Full wwPDB X-ray Structure Validation Report (i)

Mar 10, 2021 – 02:15 am GMT

PDB ID	:	6ZNT
Title	:	MaeB PTA domain, acetyl-CoA bound form
Authors	:	Lovering, A.L.; Harding, C.J.
Deposited on	:	2020-07-06
Resolution	:	1.96 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 (i) symbol.

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

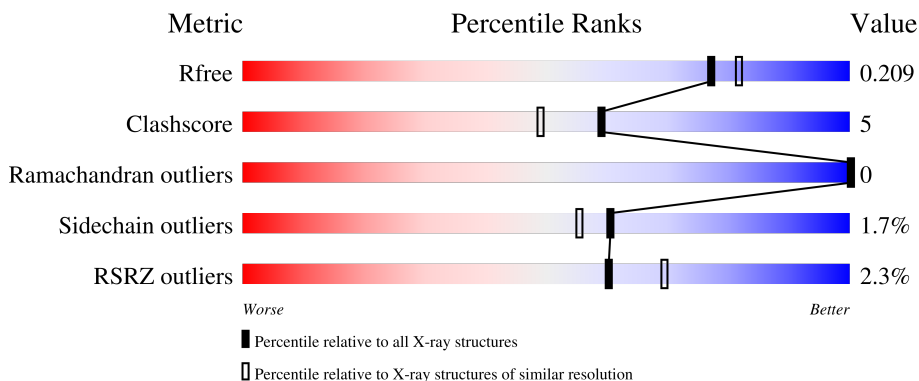|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.17.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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 1.96 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.
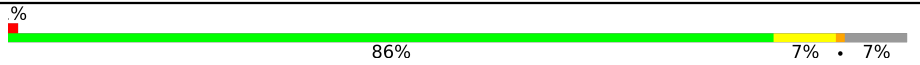
Metric	Percentile Ranks	Value
Rfree		0.209
Clashscore		5
Ramachandran outliers		0
Sidechain outliers		1.7%
RSRZ outliers		2.3%

Worse .... *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2580 (1.96-1.96)
Clashscore	141614	2705 (1.96-1.96)
Ramachandran outliers	138981	2678 (1.96-1.96)
Sidechain outliers	138945	2678 (1.96-1.96)
RSRZ outliers	127900	2539 (1.96-1.96)

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	2% 83% 10% · 7%
1	B	362	2% 82% 11% · 7%
1	C	362	4% 82% 10% · 7%
1	D	362	2% 81% 10% · 7%
1	E	362	% 86% 7% · 7%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	362	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	EDO	D	801	-	-	X	-

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 16585 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
			2583	1649	441	482	11			
1	C	336	Total	C	N	O	S	0	0	0
			2583	1649	441	482	11			
1	F	338	Total	C	N	O	S	0	0	0
			2598	1658	444	485	11			
1	D	336	Total	C	N	O	S	0	0	0
			2583	1649	441	482	11			
1	B	337	Total	C	N	O	S	0	0	0
			2592	1655	443	483	11			
1	E	338	Total	C	N	O	S	0	0	0
			2598	1658	444	485	11			

There are 120 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

Continued on next page...

Continued from previous page...

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
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
F	419	MET	-	initiating methionine	UNP Q6MM15
F	420	GLY	-	expression tag	UNP Q6MM15
F	421	SER	-	expression tag	UNP Q6MM15
F	422	SER	-	expression tag	UNP Q6MM15
F	423	HIS	-	expression tag	UNP Q6MM15
F	424	HIS	-	expression tag	UNP Q6MM15
F	425	HIS	-	expression tag	UNP Q6MM15
F	426	HIS	-	expression tag	UNP Q6MM15
F	427	HIS	-	expression tag	UNP Q6MM15
F	428	HIS	-	expression tag	UNP Q6MM15
F	429	SER	-	expression tag	UNP Q6MM15
F	430	SER	-	expression tag	UNP Q6MM15
F	431	GLY	-	expression tag	UNP Q6MM15
F	432	LEU	-	expression tag	UNP Q6MM15
F	433	VAL	-	expression tag	UNP Q6MM15
F	434	PRO	-	expression tag	UNP Q6MM15
F	435	ALA	-	expression tag	UNP Q6MM15
F	436	GLY	-	expression tag	UNP Q6MM15
F	437	SER	-	expression tag	UNP Q6MM15

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	438	HIS	-	expression tag	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
D	436	GLY	-	expression tag	UNP Q6MM15
D	437	SER	-	expression tag	UNP Q6MM15
D	438	HIS	-	expression tag	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
B	436	GLY	-	expression tag	UNP Q6MM15
B	437	SER	-	expression tag	UNP Q6MM15
B	438	HIS	-	expression tag	UNP Q6MM15
E	419	MET	-	initiating methionine	UNP Q6MM15

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
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

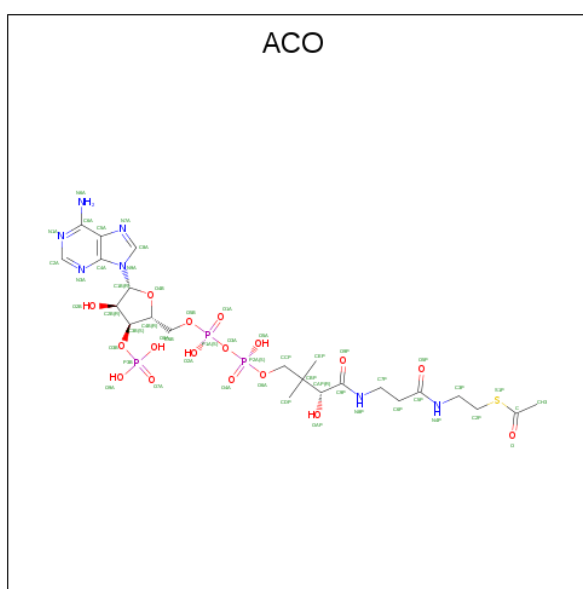- Molecule 2 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: $C_4H_{10}O_3$).
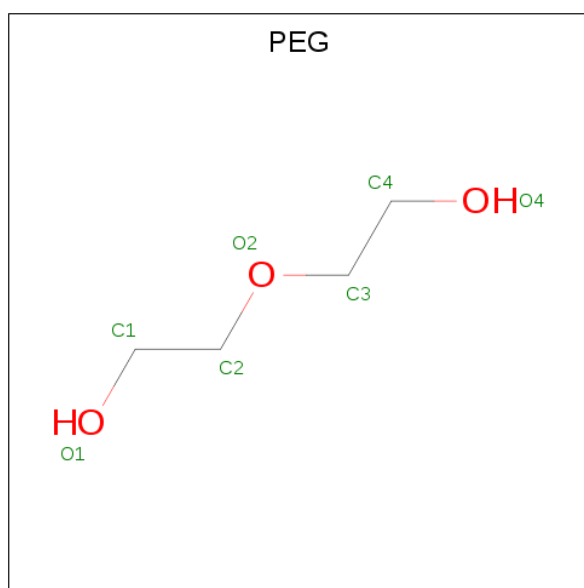
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total 7	C 4	O 3	0	0
2	C	1	Total 7	C 4	O 3	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	F	1	Total 7	C 4	O 3	0	0
2	D	1	Total 7	C 4	O 3	0	0
2	B	1	Total 7	C 4	O 3	0	0
2	E	1	Total 7	C 4	O 3	0	0

- Molecule 3 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).

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

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

EDO

O2

OH

C1

C2

HO

O1
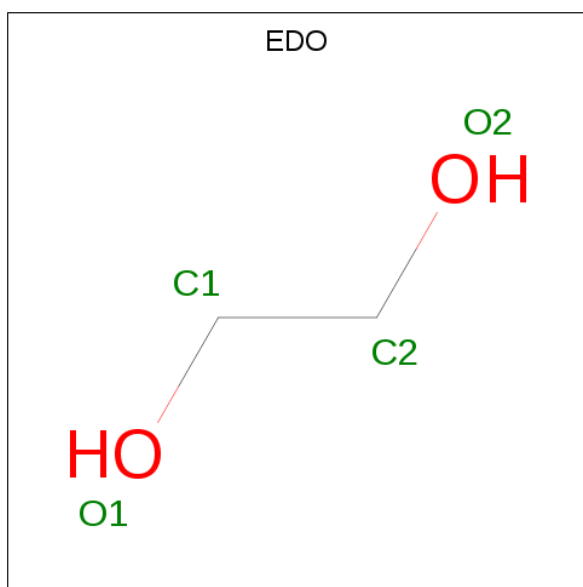
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total 4	C 2	O 2	0	0

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	109	Total 109	O 109	0	0
5	C	86	Total 86	O 86	0	0
5	F	172	Total 172	O 172	0	0
5	D	93	Total 93	O 93	0	0
5	B	85	Total 85	O 85	0	0
5	E	151	Total 151	O 151	0	0

3 Residue-property plots ⓘ

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.
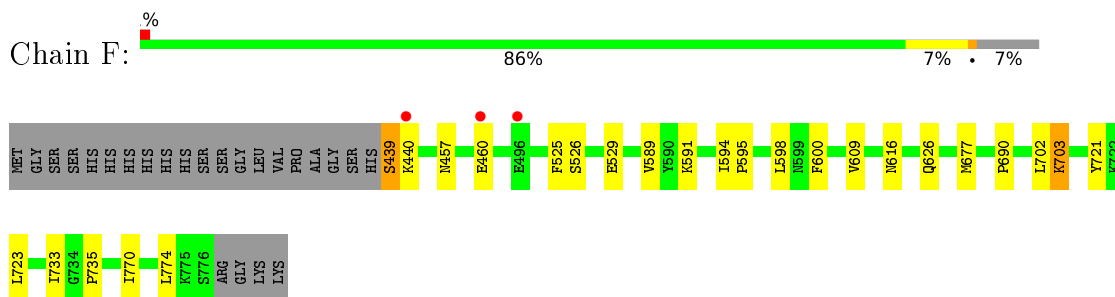
- Molecule 1: Malate dehydrogenase
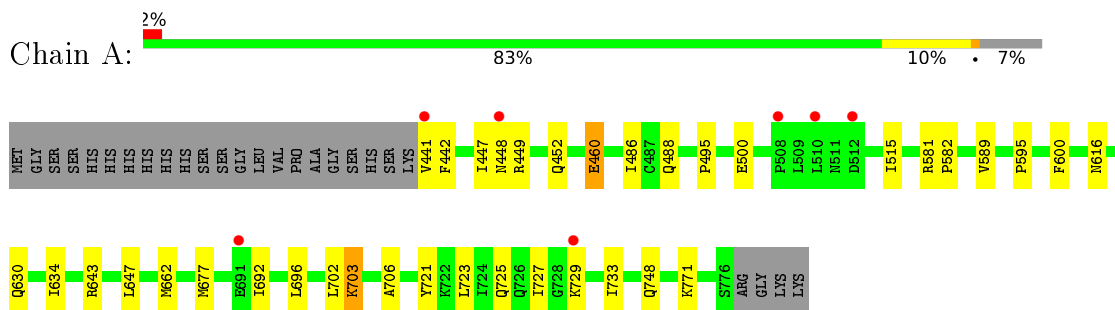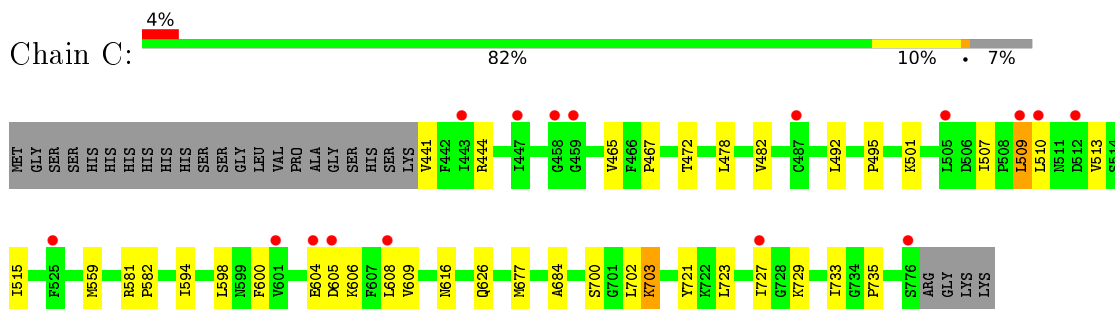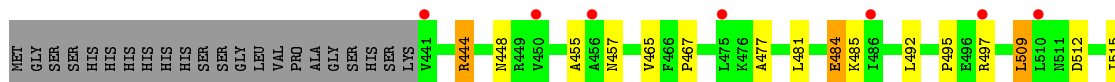

- Molecule 1: Malate dehydrogenase
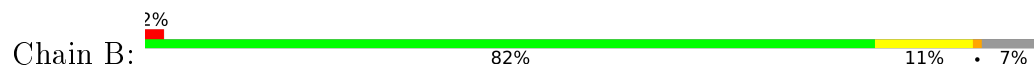

- Molecule 1: Malate dehydrogenase

- Molecule 1: Malate dehydrogenase
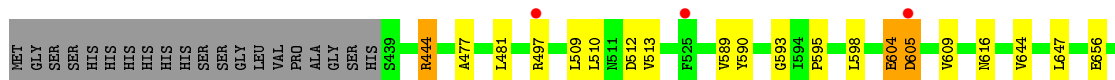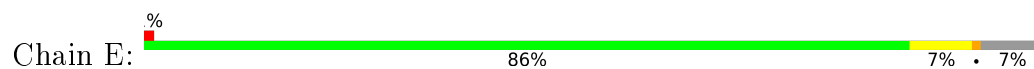
• Molecule 1: Malate dehydrogenase

Chain B:

• Molecule 1: Malate dehydrogenase

Chain E:

4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	111.19Å 60.59Å 167.75Å 90.00° 91.09° 90.00°	Depositor
Resolution (Å)	91.86 – 1.96 91.86 – 1.96	Depositor EDS
% Data completeness (in resolution range)	99.9 (91.86-1.96) 99.9 (91.86-1.96)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.52 (at 1.95Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.176 , 0.211 0.176 , 0.209	Depositor DCC
R_{free} test set	7910 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å^2)	40.8	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.30 , 49.2	EDS
L-test for twinning[2]	$< |L| > = 0.51, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	0.008 for h,-k,-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	16585	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.04% 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 (i)

5.1 Standard geometry (i)

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

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	0.47	0/2627	0.63	1/3557 (0.0%)
1	B	0.46	0/2636	0.67	4/3568 (0.1%)
1	C	0.42	0/2627	0.62	0/3557
1	D	0.46	0/2627	0.66	3/3557 (0.1%)
1	E	0.48	0/2642	0.71	8/3576 (0.2%)
1	F	0.45	0/2642	0.63	1/3576 (0.0%)
All	All	0.46	0/15801	0.65	17/21391 (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	B	0	1
1	D	0	1
1	E	0	1
All	All	0	3

There are no bond length outliers.

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	605	ASP	CB-CA-C	-7.62	95.16	110.40
1	E	604	GLU	CA-CB-CG	-7.37	97.18	113.40
1	F	591	LYS	CD-CE-NZ	-6.96	95.70	111.70
1	E	512	ASP	CB-CG-OD2	-6.86	112.13	118.30
1	B	592	GLU	CA-CB-CG	6.54	127.80	113.40
1	D	444	ARG	CB-CG-CD	6.36	128.14	111.60
1	E	512	ASP	CB-CG-OD1	5.99	123.69	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	591	LYS	CD-CE-NZ	-5.95	98.02	111.70
1	A	500	GLU	CA-CB-CG	5.85	126.27	113.40
1	E	604	GLU	N-CA-CB	-5.63	100.47	110.60
1	D	497	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	B	598	LEU	CA-CB-CG	5.52	128.00	115.30
1	E	497	ARG	CA-CB-CG	-5.51	101.28	113.40
1	D	485	LYS	CA-CB-CG	-5.50	101.31	113.40
1	E	512	ASP	CB-CA-C	-5.46	99.48	110.40
1	B	772	GLU	CA-CB-CG	5.02	124.44	113.40
1	E	444	ARG	NE-CZ-NH1	-5.02	117.79	120.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	605	ASP	Peptide
1	D	484	GLU	Sidechain
1	E	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	2583	0	2657	23	0
1	B	2592	0	2670	24	0
1	C	2583	0	2657	39	0
1	D	2583	0	2657	29	0
1	E	2598	0	2675	14	0
1	F	2598	0	2675	16	0
2	A	7	0	10	0	0
2	B	7	0	10	0	0
2	C	7	0	10	0	0
2	D	7	0	10	0	0
2	E	7	0	10	0	0
2	F	7	0	10	0	0
3	A	51	0	34	4	0
3	B	51	0	34	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	51	0	34	3	0
3	D	51	0	34	3	0
3	E	51	0	34	2	0
3	F	51	0	34	2	0
4	D	4	0	6	5	0
5	A	109	0	0	2	0
5	B	85	0	0	1	0
5	C	86	0	0	2	0
5	D	93	0	0	0	0
5	E	151	0	0	2	1
5	F	172	0	0	1	1
All	All	16585	0	16261	150	1

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 5.

All (150) 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)
3:D:803:ACO:O4B	3:D:803:ACO:C1B	1.63	1.27
3:A:802:ACO:O4B	3:A:802:ACO:C1B	1.63	1.25
3:B:802:ACO:O4B	3:B:802:ACO:C1B	1.63	1.25
3:C:802:ACO:O4B	3:C:802:ACO:C1B	1.64	1.22
1:C:482:VAL:CG1	1:C:509:LEU:CD2	2.34	1.05
1:C:482:VAL:HG12	1:C:509:LEU:CD2	1.91	1.01
1:C:482:VAL:HG12	1:C:509:LEU:HD21	1.45	0.97
1:C:482:VAL:CG1	1:C:509:LEU:HD23	1.94	0.96
1:C:482:VAL:HG11	1:C:509:LEU:HD23	1.49	0.94
1:C:465:VAL:HG21	1:C:559:MET:HE1	1.49	0.92
1:F:439:SER:N	5:F:901:HOH:O	2.03	0.90
1:B:457:ASN:ND2	1:B:460:GLU:OE1	2.04	0.90
1:C:441:VAL:N	5:C:901:HOH:O	2.08	0.85
1:D:465:VAL:HG21	1:D:559:MET:HE1	1.65	0.79
1:C:510:LEU:HD22	1:C:513:VAL:HG11	1.65	0.77
1:E:509:LEU:HD12	1:E:509:LEU:H	1.50	0.76
1:D:663:LYS:HG3	4:D:801:EDO:H12	1.70	0.72
1:D:477:ALA:O	1:D:481:LEU:HD23	1.89	0.72
1:A:630:GLN:O	1:A:634:ILE:HD13	1.95	0.67
1:D:509:LEU:HD12	1:D:509:LEU:O	1.95	0.66
4:D:801:EDO:H11	1:B:537:ARG:HD3	1.77	0.66
1:D:477:ALA:O	1:D:481:LEU:CD2	2.45	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:630:GLN:O	1:A:634:ILE:CD1	2.48	0.61
1:C:510:LEU:HA	1:C:513:VAL:HG13	1.81	0.61
1:B:677:MET:HE3	1:B:702:LEU:HD12	1.84	0.60
1:D:677:MET:HE1	1:D:703:LYS:O	2.02	0.60
1:D:677:MET:HE3	1:D:702:LEU:HD12	1.82	0.60
1:E:604:GLU:OE2	5:E:901:HOH:O	2.16	0.59
1:F:616:ASN:OD1	3:F:802:ACO:N6A	2.35	0.59
1:C:677:MET:HE3	1:C:702:LEU:HA	1.85	0.59
1:B:664:LYS:NZ	5:B:901:HOH:O	2.36	0.59
1:A:460:GLU:O	1:A:460:GLU:HG2	2.03	0.59
1:A:616:ASN:OD1	3:A:802:ACO:N6A	2.37	0.58
3:D:803:ACO:H52A	3:D:803:ACO:H8A	1.85	0.58
1:B:677:MET:HE1	1:B:703:LYS:O	2.04	0.57
1:A:488:GLN:OE1	5:A:901:HOH:O	2.16	0.57
1:C:482:VAL:CB	1:C:509:LEU:CD2	2.82	0.57
1:D:481:LEU:HD21	1:D:757:VAL:HG22	1.87	0.57
1:E:616:ASN:OD1	3:E:802:ACO:N6A	2.39	0.56
1:D:616:ASN:OD1	3:D:803:ACO:N6A	2.39	0.56
1:D:677:MET:HE3	1:D:702:LEU:HA	1.87	0.55
1:E:771:LYS:O	1:E:775:LYS:HG3	2.07	0.55
1:A:725:GLN:OE1	5:A:902:HOH:O	2.18	0.55
1:D:444:ARG:O	1:D:448:ASN:HB2	2.06	0.55
1:F:677:MET:HE1	1:F:703:LYS:O	2.07	0.54
1:A:448:ASN:O	1:A:452:GLN:HG3	2.07	0.54
1:E:589:VAL:HG12	1:E:590:TYR:O	2.07	0.54
1:F:594:ILE:HG22	1:F:626:GLN:HG3	1.89	0.54
1:A:692:ILE:HG23	1:A:696:LEU:HD12	1.89	0.54
3:B:802:ACO:H8A	3:B:802:ACO:H52A	1.89	0.54
1:F:525:PHE:O	1:F:529:GLU:HG3	2.07	0.53
1:B:449:ARG:HG2	1:B:765:LEU:HD21	1.91	0.53
1:B:702:LEU:HD21	1:B:706:ALA:HB2	1.89	0.53
1:F:677:MET:HE3	1:F:702:LEU:HA	1.89	0.53
1:E:589:VAL:HG21	1:E:595:PRO:HD3	1.90	0.53
1:D:484:GLU:HA	1:D:484:GLU:OE2	2.09	0.53
1:F:677:MET:HE3	1:F:702:LEU:HD12	1.90	0.53
1:B:700:SER:O	1:B:703:LYS:HE3	2.09	0.53
1:A:447:ILE:HG23	1:A:486:ILE:HD11	1.90	0.52
3:A:802:ACO:H52A	3:A:802:ACO:H8A	1.91	0.52
1:D:663:LYS:HE2	4:D:801:EDO:H12	1.90	0.52
1:A:677:MET:HE1	1:A:703:LYS:O	2.10	0.52
1:E:477:ALA:O	1:E:481:LEU:HD22	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:482:VAL:HB	1:C:509:LEU:CD2	2.40	0.52
1:C:467:PRO:HA	1:C:492:LEU:HB2	1.91	0.52
1:D:677:MET:CE	1:D:702:LEU:HD12	2.40	0.52
3:B:802:ACO:H8A	3:B:802:ACO:C5B	2.41	0.51
1:C:482:VAL:HB	1:C:509:LEU:HD22	1.92	0.51
1:F:457:ASN:O	1:F:460:GLU:HG2	2.11	0.50
1:C:510:LEU:O	1:C:513:VAL:HG22	2.11	0.50
1:C:729:LYS:HB2	1:D:729:LYS:HG3	1.94	0.50
1:A:634:ILE:HD12	1:A:634:ILE:N	2.26	0.50
1:C:482:VAL:CG1	1:C:509:LEU:HD21	2.18	0.50
1:B:449:ARG:HA	1:B:452:GLN:HB2	1.93	0.50
1:D:481:LEU:CD2	1:D:757:VAL:HG22	2.41	0.49
1:C:605:ASP:OD1	1:C:605:ASP:N	2.43	0.49
1:D:495:PRO:HA	1:D:515:ILE:HG21	1.94	0.49
1:D:589:VAL:HG11	1:D:595:PRO:HD3	1.94	0.49
1:E:656:GLU:O	5:E:902:HOH:O	2.20	0.49
1:C:495:PRO:HA	1:C:515:ILE:HG21	1.93	0.49
1:C:606:LYS:NZ	1:C:608:LEU:HD21	2.27	0.48
1:C:478:LEU:O	1:C:482:VAL:HG23	2.14	0.48
1:D:512:ASP:OD2	1:D:512:ASP:N	2.40	0.48
1:C:507:ILE:HG22	1:C:510:LEU:HG	1.96	0.47
1:C:482:VAL:CB	1:C:509:LEU:HD23	2.45	0.47
1:B:581:ARG:HB3	1:B:582:PRO:HD3	1.96	0.47
1:C:472:THR:OG1	1:C:501:LYS:NZ	2.47	0.47
1:A:589:VAL:HG11	1:A:595:PRO:HD3	1.95	0.47
4:D:801:EDO:O1	1:B:537:ARG:NH1	2.46	0.47
1:C:677:MET:HE1	1:C:703:LYS:O	2.15	0.46
1:F:600:PHE:HB2	1:F:733:ILE:CG1	2.46	0.46
1:B:448:ASN:O	1:B:452:GLN:HG3	2.16	0.46
1:F:677:MET:CE	1:F:702:LEU:HD12	2.46	0.45
1:B:554:TYR:CE1	1:B:582:PRO:HG3	2.51	0.45
1:A:441:VAL:HG13	1:A:442:PHE:H	1.80	0.45
1:A:643:ARG:HB3	1:A:702:LEU:HD11	1.98	0.45
1:C:684:ALA:HB1	1:D:723:LEU:HG	1.97	0.45
1:B:598:LEU:HG	1:B:609:VAL:HG13	1.99	0.45
1:E:598:LEU:HG	1:E:609:VAL:HG13	1.99	0.44
1:B:594:ILE:HG22	1:B:626:GLN:HG3	1.98	0.44
1:F:526:SER:O	1:F:529:GLU:HB2	2.17	0.44
1:F:598:LEU:HG	1:F:609:VAL:HG13	1.99	0.44
1:C:581:ARG:HB3	1:C:582:PRO:HD3	1.98	0.43
1:C:616:ASN:OD1	3:C:802:ACO:N6A	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:517:HIS:CE1	1:D:519:SER:HB2	2.53	0.43
3:E:802:ACO:H52A	3:E:802:ACO:H8A	1.99	0.43
1:D:467:PRO:HA	1:D:492:LEU:HB2	2.00	0.43
1:A:441:VAL:HG13	1:A:442:PHE:N	2.34	0.43
1:A:702:LEU:HD21	1:A:706:ALA:HB2	2.00	0.43
1:B:508:PRO:HA	1:B:511:ASN:OD1	2.18	0.43
1:F:723:LEU:HG	1:E:684:ALA:HB1	2.01	0.43
1:B:765:LEU:HD23	1:B:765:LEU:HA	1.84	0.43
1:C:594:ILE:HG22	1:C:626:GLN:HG3	2.01	0.43
1:C:604:GLU:OE1	1:D:729:LYS:NZ	2.36	0.42
1:D:681:ASP:OD1	4:D:801:EDO:H21	2.19	0.42
1:A:748:GLN:HB3	3:A:802:ACO:HH31	2.01	0.42
1:C:600:PHE:HB2	1:C:733:ILE:CG1	2.49	0.42
1:F:589:VAL:HG11	1:F:595:PRO:HD3	2.00	0.42
1:B:587:ILE:O	1:B:741:ARG:HD3	2.19	0.42
1:A:647:LEU:O	1:A:662:MET:HG3	2.20	0.42
1:F:735:PRO:HG2	3:F:802:ACO:HH33	2.02	0.42
1:D:600:PHE:HB2	1:D:733:ILE:HG12	2.01	0.42
1:C:444:ARG:NH1	5:C:906:HOH:O	2.49	0.42
1:D:455:ALA:C	1:D:457:ASN:H	2.23	0.42
1:B:616:ASN:OD1	3:B:802:ACO:N6A	2.52	0.42
1:C:507:ILE:HG21	1:C:510:LEU:CD1	2.49	0.42
1:A:495:PRO:HA	1:A:515:ILE:HG21	2.02	0.42
1:B:457:ASN:O	1:B:460:GLU:HG2	2.20	0.42
1:C:677:MET:CE	1:C:702:LEU:HD12	2.50	0.41
1:F:770:ILE:O	1:F:774:LEU:HD13	2.20	0.41
1:D:594:ILE:HG22	1:D:626:GLN:HG3	2.03	0.41
1:B:465:VAL:HG22	1:B:490:ILE:HB	2.02	0.41
1:A:677:MET:HE3	1:A:702:LEU:HA	2.01	0.41
1:B:440:LYS:NZ	1:B:440:LYS:HB3	2.35	0.41
1:D:581:ARG:HB3	1:D:582:PRO:HD3	2.03	0.41
1:A:600:PHE:HB2	1:A:733:ILE:HG12	2.01	0.41
1:C:510:LEU:HD22	1:C:513:VAL:CG1	2.44	0.41
1:C:735:PRO:HG2	3:C:802:ACO:HH33	2.03	0.41
1:C:598:LEU:HG	1:C:609:VAL:HG13	2.03	0.41
1:C:478:LEU:HD23	1:C:478:LEU:HA	1.92	0.40
1:C:723:LEU:O	1:C:727:ILE:HG12	2.21	0.40
1:D:647:LEU:O	1:D:662:MET:HG3	2.21	0.40
1:E:647:LEU:O	1:E:662:MET:HG3	2.22	0.40
1:A:581:ARG:HB3	1:A:582:PRO:HD3	2.04	0.40
1:B:633:LYS:HE2	1:B:673:ARG:NH1	2.36	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:LEU:O	1:A:727:ILE:HG12	2.22	0.40
1:B:467:PRO:HA	1:B:492:LEU:HB2	2.04	0.40
1:E:510:LEU:O	1:E:513:VAL:HG12	2.22	0.40
1:E:589:VAL:HG11	1:E:593:GLY:O	2.21	0.40
1:E:644:VAL:HB	1:E:678:ILE:HG12	2.03	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:933:HOH:O	5:E:1035:HOH:O[1_545]	2.13	0.07

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%)	332 (99%)	2 (1%)	0	100	100
1	B	335/362 (92%)	329 (98%)	6 (2%)	0	100	100
1	C	334/362 (92%)	329 (98%)	5 (2%)	0	100	100
1	D	334/362 (92%)	329 (98%)	5 (2%)	0	100	100
1	E	336/362 (93%)	331 (98%)	5 (2%)	0	100	100
1	F	336/362 (93%)	331 (98%)	5 (2%)	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%)	274 (98%)	6 (2%)	53	46
1	B	281/301 (93%)	275 (98%)	6 (2%)	53	46
1	C	280/301 (93%)	276 (99%)	4 (1%)	67	62
1	D	280/301 (93%)	275 (98%)	5 (2%)	59	53
1	E	282/301 (94%)	279 (99%)	3 (1%)	73	71
1	F	282/301 (94%)	277 (98%)	5 (2%)	59	53
All	All	1685/1806 (93%)	1656 (98%)	29 (2%)	60	55

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	449	ARG
1	A	460	GLU
1	A	703	LYS
1	A	721	TYR
1	A	729	LYS
1	A	771	LYS
1	C	509	LEU
1	C	700	SER
1	C	703	LYS
1	C	721	TYR
1	F	439	SER
1	F	440	LYS
1	F	690	PRO
1	F	703	LYS
1	F	721	TYR
1	D	509	LEU
1	D	653	SER
1	D	703	LYS
1	D	721	TYR
1	D	772	GLU
1	B	503	LYS
1	B	509	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	656	GLU
1	B	700	SER
1	B	721	TYR
1	B	729	LYS
1	E	444	ARG
1	E	703	LYS
1	E	721	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6   Ligand geometry (i)

13 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	PEG	C	801	-	6,6,6	0.49	0	5,5,5	0.31	0
2	PEG	E	801	-	6,6,6	0.48	0	5,5,5	0.19	0
2	PEG	F	801	-	6,6,6	0.46	0	5,5,5	0.32	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
3	ACO	A	802	-	45,53,53	3.94	16 (35%)	56,79,79	2.27	9 (16%)
3	ACO	F	802	-	45,53,53	3.97	16 (35%)	56,79,79	2.25	10 (17%)
3	ACO	B	802	-	45,53,53	3.94	18 (40%)	56,79,79	2.08	9 (16%)
3	ACO	D	803	-	45,53,53	3.95	16 (35%)	56,79,79	2.24	10 (17%)
4	EDO	D	801	-	3,3,3	0.46	0	2,2,2	0.21	0
2	PEG	A	801	-	6,6,6	0.48	0	5,5,5	0.26	0
2	PEG	B	801	-	6,6,6	0.46	0	5,5,5	0.20	0
3	ACO	C	802	-	45,53,53	4.06	16 (35%)	56,79,79	2.05	6 (10%)
3	ACO	E	802	-	45,53,53	3.85	18 (40%)	56,79,79	2.29	11 (19%)
2	PEG	D	802	-	6,6,6	0.45	0	5,5,5	0.25	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PEG	C	801	-	-	3/4/4/4	-
2	PEG	E	801	-	-	3/4/4/4	-
2	PEG	F	801	-	-	2/4/4/4	-
3	ACO	A	802	-	-	10/47/67/67	0/3/3/3
3	ACO	F	802	-	-	6/47/67/67	0/3/3/3
3	ACO	B	802	-	-	11/47/67/67	0/3/3/3
3	ACO	D	803	-	-	14/47/67/67	0/3/3/3
4	EDO	D	801	-	-	0/1/1/1	-
2	PEG	A	801	-	-	1/4/4/4	-
2	PEG	B	801	-	-	1/4/4/4	-
3	ACO	C	802	-	-	11/47/67/67	0/3/3/3
3	ACO	E	802	-	-	5/47/67/67	0/3/3/3
2	PEG	D	802	-	-	2/4/4/4	-

All (100) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	802	ACO	O4B-C1B	16.61	1.64	1.41
3	A	802	ACO	O4B-C1B	16.20	1.63	1.41
3	B	802	ACO	O4B-C1B	16.19	1.63	1.41
3	D	803	ACO	O4B-C1B	16.13	1.63	1.41
3	F	802	ACO	O4B-C1B	15.85	1.63	1.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	802	ACO	O4B-C1B	15.52	1.62	1.41
3	C	802	ACO	C2B-C1B	-13.36	1.33	1.53
3	F	802	ACO	C2B-C1B	-13.32	1.33	1.53
3	A	802	ACO	C2B-C1B	-12.61	1.34	1.53
3	D	803	ACO	C2B-C1B	-12.35	1.35	1.53
3	B	802	ACO	C2B-C1B	-12.34	1.35	1.53
3	E	802	ACO	C2B-C1B	-12.02	1.35	1.53
3	C	802	ACO	C9P-N8P	6.86	1.48	1.33
3	D	803	ACO	C9P-N8P	6.75	1.48	1.33
3	A	802	ACO	C9P-N8P	6.68	1.48	1.33
3	E	802	ACO	C9P-N8P	6.50	1.47	1.33
3	B	802	ACO	C9P-N8P	6.43	1.47	1.33
3	A	802	ACO	O4B-C4B	-6.32	1.30	1.45
3	E	802	ACO	O4B-C4B	-6.32	1.30	1.45
3	C	802	ACO	O4B-C4B	-6.25	1.31	1.45
3	B	802	ACO	O4B-C4B	-6.24	1.31	1.45
3	F	802	ACO	O4B-C4B	-6.23	1.31	1.45
3	F	802	ACO	C9P-N8P	6.23	1.47	1.33
3	D	803	ACO	O4B-C4B	-6.20	1.31	1.45
3	C	802	ACO	C5P-N4P	5.95	1.46	1.33
3	B	802	ACO	C5P-N4P	5.87	1.46	1.33
3	F	802	ACO	C5P-N4P	5.81	1.46	1.33
3	D	803	ACO	C5P-N4P	5.80	1.46	1.33
3	E	802	ACO	C5P-N4P	5.76	1.46	1.33
3	A	802	ACO	C5P-N4P	5.45	1.45	1.33
3	C	802	ACO	C6A-N6A	5.32	1.53	1.34
3	B	802	ACO	C6A-N6A	5.28	1.53	1.34
3	D	803	ACO	C6A-N6A	5.18	1.53	1.34
3	E	802	ACO	C6A-N6A	5.08	1.52	1.34
3	E	802	ACO	P3B-O3B	5.03	1.68	1.59
3	A	802	ACO	C6A-N6A	5.01	1.52	1.34
3	F	802	ACO	C6A-N6A	4.96	1.52	1.34
3	A	802	ACO	P3B-O3B	4.93	1.68	1.59
3	D	803	ACO	P3B-O3B	4.91	1.68	1.59
3	F	802	ACO	P3B-O3B	4.61	1.68	1.59
3	B	802	ACO	P3B-O3B	4.53	1.67	1.59
3	C	802	ACO	P3B-O3B	4.48	1.67	1.59
3	B	802	ACO	P1A-O5B	4.26	1.76	1.59
3	C	802	ACO	P1A-O5B	4.25	1.76	1.59
3	F	802	ACO	P1A-O5B	4.22	1.76	1.59
3	D	803	ACO	P1A-O5B	4.08	1.75	1.59
3	E	802	ACO	P1A-O5B	4.08	1.75	1.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	802	ACO	P1A-O5B	4.07	1.75	1.59
3	F	802	ACO	C6P-C5P	4.02	1.59	1.51
3	C	802	ACO	C6P-C5P	3.68	1.58	1.51
3	D	803	ACO	C7P-C6P	3.62	1.62	1.51
3	B	802	ACO	C6P-C5P	3.59	1.58	1.51
3	E	802	ACO	C6P-C5P	3.58	1.58	1.51
3	D	803	ACO	C6P-C5P	3.57	1.58	1.51
3	A	802	ACO	C7P-C6P	3.53	1.62	1.51
3	F	802	ACO	C2A-N3A	3.52	1.37	1.32
3	B	802	ACO	C7P-C6P	3.52	1.62	1.51
3	C	802	ACO	C2A-N3A	3.51	1.37	1.32
3	E	802	ACO	C7P-C6P	3.48	1.62	1.51
3	B	802	ACO	C2A-N3A	3.42	1.37	1.32
3	F	802	ACO	C7P-C6P	3.35	1.62	1.51
3	A	802	ACO	C2A-N3A	3.31	1.37	1.32
3	D	803	ACO	C2A-N3A	3.26	1.37	1.32
3	C	802	ACO	C7P-C6P	3.24	1.61	1.51
3	A	802	ACO	C6P-C5P	3.19	1.57	1.51
3	E	802	ACO	C2A-N3A	3.17	1.37	1.32
3	B	802	ACO	C5A-C4A	-3.04	1.32	1.40
3	D	803	ACO	C5A-C4A	-3.01	1.33	1.40
3	C	802	ACO	P2A-O6A	2.98	1.71	1.59
3	C	802	ACO	C5A-C4A	-2.97	1.33	1.40
3	D	803	ACO	P2A-O6A	2.97	1.71	1.59
3	F	802	ACO	C5A-C4A	-2.96	1.33	1.40
3	B	802	ACO	P2A-O6A	2.93	1.71	1.59
3	A	802	ACO	C5A-C4A	-2.92	1.33	1.40
3	E	802	ACO	P2A-O6A	2.90	1.71	1.59
3	D	803	ACO	O5P-C5P	-2.89	1.17	1.23
3	E	802	ACO	C5A-C4A	-2.86	1.33	1.40
3	E	802	ACO	O5P-C5P	-2.82	1.17	1.23
3	A	802	ACO	P2A-O6A	2.79	1.70	1.59
3	A	802	ACO	O5P-C5P	-2.74	1.17	1.23
3	B	802	ACO	O5P-C5P	-2.72	1.17	1.23
3	F	802	ACO	P2A-O6A	2.64	1.70	1.59
3	F	802	ACO	O5P-C5P	-2.54	1.18	1.23
3	F	802	ACO	C3P-N4P	2.53	1.51	1.46
3	F	802	ACO	O3B-C3B	-2.49	1.35	1.44
3	C	802	ACO	O3B-C3B	-2.45	1.35	1.44
3	B	802	ACO	O3B-C3B	-2.43	1.35	1.44
3	D	803	ACO	O3B-C3B	-2.39	1.35	1.44
3	C	802	ACO	O5P-C5P	-2.31	1.18	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	802	ACO	C3P-N4P	2.27	1.51	1.46
3	E	802	ACO	O3B-C3B	-2.25	1.35	1.44
3	D	803	ACO	C3P-N4P	2.22	1.51	1.46
3	B	802	ACO	O2B-C2B	2.20	1.48	1.43
3	C	802	ACO	C3P-N4P	2.17	1.51	1.46
3	A	802	ACO	O3B-C3B	-2.16	1.36	1.44
3	B	802	ACO	P3B-O8A	-2.15	1.46	1.54
3	B	802	ACO	C3P-N4P	2.14	1.51	1.46
3	E	802	ACO	P3B-O8A	-2.11	1.46	1.54
3	A	802	ACO	C3P-N4P	2.11	1.51	1.46
3	E	802	ACO	O2B-C2B	2.06	1.47	1.43

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	802	ACO	C5A-C6A-N6A	10.15	135.77	120.35
3	D	803	ACO	C5A-C6A-N6A	10.08	135.67	120.35
3	F	802	ACO	C5A-C6A-N6A	9.63	134.98	120.35
3	C	802	ACO	C5A-C6A-N6A	9.47	134.75	120.35
3	A	802	ACO	C5A-C6A-N6A	9.30	134.49	120.35
3	B	802	ACO	C5A-C6A-N6A	9.06	134.13	120.35
3	A	802	ACO	C7P-C6P-C5P	-6.72	101.17	112.36
3	D	803	ACO	N6A-C6A-N1A	-6.68	104.72	118.57
3	E	802	ACO	N6A-C6A-N1A	-6.64	104.80	118.57
3	F	802	ACO	N6A-C6A-N1A	-6.48	105.13	118.57
3	A	802	ACO	N6A-C6A-N1A	-6.20	105.71	118.57
3	C	802	ACO	N6A-C6A-N1A	-6.09	105.93	118.57
3	B	802	ACO	N6A-C6A-N1A	-5.86	106.42	118.57
3	B	802	ACO	N3A-C2A-N1A	-5.69	119.79	128.68
3	F	802	ACO	O6A-CCP-CBP	-5.69	101.40	110.55
3	D	803	ACO	N3A-C2A-N1A	-5.62	119.90	128.68
3	D	803	ACO	C7P-C6P-C5P	-5.58	103.06	112.36
3	A	802	ACO	N3A-C2A-N1A	-5.55	120.01	128.68
3	F	802	ACO	C7P-C6P-C5P	-5.39	103.38	112.36
3	E	802	ACO	N3A-C2A-N1A	-5.34	120.33	128.68
3	E	802	ACO	C7P-C6P-C5P	-5.33	103.47	112.36
3	C	802	ACO	N3A-C2A-N1A	-5.32	120.36	128.68
3	C	802	ACO	C7P-C6P-C5P	-5.24	103.62	112.36
3	F	802	ACO	N3A-C2A-N1A	-5.21	120.54	128.68
3	E	802	ACO	O6A-CCP-CBP	-5.17	102.23	110.55
3	B	802	ACO	C7P-C6P-C5P	-5.12	103.83	112.36
3	A	802	ACO	O6A-CCP-CBP	-5.01	102.49	110.55

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	D	803	ACO	C7P-N8P-C9P	-3.69	116.00	122.59
3	B	802	ACO	C7P-N8P-C9P	-3.69	116.01	122.59
3	A	802	ACO	C3P-N4P-C5P	-3.53	116.29	122.84
3	E	802	ACO	C7P-N8P-C9P	-3.26	116.77	122.59
3	E	802	ACO	CDP-CBP-CAP	2.81	113.70	108.82
3	B	802	ACO	O6A-CCP-CBP	-2.80	106.04	110.55
3	C	802	ACO	P2A-O3A-P1A	-2.79	123.25	132.83
3	F	802	ACO	P2A-O3A-P1A	-2.78	123.30	132.83
3	D	803	ACO	CDP-CBP-CAP	2.69	113.48	108.82
3	D	803	ACO	P2A-O3A-P1A	-2.67	123.66	132.83
3	C	802	ACO	O6A-CCP-CBP	-2.66	106.27	110.55
3	F	802	ACO	C7P-N8P-C9P	-2.66	117.85	122.59
3	A	802	ACO	C2P-C3P-N4P	-2.45	107.26	112.42
3	A	802	ACO	C3B-C2B-C1B	2.44	105.30	99.89
3	F	802	ACO	C3B-C2B-C1B	2.31	105.01	99.89
3	D	803	ACO	C3B-C2B-C1B	2.28	104.94	99.89
3	A	802	ACO	P2A-O3A-P1A	-2.25	125.11	132.83
3	F	802	ACO	C6P-C7P-N8P	-2.24	107.37	111.90
3	E	802	ACO	C3B-C2B-C1B	2.19	104.74	99.89
3	D	803	ACO	O6A-CCP-CBP	-2.17	107.06	110.55
3	B	802	ACO	C3B-C2B-C1B	2.13	104.60	99.89
3	F	802	ACO	CDP-CBP-CAP	2.10	112.46	108.82
3	E	802	ACO	CEP-CBP-CCP	2.10	111.66	108.23
3	B	802	ACO	P2A-O3A-P1A	-2.08	125.69	132.83
3	B	802	ACO	C3P-N4P-C5P	-2.05	119.03	122.84
3	D	803	ACO	O9P-C9P-N8P	-2.02	118.67	122.99
3	E	802	ACO	CEP-CBP-CAP	2.00	112.30	108.82
3	E	802	ACO	C1B-N9A-C4A	-2.00	123.13	126.64

There are no chirality outliers.

All (69) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802	ACO	C5B-O5B-P1A-O3A
3	A	802	ACO	CCP-O6A-P2A-O3A
3	A	802	ACO	C3P-C2P-S1P-C
3	C	802	ACO	C5B-O5B-P1A-O2A
3	C	802	ACO	C3P-C2P-S1P-C
3	F	802	ACO	C5B-O5B-P1A-O1A
3	F	802	ACO	C5B-O5B-P1A-O2A
3	F	802	ACO	C3P-C2P-S1P-C
3	D	803	ACO	C3B-O3B-P3B-O7A

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	803	ACO	C5B-O5B-P1A-O1A
3	D	803	ACO	C5B-O5B-P1A-O2A
3	D	803	ACO	C5B-O5B-P1A-O3A
3	D	803	ACO	C9P-CAP-CBP-CCP
3	D	803	ACO	C3P-C2P-S1P-C
3	B	802	ACO	C3P-C2P-S1P-C
3	E	802	ACO	C3B-O3B-P3B-O7A
3	E	802	ACO	C3P-C2P-S1P-C
2	E	801	PEG	O2-C3-C4-O4
2	C	801	PEG	O1-C1-C2-O2
3	B	802	ACO	C3B-C4B-C5B-O5B
2	F	801	PEG	O2-C3-C4-O4
3	B	802	ACO	O4B-C4B-C5B-O5B
2	D	802	PEG	O2-C3-C4-O4
2	A	801	PEG	O1-C1-C2-O2
2	E	801	PEG	O1-C1-C2-O2
3	D	803	ACO	OAP-CAP-CBP-CEP
3	B	802	ACO	C3B-O3B-P3B-O7A
2	D	802	PEG	C4-C3-O2-C2
3	A	802	ACO	C3B-O3B-P3B-O9A
3	D	803	ACO	C3B-O3B-P3B-O8A
3	B	802	ACO	C3B-O3B-P3B-O8A
3	B	802	ACO	C5B-O5B-P1A-O3A
3	A	802	ACO	C5B-O5B-P1A-O1A
3	A	802	ACO	C5B-O5B-P1A-O2A
3	A	802	ACO	CCP-O6A-P2A-O5A
3	C	802	ACO	C5B-O5B-P1A-O1A
3	B	802	ACO	C5B-O5B-P1A-O2A
2	C	801	PEG	O2-C3-C4-O4
2	F	801	PEG	O1-C1-C2-O2
3	D	803	ACO	OAP-CAP-CBP-CCP
2	E	801	PEG	C4-C3-O2-C2
3	B	802	ACO	C4B-C5B-O5B-P1A
3	A	802	ACO	P2A-O3A-P1A-O2A
3	C	802	ACO	P1A-O3A-P2A-O5A
3	F	802	ACO	P1A-O3A-P2A-O5A
3	B	802	ACO	P1A-O3A-P2A-O5A
3	E	802	ACO	P1A-O3A-P2A-O5A
3	E	802	ACO	O4B-C4B-C5B-O5B
3	C	802	ACO	O9P-C9P-CAP-OAP
3	C	802	ACO	C3B-O3B-P3B-O7A
3	D	803	ACO	C9P-CAP-CBP-CDP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	D	803	ACO	C9P-CAP-CBP-CEP
3	C	802	ACO	C3B-O3B-P3B-O8A
3	C	802	ACO	C3B-O3B-P3B-O9A
3	C	802	ACO	C5B-O5B-P1A-O3A
3	C	802	ACO	OAP-CAP-CBP-CEP
3	F	802	ACO	C3B-O3B-P3B-O8A
3	F	802	ACO	C5B-O5B-P1A-O3A
3	D	803	ACO	OAP-CAP-CBP-CDP
3	A	802	ACO	O4B-C4B-C5B-O5B
3	D	803	ACO	O4B-C4B-C5B-O5B
3	A	802	ACO	P2A-O3A-P1A-O1A
3	C	802	ACO	P1A-O3A-P2A-O4A
3	D	803	ACO	P2A-O3A-P1A-O2A
3	B	802	ACO	P1A-O3A-P2A-O4A
3	B	802	ACO	CCP-O6A-P2A-O4A
3	E	802	ACO	C3B-C4B-C5B-O5B
2	C	801	PEG	C1-C2-O2-C3
2	B	801	PEG	C1-C2-O2-C3

There are no ring outliers.

7 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802	ACO	4	0
3	F	802	ACO	2	0
3	B	802	ACO	4	0
3	D	803	ACO	3	0
4	D	801	EDO	5	0
3	C	802	ACO	3	0
3	E	802	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 A 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ACO F 802	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ACO B 802

Bond lengths

Bond angles

Torsions

Rings

Ligand ACO D 803

Bond lengths

Bond angles

Torsions

Rings

Ligand ACO C 802

Bond lengths

Bond angles

Torsions

Rings

Ligand ACO E 802

Bond lengths

Bond angles

Torsions

Rings
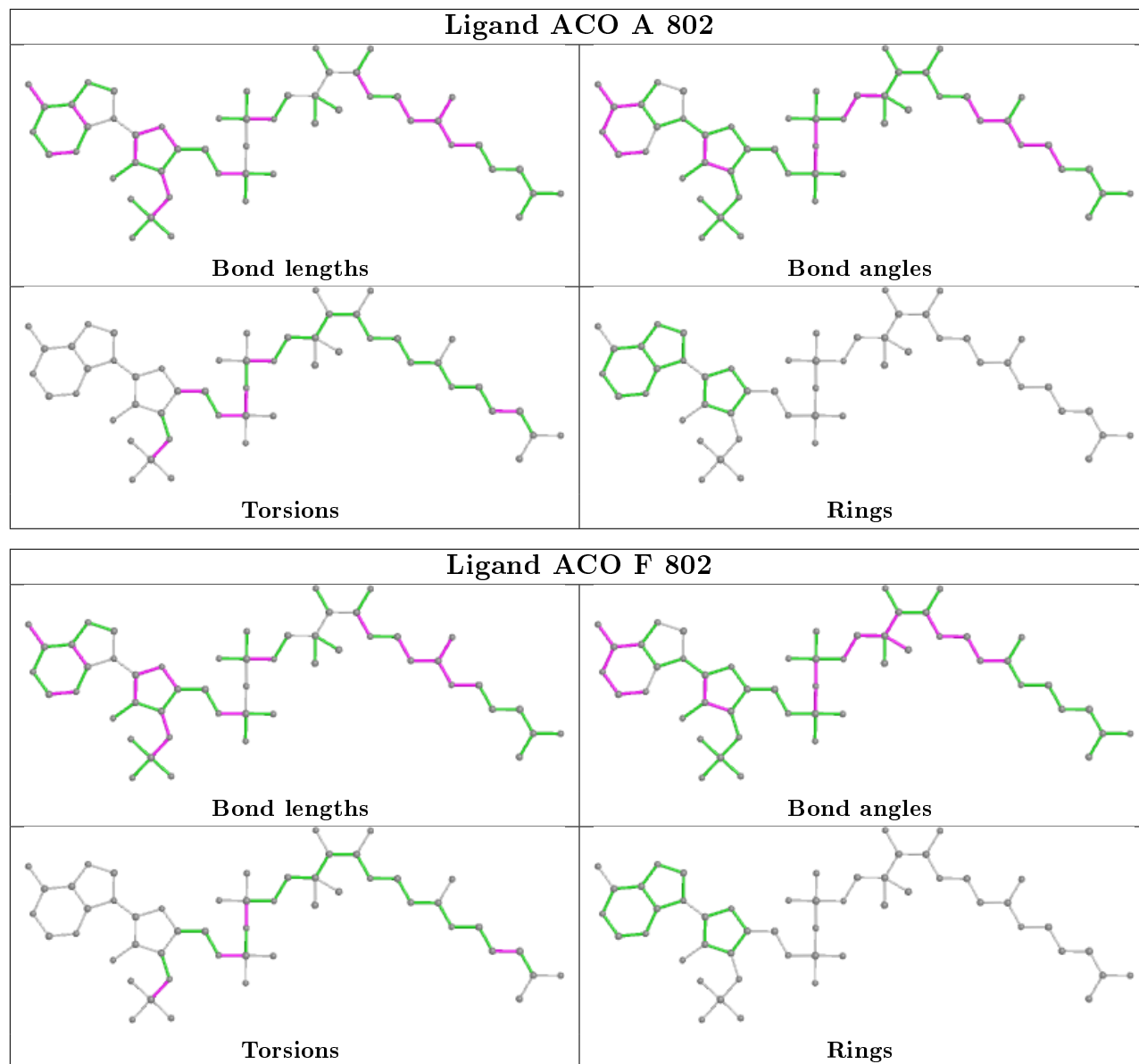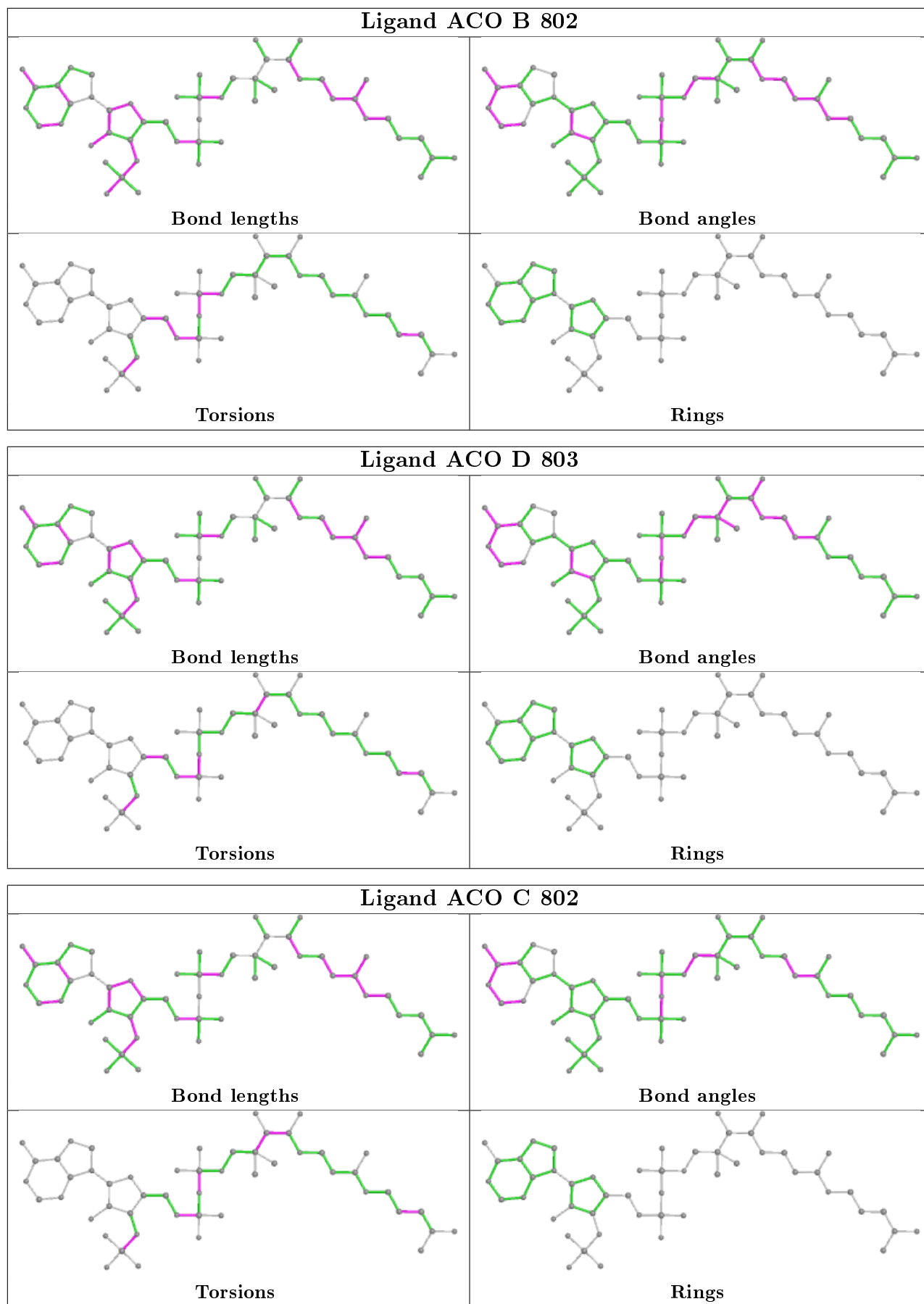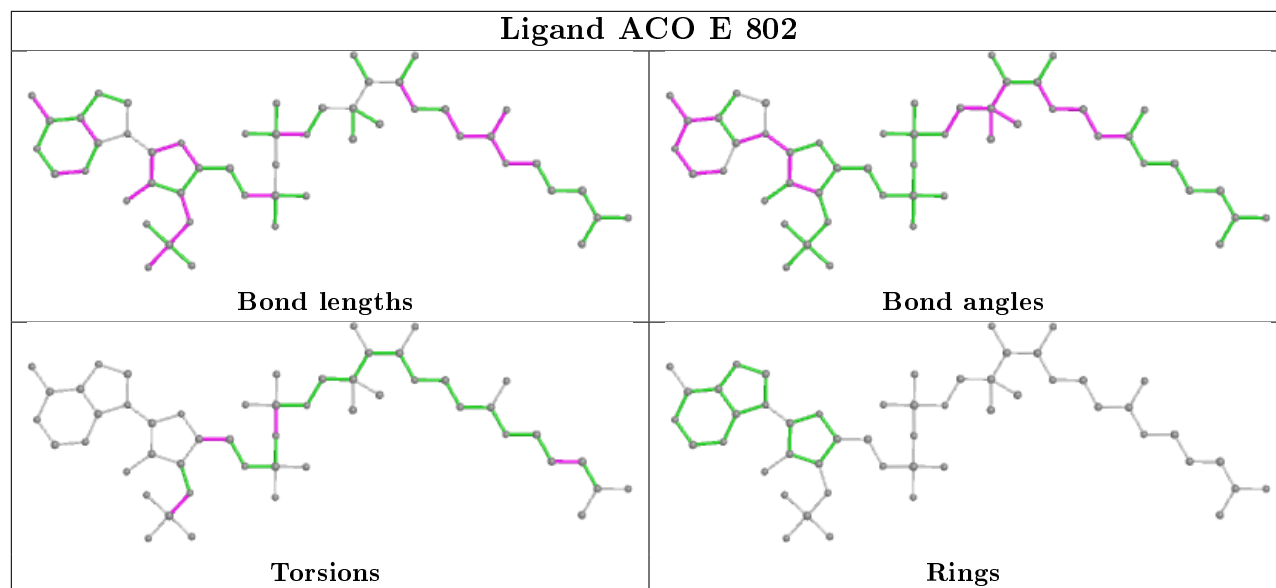
5.7 Other polymers (i)

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 (i)

6.1 Protein, DNA and RNA chains (i)

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	336/362 (92%)	0.09	7 (2%)	63	72	34, 53, 93, 118	0
1	B	337/362 (93%)	0.06	8 (2%)	59	68	39, 56, 94, 113	0
1	C	336/362 (92%)	0.23	16 (4%)	30	40	41, 64, 99, 121	0
1	D	336/362 (92%)	0.18	9 (2%)	54	63	40, 60, 102, 129	0
1	E	338/362 (93%)	0.02	3 (0%)	84	89	28, 46, 84, 101	0
1	F	338/362 (93%)	0.01	3 (0%)	84	89	30, 43, 72, 89	0
All	All	2021/2172 (93%)	0.10	46 (2%)	60	69	28, 54, 93, 129	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	510	LEU	5.0
1	C	509	LEU	4.6
1	C	604	GLU	3.9
1	D	456	ALA	3.7
1	E	525	PHE	3.6
1	A	441	VAL	3.2
1	B	512	ASP	3.1
1	B	510	LEU	3.1
1	D	510	LEU	3.0
1	D	605	ASP	2.8
1	D	450	VAL	2.8
1	C	443	ILE	2.7
1	C	727	ILE	2.7
1	A	729	LYS	2.7
1	D	486	ILE	2.6
1	C	608	LEU	2.6
1	D	497	ARG	2.5
1	F	440	LYS	2.5
1	E	605	ASP	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	487	CYS	2.5
1	A	510	LEU	2.5
1	A	448	ASN	2.5
1	C	776	SER	2.5
1	C	505	LEU	2.4
1	E	497	ARG	2.3
1	A	508	PRO	2.3
1	B	772	GLU	2.3
1	C	601	VAL	2.3
1	C	512	ASP	2.3
1	B	774	LEU	2.3
1	B	457	ASN	2.2
1	C	458	GLY	2.2
1	C	605	ASP	2.2
1	B	482	VAL	2.2
1	F	496	GLU	2.1
1	F	460	GLU	2.1
1	B	592	GLU	2.1
1	A	512	ASP	2.1
1	D	475	LEU	2.1
1	D	769	TYR	2.1
1	D	441	VAL	2.1
1	C	459	GLY	2.1
1	C	447	ILE	2.0
1	A	691	GLU	2.0
1	B	440	LYS	2.0
1	C	525	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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	PEG	D	802	7/7	0.71	0.21	70,71,76,78	0
2	PEG	C	801	7/7	0.75	0.20	79,86,87,91	0
2	PEG	E	801	7/7	0.76	0.17	57,61,65,71	0
2	PEG	A	801	7/7	0.84	0.14	68,76,82,82	0
2	PEG	F	801	7/7	0.88	0.13	59,62,69,76	0
2	PEG	B	801	7/7	0.92	0.13	65,66,72,73	0
3	ACO	C	802	51/51	0.92	0.13	38,70,87,94	0
3	ACO	B	802	51/51	0.92	0.13	41,61,83,93	0
3	ACO	A	802	51/51	0.93	0.13	34,54,77,86	0
3	ACO	E	802	51/51	0.93	0.12	36,53,78,95	0
3	ACO	F	802	51/51	0.94	0.13	37,58,75,80	0
3	ACO	D	803	51/51	0.94	0.12	44,62,82,91	0
4	EDO	D	801	4/4	0.95	0.27	56,59,60,61	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.
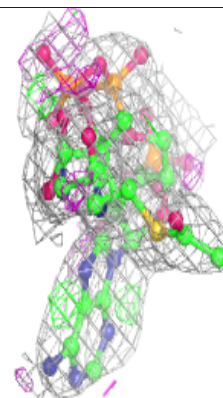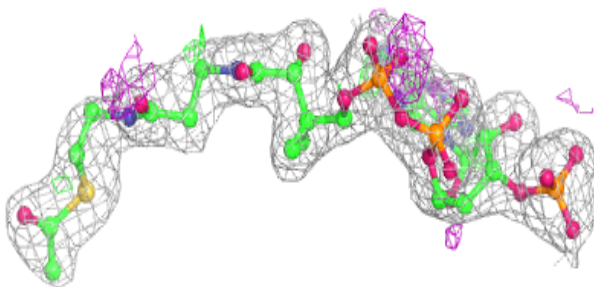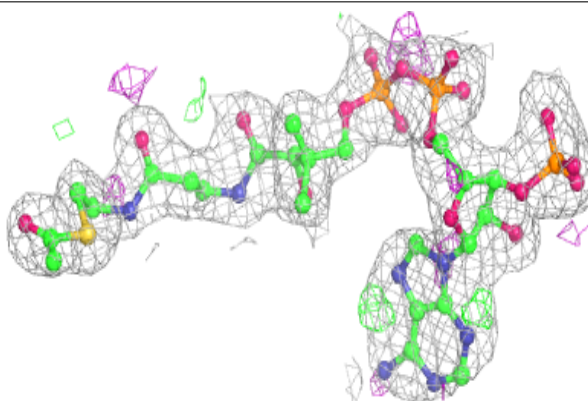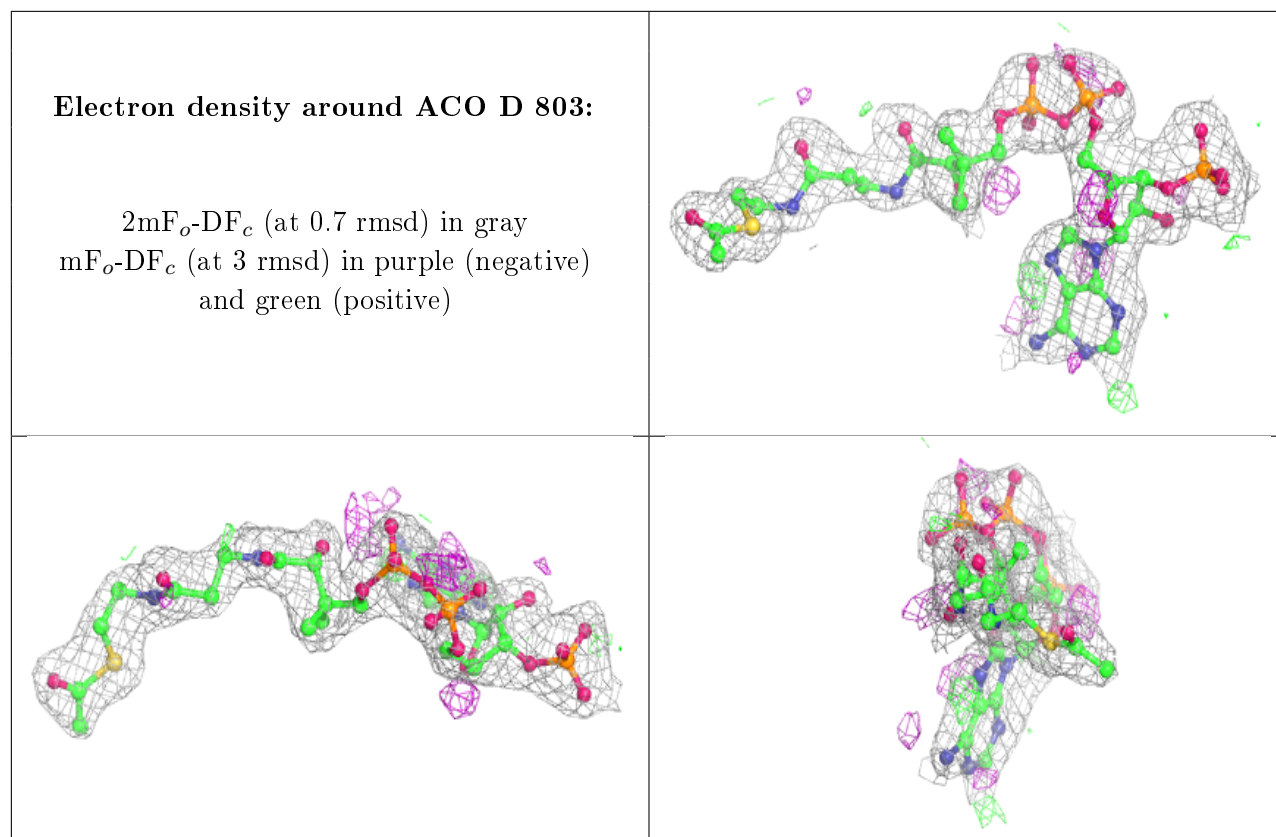

Electron density around ACO C 802:

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 802:

$2mF_o$-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 802:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
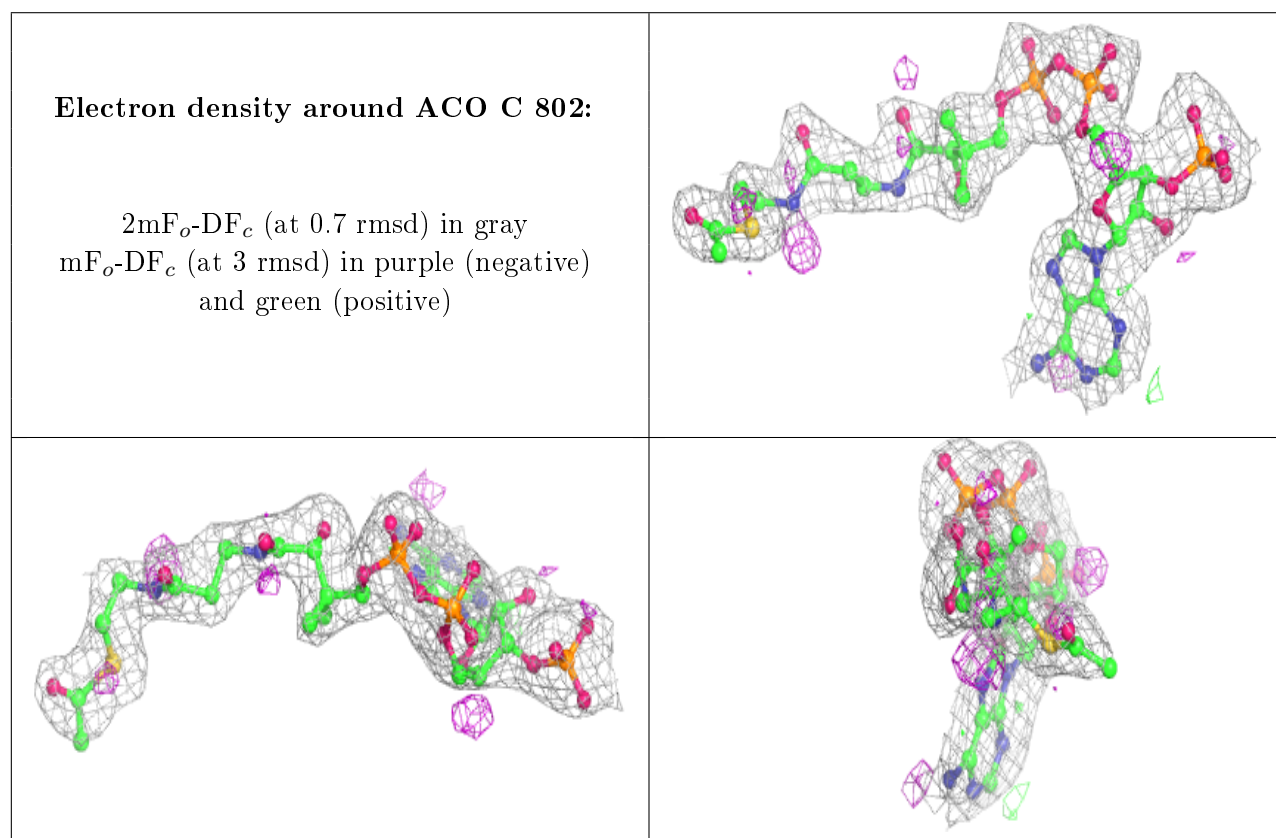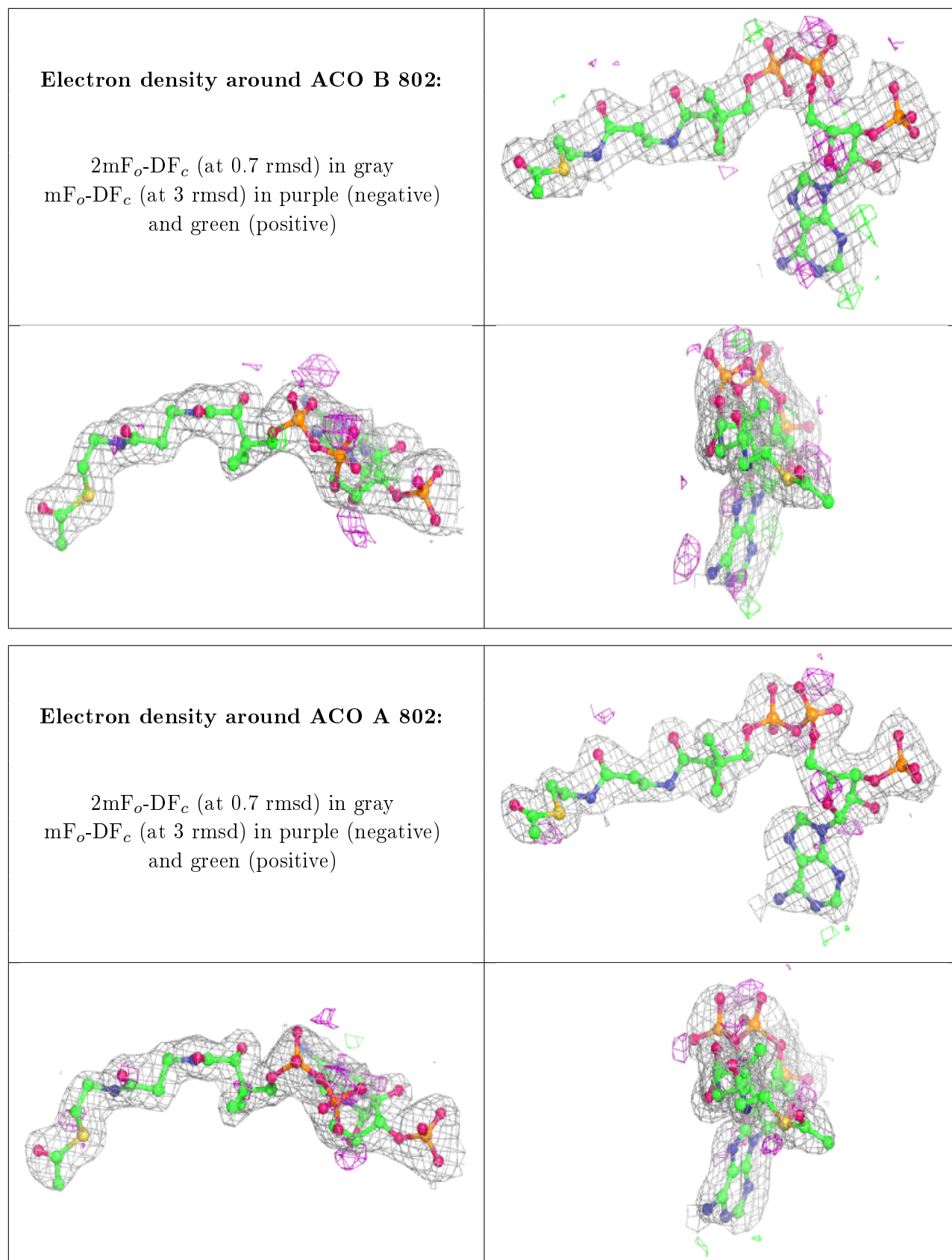
Electron density around ACO E 802:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
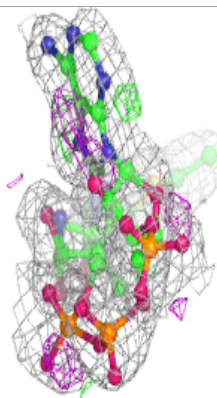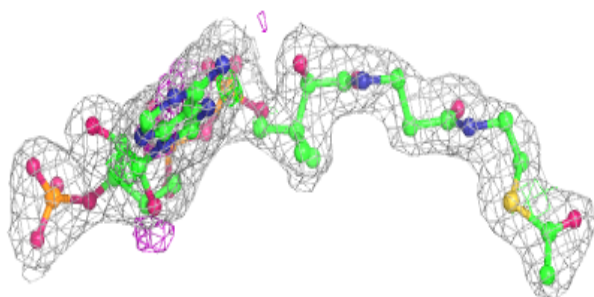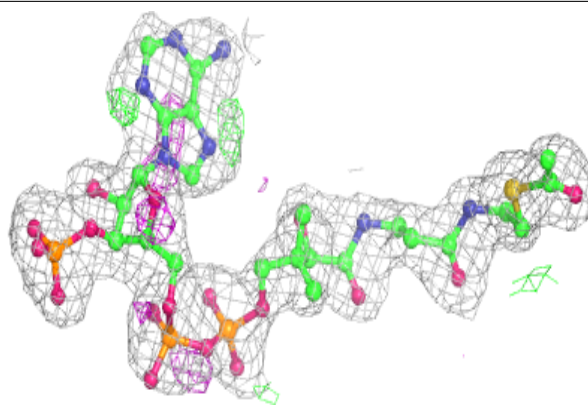
Electron density around ACO F 802:

$2mF_o$-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 803:

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

6.5 Other polymers (i)

There are no such residues in this entry.