



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:26 AM UTC

PDB ID : 6YSW / pdb_00006ysw
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

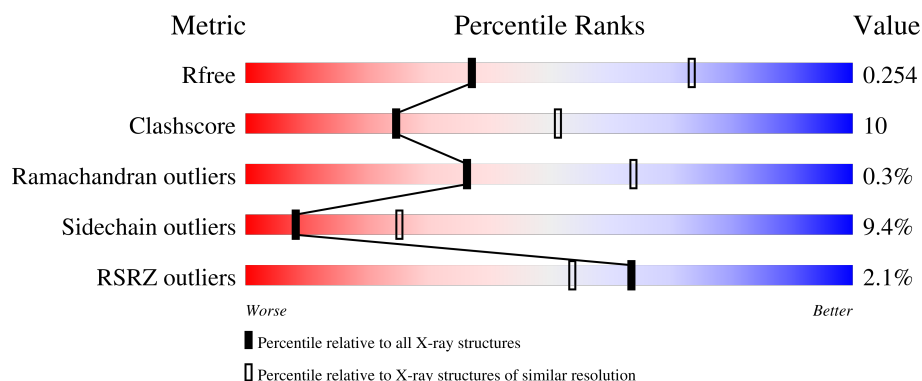
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.82 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}	180053	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (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 ≥ 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	 73% 23% . .
1	B	728	 67% 26% . .

2 Entry composition

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
1	B	698	Total	C	N	O	S	0	0	0
			5164	3261	918	962	23			
1	A	707	Total	C	N	O	S	0	0	0
			5271	3333	936	979	23			

There are 28 discrepancies between the modelled and reference sequences:

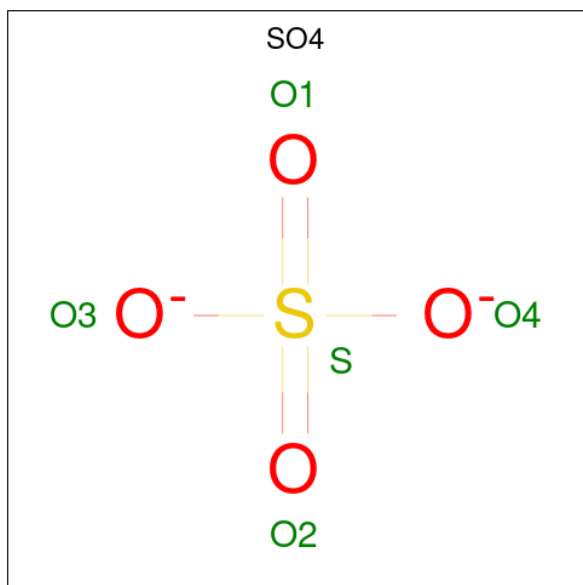
Chain	Residue	Modelled	Actual	Comment	Reference
B	-13	MET	-	initiating methionine	UNP P77399
B	-12	GLY	-	expression tag	UNP P77399
B	-11	SER	-	expression tag	UNP P77399
B	-10	SER	-	expression tag	UNP P77399
B	-9	HIS	-	expression tag	UNP P77399
B	-8	HIS	-	expression tag	UNP P77399
B	-7	HIS	-	expression 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 (CCD ID: SO4) (formula: O₄S).



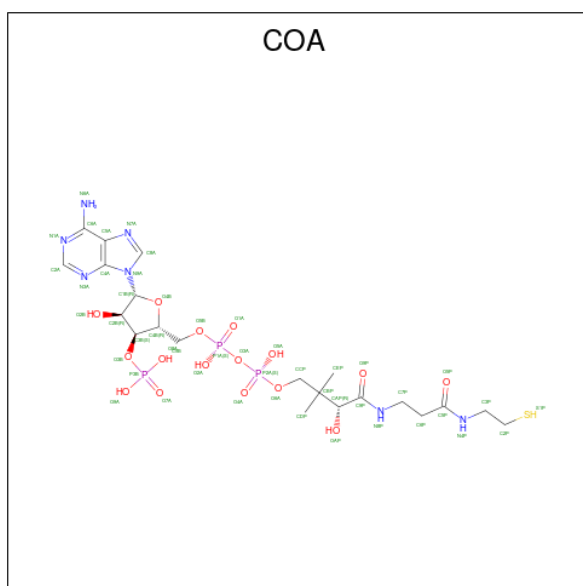
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		

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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 (CCD ID: 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		

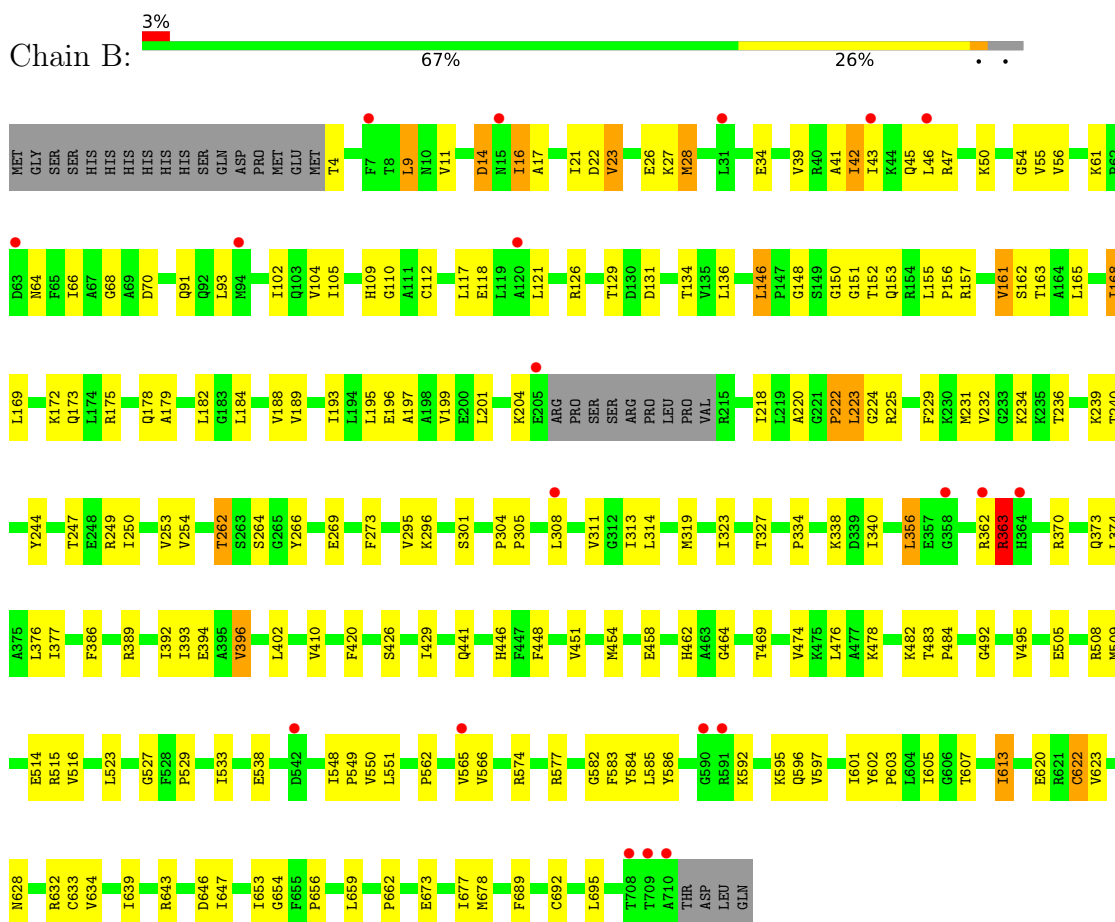
- Molecule 4 is water.

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 [i](#)

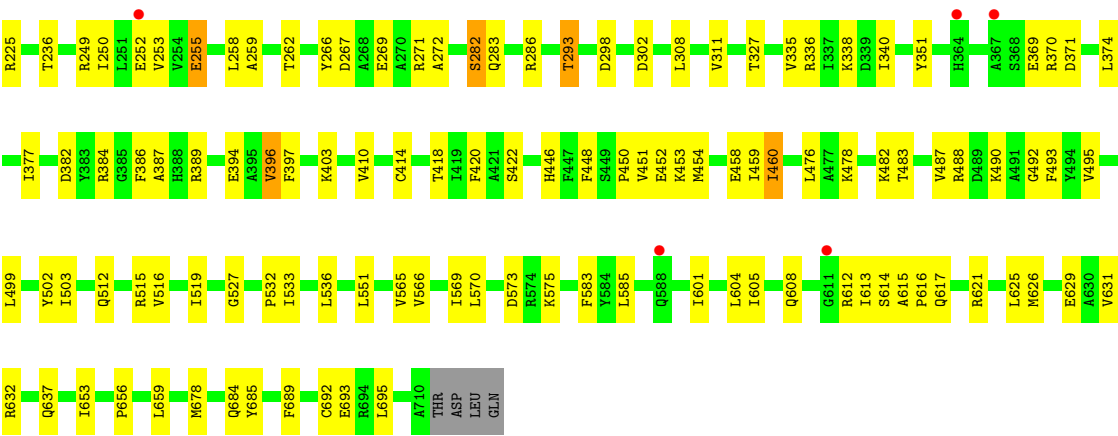
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: 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, α , β , γ	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) 59.9 (85.72-2.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.200 , 0.254 0.201 , 0.254	Depositor DCC
R_{free} test set	1428 reflections (2.97%)	wwPDB-VP
Wilson B-factor (Å ²)	62.5	Xtriage
Anisotropy	0.047	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	10567	wwPDB-VP
Average B, all atoms (Å ²)	58.0	wwPDB-VP

Xtriage'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.*

¹Intensities estimated from amplitudes.

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

5 Model quality

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	0.14	0/5361	0.34	0/7270
1	B	0.15	0/5249	0.34	0/7117
All	All	0.14	0/10610	0.34	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	94	0
1	B	5164	0	5184	112	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	207	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 10.

All (207) 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:73:MET:HE3	1:A:86:LEU:HD22	1.83	0.60
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:A:678:MET:HE1	1:A:695:LEU:HD23	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:A:450:PRO:HD2	1:A:454:MET:HE2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:64:ASN:C	1:A:64:ASN:HD22	2.27	0.43
1:A:516:VAL:HG13	1:A:533:ILE:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:110:GLY:C	1:B:134:THR:HA	2.44	0.42
1:A:129:THR:OG1	1:A:134:THR:HG21	2.18	0.42
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: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:152:THR:OG1	1:B:269:GLU:OE1	2.34	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:A:626:MET:HE3	1:A:626:MET:HB2	1.97	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:A:394:GLU:CD	1:A:403:LYS:HZ2	2.29	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:215:ARG:C	1:A:217:ARG:H	2.29	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	21	48
All	All	1399/1456 (96%)	1313 (94%)	82 (6%)	4 (0%)	36	64

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%)	498 (92%)	44 (8%)	11	32
1	B	524/583 (90%)	468 (89%)	56 (11%)	6	20
All	All	1066/1166 (91%)	966 (91%)	100 (9%)	8	25

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	4	THR
1	B	9	LEU
1	B	11	VAL
1	B	14	ASP
1	B	16	ILE
1	B	23	VAL
1	B	27	LYS
1	B	28	MET
1	B	34	GLU
1	B	42	ILE
1	B	47	ARG
1	B	50	LYS
1	B	56	VAL
1	B	91	GLN
1	B	104	VAL
1	B	105	ILE
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	178	GLN
1	B	182	LEU
1	B	188	VAL
1	B	195	LEU
1	B	196	GLU
1	B	218	ILE
1	B	223	LEU
1	B	225	ARG
1	B	231	MET
1	B	232	VAL
1	B	234	LYS
1	B	239	LYS

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Mol	Chain	Res	Type
1	B	247	THR
1	B	253	VAL
1	B	262	THR
1	B	264	SER
1	B	301	SER
1	B	319	MET
1	B	340	ILE
1	B	356	LEU
1	B	363	ARG
1	B	374	LEU
1	B	377	ILE
1	B	396	VAL
1	B	402	LEU
1	B	592	LYS
1	B	595	LYS
1	B	607	THR
1	B	613	ILE
1	B	622	CYS
1	B	633	CYS
1	B	647	ILE
1	B	653	ILE
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	127	VAL
1	A	134	THR
1	A	140	GLU
1	A	199	VAL
1	A	205	GLU
1	A	212	LEU
1	A	214	VAL
1	A	215	ARG
1	A	217	ARG
1	A	252	GLU
1	A	255	GLU

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Mol	Chain	Res	Type
1	A	282	SER
1	A	293	THR
1	A	302	ASP
1	A	369	GLU
1	A	382	ASP
1	A	396	VAL
1	A	418	THR
1	A	459	ILE
1	A	460	ILE
1	A	483	THR
1	A	487	VAL
1	A	490	LYS
1	A	566	VAL
1	A	570	LEU
1	A	573	ASP
1	A	575	LYS
1	A	585	LEU
1	A	608	GLN
1	A	613	ILE
1	A	625	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 (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	173	GLN
1	B	178	GLN
1	B	309	ASN
1	B	388	HIS
1	A	260	GLN
1	A	441	GLN
1	A	518	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	$\# Z > 2$
2	SO4	B	802	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	A	802	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	A	801	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	B	801	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	A	809	-	4,4,4	0.35	0	6,6,6	0.08	0
3	COA	A	810	-	47,50,50	2.79	9 (19%)	69,75,75	1.67	15 (21%)
2	SO4	A	806	-	4,4,4	0.32	0	6,6,6	0.07	0
2	SO4	A	803	-	4,4,4	0.31	0	6,6,6	0.07	0
2	SO4	A	807	-	4,4,4	0.33	0	6,6,6	0.07	0
2	SO4	B	803	-	4,4,4	0.33	0	6,6,6	0.07	0
2	SO4	A	808	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	A	805	-	4,4,4	0.34	0	6,6,6	0.07	0
2	SO4	B	804	-	4,4,4	0.29	0	6,6,6	0.05	0
2	SO4	A	804	-	4,4,4	0.33	0	6,6,6	0.07	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	-	-	17/48/64/64	0/3/3/3

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	810	COA	P3B-O3B	14.58	1.85	1.59
3	A	810	COA	P1A-O3A	8.84	1.69	1.59
3	A	810	COA	P2A-O6A	3.76	1.74	1.59
3	A	810	COA	O3B-C3B	-2.67	1.35	1.44
3	A	810	COA	C5A-C4A	2.63	1.43	1.39
3	A	810	COA	C5P-N4P	2.58	1.39	1.33
3	A	810	COA	C9P-N8P	2.44	1.39	1.33
3	A	810	COA	C2A-N1A	2.27	1.38	1.33
3	A	810	COA	C4A-N3A	2.13	1.38	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	810	COA	P3B-O3B-C3B	-5.23	109.46	123.43
3	A	810	COA	O3B-P3B-O7A	-4.00	95.08	109.33
3	A	810	COA	C7P-C6P-C5P	-3.17	107.11	112.39
3	A	810	COA	P1A-O5B-C5B	-3.05	103.87	121.35
3	A	810	COA	O5A-P2A-O3A	2.94	115.23	107.27
3	A	810	COA	O9A-P3B-O8A	2.78	118.23	107.80
3	A	810	COA	O3A-P1A-O1A	-2.74	102.47	110.70
3	A	810	COA	C3P-N4P-C5P	-2.72	117.75	122.82
3	A	810	COA	P2A-O6A-CCP	-2.65	106.67	121.12
3	A	810	COA	C7P-N8P-C9P	-2.53	118.00	122.55
3	A	810	COA	O6A-CCP-CBP	-2.48	106.56	110.55
3	A	810	COA	N3A-C4A-N9A	2.42	131.28	127.17
3	A	810	COA	C2A-N1A-C6A	-2.24	115.05	118.73
3	A	810	COA	C6P-C7P-N8P	-2.21	107.31	112.00
3	A	810	COA	O6A-P2A-O4A	-2.12	100.55	108.94

There are no chirality outliers.

All (17) 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

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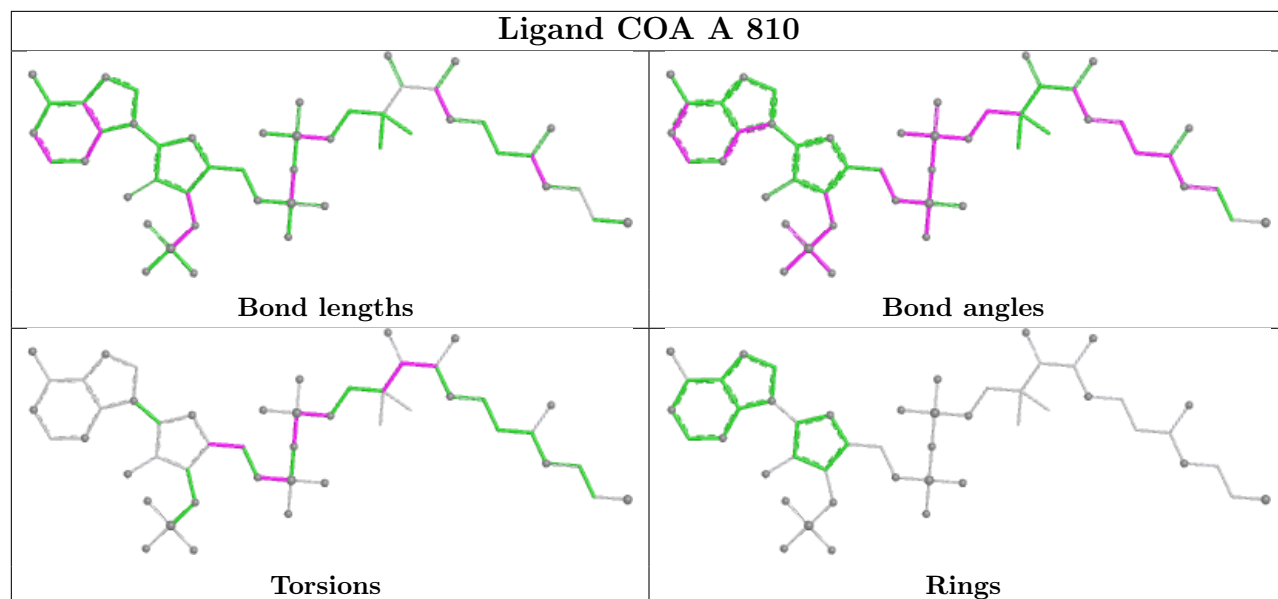
Mol	Chain	Res	Type	Atoms
3	A	810	COA	O9P-C9P-CAP-CBP
3	A	810	COA	N8P-C9P-CAP-CBP
3	A	810	COA	O4B-C4B-C5B-O5B
3	A	810	COA	C3B-C4B-C5B-O5B
3	A	810	COA	N8P-C9P-CAP-OAP
3	A	810	COA	C5B-O5B-P1A-O2A
3	A	810	COA	C5B-O5B-P1A-O3A
3	A	810	COA	CCP-O6A-P2A-O4A
3	A	810	COA	P1A-O3A-P2A-O5A

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, 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	707/728 (97%)	0.08	9 (1%) 75 66	20, 47, 97, 178	0
1	B	698/728 (95%)	0.15	20 (2%) 53 43	24, 57, 112, 164	0
All	All	1405/1456 (96%)	0.11	29 (2%) 63 54	20, 53, 105, 178	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	364	HIS	3.9
1	B	709	THR	3.3
1	A	367	ALA	3.0
1	B	63	ASP	3.0
1	B	31	LEU	2.8
1	B	710	ALA	2.7
1	B	708	THR	2.6
1	B	46	LEU	2.6
1	A	71	ILE	2.5
1	A	215	ARG	2.5
1	B	362	ARG	2.5
1	B	15	ASN	2.4
1	B	590	GLY	2.4
1	B	565	VAL	2.3
1	B	7	PHE	2.2
1	B	591	ARG	2.2
1	A	9	LEU	2.2
1	B	43	ILE	2.2
1	A	364	HIS	2.2
1	B	358	GLY	2.2
1	B	308	LEU	2.2
1	A	252	GLU	2.1
1	A	588	GLN	2.1
1	B	120	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	611	GLY	2.0
1	B	94	MET	2.0
1	A	213	PRO	2.0
1	B	205	GLU	2.0
1	B	542	ASP	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

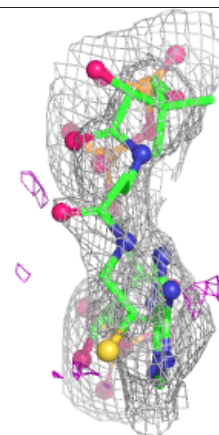
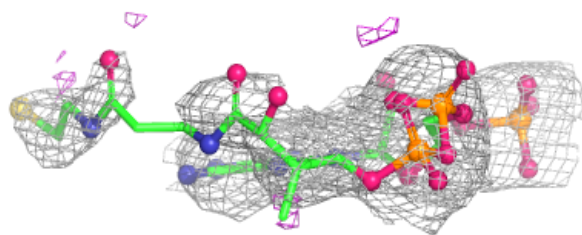
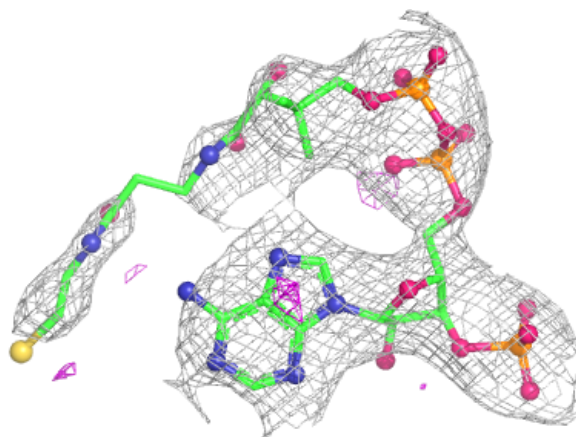
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SO4	A	807	5/5	0.55	0.13	105,110,117,119	0
2	SO4	A	804	5/5	0.68	0.12	105,108,111,112	0
2	SO4	B	801	5/5	0.76	0.14	103,107,119,121	0
2	SO4	B	803	5/5	0.80	0.16	87,100,101,112	0
2	SO4	A	808	5/5	0.81	0.08	99,109,112,113	0
2	SO4	A	801	5/5	0.82	0.12	101,101,104,104	5
2	SO4	B	804	5/5	0.82	0.08	131,134,137,138	0
2	SO4	A	809	5/5	0.84	0.15	129,132,133,136	0
3	COA	A	810	48/48	0.85	0.12	66,103,120,126	0
2	SO4	A	805	5/5	0.88	0.27	94,96,98,110	0
2	SO4	B	802	5/5	0.89	0.13	120,121,124,126	0
2	SO4	A	802	5/5	0.95	0.15	98,100,103,106	0
2	SO4	A	803	5/5	0.96	0.19	91,91,94,99	0
2	SO4	A	806	5/5	0.97	0.06	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.

Electron density around COA A 810:

$2mF_o-DF_c$ (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.