Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 10:21 AM JST

PDB ID	:	5WX6
Title	:	Alkyldiketide-CoA synthase W332Q mutant from Evodia rutaecarpa
Authors	:	Matsui, T.; Kodama, T.; Tadakoshi, T.; Morita, H.
Deposited on	:	2017-01-06
Resolution	:	1.80 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:

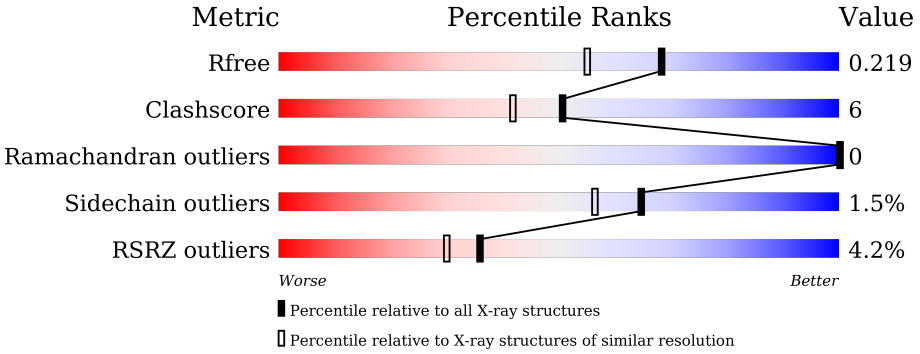
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	396	2%, 82%, 10%, 8%
1	B	396	2%, 82%, 13%, 5%
1	C	396	5%, 82%, 10%, • 7%
1	D	396	7%, 79%, 15%, • 5%

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

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SO4	C	404	-	-	X	-

2 Entry composition (i)

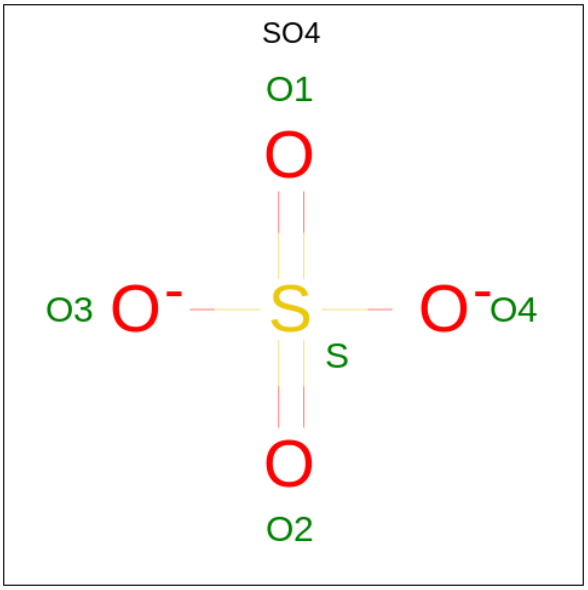
There are 4 unique types of molecules in this entry. The entry contains 12740 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Alkyldiketide-CoA synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	363	2824	1797	481	520	26	0	0	0
1	B	376	2929	1861	498	543	27	0	1	0
1	C	368	2865	1822	488	529	26	0	0	0
1	D	375	2921	1854	499	542	26	0	0	0

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	A	1	5	4	1	0	0
2	A	1	5	4	1	0	0

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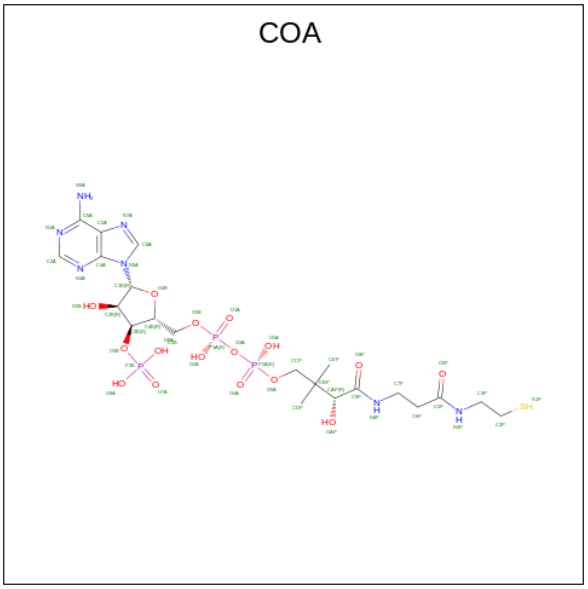
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
2	B	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	C	1	5	4	1	0	0
			Total	O	S		
2	D	1	5	4	1	0	0

- 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
			Total	C	N	O	P	S		
3	D	1	48	21	7	16	3	1	0	0

- Molecule 4 is water.

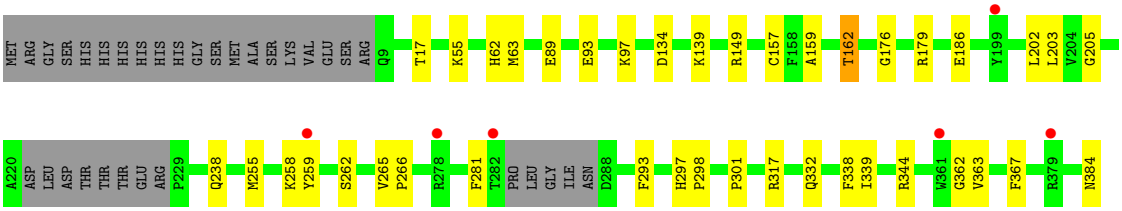
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	279	279	279	0	0
			Total	O		
4	B	315	315	315	0	0
			Total	O		
4	C	235	235	235	0	0
			Total	O		
4	D	140	140	140	0	0

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.

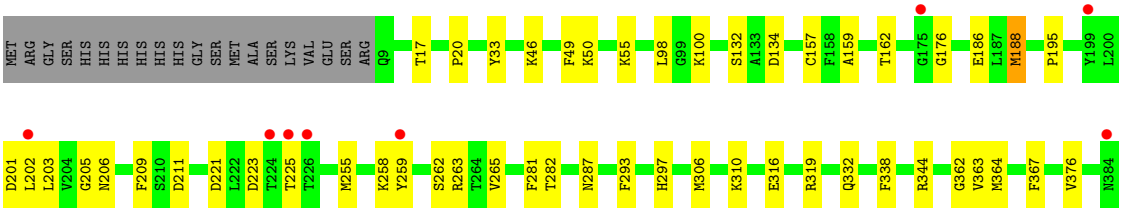
• Molecule 1: Alkyldiketide-CoA synthase

Chain A:



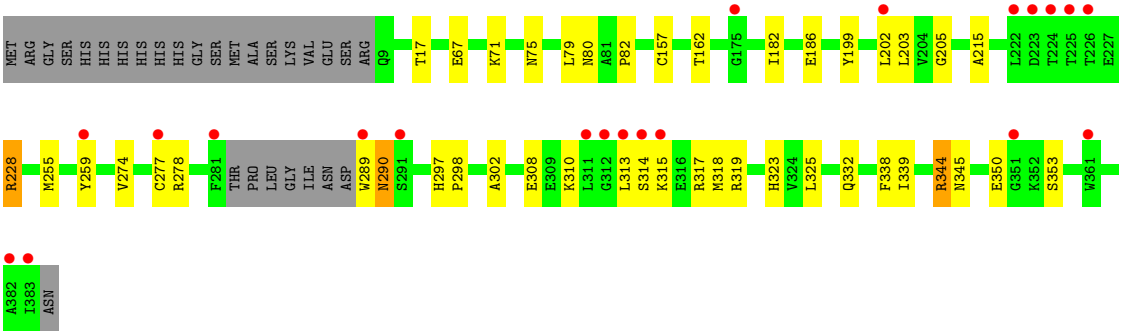
• Molecule 1: Alkyldiketide-CoA synthase

Chain B:



• Molecule 1: Alkyldiketide-CoA synthase

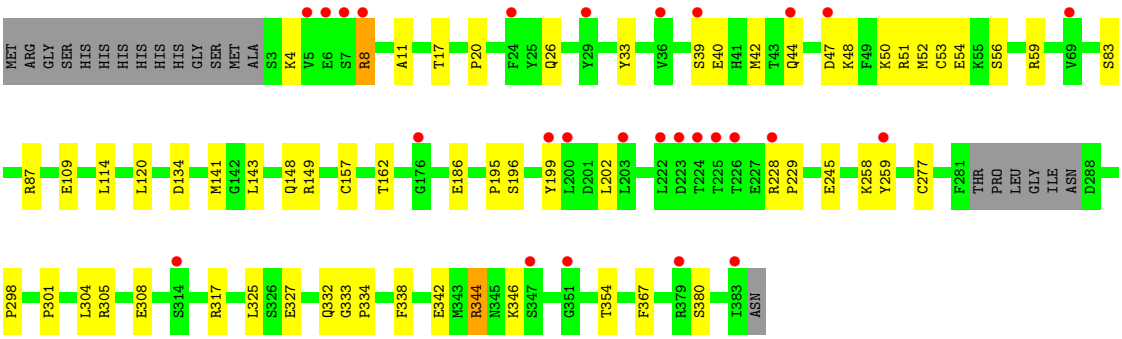
Chain C:



• Molecule 1: Alkyldiketide-CoA synthase

Chain D:

7%
79%
15%
• 5%


MET ARG GLY SER HIS HIS HIS HIS HIS HIS GLY SER MET ALA S3 K4 V5 E6 S7 R8 A11 T17 P20 F24 Y25 Q26 Y29 Y33 V36 S39 E40 H41 M42 T43 Q44 D47 K48 F49 K50 R51 M52 C53 E54 K55 S56 R59 V69 S83
R87 E109 L114 L120 D134 M141 G142 L143 Q148 R149 C157 T162 G176 E186 P195 S196 Y199 L200 D201 L202 L203 L222 D223 T224 T225 T226 E227 R228 P229 E245 K258 Y259 C277 F281 THR PRO LEU GLY ILE ASN D288
P298 P301 L304 R305 E308 S314 R317 L325 S326 E327 Q332 G333 P334 F338 E342 M343 R344 N345 K346 S347 G351 T354 F367 R379 S380 I383 ASN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	164.08Å 84.66Å 137.86Å 90.00° 124.63° 90.00°	Depositor
Resolution (Å)	47.37 – 1.80 47.37 – 1.80	Depositor EDS
% Data completeness (in resolution range)	98.4 (47.37-1.80) 98.4 (47.37-1.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.21 (at 1.79Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.183 , 0.223 0.180 , 0.219	Depositor DCC
R_{free} test set	7083 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	29.8	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 45.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.015 for h,-k,-h-l	Xtriage
Reported twinning fraction	0.020 for h,-k,-h-l	Depositor
Outliers	0 of 141647 reflections	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	12740	wwPDB-VP
Average B, all atoms (Å^2)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.99% 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: SO4, 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	0.40	0/2882	0.56	0/3894
1	B	0.43	0/2993	0.58	0/4050
1	C	0.40	0/2924	0.58	0/3955
1	D	0.39	0/2980	0.55	0/4029
All	All	0.40	0/11779	0.57	0/15928

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	2824	0	2829	25	0
1	B	2929	0	2936	34	0
1	C	2865	0	2871	25	0
1	D	2921	0	2926	40	0
2	A	10	0	0	0	0
2	B	5	0	0	1	0
2	C	20	0	0	2	0
2	D	5	0	0	1	0
3	A	48	0	32	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	48	0	32	5	0
3	C	48	0	32	5	0
3	D	48	0	32	8	0
4	A	279	0	0	2	0
4	B	315	0	0	3	0
4	C	235	0	0	0	0
4	D	140	0	0	2	0
All	All	12740	0	11690	133	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 6.

All (133) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:403:COA:O4B	3:A:403:COA:C1B	1.66	1.28
3:C:405:COA:O4B	3:C:405:COA:C1B	1.67	1.26
3:B:402:COA:C1B	3:B:402:COA:O4B	1.66	1.25
3:D:402:COA:O4B	3:D:402:COA:C1B	1.67	1.22
1:D:51:ARG:NH2	3:D:402:COA:O8A	1.72	1.22
3:C:405:COA:H8A	3:C:405:COA:H51A	1.51	0.91
1:D:199:TYR:HB3	1:D:202:LEU:HD12	1.55	0.88
1:C:323:HIS:CD2	2:C:404:SO4:O3	2.29	0.86
1:A:255:MET:SD	1:A:258:LYS:HD2	2.24	0.77
1:C:290:ASN:HD21	1:C:313:LEU:HA	1.50	0.76
3:C:405:COA:H51A	3:C:405:COA:C8A	2.23	0.69
1:D:52:MET:O	3:D:402:COA:CDP	2.42	0.68
1:B:255:MET:SD	1:B:258:LYS:HD2	2.34	0.68
1:A:301:PRO:HD2	3:A:403:COA:OAP	1.94	0.67
1:B:205:GLY:HA3	1:B:259:TYR:CZ	2.30	0.66
1:B:258:LYS:NZ	2:B:401:SO4:O4	2.23	0.65
1:D:51:ARG:CZ	3:D:402:COA:O8A	2.45	0.64
1:C:323:HIS:HD2	2:C:404:SO4:O3	1.80	0.63
1:C:67:GLU:HG2	1:C:71:LYS:HE2	1.80	0.62
1:B:188[A]:MET:HG3	1:B:211:ASP:OD1	1.99	0.62
1:D:39:SER:HB3	1:D:42:MET:SD	2.41	0.61
1:D:50:LYS:O	1:D:54:GLU:HG3	1.99	0.60
1:D:56:SER:HA	3:D:402:COA:H143	1.83	0.60
1:D:47:ASP:O	1:D:51:ARG:HG3	2.01	0.60
1:D:11:ALA:HB1	1:D:229:PRO:HB3	1.83	0.60
1:C:80:ASN:HA	1:C:255:MET:HE2	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:304:LEU:O	1:D:308:GLU:HG3	2.02	0.59
1:C:274:VAL:HG11	1:C:310:LYS:HG2	1.85	0.59
1:D:342:GLU:OE2	1:D:346:LYS:NZ	2.37	0.58
1:A:176:GLY:O	1:A:179:ARG:NH1	2.38	0.57
1:D:59:ARG:NH2	4:D:505:HOH:O	2.38	0.57
1:D:4:LYS:O	1:D:8:ARG:HD3	2.03	0.56
1:A:238:GLN:H	1:D:148:GLN:NE2	2.03	0.56
1:D:120:LEU:HD23	1:D:149:ARG:HG2	1.86	0.56
3:A:403:COA:O9P	3:A:403:COA:H133	2.05	0.55
1:B:202:LEU:O	1:B:259:TYR:OH	2.25	0.55
1:A:238:GLN:H	1:D:148:GLN:HE21	1.55	0.55
1:A:157:CYS:HB2	1:A:367:PHE:O	2.08	0.54
1:B:263:ARG:HG3	3:B:402:COA:C6A	2.37	0.54
1:D:59:ARG:NH1	1:D:327:GLU:OE1	2.41	0.54
3:D:402:COA:H121	3:D:402:COA:O9P	2.09	0.53
1:D:186:GLU:HG3	1:D:332:GLN:HB2	1.91	0.53
1:C:79:LEU:O	1:C:80:ASN:HB2	2.09	0.52
1:B:188[B]:MET:SD	1:B:209:PHE:HB3	2.48	0.52
1:D:33:TYR:CZ	1:D:195:PRO:HD3	2.43	0.52
1:C:302:ALA:HB2	3:C:405:COA:H132	1.92	0.52
3:C:405:COA:O5A	3:C:405:COA:OAP	2.27	0.51
1:A:93:GLU:HG3	1:A:97:LYS:HE2	1.93	0.51
1:C:17:THR:HB	1:C:338:PHE:CZ	2.46	0.51
1:C:319:ARG:NH2	1:C:350:GLU:OE2	2.38	0.51
1:B:132:SER:HB2	1:B:134:ASP:OD1	2.11	0.50
1:D:301:PRO:HB2	1:D:305:ARG:NH1	2.27	0.50
1:C:308:GLU:HG3	1:C:318:MET:HG3	1.93	0.50
1:D:258:LYS:NZ	2:D:401:SO4:O3	2.39	0.50
1:A:205:GLY:HA3	1:A:259:TYR:CE1	2.47	0.50
1:B:157:CYS:HB2	1:B:367:PHE:O	2.12	0.49
3:B:402:COA:O7A	3:B:402:COA:H4B	2.12	0.49
1:B:316:GLU:OE2	1:B:319:ARG:NH2	2.45	0.49
1:D:40:GLU:H	1:D:40:GLU:CD	2.15	0.49
1:D:354:THR:HB	1:D:380:SER:HB2	1.94	0.49
1:A:186:GLU:HG3	1:A:332:GLN:HB2	1.95	0.49
3:D:402:COA:H52A	3:D:402:COA:H8A	1.95	0.49
1:C:75:ASN:ND2	1:C:82:PRO:O	2.46	0.48
1:D:48:LYS:O	1:D:52:MET:HG3	2.14	0.48
1:D:317:ARG:HA	1:D:317:ARG:NE	2.27	0.48
1:B:159:ALA:O	1:B:162:THR:HG22	2.14	0.48
1:D:109:GLU:OE2	1:D:344:ARG:NH1	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:223:ASP:OD2	1:B:225:THR:HB	2.12	0.48
1:B:33:TYR:CZ	1:B:195:PRO:HD3	2.49	0.48
1:B:46:LYS:O	1:B:50:LYS:HG3	2.14	0.48
1:D:83:SER:O	1:D:87:ARG:HG3	2.14	0.47
1:A:298:PRO:HD3	1:A:339:ILE:HD11	1.97	0.47
1:B:186:GLU:HG3	1:B:332:GLN:HB2	1.97	0.47
1:D:298:PRO:HB2	1:D:325:LEU:HD13	1.96	0.47
1:D:333:GLY:HA3	4:D:556:HOH:O	2.13	0.47
1:B:17:THR:HB	1:B:338:PHE:CZ	2.50	0.47
1:A:55:LYS:HD3	3:A:403:COA:O3A	2.14	0.47
3:B:402:COA:H141	3:B:402:COA:O9P	2.15	0.47
1:A:266:PRO:HG3	3:A:403:COA:H72	1.97	0.47
1:B:205:GLY:HA3	1:B:259:TYR:CE2	2.50	0.46
1:A:293:PHE:CE1	1:A:362:GLY:HA3	2.50	0.46
1:B:49:PHE:CD1	1:B:203:LEU:HD22	2.51	0.46
1:B:282:THR:OG1	4:B:501:HOH:O	2.20	0.46
1:D:17:THR:HB	1:D:338:PHE:CZ	2.51	0.46
1:D:157:CYS:HB2	1:D:367:PHE:O	2.15	0.46
1:C:298:PRO:HB2	1:C:325:LEU:HD13	1.99	0.45
1:C:298:PRO:HD3	1:C:339:ILE:HD11	1.98	0.45
1:B:310:LYS:HB3	1:B:310:LYS:HE3	1.75	0.45
1:C:228:ARG:O	1:C:228:ARG:HD3	2.16	0.45
1:A:262:SER:HB3	1:A:265:VAL:HG23	1.99	0.45
1:A:17:THR:HB	1:A:338:PHE:CZ	2.52	0.45
1:B:176:GLY:HA2	1:B:221:ASP:HB2	1.98	0.45
1:B:287:ASN:ND2	4:B:517:HOH:O	2.50	0.44
1:C:314:SER:OG	1:C:315:LYS:N	2.51	0.43
1:D:141:MET:HE3	1:D:143:LEU:HD21	2.00	0.43
1:C:186:GLU:HG3	1:C:332:GLN:HB2	1.99	0.43
1:D:26:GLN:HG3	1:D:53:CYS:HB3	2.00	0.43
1:B:306:MET:O	1:B:310:LYS:HG2	2.17	0.43
1:A:317:ARG:NE	1:A:317:ARG:HA	2.33	0.43
1:C:199:TYR:HB3	1:C:202:LEU:HD13	1.98	0.43
1:B:159:ALA:HA	1:B:162:THR:HG22	2.00	0.43
1:C:203:LEU:HD12	1:C:203:LEU:HA	1.84	0.43
1:A:202:LEU:HA	1:A:259:TYR:CE1	2.54	0.43
1:D:134:ASP:OD2	1:D:149:ARG:HB3	2.19	0.43
1:A:134:ASP:OD2	1:A:149:ARG:HB3	2.19	0.42
1:C:157:CYS:HB3	1:C:297:HIS:CE1	2.55	0.42
1:D:44:GLN:OE1	1:D:44:GLN:N	2.47	0.42
1:C:317:ARG:NE	1:C:317:ARG:HA	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:384:ASN:ND2	4:A:518:HOH:O	2.49	0.42
1:D:51:ARG:NE	3:D:402:COA:O8A	2.53	0.42
1:B:157:CYS:HB3	1:B:297:HIS:CE1	2.54	0.42
1:B:201:ASP:O	1:B:259:TYR:HE2	2.03	0.42
1:A:89:GLU:OE2	4:A:501:HOH:O	2.22	0.42
1:C:205:GLY:HA3	1:C:259:TYR:CE1	2.56	0.41
1:D:44:GLN:CD	1:D:44:GLN:H	2.17	0.41
1:A:157:CYS:HB3	1:A:297:HIS:CE1	2.55	0.41
1:B:202:LEU:O	1:B:206:ASN:ND2	2.52	0.41
1:B:364:MET:HB3	1:B:376:VAL:HB	2.01	0.41
1:A:281:PHE:CZ	1:A:363:VAL:HB	2.55	0.41
1:B:100:LYS:NZ	4:B:505:HOH:O	2.41	0.41
1:B:293:PHE:CE1	1:B:362:GLY:HA3	2.55	0.41
1:B:281:PHE:CZ	1:B:363:VAL:HB	2.56	0.41
1:C:182:ILE:O	1:C:215:ALA:HA	2.21	0.41
1:C:344:ARG:HG3	1:C:345:ASN:N	2.35	0.41
1:D:186:GLU:HG2	1:D:334:PRO:HD2	2.02	0.41
1:A:62:HIS:O	1:A:63:MET:HG3	2.21	0.41
1:B:20:PRO:HD3	1:B:98:LEU:HD21	2.02	0.41
1:D:114:LEU:HA	1:D:114:LEU:HD23	1.85	0.41
1:C:278:ARG:HG2	1:C:289:TRP:CZ2	2.57	0.40
1:A:139:LYS:NZ	1:D:245:GLU:OE1	2.45	0.40
1:A:159:ALA:O	1:A:162:THR:HG22	2.20	0.40
1:B:55:LYS:HD3	3:B:402:COA:O3A	2.21	0.40
1:B:262:SER:HB3	1:B:265:VAL:HG23	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	357/396 (90%)	347 (97%)	10 (3%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	375/396 (95%)	363 (97%)	12 (3%)	0	100	100
1	C	364/396 (92%)	353 (97%)	11 (3%)	0	100	100
1	D	371/396 (94%)	364 (98%)	7 (2%)	0	100	100
All	All	1467/1584 (93%)	1427 (97%)	40 (3%)	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	306/335 (91%)	303 (99%)	3 (1%)	76	71
1	B	319/335 (95%)	316 (99%)	3 (1%)	78	75
1	C	311/335 (93%)	305 (98%)	6 (2%)	57	46
1	D	318/335 (95%)	310 (98%)	8 (2%)	47	34
All	All	1254/1340 (94%)	1234 (98%)	20 (2%)	65	54

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	162	THR
1	A	203	LEU
1	A	344	ARG
1	B	188[A]	MET
1	B	188[B]	MET
1	B	344	ARG
1	C	162	THR
1	C	228	ARG
1	C	277	CYS
1	C	290	ASN
1	C	344	ARG
1	C	353	SER
1	D	8	ARG

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Mol	Chain	Res	Type
1	D	20	PRO
1	D	162	THR
1	D	196	SER
1	D	228	ARG
1	D	259	TYR
1	D	277	CYS
1	D	344	ARG

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

Mol	Chain	Res	Type
1	C	323	HIS
1	D	148	GLN
1	D	174	ASN

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)

12 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	402	-	41,50,50	4.31	12 (29%)	52,75,75	1.85	6 (11%)
3	COA	D	402	-	41,50,50	4.33	12 (29%)	52,75,75	1.85	5 (9%)
2	SO4	C	403	-	4,4,4	0.15	0	6,6,6	0.09	0
2	SO4	B	401	-	4,4,4	0.30	0	6,6,6	0.05	0
3	COA	A	403	-	41,50,50	4.32	12 (29%)	52,75,75	1.86	5 (9%)
2	SO4	A	401	-	4,4,4	0.19	0	6,6,6	0.21	0
2	SO4	D	401	-	4,4,4	0.31	0	6,6,6	0.05	0
2	SO4	C	404	-	4,4,4	0.31	0	6,6,6	0.04	0
2	SO4	C	401	-	4,4,4	0.16	0	6,6,6	0.27	0
2	SO4	A	402	-	4,4,4	0.21	0	6,6,6	0.28	0
2	SO4	C	402	-	4,4,4	0.10	0	6,6,6	0.34	0
3	COA	C	405	-	41,50,50	4.32	12 (29%)	52,75,75	1.94	11 (21%)

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	402	-	-	12/44/64/64	0/3/3/3
3	COA	D	402	-	-	12/44/64/64	0/3/3/3
3	COA	A	403	-	-	10/44/64/64	0/3/3/3
3	COA	C	405	-	-	19/44/64/64	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	405	COA	O4B-C1B	19.24	1.67	1.41
3	D	402	COA	O4B-C1B	18.56	1.67	1.41
3	B	402	COA	O4B-C1B	18.49	1.66	1.41
3	A	403	COA	O4B-C1B	18.30	1.66	1.41
3	A	403	COA	C2B-C1B	-13.85	1.32	1.53
3	D	402	COA	C2B-C1B	-13.70	1.33	1.53
3	B	402	COA	C2B-C1B	-13.56	1.33	1.53
3	C	405	COA	C2B-C1B	-12.66	1.34	1.53
3	B	402	COA	C9P-N8P	6.80	1.48	1.33
3	D	402	COA	C9P-N8P	6.75	1.48	1.33
3	A	403	COA	C9P-N8P	6.73	1.48	1.33
3	C	405	COA	C9P-N8P	6.70	1.48	1.33
3	C	405	COA	O4B-C4B	-6.70	1.30	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	403	COA	C5P-N4P	6.51	1.48	1.33
3	D	402	COA	C5P-N4P	6.49	1.48	1.33
3	B	402	COA	C5P-N4P	6.49	1.48	1.33
3	C	405	COA	C5P-N4P	6.32	1.47	1.33
3	B	402	COA	O4B-C4B	-6.31	1.30	1.45
3	D	402	COA	O4B-C4B	-6.28	1.31	1.45
3	A	403	COA	O4B-C4B	-6.24	1.31	1.45
3	C	405	COA	C6A-N6A	4.83	1.51	1.34
3	D	402	COA	C6A-N6A	4.81	1.51	1.34
3	A	403	COA	C6A-N6A	4.81	1.51	1.34
3	B	402	COA	C6A-N6A	4.79	1.51	1.34
3	A	403	COA	P3B-O3B	4.43	1.67	1.59
3	B	402	COA	P3B-O3B	4.42	1.67	1.59
3	D	402	COA	P3B-O3B	4.35	1.67	1.59
3	C	405	COA	P3B-O3B	3.87	1.66	1.59
3	C	405	COA	C2A-N3A	3.04	1.37	1.32
3	C	405	COA	O3B-C3B	-2.90	1.33	1.44
3	D	402	COA	C2A-N3A	2.72	1.36	1.32
3	B	402	COA	C2A-N3A	2.70	1.36	1.32
3	A	403	COA	C2A-N3A	2.69	1.36	1.32
3	D	402	COA	O3B-C3B	-2.65	1.34	1.44
3	B	402	COA	O3B-C3B	-2.62	1.34	1.44
3	A	403	COA	O3B-C3B	-2.61	1.34	1.44
3	D	402	COA	O9P-C9P	-2.58	1.18	1.23
3	B	402	COA	O9P-C9P	-2.56	1.18	1.23
3	A	403	COA	O9P-C9P	-2.56	1.18	1.23
3	A	403	COA	C3B-C4B	2.40	1.59	1.52
3	C	405	COA	O9P-C9P	-2.32	1.18	1.23
3	C	405	COA	C2A-N1A	2.31	1.38	1.33
3	D	402	COA	P2A-O6A	2.29	1.68	1.59
3	A	403	COA	P2A-O6A	2.28	1.68	1.59
3	B	402	COA	P2A-O6A	2.27	1.68	1.59
3	C	405	COA	P2A-O6A	2.24	1.68	1.59
3	D	402	COA	C3B-C4B	2.22	1.58	1.52
3	B	402	COA	C3B-C4B	2.16	1.58	1.52

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	403	COA	C5A-C6A-N6A	8.46	133.21	120.35
3	B	402	COA	C5A-C6A-N6A	8.45	133.20	120.35
3	D	402	COA	C5A-C6A-N6A	8.44	133.18	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	405	COA	C5A-C6A-N6A	7.11	131.16	120.35
3	B	402	COA	N6A-C6A-N1A	-5.64	106.86	118.57
3	A	403	COA	N6A-C6A-N1A	-5.63	106.88	118.57
3	D	402	COA	N6A-C6A-N1A	-5.63	106.90	118.57
3	B	402	COA	N3A-C2A-N1A	-5.49	120.10	128.68
3	A	403	COA	N3A-C2A-N1A	-5.48	120.11	128.68
3	D	402	COA	N3A-C2A-N1A	-5.47	120.13	128.68
3	C	405	COA	N3A-C2A-N1A	-5.46	120.15	128.68
3	C	405	COA	N6A-C6A-N1A	-4.48	109.28	118.57
3	C	405	COA	C5B-C4B-C3B	-3.90	101.46	114.40
3	C	405	COA	C7P-C6P-C5P	-3.20	107.03	112.36
3	C	405	COA	CDP-CBP-CAP	3.15	114.28	108.82
3	C	405	COA	P2A-O3A-P1A	-2.87	122.96	132.83
3	A	403	COA	P2A-O3A-P1A	-2.82	123.16	132.83
3	D	402	COA	P2A-O3A-P1A	-2.73	123.46	132.83
3	B	402	COA	P2A-O3A-P1A	-2.67	123.67	132.83
3	C	405	COA	C7P-N8P-C9P	-2.51	118.11	122.59
3	C	405	COA	C6P-C5P-N4P	2.32	120.33	116.42
3	C	405	COA	C3P-N4P-C5P	-2.29	118.59	122.84
3	B	402	COA	C6P-C5P-N4P	2.26	120.23	116.42
3	B	402	COA	C3B-C2B-C1B	2.21	104.78	99.89
3	D	402	COA	C6P-C5P-N4P	2.18	120.09	116.42
3	A	403	COA	C6P-C5P-N4P	2.17	120.08	116.42
3	C	405	COA	C3B-C2B-C1B	2.14	104.63	99.89

There are no chirality outliers.

All (53) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	403	COA	CAP-CBP-CCP-O6A
3	A	403	COA	C5P-C6P-C7P-N8P
3	A	403	COA	S1P-C2P-C3P-N4P
3	B	402	COA	S1P-C2P-C3P-N4P
3	C	405	COA	C5B-O5B-P1A-O3A
3	C	405	COA	CCP-O6A-P2A-O3A
3	C	405	COA	CCP-O6A-P2A-O4A
3	C	405	COA	CCP-O6A-P2A-O5A
3	C	405	COA	CBP-CCP-O6A-P2A
3	C	405	COA	CAP-CBP-CCP-O6A
3	C	405	COA	C5P-C6P-C7P-N8P
3	C	405	COA	S1P-C2P-C3P-N4P
3	D	402	COA	C5B-O5B-P1A-O1A

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Mol	Chain	Res	Type	Atoms
3	D	402	COA	C5B-O5B-P1A-O2A
3	D	402	COA	C5B-O5B-P1A-O3A
3	D	402	COA	CCP-O6A-P2A-O3A
3	D	402	COA	CCP-O6A-P2A-O4A
3	D	402	COA	C5P-C6P-C7P-N8P
3	D	402	COA	S1P-C2P-C3P-N4P
3	B	402	COA	C6P-C7P-N8P-C9P
3	C	405	COA	C3B-C4B-C5B-O5B
3	B	402	COA	C4B-C3B-O3B-P3B
3	C	405	COA	CDP-CBP-CCP-O6A
3	B	402	COA	C2B-C3B-O3B-P3B
3	C	405	COA	O4B-C4B-C5B-O5B
3	D	402	COA	O4B-C4B-C5B-O5B
3	C	405	COA	CEP-CBP-CCP-O6A
3	C	405	COA	P1A-O3A-P2A-O4A
3	A	403	COA	O9P-C9P-CAP-CBP
3	A	403	COA	N8P-C9P-CAP-CBP
3	C	405	COA	N8P-C9P-CAP-CBP
3	C	405	COA	P1A-O3A-P2A-O6A
3	A	403	COA	CEP-CBP-CCP-O6A
3	B	402	COA	C5P-C6P-C7P-N8P
3	B	402	COA	CCP-O6A-P2A-O3A
3	A	403	COA	P1A-O3A-P2A-O5A
3	B	402	COA	P1A-O3A-P2A-O5A
3	B	402	COA	CCP-O6A-P2A-O4A
3	C	405	COA	C5B-O5B-P1A-O2A
3	C	405	COA	O9P-C9P-CAP-OAP
3	D	402	COA	P2A-O3A-P1A-O1A
3	D	402	COA	O9P-C9P-CAP-CBP
3	A	403	COA	CDP-CBP-CCP-O6A
3	D	402	COA	N8P-C9P-CAP-CBP
3	A	403	COA	O9P-C9P-CAP-OAP
3	B	402	COA	O5P-C5P-C6P-C7P
3	C	405	COA	N8P-C9P-CAP-OAP
3	B	402	COA	C5B-O5B-P1A-O3A
3	D	402	COA	P2A-O3A-P1A-O2A
3	B	402	COA	CBP-CCP-O6A-P2A
3	A	403	COA	CCP-O6A-P2A-O4A
3	C	405	COA	O9P-C9P-CAP-CBP
3	B	402	COA	N4P-C5P-C6P-C7P

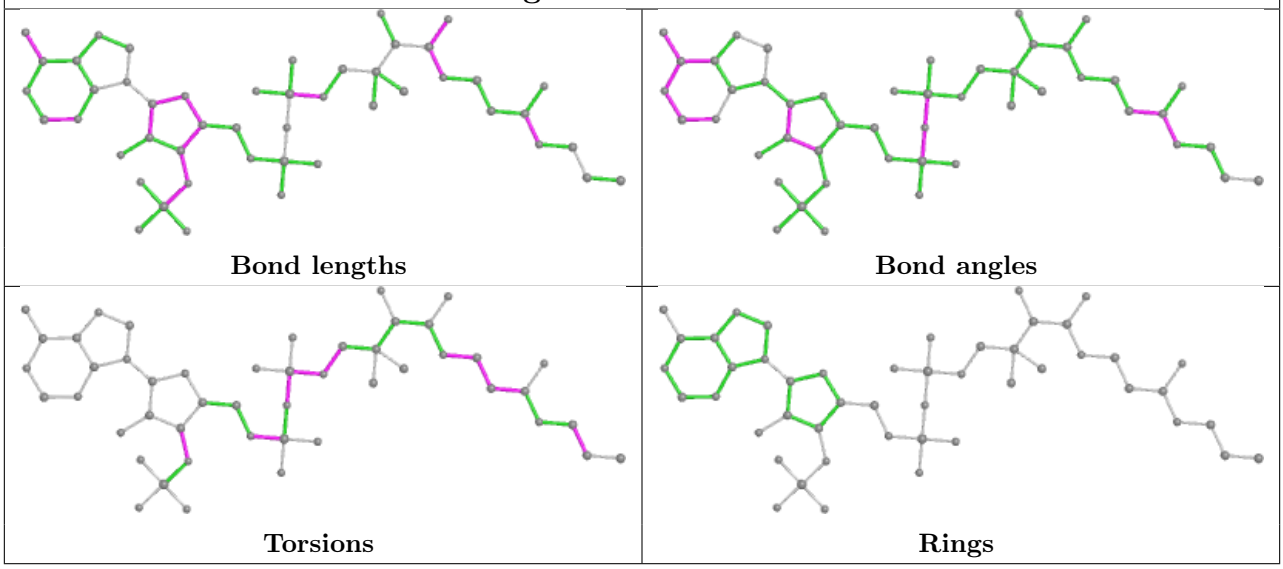
There are no ring outliers.

7 monomers are involved in 27 short contacts:

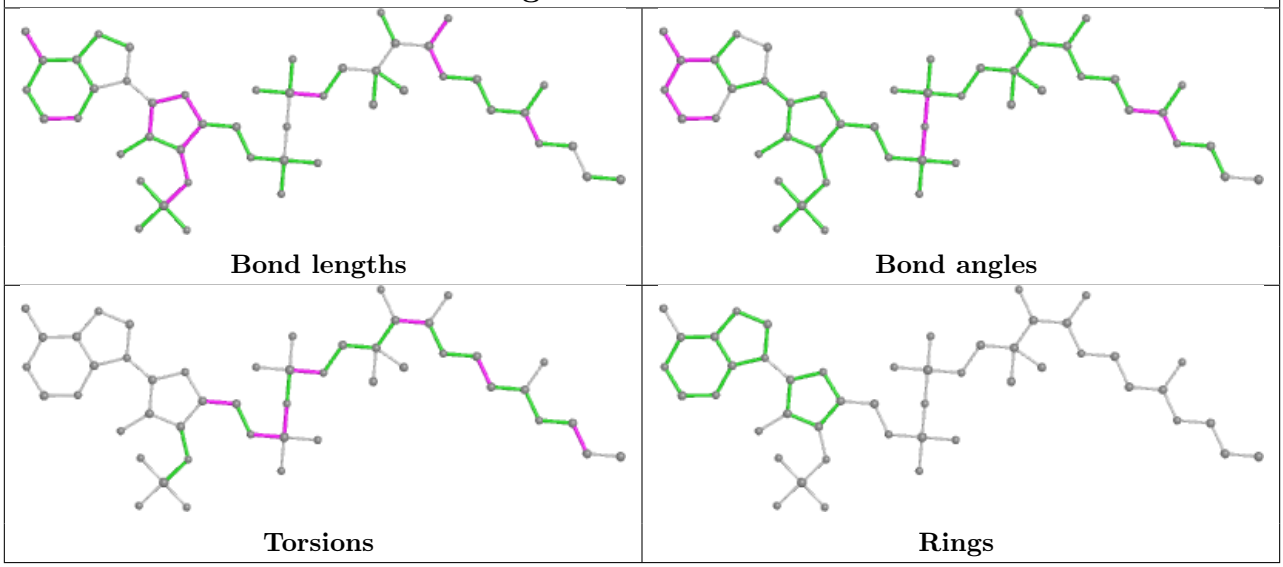
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	402	COA	5	0
3	D	402	COA	8	0
2	B	401	SO4	1	0
3	A	403	COA	5	0
2	D	401	SO4	1	0
2	C	404	SO4	2	0
3	C	405	COA	5	0

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.

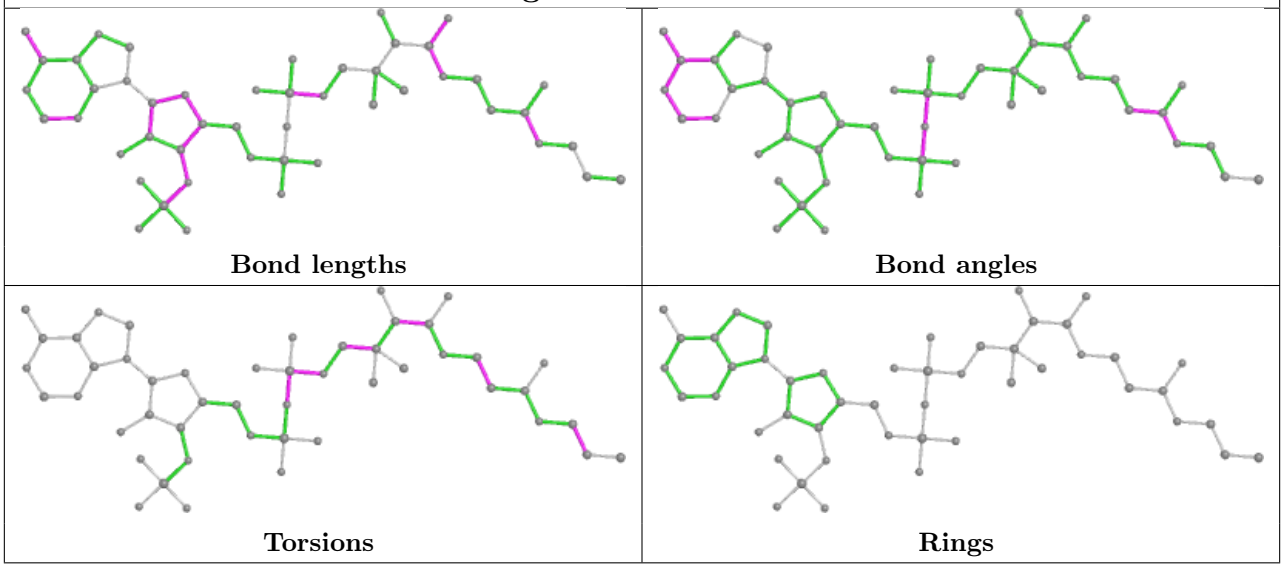
Ligand COA B 402



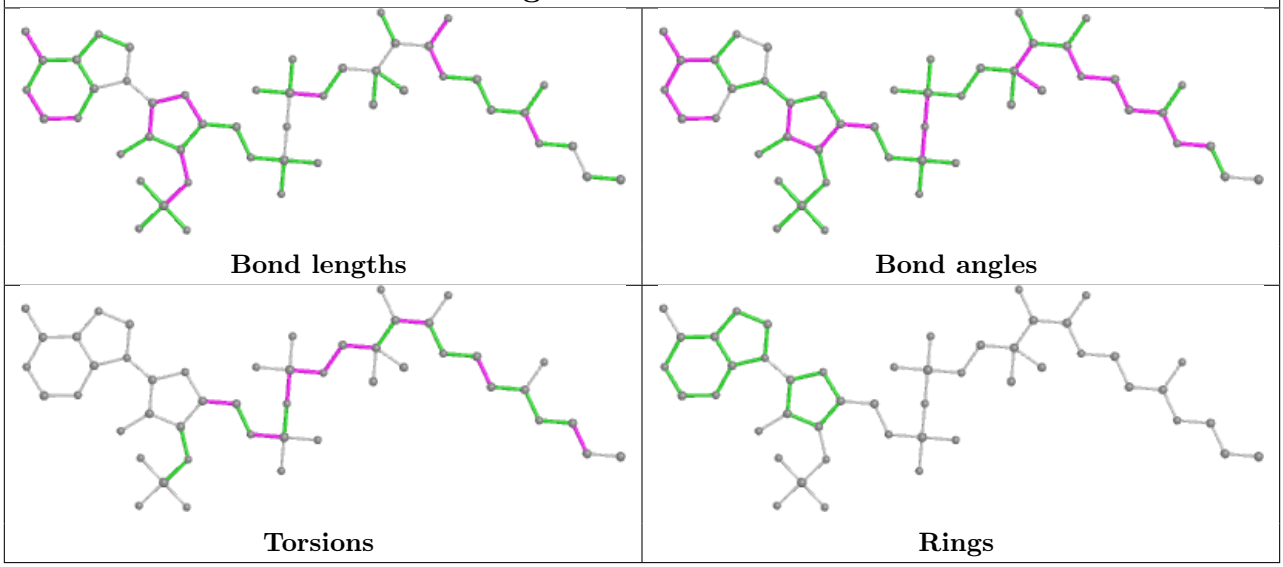
Ligand COA D 402



Ligand COA A 403



Ligand COA C 405



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	363/396 (91%)	-0.07	6 (1%)	70	66	19, 29, 51, 84	0
1	B	376/396 (94%)	-0.16	8 (2%)	63	59	20, 28, 48, 78	0
1	C	368/396 (92%)	0.07	21 (5%)	23	19	21, 31, 59, 92	0
1	D	375/396 (94%)	0.42	27 (7%)	15	12	25, 42, 72, 114	0
All	All	1482/1584 (93%)	0.07	62 (4%)	36	30	19, 32, 63, 114	0

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	199	TYR	8.2
1	D	199	TYR	7.3
1	D	224	THR	6.2
1	D	176	GLY	5.2
1	B	199	TYR	4.5
1	B	225	THR	4.4
1	D	225	THR	4.3
1	D	226	THR	4.1
1	D	5	VAL	4.1
1	D	351	GLY	4.0
1	D	36	VAL	3.8
1	C	225	THR	3.7
1	C	281	PHE	3.7
1	B	226	THR	3.6
1	D	259	TYR	3.4
1	C	259	TYR	3.4
1	B	175	GLY	3.4
1	B	259	TYR	3.3
1	B	224	THR	3.2
1	D	223	ASP	3.2
1	A	361	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	223	ASP	3.1
1	D	8	ARG	3.0
1	B	384	ASN	3.0
1	B	202	LEU	3.0
1	D	6	GLU	2.9
1	C	382	ALA	2.9
1	C	311	LEU	2.8
1	D	222	LEU	2.8
1	C	202	LEU	2.8
1	C	291	SER	2.8
1	C	315	LYS	2.7
1	D	200	LEU	2.7
1	C	277	CYS	2.6
1	C	313	LEU	2.6
1	D	39	SER	2.6
1	C	224	THR	2.6
1	D	228	ARG	2.6
1	D	44	GLN	2.5
1	C	361	TRP	2.5
1	C	289	TRP	2.5
1	C	314	SER	2.5
1	C	351	GLY	2.5
1	A	379	ARG	2.4
1	D	47	ASP	2.3
1	C	222	LEU	2.3
1	D	29	TYR	2.3
1	D	203	LEU	2.2
1	D	383	ILE	2.2
1	A	259	TYR	2.2
1	D	69	VAL	2.2
1	C	383	ILE	2.1
1	C	175	GLY	2.1
1	C	312	GLY	2.1
1	D	7	SER	2.1
1	D	24	PHE	2.1
1	A	282	THR	2.1
1	A	278	ARG	2.1
1	D	379	ARG	2.0
1	D	347	SER	2.0
1	D	314	SER	2.0
1	C	226	THR	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)

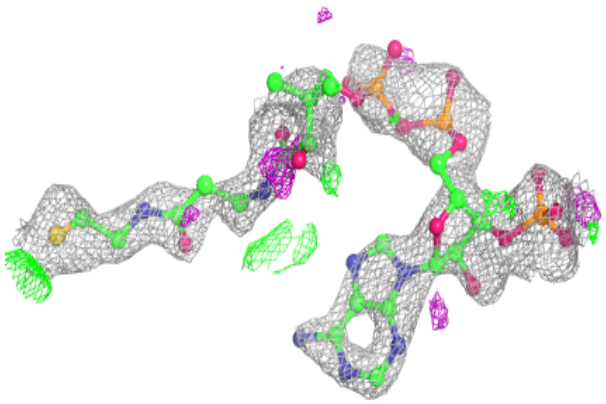
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

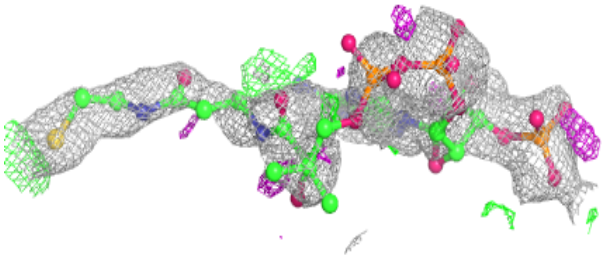
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	COA	D	402	48/48	0.76	0.25	72,105,116,116	0
2	SO4	C	404	5/5	0.81	0.38	119,120,122,123	0
3	COA	B	402	48/48	0.82	0.15	38,70,85,88	0
2	SO4	C	402	5/5	0.84	0.15	70,73,77,79	0
3	COA	A	403	48/48	0.85	0.14	54,73,87,101	0
3	COA	C	405	48/48	0.88	0.16	44,71,91,97	0
2	SO4	C	403	5/5	0.90	0.26	100,100,105,106	0
2	SO4	C	401	5/5	0.95	0.09	50,61,64,74	0
2	SO4	A	402	5/5	0.95	0.11	47,51,53,63	0
2	SO4	A	401	5/5	0.97	0.07	61,63,66,66	0
2	SO4	B	401	5/5	0.98	0.10	60,61,62,65	0
2	SO4	D	401	5/5	0.98	0.10	68,69,74,76	0

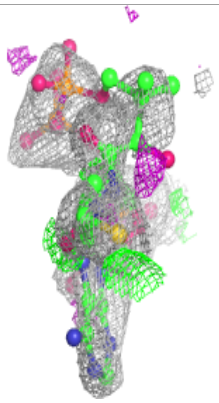
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around COA D 402:

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

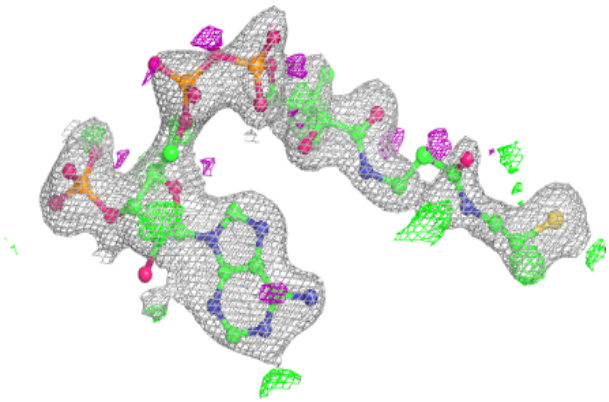


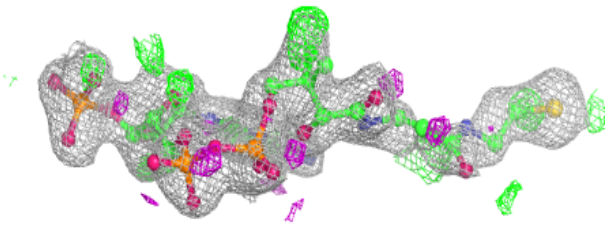




Electron density around COA B 402:

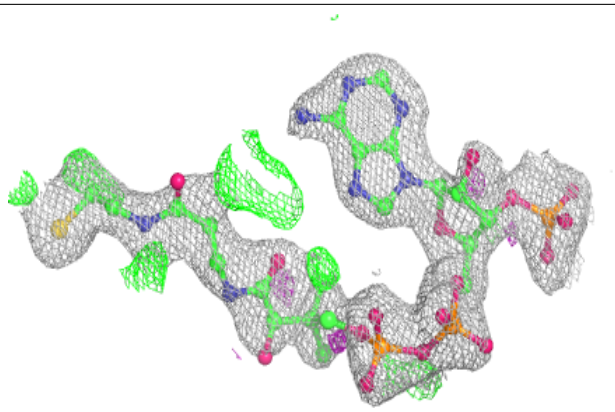
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

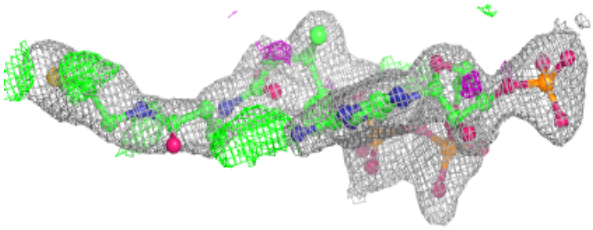


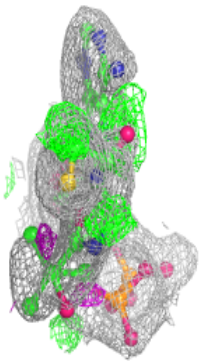


Electron density around COA A 403:

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

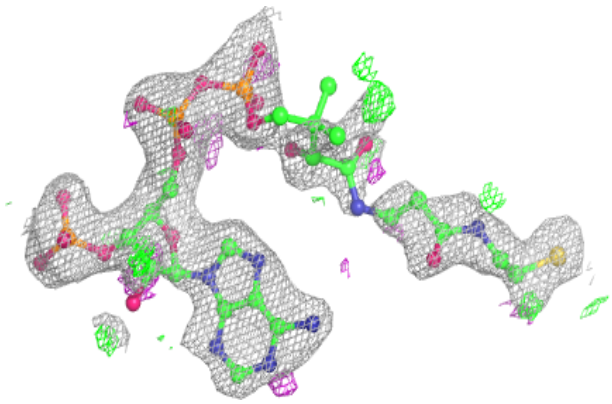


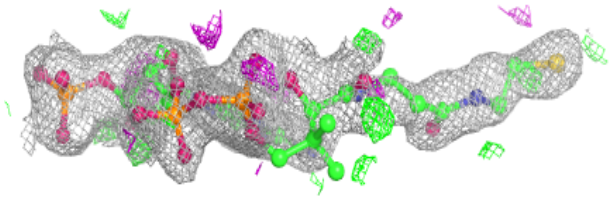


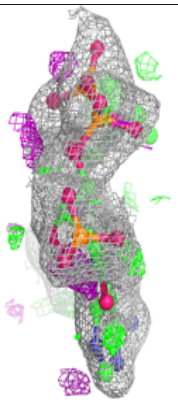


Electron density around COA C 405:

$2mF_o$-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.