



# Full wwPDB X-ray Structure Validation Report ⓘ

May 5, 2021 – 03:12 pm BST

PDB ID : 6YSW  
Title : E. coli anaerobic trifunctional enzyme subunit-alpha in complex with coenzyme A  
Authors : Sah-Teli, S.K.; Hynonen, M.J.; Wierenga, R.K.; Venkatesan, R.  
Deposited on : 2020-04-23  
Resolution : 2.82 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](mailto: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.

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The following versions of software and data (see [references ⓘ](#)) 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 : 2.18  
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) : 2.18

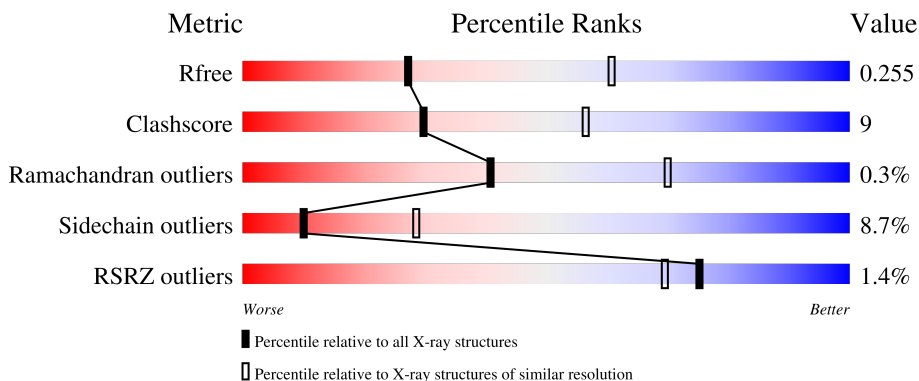
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.82 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	3617 (2.84-2.80)
Clashscore	141614	4060 (2.84-2.80)
Ramachandran outliers	138981	3978 (2.84-2.80)
Sidechain outliers	138945	3980 (2.84-2.80)
RSRZ outliers	127900	3552 (2.84-2.80)

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  $\geq 3$ , 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	728	
1	B	728	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 10567 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 Fatty acid oxidation complex subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	B	698	5164	3261	918	962	23	0	0	0
1	A	707	5271	3333	936	979	23	0	0	0

There are 28 discrepancies between the modelled and reference sequences:

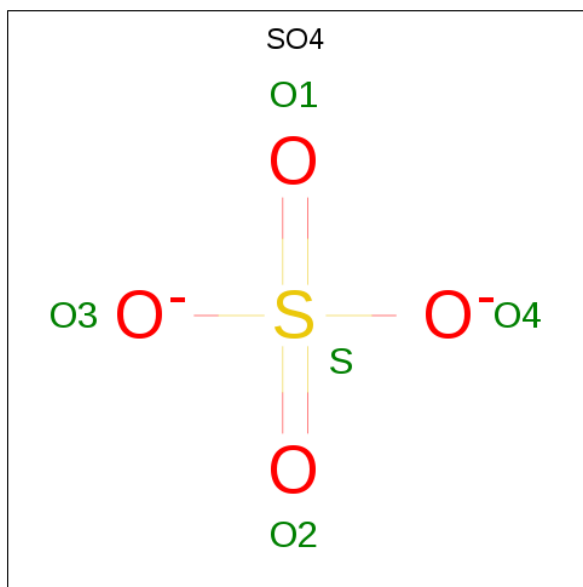
Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	MET	-	initiating methionine	UNP P77399
B	-12	GLY	-	expression tag	UNP P77399
B	-11	SER	-	expression tag	UNP P77399
B	-10	SER	-	expression tag	UNP P77399
B	-9	HIS	-	expression tag	UNP P77399
B	-8	HIS	-	expression tag	UNP P77399
B	-7	HIS	-	expression tag	UNP P77399
B	-6	HIS	-	expression tag	UNP P77399
B	-5	HIS	-	expression tag	UNP P77399
B	-4	HIS	-	expression tag	UNP P77399
B	-3	SER	-	expression tag	UNP P77399
B	-2	GLN	-	expression tag	UNP P77399
B	-1	ASP	-	expression tag	UNP P77399
B	0	PRO	-	expression tag	UNP P77399
A	-13	MET	-	initiating methionine	UNP P77399
A	-12	GLY	-	expression tag	UNP P77399
A	-11	SER	-	expression tag	UNP P77399
A	-10	SER	-	expression tag	UNP P77399
A	-9	HIS	-	expression tag	UNP P77399
A	-8	HIS	-	expression tag	UNP P77399
A	-7	HIS	-	expression tag	UNP P77399
A	-6	HIS	-	expression tag	UNP P77399
A	-5	HIS	-	expression tag	UNP P77399
A	-4	HIS	-	expression tag	UNP P77399
A	-3	SER	-	expression tag	UNP P77399

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLN	-	expression tag	UNP P77399
A	-1	ASP	-	expression tag	UNP P77399
A	0	PRO	-	expression tag	UNP P77399

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



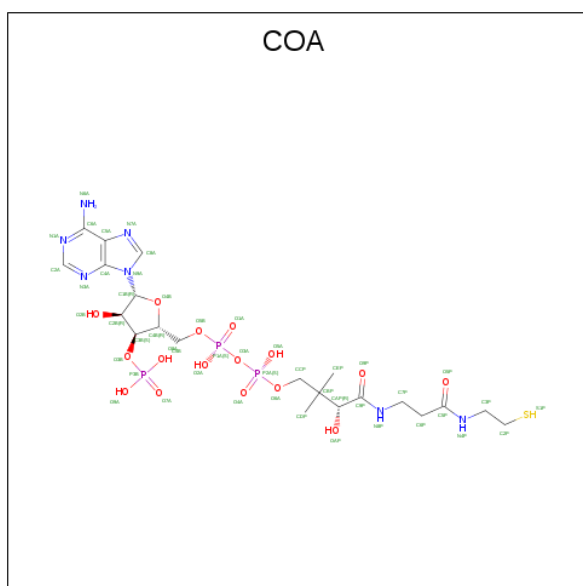
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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

- Molecule 3 is COENZYME A (three-letter code: COA) (formula:  $C_{21}H_{36}N_7O_{16}P_3S$ ) (labeled as "Ligand of Interest" by depositor).



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

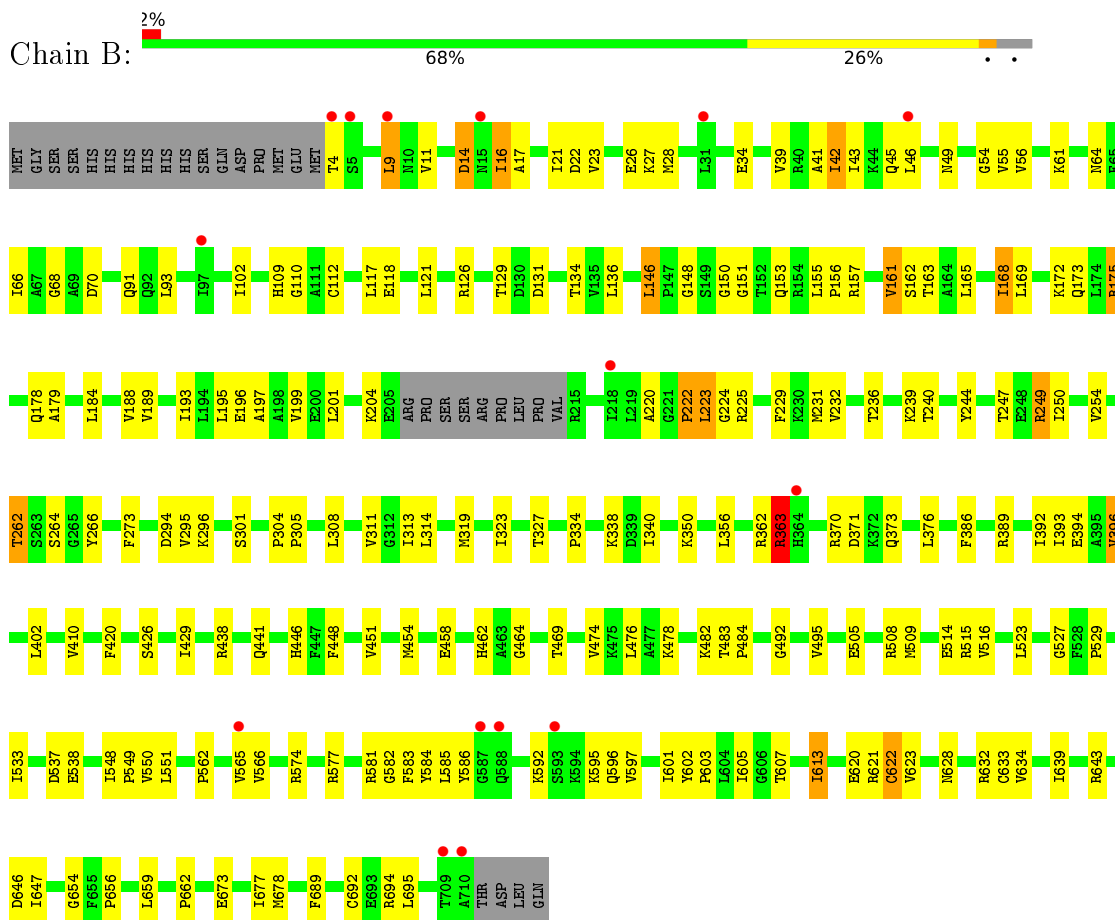
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	8	Total	O	0	0
			8	8		
4	A	11	Total	O	0	0
			11	11		

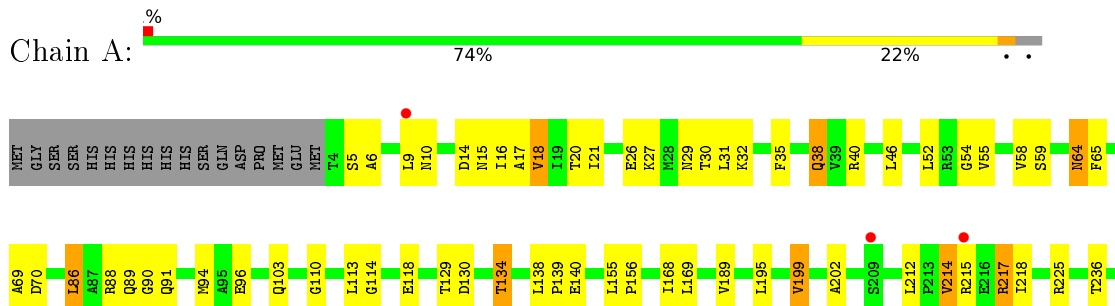
### 3 Residue-property plots

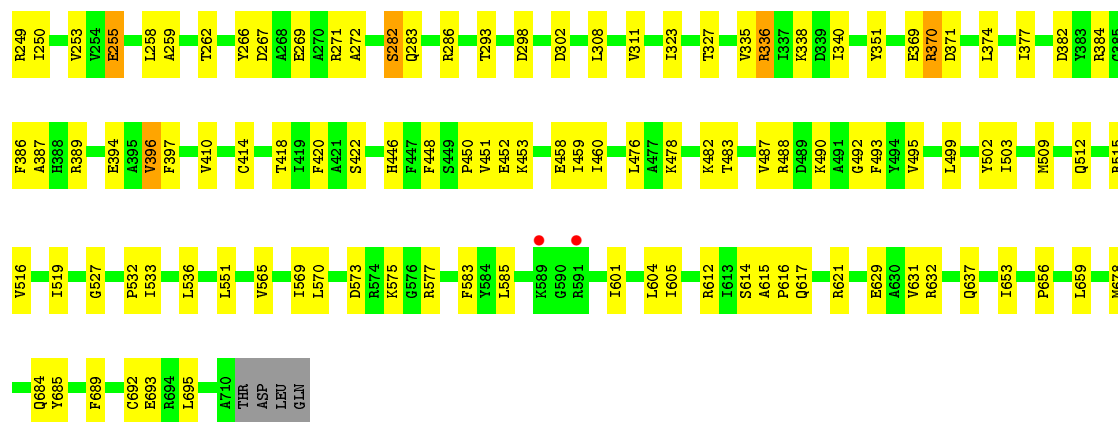
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Fatty acid oxidation complex subunit alpha



- Molecule 1: Fatty acid oxidation complex subunit alpha





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	204.79Å 90.72Å 128.62Å 90.00° 123.17° 90.00°	Depositor
Resolution (Å)	85.72 – 2.82 85.72 – 2.82	Depositor EDS
% Data completeness (in resolution range)	59.6 (85.72-2.82) 59.6 (85.72-2.82)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.36 (at 2.82Å)	Xtrriage
Refinement program	PHENIX 1.16_3549	Depositor
R, $R_{free}$	0.200 , 0.254 0.200 , 0.255	Depositor DCC
$R_{free}$ test set	1417 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.5	Xtrriage
Anisotropy	0.047	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 38.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	10567	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	58.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.80% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

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	0.26	0/5361	0.45	0/7270
1	B	0.26	0/5249	0.45	0/7117
All	All	0.26	0/10610	0.45	0/14387

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

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	5271	0	5330	88	0
1	B	5164	0	5184	110	0
2	A	45	0	0	0	0
2	B	20	0	0	0	0
3	A	48	0	32	3	0
4	A	11	0	0	0	0
4	B	8	0	0	1	0
All	All	10567	0	10546	199	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 9.

All (199) 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:B:586:TYR:H	1:B:596:GLN:HG2	1.41	0.86
1:B:165:LEU:HD21	1:B:254:VAL:HG11	1.59	0.85
1:A:46:LEU:HD21	1:A:55:VAL:HG11	1.68	0.75
1:B:222:PRO:HG2	1:B:223:LEU:HD23	1.68	0.73
1:B:548:ILE:HG13	1:B:549:PRO:HD3	1.71	0.71
1:B:28:MET:HB2	1:B:64:ASN:HD21	1.55	0.70
1:B:296:LYS:HE2	1:B:483:THR:HG22	1.73	0.70
1:A:21:ILE:O	1:A:29:ASN:ND2	2.25	0.69
1:A:253:VAL:HG11	1:A:269:GLU:HB3	1.76	0.67
1:A:169:LEU:HD23	1:A:236:THR:HG21	1.74	0.67
1:B:574:ARG:HG2	1:B:582:GLY:HA2	1.76	0.67
1:B:43:ILE:HA	1:B:46:LEU:HD12	1.76	0.66
1:B:585:LEU:HB2	1:B:596:GLN:HB3	1.77	0.66
1:B:64:ASN:HA	1:B:110:GLY:HA3	1.79	0.65
1:B:565:VAL:HG23	1:B:605:ILE:HG21	1.78	0.65
1:A:15:ASN:HB3	1:A:52:LEU:HA	1.79	0.65
1:A:446:HIS:HB3	1:A:458:GLU:HB2	1.78	0.65
1:A:450:PRO:HG2	1:A:453:LYS:HB2	1.79	0.65
1:B:527:GLY:HA3	1:B:656:PRO:HB3	1.79	0.65
1:B:585:LEU:H	1:B:596:GLN:HB3	1.61	0.64
1:B:514:GLU:HG2	1:B:613:ILE:HD13	1.78	0.63
1:A:394:GLU:HG2	1:A:396:VAL:HG23	1.80	0.63
1:A:17:ALA:HB3	1:A:55:VAL:HG12	1.79	0.63
1:A:336:ARG:NH1	1:A:384:ARG:O	2.32	0.62
1:B:451:VAL:O	1:B:482:LYS:NZ	2.33	0.61
1:A:298:ASP:O	1:A:478:LYS:NZ	2.29	0.61
1:A:5:SER:OG	1:A:38:GLN:NE2	2.34	0.61
1:A:351:TYR:OH	1:A:452:GLU:OE1	2.19	0.61
1:B:446:HIS:HB3	1:B:458:GLU:HB2	1.83	0.61
1:A:59:SER:HB3	1:A:65:PHE:HA	1.83	0.60
1:A:40:ARG:NH1	1:A:96:GLU:OE1	2.35	0.60
1:B:516:VAL:HB	1:B:533:ILE:HD11	1.84	0.59
1:A:338:LYS:HB2	1:A:386:PHE:CZ	2.37	0.59
1:A:10:ASN:HB3	1:A:18:VAL:HG12	1.83	0.59
1:B:220:ALA:HB3	1:B:224:GLY:H	1.67	0.58
1:B:117:LEU:HD13	1:B:136:LEU:HD22	1.84	0.58
1:B:311:VAL:HG21	1:B:327:THR:HG21	1.86	0.57
1:B:508:ARG:HG3	1:B:562:PRO:HG3	1.86	0.57
3:A:810:COA:H62A	3:A:810:COA:H71	1.70	0.56
1:A:91:GLN:NE2	1:A:266:TYR:O	2.33	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:28:MET:HB2	1:B:64:ASN:ND2	2.20	0.56
1:B:157:ARG:HH22	1:B:262:THR:HB	1.71	0.55
1:B:334:PRO:HA	1:B:376:LEU:HB3	1.87	0.55
1:B:66:ILE:HG22	1:B:68:GLY:H	1.70	0.55
1:A:64:ASN:HA	1:A:110:GLY:HA3	1.88	0.55
1:A:488:ARG:NH1	1:A:637:GLN:O	2.40	0.55
1:B:109:HIS:ND1	1:B:129:THR:HG21	2.22	0.54
1:A:615:ALA:HB3	1:A:616:PRO:HD3	1.90	0.54
1:B:410:VAL:HG11	1:B:420:PHE:HD2	1.73	0.54
1:B:613:ILE:HD12	1:B:613:ILE:H	1.73	0.53
1:A:9:LEU:HD11	1:A:46:LEU:HD13	1.90	0.53
1:B:386:PHE:HA	1:B:389:ARG:HG2	1.90	0.53
1:A:374:LEU:HD22	1:A:377:ILE:HD11	1.90	0.53
1:B:14:ASP:OD1	1:B:14:ASP:N	2.35	0.53
1:B:175:ARG:HH12	1:B:363:ARG:HG2	1.73	0.53
1:B:17:ALA:HB3	1:B:55:VAL:HG23	1.91	0.53
1:A:113:LEU:HD22	1:A:139:PRO:HG3	1.91	0.53
1:B:323:ILE:HD13	1:B:451:VAL:HG11	1.91	0.52
1:A:492:GLY:HA3	1:A:551:LEU:HD21	1.91	0.52
1:A:565:VAL:HG21	1:A:605:ILE:HG23	1.90	0.52
1:B:508:ARG:NH1	4:B:901:HOH:O	2.43	0.51
1:B:9:LEU:HD12	1:B:17:ALA:HB1	1.93	0.51
1:A:451:VAL:O	1:A:482:LYS:NZ	2.38	0.50
1:B:131:ASP:O	1:B:134:THR:HG22	2.11	0.50
1:B:584:TYR:HB3	1:B:596:GLN:HB2	1.93	0.50
1:A:35:PHE:HD1	1:A:38:GLN:HE22	1.60	0.50
1:A:583:PHE:HA	1:A:601:ILE:HD13	1.94	0.50
1:B:26:GLU:O	1:B:61:LYS:HE2	2.11	0.50
1:A:168:ILE:HG22	1:A:250:ILE:HD13	1.94	0.50
1:B:492:GLY:HA3	1:B:551:LEU:HD21	1.92	0.50
1:A:488:ARG:HH11	1:A:488:ARG:HB2	1.76	0.50
1:A:614:SER:HB3	1:A:617:GLN:HB2	1.93	0.49
1:A:282:SER:OG	1:A:286:ARG:NH1	2.46	0.49
1:B:394:GLU:HG2	1:B:396:VAL:HG23	1.94	0.49
1:B:538:GLU:OE2	1:B:577:ARG:NH1	2.46	0.49
1:A:54:GLY:HA3	1:A:202:ALA:HB1	1.95	0.49
1:A:58:VAL:HG11	1:A:195:LEU:HD13	1.93	0.49
1:A:371:ASP:HA	1:A:374:LEU:HB2	1.95	0.49
1:A:308:LEU:HD21	1:A:476:LEU:HB2	1.94	0.49
1:A:249:ARG:HH21	1:A:272:ALA:HA	1.77	0.49
1:B:22:ASP:OD1	1:B:61:LYS:NZ	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:585:LEU:N	1:B:596:GLN:HB3	2.27	0.49
1:B:70:ASP:N	1:B:70:ASP:OD1	2.41	0.49
1:B:146:LEU:HB2	1:B:250:ILE:HD11	1.95	0.49
1:A:293:THR:HG21	3:A:810:COA:H3B	1.96	0.48
1:A:370:ARG:HG2	1:A:371:ASP:N	2.28	0.48
1:A:370:ARG:O	1:A:374:LEU:HG	2.13	0.48
1:B:620:GLU:HA	1:B:623:VAL:HG12	1.95	0.48
1:B:311:VAL:O	1:B:389:ARG:NH2	2.45	0.48
1:B:426:SER:HB2	1:B:550:VAL:HG21	1.95	0.48
1:A:262:THR:O	1:A:266:TYR:N	2.47	0.48
1:B:313:ILE:HD13	1:B:393:ILE:HB	1.96	0.48
1:B:295:VAL:HG23	1:B:643:ARG:HD3	1.96	0.47
1:A:138:LEU:HD12	1:A:168:ILE:HG12	1.95	0.47
1:A:396:VAL:HG12	1:A:397:PHE:H	1.80	0.47
1:B:54:GLY:HA2	1:B:102:ILE:HG22	1.96	0.47
1:A:16:ILE:HD12	1:A:199:VAL:HG22	1.95	0.47
1:A:394:GLU:HB3	1:A:422:SER:HA	1.96	0.47
1:B:157:ARG:HH12	1:B:262:THR:HB	1.79	0.47
1:B:656:PRO:HG2	1:B:659:LEU:HD12	1.97	0.47
1:A:601:ILE:O	1:A:605:ILE:HG12	2.15	0.47
1:B:462:HIS:CE1	1:B:464:GLY:H	2.32	0.47
1:A:255:GLU:HA	1:A:258:LEU:HB2	1.97	0.47
1:A:527:GLY:HA3	1:A:656:PRO:HB3	1.95	0.47
1:A:629:GLU:OE2	1:A:632:ARG:NE	2.47	0.47
1:A:678:MET:HB3	1:A:689:PHE:O	2.15	0.47
1:B:175:ARG:O	1:B:179:ALA:N	2.43	0.47
1:B:392:ILE:HD12	1:B:410:VAL:HG23	1.97	0.47
1:B:169:LEU:HD23	1:B:236:THR:HG21	1.96	0.46
1:B:172:LYS:HA	1:B:172:LYS:HD3	1.62	0.46
1:A:267:ASP:OD2	1:A:271:ARG:NH2	2.49	0.46
1:B:112:CYS:HB3	1:B:136:LEU:HD23	1.97	0.46
1:B:586:TYR:N	1:B:596:GLN:HG2	2.21	0.46
1:B:583:PHE:HA	1:B:601:ILE:HG13	1.97	0.46
1:A:656:PRO:HG2	1:A:659:LEU:HD12	1.98	0.46
1:A:311:VAL:HG23	1:A:335:VAL:HG23	1.98	0.46
1:A:631:VAL:HG21	1:A:695:LEU:HD22	1.98	0.46
1:B:193:ILE:HG22	1:B:197:ALA:HB2	1.98	0.46
1:A:86:LEU:HA	1:A:89:GLN:HB3	1.98	0.46
1:B:678:MET:HB3	1:B:689:PHE:O	2.16	0.45
1:B:129:THR:HA	1:B:189:VAL:O	2.16	0.45
1:B:148:GLY:HA3	1:B:273:PHE:CD2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:314:LEU:HB2	1:B:394:GLU:HA	1.97	0.45
1:B:168:ILE:HG22	1:B:250:ILE:HD12	1.99	0.45
1:B:16:ILE:HD13	1:B:199:VAL:HG21	1.98	0.45
1:B:308:LEU:HD13	1:B:476:LEU:HB2	1.98	0.45
1:A:503:ILE:HG21	1:A:536:LEU:HD13	1.99	0.45
1:A:14:ASP:O	1:A:16:ILE:N	2.47	0.45
1:A:283:GLN:HG2	1:A:286:ARG:HH22	1.80	0.45
1:B:448:PHE:CZ	1:B:495:VAL:HG11	2.52	0.44
1:B:448:PHE:HB2	1:B:454:MET:HG2	1.98	0.44
1:A:394:GLU:OE2	1:A:422:SER:OG	2.22	0.44
1:B:118:GLU:OE2	1:B:151:GLY:N	2.50	0.44
1:B:126:ARG:NE	1:B:184:LEU:O	2.44	0.44
1:B:373:GLN:HA	1:B:376:LEU:HD12	1.99	0.44
1:B:121:LEU:HD21	1:B:155:LEU:HD12	1.98	0.44
1:B:220:ALA:HB3	1:B:224:GLY:N	2.32	0.44
1:B:628:ASN:HD21	1:B:632:ARG:NH2	2.15	0.44
1:B:41:ALA:O	1:B:45:GLN:HG2	2.18	0.44
1:A:311:VAL:HG21	1:A:327:THR:HG21	1.99	0.44
1:A:386:PHE:HA	1:A:389:ARG:HG2	2.00	0.44
1:B:474:VAL:HG23	1:B:484:PRO:HG3	2.00	0.44
1:B:515:ARG:HA	1:B:602:TYR:HE2	1.82	0.44
1:B:646:ASP:HA	1:B:662:PRO:HD2	1.99	0.43
1:A:5:SER:OG	1:A:6:ALA:N	2.50	0.43
1:B:304:PRO:HA	1:B:305:PRO:HD3	1.91	0.43
1:A:387:ALA:HA	1:A:414:CYS:HA	2.00	0.43
1:B:175:ARG:HH12	1:B:363:ARG:CG	2.31	0.43
1:A:340:ILE:H	1:A:340:ILE:HG13	1.68	0.43
1:A:569:ILE:HD13	1:A:604:LEU:HD23	2.00	0.43
1:B:240:THR:HB	1:B:244:TYR:HD1	1.83	0.43
1:B:338:LYS:HB2	1:B:386:PHE:CZ	2.53	0.43
1:A:283:GLN:HG2	1:A:286:ARG:NH2	2.34	0.43
1:B:356:LEU:HB3	1:B:370:ARG:HG3	1.99	0.43
1:B:529:PRO:HD3	1:B:654:GLY:O	2.19	0.43
1:B:201:LEU:HA	1:B:204:LYS:HD3	2.00	0.43
1:B:634:VAL:HB	1:B:639:ILE:HD11	2.01	0.43
1:A:515:ARG:O	1:A:519:ILE:HG12	2.19	0.43
1:A:516:VAL:HG13	1:A:533:ILE:HG21	2.00	0.43
1:B:474:VAL:HG22	1:B:478:LYS:HE2	1.99	0.43
1:B:673:GLU:O	1:B:677:ILE:HG13	2.19	0.43
1:A:460:ILE:HG21	1:A:493:PHE:CE1	2.53	0.43
1:A:129:THR:OG1	1:A:134:THR:HG21	2.18	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:21:ILE:HD13	1:B:66:ILE:HD11	2.01	0.42
1:B:39:VAL:HG11	1:B:93:LEU:HD21	2.01	0.42
1:B:441:GLN:HA	1:B:469:THR:HG21	2.02	0.42
1:A:70:ASP:HA	3:A:810:COA:N1A	2.34	0.42
1:B:429:ILE:HB	1:B:462:HIS:HB3	2.02	0.42
1:A:448:PHE:CZ	1:A:495:VAL:HG11	2.54	0.42
1:A:323:ILE:O	1:A:327:THR:OG1	2.28	0.42
1:B:602:TYR:HB2	1:B:603:PRO:HD3	2.01	0.42
1:B:9:LEU:HD22	1:B:42:ILE:HG13	2.02	0.42
1:B:565:VAL:HG13	1:B:566:VAL:H	1.85	0.42
1:B:628:ASN:HD21	1:B:632:ARG:HH21	1.68	0.42
1:A:499:LEU:HD13	1:A:653:ILE:HG23	2.01	0.42
1:A:410:VAL:HG21	1:A:420:PHE:HD2	1.85	0.41
1:A:502:TYR:CZ	1:A:532:PRO:HG3	2.55	0.41
1:B:161:VAL:HG21	1:B:229:PHE:HE1	1.85	0.41
1:B:161:VAL:HG21	1:B:229:PHE:CE1	2.56	0.41
1:A:218:ILE:H	1:A:218:ILE:HG13	1.72	0.41
1:B:692:CYS:HB3	1:B:695:LEU:HB2	2.03	0.41
1:A:155:LEU:HB3	1:A:156:PRO:HD3	2.03	0.41
1:B:505:GLU:HB3	1:B:622:CYS:HB3	2.02	0.41
1:A:31:LEU:HB3	1:A:69:ALA:HA	2.03	0.41
1:A:225:ARG:HH12	1:A:259:ALA:HA	1.84	0.41
1:B:23:VAL:O	1:B:61:LYS:NZ	2.49	0.41
1:B:523:LEU:HD21	1:B:622:CYS:SG	2.61	0.41
1:A:129:THR:HA	1:A:189:VAL:O	2.21	0.41
1:A:512:GLN:HB3	1:A:612:ARG:HH21	1.85	0.41
1:B:155:LEU:HB3	1:B:156:PRO:HD3	2.03	0.41
1:B:249:ARG:HE	1:B:249:ARG:HB3	1.54	0.41
1:B:505:GLU:O	1:B:509:MET:HG3	2.21	0.41
1:A:621:ARG:HD2	1:A:685:TYR:CZ	2.56	0.41
1:A:88:ARG:HH12	1:A:267:ASP:HB2	1.85	0.40
1:A:90:GLY:O	1:A:94:MET:HG2	2.22	0.40
1:A:114:GLY:O	1:A:118:GLU:HG3	2.21	0.40
1:A:214:VAL:O	1:A:217:ARG:HG2	2.21	0.40
1:B:150:GLY:HA2	1:B:266:TYR:HE1	1.86	0.40
1:B:389:ARG:HA	1:B:389:ARG:HD2	1.79	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	705/728 (97%)	659 (94%)	46 (6%)	0	100	100
1	B	694/728 (95%)	654 (94%)	36 (5%)	4 (1%)	25	54
All	All	1399/1456 (96%)	1313 (94%)	82 (6%)	4 (0%)	41	70

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	362	ARG
1	B	363	ARG
1	B	597	VAL
1	B	222	PRO

### 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	542/583 (93%)	502 (93%)	40 (7%)	13	36
1	B	524/583 (90%)	471 (90%)	53 (10%)	7	21
All	All	1066/1166 (91%)	973 (91%)	93 (9%)	10	28

All (93) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4	THR
1	B	9	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	11	VAL
1	B	14	ASP
1	B	16	ILE
1	B	27	LYS
1	B	34	GLU
1	B	42	ILE
1	B	49	ASN
1	B	56	VAL
1	B	91	GLN
1	B	146	LEU
1	B	153	GLN
1	B	161	VAL
1	B	162	SER
1	B	163	THR
1	B	168	ILE
1	B	173	GLN
1	B	175	ARG
1	B	178	GLN
1	B	188	VAL
1	B	195	LEU
1	B	196	GLU
1	B	223	LEU
1	B	225	ARG
1	B	231	MET
1	B	232	VAL
1	B	239	LYS
1	B	247	THR
1	B	249	ARG
1	B	262	THR
1	B	264	SER
1	B	294	ASP
1	B	301	SER
1	B	319	MET
1	B	340	ILE
1	B	350	LYS
1	B	363	ARG
1	B	371	ASP
1	B	396	VAL
1	B	402	LEU
1	B	438	ARG
1	B	537	ASP
1	B	581	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	592	LYS
1	B	595	LYS
1	B	607	THR
1	B	613	ILE
1	B	621	ARG
1	B	622	CYS
1	B	633	CYS
1	B	647	ILE
1	B	694	ARG
1	A	18	VAL
1	A	20	THR
1	A	26	GLU
1	A	27	LYS
1	A	30	THR
1	A	32	LYS
1	A	38	GLN
1	A	64	ASN
1	A	86	LEU
1	A	103	GLN
1	A	130	ASP
1	A	134	THR
1	A	140	GLU
1	A	199	VAL
1	A	212	LEU
1	A	214	VAL
1	A	215	ARG
1	A	217	ARG
1	A	255	GLU
1	A	282	SER
1	A	302	ASP
1	A	336	ARG
1	A	369	GLU
1	A	370	ARG
1	A	382	ASP
1	A	396	VAL
1	A	418	THR
1	A	459	ILE
1	A	483	THR
1	A	487	VAL
1	A	490	LYS
1	A	509	MET
1	A	570	LEU

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Mol	Chain	Res	Type
1	A	573	ASP
1	A	575	LYS
1	A	577	ARG
1	A	585	LEU
1	A	684	GLN
1	A	692	CYS
1	A	693	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	64	ASN
1	A	412	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

14 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	A	810	-	41,50,50	2.49	6 (14%)	52,75,75	1.86	12 (23%)
2	SO4	A	806	-	4,4,4	0.36	0	6,6,6	0.05	0
2	SO4	B	801	-	4,4,4	0.38	0	6,6,6	0.05	0
2	SO4	A	807	-	4,4,4	0.38	0	6,6,6	0.04	0
2	SO4	A	805	-	4,4,4	0.39	0	6,6,6	0.05	0
2	SO4	A	808	-	4,4,4	0.39	0	6,6,6	0.05	0
2	SO4	A	809	-	4,4,4	0.39	0	6,6,6	0.05	0
2	SO4	A	801	-	4,4,4	0.38	0	6,6,6	0.05	0
2	SO4	A	804	-	4,4,4	0.37	0	6,6,6	0.05	0
2	SO4	A	802	-	4,4,4	0.39	0	6,6,6	0.05	0
2	SO4	B	802	-	4,4,4	0.38	0	6,6,6	0.05	0
2	SO4	A	803	-	4,4,4	0.35	0	6,6,6	0.05	0
2	SO4	B	804	-	4,4,4	0.32	0	6,6,6	0.08	0
2	SO4	B	803	-	4,4,4	0.38	0	6,6,6	0.05	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	A	810	-	-	19/44/64/64	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	810	COA	P3B-O3B	13.64	1.85	1.59
3	A	810	COA	P2A-O6A	3.66	1.74	1.59
3	A	810	COA	C5P-N4P	2.69	1.39	1.33
3	A	810	COA	C9P-N8P	2.63	1.39	1.33
3	A	810	COA	O3B-C3B	-2.51	1.35	1.44
3	A	810	COA	C2A-N1A	2.18	1.38	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	810	COA	P2A-O3A-P1A	-7.32	107.72	132.83
3	A	810	COA	O3B-P3B-O7A	-3.71	95.08	109.39
3	A	810	COA	C7P-C6P-C5P	-3.15	107.11	112.36
3	A	810	COA	P1A-O5B-C5B	-3.04	103.88	121.68
3	A	810	COA	O9A-P3B-O8A	2.77	118.23	107.64
3	A	810	COA	C3P-N4P-C5P	-2.74	117.75	122.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	810	COA	P2A-O6A-CCP	-2.58	106.67	121.56
3	A	810	COA	C7P-N8P-C9P	-2.57	118.00	122.59
3	A	810	COA	O6A-CCP-CBP	-2.48	106.56	110.55
3	A	810	COA	C6P-C7P-N8P	-2.27	107.31	111.90
3	A	810	COA	O6A-P2A-O4A	-2.18	100.55	109.07
3	A	810	COA	C2A-N1A-C6A	-2.17	115.05	118.75

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	810	COA	C5B-O5B-P1A-O1A
3	A	810	COA	CCP-O6A-P2A-O3A
3	A	810	COA	OAP-CAP-CBP-CCP
3	A	810	COA	C9P-CAP-CBP-CCP
3	A	810	COA	OAP-CAP-CBP-CDP
3	A	810	COA	C9P-CAP-CBP-CDP
3	A	810	COA	OAP-CAP-CBP-CEP
3	A	810	COA	C9P-CAP-CBP-CEP
3	A	810	COA	O9P-C9P-CAP-CBP
3	A	810	COA	N8P-C9P-CAP-CBP
3	A	810	COA	C3B-C4B-C5B-O5B
3	A	810	COA	O4B-C4B-C5B-O5B
3	A	810	COA	N8P-C9P-CAP-OAP
3	A	810	COA	C5B-O5B-P1A-O3A
3	A	810	COA	C5B-O5B-P1A-O2A
3	A	810	COA	CCP-O6A-P2A-O4A
3	A	810	COA	C3B-O3B-P3B-O7A
3	A	810	COA	C3B-O3B-P3B-O8A
3	A	810	COA	P1A-O3A-P2A-O5A

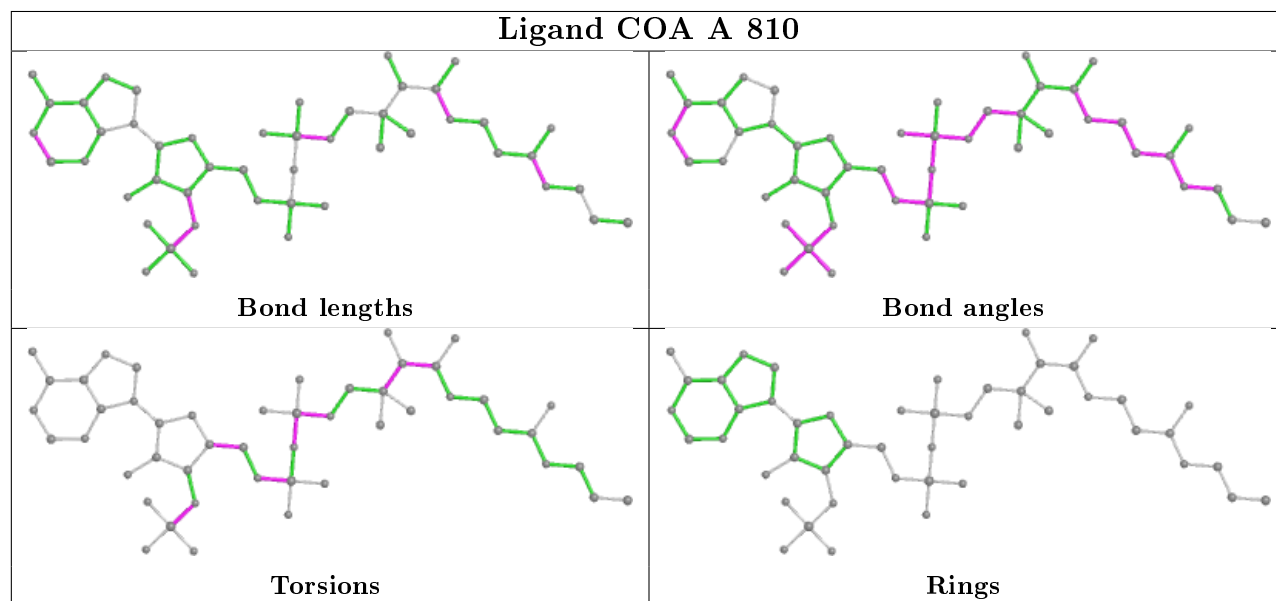
There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	810	COA	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 [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

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	707/728 (97%)	-0.03	5 (0%) 87 84	20, 47, 97, 178	0
1	B	698/728 (95%)	0.04	15 (2%) 63 54	24, 57, 112, 164	0
All	All	1405/1456 (96%)	0.00	20 (1%) 75 69	20, 53, 105, 178	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	364	HIS	4.6
1	B	4	THR	4.4
1	B	710	ALA	4.2
1	A	589	LYS	3.6
1	A	209	SER	3.2
1	B	709	THR	3.1
1	B	218	ILE	2.6
1	A	215	ARG	2.5
1	B	15	ASN	2.5
1	B	565	VAL	2.4
1	B	46	LEU	2.4
1	B	31	LEU	2.3
1	B	588	GLN	2.3
1	B	97	ILE	2.2
1	B	587	GLY	2.2
1	A	591	ARG	2.1
1	A	9	LEU	2.1
1	B	5	SER	2.0
1	B	593	SER	2.0
1	B	9	LEU	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](#)

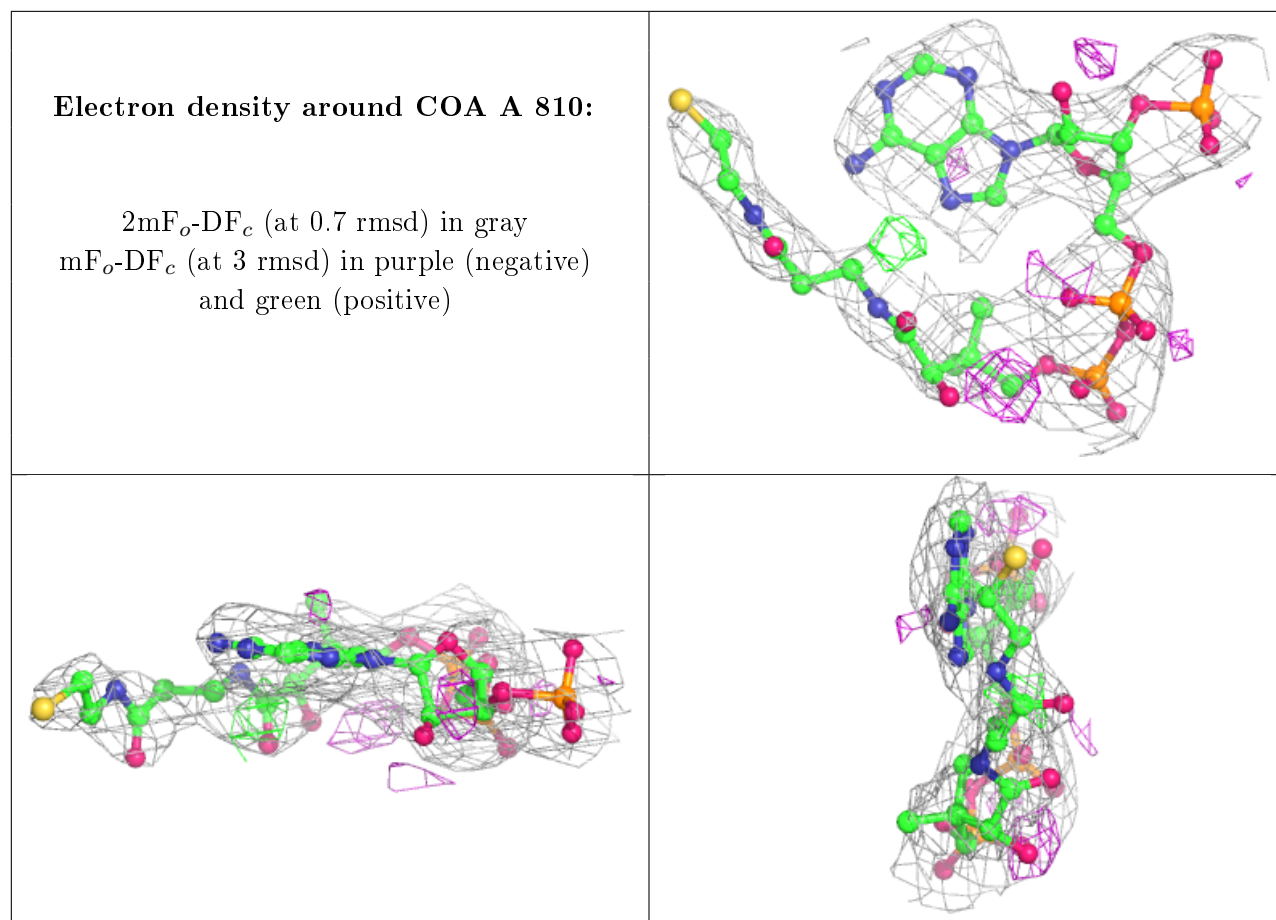
There are no monosaccharides in this entry.

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	SO4	A	807	5/5	0.81	0.21	105,110,117,119	0
2	SO4	B	804	5/5	0.89	0.12	131,134,137,138	0
2	SO4	A	804	5/5	0.90	0.14	105,108,111,112	0
2	SO4	B	803	5/5	0.91	0.18	87,100,101,112	0
2	SO4	B	802	5/5	0.91	0.26	120,121,124,126	0
2	SO4	A	809	5/5	0.91	0.60	129,132,133,136	0
3	COA	A	810	48/48	0.91	0.23	66,103,120,126	0
2	SO4	A	805	5/5	0.92	0.26	94,96,98,110	0
2	SO4	A	808	5/5	0.93	0.12	99,109,112,113	0
2	SO4	A	803	5/5	0.94	0.24	91,91,94,99	0
2	SO4	B	801	5/5	0.96	0.29	103,107,119,121	0
2	SO4	A	802	5/5	0.98	0.21	98,100,103,106	0
2	SO4	A	801	5/5	0.98	0.13	101,101,104,104	5
2	SO4	A	806	5/5	0.99	0.13	47,55,62,65	5

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.



## 6.5 Other polymers [i](#)

There are no such residues in this entry.