A	801	ACO	O4B-C1B-N9A	2.98	113.80	108.09
2	A	801	ACO	C2B-C1B-N9A	-2.95	105.98	113.30
2	D	801	ACO	C4A-N9A-C8A	2.92	108.81	105.74
2	B	801	ACO	C4A-C5A-N7A	-2.78	107.40	110.58
2	A	801	ACO	N9A-C8A-N7A	-2.72	110.08	113.94
2	C	801	ACO	CEP-CBP-CAP	2.71	113.39	108.77
2	B	801	ACO	C2A-N1A-C6A	2.59	122.99	118.73
2	A	801	ACO	C5A-N7A-C8A	2.58	107.51	103.45
2	B	801	ACO	O6A-CCP-CBP	-2.56	106.43	110.55
2	D	801	ACO	C4A-C5A-N7A	-2.49	107.74	110.58
2	C	801	ACO	C5A-N7A-C8A	2.48	107.35	103.45
2	B	801	ACO	O9A-P3B-O8A	2.38	116.73	107.80
2	A	801	ACO	C2A-N1A-C6A	2.37	122.62	118.73
2	A	801	ACO	C2P-C3P-N4P	2.36	117.33	112.41
2	A	801	ACO	C6A-C5A-N7A	2.28	136.49	132.09
2	D	801	ACO	C2A-N1A-C6A	2.26	122.45	118.73
2	B	801	ACO	C6A-C5A-N7A	2.26	136.45	132.09
2	D	801	ACO	C5A-N7A-C8A	2.22	106.94	103.45
2	B	801	ACO	CEP-CBP-CAP	2.21	112.54	108.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	801	ACO	N9A-C8A-N7A	-2.17	110.86	113.94
2	C	801	ACO	C2A-N1A-C6A	2.14	122.24	118.73
2	D	801	ACO	N9A-C8A-N7A	-2.13	110.91	113.94
2	A	801	ACO	C3P-N4P-C5P	2.07	126.68	122.82
2	D	801	ACO	N6A-C6A-N1A	2.04	122.93	118.38
2	B	801	ACO	C5A-N7A-C8A	2.01	106.61	103.45

There are no chirality outliers.

All (35) torsion outliers are listed below:

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	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	C5B-O5B-P1A-O3A
2	C	801	ACO	N8P-C9P-CAP-OAP
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	A	801	ACO	C2P-C3P-N4P-C5P
2	B	801	ACO	P2A-O3A-P1A-O1A
2	C	801	ACO	O9P-C9P-CAP-OAP
2	B	801	ACO	C3P-C2P-S1P-C
2	C	801	ACO	O4B-C4B-C5B-O5B
2	B	801	ACO	C5B-O5B-P1A-O1A
2	D	801	ACO	C5B-O5B-P1A-O1A
2	B	801	ACO	C3B-O3B-P3B-O9A
2	C	801	ACO	C2B-C3B-O3B-P3B
2	C	801	ACO	C4B-C3B-O3B-P3B
2	A	801	ACO	P2A-O3A-P1A-O2A
2	C	801	ACO	C3B-O3B-P3B-O8A
2	D	801	ACO	C3B-O3B-P3B-O8A
2	D	801	ACO	C4B-C3B-O3B-P3B

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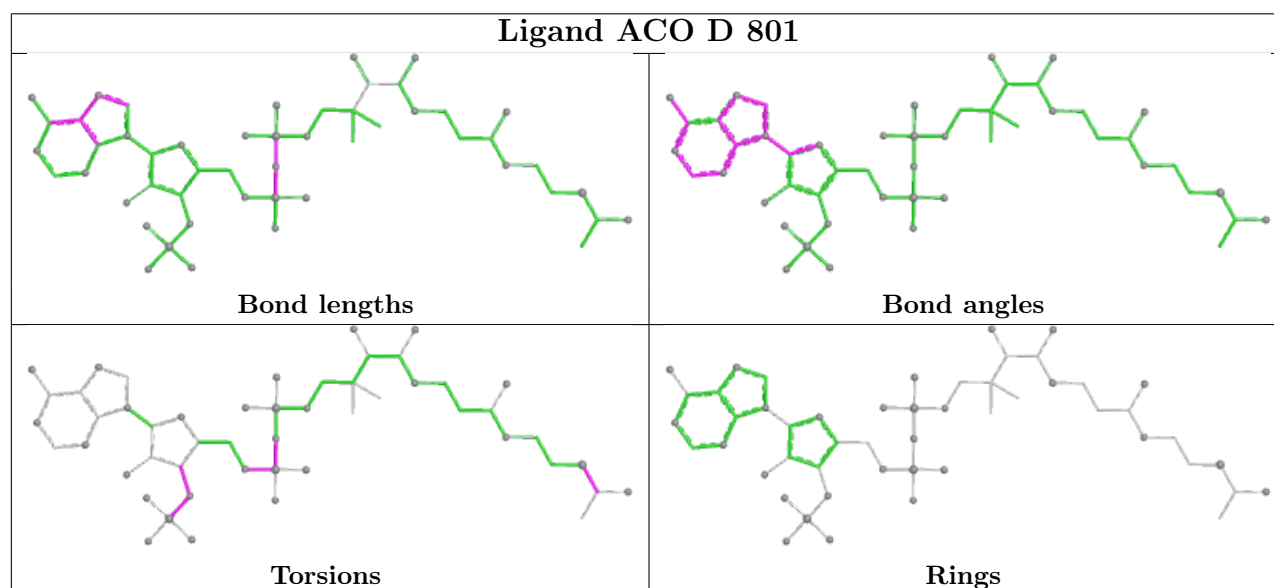
Mol	Chain	Res	Type	Atoms
2	C	801	ACO	C3B-C4B-C5B-O5B
2	D	801	ACO	C2B-C3B-O3B-P3B
2	B	801	ACO	P2A-O3A-P1A-O2A
2	D	801	ACO	P2A-O3A-P1A-O2A

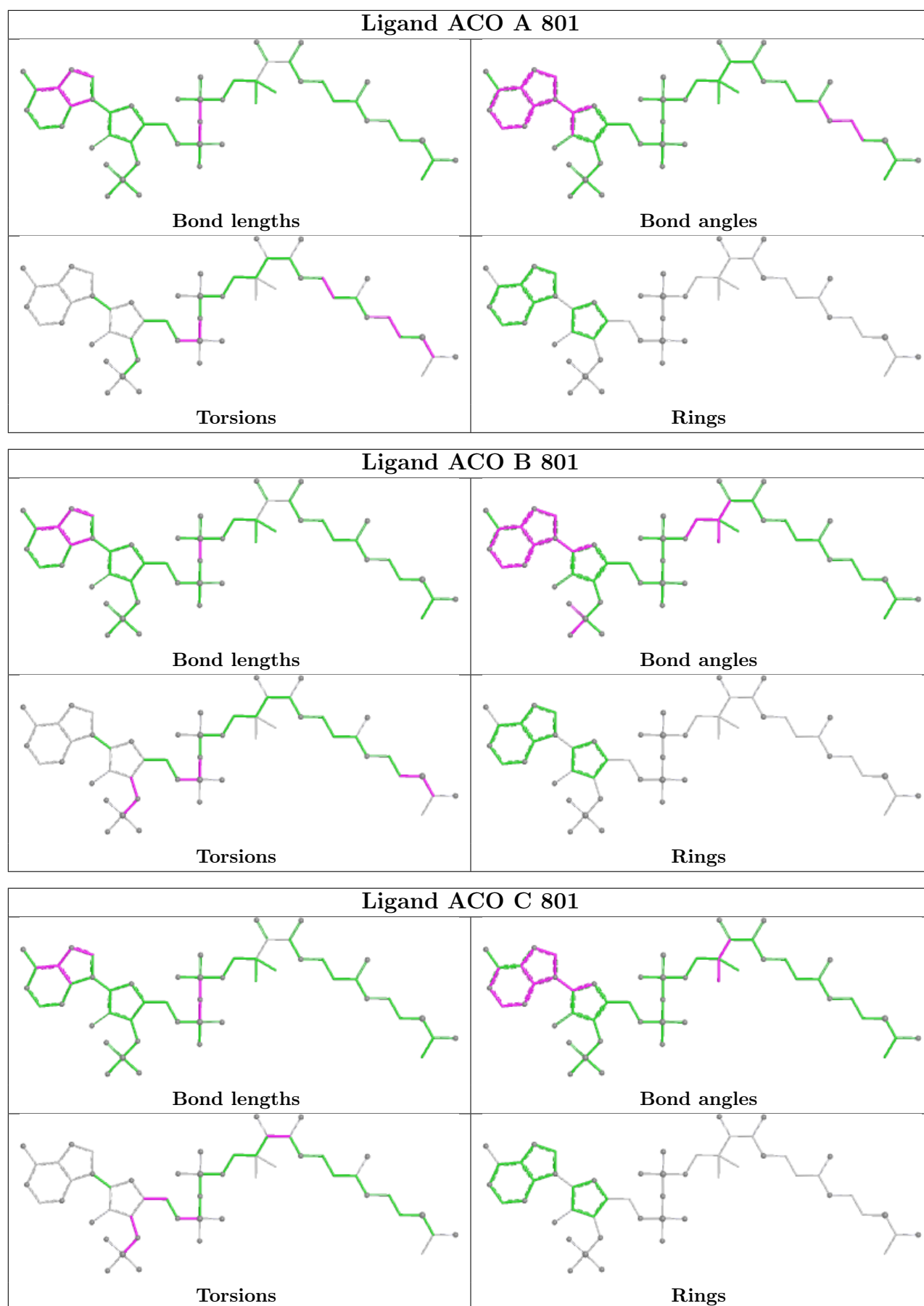
There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	801	ACO	6	0
2	A	801	ACO	2	0
2	B	801	ACO	4	0
2	C	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%)	0.24	18 (2%) 58 64	35, 59, 98, 134	0
1	B	729/786 (92%)	0.40	32 (4%) 39 45	37, 62, 104, 137	0
1	C	722/786 (91%)	0.36	36 (4%) 34 40	37, 60, 100, 130	0
1	D	730/786 (92%)	0.41	20 (2%) 56 63	41, 61, 104, 133	0
All	All	2900/3144 (92%)	0.35	106 (3%) 45 51	35, 61, 102, 137	0

All (106) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	216	GLY	6.8
1	B	219	GLY	6.2
1	B	216	GLY	5.8
1	A	216	GLY	5.4
1	D	216	GLY	5.2
1	C	279	LEU	4.4
1	C	219	GLY	4.0
1	D	392	ALA	4.0
1	B	602	VAL	4.0
1	D	219	GLY	3.9
1	A	732	GLN	3.9
1	B	382	GLY	3.8
1	C	417	ALA	3.8
1	A	602	VAL	3.8
1	D	381	PHE	3.7
1	C	764	LYS	3.7
1	D	602	VAL	3.6
1	C	215	CYS	3.4
1	C	366	ALA	3.4
1	A	392	ALA	3.3
1	A	416	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	762	ILE	3.2
1	D	732	GLN	3.1
1	B	393	PRO	3.1
1	B	392	ALA	3.1
1	B	588	THR	3.1
1	A	343	GLY	3.1
1	C	461	LYS	3.1
1	B	350	ILE	3.0
1	D	393	PRO	2.9
1	B	396	TRP	2.9
1	B	379	LEU	2.9
1	A	220	GLY	2.9
1	B	753	PRO	2.9
1	B	11	HIS	2.8
1	B	415	LEU	2.8
1	D	379	LEU	2.8
1	B	338	ALA	2.8
1	C	716	TYR	2.8
1	B	417	ALA	2.8
1	C	276	ALA	2.8
1	B	331	LEU	2.7
1	C	732	GLN	2.7
1	D	220	GLY	2.7
1	C	578	LEU	2.7
1	B	347	ILE	2.6
1	B	638	GLY	2.6
1	C	300	VAL	2.6
1	C	587	THR	2.6
1	D	376	ALA	2.6
1	D	166	PRO	2.6
1	B	622	TYR	2.6
1	A	624	LEU	2.5
1	B	715	LEU	2.5
1	D	400	ALA	2.5
1	A	393	PRO	2.5
1	C	602	VAL	2.5
1	C	415	LEU	2.5
1	C	420	PRO	2.5
1	D	378	VAL	2.5
1	C	350	ILE	2.5
1	C	682	GLU	2.5
1	C	405	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	280	ASP	2.4
1	C	351	PHE	2.4
1	C	399	PHE	2.4
1	D	11	HIS	2.4
1	A	586	ALA	2.4
1	B	637	ALA	2.4
1	B	381	PHE	2.4
1	C	724	HIS	2.4
1	C	367	GLY	2.4
1	A	310	ALA	2.3
1	C	375	VAL	2.3
1	C	737	ILE	2.3
1	C	378	VAL	2.3
1	A	400	ALA	2.3
1	A	587	THR	2.2
1	B	752	THR	2.2
1	D	588	THR	2.2
1	B	618	TRP	2.2
1	D	682	GLU	2.2
1	D	361	ALA	2.2
1	B	764	LYS	2.2
1	C	12	THR	2.2
1	C	740	ALA	2.2
1	D	766	ALA	2.2
1	C	618	TRP	2.2
1	C	301	LYS	2.2
1	B	655	ALA	2.2
1	B	298	LEU	2.1
1	A	406	HIS	2.1
1	A	724	HIS	2.1
1	A	346	SER	2.1
1	A	753	PRO	2.1
1	B	601	LEU	2.1
1	C	425	LEU	2.1
1	D	716	TYR	2.1
1	B	702	ALA	2.1
1	C	392	ALA	2.1
1	C	220	GLY	2.0
1	C	312	GLY	2.0
1	B	346	SER	2.0
1	B	179	ASP	2.0
1	B	624	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	D	342	ASP	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](#)

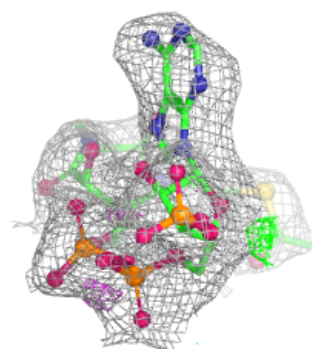
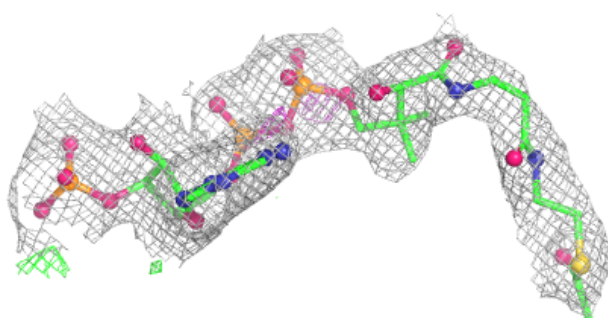
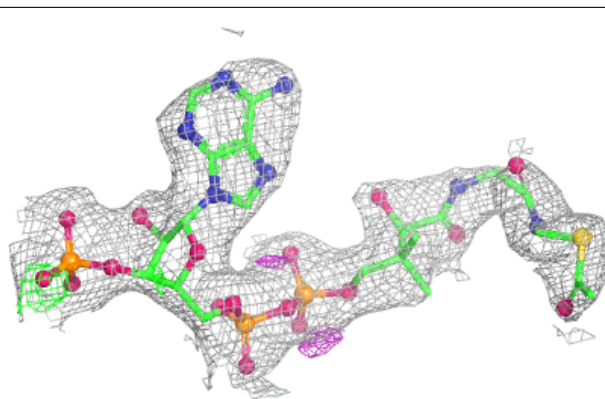
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	ACO	C	801	51/51	0.88	0.11	81,95,107,117	0
2	ACO	D	801	51/51	0.94	0.09	60,71,86,89	0
2	ACO	A	801	51/51	0.95	0.08	65,75,89,93	0
2	ACO	B	801	51/51	0.95	0.08	56,69,77,79	0
3	MG	B	802	1/1	0.96	0.21	30,30,30,30	0
3	MG	C	802	1/1	0.96	0.22	30,30,30,30	0
3	MG	D	802	1/1	0.98	0.16	30,30,30,30	0
3	MG	A	802	1/1	0.99	0.19	30,30,30,30	0

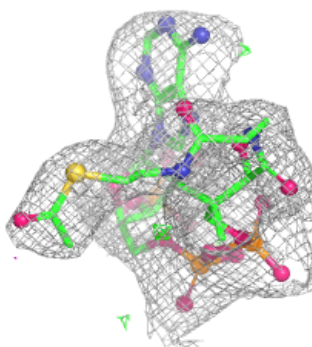
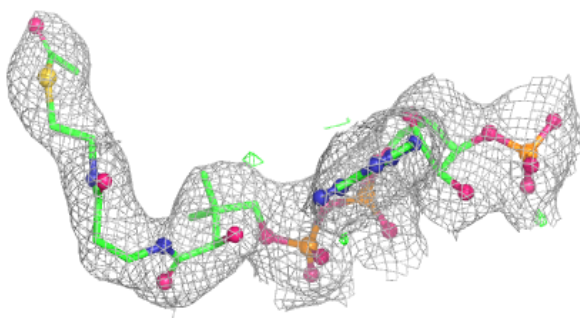
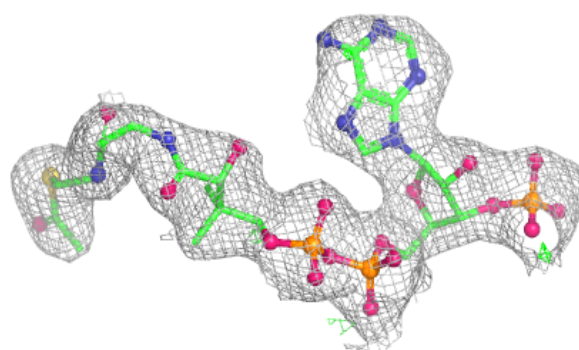
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around ACO C 801:

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

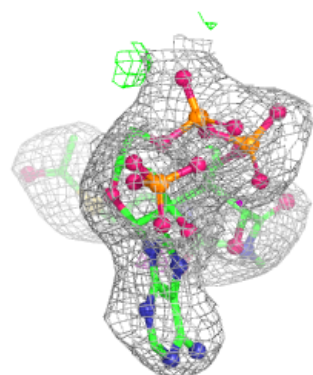
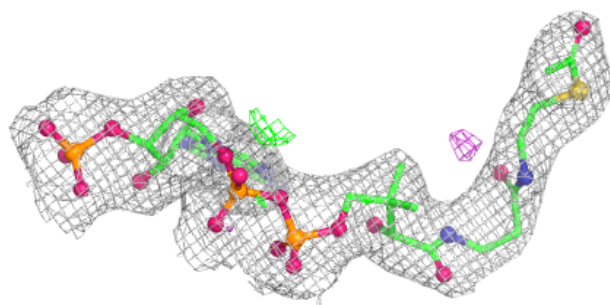
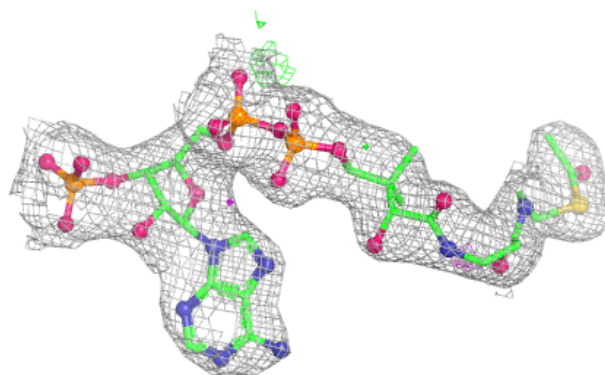
**Electron density around ACO D 801:**

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

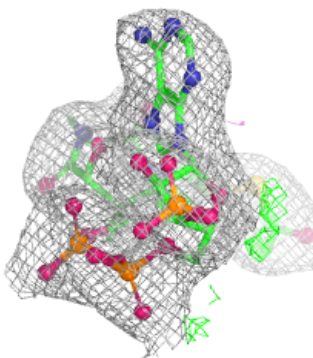
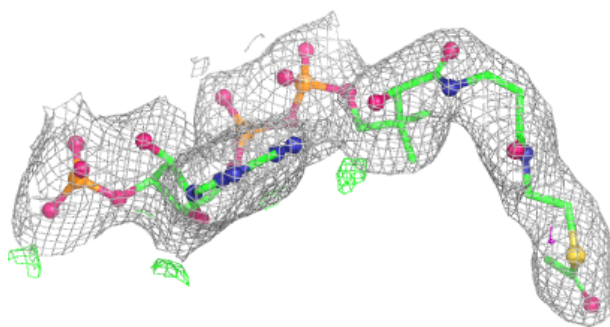
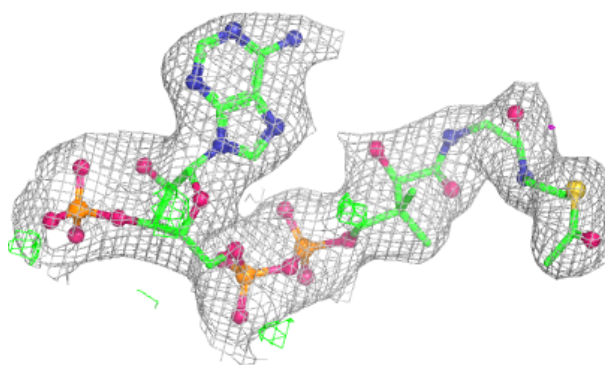


Electron density around ACO A 801:

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

**Electron density around ACO B 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.