



Full wwPDB X-ray Structure Validation Report

Mar 1, 2014 – 12:52 AM GMT

PDB ID : 2IBY
Title : Crystallographic and kinetic studies of human mitochondrial acetoacetyl-CoA thiolase (T2): the importance of potassium and chloride for its structure and function
Authors : Haapalainen, A.M.; Wierenga, R.K.
Deposited on : 2006-09-12
Resolution : 1.85 Å(reported)

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

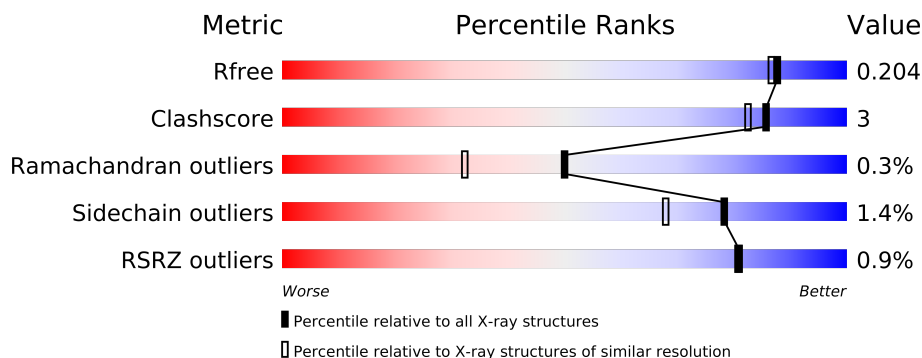
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

The reported resolution of this entry is 1.85 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	1269 (1.86-1.86)
Clashscore	79885	1470 (1.86-1.86)
Ramachandran outliers	78287	1451 (1.86-1.86)
Sidechain outliers	78261	1451 (1.86-1.86)
RSRZ outliers	66119	1269 (1.86-1.86)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	395	
1	B	395	
1	C	395	
1	D	395	

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

Mol	Type	Chain	Res	Geometry	Electron density
2	CL	B	2001	-	X
4	COA	A	6001	-	X
4	COA	B	6002	-	X
5	MES	A	5001	-	X

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Geometry	Electron density
6	GOL	A	4001	-	X
6	GOL	B	4002	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13011 atoms, of which 0 are hydrogen and 0 are deuterium.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Acetyl-CoA acetyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	11	0
			2913	1842	491	559	21			
1	B	391	Total	C	N	O	S	0	14	0
			2921	1851	492	557	21			
1	C	393	Total	C	N	O	S	0	3	0
			2900	1830	494	555	21			
1	D	393	Total	C	N	O	S	0	1	0
			2891	1823	493	554	21			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	33	MET	-	INITIATING METHIONINE	UNP P24752
A	34	ALA	VAL	ENGINEERED	UNP P24752
A	126	CSO	CYS	MODIFIED RESIDUE	UNP P24752
B	33	MET	-	INITIATING METHIONINE	UNP P24752
B	34	ALA	VAL	ENGINEERED	UNP P24752
B	126	CSO	CYS	MODIFIED RESIDUE	UNP P24752
C	33	MET	-	INITIATING METHIONINE	UNP P24752
C	34	ALA	VAL	ENGINEERED	UNP P24752
C	126	CSO	CYS	MODIFIED RESIDUE	UNP P24752
D	33	MET	-	INITIATING METHIONINE	UNP P24752
D	34	ALA	VAL	ENGINEERED	UNP P24752
D	126	CSO	CYS	MODIFIED RESIDUE	UNP P24752

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Cl	0	0
			1	1		
2	A	1	Total	Cl	0	0
			1	1		

Continued on next page...

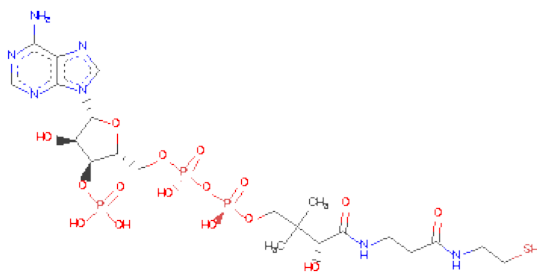
Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	K	0	0
			1	1		
3	A	1	Total	K	0	0
			1	1		
3	D	1	Total	K	0	0
			1	1		
3	C	1	Total	K	0	0
			1	1		

- Molecule 4 is COENZYME A (three-letter code: COA) (formula: C₂₁H₃₆N₇O₁₆P₃S).



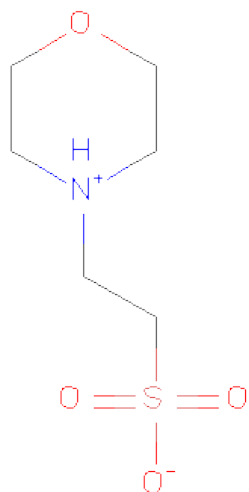
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
4	B	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0
4	C	1	Total 48	C 21	N 7	O 16	P 3	S 1	0	0

Continued on next page...

Continued from previous page...

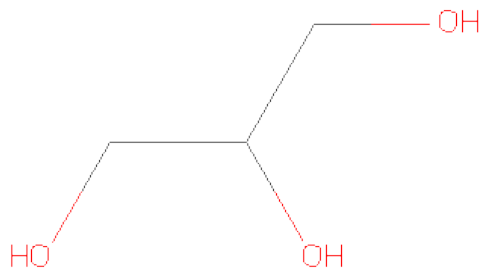
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	N	O	P	S		
4	D	1	48	21	7	16	3	1	0	0

- Molecule 5 is 2-(N-MORPHOLINO)-ETHANESULFONICACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
5	A	1	12	6	1	4	1	0	0

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	410	Total	O	0	0
			410	410		
7	B	376	Total	O	0	0
			376	376		
7	C	176	Total	O	0	0
			176	176		
7	D	200	Total	O	0	0
			200	200		

3 Residue-property plots

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

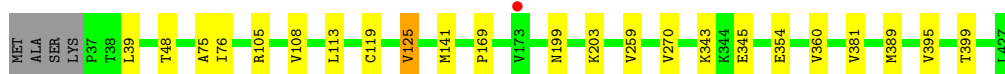
- Molecule 1: Acetyl-CoA acetyltransferase

Chain A: 



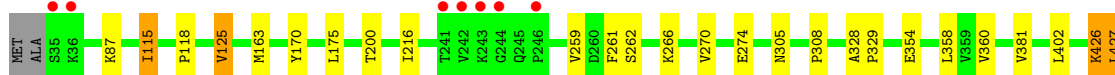
- Molecule 1: Acetyl-CoA acetyltransferase

Chain B: 



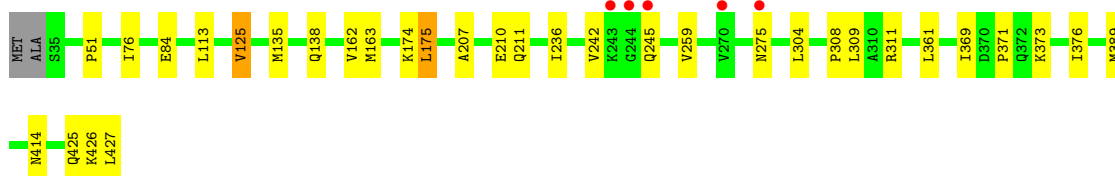
- Molecule 1: Acetyl-CoA acetyltransferase

Chain C: 



- Molecule 1: Acetyl-CoA acetyltransferase

Chain D: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	75.35Å 106.75Å 101.66Å 90.00° 103.06° 90.00°	Depositor
Resolution (Å)	73.32 – 1.85 73.40 – 1.85	Depositor EDS
% Data completeness (in resolution range)	100.0 (73.32-1.85) 99.9 (73.40-1.85)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.96 (at 1.86Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.164 , 0.203 0.165 , 0.204	Depositor DCC
R_{free} test set	6668 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 133366 reflections	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	13011	wwPDB-VP
Average B, all atoms (Å ²)	25.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, CSO, CL, K, COA, MES

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	0.59	0/2991	0.65	0/4048
1	B	0.57	0/3014	0.64	0/4082
1	C	0.41	0/2946	0.56	0/3984
1	D	0.43	0/2929	0.56	0/3962
All	All	0.51	0/11880	0.60	0/16076

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2913	0	3005	15	0
1	B	2921	0	3027	16	0
1	C	2900	0	2994	14	0
1	D	2891	0	2980	19	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	48	0	32	3	0
4	B	48	0	32	2	0
4	C	48	0	32	1	0
4	D	48	0	32	1	0
5	A	12	0	12	2	0
6	A	6	0	8	0	0
6	B	6	0	8	0	0
7	A	410	0	0	4	0
7	B	376	0	0	3	0
7	C	176	0	0	0	0
7	D	200	0	0	0	0
All	All	13011	0	12162	66	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (66) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:108[A]:VAL:HG21	1:B:119:CYS:SG	1.99	1.01
1:B:48[A]:THR:HG22	7:B:6191:HOH:O	1.81	0.81
1:B:343[A]:LYS:HD2	1:B:345:GLU:OE1	1.84	0.76
1:A:48[A]:THR:HG22	7:A:6155:HOH:O	1.89	0.71
1:B:395:VAL:O	1:B:399[B]:THR:HG23	1.96	0.66
1:A:395:VAL:O	1:A:399[B]:THR:HG23	2.00	0.61
4:A:6001:COA:O5A	5:A:5001:MES:H52	2.02	0.59
1:A:336[A]:VAL:HG11	1:A:423:LEU:HB2	1.84	0.59
1:A:223:LYS:HE3	1:A:227:GLU:OE2	2.03	0.59
1:B:108[A]:VAL:CG2	1:B:119:CYS:SG	2.84	0.57
1:B:39:LEU:HD13	1:B:141:MET:HE2	1.89	0.54
1:D:76:ILE:CD1	1:D:113:LEU:HD11	2.37	0.54
1:B:76:ILE:CD1	1:B:113[A]:LEU:HD11	2.38	0.54
1:D:210:GLU:HG2	1:D:361:LEU:HD13	1.91	0.52
1:D:373:LYS:C	1:D:376:ILE:HD11	2.29	0.52
1:B:270:VAL:HG11	7:B:6317:HOH:O	2.07	0.52
1:D:311:ARG:NH2	1:D:425:GLN:OE1	2.31	0.52
1:B:39:LEU:HD13	1:B:141:MET:CE	2.41	0.51
1:C:308:PRO:HB2	1:C:427:LEU:HD23	1.92	0.51
1:A:313:VAL:HG12	1:A:340:VAL:HG11	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:D:51:PRO:HD3	1:D:236:ILE:O	2.13	0.49
4:A:6001:COA:H52A	7:A:6243:HOH:O	2.11	0.49
1:C:115:ILE:H	1:C:115:ILE:HD13	1.78	0.48
1:A:76:ILE:CD1	1:A:113:LEU:HD11	2.43	0.48
1:D:125:VAL:HB	1:D:414:ASN:HB2	1.96	0.48
4:B:6002:COA:H52A	7:B:6317:HOH:O	2.13	0.48
1:B:354:GLU:HB3	1:B:381:VAL:HG23	1.95	0.48
1:B:259:VAL:HG23	4:B:6002:COA:H61A	1.79	0.47
1:A:309:LEU:O	1:A:426:LYS:HD2	2.15	0.47
1:A:354:GLU:HG2	1:A:360:VAL:HG21	1.96	0.47
1:D:309:LEU:O	1:D:426:LYS:HD2	2.15	0.46
1:C:354:GLU:HB3	1:C:381:VAL:HG23	1.98	0.46
1:C:354:GLU:HG2	1:C:360:VAL:HG21	1.97	0.46
1:D:373:LYS:CA	1:D:376:ILE:HD11	2.46	0.46
1:C:163:MET:HE2	1:D:175:LEU:HD12	1.97	0.46
1:A:336[A]:VAL:CG1	1:A:423:LEU:HB2	2.46	0.45
1:C:259:VAL:HG23	4:C:6003:COA:H61A	1.81	0.45
1:A:354:GLU:HB3	1:A:381:VAL:HG23	1.98	0.45
1:B:354:GLU:HG2	1:B:360:VAL:HG21	1.99	0.45
1:D:163:MET:CE	1:D:175:LEU:HD21	2.46	0.45
1:D:259:VAL:HG23	4:D:6004:COA:H61A	1.83	0.44
1:D:84:GLU:H	1:D:84:GLU:CD	2.20	0.44
1:C:200:THR:HB	1:C:358:LEU:HD11	1.98	0.44
1:A:73:GLN:NE2	7:A:6294:HOH:O	2.50	0.44
1:B:105:ARG:HA	1:B:108[A]:VAL:HG22	2.00	0.43
1:D:373:LYS:HA	1:D:376:ILE:HD11	1.99	0.43
1:A:77[B]:GLU:HG3	7:A:6122:HOH:O	2.17	0.43
1:A:125:VAL:HB	1:A:414:ASN:HB2	2.01	0.43
5:A:5001:MES:H62	1:C:170:TYR:CE2	2.55	0.42
1:D:135:MET:HA	1:D:138:GLN:HE21	1.84	0.42
1:C:216:ILE:HG23	1:C:261:PHE:CE2	2.54	0.42
1:D:242:VAL:HB	1:D:245:GLN:HB2	2.00	0.42
1:B:199:ASN:ND2	1:B:203:LYS:HE2	2.34	0.42
1:D:308:PRO:HG2	1:D:427:LEU:HD23	2.01	0.42
1:B:48[A]:THR:CG2	1:B:75:ALA:HA	2.50	0.41
1:C:87:LYS:O	1:C:118:PRO:HD2	2.21	0.41
1:D:163:MET:HE3	1:D:175:LEU:HD21	2.01	0.41
1:C:328:ALA:N	1:C:329:PRO:CD	2.83	0.41
1:A:259:VAL:HG23	4:A:6001:COA:H61A	1.85	0.41
1:D:369:ILE:O	1:D:371:PRO:HD3	2.20	0.41
1:D:207:ALA:O	1:D:211:GLN:HG3	2.20	0.41
1:A:242:VAL:HB	1:A:245:GLN:HB2	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:163:MET:HB2	1:C:175:LEU:HD22	2.02	0.41
1:C:402:LEU:HB2	1:C:426:LYS:HG3	2.03	0.40
1:C:262:SER:O	1:C:266:LYS:HE2	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	399/395 (101%)	395 (99%)	3 (1%)	1 (0%)	50	32
1	B	402/395 (102%)	396 (98%)	5 (1%)	1 (0%)	56	38
1	C	393/395 (100%)	382 (97%)	10 (2%)	1 (0%)	50	32
1	D	391/395 (99%)	383 (98%)	7 (2%)	1 (0%)	50	32
All	All	1585/1580 (100%)	1556 (98%)	25 (2%)	4 (0%)	50	32

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	VAL
1	B	125	VAL
1	C	125	VAL
1	D	125	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution. The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	316/308 (103%)	314 (99%)	2 (1%)	92	89

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	319/308 (104%)	317 (99%)	2 (1%)	92	89
1	C	310/308 (101%)	303 (98%)	7 (2%)	63	46
1	D	308/308 (100%)	301 (98%)	7 (2%)	63	46
All	All	1253/1232 (102%)	1235 (99%)	18 (1%)	78	68

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	175	LEU
1	A	389	MET
1	B	125	VAL
1	B	389	MET
1	C	115	ILE
1	C	125	VAL
1	C	270	VAL
1	C	274	GLU
1	C	305	ASN
1	C	426	LYS
1	C	427	LEU
1	D	162[A]	VAL
1	D	162[B]	VAL
1	D	174	LYS
1	D	175	LEU
1	D	275	ASN
1	D	304	LEU
1	D	389	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	B	93	ASN
1	B	138	GLN
1	B	199	ASN
1	C	93	ASN
1	D	93	ASN
1	D	138	GLN

5.3.3 RNA ⓘ

There are no RNA chains in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
1	CSO	A	126	1	6,6,7	6.96	4 (66%)	3,6,8	1.18	0
1	CSO	B	126	1	6,6,7	6.72	4 (66%)	3,6,8	1.24	0
1	CSO	C	126	1	6,6,7	7.74	3 (50%)	3,6,8	1.48	0
1	CSO	D	126	1	6,6,7	7.42	3 (50%)	3,6,8	0.99	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
1	CSO	A	126	1	-	0/2/5/7	0/0/0/0
1	CSO	B	126	1	-	0/2/5/7	0/0/0/0
1	CSO	C	126	1	-	0/2/5/7	0/0/0/0
1	CSO	D	126	1	-	0/2/5/7	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	126	CSO	O-C	18.19	1.23	1.11
1	D	126	CSO	O-C	17.40	1.23	1.11
1	A	126	CSO	O-C	15.82	1.22	1.11
1	B	126	CSO	O-C	15.48	1.22	1.11
1	B	126	CSO	OD-SG	4.42	1.81	1.62
1	D	126	CSO	OD-SG	3.96	1.79	1.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	126	CSO	OD-SG	3.94	1.79	1.62
1	A	126	CSO	CB-SG	-3.85	1.77	1.82
1	A	126	CSO	OD-SG	3.74	1.78	1.62
1	C	126	CSO	CA-C	3.27	1.54	1.48
1	A	126	CSO	CA-C	3.15	1.54	1.48
1	D	126	CSO	CA-C	2.71	1.53	1.48
1	B	126	CSO	CA-C	2.28	1.52	1.48
1	B	126	CSO	CB-SG	-2.10	1.80	1.82

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	GOL	A	4001	-	5,5,5	0.35	0	5,5,5	0.24	0
5	MES	A	5001	-	12,12,12	2.19	1 (8%)	16,16,16	2.58	7 (43%)
4	COA	A	6001	-	50,50,50	1.48	6 (12%)	75,75,75	1.42	9 (12%)
6	GOL	B	4002	-	5,5,5	0.35	0	5,5,5	0.34	0
4	COA	B	6002	-	50,50,50	1.46	6 (12%)	75,75,75	1.47	7 (9%)
4	COA	C	6003	-	50,50,50	1.50	6 (12%)	75,75,75	1.41	6 (8%)
4	COA	D	6004	-	50,50,50	1.50	6 (12%)	75,75,75	1.42	6 (8%)

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
6	GOL	A	4001	-	-	0/4/4/4	0/0/0/0
5	MES	A	5001	-	-	0/6/14/14	1/1/1/1
4	COA	A	6001	-	-	0/48/64/64	0/1/3/3
6	GOL	B	4002	-	-	0/4/4/4	0/0/0/0
4	COA	B	6002	-	-	0/48/64/64	0/1/3/3
4	COA	C	6003	-	-	0/48/64/64	0/1/3/3
4	COA	D	6004	-	-	0/48/64/64	0/1/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	5001	MES	C8-S	-6.68	1.66	1.78
4	C	6003	COA	P3B-O7A	5.84	1.70	1.51
4	B	6002	COA	P3B-O7A	5.83	1.70	1.51
4	D	6004	COA	P3B-O7A	5.80	1.70	1.51
4	A	6001	COA	P3B-O7A	5.76	1.70	1.51
4	C	6003	COA	P3B-O8A	4.35	1.70	1.54
4	D	6004	COA	P3B-O8A	4.32	1.70	1.54
4	A	6001	COA	P3B-O8A	4.27	1.70	1.54
4	B	6002	COA	P3B-O8A	4.00	1.69	1.54
4	C	6003	COA	P1A-O2A	3.57	1.71	1.55
4	D	6004	COA	P1A-O2A	3.56	1.70	1.55
4	A	6001	COA	P1A-O2A	3.49	1.70	1.55
4	D	6004	COA	P2A-O5A	3.48	1.70	1.55
4	B	6002	COA	P1A-O2A	3.43	1.70	1.55
4	C	6003	COA	P2A-O5A	3.41	1.70	1.55
4	B	6002	COA	P2A-O5A	3.30	1.69	1.55
4	A	6001	COA	P2A-O5A	3.18	1.69	1.55
4	A	6001	COA	C4A-N9A	-2.82	1.33	1.37
4	B	6002	COA	C4A-N9A	-2.80	1.33	1.37
4	C	6003	COA	C5A-C4A	2.74	1.46	1.40
4	C	6003	COA	C4A-N9A	-2.67	1.33	1.37
4	A	6001	COA	C5A-C4A	2.67	1.46	1.40
4	D	6004	COA	C4A-N9A	-2.66	1.33	1.37
4	D	6004	COA	C5A-C4A	2.63	1.46	1.40
4	B	6002	COA	C5A-C4A	2.58	1.46	1.40

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	6002	COA	N3A-C4A-N9A	6.67	137.47	125.43
4	A	6001	COA	N3A-C4A-N9A	6.66	137.46	125.43
4	D	6004	COA	N3A-C4A-N9A	6.58	137.31	125.43
4	C	6003	COA	N3A-C4A-N9A	6.53	137.23	125.43
4	B	6002	COA	N3A-C2A-N1A	-6.46	123.31	128.71
5	A	5001	MES	C5-N4-C3	6.02	121.68	109.75
4	C	6003	COA	N3A-C2A-N1A	-5.84	123.83	128.71
4	D	6004	COA	N3A-C2A-N1A	-5.72	123.93	128.71
4	A	6001	COA	N3A-C2A-N1A	-5.35	124.24	128.71
5	A	5001	MES	C8-C7-N4	-3.96	105.67	112.44
4	D	6004	COA	P2A-O3A-P1A	-3.86	120.37	131.68
5	A	5001	MES	C6-C5-N4	-3.64	105.29	109.96
4	C	6003	COA	P2A-O3A-P1A	-3.46	121.53	131.68
4	D	6004	COA	C5A-C4A-N3A	-3.44	118.21	125.70
4	B	6002	COA	C5A-C4A-N3A	-3.43	118.24	125.70
4	A	6001	COA	C5A-C4A-N3A	-3.38	118.34	125.70
4	C	6003	COA	C5A-C4A-N3A	-3.36	118.38	125.70
4	A	6001	COA	P2A-O3A-P1A	-3.23	122.20	131.68
5	A	5001	MES	C7-N4-C5	3.16	119.91	111.66
4	A	6001	COA	C8A-N9A-C4A	2.96	109.16	106.90
4	B	6002	COA	C8A-N9A-C4A	2.95	109.15	106.90
5	A	5001	MES	C2-C3-N4	-2.90	106.25	109.96
4	C	6003	COA	C8A-N9A-C4A	2.69	108.95	106.90
5	A	5001	MES	O1-C6-C5	-2.58	108.26	111.34
5	A	5001	MES	C7-N4-C3	2.58	118.41	111.66
4	B	6002	COA	P2A-O3A-P1A	-2.57	124.16	131.68
4	B	6002	COA	C2A-N3A-C4A	2.44	120.95	114.01
4	D	6004	COA	C8A-N9A-C4A	2.43	108.75	106.90
4	C	6003	COA	C2A-N3A-C4A	2.26	120.43	114.01
4	D	6004	COA	C2A-N3A-C4A	2.25	120.40	114.01
4	A	6001	COA	C2A-N3A-C4A	2.13	120.08	114.01
4	A	6001	COA	C7P-C6P-C5P	-2.09	108.69	112.25
4	A	6001	COA	C5A-C4A-N9A	-2.05	104.21	107.16
4	B	6002	COA	C2A-N1A-C6A	2.00	122.39	118.77
4	A	6001	COA	CBP-CAP-C9P	-2.00	110.79	112.73

There are no chirality outliers.

There are no torsion outliers.

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	5001	MES	C2-C3-C5-C6-N4-O1

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	391/395 (98%)	-0.52	2 (0%) 88 89	7, 14, 28, 56	14 (3%)
1	B	391/395 (98%)	-0.47	1 (0%) 91 92	8, 15, 30, 53	20 (5%)
1	C	393/395 (99%)	-0.03	7 (1%) 65 64	17, 30, 47, 70	20 (5%)
1	D	393/395 (99%)	-0.05	5 (1%) 74 72	17, 29, 44, 65	31 (7%)
All	All	1568/1580 (99%)	-0.27	15 (0%) 81 78	7, 23, 43, 70	85 (5%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	244	GLY	8.2
1	C	243	LYS	5.2
1	D	243	LYS	3.6
1	C	35	SER	2.8
1	D	244	GLY	2.6
1	A	243	LYS	2.6
1	B	173	VAL	2.6
1	D	270	VAL	2.4
1	C	241	THR	2.3
1	A	37	PRO	2.2
1	C	242	VAL	2.2
1	C	36	LYS	2.1
1	D	275	ASN	2.1
1	D	245	GLN	2.0
1	C	246	PRO	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains.

The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	CSO	B	126	7/8	0.09	1.27	10,11,20,23	0
1	CSO	A	126	7/8	0.08	0.09	8,10,17,21	0
1	CSO	D	126	7/8	0.08	-0.27	20,21,26,32	0
1	CSO	C	126	7/8	0.06	-1.02	19,20,24,28	0

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	MES	A	5001	12/12	0.32	51.14	75,76,76,76	4
2	CL	B	2001	1/1	0.10	5.59	43,43,43,43	0
6	GOL	B	4002	6/6	0.14	3.79	40,41,41,41	6
4	COA	B	6002	48/48	0.13	3.28	27,33,43,44	0
4	COA	A	6001	48/48	0.14	3.16	20,35,45,46	1
6	GOL	A	4001	6/6	0.13	2.77	30,33,34,35	0
4	COA	D	6004	48/48	0.19	1.76	40,59,62,63	1
4	COA	C	6003	48/48	0.15	1.52	29,50,55,56	1
2	CL	A	2002	1/1	0.09	0.97	43,43,43,43	0
2	CL	C	2004	1/1	0.09	0.73	54,54,54,54	0
3	K	A	3001	1/1	0.07	-0.27	12,12,12,12	0
3	K	B	3002	1/1	0.07	-0.58	15,15,15,15	0
2	CL	D	2003	1/1	0.06	-0.64	55,55,55,55	0
3	K	D	3004	1/1	0.05	-2.08	26,26,26,26	0
3	K	C	3003	1/1	0.04	-4.56	28,28,28,28	0

6.5 Other polymers ⓘ

There are no such residues in this entry.