



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 1, 2026 – 07:48 AM UTC

PDB ID : 7L3Q / pdb_0000713q
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

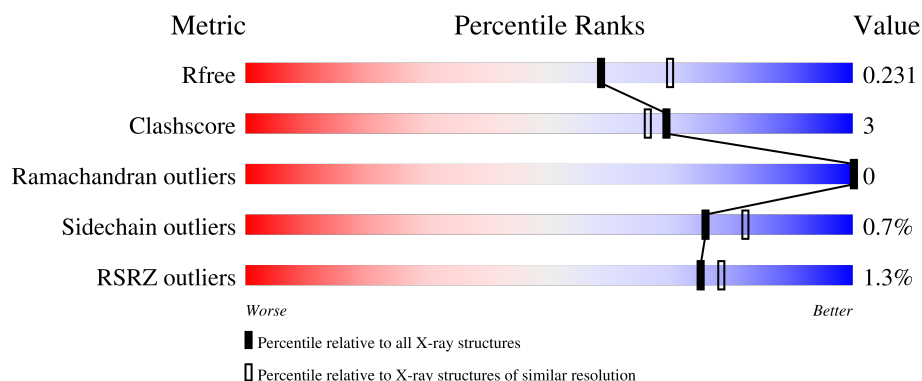
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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}	180053	2057 (2.16-2.16)
Clashscore	190562	2159 (2.16-2.16)
Ramachandran outliers	187476	2134 (2.16-2.16)
Sidechain outliers	187428	2133 (2.16-2.16)
RSRZ outliers	180081	2059 (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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	706	% 82% 7% 11%
1	B	706	% 80% 9% 11%
1	C	706	% 82% 8% 11%

2 Entry composition

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
1	A	631	Total	C	N	O	S	0	4	0
			4842	3095	838	890	19			
1	B	629	Total	C	N	O	S	0	3	0
			4820	3084	833	885	18			
1	C	629	Total	C	N	O	S	0	4	0
			4785	3060	825	882	18			

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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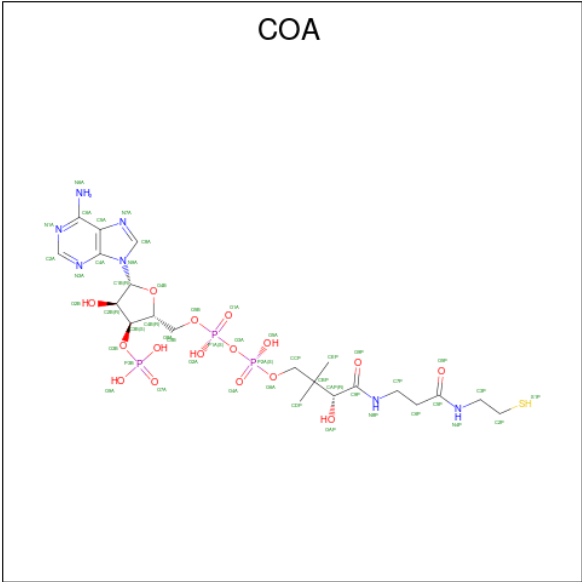
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	HIS	-	expression tag	UNP J3KJC6
B	-6	HIS	-	expression tag	UNP J3KJC6
B	-5	GLU	-	expression tag	UNP J3KJC6
B	-4	ASN	-	expression tag	UNP J3KJC6
B	-3	LEU	-	expression tag	UNP J3KJC6
B	-2	TYR	-	expression tag	UNP J3KJC6
B	-1	PHE	-	expression tag	UNP J3KJC6
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 (CCD ID: EDO) (formula: C₂H₆O₂).



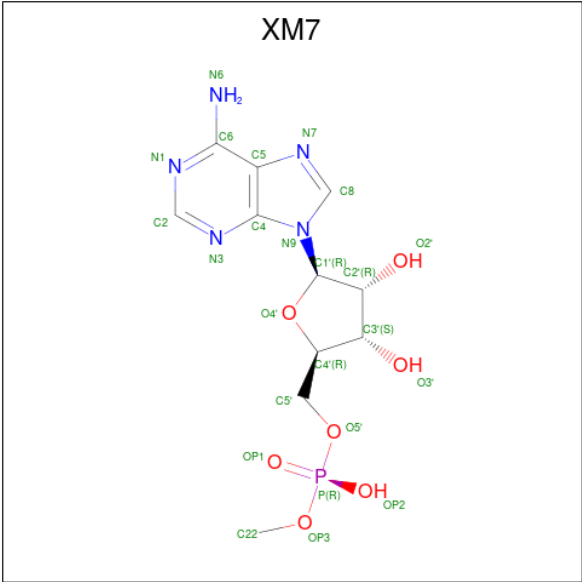
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	A	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0
2	B	1	Total C O 4 2 2	0	0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

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



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

- Molecule 4 is 5'-O-[(R)-hydroxy(methoxy)phosphoryl]adenosine (CCD ID: XM7) (formula: C₁₁H₁₆N₅O₇P).



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

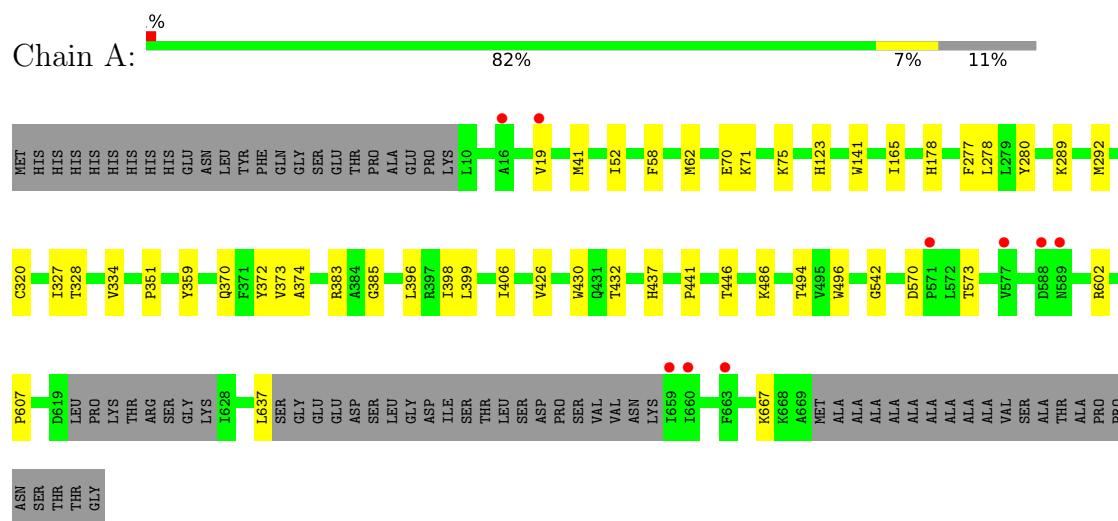
- Molecule 5 is water.

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

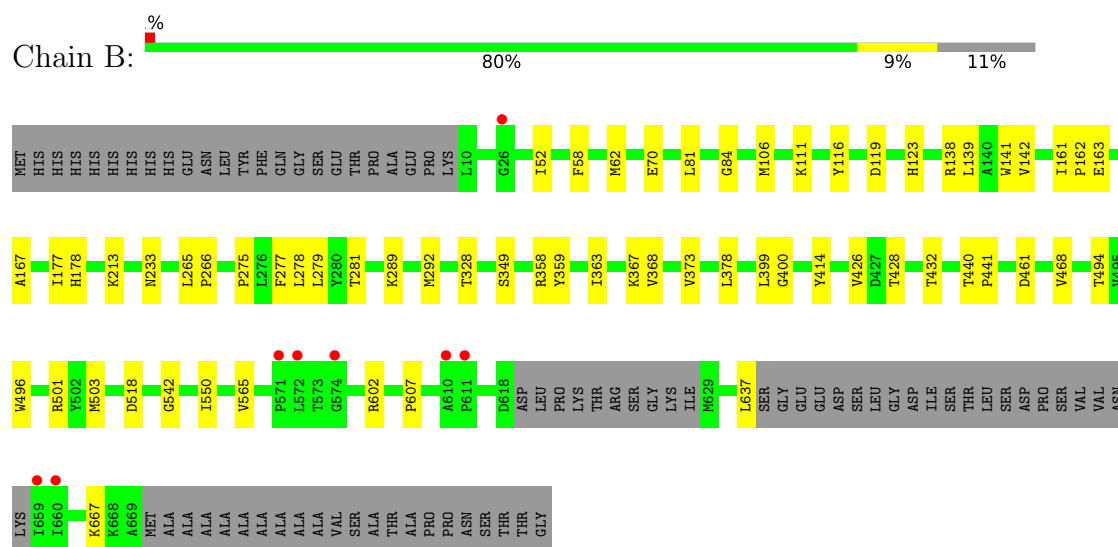
3 Residue-property plots [i](#)

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.

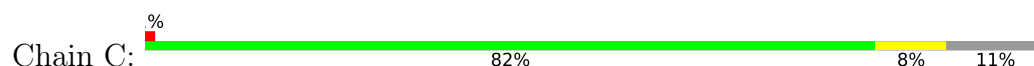
• Molecule 1: Acetyl-coenzyme A synthetase



• Molecule 1: Acetyl-coenzyme A synthetase



• Molecule 1: Acetyl-coenzyme A synthetase





4 Data and refinement statistics

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 46.38 – 2.15	Depositor EDS
% Data completeness (in resolution range)	94.1 (46.38-2.15) 92.6 (46.38-2.15)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ 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 (1.68%)	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)	0.33 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: XM7, EDO, 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	0.33	0/4981	0.49	0/6787
1	B	0.33	0/4963	0.49	0/6767
1	C	0.32	0/4930	0.49	0/6726
All	All	0.33	0/14874	0.49	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	31	0
1	B	4820	0	4551	40	0
1	C	4785	0	4491	30	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	99	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 (99) 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:292[A]:MET:HE2	1:A:494:THR:HG22	1.88	0.55
1:A:41:MET:HE1	1:A:446:THR:HG23	1.88	0.54
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:292[B]:MET:HE3	1:C:494:THR:HG22	1.95	0.48
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:A:62:MET:HE2	1:A:62:MET:HB2	1.79	0.46
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:58:PHE:CZ	1:A:62:MET:HE3	2.52	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:B:58:PHE:CZ	1:B:62:MET:HE3	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:292[A]:MET:HE3	1:B:494:THR:HG22	2.03	0.40
1:B:328:THR:HG21	3:B:706:COA:S1P	2.61	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
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 ⓘ

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%)	482 (100%)	2 (0%)	84	89
1	B	482/584 (82%)	478 (99%)	4 (1%)	73	79
1	C	475/584 (81%)	471 (99%)	4 (1%)	73	79
All	All	1441/1752 (82%)	1431 (99%)	10 (1%)	76	82

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	383	ARG
1	A	406	ILE
1	B	213	LYS
1	B	359	TYR
1	B	367	LYS
1	B	468	VAL
1	C	62	MET
1	C	394	LYS
1	C	406	ILE
1	C	468	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	388	HIS
1	A	575	GLN
1	A	600	GLN
1	B	123	HIS
1	B	388	HIS
1	B	431	GLN
1	B	558	HIS
1	C	31	ASN
1	C	34	HIS
1	C	123	HIS
1	C	422	GLN
1	C	524	HIS
1	C	578	HIS
1	C	600	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 oligosaccharides 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	-	47,50,50	3.24	17 (36%)	69,75,75	1.61	15 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	EDO	A	705	-	3,3,3	0.52	0	2,2,2	0.12	0
2	EDO	A	701	-	3,3,3	0.56	0	2,2,2	0.18	0
2	EDO	B	702	-	3,3,3	0.51	0	2,2,2	0.57	0
2	EDO	C	802	-	3,3,3	0.51	0	2,2,2	0.21	0
2	EDO	C	801	-	3,3,3	0.49	0	2,2,2	0.38	0
2	EDO	B	701	-	3,3,3	0.58	0	2,2,2	0.24	0
2	EDO	A	704	-	3,3,3	0.46	0	2,2,2	0.32	0
2	EDO	B	703	-	3,3,3	0.48	0	2,2,2	0.12	0
2	EDO	B	708	-	3,3,3	0.51	0	2,2,2	0.58	0
2	EDO	A	703	-	3,3,3	0.50	0	2,2,2	0.47	0
4	XM7	A	707	-	26,26,26	0.88	2 (7%)	38,39,39	0.90	1 (2%)
2	EDO	C	804	-	3,3,3	0.42	0	2,2,2	0.21	0
3	COA	A	706	-	47,50,50	3.27	19 (40%)	69,75,75	1.63	13 (18%)
2	EDO	A	708	-	3,3,3	0.45	0	2,2,2	0.72	0
4	XM7	C	806	-	26,26,26	0.80	1 (3%)	38,39,39	0.84	0
2	EDO	B	704	-	3,3,3	0.50	0	2,2,2	0.37	0
3	COA	C	805	-	47,50,50	3.20	16 (34%)	69,75,75	1.58	12 (17%)
2	EDO	A	702	-	3,3,3	0.49	0	2,2,2	0.45	0
2	EDO	B	705	-	3,3,3	0.63	0	2,2,2	0.25	0
4	XM7	B	707	-	26,26,26	0.85	1 (3%)	38,39,39	0.79	0
2	EDO	C	803	-	3,3,3	0.51	0	2,2,2	0.15	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
3	COA	B	706	-	-	14/48/64/64	0/3/3/3
2	EDO	A	705	-	-	0/1/1/1	-
2	EDO	A	701	-	-	0/1/1/1	-
2	EDO	B	702	-	-	0/1/1/1	-
2	EDO	C	802	-	-	0/1/1/1	-
2	EDO	C	801	-	-	0/1/1/1	-
2	EDO	B	701	-	-	0/1/1/1	-
2	EDO	A	704	-	-	0/1/1/1	-
2	EDO	B	703	-	-	0/1/1/1	-
2	EDO	B	708	-	-	0/1/1/1	-
2	EDO	A	703	-	-	0/1/1/1	-
4	XM7	A	707	-	-	6/13/29/29	0/3/3/3
2	EDO	C	804	-	-	0/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COA	A	706	-	-	8/48/64/64	0/3/3/3
2	EDO	A	708	-	-	1/1/1/1	-
4	XM7	C	806	-	-	2/13/29/29	0/3/3/3
2	EDO	B	704	-	-	1/1/1/1	-
3	COA	C	805	-	-	14/48/64/64	0/3/3/3
2	EDO	A	702	-	-	1/1/1/1	-
2	EDO	B	705	-	-	1/1/1/1	-
4	XM7	B	707	-	-	2/13/29/29	0/3/3/3
2	EDO	C	803	-	-	0/1/1/1	-

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	706	COA	C2B-C3B	-12.36	1.26	1.53
3	B	706	COA	C2B-C3B	-12.33	1.26	1.53
3	C	805	COA	C2B-C3B	-12.23	1.26	1.53
3	B	706	COA	C5P-N4P	7.04	1.50	1.33
3	A	706	COA	C9P-N8P	7.02	1.50	1.33
3	B	706	COA	C9P-N8P	6.98	1.50	1.33
3	C	805	COA	C9P-N8P	6.94	1.49	1.33
3	C	805	COA	C5P-N4P	6.91	1.49	1.33
3	A	706	COA	C5P-N4P	6.81	1.49	1.33
3	B	706	COA	P2A-O3A	6.71	1.66	1.59
3	A	706	COA	P2A-O3A	6.46	1.66	1.59
3	C	805	COA	P2A-O3A	6.08	1.66	1.59
3	C	805	COA	O4B-C1B	-5.93	1.28	1.42
3	B	706	COA	O4B-C1B	-5.78	1.28	1.42
3	A	706	COA	O4B-C1B	-5.70	1.28	1.42
3	A	706	COA	O4B-C4B	4.99	1.56	1.45
3	A	706	COA	C2B-C1B	4.81	1.68	1.53
3	B	706	COA	O4B-C4B	4.76	1.55	1.45
3	C	805	COA	O4B-C4B	4.59	1.55	1.45
3	C	805	COA	C2B-C1B	4.58	1.67	1.53
3	B	706	COA	C2B-C1B	4.50	1.67	1.53
3	C	805	COA	C5B-C4B	-4.35	1.38	1.51
3	B	706	COA	C5B-C4B	-4.31	1.38	1.51
3	A	706	COA	C6A-N6A	4.22	1.45	1.34
3	A	706	COA	C5B-C4B	-4.20	1.38	1.51
3	A	706	COA	P3B-O3B	3.96	1.66	1.59
3	B	706	COA	C6A-N6A	3.95	1.44	1.34
3	B	706	COA	P3B-O3B	3.91	1.66	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	805	COA	C6A-N6A	3.89	1.44	1.34
3	A	706	COA	P1A-O3A	3.89	1.63	1.59
3	C	805	COA	P3B-O3B	3.58	1.65	1.59
3	B	706	COA	P1A-O3A	3.25	1.63	1.59
3	C	805	COA	C8A-N9A	-3.09	1.32	1.37
3	C	805	COA	P1A-O3A	2.97	1.62	1.59
3	A	706	COA	C8A-N9A	-2.80	1.32	1.37
3	A	706	COA	CCP-CBP	2.73	1.57	1.52
4	A	707	XM7	P-OP3	2.73	1.67	1.58
3	B	706	COA	C8A-N9A	-2.72	1.32	1.37
4	B	707	XM7	P-OP3	2.70	1.67	1.58
3	C	805	COA	CCP-CBP	2.65	1.56	1.52
3	C	805	COA	OAP-CAP	-2.57	1.37	1.42
4	C	806	XM7	P-OP3	2.55	1.67	1.58
3	B	706	COA	OAP-CAP	-2.50	1.37	1.42
3	B	706	COA	CCP-CBP	2.41	1.56	1.52
3	A	706	COA	OAP-CAP	-2.41	1.38	1.42
3	A	706	COA	O3B-C3B	2.34	1.52	1.44
3	B	706	COA	C5A-N7A	-2.32	1.34	1.39
4	A	707	XM7	P-O5'	2.25	1.68	1.59
3	B	706	COA	O3B-C3B	2.22	1.51	1.44
3	A	706	COA	C6P-C5P	2.22	1.55	1.51
3	C	805	COA	O3B-C3B	2.17	1.51	1.44
3	A	706	COA	C5A-N7A	-2.11	1.35	1.39
3	C	805	COA	C5A-N7A	-2.10	1.35	1.39
3	A	706	COA	P1A-O5B	2.08	1.67	1.59
3	B	706	COA	O2B-C2B	2.02	1.48	1.43
3	A	706	COA	O2B-C2B	2.01	1.47	1.43

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	706	COA	C5A-C4A-N3A	-5.50	119.15	126.72
3	A	706	COA	C5A-C4A-N3A	-5.27	119.46	126.72
3	C	805	COA	C5A-C4A-N3A	-4.99	119.85	126.72
3	B	706	COA	N3A-C4A-N9A	4.54	134.88	127.17
3	A	706	COA	N3A-C2A-N1A	-4.44	121.86	128.58
3	B	706	COA	N3A-C2A-N1A	-4.29	122.09	128.58
3	C	805	COA	N3A-C2A-N1A	-4.12	122.34	128.58
3	A	706	COA	N3A-C4A-N9A	3.82	133.67	127.17
3	C	805	COA	N3A-C4A-N9A	3.68	133.42	127.17
3	A	706	COA	C2P-C3P-N4P	-3.59	104.17	112.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	706	COA	C2A-N3A-C4A	3.48	120.34	111.83
3	A	706	COA	C2A-N3A-C4A	3.46	120.28	111.83
3	C	805	COA	C3P-N4P-C5P	-3.44	116.43	122.82
3	C	805	COA	C2A-N3A-C4A	3.31	119.91	111.83
3	C	805	COA	N9A-C8A-N7A	-3.17	109.43	113.94
3	C	805	COA	C5A-N7A-C8A	3.07	108.28	103.45
3	A	706	COA	N9A-C8A-N7A	-2.97	109.72	113.94
3	C	805	COA	C4A-C5A-N7A	-2.96	107.20	110.58
3	B	706	COA	O6A-CCP-CBP	-2.93	105.84	110.55
3	B	706	COA	N9A-C8A-N7A	-2.86	109.87	113.94
3	A	706	COA	C5A-N7A-C8A	2.80	107.85	103.45
3	A	706	COA	O6A-CCP-CBP	-2.75	106.13	110.55
3	B	706	COA	C5A-N7A-C8A	2.74	107.76	103.45
3	A	706	COA	C4A-C5A-N7A	-2.72	107.47	110.58
3	B	706	COA	C2P-C3P-N4P	-2.70	106.17	112.31
3	A	706	COA	C6P-C7P-N8P	2.69	117.73	112.00
4	A	707	XM7	O4'-C4'-C3'	-2.59	100.00	105.15
3	C	805	COA	C4A-N9A-C8A	2.49	108.36	105.74
3	B	706	COA	CEP-CBP-CAP	2.41	112.87	108.77
3	B	706	COA	P3B-O3B-C3B	-2.36	117.12	123.43
3	B	706	COA	C5A-C6A-N6A	-2.35	117.47	123.29
3	B	706	COA	C4A-N9A-C8A	2.34	108.19	105.74
3	A	706	COA	C3P-N4P-C5P	-2.25	118.63	122.82
3	A	706	COA	C4A-N9A-C8A	2.24	108.09	105.74
3	C	805	COA	C2P-C3P-N4P	-2.21	107.28	112.31
3	C	805	COA	CEP-CBP-CAP	2.20	112.51	108.77
3	A	706	COA	P3B-O3B-C3B	-2.19	117.59	123.43
3	B	706	COA	C2B-C3B-C4B	2.13	106.96	103.24
3	B	706	COA	C4A-C5A-N7A	-2.08	108.21	110.58
3	C	805	COA	P3B-O3B-C3B	-2.06	117.94	123.43
3	B	706	COA	C3B-C2B-C1B	2.03	104.34	99.89

There are no chirality outliers.

All (50) 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	CCP-O6A-P2A-O3A
3	B	706	COA	CCP-O6A-P2A-O4A
3	B	706	COA	S1P-C2P-C3P-N4P
3	C	805	COA	C5B-O5B-P1A-O1A

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Mol	Chain	Res	Type	Atoms
3	C	805	COA	C5B-O5B-P1A-O2A
3	C	805	COA	C5B-O5B-P1A-O3A
3	C	805	COA	N8P-C9P-CAP-OAP
3	C	805	COA	S1P-C2P-C3P-N4P
4	A	707	XM7	C5'-O5'-P-OP3
4	A	707	XM7	C5'-O5'-P-OP1
4	A	707	XM7	C3'-C4'-C5'-O5'
4	A	707	XM7	O4'-C4'-C5'-O5'
3	B	706	COA	O4B-C4B-C5B-O5B
4	C	806	XM7	C3'-C4'-C5'-O5'
4	C	806	XM7	O4'-C4'-C5'-O5'
4	B	707	XM7	C3'-C4'-C5'-O5'
3	A	706	COA	C3B-C4B-C5B-O5B
2	B	705	EDO	O1-C1-C2-O2
3	B	706	COA	N8P-C9P-CAP-OAP
3	C	805	COA	P2A-O3A-P1A-O5B
3	C	805	COA	O9P-C9P-CAP-OAP
3	B	706	COA	CDP-CBP-CCP-O6A
3	C	805	COA	CDP-CBP-CCP-O6A
3	C	805	COA	CEP-CBP-CCP-O6A
3	A	706	COA	CCP-O6A-P2A-O4A
3	B	706	COA	C5B-O5B-P1A-O1A
3	B	706	COA	C5B-O5B-P1A-O3A
3	C	805	COA	CCP-O6A-P2A-O3A
3	C	805	COA	CCP-O6A-P2A-O4A
3	C	805	COA	CCP-O6A-P2A-O5A
4	A	707	XM7	C5'-O5'-P-OP2
4	A	707	XM7	C22-OP3-P-OP2
3	B	706	COA	C3B-C4B-C5B-O5B
3	B	706	COA	C3B-O3B-P3B-O8A
3	C	805	COA	C3B-O3B-P3B-O7A
4	B	707	XM7	O4'-C4'-C5'-O5'
3	A	706	COA	O5P-C5P-C6P-C7P
3	B	706	COA	O5P-C5P-C6P-C7P
2	A	702	EDO	O1-C1-C2-O2
3	B	706	COA	N4P-C5P-C6P-C7P
3	C	805	COA	O4B-C4B-C5B-O5B
3	A	706	COA	N4P-C5P-C6P-C7P
2	B	704	EDO	O1-C1-C2-O2
2	A	708	EDO	O1-C1-C2-O2
3	A	706	COA	CDP-CBP-CCP-O6A
3	A	706	COA	CEP-CBP-CCP-O6A

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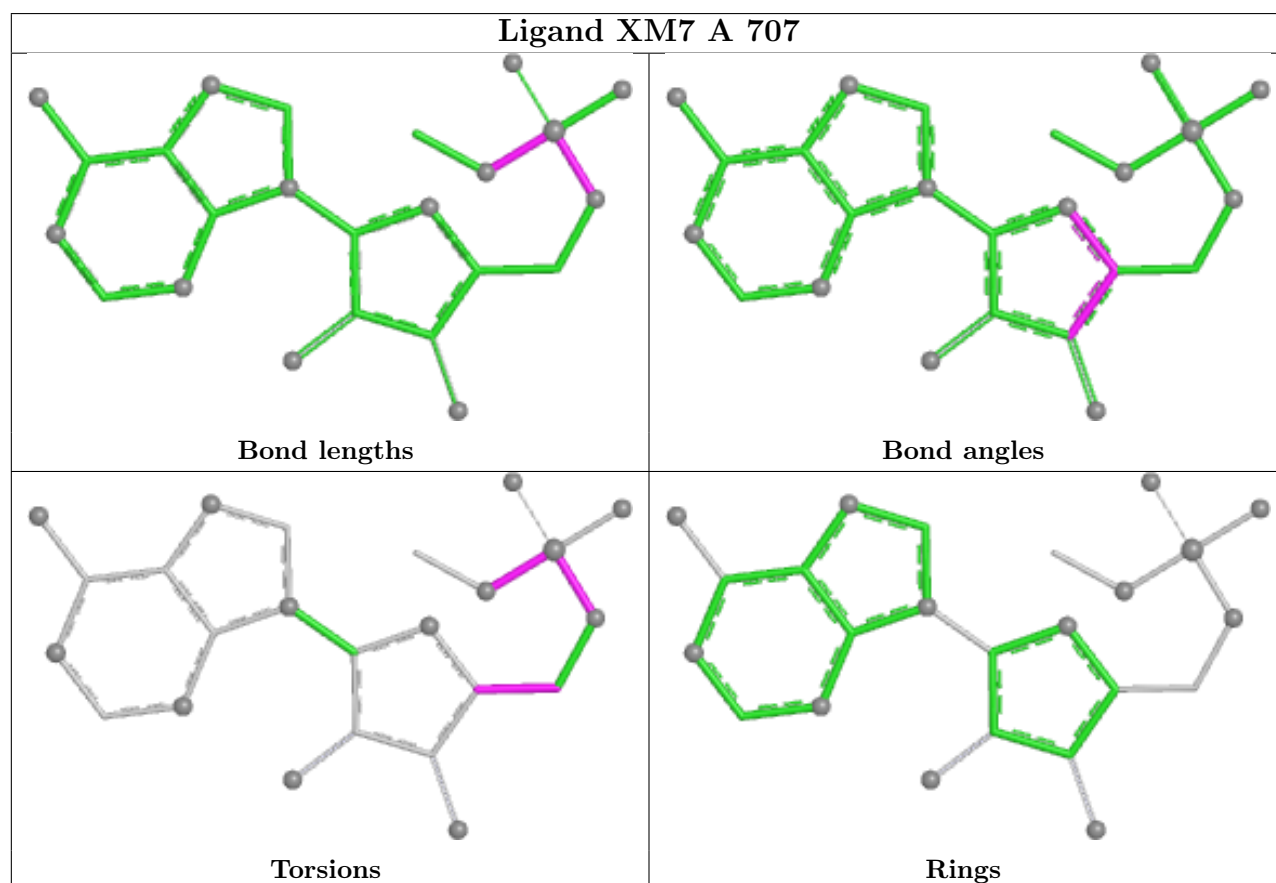
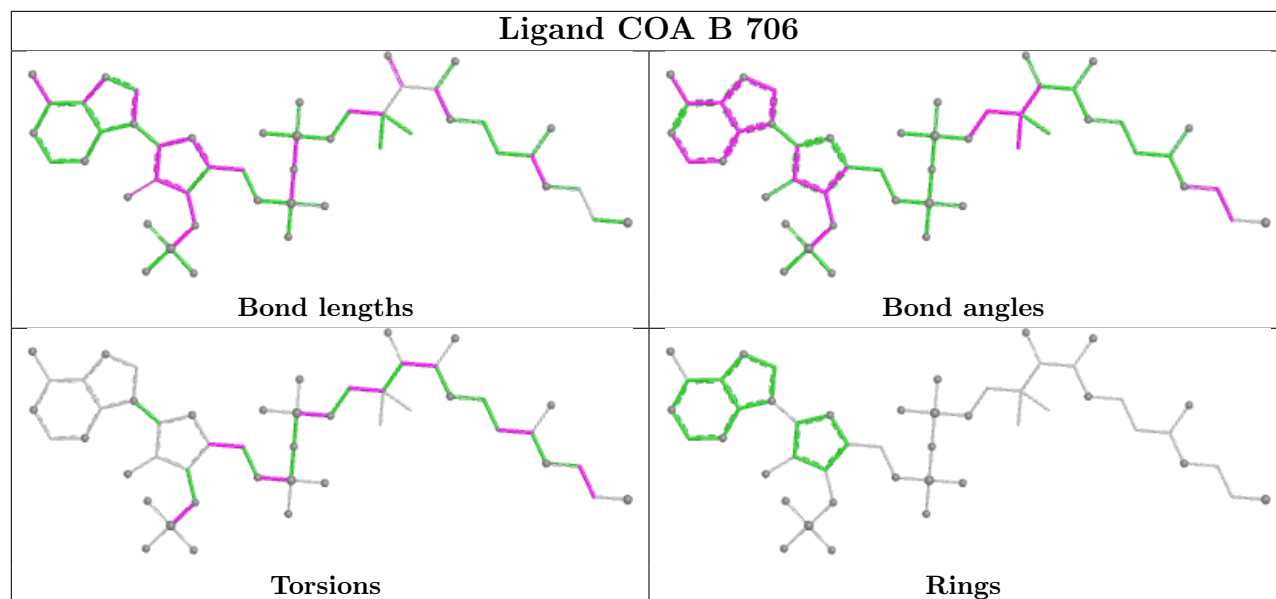
Mol	Chain	Res	Type	Atoms
3	B	706	COA	CEP-CBP-CCP-O6A
3	B	706	COA	C3B-O3B-P3B-O7A

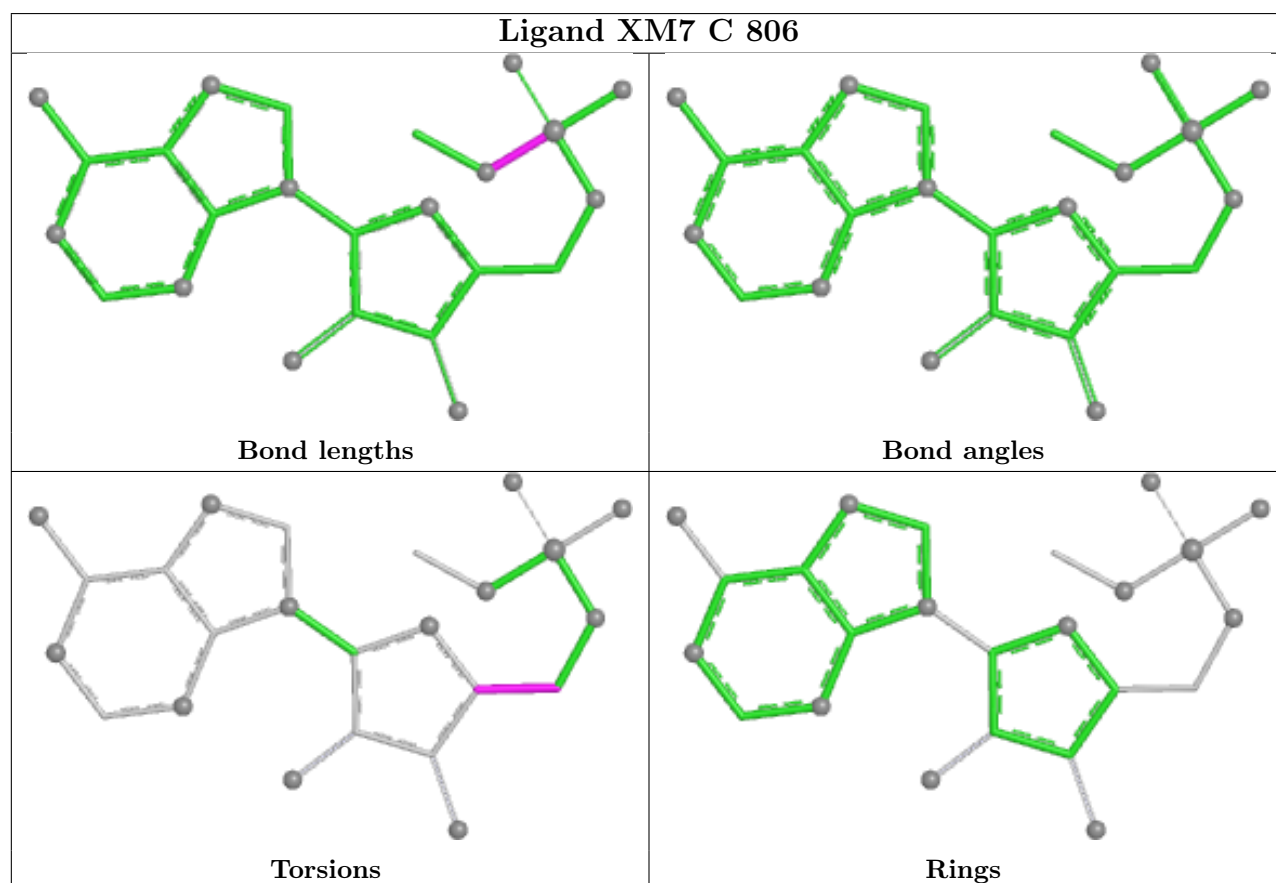
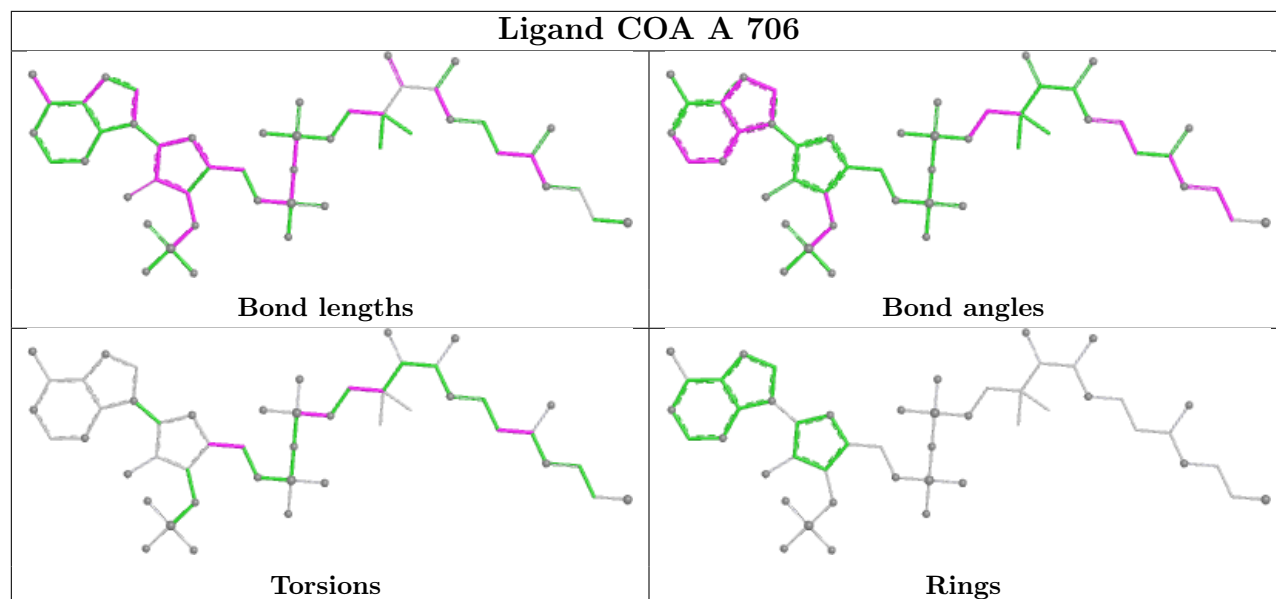
There are no ring outliers.

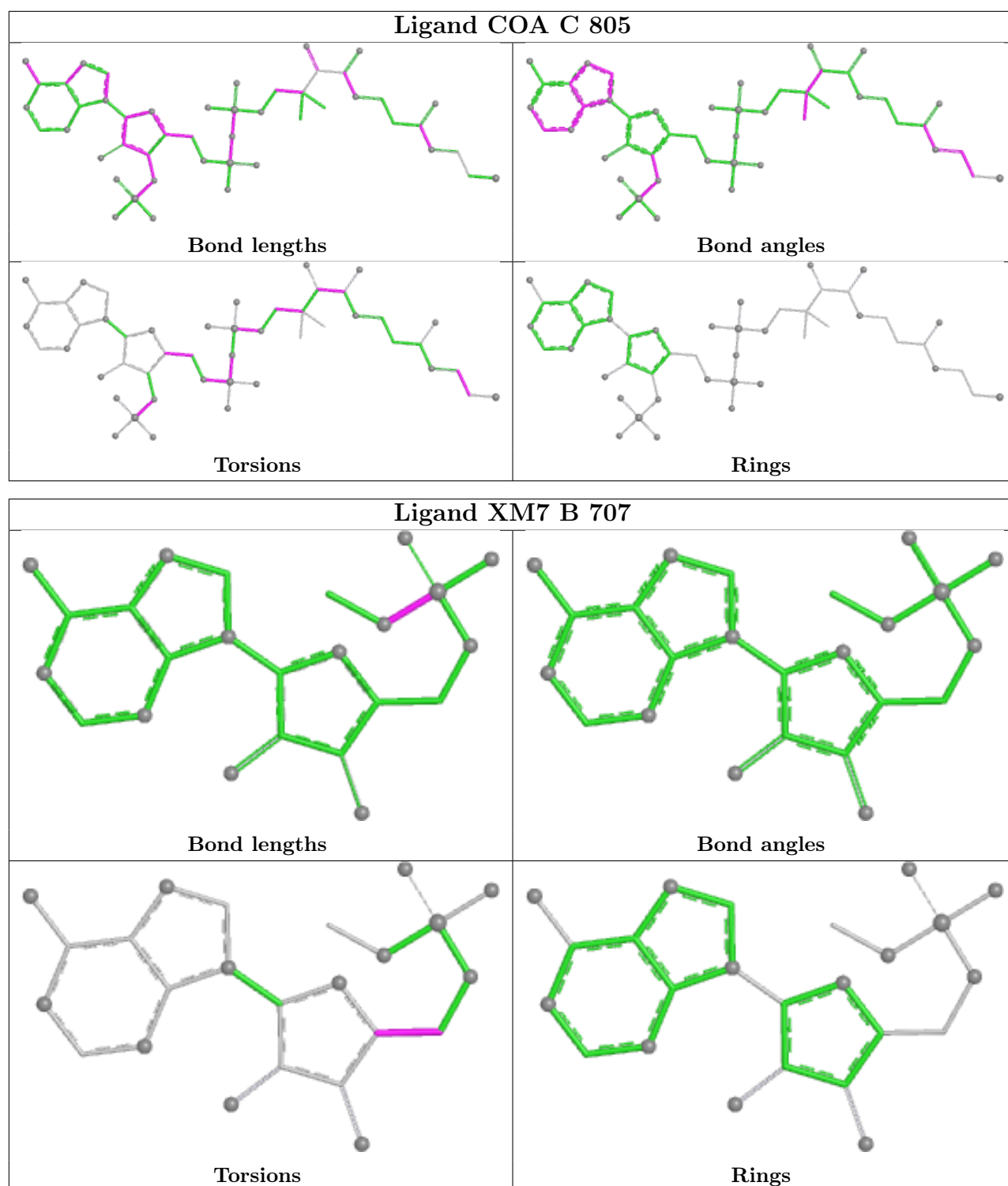
11 monomers are involved in 17 short contacts:

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

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers ⓘ

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, 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%)	-0.63	9 (1%) 73 77	17, 45, 102, 135	4 (0%)
1	B	629/706 (89%)	-0.68	8 (1%) 75 78	18, 45, 99, 120	3 (0%)
1	C	629/706 (89%)	-0.60	7 (1%) 78 80	18, 47, 103, 140	4 (0%)
All	All	1889/2118 (89%)	-0.64	24 (1%) 75 78	17, 46, 101, 140	11 (0%)

All (24) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	571	PRO	3.5
1	B	611	PRO	3.5
1	C	637	LEU	3.1
1	A	16	ALA	3.0
1	A	659	ILE	2.8
1	B	660	ILE	2.7
1	A	589	ASN	2.6
1	B	26	GLY	2.6
1	A	660	ILE	2.6
1	C	16	ALA	2.6
1	C	663	PHE	2.5
1	B	659	ILE	2.4
1	C	27	VAL	2.4
1	B	572	LEU	2.4
1	B	574	GLY	2.3
1	A	19	VAL	2.1
1	B	610	ALA	2.1
1	A	663	PHE	2.1
1	A	588	ASP	2.1
1	B	571	PRO	2.1
1	C	611	PRO	2.0
1	C	662	THR	2.0
1	A	577	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	567	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

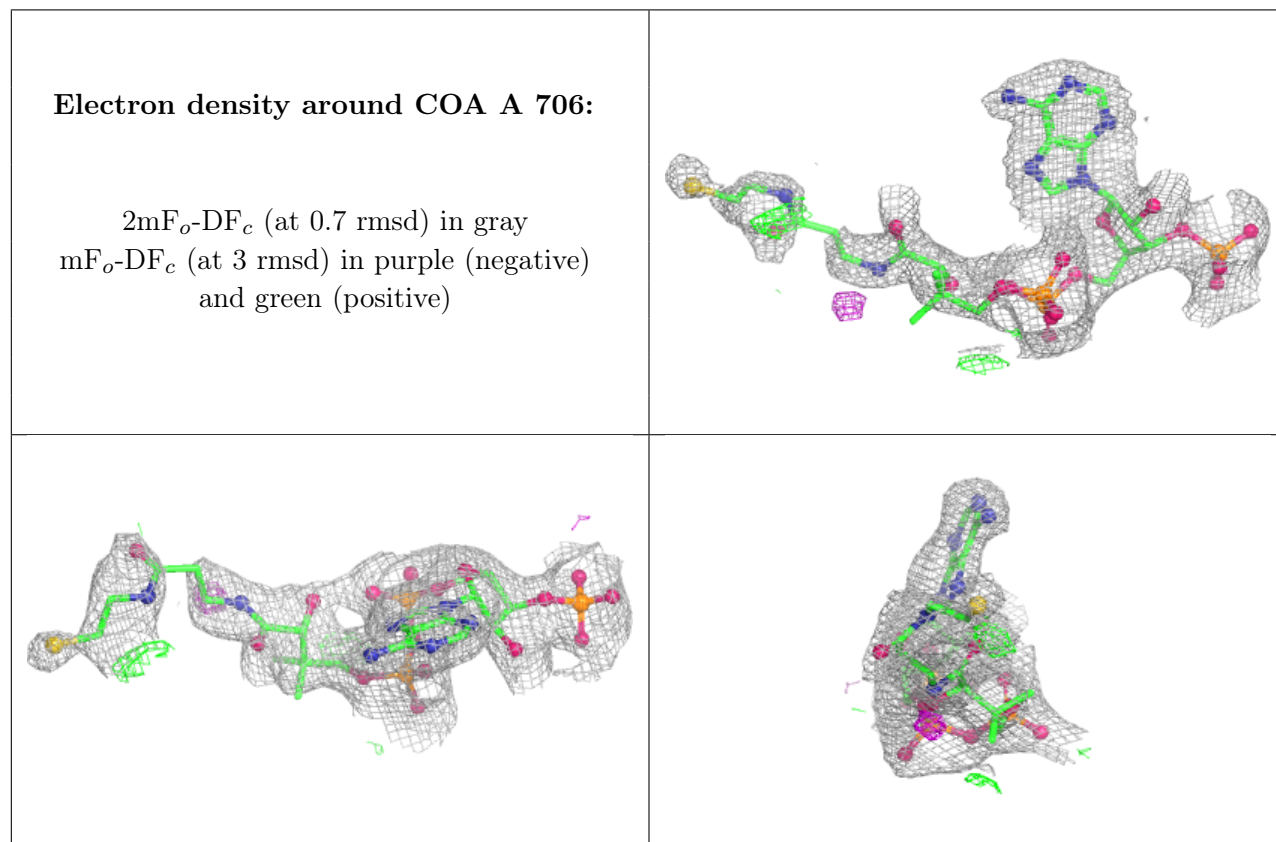
There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

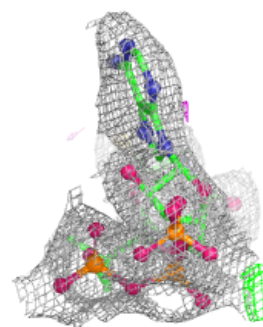
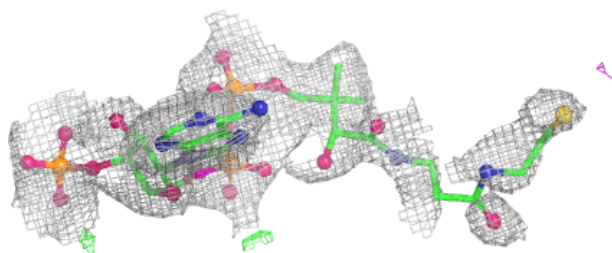
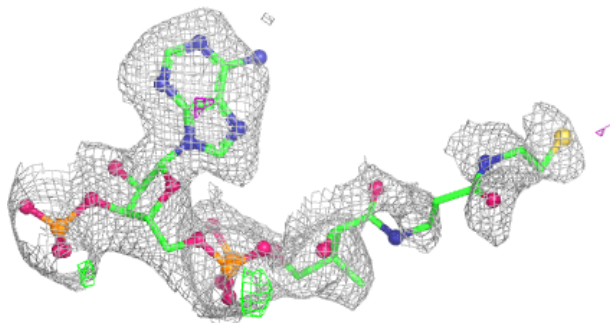
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	EDO	B	705	4/4	0.96	0.08	42,46,46,52	0
2	EDO	C	804	4/4	0.96	0.07	41,42,42,43	0
2	EDO	A	702	4/4	0.97	0.06	40,41,42,43	0
2	EDO	A	708	4/4	0.98	0.07	38,40,42,46	0
2	EDO	B	701	4/4	0.98	0.06	40,41,43,48	0
2	EDO	B	702	4/4	0.98	0.05	38,38,40,42	0
2	EDO	B	704	4/4	0.98	0.05	36,38,40,42	0
2	EDO	A	701	4/4	0.98	0.08	37,37,43,44	0
2	EDO	B	708	4/4	0.98	0.07	41,42,44,48	0
2	EDO	C	801	4/4	0.98	0.07	41,41,42,46	0
2	EDO	A	705	4/4	0.98	0.05	38,38,40,41	0
3	COA	A	706	48/48	0.98	0.05	50,66,73,77	0
3	COA	B	706	48/48	0.98	0.06	50,66,72,74	0
3	COA	C	805	48/48	0.98	0.05	54,69,78,78	0
2	EDO	C	803	4/4	0.99	0.03	35,37,37,38	0
2	EDO	A	704	4/4	0.99	0.04	38,40,42,48	0
2	EDO	B	703	4/4	0.99	0.04	35,37,39,40	0
2	EDO	A	703	4/4	0.99	0.05	38,38,40,41	0
2	EDO	C	802	4/4	0.99	0.06	41,41,43,44	0
4	XM7	A	707	24/24	0.99	0.04	36,41,46,48	0
4	XM7	B	707	24/24	0.99	0.04	32,42,44,45	0
4	XM7	C	806	24/24	0.99	0.03	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.

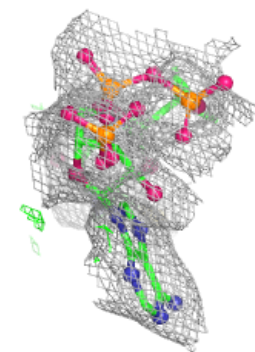
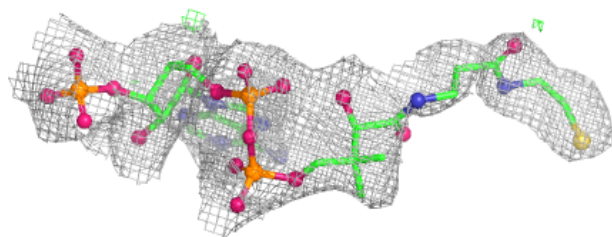
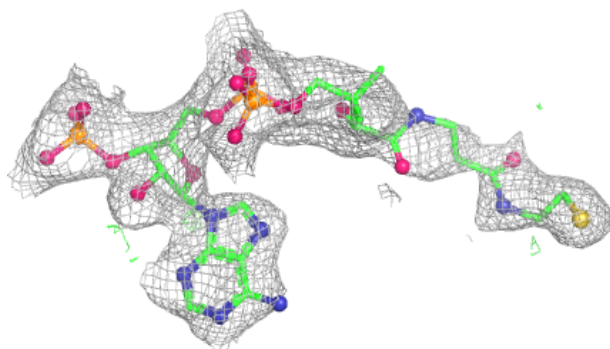


Electron density around COA B 706:

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

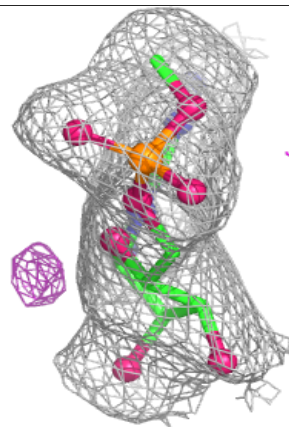
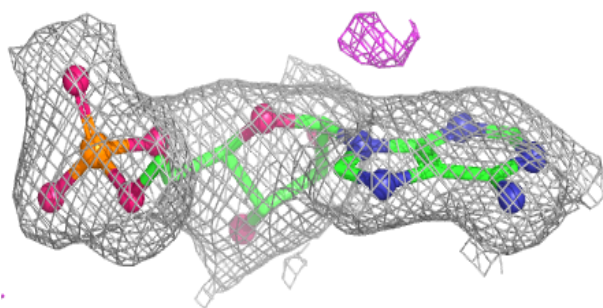
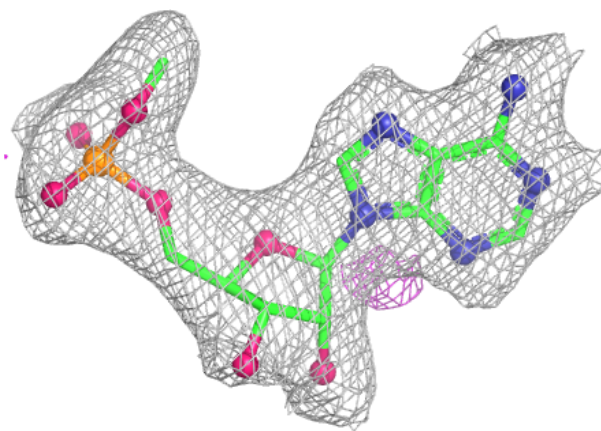
**Electron density around COA C 805:**

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



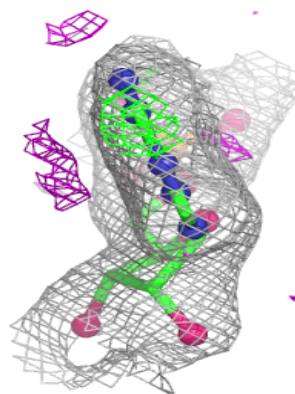
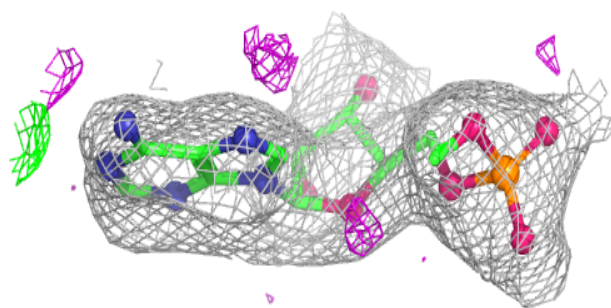
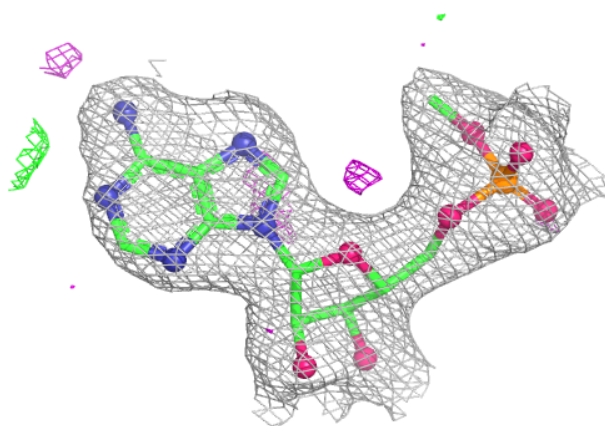
Electron density around XM7 A 707:

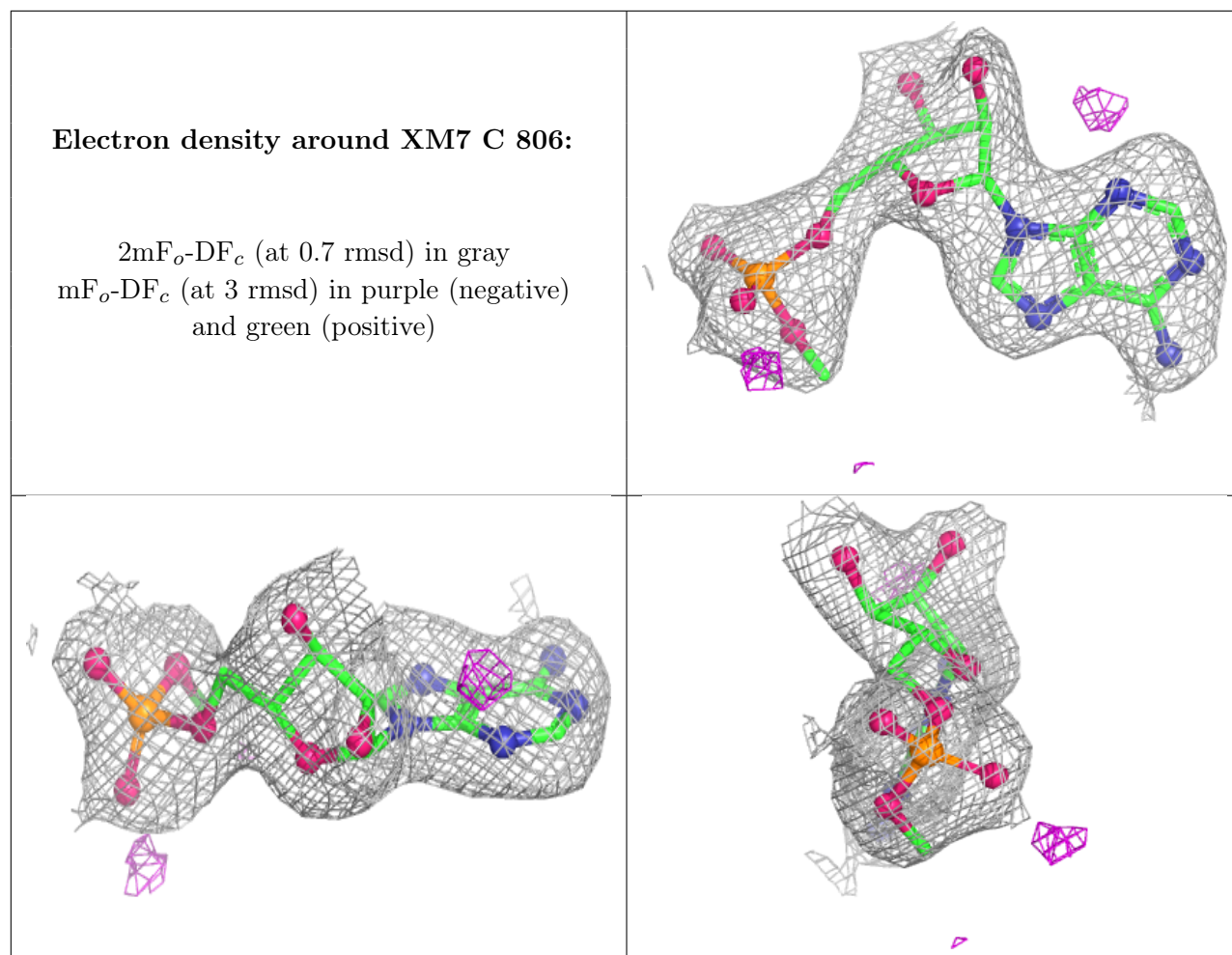
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.