Full wwPDB X-ray Structure Validation Report (i)

Oct 11, 2023 – 03:51 AM EDT

PDB ID	:	7L3Q
Title	:	Crystal Structure of Acetyl-CoA synthetase in complex with adenosine-5'-methylphosphate and Co-enzyme A from Coccidioides immitis RS
Authors	:	Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on	:	2020-12-18
Resolution	:	2.15 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 types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

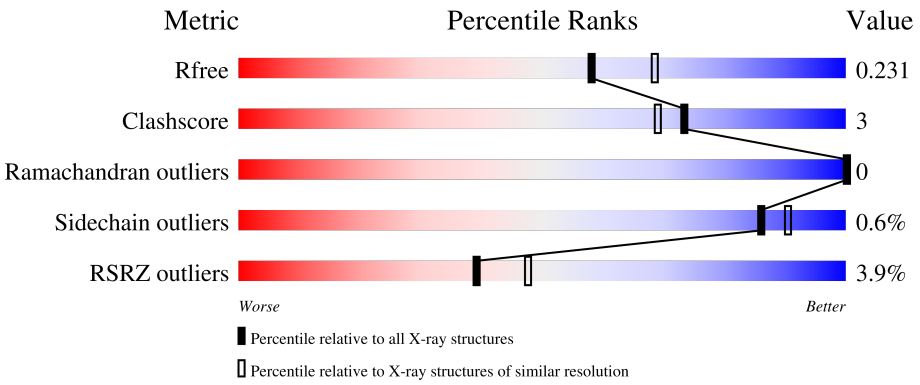
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

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 2.15 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	1479 (2.16-2.16)
Clashscore	141614	1585 (2.16-2.16)
Ramachandran outliers	138981	1560 (2.16-2.16)
Sidechain outliers	138945	1559 (2.16-2.16)
RSRZ outliers	127900	1456 (2.16-2.16)

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	706	5% 83% 6% 11%
1	B	706	2% 81% 8% 11%
1	C	706	3% 82% 7% 11%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 15268 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 Acetyl-coenzyme A synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	631	4842	3095	838	890	19	0	4	0
1	B	629	4820	3084	833	885	18	0	3	0
1	C	629	4785	3060	825	882	18	0	4	0

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-14	MET	-	initiating methionine	UNP J3KJC6
A	-13	HIS	-	expression tag	UNP J3KJC6
A	-12	HIS	-	expression tag	UNP J3KJC6
A	-11	HIS	-	expression tag	UNP J3KJC6
A	-10	HIS	-	expression tag	UNP J3KJC6
A	-9	HIS	-	expression tag	UNP J3KJC6
A	-8	HIS	-	expression tag	UNP J3KJC6
A	-7	HIS	-	expression tag	UNP J3KJC6
A	-6	HIS	-	expression tag	UNP J3KJC6
A	-5	GLU	-	expression tag	UNP J3KJC6
A	-4	ASN	-	expression tag	UNP J3KJC6
A	-3	LEU	-	expression tag	UNP J3KJC6
A	-2	TYR	-	expression tag	UNP J3KJC6
A	-1	PHE	-	expression tag	UNP J3KJC6
A	0	GLN	-	expression tag	UNP J3KJC6
A	1	GLY	-	expression tag	UNP J3KJC6
B	-14	MET	-	initiating methionine	UNP J3KJC6
B	-13	HIS	-	expression tag	UNP J3KJC6
B	-12	HIS	-	expression tag	UNP J3KJC6
B	-11	HIS	-	expression tag	UNP J3KJC6
B	-10	HIS	-	expression tag	UNP J3KJC6
B	-9	HIS	-	expression tag	UNP J3KJC6
B	-8	HIS	-	expression tag	UNP J3KJC6

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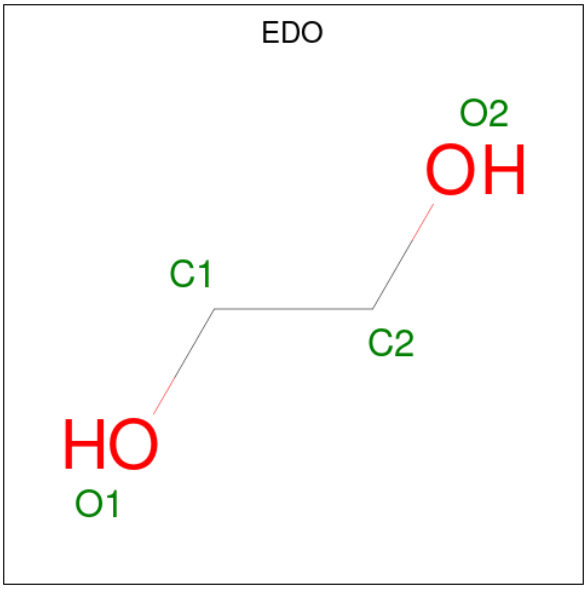
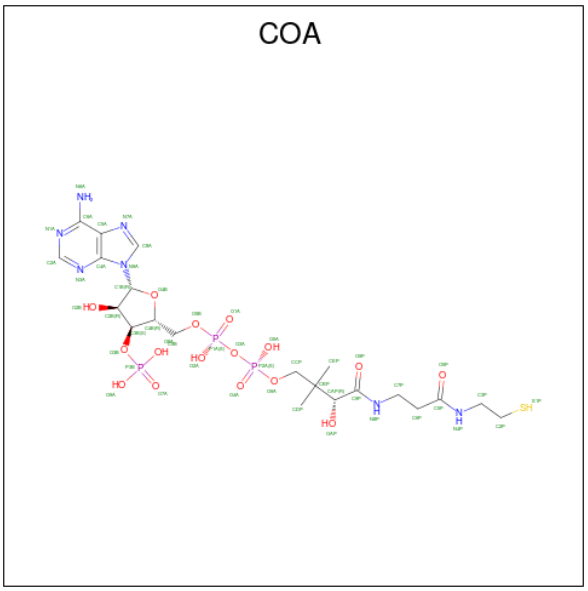
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP J3KJC6
B	-6	HIS	-	expression tag	UNP J3KJC6
B	-5	GLU	-	expression tag	UNP J3KJC6
B	-4	ASN	-	expression tag	UNP J3KJC6
B	-3	LEU	-	expression tag	UNP J3KJC6
B	-2	TYR	-	expression tag	UNP J3KJC6
B	-1	PHE	-	expression tag	UNP J3KJC6
B	0	GLN	-	expression tag	UNP J3KJC6
B	1	GLY	-	expression tag	UNP J3KJC6
C	-14	MET	-	initiating methionine	UNP J3KJC6
C	-13	HIS	-	expression tag	UNP J3KJC6
C	-12	HIS	-	expression tag	UNP J3KJC6
C	-11	HIS	-	expression tag	UNP J3KJC6
C	-10	HIS	-	expression tag	UNP J3KJC6
C	-9	HIS	-	expression tag	UNP J3KJC6
C	-8	HIS	-	expression tag	UNP J3KJC6
C	-7	HIS	-	expression tag	UNP J3KJC6
C	-6	HIS	-	expression tag	UNP J3KJC6
C	-5	GLU	-	expression tag	UNP J3KJC6
C	-4	ASN	-	expression tag	UNP J3KJC6
C	-3	LEU	-	expression tag	UNP J3KJC6
C	-2	TYR	-	expression tag	UNP J3KJC6
C	-1	PHE	-	expression tag	UNP J3KJC6
C	0	GLN	-	expression tag	UNP J3KJC6
C	1	GLY	-	expression tag	UNP J3KJC6

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



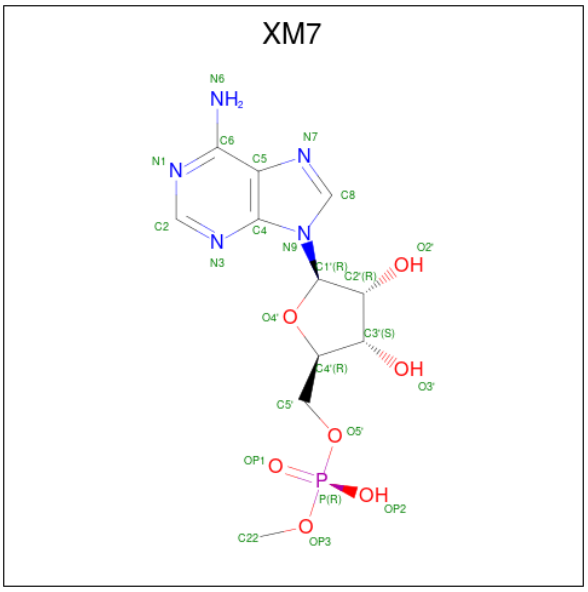
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	4	2	2	0	0
			Total	C	O		
2	A	1	4	2	2	0	0
			Total	C	O		
2	A	1	4	2	2	0	0
			Total	C	O		
2	A	1	4	2	2	0	0
			Total	C	O		
2	A	1	4	2	2	0	0
			Total	C	O		
2	A	1	4	2	2	0	0
			Total	C	O		
2	B	1	4	2	2	0	0
			Total	C	O		
2	B	1	4	2	2	0	0
			Total	C	O		
2	B	1	4	2	2	0	0
			Total	C	O		
2	B	1	4	2	2	0	0
			Total	C	O		
2	B	1	4	2	2	0	0
			Total	C	O		
2	B	1	4	2	2	0	0
			Total	C	O		
2	C	1	4	2	2	0	0
			Total	C	O		
2	C	1	4	2	2	0	0
			Total	C	O		
2	C	1	4	2	2	0	0
			Total	C	O		
2	C	1	4	2	2	0	0

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
3	A	1	48	21	7	16	3	1	0	0
			Total	C	N	O	P	S		
3	B	1	48	21	7	16	3	1	0	0
			Total	C	N	O	P	S		
3	C	1	48	21	7	16	3	1	0	0

- Molecule 4 is 5'-O-[(R)-hydroxy(methoxy)phosphoryl]adenosine (three-letter code: XM7) (formula: $C_{11}H_{16}N_5O_7P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
4	A	1	24	11	5	7	1	0	0
			Total	C	N	O	P		
4	B	1	24	11	5	7	1	0	0
			Total	C	N	O	P		
4	C	1	24	11	5	7	1	0	0

- Molecule 5 is water.

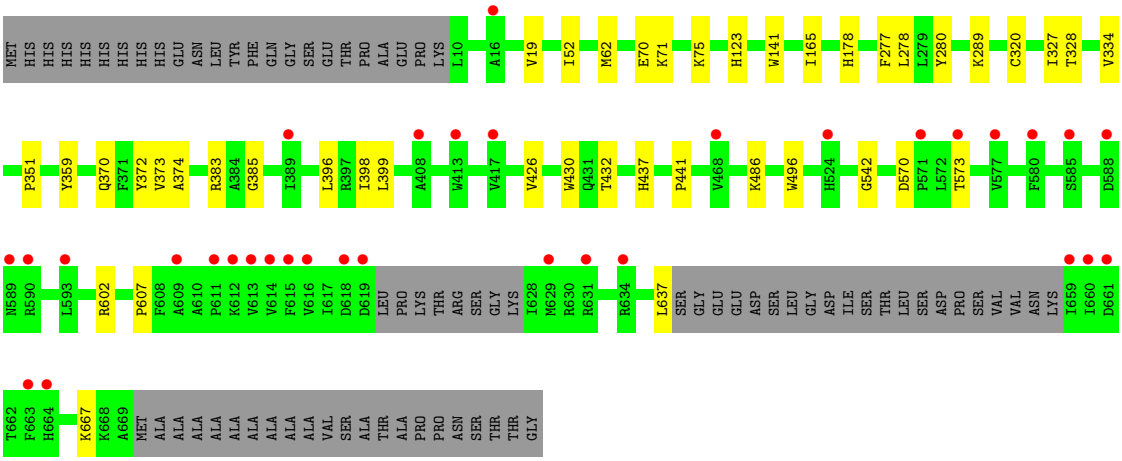
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
5	A	182	182	182	0	0
			Total	O		
5	B	197	198	198	0	1
			Total	O		
5	C	161	161	161	0	0

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.

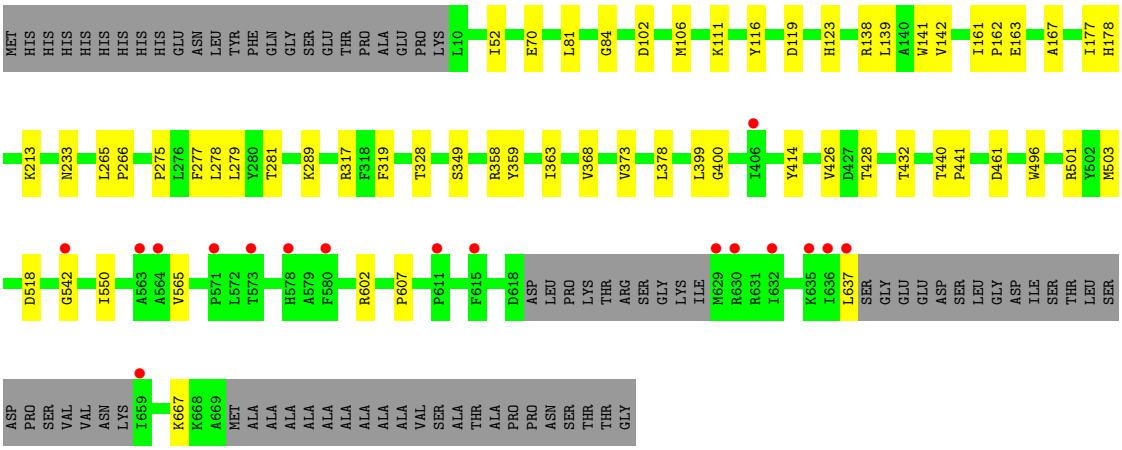
• Molecule 1: Acetyl-coenzyme A synthetase

Chain A: 5% 83% 6% 11%



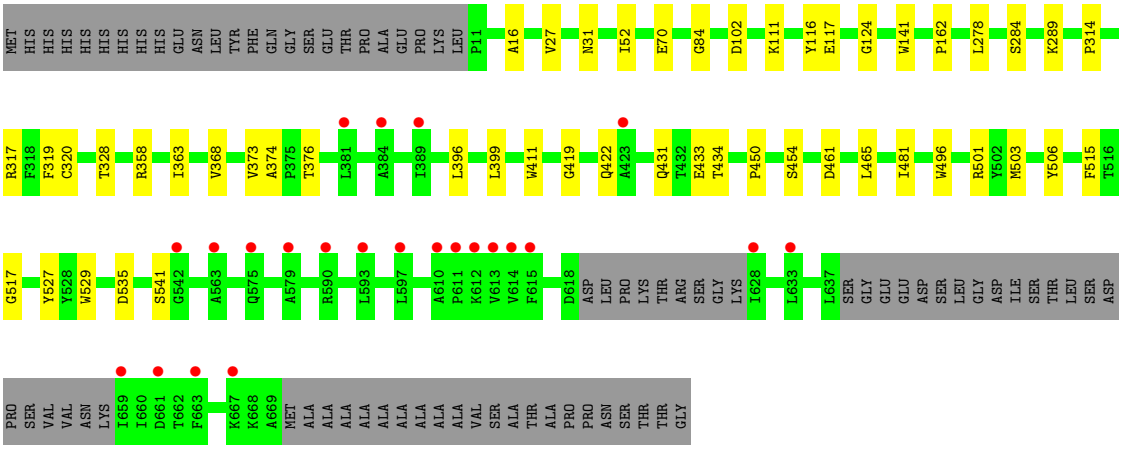
• Molecule 1: Acetyl-coenzyme A synthetase

Chain B: 2% 81% 8% 11%



• Molecule 1: Acetyl-coenzyme A synthetase

Chain C: 3% 82% 7% 11%


MET HIS HIS HIS HIS HIS HIS HIS HIS GLU ASN LEU TYR PHE GLN GLY SER GLU THR PRO ALA GLU PRO LYS LEU P11
A16
V27
N31
I52
E70
G84
D102
K111
Y116 E117
G124
W141
P162
L278
S284
K289
P314
R317 E318 F319 C320
T328
R358
I363
V368
V373 A374
P375 T376
L381
A384
I389
L396
L399
W411
G419
Q422 A423
Q431 T432 E433 T434
P450
S454
D461
L465
I481
W496
R501 Y502 M503
Y506
F515 T516
G517
Y527 Y528 W529
D535
S541 G542
A553
Q575
A579
R590
L593
L597
A610 P611 K612 V613 V614 F615
D618 ASP LEU PRO LYS THR ARG SER GLY LYS
I628
L633
L637 SER GLY GLU GLU ASP SER LEU GLY ASP ILE SER THR LEU SER ASP
PRO SER VAL VAL ASN LYS
I659 I660 D661 T662 F663
K667 K668 A669
MET ALA ALA ALA ALA ALA ALA ALA ALA ALA ALA VAL SER ALA THR ALA PRO PRO ASN SER THR THR GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	106.44Å 116.27Å 106.82Å 90.00° 119.73° 90.00°	Depositor
Resolution (Å)	46.38 – 2.15 48.53 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.1 (46.38-2.15) 92.6 (48.53-2.15)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.16Å)	Xtriage
Refinement program	PHENIX 1.19RC4-4035	Depositor
R, R_{free}	0.187 , 0.233 0.187 , 0.231	Depositor DCC
R_{free} test set	2058 reflections (1.78%)	wwPDB-VP
Wilson B-factor (Å^2)	38.2	Xtriage
Anisotropy	0.323	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 39.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Estimated twinning fraction	0.378 for -h-l,k,h 0.378 for l,k,-h-l 0.064 for h,-k,-h-l 0.057 for -h-l,-k,l 0.055 for l,-k,h	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	15268	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.49% 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: EDO, XM7, COA

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	0.39	0/4981	0.59	0/6787
1	B	0.40	0/4963	0.60	0/6767
1	C	0.39	0/4930	0.58	0/6726
All	All	0.40	0/14874	0.59	0/20280

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4842	0	4576	28	0
1	B	4820	0	4551	38	0
1	C	4785	0	4491	29	0
2	A	24	0	36	3	0
2	B	24	0	36	4	0
2	C	16	0	24	4	0
3	A	48	0	32	2	0
3	B	48	0	32	2	0
3	C	48	0	32	1	0
4	A	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	24	0	0	1	0
4	C	24	0	0	0	0
5	A	182	0	0	2	0
5	B	198	0	0	4	0
5	C	161	0	0	1	0
All	All	15268	0	13810	93	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 3.

All (93) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:LYS:HE3	1:B:70[A]:GLU:HG3	1.62	0.81
1:C:289:LYS:NZ	5:C:903:HOH:O	2.28	0.66
1:B:123:HIS:HB3	5:B:803:HOH:O	1.95	0.66
2:A:708:EDO:H21	1:B:70[B]:GLU:HG2	1.77	0.66
1:B:281:THR:HG21	1:B:432:THR:HG21	1.78	0.65
1:A:123:HIS:HB3	5:A:805:HOH:O	1.98	0.64
1:B:542:GLY:HA3	3:B:706:COA:H61	1.81	0.63
1:B:111:LYS:NZ	5:B:804:HOH:O	2.31	0.61
1:A:278:LEU:HD21	1:A:496:TRP:CE3	2.35	0.61
1:A:426:VAL:HG13	1:A:441:PRO:HG2	1.83	0.61
1:B:496:TRP:CZ3	2:B:703:EDO:H21	2.36	0.61
1:B:363:ILE:HG23	1:B:368:VAL:HB	1.83	0.60
1:C:117:GLU:OE2	1:C:358:ARG:NH1	2.31	0.59
1:B:637:LEU:HD23	1:B:667:LYS:HD2	1.84	0.58
2:A:705:EDO:H22	1:B:141:TRP:CZ3	2.39	0.58
1:B:233:ASN:OD1	5:B:801:HOH:O	2.17	0.57
1:C:496:TRP:CZ3	2:C:803:EDO:H21	2.39	0.57
1:B:161:ILE:HG13	1:B:163:GLU:HB2	1.85	0.57
2:B:708:EDO:H21	1:C:70:GLU:HG2	1.86	0.57
1:A:637:LEU:HD22	1:A:667:LYS:HD3	1.86	0.56
1:B:111:LYS:HD3	2:B:704:EDO:H21	1.88	0.56
1:A:496:TRP:CZ3	2:A:705:EDO:H21	2.44	0.53
1:B:279:LEU:O	1:B:281:THR:HG23	2.09	0.53
1:B:289:LYS:HG2	1:B:501:ARG:CZ	2.39	0.53
1:B:111:LYS:NZ	5:B:802:HOH:O	2.24	0.52
1:A:373:VAL:HG22	1:A:374:ALA:H	1.75	0.52
1:B:119:ASP:HA	1:B:349:SER:HB2	1.92	0.51
1:A:52:ILE:O	1:A:486:LYS:NZ	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:278:LEU:HD21	1:C:496:TRP:CE3	2.46	0.51
1:C:373:VAL:HG22	1:C:374:ALA:H	1.74	0.51
1:C:465:LEU:HB2	1:C:481:ILE:HB	1.92	0.50
1:C:111:LYS:NZ	1:C:314:PRO:O	2.38	0.50
1:A:396:LEU:HD21	1:A:399:LEU:HD21	1.94	0.50
1:C:396:LEU:HD21	1:C:399:LEU:HD21	1.94	0.49
1:A:602:ARG:HG2	1:A:607:PRO:HA	1.96	0.48
1:C:284:SER:OG	1:C:535:ASP:HB2	2.14	0.48
1:A:70:GLU:HG2	2:C:801:EDO:H12	1.96	0.47
1:A:327:ILE:HG12	1:A:432:THR:HA	1.96	0.47
1:C:363:ILE:HG23	1:C:368:VAL:HB	1.96	0.47
1:A:178:HIS:CE1	1:A:277:PHE:HB3	2.49	0.47
1:C:515:PHE:CZ	1:C:517:GLY:HA2	2.50	0.47
1:C:116:TYR:CD2	1:C:124:GLY:HA2	2.50	0.46
1:C:52:ILE:HD12	1:C:461:ASP:HB2	1.96	0.46
1:C:496:TRP:CE3	2:C:803:EDO:H21	2.51	0.46
1:A:328:THR:HG21	3:A:706:COA:S1P	2.56	0.46
1:B:428:THR:HG22	1:B:440:THR:OG1	2.15	0.46
1:A:430:TRP:HB3	1:A:437:HIS:HA	1.98	0.45
1:B:399:LEU:HB3	1:B:414:TYR:CZ	2.52	0.45
1:C:116:TYR:CD1	1:C:162:PRO:HD3	2.51	0.45
1:B:518:ASP:OD2	4:B:707:XM7:O3'	2.35	0.45
1:B:550:ILE:HG22	1:B:565:VAL:HG21	1.99	0.45
1:A:351:PRO:HB3	1:A:359:TYR:CE2	2.52	0.44
1:C:289:LYS:HG2	1:C:501:ARG:CZ	2.47	0.44
1:A:75:LYS:HE2	1:B:106:MET:O	2.18	0.44
1:A:280:TYR:HA	1:A:289:LYS:O	2.17	0.44
1:C:374:ALA:HB2	3:C:805:COA:H21	1.99	0.44
1:C:84:GLY:HA3	1:C:503:MET:SD	2.57	0.44
1:C:431:GLN:HG2	1:C:434:THR:HG23	1.99	0.44
1:A:141:TRP:CZ3	2:C:803:EDO:H22	2.52	0.44
1:A:570:ASP:OD2	1:A:573:THR:N	2.40	0.43
1:B:426:VAL:HA	1:B:441:PRO:HG2	1.98	0.43
1:C:454:SER:HA	1:C:527:TYR:CD2	2.53	0.43
1:A:370:GLN:HG3	1:A:398:ILE:HB	2.00	0.43
1:B:265:LEU:HD12	1:B:266:PRO:HD2	2.01	0.43
1:B:278:LEU:HD21	1:B:496:TRP:CE3	2.54	0.43
1:C:411:TRP:CD2	1:C:450:PRO:HB3	2.53	0.43
1:A:19:VAL:O	1:A:19:VAL:HG23	2.19	0.43
1:B:52:ILE:HD12	1:B:461:ASP:HB2	2.01	0.43
1:B:84:GLY:HA3	1:B:503:MET:SD	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:542:GLY:HA3	3:A:706:COA:H61	2.01	0.42
2:B:703:EDO:H22	1:C:141:TRP:CZ3	2.54	0.42
1:B:400:GLY:HA2	1:B:426:VAL:HG23	2.01	0.42
1:B:373:VAL:HG11	1:B:378:LEU:HD21	2.02	0.42
1:C:27:VAL:HG12	1:C:31:ASN:ND2	2.35	0.42
1:A:426:VAL:HA	1:A:441:PRO:HG2	2.02	0.42
1:C:376:THR:HG21	1:C:541:SER:HA	2.01	0.42
1:C:433:GLU:HG2	1:C:506:TYR:CZ	2.55	0.41
1:B:139:LEU:HD21	1:B:167:ALA:HA	2.02	0.41
1:C:16:ALA:HB2	1:C:529:TRP:CE2	2.55	0.41
1:C:320:CYS:SG	1:C:328:THR:HG22	2.60	0.41
1:B:116:TYR:CD1	1:B:162:PRO:HD3	2.56	0.41
1:A:320:CYS:HA	1:A:372:TYR:HB3	2.03	0.41
1:B:602:ARG:HG2	1:B:607:PRO:HA	2.03	0.41
1:B:358:ARG:HD2	1:B:358:ARG:HA	1.89	0.41
1:A:385:GLY:HA2	5:A:930:HOH:O	2.21	0.41
1:B:81:LEU:HD23	1:B:81:LEU:HA	1.87	0.41
1:B:138:ARG:O	1:B:142:VAL:HG23	2.21	0.41
1:C:419:GLY:O	1:C:422:GLN:HB2	2.21	0.41
1:B:177:ILE:HD13	1:B:275:PRO:HB2	2.03	0.40
1:B:328:THR:HG21	3:B:706:COA:S1P	2.61	0.40
1:A:62:MET:HE3	1:A:62:MET:HB2	1.91	0.40
1:B:178:HIS:CE1	1:B:277:PHE:HB3	2.57	0.40
1:A:165:ILE:HG12	1:A:334:VAL:HG22	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	629/706 (89%)	605 (96%)	24 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	626/706 (89%)	600 (96%)	26 (4%)	0	100	100
1	C	627/706 (89%)	597 (95%)	30 (5%)	0	100	100
All	All	1882/2118 (89%)	1802 (96%)	80 (4%)	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	484/584 (83%)	483 (100%)	1 (0%)	93	96
1	B	482/584 (82%)	477 (99%)	5 (1%)	76	81
1	C	475/584 (81%)	472 (99%)	3 (1%)	86	90
All	All	1441/1752 (82%)	1432 (99%)	9 (1%)	86	90

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	383	ARG
1	B	102	ASP
1	B	213	LYS
1	B	317	ARG
1	B	319	PHE
1	B	359	TYR
1	C	102	ASP
1	C	317	ARG
1	C	319	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	558	HIS
1	C	31	ASN

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Mol	Chain	Res	Type
1	C	422	GLN

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)

22 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	COA	B	706	-	41,50,50	3.58	12 (29%)	52,75,75	1.21	7 (13%)
3	COA	A	706	-	41,50,50	3.62	14 (34%)	52,75,75	1.32	6 (11%)
2	EDO	B	704	-	3,3,3	0.53	0	2,2,2	0.33	0
2	EDO	B	701	-	3,3,3	0.60	0	2,2,2	0.20	0
2	EDO	A	708	-	3,3,3	0.47	0	2,2,2	0.70	0
2	EDO	C	801	-	3,3,3	0.52	0	2,2,2	0.35	0
2	EDO	B	703	-	3,3,3	0.52	0	2,2,2	0.09	0
2	EDO	A	705	-	3,3,3	0.55	0	2,2,2	0.11	0
2	EDO	C	803	-	3,3,3	0.55	0	2,2,2	0.14	0
4	XM7	C	806	-	23,26,26	0.96	2 (8%)	25,39,39	0.93	0
4	XM7	B	707	-	23,26,26	0.99	2 (8%)	25,39,39	0.90	0
4	XM7	A	707	-	23,26,26	1.07	3 (13%)	25,39,39	1.03	1 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	EDO	A	702	-	3,3,3	0.52	0	2,2,2	0.41	0
2	EDO	A	701	-	3,3,3	0.60	0	2,2,2	0.12	0
2	EDO	B	702	-	3,3,3	0.54	0	2,2,2	0.54	0
2	EDO	A	703	-	3,3,3	0.53	0	2,2,2	0.43	0
2	EDO	A	704	-	3,3,3	0.50	0	2,2,2	0.29	0
2	EDO	C	804	-	3,3,3	0.45	0	2,2,2	0.16	0
2	EDO	B	705	-	3,3,3	0.65	0	2,2,2	0.21	0
2	EDO	B	708	-	3,3,3	0.53	0	2,2,2	0.55	0
2	EDO	C	802	-	3,3,3	0.54	0	2,2,2	0.16	0
3	COA	C	805	-	41,50,50	3.58	12 (29%)	52,75,75	1.23	6 (11%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COA	B	706	-	-	16/44/64/64	0/3/3/3
3	COA	A	706	-	-	8/44/64/64	0/3/3/3
2	EDO	B	704	-	-	1/1/1/1	-
2	EDO	B	701	-	-	0/1/1/1	-
2	EDO	A	708	-	-	1/1/1/1	-
2	EDO	C	801	-	-	0/1/1/1	-
2	EDO	B	703	-	-	0/1/1/1	-
2	EDO	A	705	-	-	0/1/1/1	-
2	EDO	C	803	-	-	0/1/1/1	-
4	XM7	C	806	-	-	3/9/29/29	0/3/3/3
4	XM7	B	707	-	-	2/9/29/29	0/3/3/3
4	XM7	A	707	-	-	6/9/29/29	0/3/3/3
2	EDO	A	702	-	-	1/1/1/1	-
2	EDO	A	701	-	-	0/1/1/1	-
2	EDO	B	702	-	-	0/1/1/1	-
2	EDO	A	703	-	-	0/1/1/1	-
2	EDO	A	704	-	-	0/1/1/1	-
2	EDO	C	804	-	-	0/1/1/1	-
2	EDO	B	705	-	-	1/1/1/1	-
2	EDO	B	708	-	-	0/1/1/1	-
2	EDO	C	802	-	-	0/1/1/1	-
3	COA	C	805	-	-	14/44/64/64	0/3/3/3

All (45) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	706	COA	C2B-C3B	-12.11	1.26	1.52
3	B	706	COA	C2B-C3B	-12.07	1.26	1.52
3	C	805	COA	C2B-C3B	-11.97	1.26	1.52
3	A	706	COA	C2B-C1B	9.78	1.68	1.53
3	C	805	COA	C2B-C1B	9.31	1.67	1.53
3	C	805	COA	O4B-C1B	-9.16	1.28	1.41
3	B	706	COA	C2B-C1B	9.14	1.67	1.53
3	B	706	COA	O4B-C1B	-8.91	1.28	1.41
3	A	706	COA	O4B-C1B	-8.77	1.28	1.41
3	A	706	COA	C9P-N8P	7.53	1.50	1.33
3	B	706	COA	C9P-N8P	7.50	1.50	1.33
3	C	805	COA	C9P-N8P	7.45	1.49	1.33
3	B	706	COA	C5P-N4P	7.34	1.50	1.33
3	C	805	COA	C5P-N4P	7.21	1.49	1.33
3	A	706	COA	C5P-N4P	7.10	1.49	1.33
3	A	706	COA	O4B-C4B	4.96	1.56	1.45
3	B	706	COA	O4B-C4B	4.73	1.55	1.45
3	C	805	COA	O4B-C4B	4.56	1.55	1.45
3	C	805	COA	C5B-C4B	-4.21	1.38	1.51
3	B	706	COA	C5B-C4B	-4.17	1.38	1.51
3	A	706	COA	C5B-C4B	-4.06	1.38	1.51
3	A	706	COA	P3B-O3B	3.79	1.66	1.59
3	B	706	COA	P3B-O3B	3.74	1.66	1.59
3	C	805	COA	P3B-O3B	3.44	1.65	1.59
3	A	706	COA	C6A-N6A	3.00	1.45	1.34
3	B	706	COA	C6A-N6A	2.81	1.44	1.34
3	C	805	COA	C6A-N6A	2.77	1.44	1.34
3	C	805	COA	OAP-CAP	-2.47	1.37	1.42
3	B	706	COA	OAP-CAP	-2.39	1.37	1.42
4	A	707	XM7	P-OP3	2.38	1.67	1.59
4	B	707	XM7	P-OP3	2.35	1.67	1.59
3	A	706	COA	C6P-C5P	2.33	1.55	1.51
4	A	707	XM7	C8-N7	-2.31	1.30	1.34
3	A	706	COA	OAP-CAP	-2.31	1.38	1.42
4	C	806	XM7	C8-N7	-2.25	1.30	1.34
4	C	806	XM7	P-OP3	2.21	1.67	1.59
4	A	707	XM7	P-O5'	2.20	1.68	1.59
3	A	706	COA	O3B-C3B	2.18	1.52	1.44
3	B	706	COA	O2B-C2B	2.12	1.48	1.43
3	A	706	COA	O2B-C2B	2.11	1.47	1.43
3	B	706	COA	O3B-C3B	2.08	1.51	1.44
4	B	707	XM7	C8-N7	-2.07	1.31	1.34
3	A	706	COA	P1A-O5B	2.04	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	805	COA	O3B-C3B	2.03	1.51	1.44
3	C	805	COA	O2B-C2B	2.02	1.47	1.43

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	706	COA	N3A-C2A-N1A	-4.36	121.86	128.68
3	B	706	COA	N3A-C2A-N1A	-4.21	122.09	128.68
3	C	805	COA	N3A-C2A-N1A	-4.06	122.34	128.68
3	A	706	COA	C2P-C3P-N4P	-3.56	104.17	112.31
3	C	805	COA	C3P-N4P-C5P	-3.45	116.43	122.84
3	B	706	COA	O6A-CCP-CBP	-2.93	105.84	110.55
3	A	706	COA	C6P-C7P-N8P	2.89	117.73	111.90
3	A	706	COA	O6A-CCP-CBP	-2.75	106.13	110.55
3	B	706	COA	C2P-C3P-N4P	-2.68	106.17	112.31
4	A	707	XM7	O4'-C4'-C3'	-2.58	100.00	105.11
3	C	805	COA	P2A-O3A-P1A	-2.46	124.38	132.83
3	B	706	COA	CEP-CBP-CAP	2.33	112.87	108.82
3	A	706	COA	C3P-N4P-C5P	-2.27	118.63	122.84
3	B	706	COA	P2A-O3A-P1A	-2.25	125.12	132.83
3	C	805	COA	C2P-C3P-N4P	-2.20	107.28	112.31
3	A	706	COA	P2A-O3A-P1A	-2.13	125.51	132.83
3	C	805	COA	CEP-CBP-CAP	2.13	112.51	108.82
3	C	805	COA	C4A-C5A-N7A	-2.11	107.20	109.40
3	B	706	COA	C2B-C3B-C4B	2.11	106.96	103.22
3	B	706	COA	C3B-C2B-C1B	2.01	104.34	99.89

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	706	COA	O4B-C4B-C5B-O5B
3	A	706	COA	CCP-O6A-P2A-O3A
3	B	706	COA	C3B-O3B-P3B-O7A
3	B	706	COA	CCP-O6A-P2A-O3A
3	B	706	COA	CCP-O6A-P2A-O4A
3	B	706	COA	S1P-C2P-C3P-N4P
3	C	805	COA	C3B-O3B-P3B-O7A
3	C	805	COA	C5B-O5B-P1A-O1A
3	C	805	COA	C5B-O5B-P1A-O2A
3	C	805	COA	CCP-O6A-P2A-O3A
3	C	805	COA	O9P-C9P-CAP-OAP

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Mol	Chain	Res	Type	Atoms
3	C	805	COA	N8P-C9P-CAP-OAP
3	C	805	COA	S1P-C2P-C3P-N4P
4	A	707	XM7	C3'-C4'-C5'-O5'
4	A	707	XM7	C5'-O5'-P-OP1
4	A	707	XM7	O4'-C4'-C5'-O5'
4	C	806	XM7	C3'-C4'-C5'-O5'
3	A	706	COA	C3B-C4B-C5B-O5B
3	B	706	COA	O4B-C4B-C5B-O5B
4	C	806	XM7	O4'-C4'-C5'-O5'
4	B	707	XM7	C3'-C4'-C5'-O5'
2	B	705	EDO	O1-C1-C2-O2
4	A	707	XM7	C5'-O5'-P-OP3
3	C	805	COA	P2A-O3A-P1A-O5B
3	B	706	COA	N8P-C9P-CAP-OAP
3	B	706	COA	C3B-O3B-P3B-O8A
3	B	706	COA	C5B-O5B-P1A-O3A
3	A	706	COA	CCP-O6A-P2A-O4A
3	B	706	COA	C5B-O5B-P1A-O1A
3	C	805	COA	CCP-O6A-P2A-O4A
3	C	805	COA	CCP-O6A-P2A-O5A
4	A	707	XM7	C5'-O5'-P-OP2
3	B	706	COA	C3B-C4B-C5B-O5B
3	C	805	COA	CDP-CBP-CCP-O6A
3	C	805	COA	CEP-CBP-CCP-O6A
2	A	702	EDO	O1-C1-C2-O2
4	A	707	XM7	C22-OP3-P-OP2
4	C	806	XM7	C22-OP3-P-OP2
3	B	706	COA	O5P-C5P-C6P-C7P
3	B	706	COA	CDP-CBP-CCP-O6A
3	A	706	COA	O5P-C5P-C6P-C7P
3	B	706	COA	N4P-C5P-C6P-C7P
3	B	706	COA	O9P-C9P-CAP-OAP
4	B	707	XM7	O4'-C4'-C5'-O5'
3	B	706	COA	CEP-CBP-CCP-O6A
3	A	706	COA	N4P-C5P-C6P-C7P
3	C	805	COA	O4B-C4B-C5B-O5B
3	C	805	COA	C5B-O5B-P1A-O3A
3	A	706	COA	C5B-O5B-P1A-O1A
3	A	706	COA	CCP-O6A-P2A-O5A
3	B	706	COA	C5B-O5B-P1A-O2A
2	A	708	EDO	O1-C1-C2-O2
2	B	704	EDO	O1-C1-C2-O2

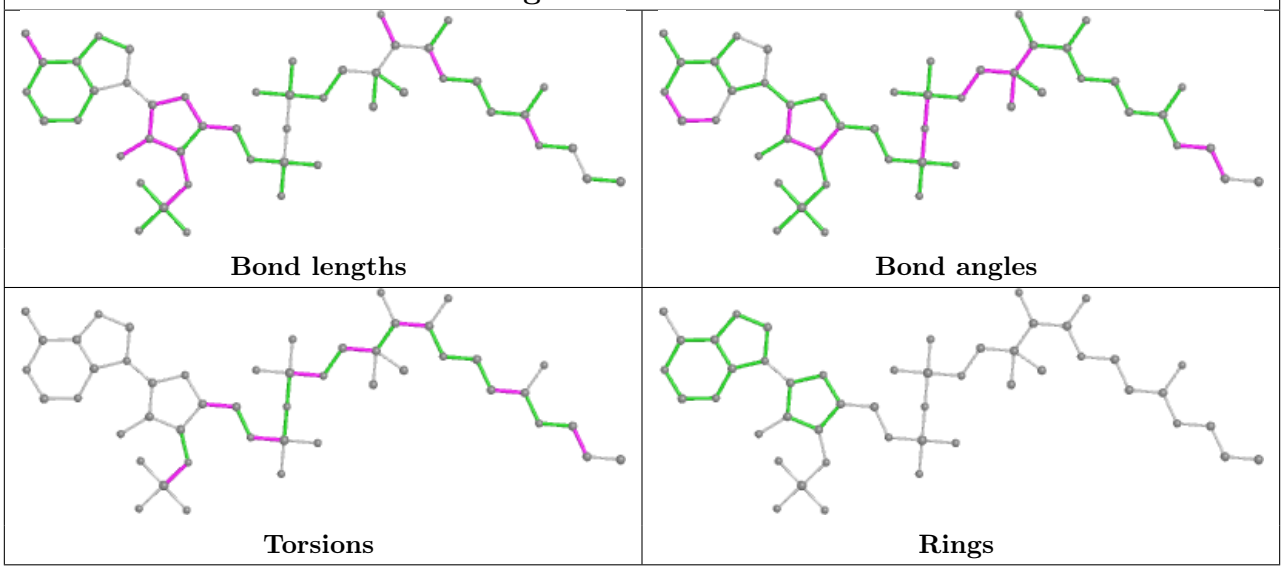
There are no ring outliers.

11 monomers are involved in 17 short contacts:

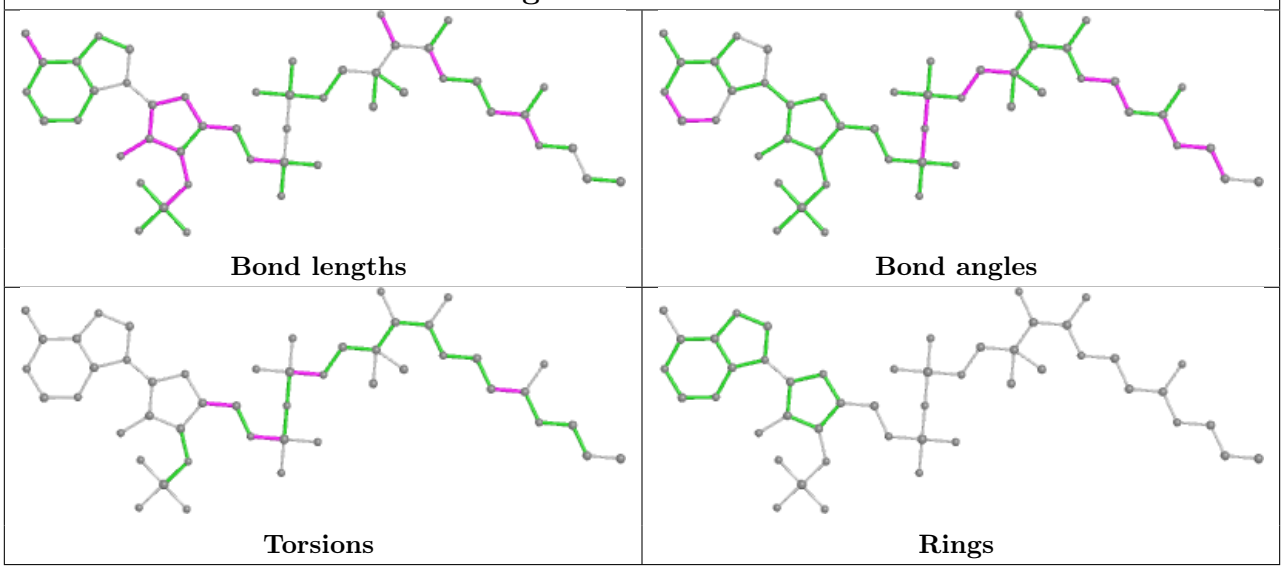
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	706	COA	2	0
3	A	706	COA	2	0
2	B	704	EDO	1	0
2	A	708	EDO	1	0
2	C	801	EDO	1	0
2	B	703	EDO	2	0
2	A	705	EDO	2	0
2	C	803	EDO	3	0
4	B	707	XM7	1	0
2	B	708	EDO	1	0
3	C	805	COA	1	0

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.

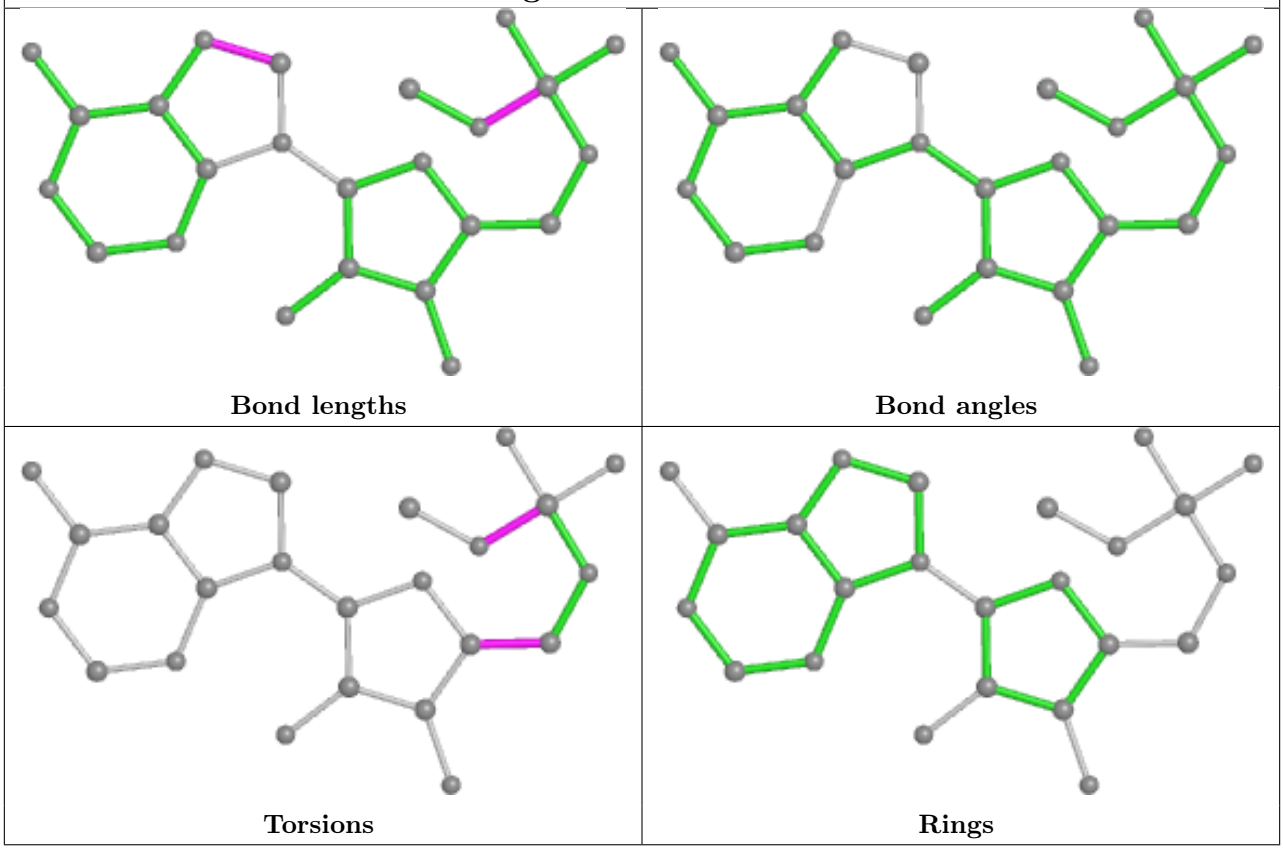
Ligand COA B 706



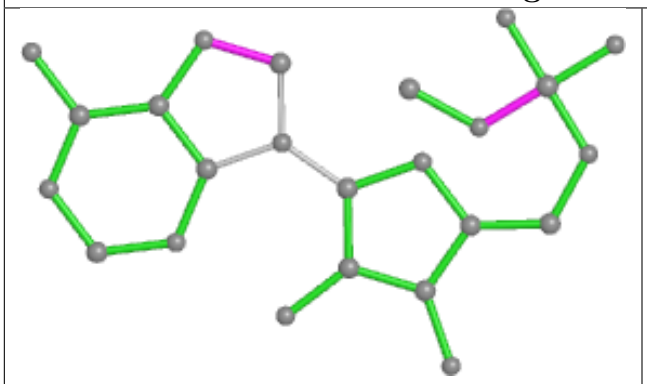
Ligand COA A 706



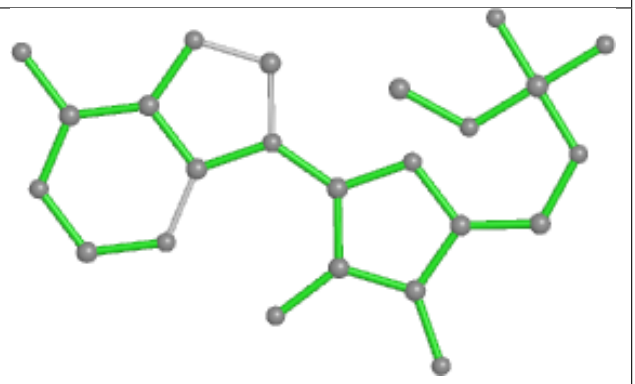
Ligand XM7 C 806



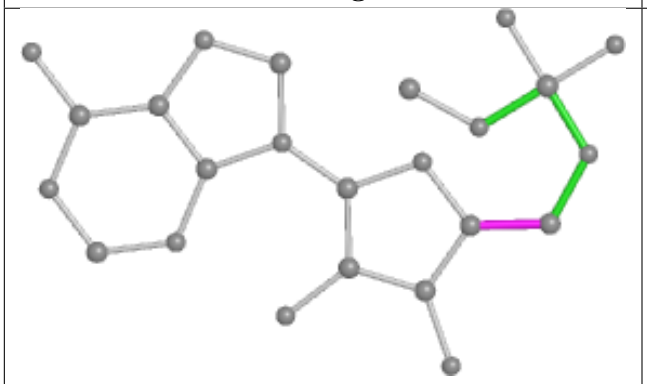
Ligand XM7 B 707



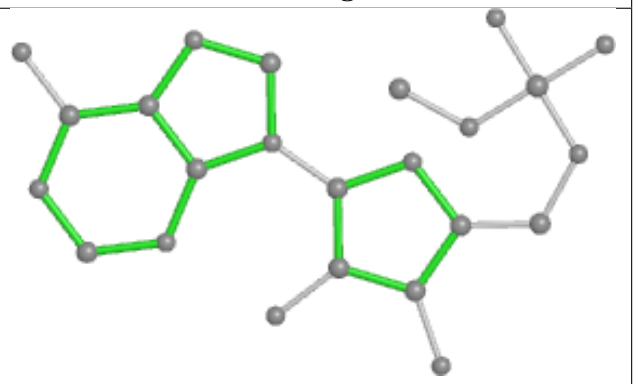
Bond lengths



Bond angles

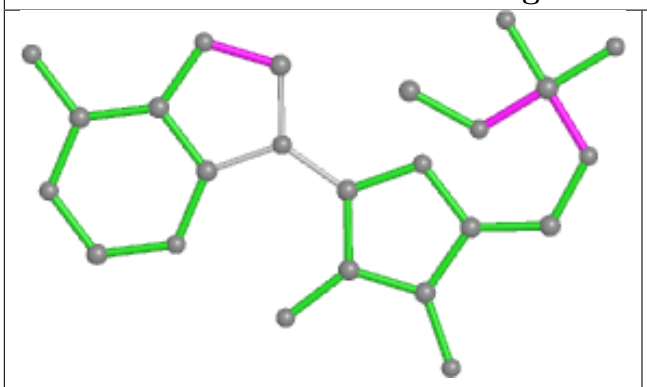


Torsions

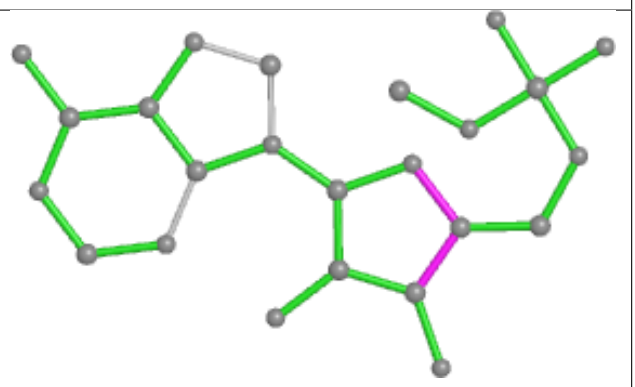


Rings

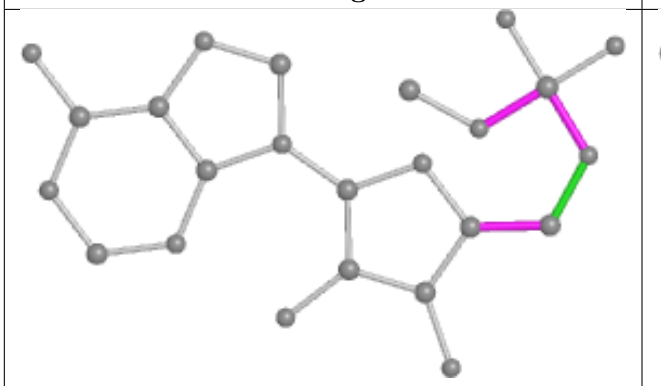
Ligand XM7 A 707



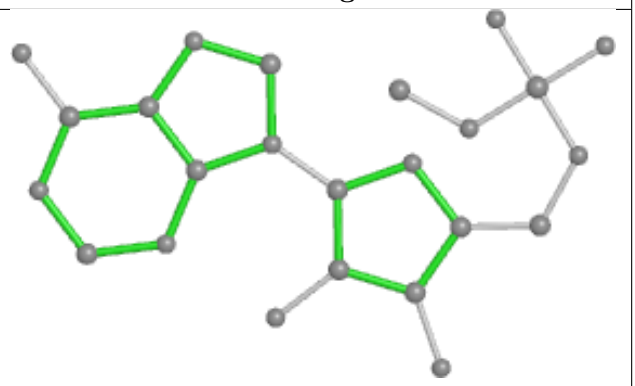
Bond lengths



Bond angles

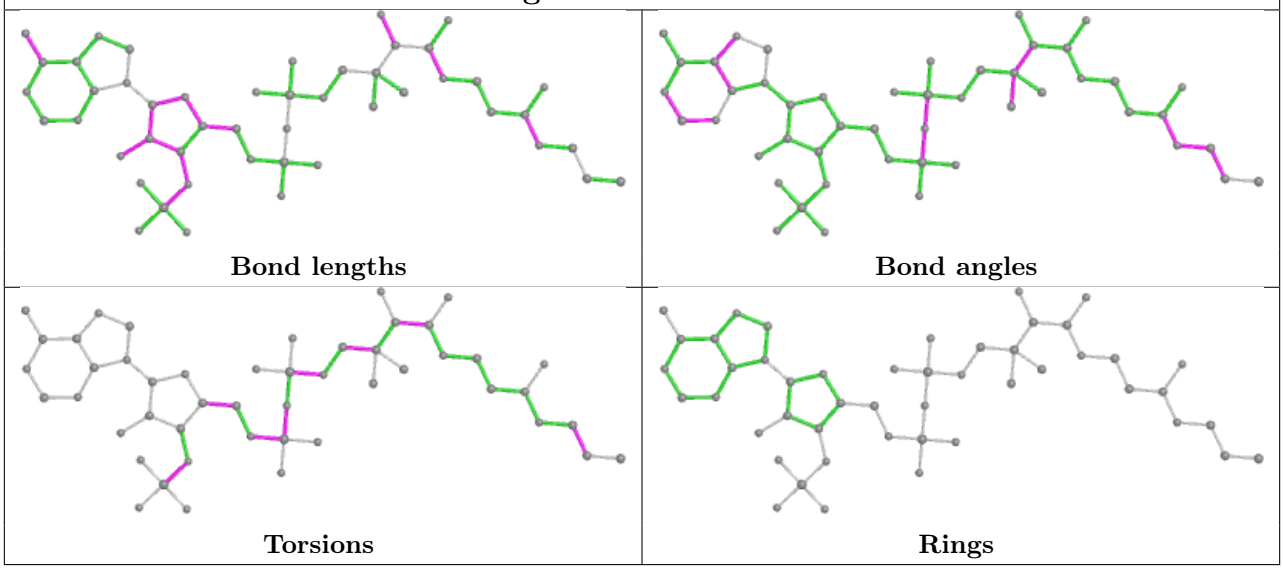


Torsions



Rings

Ligand COA C 805



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	631/706 (89%)	0.16	33 (5%)	27	35	24, 45, 102, 135	0
1	B	629/706 (89%)	0.06	17 (2%)	54	63	24, 45, 99, 120	0
1	C	629/706 (89%)	0.15	23 (3%)	41	49	25, 47, 103, 140	0
All	All	1889/2118 (89%)	0.12	73 (3%)	39	48	24, 46, 101, 140	0

All (73) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	613	VAL	6.2
1	B	635	LYS	5.8
1	B	629	MET	5.8
1	A	659	ILE	5.7
1	C	613	VAL	5.7
1	A	660	ILE	5.4
1	C	615	PHE	5.3
1	A	16	ALA	5.2
1	A	661	ASP	4.4
1	B	637	LEU	4.1
1	B	615	PHE	3.8
1	A	663	PHE	3.7
1	C	661	ASP	3.6
1	A	615	PHE	3.5
1	C	659	ILE	3.4
1	A	614	VAL	3.4
1	A	590	ARG	3.4
1	B	659	ILE	3.3
1	A	593	LEU	3.3
1	B	406	ILE	3.3
1	A	577	VAL	3.3
1	B	542	GLY	3.2
1	C	563	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	588	ASP	3.2
1	B	611	PRO	3.1
1	A	618	ASP	3.1
1	A	413	TRP	3.0
1	B	564	ALA	3.0
1	C	579	ALA	2.9
1	C	593	LEU	2.9
1	C	628	ILE	2.8
1	C	590	ARG	2.8
1	C	612	LYS	2.8
1	C	610	ALA	2.7
1	A	524	HIS	2.7
1	A	585	SER	2.7
1	C	542	GLY	2.7
1	C	633	LEU	2.7
1	C	663	PHE	2.6
1	A	571	PRO	2.6
1	C	614	VAL	2.6
1	A	589	ASN	2.6
1	A	417	VAL	2.5
1	C	381	LEU	2.4
1	C	389	ILE	2.4
1	A	580	PHE	2.4
1	C	423	ALA	2.4
1	C	611	PRO	2.4
1	A	611	PRO	2.4
1	A	664	HIS	2.4
1	C	384	ALA	2.3
1	C	667	LYS	2.3
1	B	630	ARG	2.3
1	A	389	ILE	2.3
1	B	632	ILE	2.3
1	C	597	LEU	2.3
1	B	580	PHE	2.3
1	A	629	MET	2.2
1	A	468	VAL	2.2
1	B	563	ALA	2.2
1	A	634	ARG	2.2
1	A	612	LYS	2.2
1	B	636	ILE	2.2
1	B	578	HIS	2.2
1	A	573	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	573	THR	2.1
1	A	619	ASP	2.1
1	A	408	ALA	2.1
1	C	575	GLN	2.0
1	A	609	ALA	2.0
1	A	631	ARG	2.0
1	B	571	PRO	2.0
1	A	616	VAL	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, 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	EDO	B	701	4/4	0.76	0.20	40,41,43,48	0
2	EDO	A	708	4/4	0.87	0.25	38,40,42,46	0
3	COA	B	706	48/48	0.87	0.15	50,66,72,74	0
3	COA	A	706	48/48	0.88	0.15	50,66,73,77	0
2	EDO	B	705	4/4	0.89	0.12	42,46,46,52	0
2	EDO	B	704	4/4	0.90	0.13	36,38,40,42	0
2	EDO	C	804	4/4	0.90	0.14	41,42,42,43	0
3	COA	C	805	48/48	0.90	0.14	54,69,78,78	0
2	EDO	B	702	4/4	0.91	0.15	38,38,40,42	0
2	EDO	A	701	4/4	0.91	0.17	37,37,43,44	0
2	EDO	A	705	4/4	0.91	0.15	38,38,40,41	0
2	EDO	C	802	4/4	0.91	0.20	41,41,43,44	0
2	EDO	A	702	4/4	0.92	0.08	40,41,42,43	0
2	EDO	B	703	4/4	0.93	0.11	35,37,39,40	0
2	EDO	C	803	4/4	0.93	0.15	35,37,37,38	0

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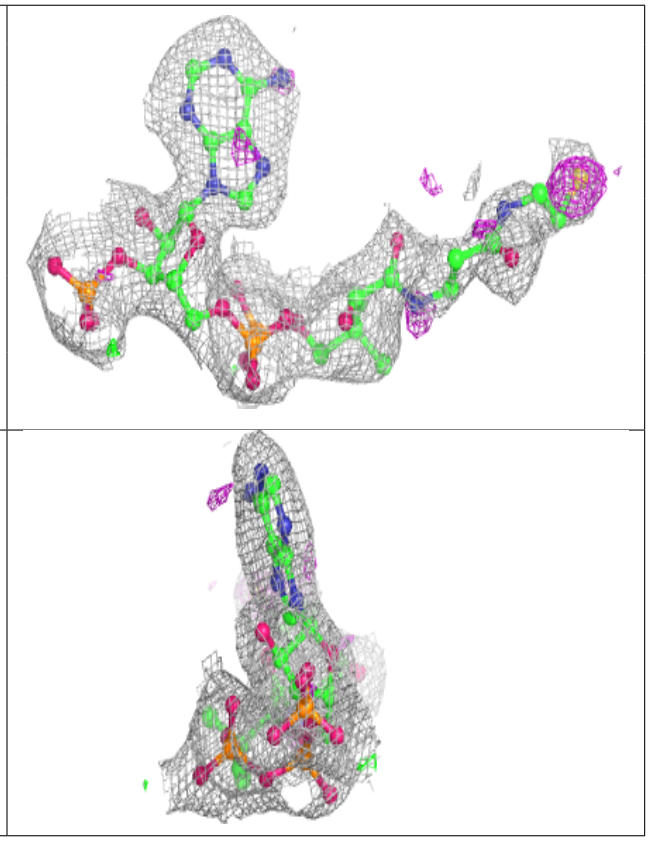
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	EDO	C	801	4/4	0.94	0.16	41,41,42,46	0
4	XM7	A	707	24/24	0.94	0.12	36,41,46,48	0
2	EDO	B	708	4/4	0.95	0.25	41,42,44,48	0
2	EDO	A	704	4/4	0.95	0.16	38,40,42,48	0
2	EDO	A	703	4/4	0.95	0.13	38,38,40,41	0
4	XM7	B	707	24/24	0.96	0.11	32,42,44,45	0
4	XM7	C	806	24/24	0.96	0.11	37,45,48,50	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.

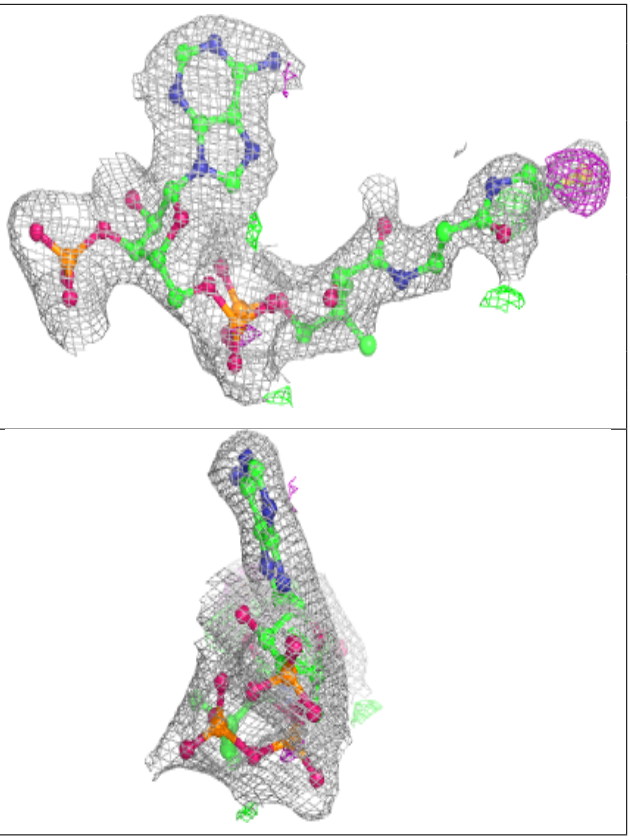
Electron density around COA B 706:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



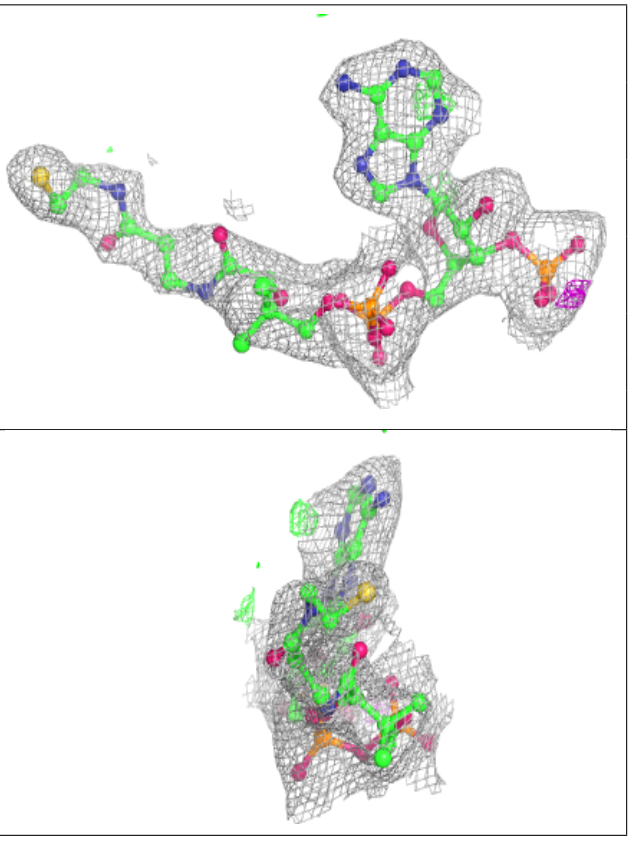
Electron density around COA A 706:

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



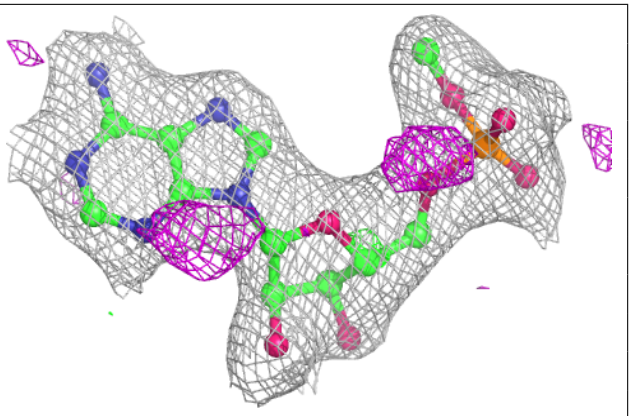
Electron density around COA C 805:

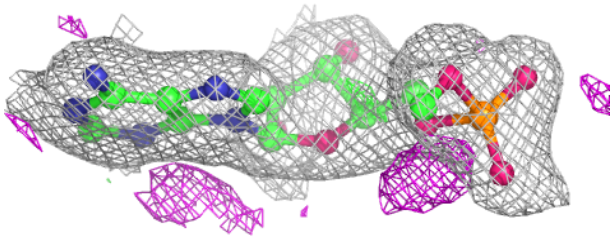
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

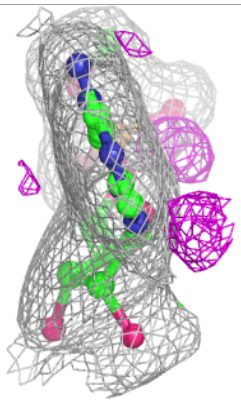


Electron density around XM7 A 707:

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

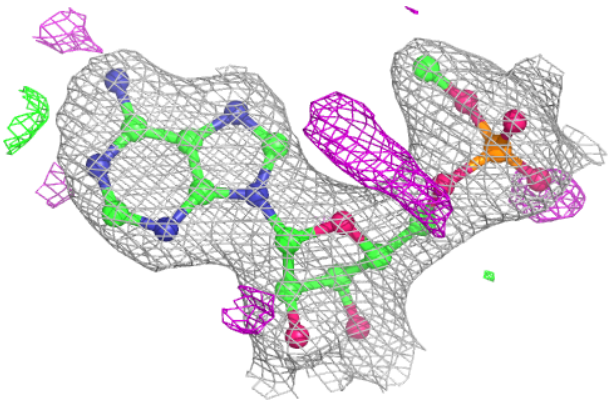


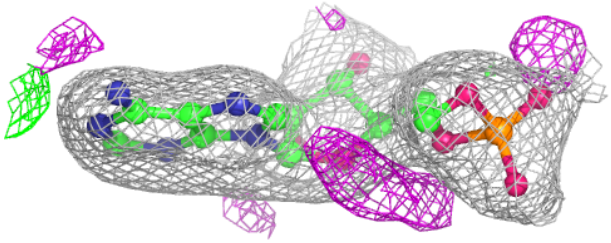


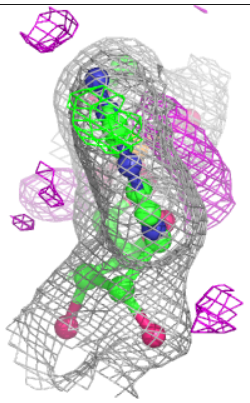


Electron density around XM7 B 707:

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







Electron density around XM7 C 806:

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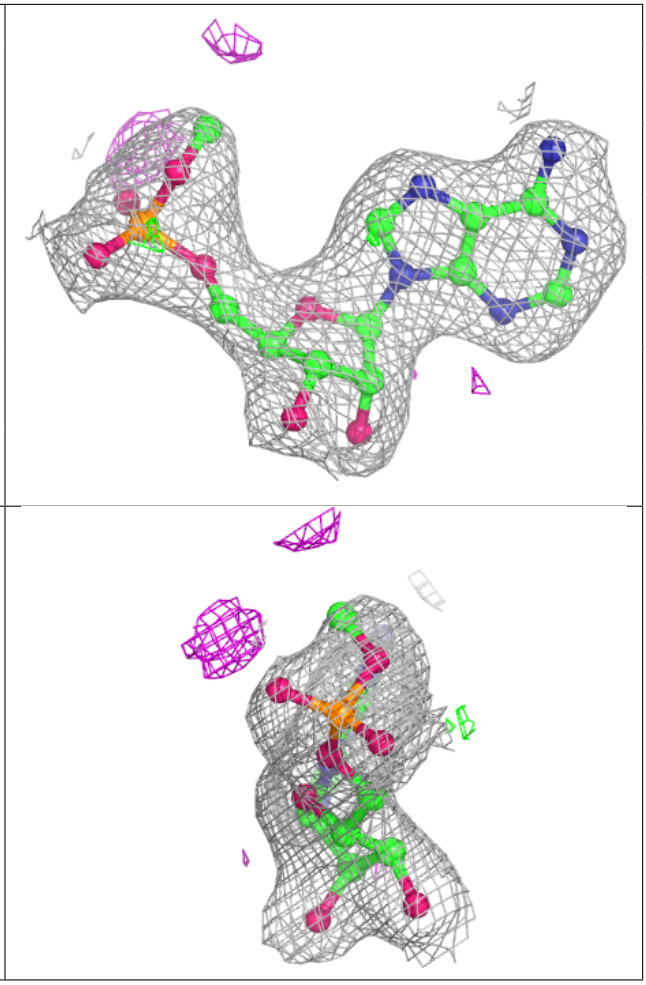
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.