Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2021 – 02:15 am GMT

PDB ID	:	6ZNU
Title	:	MaeB PTA domain E544R mutant
Authors	:	Lovering, A.L.; Harding, C.J.
Deposited on	:	2020-07-06
Resolution	:	2.33 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:

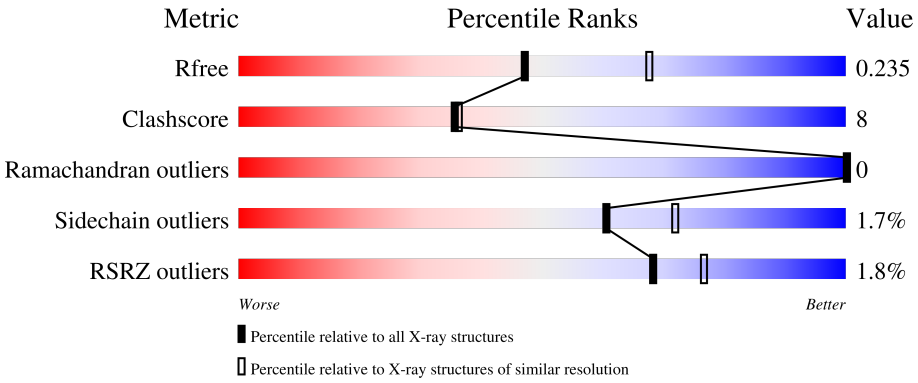
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.17.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.17.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

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 <=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	362	80% 11% 7%
1	B	362	4% 75% 15% 7%
1	C	362	2% 80% 13% 7%
1	D	362	76% 17% 7%
1	E	362	77% 15% 7%

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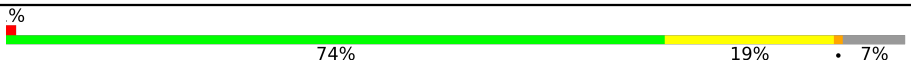
Mol	Chain	Length	Quality of chain
1	G	362	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15858 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 Malate dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	336	Total	C	N	O	S	0	0	0
			2585	1650	444	480	11			
1	G	337	Total	C	N	O	S	0	0	0
			2594	1656	446	481	11			
1	B	336	Total	C	N	O	S	0	0	0
			2585	1650	444	480	11			
1	C	337	Total	C	N	O	S	0	0	0
			2594	1656	446	481	11			
1	D	338	Total	C	N	O	S	0	0	0
			2594	1655	446	482	11			
1	E	337	Total	C	N	O	S	0	0	0
			2594	1656	446	481	11			

There are 126 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	419	MET	-	initiating methionine	UNP Q6MM15
A	420	GLY	-	expression tag	UNP Q6MM15
A	421	SER	-	expression tag	UNP Q6MM15
A	422	SER	-	expression tag	UNP Q6MM15
A	423	HIS	-	expression tag	UNP Q6MM15
A	424	HIS	-	expression tag	UNP Q6MM15
A	425	HIS	-	expression tag	UNP Q6MM15
A	426	HIS	-	expression tag	UNP Q6MM15
A	427	HIS	-	expression tag	UNP Q6MM15
A	428	HIS	-	expression tag	UNP Q6MM15
A	429	SER	-	expression tag	UNP Q6MM15
A	430	SER	-	expression tag	UNP Q6MM15
A	431	GLY	-	expression tag	UNP Q6MM15
A	432	LEU	-	expression tag	UNP Q6MM15
A	433	VAL	-	expression tag	UNP Q6MM15
A	434	PRO	-	expression tag	UNP Q6MM15
A	435	ALA	-	expression tag	UNP Q6MM15

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Chain	Residue	Modelled	Actual	Comment	Reference
A	436	GLY	-	expression tag	UNP Q6MM15
A	437	SER	-	expression tag	UNP Q6MM15
A	438	HIS	-	expression tag	UNP Q6MM15
A	544	ARG	GLU	engineered mutation	UNP Q6MM15
G	419	MET	-	initiating methionine	UNP Q6MM15
G	420	GLY	-	expression tag	UNP Q6MM15
G	421	SER	-	expression tag	UNP Q6MM15
G	422	SER	-	expression tag	UNP Q6MM15
G	423	HIS	-	expression tag	UNP Q6MM15
G	424	HIS	-	expression tag	UNP Q6MM15
G	425	HIS	-	expression tag	UNP Q6MM15
G	426	HIS	-	expression tag	UNP Q6MM15
G	427	HIS	-	expression tag	UNP Q6MM15
G	428	HIS	-	expression tag	UNP Q6MM15
G	429	SER	-	expression tag	UNP Q6MM15
G	430	SER	-	expression tag	UNP Q6MM15
G	431	GLY	-	expression tag	UNP Q6MM15
G	432	LEU	-	expression tag	UNP Q6MM15
G	433	VAL	-	expression tag	UNP Q6MM15
G	434	PRO	-	expression tag	UNP Q6MM15
G	435	ALA	-	expression tag	UNP Q6MM15
G	436	GLY	-	expression tag	UNP Q6MM15
G	437	SER	-	expression tag	UNP Q6MM15
G	438	HIS	-	expression tag	UNP Q6MM15
G	544	ARG	GLU	engineered mutation	UNP Q6MM15
B	419	MET	-	initiating methionine	UNP Q6MM15
B	420	GLY	-	expression tag	UNP Q6MM15
B	421	SER	-	expression tag	UNP Q6MM15
B	422	SER	-	expression tag	UNP Q6MM15
B	423	HIS	-	expression tag	UNP Q6MM15
B	424	HIS	-	expression tag	UNP Q6MM15
B	425	HIS	-	expression tag	UNP Q6MM15
B	426	HIS	-	expression tag	UNP Q6MM15
B	427	HIS	-	expression tag	UNP Q6MM15
B	428	HIS	-	expression tag	UNP Q6MM15
B	429	SER	-	expression tag	UNP Q6MM15
B	430	SER	-	expression tag	UNP Q6MM15
B	431	GLY	-	expression tag	UNP Q6MM15
B	432	LEU	-	expression tag	UNP Q6MM15
B	433	VAL	-	expression tag	UNP Q6MM15
B	434	PRO	-	expression tag	UNP Q6MM15
B	435	ALA	-	expression tag	UNP Q6MM15

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Chain	Residue	Modelled	Actual	Comment	Reference
B	436	GLY	-	expression tag	UNP Q6MM15
B	437	SER	-	expression tag	UNP Q6MM15
B	438	HIS	-	expression tag	UNP Q6MM15
B	544	ARG	GLU	engineered mutation	UNP Q6MM15
C	419	MET	-	initiating methionine	UNP Q6MM15
C	420	GLY	-	expression tag	UNP Q6MM15
C	421	SER	-	expression tag	UNP Q6MM15
C	422	SER	-	expression tag	UNP Q6MM15
C	423	HIS	-	expression tag	UNP Q6MM15
C	424	HIS	-	expression tag	UNP Q6MM15
C	425	HIS	-	expression tag	UNP Q6MM15
C	426	HIS	-	expression tag	UNP Q6MM15
C	427	HIS	-	expression tag	UNP Q6MM15
C	428	HIS	-	expression tag	UNP Q6MM15
C	429	SER	-	expression tag	UNP Q6MM15
C	430	SER	-	expression tag	UNP Q6MM15
C	431	GLY	-	expression tag	UNP Q6MM15
C	432	LEU	-	expression tag	UNP Q6MM15
C	433	VAL	-	expression tag	UNP Q6MM15
C	434	PRO	-	expression tag	UNP Q6MM15
C	435	ALA	-	expression tag	UNP Q6MM15
C	436	GLY	-	expression tag	UNP Q6MM15
C	437	SER	-	expression tag	UNP Q6MM15
C	438	HIS	-	expression tag	UNP Q6MM15
C	544	ARG	GLU	engineered mutation	UNP Q6MM15
D	419	MET	-	initiating methionine	UNP Q6MM15
D	420	GLY	-	expression tag	UNP Q6MM15
D	421	SER	-	expression tag	UNP Q6MM15
D	422	SER	-	expression tag	UNP Q6MM15
D	423	HIS	-	expression tag	UNP Q6MM15
D	424	HIS	-	expression tag	UNP Q6MM15
D	425	HIS	-	expression tag	UNP Q6MM15
D	426	HIS	-	expression tag	UNP Q6MM15
D	427	HIS	-	expression tag	UNP Q6MM15
D	428	HIS	-	expression tag	UNP Q6MM15
D	429	SER	-	expression tag	UNP Q6MM15
D	430	SER	-	expression tag	UNP Q6MM15
D	431	GLY	-	expression tag	UNP Q6MM15
D	432	LEU	-	expression tag	UNP Q6MM15
D	433	VAL	-	expression tag	UNP Q6MM15
D	434	PRO	-	expression tag	UNP Q6MM15
D	435	ALA	-	expression tag	UNP Q6MM15

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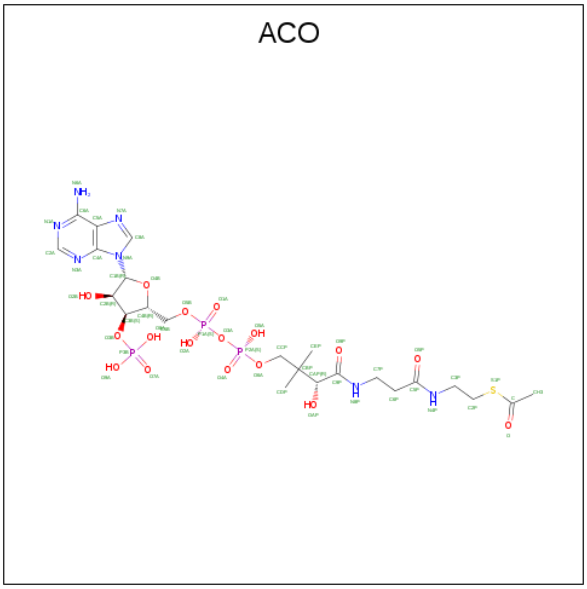
Chain	Residue	Modelled	Actual	Comment	Reference
D	436	GLY	-	expression tag	UNP Q6MM15
D	437	SER	-	expression tag	UNP Q6MM15
D	438	HIS	-	expression tag	UNP Q6MM15
D	544	ARG	GLU	engineered mutation	UNP Q6MM15
E	419	MET	-	initiating methionine	UNP Q6MM15
E	420	GLY	-	expression tag	UNP Q6MM15
E	421	SER	-	expression tag	UNP Q6MM15
E	422	SER	-	expression tag	UNP Q6MM15
E	423	HIS	-	expression tag	UNP Q6MM15
E	424	HIS	-	expression tag	UNP Q6MM15
E	425	HIS	-	expression tag	UNP Q6MM15
E	426	HIS	-	expression tag	UNP Q6MM15
E	427	HIS	-	expression tag	UNP Q6MM15
E	428	HIS	-	expression tag	UNP Q6MM15
E	429	SER	-	expression tag	UNP Q6MM15
E	430	SER	-	expression tag	UNP Q6MM15
E	431	GLY	-	expression tag	UNP Q6MM15
E	432	LEU	-	expression tag	UNP Q6MM15
E	433	VAL	-	expression tag	UNP Q6MM15
E	434	PRO	-	expression tag	UNP Q6MM15
E	435	ALA	-	expression tag	UNP Q6MM15
E	436	GLY	-	expression tag	UNP Q6MM15
E	437	SER	-	expression tag	UNP Q6MM15
E	438	HIS	-	expression tag	UNP Q6MM15
E	544	ARG	GLU	engineered mutation	UNP Q6MM15

- Molecule 2 is ACETYL COENZYME *A (three-letter code: 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	G	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		
2	D	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

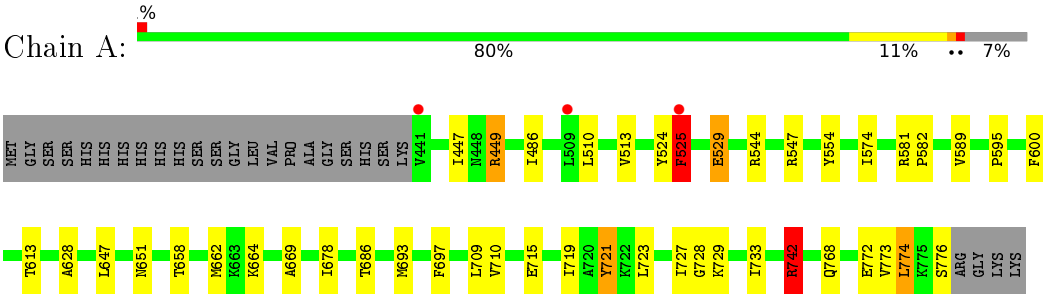
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Cl	0	0
			2	2		
3	B	1	Total	Cl	0	0
			1	1		
3	C	1	Total	Cl	0	0
			1	1		
3	D	1	Total	Cl	0	0
			1	1		
3	E	1	Total	Cl	0	0
			1	1		

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.

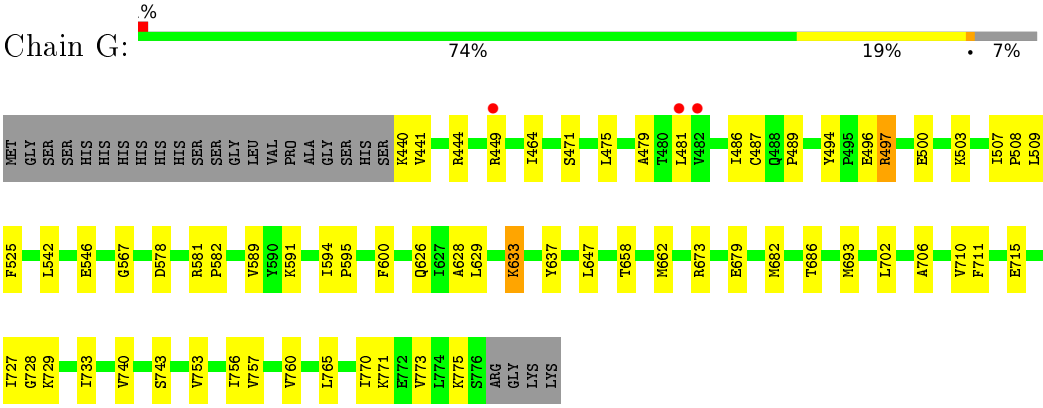
- Molecule 1: Malate dehydrogenase

Chain A:



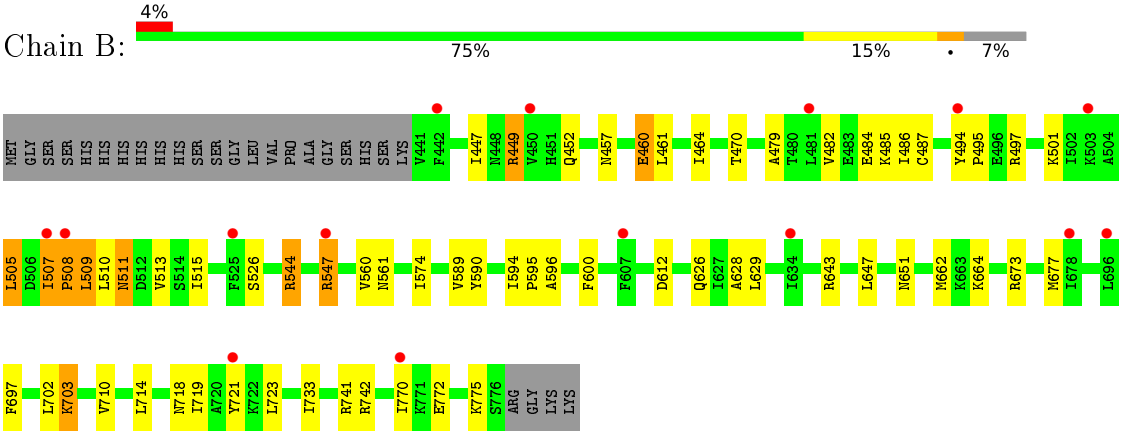
- Molecule 1: Malate dehydrogenase

Chain G:



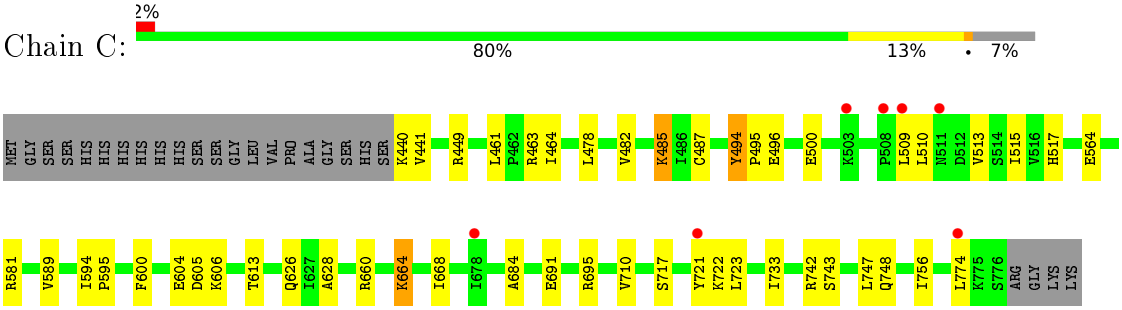
- Molecule 1: Malate dehydrogenase

Chain B:



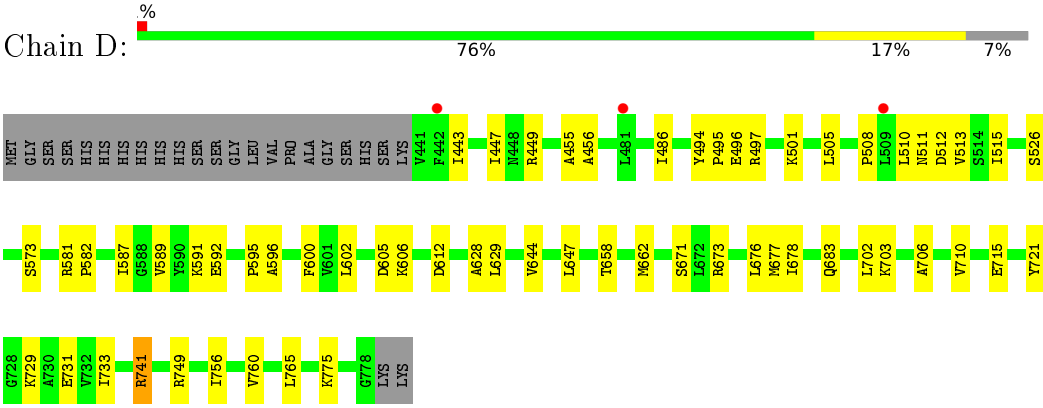
• Molecule 1: Malate dehydrogenase

Chain C:



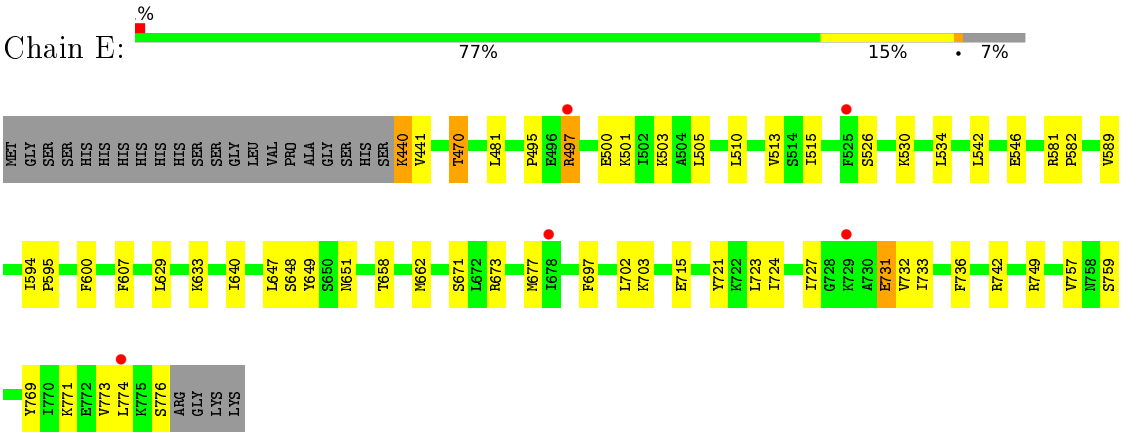
• Molecule 1: Malate dehydrogenase

Chain D:



• Molecule 1: Malate dehydrogenase

Chain E:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	129.09Å 182.85Å 119.66Å 90.00° 117.69° 90.00°	Depositor
Resolution (Å)	56.86 – 2.33 69.22 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.7 (56.86-2.33) 99.7 (69.22-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.62 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.196 , 0.236 0.195 , 0.235	Depositor DCC
R_{free} test set	5234 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	49.7	Xtriage
Anisotropy	0.558	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 36.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.51$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15858	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.00% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ACO, CL

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	0.46	0/2629	0.76	7/3559 (0.2%)
1	B	0.46	0/2629	0.79	10/3559 (0.3%)
1	C	0.53	3/2638 (0.1%)	0.70	2/3570 (0.1%)
1	D	0.46	0/2638	0.68	5/3571 (0.1%)
1	E	0.49	0/2638	0.72	3/3570 (0.1%)
1	G	0.52	0/2638	0.72	4/3570 (0.1%)
All	All	0.49	3/15810 (0.0%)	0.73	31/21399 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	D	0	2
All	All	0	3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	485	LYS	CD-CE	6.90	1.68	1.51
1	C	494	TYR	CD2-CE2	-5.99	1.30	1.39
1	C	485	LYS	CE-NZ	5.48	1.62	1.49

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	547	ARG	NE-CZ-NH1	-14.06	113.27	120.30
1	A	742	ARG	NE-CZ-NH1	-10.08	115.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	703	LYS	CD-CE-NZ	-9.58	89.66	111.70
1	G	497	ARG	CB-CG-CD	8.83	134.55	111.60
1	G	497	ARG	CA-CB-CG	8.57	132.26	113.40
1	A	729	LYS	CD-CE-NZ	-8.55	92.02	111.70
1	D	512	ASP	CB-CG-OD2	-8.40	110.74	118.30
1	D	606	LYS	CD-CE-NZ	-8.08	93.12	111.70
1	A	529	GLU	CA-CB-CG	-7.50	96.90	113.40
1	D	512	ASP	CB-CG-OD1	6.91	124.52	118.30
1	A	605	ASP	CB-CG-OD2	-6.86	112.12	118.30
1	G	512	ASP	CB-CG-OD2	-6.42	112.52	118.30
1	B	460	GLU	C-N-CA	-6.39	105.72	121.70
1	E	470	THR	CA-CB-CG2	-6.34	103.52	112.40
1	A	449	ARG	NE-CZ-NH2	-6.03	117.29	120.30
1	A	774	LEU	CA-CB-CG	-6.00	101.50	115.30
1	E	497	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	B	741	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	E	731	GLU	CA-CB-CG	-5.79	100.67	113.40
1	C	604	GLU	CB-CA-C	5.72	121.85	110.40
1	B	460	GLU	CB-CA-C	-5.70	98.99	110.40
1	B	547	ARG	CB-CG-CD	5.60	126.15	111.60
1	G	525	PHE	CB-CG-CD2	-5.53	116.93	120.80
1	B	508	PRO	N-CA-CB	-5.38	96.69	102.60
1	B	703	LYS	CB-CG-CD	5.36	125.53	111.60
1	D	449	ARG	CB-CG-CD	-5.34	97.70	111.60
1	B	547	ARG	CD-NE-CZ	-5.16	116.38	123.60
1	B	544	ARG	CG-CD-NE	5.15	122.62	111.80
1	C	604	GLU	CA-CB-CG	5.14	124.72	113.40
1	A	525	PHE	N-CA-CB	-5.07	101.47	110.60
1	D	741	ARG	CA-CB-CG	5.03	124.46	113.40

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	525	PHE	Sidechain
1	D	496	GLU	Sidechain
1	D	605	ASP	Peptide

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	2585	0	2664	34	0
1	B	2585	0	2664	67	0
1	C	2594	0	2677	38	0
1	D	2594	0	2669	40	0
1	E	2594	0	2677	42	0
1	G	2594	0	2677	44	0
2	A	51	0	34	2	0
2	B	51	0	34	2	0
2	C	51	0	34	3	0
2	D	51	0	34	1	0
2	E	51	0	34	3	0
2	G	51	0	34	3	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
All	All	15858	0	16232	259	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 8.

All (259) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:801:ACO:O4B	2:G:801:ACO:C1B	1.64	1.27
2:A:801:ACO:O4B	2:A:801:ACO:C1B	1.64	1.23
2:E:801:ACO:O4B	2:E:801:ACO:C1B	1.64	1.21
2:D:801:ACO:O4B	2:D:801:ACO:C1B	1.64	1.19
2:B:801:ACO:O4B	2:B:801:ACO:C1B	1.64	1.18
1:C:463:ARG:NH2	1:C:564:GLU:O	1.80	1.15
2:C:801:ACO:O4B	2:C:801:ACO:C1B	1.64	1.10
1:B:482:VAL:HG11	1:B:509:LEU:HB3	1.45	0.99
1:B:544:ARG:HA	1:B:547:ARG:HD2	1.57	0.85
1:B:485:LYS:HA	1:B:485:LYS:CE	2.08	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:463:ARG:NH2	1:C:564:GLU:C	2.34	0.81
1:B:485:LYS:HA	1:B:485:LYS:HE3	1.65	0.78
1:E:742:ARG:HH12	1:E:774:LEU:HD11	1.49	0.76
1:B:461:LEU:HD11	1:B:485:LYS:HE3	1.67	0.75
1:D:600:PHE:HB2	1:D:733:ILE:HG12	1.71	0.73
1:B:677:MET:CE	1:B:703:LYS:H	2.02	0.73
1:E:600:PHE:HB2	1:E:733:ILE:HG12	1.71	0.72
1:C:613:THR:HB	1:C:721:TYR:CE2	2.26	0.71
1:D:677:MET:CE	1:D:703:LYS:H	2.04	0.71
1:B:505:LEU:HD12	1:B:507:ILE:HD11	1.71	0.71
1:D:494:TYR:H	1:D:497:ARG:HH21	1.39	0.70
1:B:505:LEU:HB2	1:B:507:ILE:HD11	1.73	0.70
1:B:600:PHE:HB2	1:B:733:ILE:HG12	1.74	0.70
1:B:505:LEU:CD1	1:B:507:ILE:HD11	2.21	0.70
1:C:600:PHE:HB2	1:C:733:ILE:HG12	1.74	0.70
1:G:481:LEU:HD11	1:G:757:VAL:HA	1.74	0.69
1:B:560:VAL:O	1:B:742:ARG:NH1	2.26	0.68
1:C:589:VAL:HG11	1:C:595:PRO:HD3	1.75	0.68
1:A:600:PHE:HB2	1:A:733:ILE:HG12	1.76	0.68
1:B:544:ARG:HD3	1:B:547:ARG:HD2	1.76	0.68
1:E:773:VAL:O	1:E:776:SER:OG	2.11	0.68
1:B:561:ASN:O	1:B:742:ARG:NH1	2.26	0.67
1:C:461:LEU:HD11	1:C:485:LYS:HD3	1.77	0.67
1:G:440:LYS:HG3	1:G:441:VAL:H	1.60	0.67
1:E:500:GLU:HA	1:E:503:LYS:HG2	1.77	0.67
1:E:607:PHE:CE2	1:E:640:ILE:HD13	2.31	0.66
1:A:574:ILE:HG21	1:B:547:ARG:HH12	1.60	0.65
1:C:478:LEU:O	1:C:482:VAL:HG23	1.97	0.65
1:E:530:LYS:HZ3	1:E:534:LEU:HD21	1.61	0.65
1:E:607:PHE:CZ	1:E:640:ILE:HD13	2.31	0.65
1:D:677:MET:HE3	1:D:703:LYS:H	1.62	0.64
1:B:544:ARG:CD	1:B:547:ARG:HD2	2.27	0.63
1:E:440:LYS:HG2	1:E:441:VAL:H	1.62	0.63
1:E:530:LYS:NZ	1:E:534:LEU:HD11	2.14	0.62
1:E:677:MET:HE3	1:E:703:LYS:H	1.64	0.62
1:C:664:LYS:O	1:C:664:LYS:HG3	1.99	0.62
1:E:742:ARG:NH1	1:E:774:LEU:HD11	2.16	0.61
1:G:723:LEU:O	1:G:727:ILE:HG12	2.00	0.60
1:B:457:ASN:HD21	1:B:775:LYS:NZ	1.98	0.60
1:B:501:LYS:HE2	1:B:505:LEU:HD21	1.83	0.60
1:B:461:LEU:CD1	1:B:485:LYS:HE3	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:613:THR:HB	1:C:721:TYR:CD2	2.36	0.60
1:G:629:LEU:O	1:G:633:LYS:HD2	2.02	0.59
1:B:482:VAL:CG1	1:B:509:LEU:HB3	2.28	0.59
1:E:481:LEU:HD21	1:E:757:VAL:HA	1.83	0.59
1:D:587:ILE:O	1:D:741:ARG:CZ	2.50	0.59
1:D:591:LYS:HE2	1:D:592:GLU:OE2	2.03	0.59
1:B:677:MET:HE2	1:B:703:LYS:H	1.66	0.59
1:A:449:ARG:O	1:A:449:ARG:HG2	2.03	0.59
1:G:647:LEU:O	1:G:662:MET:HG3	2.03	0.59
1:E:677:MET:CE	1:E:703:LYS:H	2.15	0.59
1:B:505:LEU:HD12	1:B:507:ILE:CD1	2.33	0.58
1:B:501:LYS:O	1:B:505:LEU:HG	2.03	0.58
1:E:497:ARG:HA	1:E:500:GLU:HB3	1.86	0.58
1:B:643:ARG:HB3	1:B:702:LEU:HD11	1.85	0.57
1:C:496:GLU:O	1:C:500:GLU:HB2	2.03	0.57
1:C:605:ASP:OD1	1:C:606:LYS:HD3	2.04	0.57
1:B:447:ILE:HG23	1:B:486:ILE:HD11	1.87	0.57
1:C:581:ARG:HG3	2:C:801:ACO:O2A	2.05	0.57
2:A:801:ACO:H8A	2:A:801:ACO:H52A	1.87	0.56
1:G:600:PHE:HB2	1:G:733:ILE:HG12	1.87	0.56
1:A:589:VAL:HG11	1:A:595:PRO:HD3	1.87	0.56
1:A:742:ARG:HH12	1:A:774:LEU:CD1	2.18	0.56
1:E:731:GLU:HG3	1:E:732:VAL:N	2.21	0.56
1:E:647:LEU:O	1:E:662:MET:HG3	2.06	0.56
1:B:544:ARG:HA	1:B:547:ARG:CD	2.30	0.56
1:A:719:ILE:HG21	1:G:711:PHE:HE2	1.71	0.56
1:C:495:PRO:HD3	1:C:517:HIS:HB2	1.88	0.56
1:A:628:ALA:HB2	1:A:710:VAL:HG21	1.88	0.55
1:D:647:LEU:O	1:D:662:MET:HG3	2.06	0.55
1:A:719:ILE:HG21	1:G:711:PHE:CE2	2.42	0.55
1:E:497:ARG:O	1:E:501:LYS:N	2.35	0.55
1:G:479:ALA:HB2	1:G:507:ILE:HG12	1.88	0.54
1:G:756:ILE:O	1:G:760:VAL:HG23	2.08	0.54
1:G:494:TYR:HB2	1:G:497:ARG:HG2	1.90	0.54
1:B:647:LEU:O	1:B:662:MET:HG3	2.08	0.54
1:E:542:LEU:O	1:E:546:GLU:HG3	2.07	0.54
1:A:742:ARG:HH12	1:A:774:LEU:HD11	1.72	0.53
1:A:715:GLU:OE2	1:G:658:THR:HG21	2.09	0.53
1:E:495:PRO:HA	1:E:515:ILE:HG21	1.90	0.53
1:E:769:TYR:O	1:E:773:VAL:HG23	2.07	0.53
1:B:714:LEU:HD21	2:B:801:ACO:H32	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:561:ASN:C	1:B:742:ARG:HH12	2.12	0.53
1:E:589:VAL:HG11	1:E:595:PRO:HD3	1.90	0.53
1:D:702:LEU:HD21	1:D:706:ALA:HB2	1.90	0.53
1:D:510:LEU:O	1:D:513:VAL:HG12	2.09	0.53
1:E:651:ASN:HB3	1:E:697:PHE:CZ	2.43	0.53
1:C:605:ASP:OD1	1:C:606:LYS:CD	2.57	0.52
1:D:443:ILE:HD11	1:D:731:GLU:OE2	2.09	0.52
1:A:723:LEU:O	1:A:727:ILE:HG12	2.10	0.52
1:G:729:LYS:H	1:G:729:LYS:HE2	1.74	0.52
1:C:495:PRO:HA	1:C:515:ILE:HG21	1.92	0.52
1:C:721:TYR:CE1	1:C:722:LYS:HG3	2.45	0.51
1:A:658:THR:HG21	1:G:715:GLU:OE2	2.10	0.51
1:B:461:LEU:HD11	1:B:485:LYS:CE	2.38	0.51
1:D:495:PRO:HA	1:D:515:ILE:HG21	1.92	0.51
1:E:677:MET:HE3	1:E:702:LEU:HA	1.91	0.51
1:G:702:LEU:HD21	1:G:706:ALA:HB2	1.93	0.51
1:A:613:THR:HB	1:A:721:TYR:CE2	2.46	0.51
1:C:747:LEU:HD13	1:C:756:ILE:HG12	1.92	0.51
1:D:508:PRO:HA	1:D:511:ASN:HD21	1.76	0.51
1:B:511:ASN:HD22	1:B:511:ASN:H	1.59	0.51
1:C:509:LEU:HD12	1:C:509:LEU:H	1.76	0.51
1:E:629:LEU:O	1:E:633:LYS:HG3	2.11	0.51
1:B:511:ASN:N	1:B:511:ASN:ND2	2.59	0.50
1:B:511:ASN:HD22	1:B:511:ASN:N	2.09	0.50
1:D:508:PRO:HA	1:D:511:ASN:ND2	2.26	0.50
1:D:715:GLU:OE2	1:E:658:THR:HG21	2.12	0.50
1:E:530:LYS:HZ3	1:E:534:LEU:HD11	1.75	0.50
1:A:529:GLU:O	1:A:529:GLU:HG3	2.11	0.50
1:B:501:LYS:CE	1:B:505:LEU:HD21	2.42	0.50
1:C:464:ILE:HG12	1:C:487:CYS:HB2	1.94	0.50
1:D:703:LYS:HE3	1:D:703:LYS:HA	1.94	0.50
1:A:647:LEU:O	1:A:662:MET:HG3	2.11	0.50
1:G:464:ILE:HG12	1:G:487:CYS:HB2	1.94	0.50
1:C:605:ASP:OD1	1:C:606:LYS:CG	2.60	0.50
1:D:573:SER:HA	1:D:749:ARG:NH1	2.27	0.50
1:D:602:LEU:HD12	1:D:731:GLU:HB3	1.93	0.50
1:G:449:ARG:HG2	1:G:765:LEU:HD21	1.93	0.49
1:A:574:ILE:CG2	1:B:547:ARG:HH12	2.25	0.49
1:E:594:ILE:HG13	2:E:801:ACO:N6A	2.28	0.49
1:A:773:VAL:O	1:A:776:SER:OG	2.19	0.49
1:B:742:ARG:HA	1:B:770:ILE:HD13	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:495:PRO:HA	1:B:515:ILE:HG21	1.95	0.49
1:D:447:ILE:HG23	1:D:486:ILE:HD11	1.95	0.49
1:D:589:VAL:HG11	1:D:595:PRO:HD3	1.94	0.49
1:B:561:ASN:C	1:B:742:ARG:NH1	2.66	0.48
1:D:591:LYS:HG3	1:D:592:GLU:HG2	1.94	0.48
1:D:587:ILE:O	1:D:741:ARG:NH1	2.46	0.48
1:G:542:LEU:O	1:G:546:GLU:HG3	2.13	0.48
1:G:581:ARG:HB3	1:G:582:PRO:HD3	1.95	0.48
1:G:589:VAL:HG11	1:G:595:PRO:HD3	1.94	0.48
1:A:544:ARG:HA	1:A:547:ARG:HG2	1.95	0.48
1:E:440:LYS:HG2	1:E:441:VAL:N	2.29	0.48
1:G:578:ASP:OD2	1:D:544:ARG:NH1	2.47	0.48
1:B:505:LEU:HB2	1:B:507:ILE:CD1	2.42	0.48
1:C:742:ARG:CZ	1:C:774:LEU:HD11	2.44	0.48
1:G:770:ILE:O	1:G:773:VAL:HG12	2.14	0.47
1:B:629:LEU:HD22	1:B:673:ARG:HG3	1.95	0.47
1:G:496:GLU:OE1	1:G:496:GLU:N	2.47	0.47
1:B:460:GLU:O	1:B:461:LEU:HD23	2.14	0.47
1:G:503:LYS:NZ	1:G:508:PRO:HA	2.30	0.47
1:B:509:LEU:HD12	1:B:509:LEU:HA	1.78	0.47
1:C:594:ILE:HG22	1:C:626:GLN:HG3	1.97	0.47
1:C:748:GLN:HB3	2:C:801:ACO:HH31	1.97	0.47
1:B:494:TYR:HB2	1:B:497:ARG:HE	1.80	0.47
1:B:505:LEU:HD12	1:B:507:ILE:CG1	2.45	0.46
1:B:457:ASN:HD21	1:B:775:LYS:HZ3	1.62	0.46
1:E:510:LEU:O	1:E:513:VAL:HG12	2.15	0.46
1:A:547:ARG:HH12	1:B:574:ILE:HG22	1.80	0.46
1:C:664:LYS:HD2	1:C:668:ILE:HG13	1.98	0.46
1:G:494:TYR:HD1	1:G:497:ARG:HH11	1.63	0.46
1:G:496:GLU:O	1:G:500:GLU:HG2	2.16	0.46
1:C:494:TYR:HD2	1:C:496:GLU:H	1.63	0.46
1:E:723:LEU:O	1:E:727:ILE:HG12	2.15	0.46
1:E:731:GLU:HG3	1:E:732:VAL:H	1.80	0.46
1:A:524:TYR:HD2	1:A:525:PHE:CD1	2.34	0.46
1:D:455:ALA:O	1:D:456:ALA:HB3	2.15	0.46
1:D:596:ALA:HB1	1:D:612:ASP:HB2	1.98	0.46
1:E:736:PHE:HE1	1:E:759:SER:HA	1.81	0.45
1:B:510:LEU:HA	1:B:513:VAL:HG13	1.98	0.45
1:C:510:LEU:O	1:C:513:VAL:HG12	2.16	0.45
1:G:753:VAL:O	1:G:757:VAL:HG23	2.16	0.45
1:A:664:LYS:O	1:A:664:LYS:HG3	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:718:ASN:HA	1:B:721:TYR:CE2	2.51	0.45
1:G:628:ALA:HB2	1:G:710:VAL:HG21	1.98	0.45
1:C:660:ARG:HG3	1:C:660:ARG:HH11	1.82	0.45
1:D:628:ALA:HB2	1:D:710:VAL:HG21	1.99	0.45
1:E:629:LEU:HD22	1:E:673:ARG:HG3	2.00	0.44
1:E:648:SER:OG	1:E:649:TYR:N	2.49	0.44
1:A:686:THR:HG22	1:A:693:MET:HE1	1.99	0.44
1:B:589:VAL:HG21	1:B:595:PRO:HD3	1.99	0.44
1:B:485:LYS:HE3	1:B:485:LYS:CA	2.34	0.44
1:B:544:ARG:HD2	1:B:547:ARG:HD2	1.99	0.44
1:B:461:LEU:CD1	1:B:485:LYS:CE	2.95	0.44
1:B:479:ALA:O	1:B:482:VAL:HG12	2.17	0.44
1:B:547:ARG:H	1:B:547:ARG:HG2	1.39	0.44
1:A:669:ALA:HB1	1:A:678:ILE:HD13	2.00	0.44
1:B:589:VAL:HG12	1:B:590:TYR:O	2.17	0.44
1:C:691:GLU:OE1	1:C:695:ARG:NH1	2.50	0.44
1:B:447:ILE:HD13	1:B:484:GLU:HG2	2.00	0.44
1:G:771:LYS:O	1:G:775:LYS:HG2	2.18	0.44
1:B:494:TYR:H	1:B:497:ARG:NH2	2.14	0.44
1:G:489:PRO:HB2	1:G:513:VAL:HG21	2.00	0.43
1:G:729:LYS:HE2	1:G:729:LYS:N	2.32	0.43
1:A:510:LEU:O	1:A:513:VAL:HG12	2.18	0.43
1:A:651:ASN:HB3	1:A:697:PHE:CZ	2.54	0.43
1:C:463:ARG:CZ	1:C:564:GLU:O	2.60	0.43
1:C:605:ASP:OD1	1:C:606:LYS:HG2	2.18	0.43
1:G:686:THR:HG22	1:G:693:MET:HE1	1.98	0.43
1:C:463:ARG:HH21	1:C:564:GLU:C	2.19	0.43
1:D:724:ILE:HD13	1:E:727:ILE:HD11	2.01	0.43
1:D:775:LYS:HB2	1:D:775:LYS:HE2	1.72	0.43
1:A:581:ARG:HB3	1:A:582:PRO:HD3	2.01	0.43
1:D:644:VAL:HB	1:D:678:ILE:HG12	2.01	0.43
1:A:544:ARG:HD2	1:A:547:ARG:HD2	2.00	0.43
1:D:676:LEU:HD23	1:D:676:LEU:HA	1.78	0.43
1:A:610:LEU:CD2	1:A:709:LEU:HD12	2.49	0.43
1:A:768:GLN:O	1:A:772:GLU:OE2	2.36	0.43
1:B:651:ASN:HB3	1:B:697:PHE:CZ	2.54	0.42
1:C:494:TYR:CE2	1:C:496:GLU:HB2	2.55	0.42
1:C:628:ALA:HB2	1:C:710:VAL:HG21	2.01	0.42
1:B:628:ALA:HB2	1:B:710:VAL:HG21	2.01	0.42
1:C:723:LEU:HD23	1:C:723:LEU:HA	1.92	0.42
1:E:731:GLU:CG	1:E:732:VAL:N	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:567:GLY:HA2	1:G:743:SER:O	2.20	0.42
1:G:633:LYS:HE3	1:G:673:ARG:HH11	1.84	0.42
1:D:581:ARG:HB3	1:D:582:PRO:HD3	2.01	0.42
1:E:581:ARG:HB3	1:E:582:PRO:HD3	2.02	0.42
1:E:530:LYS:HZ2	1:E:534:LEU:HD11	1.82	0.42
1:D:729:LYS:HD2	1:D:729:LYS:HA	1.87	0.42
1:A:447:ILE:HG23	1:A:486:ILE:HD11	2.02	0.42
1:D:629:LEU:HD22	1:D:673:ARG:HG3	2.01	0.42
1:A:613:THR:HB	1:A:721:TYR:CD2	2.54	0.41
2:G:801:ACO:H52A	2:G:801:ACO:H8A	2.02	0.41
1:B:505:LEU:HG	1:B:505:LEU:H	1.49	0.41
1:D:756:ILE:O	1:D:760:VAL:HG23	2.20	0.41
1:A:742:ARG:NH1	1:A:774:LEU:HD12	2.35	0.41
1:B:719:ILE:HG23	1:C:684:ALA:HB2	2.02	0.41
1:D:727:ILE:HD11	1:E:724:ILE:HD13	2.01	0.41
1:G:507:ILE:HD11	1:G:509:LEU:HD12	2.01	0.41
1:D:501:LYS:HE2	1:D:505:LEU:HD11	2.03	0.41
1:G:449:ARG:NH1	1:G:637:TYR:CE2	2.89	0.41
1:D:526:SER:O	1:D:530:LYS:HG3	2.21	0.41
1:B:464:ILE:HG12	1:B:487:CYS:HB2	2.01	0.41
1:D:658:THR:HG21	1:E:715:GLU:OE2	2.20	0.41
1:E:470:THR:HG21	1:E:497:ARG:HG3	2.03	0.41
1:G:503:LYS:HE2	1:G:503:LYS:HA	2.03	0.41
1:G:589:VAL:HA	1:G:740:VAL:HA	2.02	0.41
1:B:449:ARG:HH11	1:B:449:ARG:HD3	1.64	0.41
1:B:505:LEU:HD12	1:B:507:ILE:HG13	2.02	0.41
1:D:683:GLN:NE2	2:E:801:ACO:H21	2.35	0.41
1:A:728:GLY:HA2	1:G:728:GLY:HA2	2.02	0.40
1:B:594:ILE:HG22	1:B:626:GLN:HG3	2.02	0.40
1:B:596:ALA:HB1	1:B:612:ASP:HB2	2.02	0.40
1:B:723:LEU:HG	1:C:684:ALA:HB1	2.03	0.40
1:D:494:TYR:H	1:D:497:ARG:NH2	2.13	0.40
1:D:765:LEU:HA	1:D:765:LEU:HD23	1.89	0.40
1:G:594:ILE:HG22	1:G:626:GLN:HG3	2.04	0.40
1:G:481:LEU:HD21	1:G:757:VAL:HG13	2.02	0.40
1:E:501:LYS:O	1:E:505:LEU:HG	2.21	0.40
1:A:554:TYR:CE2	1:A:582:PRO:HG3	2.56	0.40
1:G:471:SER:O	1:G:475:LEU:HG	2.22	0.40
1:G:481:LEU:HD22	1:G:486:ILE:CD1	2.52	0.40
1:G:679:GLU:HB3	1:G:682:MET:HE3	2.04	0.40
2:G:801:ACO:H8A	2:G:801:ACO:C5B	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:470:THR:HG21	1:B:497:ARG:HD2	2.03	0.40
1:C:440:LYS:HB2	1:C:441:VAL:H	1.70	0.40
1:C:613:THR:HA	1:C:717:SER:OG	2.22	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	334/362 (92%)	330 (99%)	4 (1%)	0	100	100
1	B	334/362 (92%)	329 (98%)	5 (2%)	0	100	100
1	C	335/362 (92%)	330 (98%)	5 (2%)	0	100	100
1	D	336/362 (93%)	330 (98%)	6 (2%)	0	100	100
1	E	335/362 (92%)	330 (98%)	5 (2%)	0	100	100
1	G	335/362 (92%)	332 (99%)	3 (1%)	0	100	100
All	All	2009/2172 (92%)	1981 (99%)	28 (1%)	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	280/301 (93%)	277 (99%)	3 (1%)	73 83
1	B	280/301 (93%)	270 (96%)	10 (4%)	35 44
1	C	281/301 (93%)	278 (99%)	3 (1%)	73 83
1	D	280/301 (93%)	278 (99%)	2 (1%)	84 90
1	E	281/301 (93%)	275 (98%)	6 (2%)	53 65
1	G	281/301 (93%)	277 (99%)	4 (1%)	67 78
All	All	1683/1806 (93%)	1655 (98%)	28 (2%)	60 72

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	525	PHE
1	A	721	TYR
1	A	742	ARG
1	G	444	ARG
1	G	591	LYS
1	G	633	LYS
1	G	721	TYR
1	B	449	ARG
1	B	452	GLN
1	B	505	LEU
1	B	507	ILE
1	B	508	PRO
1	B	509	LEU
1	B	511	ASN
1	B	526	SER
1	B	664	LYS
1	B	772	GLU
1	C	449	ARG
1	C	664	LYS
1	C	743	SER
1	D	671	SER
1	D	721	TYR
1	E	440	LYS
1	E	526	SER
1	E	671	SER
1	E	721	TYR
1	E	749	ARG
1	E	771	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	457	ASN
1	B	457	ASN
1	B	511	ASN
1	B	561	ASN
1	B	562	GLN
1	D	511	ASN
1	D	561	ASN
1	D	562	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	E	801	-	45,53,53	4.13	17 (37%)	56,79,79	2.14	6 (10%)
2	ACO	D	801	-	45,53,53	4.09	18 (40%)	56,79,79	2.09	8 (14%)
2	ACO	G	801	-	45,53,53	4.05	17 (37%)	56,79,79	2.04	5 (8%)
2	ACO	A	801	-	45,53,53	4.01	17 (37%)	56,79,79	2.14	11 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ACO	C	801	-	45,53,53	4.11	16 (35%)	56,79,79	2.14	7 (12%)
2	ACO	B	801	-	45,53,53	4.06	16 (35%)	56,79,79	2.08	10 (17%)

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	E	801	-	-	15/47/67/67	0/3/3/3
2	ACO	D	801	-	-	10/47/67/67	0/3/3/3
2	ACO	G	801	-	-	11/47/67/67	0/3/3/3
2	ACO	A	801	-	-	14/47/67/67	0/3/3/3
2	ACO	C	801	-	-	5/47/67/67	0/3/3/3
2	ACO	B	801	-	-	16/47/67/67	0/3/3/3

All (101) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	801	ACO	O4B-C1B	16.99	1.64	1.41
2	G	801	ACO	O4B-C1B	16.91	1.64	1.41
2	C	801	ACO	O4B-C1B	16.67	1.64	1.41
2	B	801	ACO	O4B-C1B	16.65	1.64	1.41
2	D	801	ACO	O4B-C1B	16.53	1.64	1.41
2	A	801	ACO	O4B-C1B	16.43	1.64	1.41
2	B	801	ACO	C2B-C1B	-13.22	1.33	1.53
2	C	801	ACO	C2B-C1B	-13.21	1.33	1.53
2	D	801	ACO	C2B-C1B	-13.09	1.33	1.53
2	E	801	ACO	C2B-C1B	-12.99	1.34	1.53
2	A	801	ACO	C2B-C1B	-12.64	1.34	1.53
2	G	801	ACO	C2B-C1B	-12.38	1.35	1.53
2	B	801	ACO	C9P-N8P	7.21	1.49	1.33
2	A	801	ACO	C9P-N8P	7.09	1.49	1.33
2	D	801	ACO	C9P-N8P	7.05	1.49	1.33
2	G	801	ACO	C9P-N8P	7.00	1.48	1.33
2	E	801	ACO	C9P-N8P	6.96	1.48	1.33
2	C	801	ACO	C9P-N8P	6.94	1.48	1.33
2	A	801	ACO	O4B-C4B	-6.53	1.30	1.45
2	D	801	ACO	C5P-N4P	6.33	1.47	1.33
2	B	801	ACO	O4B-C4B	-6.32	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	801	ACO	O4B-C4B	-6.22	1.31	1.45
2	G	801	ACO	O4B-C4B	-6.19	1.31	1.45
2	D	801	ACO	O4B-C4B	-6.14	1.31	1.45
2	E	801	ACO	O4B-C4B	-6.08	1.31	1.45
2	C	801	ACO	C5P-N4P	6.01	1.47	1.33
2	E	801	ACO	C5P-N4P	5.99	1.47	1.33
2	G	801	ACO	C5P-N4P	5.85	1.46	1.33
2	E	801	ACO	P3B-O3B	5.70	1.70	1.59
2	C	801	ACO	P3B-O3B	5.58	1.69	1.59
2	D	801	ACO	P3B-O3B	5.53	1.69	1.59
2	A	801	ACO	C5P-N4P	5.52	1.45	1.33
2	B	801	ACO	C6A-N6A	5.43	1.53	1.34
2	E	801	ACO	C6A-N6A	5.41	1.53	1.34
2	D	801	ACO	C6A-N6A	5.35	1.53	1.34
2	C	801	ACO	C6A-N6A	5.32	1.53	1.34
2	G	801	ACO	P3B-O3B	5.30	1.69	1.59
2	G	801	ACO	C6A-N6A	5.29	1.53	1.34
2	A	801	ACO	C6A-N6A	5.19	1.53	1.34
2	A	801	ACO	P3B-O3B	5.15	1.69	1.59
2	B	801	ACO	P3B-O3B	5.10	1.68	1.59
2	B	801	ACO	C5P-N4P	4.75	1.44	1.33
2	E	801	ACO	P1A-O5B	4.50	1.77	1.59
2	C	801	ACO	P1A-O5B	4.37	1.77	1.59
2	D	801	ACO	P1A-O5B	4.26	1.76	1.59
2	G	801	ACO	P1A-O5B	4.26	1.76	1.59
2	B	801	ACO	P1A-O5B	4.24	1.76	1.59
2	E	801	ACO	C6P-C5P	4.03	1.59	1.51
2	A	801	ACO	P1A-O5B	4.02	1.75	1.59
2	C	801	ACO	C6P-C5P	3.91	1.58	1.51
2	B	801	ACO	C6P-C5P	3.89	1.58	1.51
2	D	801	ACO	C6P-C5P	3.86	1.58	1.51
2	G	801	ACO	C6P-C5P	3.75	1.58	1.51
2	B	801	ACO	C2A-N3A	3.67	1.38	1.32
2	A	801	ACO	C2A-N3A	3.62	1.37	1.32
2	D	801	ACO	C2A-N3A	3.61	1.37	1.32
2	C	801	ACO	C2A-N3A	3.58	1.37	1.32
2	C	801	ACO	C7P-C6P	3.57	1.62	1.51
2	E	801	ACO	C7P-C6P	3.56	1.62	1.51
2	A	801	ACO	C6P-C5P	3.54	1.58	1.51
2	G	801	ACO	C2A-N3A	3.51	1.37	1.32
2	E	801	ACO	C2A-N3A	3.48	1.37	1.32
2	G	801	ACO	C7P-C6P	3.47	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	801	ACO	C7P-C6P	3.45	1.62	1.51
2	A	801	ACO	C7P-C6P	3.38	1.62	1.51
2	B	801	ACO	C7P-C6P	3.30	1.61	1.51
2	C	801	ACO	P2A-O6A	3.25	1.72	1.59
2	B	801	ACO	O5P-C5P	-3.23	1.16	1.23
2	E	801	ACO	P2A-O6A	3.22	1.72	1.59
2	G	801	ACO	P2A-O6A	3.10	1.71	1.59
2	A	801	ACO	P2A-O6A	3.03	1.71	1.59
2	B	801	ACO	P2A-O6A	2.96	1.71	1.59
2	A	801	ACO	C5A-C4A	-2.92	1.33	1.40
2	D	801	ACO	P2A-O6A	2.90	1.71	1.59
2	E	801	ACO	C5A-C4A	-2.90	1.33	1.40
2	C	801	ACO	C5A-C4A	-2.88	1.33	1.40
2	G	801	ACO	C5A-C4A	-2.80	1.33	1.40
2	D	801	ACO	C5A-C4A	-2.79	1.33	1.40
2	B	801	ACO	C5A-C4A	-2.74	1.33	1.40
2	C	801	ACO	O5P-C5P	-2.67	1.17	1.23
2	E	801	ACO	O5P-C5P	-2.63	1.17	1.23
2	A	801	ACO	O5P-C5P	-2.55	1.18	1.23
2	D	801	ACO	O5P-C5P	-2.50	1.18	1.23
2	G	801	ACO	O5P-C5P	-2.43	1.18	1.23
2	A	801	ACO	O3B-C3B	-2.22	1.36	1.44
2	D	801	ACO	C3P-N4P	2.17	1.51	1.46
2	G	801	ACO	O3B-C3B	-2.15	1.36	1.44
2	D	801	ACO	O3B-C3B	-2.15	1.36	1.44
2	A	801	ACO	C3P-N4P	2.14	1.51	1.46
2	G	801	ACO	O2B-C2B	2.14	1.48	1.43
2	B	801	ACO	O3B-C3B	-2.13	1.36	1.44
2	A	801	ACO	P3B-O8A	-2.13	1.46	1.54
2	G	801	ACO	P3B-O8A	-2.10	1.46	1.54
2	D	801	ACO	P3B-O8A	-2.10	1.46	1.54
2	E	801	ACO	C3B-C4B	2.09	1.58	1.52
2	E	801	ACO	C3P-N4P	2.08	1.50	1.46
2	E	801	ACO	P3B-O8A	-2.06	1.46	1.54
2	C	801	ACO	C3P-N4P	2.06	1.50	1.46
2	D	801	ACO	O2B-C2B	2.05	1.47	1.43
2	B	801	ACO	O2B-C2B	2.01	1.47	1.43
2	C	801	ACO	O3B-C3B	-2.01	1.36	1.44

All (47) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	801	ACO	C5A-C6A-N6A	10.57	136.41	120.35
2	G	801	ACO	C5A-C6A-N6A	10.27	135.97	120.35
2	C	801	ACO	C5A-C6A-N6A	10.25	135.94	120.35
2	D	801	ACO	C5A-C6A-N6A	10.02	135.59	120.35
2	B	801	ACO	C5A-C6A-N6A	9.95	135.47	120.35
2	A	801	ACO	C5A-C6A-N6A	9.37	134.59	120.35
2	E	801	ACO	N6A-C6A-N1A	-6.95	104.14	118.57
2	C	801	ACO	N6A-C6A-N1A	-6.89	104.28	118.57
2	G	801	ACO	N6A-C6A-N1A	-6.73	104.60	118.57
2	D	801	ACO	N6A-C6A-N1A	-6.60	104.88	118.57
2	B	801	ACO	N6A-C6A-N1A	-6.22	105.66	118.57
2	A	801	ACO	N6A-C6A-N1A	-6.12	105.87	118.57
2	A	801	ACO	N3A-C2A-N1A	-5.76	119.68	128.68
2	C	801	ACO	N3A-C2A-N1A	-5.56	120.00	128.68
2	G	801	ACO	N3A-C2A-N1A	-5.43	120.19	128.68
2	D	801	ACO	N3A-C2A-N1A	-5.36	120.30	128.68
2	E	801	ACO	N3A-C2A-N1A	-5.29	120.41	128.68
2	B	801	ACO	N3A-C2A-N1A	-5.23	120.50	128.68
2	A	801	ACO	C7P-C6P-C5P	-4.94	104.13	112.36
2	C	801	ACO	C7P-C6P-C5P	-4.18	105.39	112.36
2	B	801	ACO	C7P-C6P-C5P	-3.93	105.81	112.36
2	D	801	ACO	C7P-C6P-C5P	-3.72	106.15	112.36
2	E	801	ACO	C3B-C2B-C1B	3.52	107.69	99.89
2	G	801	ACO	C7P-C6P-C5P	-3.36	106.76	112.36
2	E	801	ACO	C7P-C6P-C5P	-3.35	106.78	112.36
2	C	801	ACO	C3B-C2B-C1B	3.23	107.04	99.89
2	G	801	ACO	C3B-C2B-C1B	3.04	106.62	99.89
2	D	801	ACO	O6A-CCP-CBP	-3.03	105.68	110.55
2	A	801	ACO	C3P-N4P-C5P	-2.94	117.38	122.84
2	B	801	ACO	C2P-C3P-N4P	-2.88	106.36	112.42
2	A	801	ACO	P2A-O3A-P1A	-2.77	123.32	132.83
2	B	801	ACO	C6P-C5P-N4P	2.71	120.99	116.42
2	D	801	ACO	C7P-N8P-C9P	-2.68	117.81	122.59
2	A	801	ACO	C7P-N8P-C9P	-2.66	117.85	122.59
2	A	801	ACO	C2P-C3P-N4P	-2.58	107.00	112.42
2	A	801	ACO	C6P-C7P-N8P	-2.57	106.71	111.90
2	B	801	ACO	O5P-C5P-N4P	-2.53	118.24	123.01
2	C	801	ACO	C7P-N8P-C9P	-2.46	118.20	122.59
2	A	801	ACO	C3B-C2B-C1B	2.45	105.32	99.89
2	B	801	ACO	O6A-CCP-CBP	-2.38	106.71	110.55
2	B	801	ACO	P2A-O3A-P1A	-2.35	124.76	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	801	ACO	C3B-C2B-C1B	2.24	104.84	99.89
2	A	801	ACO	O6A-CCP-CBP	-2.22	106.98	110.55
2	D	801	ACO	O4B-C1B-C2B	-2.20	103.71	106.93
2	C	801	ACO	C6P-C7P-N8P	-2.18	107.49	111.90
2	D	801	ACO	C6P-C7P-N8P	-2.13	107.59	111.90
2	E	801	ACO	C7P-N8P-C9P	-2.07	118.90	122.59

There are no chirality outliers.

All (71) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	801	ACO	CCP-O6A-P2A-O3A
2	A	801	ACO	CEP-CBP-CCP-O6A
2	A	801	ACO	CAP-CBP-CCP-O6A
2	A	801	ACO	O9P-C9P-CAP-OAP
2	A	801	ACO	N8P-C9P-CAP-OAP
2	A	801	ACO	C3P-C2P-S1P-C
2	G	801	ACO	O4B-C4B-C5B-O5B
2	G	801	ACO	C5B-O5B-P1A-O1A
2	G	801	ACO	CAP-CBP-CCP-O6A
2	G	801	ACO	C3P-C2P-S1P-C
2	B	801	ACO	C3B-O3B-P3B-O7A
2	B	801	ACO	C5B-O5B-P1A-O1A
2	B	801	ACO	C5B-O5B-P1A-O2A
2	B	801	ACO	C5P-C6P-C7P-N8P
2	B	801	ACO	S1P-C2P-C3P-N4P
2	C	801	ACO	P1A-O3A-P2A-O6A
2	C	801	ACO	C3P-C2P-S1P-C
2	D	801	ACO	C5B-O5B-P1A-O1A
2	D	801	ACO	C3P-C2P-S1P-C
2	E	801	ACO	CCP-O6A-P2A-O3A
2	E	801	ACO	CCP-O6A-P2A-O5A
2	E	801	ACO	CEP-CBP-CCP-O6A
2	E	801	ACO	CAP-CBP-CCP-O6A
2	E	801	ACO	C3P-C2P-S1P-C
2	E	801	ACO	O-C-S1P-C2P
2	E	801	ACO	CH3-C-S1P-C2P
2	B	801	ACO	C6P-C5P-N4P-C3P
2	G	801	ACO	C3B-C4B-C5B-O5B
2	C	801	ACO	O4B-C4B-C5B-O5B
2	E	801	ACO	C3B-C4B-C5B-O5B
2	E	801	ACO	O4B-C4B-C5B-O5B

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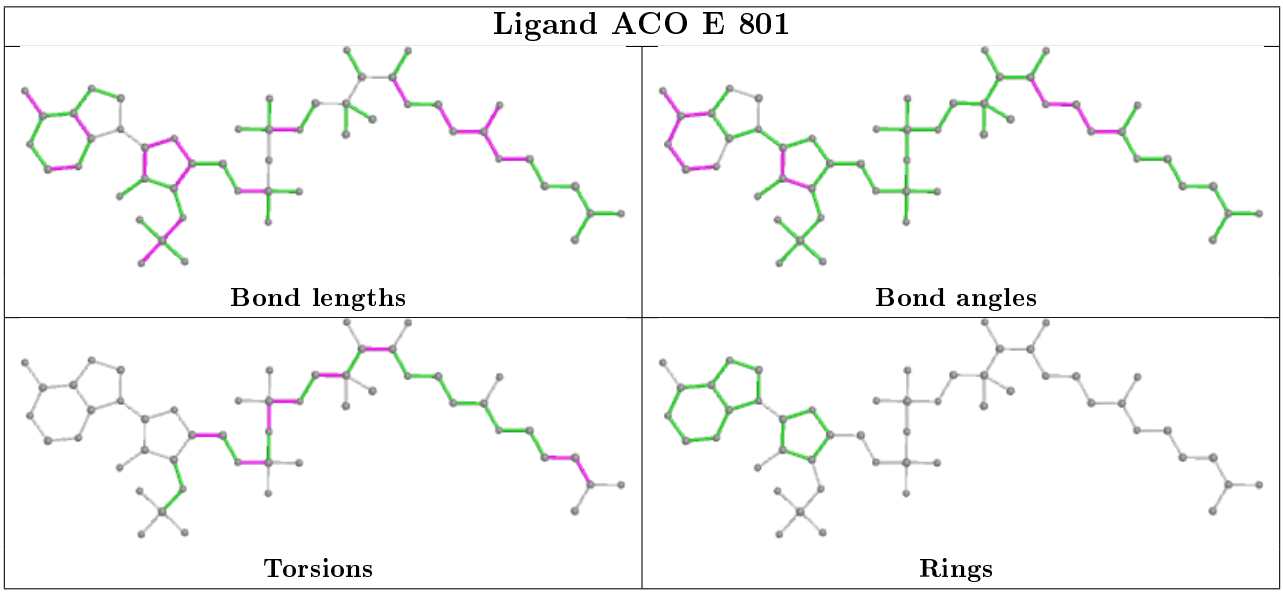
Mol	Chain	Res	Type	Atoms
2	B	801	ACO	O5P-C5P-N4P-C3P
2	A	801	ACO	CDP-CBP-CCP-O6A
2	G	801	ACO	CDP-CBP-CCP-O6A
2	G	801	ACO	CEP-CBP-CCP-O6A
2	E	801	ACO	CDP-CBP-CCP-O6A
2	C	801	ACO	C3B-C4B-C5B-O5B
2	E	801	ACO	P1A-O3A-P2A-O4A
2	A	801	ACO	C3B-O3B-P3B-O9A
2	G	801	ACO	C5B-O5B-P1A-O3A
2	B	801	ACO	C5B-O5B-P1A-O3A
2	B	801	ACO	CCP-O6A-P2A-O3A
2	D	801	ACO	C3B-O3B-P3B-O8A
2	D	801	ACO	C5B-O5B-P1A-O3A
2	E	801	ACO	C5B-O5B-P1A-O3A
2	G	801	ACO	P2A-O3A-P1A-O1A
2	B	801	ACO	P1A-O3A-P2A-O5A
2	D	801	ACO	P2A-O3A-P1A-O1A
2	A	801	ACO	CCP-O6A-P2A-O4A
2	A	801	ACO	CCP-O6A-P2A-O5A
2	E	801	ACO	C5B-O5B-P1A-O2A
2	E	801	ACO	CCP-O6A-P2A-O4A
2	G	801	ACO	C6P-C7P-N8P-C9P
2	B	801	ACO	O-C-S1P-C2P
2	A	801	ACO	P1A-O3A-P2A-O5A
2	G	801	ACO	C4B-C5B-O5B-P1A
2	D	801	ACO	CDP-CBP-CCP-O6A
2	B	801	ACO	C3P-C2P-S1P-C
2	D	801	ACO	O5P-C5P-C6P-C7P
2	E	801	ACO	O9P-C9P-CAP-OAP
2	B	801	ACO	CH3-C-S1P-C2P
2	A	801	ACO	C3B-O3B-P3B-O8A
2	B	801	ACO	OAP-CAP-CBP-CEP
2	D	801	ACO	C3B-O3B-P3B-O9A
2	A	801	ACO	O4B-C4B-C5B-O5B
2	D	801	ACO	O4B-C4B-C5B-O5B
2	A	801	ACO	P1A-O3A-P2A-O4A
2	B	801	ACO	CCP-O6A-P2A-O4A
2	C	801	ACO	C5B-O5B-P1A-O1A
2	D	801	ACO	N4P-C5P-C6P-C7P
2	B	801	ACO	C9P-CAP-CBP-CCP

There are no ring outliers.

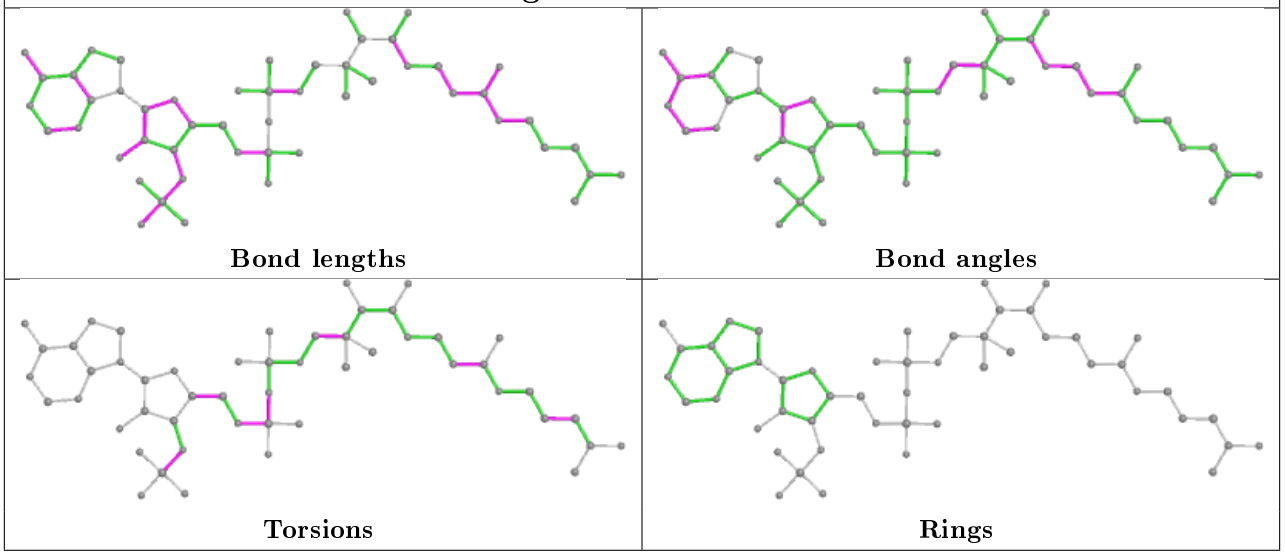
6 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	801	ACO	3	0
2	D	801	ACO	1	0
2	G	801	ACO	3	0
2	A	801	ACO	2	0
2	C	801	ACO	3	0
2	B	801	ACO	2	0

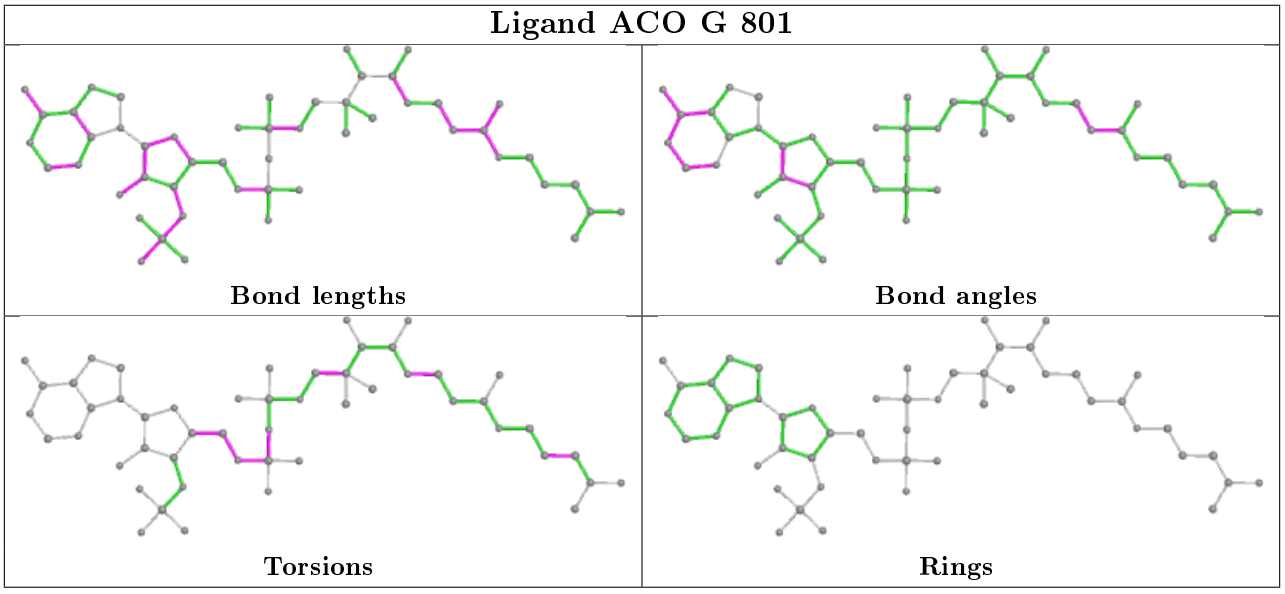
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



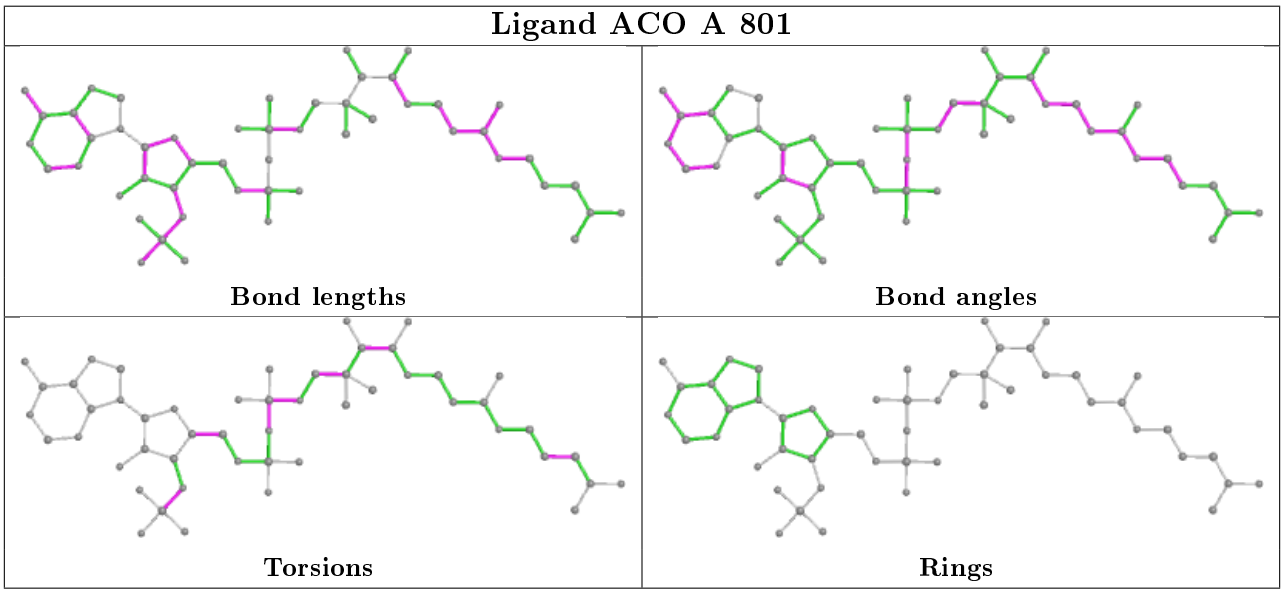
Ligand ACO D 801

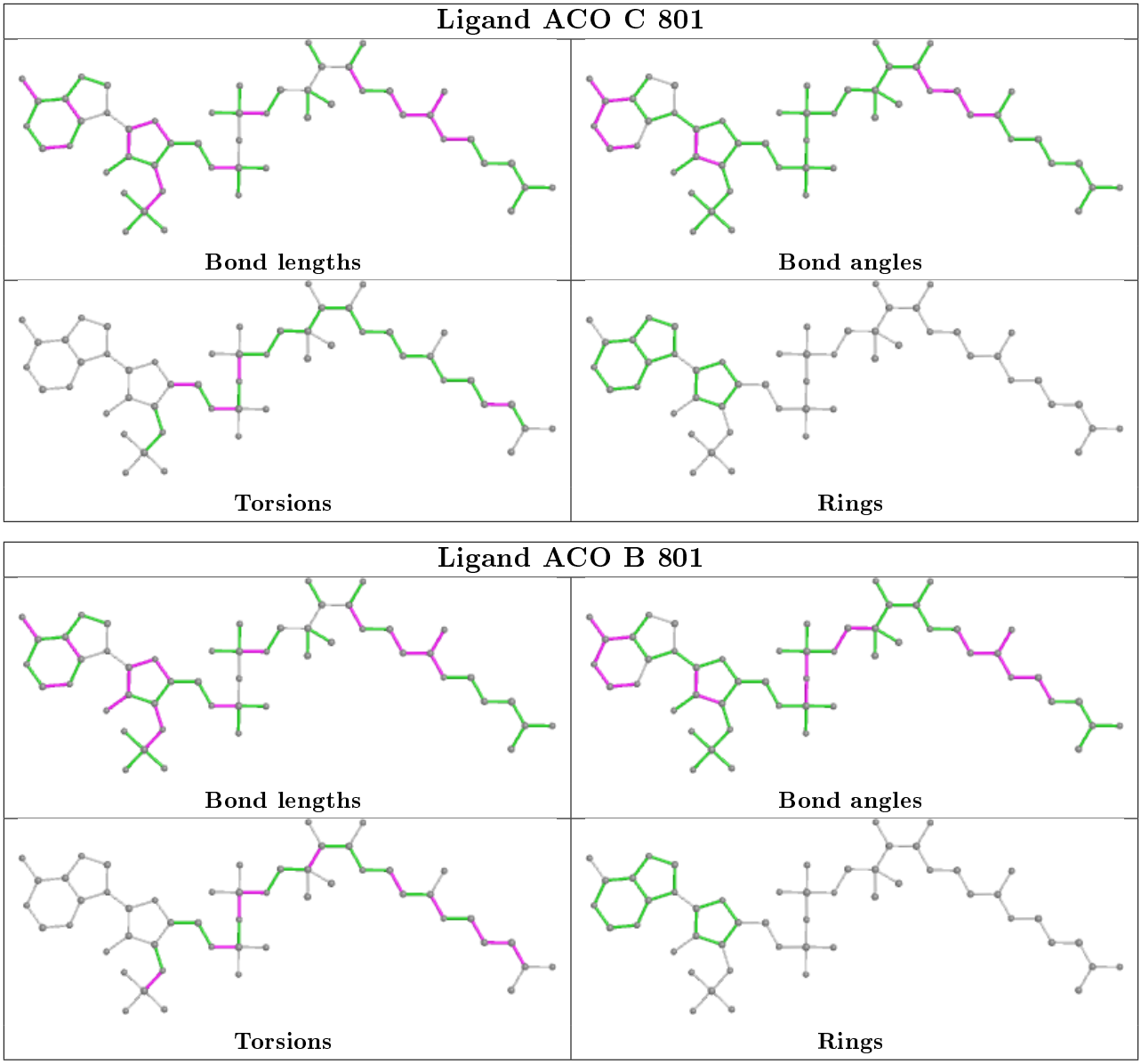


Ligand ACO G 801



Ligand ACO A 801





5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	336/362 (92%)	0.12	3 (0%) 84 89	39, 57, 89, 112	0
1	B	336/362 (92%)	0.28	15 (4%) 33 44	37, 64, 109, 149	0
1	C	337/362 (93%)	0.18	7 (2%) 63 73	33, 52, 92, 105	0
1	D	338/362 (93%)	0.11	3 (0%) 84 89	36, 52, 81, 116	0
1	E	337/362 (93%)	0.18	5 (1%) 73 81	35, 57, 105, 155	0
1	G	337/362 (93%)	0.15	3 (0%) 84 89	40, 57, 100, 134	0
All	All	2021/2172 (93%)	0.17	36 (1%) 68 76	33, 56, 98, 155	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	525	PHE	4.6
1	C	508	PRO	4.5
1	E	729	LYS	4.3
1	E	774	LEU	4.3
1	B	547	ARG	3.7
1	C	511	ASN	3.3
1	B	507	ILE	3.1
1	C	721	TYR	3.1
1	A	525	PHE	3.0
1	B	442	PHE	3.0
1	B	503	LYS	3.0
1	B	450	VAL	2.9
1	D	509	LEU	2.8
1	B	508	PRO	2.7
1	B	494	TYR	2.7
1	G	482	VAL	2.7
1	D	481	LEU	2.7
1	C	509	LEU	2.6
1	C	503	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	509	LEU	2.4
1	B	481	LEU	2.3
1	B	607	PHE	2.3
1	C	774	LEU	2.3
1	A	441	VAL	2.3
1	E	497	ARG	2.2
1	B	721	TYR	2.2
1	G	481	LEU	2.2
1	D	442	PHE	2.2
1	B	525	PHE	2.2
1	B	634	ILE	2.2
1	B	770	ILE	2.2
1	C	678	ILE	2.2
1	E	678	ILE	2.1
1	B	678	ILE	2.1
1	B	696	LEU	2.1
1	G	449	ARG	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 monosaccharides 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, 95^{th} 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	E	801	51/51	0.76	0.30	89,132,160,163	0
2	ACO	G	801	51/51	0.87	0.31	61,106,124,128	0
2	ACO	C	801	51/51	0.88	0.31	62,105,125,128	0
3	CL	E	802	1/1	0.90	0.09	65,65,65,65	0
2	ACO	D	801	51/51	0.91	0.19	51,96,109,116	0
2	ACO	A	801	51/51	0.92	0.13	49,77,96,98	0

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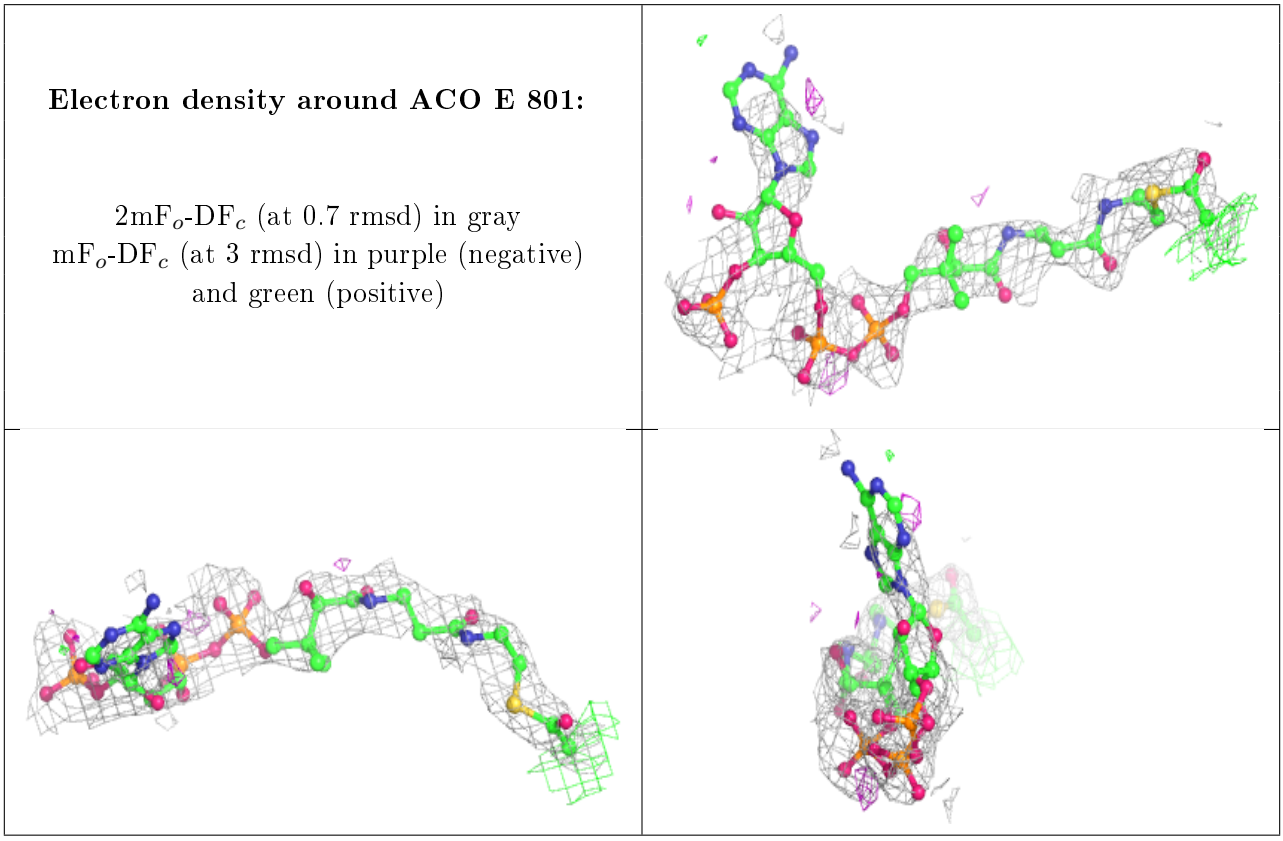
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ACO	B	801	51/51	0.93	0.17	48,78,89,93	0
3	CL	D	802	1/1	0.94	0.08	52,52,52,52	0
3	CL	A	802	1/1	0.94	0.10	47,47,47,47	0
3	CL	A	803	1/1	0.96	0.06	50,50,50,50	0
3	CL	C	802	1/1	0.97	0.10	59,59,59,59	0
3	CL	B	802	1/1	0.98	0.07	48,48,48,48	0

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.

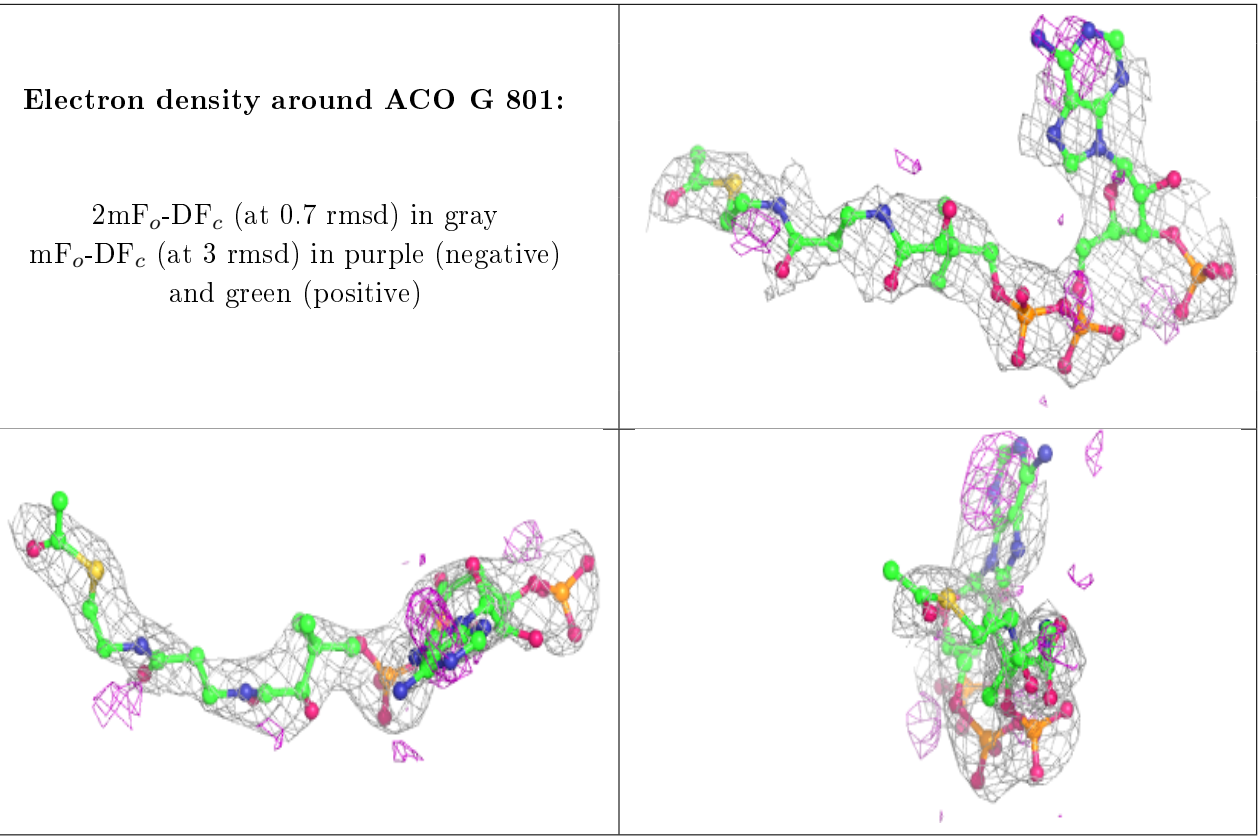
Electron density around ACO E 801:

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



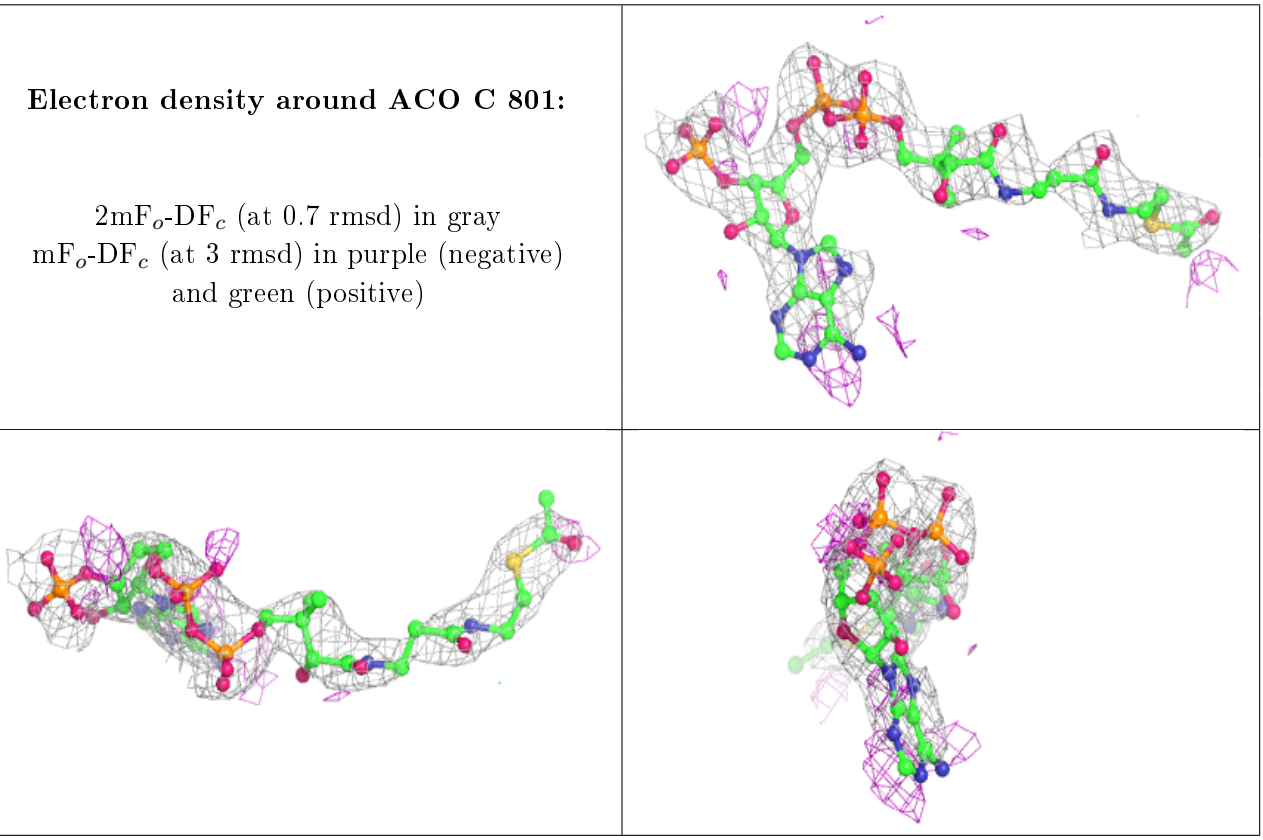
Electron density around ACO G 801:

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



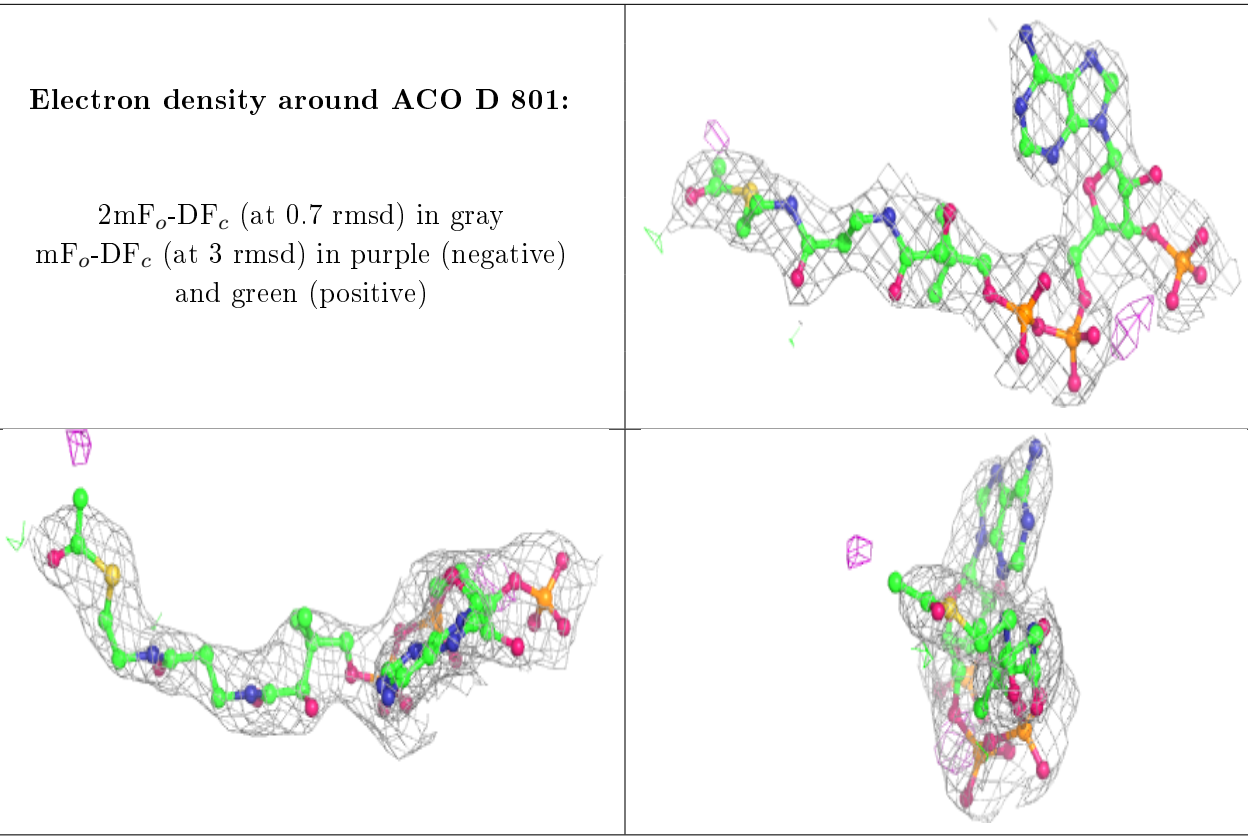
Electron density around ACO C 801:

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



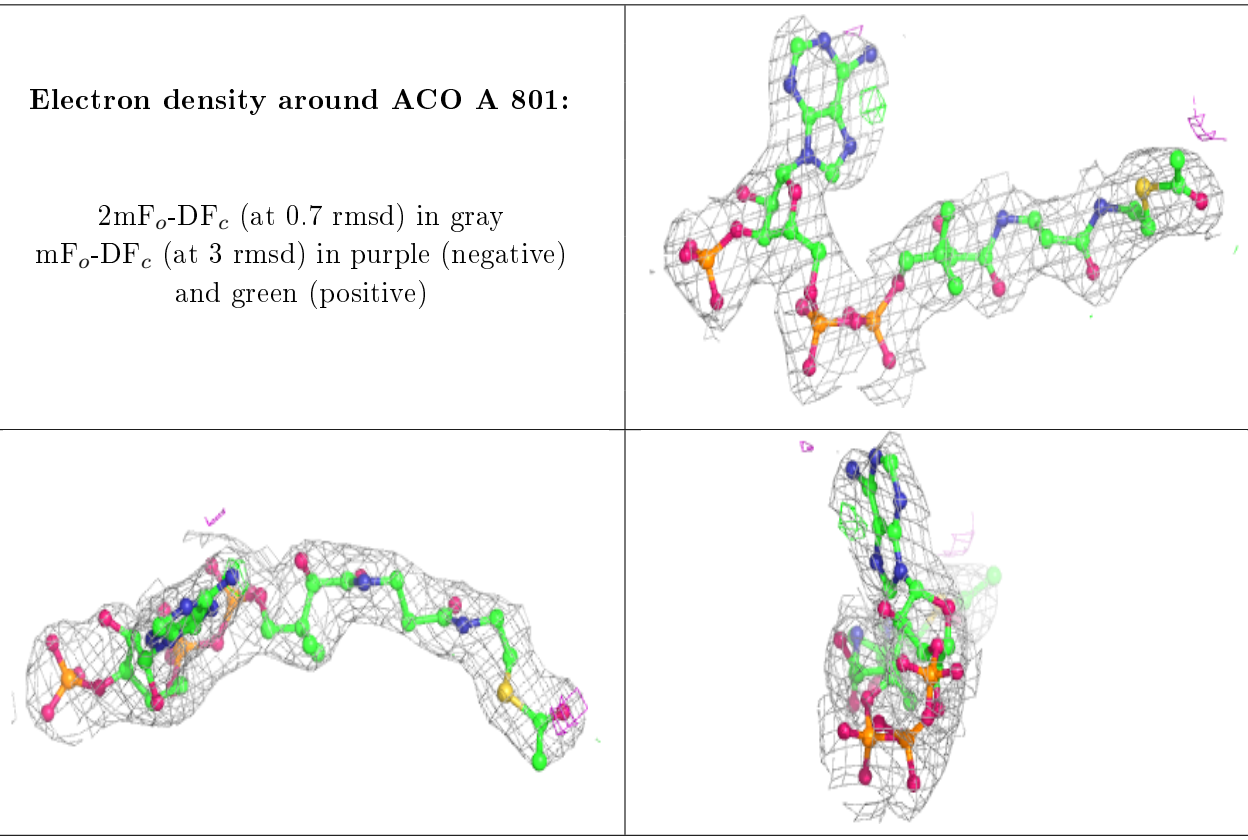
Electron density around ACO D 801:

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



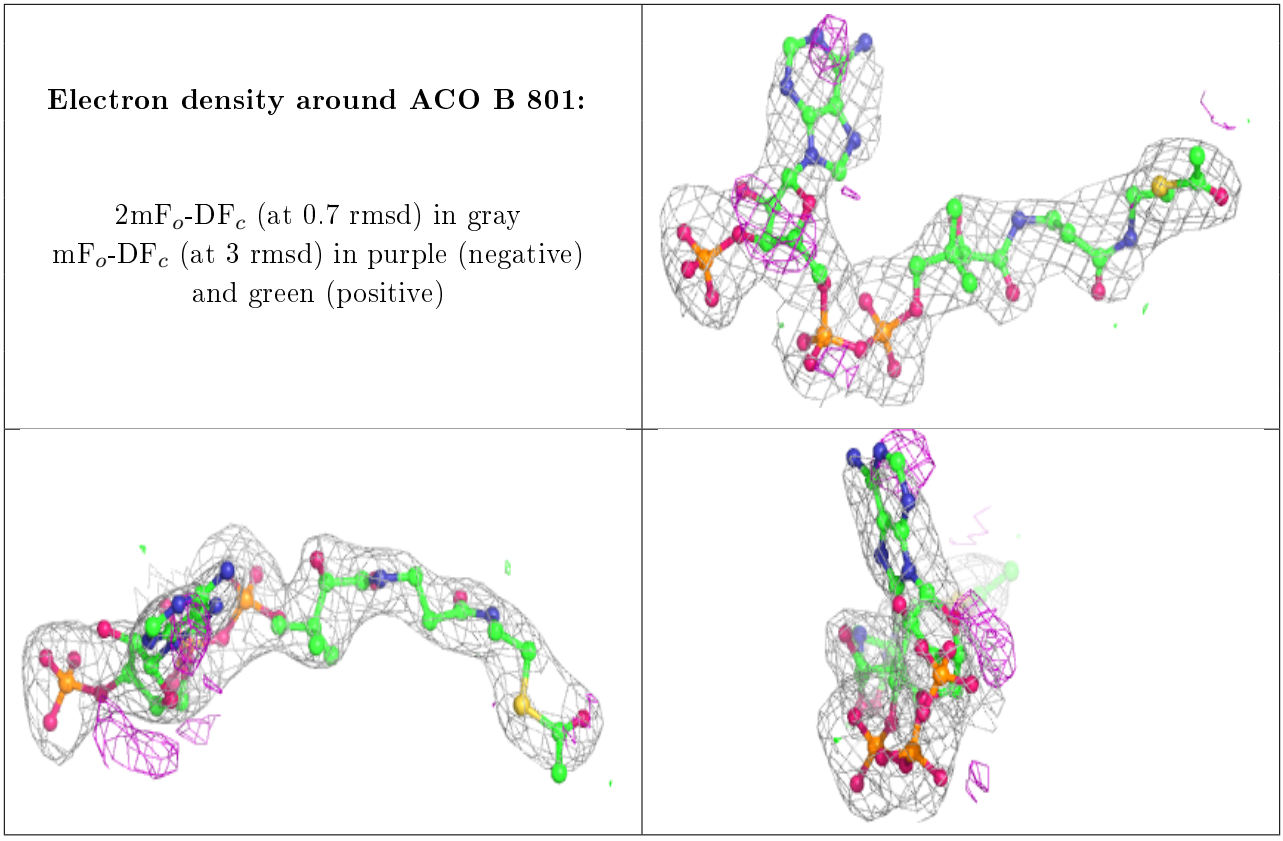
Electron density around ACO A 801:

$2mF_o$-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.