



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 26, 2014 – 12:00 PM EST

PDB ID : 4X0O
Title : Beta-ketoacyl-(acyl carrier protein) synthase III-2 (FabH2) from *Vibrio cholerae* soaked with Acetyl-CoA
Authors : Hou, J.; Chruszcz, M.; Zheng, H.; Cooper, D.R.; Chordia, M.D.; Zimmerman, M.D.; Anderson, W.F.; Minor, W.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on : 2014-11-21
Resolution : 2.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

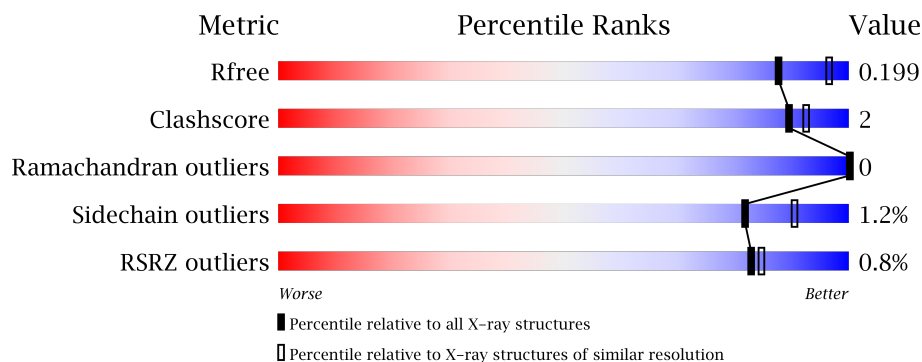
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.16 November 2013
Xtriage (Phenix) : dev-1439
EDS : stable24195
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.1.3
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable24195

1 Overall quality at a glance

The reported resolution of this entry is 2.20 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}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (2.20-2.20)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	362	
1	B	362	
1	C	362	
1	E	362	
1	F	362	
1	G	362	
1	H	362	
2	D	362	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	COA	H	401	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22469 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

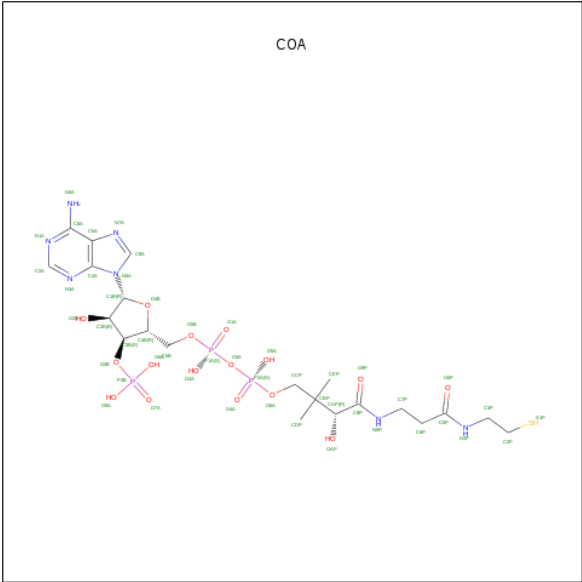
- Molecule 1 is a protein called 3-oxoacyl-[acyl-carrier-protein]synthase 3 protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	359	Total	C	N	O	S	0	1	0
			2671	1682	468	508	13			
1	B	359	Total	C	N	O	S	0	0	0
			2669	1682	468	506	13			
1	C	359	Total	C	N	O	S	0	2	0
			2694	1694	474	513	13			
1	E	360	Total	C	N	O	S	0	1	0
			2679	1685	468	513	13			
1	F	359	Total	C	N	O	S	0	1	0
			2689	1691	472	513	13			
1	G	359	Total	C	N	O	S	0	1	0
			2701	1701	475	512	13			
1	H	358	Total	C	N	O	S	0	3	0
			2709	1704	480	512	13			

- Molecule 2 is a protein called 3-oxoacyl-[acyl-carrier-protein]synthase 3 protein 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	359	Total	C	N	O	S	0	3	0
			2712	1706	479	514	13			

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			21	9	5	6	1		
3	D	1	Total	C	N	O	P	0	0
			21	9	5	6	1		
3	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	F	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	G	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
3	H	1	Total	C	N	O	P	0	0
			48	21	7	16	3		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

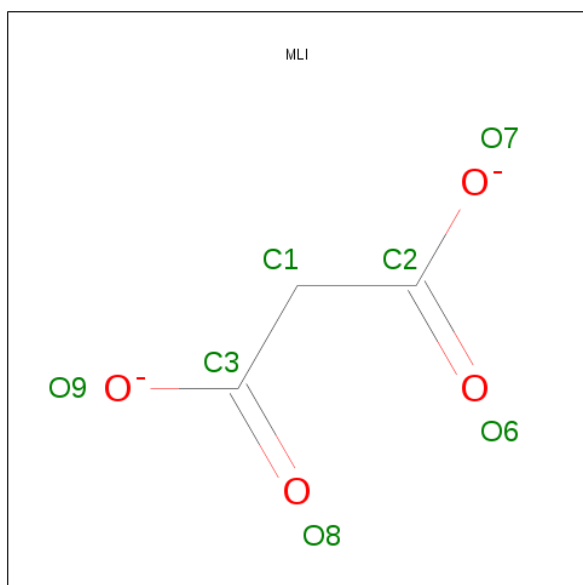
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total	Na	0	0
			1	1		
4	D	1	Total	Na	0	0
			1	1		
4	H	1	Total	Na	0	0
			1	1		
4	B	1	Total	Na	0	0
			1	1		
4	C	1	Total	Na	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		
4	F	1	Total	Na	0	0
			1	1		

- Molecule 5 is MALONATE ION (three-letter code: MLI) (formula: $C_3H_2O_4$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	G	1	Total	C	O	0	0
			7	3	4		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	80	Total	O	0	1
			81	81		
6	B	86	Total	O	0	1
			87	87		
6	C	101	Total	O	0	0
			101	101		
6	D	106	Total	O	0	0
			106	106		
6	E	75	Total	O	0	1
			76	76		
6	F	100	Total	O	0	0
			100	100		

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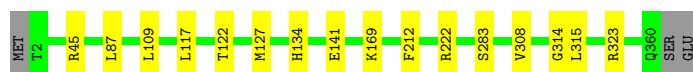
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	G	90	Total	O	0	0
			90	90		
6	H	84	Total	O	0	0
			84	84		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: 3-oxoacyl-[acyl-carrier-protein]synthase 3 protein 2

Chain A: 



- Molecule 1: 3-oxoacyl-[acyl-carrier-protein]synthase 3 protein 2

Chain B: 



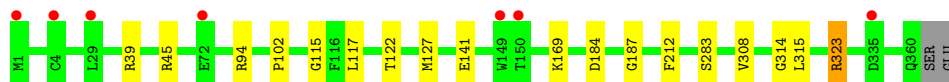
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein]synthase 3 protein 2

Chain C: 



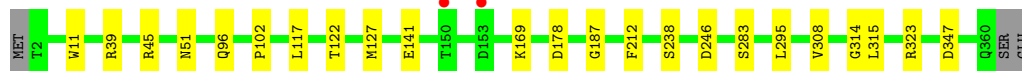
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein]synthase 3 protein 2

Chain E: 



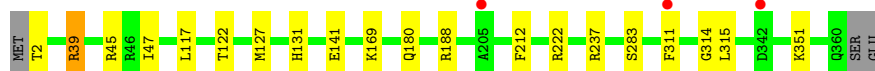
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein]synthase 3 protein 2

Chain F: 



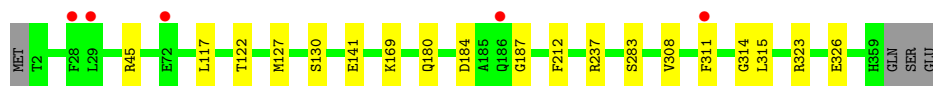
- Molecule 1: 3-oxoacyl-[acyl-carrier-protein]synthase 3 protein 2

Chain G: 



- Molecule 1: 3-oxoacyl-[acyl-carrier-protein]synthase 3 protein 2

Chain H: 



- Molecule 2: 3-oxoacyl-[acyl-carrier-protein]synthase 3 protein 2

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.76Å 86.98Å 157.34Å 90.06° 89.96° 90.08°	Depositor
Resolution (Å)	26.70 – 2.20 26.68 – 2.19	Depositor EDS
% Data completeness (in resolution range)	95.9 (26.70-2.20) 95.9 (26.68-2.19)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.20Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.173 , 0.201 0.177 , 0.199	Depositor DCC
R_{free} test set	8101 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	30.5	Xtriage
Anisotropy	0.865	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 23.3	EDS
Estimated twinning fraction	0.394 for H, K, L 0.233 for -H, -K, L 0.224 for H, -K, -L 0.148 for -H, K, -L 0.367 for h,-k,-l 0.367 for -h,k,-l 0.450 for -h,-k,l	Xtriage
Reported twinning fraction	0.394 for H, K, L 0.233 for -H, -K, L 0.224 for H, -K, -L 0.148 for -H, K, -L	Depositor
L-test for twinning	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	0 of 161071 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	22469	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.91 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.2078e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: COA, NA, MLI, SCY

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.46	0/2716	0.64	1/3700 (0.0%)
1	B	0.52	0/2711	0.66	1/3692 (0.0%)
1	C	0.46	0/2737	0.63	1/3727 (0.0%)
1	E	0.45	0/2721	0.65	2/3707 (0.1%)
1	F	0.51	0/2731	0.64	0/3717
1	G	0.45	0/2747	0.67	2/3736 (0.1%)
1	H	0.48	0/2751	0.64	0/3741
2	D	0.53	0/2774	0.70	4/3775 (0.1%)
All	All	0.48	0/21888	0.65	11/29795 (0.0%)

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	39	ARG	NE-CZ-NH1	11.49	126.05	120.30
2	D	323	ARG	NE-CZ-NH2	8.39	124.50	120.30
1	E	323	ARG	NE-CZ-NH2	8.37	124.48	120.30
2	D	117	LEU	CB-CG-CD2	7.41	123.60	111.00
1	G	39	ARG	NE-CZ-NH2	-7.05	116.77	120.30
1	C	323	ARG	NE-CZ-NH2	7.01	123.80	120.30
1	A	323	ARG	NE-CZ-NH1	6.81	123.70	120.30
1	B	39	ARG	NE-CZ-NH2	5.99	123.29	120.30
2	D	323	ARG	NE-CZ-NH1	-5.66	117.47	120.30
2	D	113	CYS	N-CA-CB	5.49	120.48	110.60
1	E	323	ARG	NE-CZ-NH1	-5.42	117.59	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts ⓘ

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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2671	0	2591	9	0
1	B	2669	0	2593	12	0
1	C	2694	0	2602	8	0
1	E	2679	0	2592	12	0
1	F	2689	0	2617	19	0
1	G	2701	0	2645	14	0
1	H	2709	0	2644	14	0
2	D	2712	0	2653	9	0
3	A	27	0	11	0	0
3	B	21	0	8	0	0
3	D	21	0	8	0	0
3	E	27	0	11	1	0
3	F	31	0	11	0	0
3	G	31	0	11	0	0
3	H	48	0	32	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	G	7	0	2	0	0
6	A	81	0	0	2	0
6	B	87	0	0	4	0
6	C	101	0	0	2	0
6	D	106	0	0	3	0
6	E	76	0	0	4	0
6	F	100	0	0	6	0
6	G	90	0	0	4	0
6	H	84	0	0	4	0
All	All	22469	0	21031	92	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 2.

All (92) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:180:GLN:OE1	2:D:237:ARG:NH2	2.06	0.88
1:H:180:GLN:OE1	1:H:237:ARG:NH2	2.07	0.86
1:G:180:GLN:OE1	1:G:237:ARG:NH2	2.07	0.85
1:A:87:LEU:O	6:A:579:HOH:O	1.95	0.83
1:H:311[A]:PHE:CE1	1:H:315:LEU:HD12	2.17	0.78
1:B:153:ASP:CB	6:B:558:HOH:O	2.34	0.75
1:H:184[A]:ASP:OD1	6:H:532:HOH:O	2.09	0.71
1:F:323:ARG:NH2	6:F:511:HOH:O	2.25	0.69
1:F:178[B]:ASP:OD2	1:F:238:SER:HB3	1.94	0.68
1:E:115:GLY:HA3	6:E:570:HOH:O	1.95	0.65
1:F:96:GLN:NE2	6:F:540:HOH:O	2.30	0.65
1:G:2:THR:N	6:G:551:HOH:O	2.30	0.64
1:F:102:PRO:O	6:F:514:HOH:O	2.15	0.64
1:G:131:HIS:CD2	1:G:131:HIS:O	2.51	0.62
2:D:323:ARG:HG2	6:D:577:HOH:O	2.00	0.62
1:E:187:GLY:O	1:E:315:LEU:CD2	2.49	0.61
1:B:187:GLY:O	1:B:315:LEU:CD2	2.49	0.61
1:F:187:GLY:O	1:F:315:LEU:CD2	2.49	0.61
1:H:187:GLY:O	1:H:315:LEU:CD2	2.49	0.61
1:G:131:HIS:O	1:G:131:HIS:HD2	1.86	0.58
1:C:35:TRP:CZ2	1:C:39:ARG:HD2	2.38	0.58
1:E:323:ARG:NH2	6:E:536:HOH:O	2.36	0.58
1:C:141:GLU:HG3	1:C:283:SER:HB3	1.86	0.57
1:B:141:GLU:HG3	1:B:283:SER:HB3	1.87	0.57
2:D:141:GLU:HG3	2:D:283:SER:HB3	1.87	0.57
1:F:51:ASN:HA	6:F:548:HOH:O	2.03	0.57
1:E:141:GLU:HG3	1:E:283:SER:HB3	1.88	0.55
1:H:141:GLU:HG3	1:H:283:SER:HB3	1.89	0.55
1:A:141:GLU:HG3	1:A:283:SER:HB3	1.89	0.55
1:F:141:GLU:HG3	1:F:283:SER:HB3	1.89	0.54
1:G:141:GLU:HG3	1:G:283:SER:HB3	1.90	0.54
1:H:311[A]:PHE:CZ	1:H:315:LEU:HD12	2.42	0.54
1:H:323:ARG:NH2	6:H:536:HOH:O	2.42	0.53
1:A:134:HIS:HD2	6:A:576:HOH:O	1.90	0.53
1:B:178:ASP:HB2	6:B:523:HOH:O	2.08	0.52
1:C:148:ASP:N	6:C:590:HOH:O	2.36	0.52
1:F:246:ASP:OD1	6:F:573:HOH:O	2.19	0.51
1:B:323:ARG:NH2	6:B:507:HOH:O	2.43	0.50
1:F:347:ASP:HB3	6:F:544:HOH:O	2.11	0.49
1:C:314:GLY:N	1:C:315:LEU:HA	2.28	0.49
2:D:314:GLY:N	2:D:315:LEU:HA	2.28	0.49
1:G:222:ARG:HD3	1:G:315:LEU:CD1	2.43	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:F:187:GLY:O	1:F:315:LEU:HD23	2.13	0.48
1:B:187:GLY:O	1:B:315:LEU:HD23	2.13	0.48
1:H:187:GLY:O	1:H:315:LEU:HD23	2.13	0.48
1:E:187:GLY:O	1:E:315:LEU:HD23	2.13	0.48
1:B:212:PHE:HB3	6:B:525:HOH:O	2.14	0.48
1:E:122:THR:HG23	1:G:122:THR:HG23	1.96	0.47
1:C:194:PRO:HD2	6:C:527:HOH:O	2.14	0.47
1:H:326:GLU:HG2	6:H:504:HOH:O	2.14	0.47
1:F:117:LEU:HD11	1:F:308:VAL:HG11	1.97	0.47
1:H:130:SER:OG	6:H:582:HOH:O	2.06	0.47
1:A:222:ARG:HD3	1:A:315:LEU:CD1	2.45	0.46
3:H:401:COA:OAP	3:H:401:COA:O6A	2.33	0.46
1:G:314:GLY:N	1:G:315:LEU:HA	2.31	0.46
1:A:314:GLY:N	1:A:315:LEU:HA	2.31	0.45
1:F:117:LEU:HD13	1:F:117:LEU:HA	1.70	0.45
1:E:314:GLY:N	1:E:315:LEU:HA	2.32	0.45
1:H:314:GLY:N	1:H:315:LEU:HA	2.32	0.44
2:D:184[A]:ASP:OD2	6:D:573:HOH:O	2.21	0.44
1:E:117:LEU:HD11	1:E:308:VAL:CG1	2.48	0.44
1:G:2:THR:HA	6:G:545:HOH:O	2.16	0.44
1:F:314:GLY:N	1:F:315:LEU:HA	2.33	0.44
1:C:127:MET:O	1:C:169:LYS:CE	2.66	0.44
1:A:127:MET:O	1:A:169:LYS:CE	2.66	0.44
1:E:184:ASP:HB2	6:E:565:HOH:O	2.17	0.44
2:D:127:MET:O	2:D:169:LYS:CE	2.67	0.43
1:A:122:THR:HG23	1:C:122:THR:HG23	2.01	0.43
1:G:311[B]:PHE:HZ	1:G:315:LEU:HD13	1.84	0.43
1:B:314:GLY:N	1:B:315:LEU:HA	2.33	0.43
1:E:127:MET:O	1:E:169:LYS:CE	2.67	0.43
1:A:117:LEU:HD11	1:A:308:VAL:CG1	2.48	0.43
1:F:117:LEU:HD11	1:F:308:VAL:CG1	2.49	0.43
1:F:117:LEU:HD21	1:F:308:VAL:CG1	2.48	0.43
1:G:127:MET:O	1:G:169:LYS:CE	2.67	0.43
1:B:127:MET:O	1:B:169:LYS:CE	2.67	0.43
1:H:117:LEU:HD11	1:H:308:VAL:CG1	2.48	0.43
1:F:127:MET:O	1:F:169:LYS:CE	2.68	0.42
1:H:127:MET:O	1:H:169:LYS:CE	2.67	0.42
3:E:400:COA:H4B	3:E:400:COA:O2A	2.19	0.42
1:G:47:ILE:O	6:G:581:HOH:O	2.21	0.42
1:B:117:LEU:HD11	1:B:308:VAL:CG1	2.49	0.42
2:D:115:GLY:HA3	6:D:570:HOH:O	2.18	0.42
1:B:122:THR:HG23	2:D:122:THR:HG23	2.01	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:102:PRO:HA	6:E:571:HOH:O	2.20	0.42
1:F:117:LEU:N	1:F:117:LEU:HD22	2.35	0.42
1:F:122:THR:HG23	1:H:122:THR:HG23	2.02	0.41
1:B:109:LEU:HG	2:D:107:PHE:CD2	2.55	0.41
1:F:11:TRP:CD2	1:F:295:LEU:HD13	2.55	0.41
1:G:351:LYS:NZ	6:G:559:HOH:O	2.46	0.41
1:A:109:LEU:HG	1:C:107:PHE:CD2	2.56	0.41
1:E:94:ARG:HB2	1:G:188:ARG:CZ	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

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	357/362 (99%)	345 (97%)	12 (3%)	0	100	100
1	B	356/362 (98%)	343 (96%)	13 (4%)	0	100	100
1	C	358/362 (99%)	345 (96%)	13 (4%)	0	100	100
1	E	358/362 (99%)	345 (96%)	13 (4%)	0	100	100
1	F	357/362 (99%)	345 (97%)	12 (3%)	0	100	100
1	G	357/362 (99%)	345 (97%)	12 (3%)	0	100	100
1	H	358/362 (99%)	345 (96%)	13 (4%)	0	100	100
2	D	360/362 (99%)	347 (96%)	13 (4%)	0	100	100
All	All	2861/2896 (99%)	2760 (96%)	101 (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	268/284 (94%)	266 (99%)	2 (1%)	91	96
1	B	267/284 (94%)	264 (99%)	3 (1%)	84	92
1	C	270/284 (95%)	265 (98%)	5 (2%)	69	81
1	E	269/284 (95%)	266 (99%)	3 (1%)	84	92
1	F	272/284 (96%)	269 (99%)	3 (1%)	84	92
1	G	275/284 (97%)	271 (98%)	4 (2%)	76	86
1	H	274/284 (96%)	272 (99%)	2 (1%)	91	96
2	D	277/285 (97%)	273 (99%)	4 (1%)	78	88
All	All	2172/2273 (96%)	2146 (99%)	26 (1%)	82	90

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
1	A	212	PHE
1	B	39	ARG
1	B	45	ARG
1	B	212	PHE
1	C	45	ARG
1	C	117	LEU
1	C	153[A]	ASP
1	C	153[B]	ASP
1	C	212	PHE
2	D	39	ARG
2	D	45	ARG
2	D	117	LEU
2	D	212	PHE
1	E	39	ARG
1	E	45	ARG
1	E	212	PHE
1	F	39	ARG
1	F	45	ARG
1	F	212	PHE
1	G	39	ARG
1	G	45	ARG
1	G	117	LEU
1	G	212	PHE

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Mol	Chain	Res	Type
1	H	45	ARG
1	H	212	PHE

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

Mol	Chain	Res	Type
1	A	37	GLN
1	A	134	HIS
1	B	37	GLN
1	B	180	GLN
1	B	186	GLN
1	C	37	GLN
2	D	37	GLN
1	E	37	GLN
1	F	3	GLN
1	F	37	GLN
1	G	37	GLN
1	G	131	HIS
1	H	3	GLN
1	H	37	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

7 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	SCY	A	113	1	8,8,9	6.42	3 (37%)	7,9,11	4.39	1 (14%)
1	SCY	B	113	1	8,8,9	6.40	3 (37%)	7,9,11	4.28	1 (14%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	SCY	C	113	1	8,8,9	6.15	2 (25%)	7,9,11	4.50	1 (14%)
1	SCY	E	113	1	8,8,9	6.48	2 (25%)	7,9,11	4.43	1 (14%)
1	SCY	F	113	1	8,8,9	6.98	3 (37%)	7,9,11	4.02	1 (14%)
1	SCY	G	113	1	8,8,9	6.38	3 (37%)	7,9,11	4.44	1 (14%)
1	SCY	H	113	1	8,8,9	6.88	3 (37%)	7,9,11	4.63	1 (14%)

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
1	SCY	A	113	1	-	0/5/7/9	0/0/0/0
1	SCY	B	113	1	-	0/5/7/9	0/0/0/0
1	SCY	C	113	1	-	0/5/7/9	0/0/0/0
1	SCY	E	113	1	-	0/5/7/9	0/0/0/0
1	SCY	F	113	1	-	0/5/7/9	0/0/0/0
1	SCY	G	113	1	-	0/5/7/9	0/0/0/0
1	SCY	H	113	1	-	0/5/7/9	0/0/0/0

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	113	SCY	O-C	19.41	1.24	1.11
1	H	113	SCY	O-C	19.13	1.24	1.11
1	E	113	SCY	O-C	18.06	1.23	1.11
1	A	113	SCY	O-C	17.71	1.23	1.11
1	B	113	SCY	O-C	17.68	1.23	1.11
1	G	113	SCY	O-C	17.62	1.23	1.11
1	C	113	SCY	O-C	17.14	1.23	1.11
1	A	113	SCY	CB-SG	-2.95	1.78	1.81
1	B	113	SCY	CB-SG	-2.78	1.78	1.81
1	H	113	SCY	CB-SG	-2.47	1.78	1.81
1	G	113	SCY	CB-SG	-2.34	1.78	1.81
1	B	113	SCY	CD-SG	-2.32	1.66	1.75
1	A	113	SCY	CD-SG	-2.27	1.66	1.75
1	F	113	SCY	CD-SG	-2.26	1.66	1.75
1	C	113	SCY	CD-SG	-2.21	1.66	1.75
1	F	113	SCY	CB-CA	2.18	1.55	1.53
1	E	113	SCY	CD-SG	-2.16	1.66	1.75
1	H	113	SCY	CD-SG	-2.11	1.66	1.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	113	SCY	CD-SG	-2.04	1.67	1.75

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	113	SCY	CB-SG-CD	12.09	108.58	100.87
1	C	113	SCY	CB-SG-CD	11.74	108.35	100.87
1	G	113	SCY	CB-SG-CD	11.60	108.26	100.87
1	E	113	SCY	CB-SG-CD	11.57	108.24	100.87
1	A	113	SCY	CB-SG-CD	11.42	108.14	100.87
1	B	113	SCY	CB-SG-CD	11.14	107.97	100.87
1	F	113	SCY	CB-SG-CD	10.48	107.55	100.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	COA	A	400	-	29,29,50	1.22	4 (13%)	45,45,75	2.13	8 (17%)
3	COA	B	400	-	21,23,50	1.26	3 (14%)	31,35,75	2.44	7 (22%)
3	COA	D	400	-	21,23,50	1.27	3 (14%)	31,35,75	2.57	7 (22%)
3	COA	E	400	-	29,29,50	1.32	4 (13%)	45,45,75	2.25	8 (17%)
3	COA	F	401	-	33,33,50	1.36	5 (15%)	52,52,75	1.91	8 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	COA	G	401	-	33,33,50	1.34	5 (15%)	52,52,75	1.87	8 (15%)
5	MLI	G	403	-	2,6,6	4.08	2 (100%)	0,7,7	0.00	-
3	COA	H	401	-	50,50,50	0.92	3 (6%)	75,75,75	1.87	15 (20%)

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	A	400	-	-	0/15/31/64	0/3/3/3
3	COA	B	400	-	-	0/9/22/64	0/3/3/3
3	COA	D	400	-	-	0/9/22/64	0/3/3/3
3	COA	E	400	-	-	0/15/31/64	0/3/3/3
3	COA	F	401	-	-	0/21/37/64	0/3/3/3
3	COA	G	401	-	-	0/21/37/64	0/3/3/3
5	MLI	G	403	-	-	0/0/4/4	0/0/0/0
3	COA	H	401	-	-	1/48/64/64	0/3/3/3

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	G	403	MLI	C1-C2	4.34	1.52	1.49
3	G	401	COA	P2A-O4A	3.95	1.63	1.50
5	G	403	MLI	C1-C3	3.80	1.52	1.49
3	F	401	COA	P2A-O4A	3.62	1.61	1.50
3	E	400	COA	P1A-O1A	3.57	1.61	1.50
3	G	401	COA	C5A-C4A	3.46	1.48	1.40
3	A	400	COA	P1A-O3A	3.38	1.61	1.50
3	F	401	COA	C5A-C4A	3.32	1.48	1.40
3	B	400	COA	C5A-C4A	3.20	1.47	1.40
3	A	400	COA	C5A-C4A	3.18	1.47	1.40
3	H	401	COA	C5A-C4A	3.13	1.47	1.40
3	E	400	COA	C5A-C4A	3.13	1.47	1.40
3	F	401	COA	C4A-N9A	-3.07	1.33	1.37
3	G	401	COA	O4B-C1B	2.89	1.44	1.41
3	E	400	COA	O4B-C1B	2.84	1.44	1.41
3	F	401	COA	O4B-C1B	2.72	1.44	1.41
3	B	400	COA	C4A-N9A	-2.70	1.33	1.37
3	D	400	COA	C5A-C4A	2.65	1.46	1.40
3	E	400	COA	C4A-N9A	-2.61	1.33	1.37
3	G	401	COA	C4A-N9A	-2.57	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	400	COA	C4A-N9A	-2.55	1.34	1.37
3	H	401	COA	C4A-N9A	-2.32	1.34	1.37
3	F	401	COA	C2A-N3A	2.23	1.36	1.32
3	H	401	COA	O4B-C1B	2.21	1.44	1.41
3	D	400	COA	O4B-C1B	2.10	1.44	1.40
3	A	400	COA	O4B-C1B	2.09	1.43	1.41
3	B	400	COA	O4B-C1B	2.09	1.44	1.40
3	A	400	COA	C4A-N9A	-2.08	1.34	1.37
3	G	401	COA	C2A-N3A	2.02	1.35	1.32

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	400	COA	C5A-C4A-N3A	-8.11	118.07	125.98
3	B	400	COA	C5A-C4A-N3A	-7.83	118.34	125.98
3	D	400	COA	N3A-C2A-N1A	-7.65	122.16	128.89
3	D	400	COA	C5A-C4A-N3A	-7.47	118.70	125.98
3	H	401	COA	C5A-C4A-N3A	-7.37	118.79	125.98
3	F	401	COA	N3A-C2A-N1A	-7.07	122.67	128.89
3	E	400	COA	N3A-C2A-N1A	-7.06	122.68	128.89
3	G	401	COA	C5A-C4A-N3A	-6.95	119.20	125.98
3	E	400	COA	C5A-C4A-N3A	-6.86	119.29	125.98
3	G	401	COA	N3A-C2A-N1A	-6.83	122.89	128.89
3	H	401	COA	N3A-C2A-N1A	-6.82	122.89	128.89
3	F	401	COA	C5A-C4A-N3A	-6.76	119.39	125.98
3	B	400	COA	N3A-C2A-N1A	-6.46	123.21	128.89
3	A	400	COA	N3A-C2A-N1A	-6.33	123.32	128.89
3	A	400	COA	N3A-C4A-N9A	5.94	135.58	125.39
3	B	400	COA	N3A-C4A-N9A	5.89	135.50	125.39
3	D	400	COA	N3A-C4A-N9A	5.58	134.96	125.39
3	H	401	COA	N3A-C4A-N9A	5.51	134.84	125.39
3	E	400	COA	C4B-O4B-C1B	-5.46	103.72	109.72
3	E	400	COA	N3A-C4A-N9A	5.40	134.66	125.39
3	F	401	COA	N3A-C4A-N9A	5.33	134.54	125.39
3	G	401	COA	N3A-C4A-N9A	5.25	134.39	125.39
3	H	401	COA	C6P-C7P-N8P	-3.84	103.48	111.94
3	H	401	COA	CDP-CBP-CAP	3.20	114.38	108.82
3	H	401	COA	O4B-C1B-N9A	3.09	114.82	108.10
3	D	400	COA	C4A-C5A-N7A	-3.05	106.47	109.41
3	D	400	COA	C2A-N3A-C4A	2.93	121.70	113.27
3	H	401	COA	O4B-C1B-C2B	-2.89	102.48	106.69
3	H	401	COA	C4A-C5A-N7A	-2.88	106.63	109.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	400	COA	C2A-N3A-C4A	2.87	121.53	113.27
3	E	400	COA	C2A-N3A-C4A	2.85	121.47	113.27
3	B	400	COA	C2A-N3A-C4A	2.84	121.45	113.27
3	A	400	COA	C3B-C2B-C1B	2.82	106.74	99.96
3	H	401	COA	C2A-N3A-C4A	2.80	121.33	113.27
3	B	400	COA	C1B-C2B-C3B	2.78	105.20	101.09
3	B	400	COA	C4A-C5A-N7A	-2.71	106.79	109.41
3	A	400	COA	C4A-C5A-N7A	-2.69	106.81	109.41
3	A	400	COA	O2A-P1A-O1A	2.66	120.50	110.88
3	F	401	COA	C2A-N3A-C4A	2.65	120.91	113.27
3	G	401	COA	C2A-N3A-C4A	2.65	120.89	113.27
3	G	401	COA	C4A-C5A-N7A	-2.51	106.99	109.41
3	G	401	COA	P2A-O3A-P1A	-2.50	123.12	133.17
3	H	401	COA	P2A-O3A-P1A	-2.50	125.02	131.93
3	E	400	COA	C4A-C5A-N7A	-2.42	107.07	109.41
3	H	401	COA	O5P-C5P-C6P	-2.42	117.29	121.92
3	F	401	COA	O5A-P2A-O6A	2.39	120.13	110.63
3	A	400	COA	C4B-O4B-C1B	2.38	112.33	109.72
3	H	401	COA	CDP-CBP-CCP	-2.37	105.43	108.71
3	E	400	COA	O4B-C1B-N9A	2.34	113.20	108.10
3	E	400	COA	C8A-N9A-C4A	2.34	108.86	106.96
3	D	400	COA	C8A-N9A-C4A	2.31	108.83	106.96
3	G	401	COA	O5A-P2A-O6A	2.31	119.83	110.63
3	B	400	COA	C8A-N9A-C4A	2.21	108.75	106.96
3	D	400	COA	C2A-N1A-C6A	2.21	122.69	118.76
3	H	401	COA	O9A-P3B-O8A	2.19	115.59	107.38
3	F	401	COA	C4A-C5A-N7A	-2.18	107.30	109.41
3	G	401	COA	C2A-N1A-C6A	2.18	122.63	118.76
3	F	401	COA	C2A-N1A-C6A	2.16	122.61	118.76
3	F	401	COA	C3B-C2B-C1B	2.11	105.02	99.96
3	H	401	COA	C2A-N1A-C6A	2.02	122.36	118.76
3	H	401	COA	O9P-C9P-CAP	2.00	122.82	120.05

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	H	401	COA	C2B-C1B-N9A-C8A

There are no ring outliers.

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	359/362 (99%)	0.08	0 100 100	28, 44, 71, 86	0
1	B	359/362 (99%)	0.04	3 (0%) 83 85	24, 40, 69, 78	0
1	C	359/362 (99%)	0.05	1 (0%) 91 93	27, 43, 63, 70	0
1	E	360/362 (99%)	0.09	7 (1%) 64 64	29, 45, 69, 84	0
1	F	359/362 (99%)	-0.03	2 (0%) 86 88	23, 40, 61, 83	0
1	G	359/362 (99%)	0.07	3 (0%) 83 85	29, 45, 70, 93	0
1	H	358/362 (98%)	0.08	5 (1%) 72 72	25, 42, 66, 76	0
2	D	359/362 (99%)	0.04	2 (0%) 86 88	21, 39, 61, 74	0
All	All	2872/2896 (99%)	0.05	23 (0%) 83 85	21, 42, 67, 93	0

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	1	MET	4.4
1	E	4	CYS	3.7
1	E	29	LEU	3.5
1	G	342	ASP	3.2
1	C	240	LEU	3.0
1	E	335	ASP	2.9
1	H	28	PHE	2.7
2	D	29	LEU	2.7
2	D	311[A]	PHE	2.7
1	E	150	THR	2.6
1	F	153	ASP	2.5
1	H	29	LEU	2.5
1	F	150	THR	2.4
1	B	240	LEU	2.4
1	G	311[A]	PHE	2.4
1	B	342	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	E	149	TRP	2.1
1	H	311[A]	PHE	2.1
1	G	205	ALA	2.1
1	H	72	GLU	2.1
1	B	2	THR	2.1
1	H	186	GLN	2.0
1	E	72	GLU	2.0

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

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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	SCY	B	113	9/10	0.12	0.14	32,34,44,47	0
1	SCY	G	113	9/10	0.13	-0.09	37,39,42,43	0
1	SCY	H	113	9/10	0.12	-0.27	37,40,44,48	0
1	SCY	C	113	9/10	0.12	-0.30	36,39,47,48	0
1	SCY	A	113	9/10	0.11	-0.55	33,37,46,49	0
1	SCY	E	113	9/10	0.10	-0.82	39,42,46,48	0
1	SCY	F	113	9/10	0.08	-1.75	31,33,40,40	0

6.3 Carbohydrates ⓘ

There are no carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
3	COA	H	401	48/48	0.26	2.85	50,63,76,82	48

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	COA	A	400	27/48	0.28	1.90	55,74,88,91	27
3	COA	B	400	21/48	0.21	1.46	45,49,53,54	21
3	COA	D	400	21/48	0.23	1.33	39,48,59,66	21
3	COA	G	401	31/48	0.17	0.53	53,69,78,83	0
3	COA	F	401	31/48	0.17	0.45	53,70,92,96	0
3	COA	E	400	27/48	0.19	0.43	48,51,56,59	27
5	MLI	G	403	7/7	0.15	-0.22	66,67,71,71	0
4	NA	F	402	1/1	0.12	-0.78	34,34,34,34	0
4	NA	C	401	1/1	0.10	-1.47	39,39,39,39	0
4	NA	A	401	1/1	0.07	-2.00	42,42,42,42	0
4	NA	H	402	1/1	0.08	-2.06	45,45,45,45	0
4	NA	G	402	1/1	0.06	-2.54	51,51,51,51	0
4	NA	B	401	1/1	0.07	-3.05	32,32,32,32	0
4	NA	D	401	1/1	0.05	-3.87	36,36,36,36	0

6.5 Other polymers ⓘ

There are no such residues in this entry.