W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:16 am BST

PDB ID	:	4C2K
Title	:	Crystal structure of human mitochondrial 3-ketoacyl-CoA thiolase
Authors	:	Kiema, T.-R.; Harijan, R.K.; Wierenga, R.K.
Deposited on	:	2013-08-19
Resolution	:	2.00 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 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	:	2.11
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)	:	2.11

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 2.00 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.
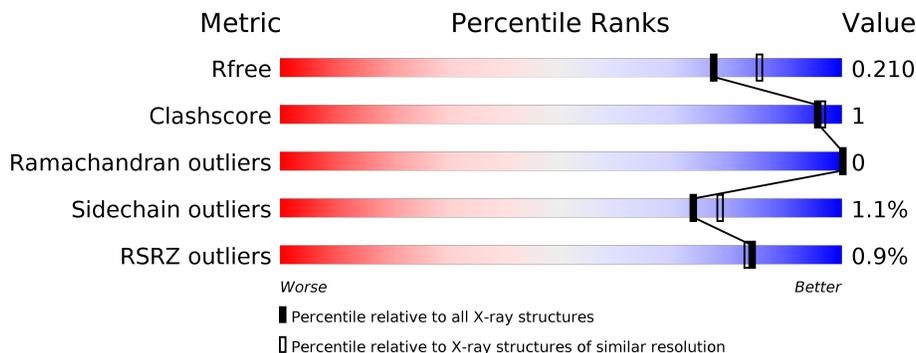
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 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	417	92% • 5%
1	B	417	94% • 5%
1	C	417	91% • 6%
1	D	417	93% • •

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 12340 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 3-KETOACYL-COA THIOLASE, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	395	Total	C	N	O	S	0	0	0
			2925	1835	516	558	16			
1	B	395	Total	C	N	O	S	0	0	0
			2921	1831	514	559	17			
1	C	394	Total	C	N	O	S	0	0	0
			2913	1826	513	558	16			
1	D	399	Total	C	N	O	S	0	0	0
			2953	1851	522	563	17			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P42765
A	-18	GLY	-	expression tag	UNP P42765
A	-17	SER	-	expression tag	UNP P42765
A	-16	SER	-	expression tag	UNP P42765
A	-15	HIS	-	expression tag	UNP P42765
A	-14	HIS	-	expression tag	UNP P42765
A	-13	HIS	-	expression tag	UNP P42765
A	-12	HIS	-	expression tag	UNP P42765
A	-11	HIS	-	expression tag	UNP P42765
A	-10	HIS	-	expression tag	UNP P42765
A	-9	SER	-	expression tag	UNP P42765
A	-8	SER	-	expression tag	UNP P42765
A	-7	GLY	-	expression tag	UNP P42765
A	-6	LEU	-	expression tag	UNP P42765
A	-5	VAL	-	expression tag	UNP P42765
A	-4	PRO	-	expression tag	UNP P42765
A	-3	ARG	-	expression tag	UNP P42765
A	-2	GLY	-	expression tag	UNP P42765
A	-1	SER	-	expression tag	UNP P42765
A	0	HIS	-	expression tag	UNP P42765
B	-19	MET	-	expression tag	UNP P42765

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	expression tag	UNP P42765
B	-17	SER	-	expression tag	UNP P42765
B	-16	SER	-	expression tag	UNP P42765
B	-15	HIS	-	expression tag	UNP P42765
B	-14	HIS	-	expression tag	UNP P42765
B	-13	HIS	-	expression tag	UNP P42765
B	-12	HIS	-	expression tag	UNP P42765
B	-11	HIS	-	expression tag	UNP P42765
B	-10	HIS	-	expression tag	UNP P42765
B	-9	SER	-	expression tag	UNP P42765
B	-8	SER	-	expression tag	UNP P42765
B	-7	GLY	-	expression tag	UNP P42765
B	-6	LEU	-	expression tag	UNP P42765
B	-5	VAL	-	expression tag	UNP P42765
B	-4	PRO	-	expression tag	UNP P42765
B	-3	ARG	-	expression tag	UNP P42765
B	-2	GLY	-	expression tag	UNP P42765
B	-1	SER	-	expression tag	UNP P42765
B	0	HIS	-	expression tag	UNP P42765
C	-19	MET	-	expression tag	UNP P42765
C	-18	GLY	-	expression tag	UNP P42765
C	-17	SER	-	expression tag	UNP P42765
C	-16	SER	-	expression tag	UNP P42765
C	-15	HIS	-	expression tag	UNP P42765
C	-14	HIS	-	expression tag	UNP P42765
C	-13	HIS	-	expression tag	UNP P42765
C	-12	HIS	-	expression tag	UNP P42765
C	-11	HIS	-	expression tag	UNP P42765
C	-10	HIS	-	expression tag	UNP P42765
C	-9	SER	-	expression tag	UNP P42765
C	-8	SER	-	expression tag	UNP P42765
C	-7	GLY	-	expression tag	UNP P42765
C	-6	LEU	-	expression tag	UNP P42765
C	-5	VAL	-	expression tag	UNP P42765
C	-4	PRO	-	expression tag	UNP P42765
C	-3	ARG	-	expression tag	UNP P42765
C	-2	GLY	-	expression tag	UNP P42765
C	-1	SER	-	expression tag	UNP P42765
C	0	HIS	-	expression tag	UNP P42765
D	-19	MET	-	expression tag	UNP P42765
D	-18	GLY	-	expression tag	UNP P42765
D	-17	SER	-	expression tag	UNP P42765

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	expression tag	UNP P42765
D	-15	HIS	-	expression tag	UNP P42765
D	-14	HIS	-	expression tag	UNP P42765
D	-13	HIS	-	expression tag	UNP P42765
D	-12	HIS	-	expression tag	UNP P42765
D	-11	HIS	-	expression tag	UNP P42765
D	-10	HIS	-	expression tag	UNP P42765
D	-9	SER	-	expression tag	UNP P42765
D	-8	SER	-	expression tag	UNP P42765
D	-7	GLY	-	expression tag	UNP P42765
D	-6	LEU	-	expression tag	UNP P42765
D	-5	VAL	-	expression tag	UNP P42765
D	-4	PRO	-	expression tag	UNP P42765
D	-3	ARG	-	expression tag	UNP P42765
D	-2	GLY	-	expression tag	UNP P42765
D	-1	SER	-	expression tag	UNP P42765
D	0	HIS	-	expression tag	UNP P42765

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).
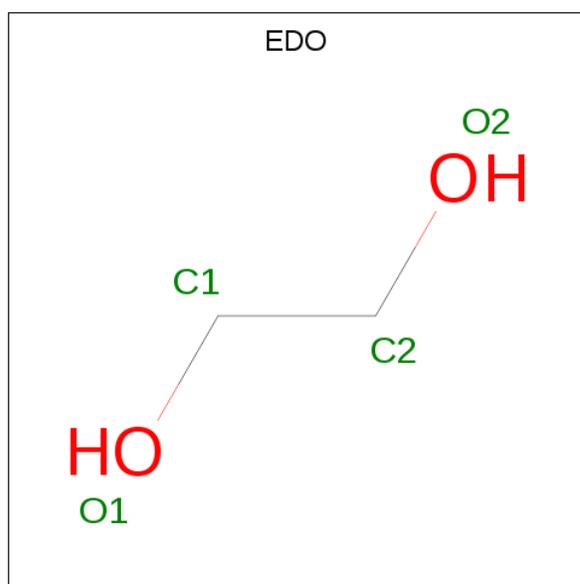
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		
2	A	1	Total	C	O	0	0
			4	2	2		

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

- Molecule 3 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (three-letter code: DTT) (formula: $C_4H_{10}O_2S_2$).

DTT

O3   S4
HO   SH

C3(R)   C4

C1   C2(R)

HS   OH
S1   O2
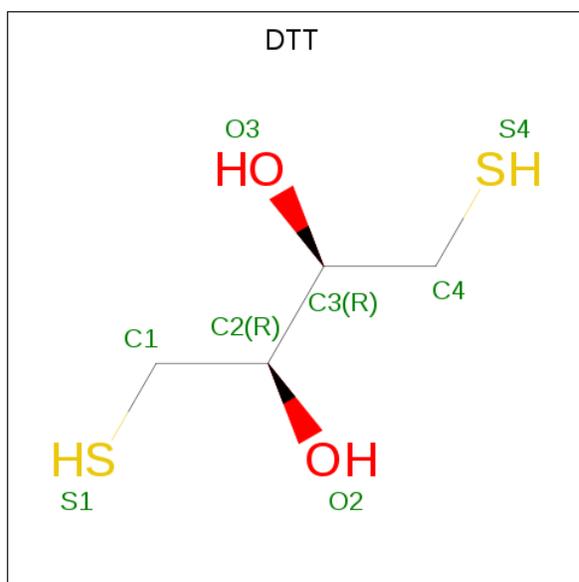
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 8	C 4	O 2	S 2	0	0

- Molecule 4 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).
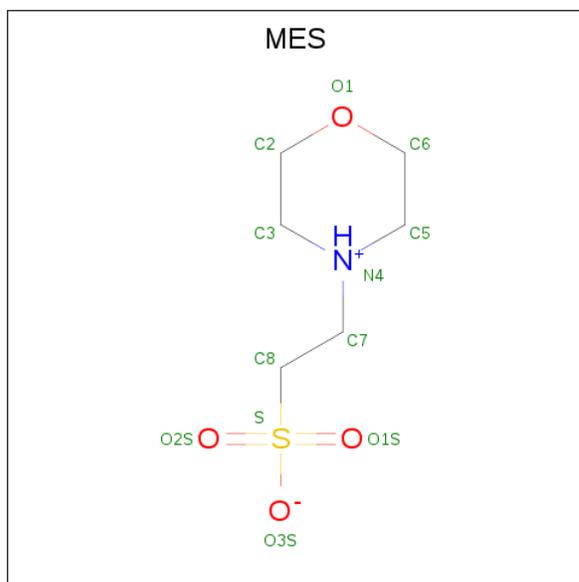
MES

O1
O

C2   C6

C3   H   C5
N+
N4

C7

C8

S

O2S   S   O1S

O-
O3S

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

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

- Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	141	Total	O	0	0
			141	141		
5	B	108	Total	O	0	0
			108	108		
5	C	138	Total	O	0	0
			138	138		
5	D	101	Total	O	0	0
			101	101		

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 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: 3-KETOACYL-COA THIOLASE, MITOCHONDRIAL
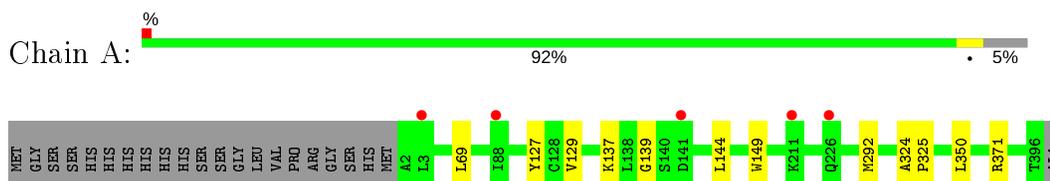
- Molecule 1: 3-KETOACYL-COA THIOLASE, MITOCHONDRIAL
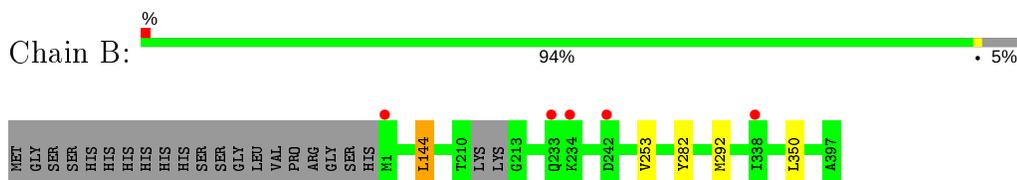
- Molecule 1: 3-KETOACYL-COA THIOLASE, MITOCHONDRIAL
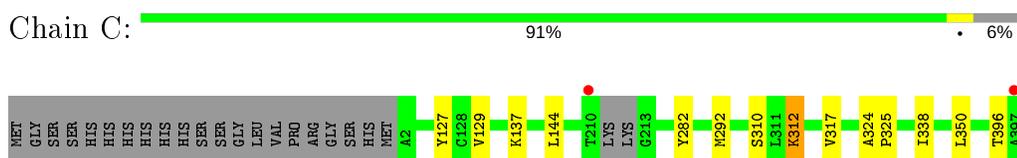
- Molecule 1: 3-KETOACYL-COA THIOLASE, MITOCHONDRIAL
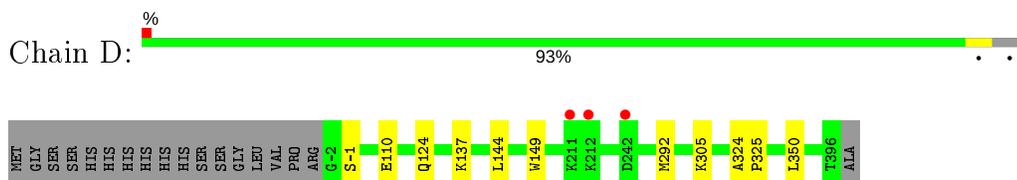
4   Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	54.73Å 196.77Å 79.65Å 90.00° 103.78° 90.00°	Depositor
Resolution (Å)	48.17 – 2.00	Depositor
	48.17 – 2.00	EDS
% Data completeness	99.7 (48.17-2.00)	Depositor
(in resolution range)	99.7 (48.17-2.00)	EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.84 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.195 , 0.229	Depositor
	0.181 , 0.210	DCC
R_{free} test set	5461 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å^2)	21.8	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 51.7	EDS
L-test for twinning[2]	$<|L|> = 0.46$, $<L^2> = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	12340	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.46% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: EDO, MES, DTT

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	0.75	0/2971	0.73	0/4017
1	B	0.72	0/2966	0.74	0/4009
1	C	0.76	0/2958	0.75	0/3999
1	D	0.68	0/3000	0.72	0/4055
All	All	0.73	0/11895	0.74	0/16080

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	396	THR	Peptide

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	2925	0	2974	10	0
1	B	2921	0	2964	3	0
1	C	2913	0	2952	10	0
1	D	2953	0	3001	7	0
2	A	12	0	18	1	0
2	B	20	0	30	1	0
2	C	28	0	42	5	0
2	D	24	0	36	0	0
3	A	8	0	10	3	0
4	A	12	0	13	0	0
4	B	24	0	26	1	0
4	D	12	0	13	0	0
5	A	141	0	0	0	0
5	B	108	0	0	0	0
5	C	138	0	0	0	0
5	D	101	0	0	0	0
All	All	12340	0	12079	27	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 1.

All (27) 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:A:371:ARG:HH12	3:A:1400:DTT:H42	1.17	1.06
1:A:371:ARG:NH1	3:A:1400:DTT:H42	1.85	0.90
1:A:371:ARG:HH12	3:A:1400:DTT:C4	1.96	0.78
1:C:338:ILE:HG12	2:C:1403:EDO:H12	1.68	0.73
1:C:338:ILE:HG12	2:C:1403:EDO:C1	2.22	0.69
1:C:310:SER:OG	1:C:312:LYS:HE2	1.92	0.68
1:D:-1:SER:CB	1:D:305:LYS:HE2	2.32	0.60
1:D:-1:SER:HB3	1:D:305:LYS:HE2	1.87	0.55
1:B:144:LEU:CD1	1:C:144:LEU:HD13	2.39	0.52
1:C:127:TYR:HB3	1:C:144:LEU:HG	1.93	0.51
1:A:149:TRP:CE2	2:A:1397:EDO:H12	2.47	0.50
1:A:127:TYR:HB3	1:A:144:LEU:HG	1.93	0.49
1:C:317:VAL:HG21	2:C:1400:EDO:H21	1.98	0.46
2:C:1402:EDO:H11	1:D:124:GLN:HG2	1.98	0.45
1:B:253:VAL:HB	4:B:1403:MES:H21	1.99	0.45
1:C:282:TYR:OH	1:D:110:GLU:OE2	2.27	0.45
1:C:317:VAL:HG21	2:C:1400:EDO:C2	2.48	0.43
1:A:129:VAL:CG2	1:A:144:LEU:HD12	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:ALA:N	1:C:325:PRO:HD2	2.34	0.43
1:A:324:ALA:N	1:A:325:PRO:HD2	2.34	0.42
1:C:129:VAL:CG2	1:C:144:LEU:HD12	2.50	0.41
1:D:324:ALA:N	1:D:325:PRO:HD2	2.35	0.41
1:A:69:LEU:HD23	1:A:69:LEU:C	2.41	0.41
1:A:129:VAL:HG22	1:A:144:LEU:HD12	2.03	0.41
1:A:139:GLY:HA2	1:D:149:TRP:CG	2.56	0.41
1:B:282:TYR:CZ	2:B:1400:EDO:H21	2.56	0.40
1:D:-1:SER:HB2	1:D:305:LYS:HE2	2.04	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	393/417 (94%)	387 (98%)	6 (2%)	0	100	100
1	B	391/417 (94%)	385 (98%)	6 (2%)	0	100	100
1	C	390/417 (94%)	383 (98%)	7 (2%)	0	100	100
1	D	397/417 (95%)	391 (98%)	6 (2%)	0	100	100
All	All	1571/1668 (94%)	1546 (98%)	25 (2%)	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	310/328 (94%)	307 (99%)	3 (1%)	76	81
1	B	309/328 (94%)	306 (99%)	3 (1%)	76	81
1	C	308/328 (94%)	304 (99%)	4 (1%)	69	74
1	D	313/328 (95%)	309 (99%)	4 (1%)	69	74
All	All	1240/1312 (94%)	1226 (99%)	14 (1%)	73	78

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	LYS
1	A	292	MET
1	A	350	LEU
1	B	144	LEU
1	B	292	MET
1	B	350	LEU
1	C	137	LYS
1	C	292	MET
1	C	312	LYS
1	C	350	LEU
1	D	137	LYS
1	D	144	LEU
1	D	292	MET
1	D	350	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

26 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	EDO	C	1400	-	3,3,3	0.32	0	2,2,2	0.31	0
2	EDO	B	1402	-	3,3,3	0.45	0	2,2,2	0.29	0
2	EDO	C	1401	-	3,3,3	0.75	0	2,2,2	0.36	0
4	MES	D	1403	-	12,12,12	1.77	1 (8%)	14,16,16	1.80	1 (7%)
2	EDO	D	1402	-	3,3,3	0.43	0	2,2,2	0.62	0
2	EDO	C	1403	-	3,3,3	0.51	0	2,2,2	0.51	0
2	EDO	C	1404	-	3,3,3	0.37	0	2,2,2	0.33	0
2	EDO	B	1398	-	3,3,3	0.58	0	2,2,2	0.27	0
2	EDO	A	1398	-	3,3,3	0.30	0	2,2,2	0.34	0
2	EDO	C	1398	-	3,3,3	0.44	0	2,2,2	0.41	0
4	MES	B	1404	-	12,12,12	1.94	1 (8%)	14,16,16	1.61	2 (14%)
2	EDO	C	1399	-	3,3,3	0.43	0	2,2,2	0.39	0
2	EDO	B	1401	-	3,3,3	0.66	0	2,2,2	0.22	0
2	EDO	B	1400	-	3,3,3	0.56	0	2,2,2	0.72	0
2	EDO	A	1399	-	3,3,3	0.24	0	2,2,2	0.55	0
2	EDO	B	1399	-	3,3,3	0.39	0	2,2,2	0.30	0
2	EDO	D	1399	-	3,3,3	0.44	0	2,2,2	0.24	0
3	DTT	A	1400	-	7,7,7	0.73	0	4,8,8	1.52	1 (25%)
2	EDO	D	1401	-	3,3,3	0.42	0	2,2,2	0.27	0
4	MES	A	1401	-	12,12,12	2.09	1 (8%)	14,16,16	2.01	5 (35%)
2	EDO	D	1398	-	3,3,3	0.35	0	2,2,2	0.47	0
4	MES	B	1403	-	12,12,12	1.64	1 (8%)	14,16,16	2.04	5 (35%)
2	EDO	D	1400	-	3,3,3	0.23	0	2,2,2	0.21	0
2	EDO	C	1402	-	3,3,3	0.49	0	2,2,2	0.48	0
2	EDO	A	1397	-	3,3,3	0.54	0	2,2,2	0.42	0
2	EDO	D	1397	-	3,3,3	0.67	0	2,2,2	0.16	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
2	EDO	C	1400	-	-	1/1/1/1	-
2	EDO	B	1402	-	-	0/1/1/1	-
2	EDO	C	1401	-	-	1/1/1/1	-
4	MES	D	1403	-	-	0/6/14/14	0/1/1/1
2	EDO	D	1402	-	-	0/1/1/1	-
2	EDO	C	1403	-	-	0/1/1/1	-
2	EDO	C	1404	-	-	1/1/1/1	-
2	EDO	B	1398	-	-	1/1/1/1	-
2	EDO	A	1398	-	-	0/1/1/1	-
2	EDO	C	1398	-	-	1/1/1/1	-
4	MES	B	1404	-	-	0/6/14/14	0/1/1/1
2	EDO	C	1399	-	-	1/1/1/1	-
2	EDO	B	1401	-	-	1/1/1/1	-
2	EDO	B	1400	-	-	0/1/1/1	-
2	EDO	A	1399	-	-	0/1/1/1	-
2	EDO	B	1399	-	-	1/1/1/1	-
2	EDO	D	1399	-	-	0/1/1/1	-
3	DTT	A	1400	-	-	4/8/8/8	-
2	EDO	D	1401	-	-	0/1/1/1	-
4	MES	A	1401	-	-	2/6/14/14	0/1/1/1
2	EDO	D	1398	-	-	0/1/1/1	-
4	MES	B	1403	-	-	4/6/14/14	0/1/1/1
2	EDO	D	1400	-	-	0/1/1/1	-
2	EDO	C	1402	-	-	1/1/1/1	-
2	EDO	A	1397	-	-	1/1/1/1	-
2	EDO	D	1397	-	-	0/1/1/1	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1401	MES	C8-S	-6.76	1.67	1.77
4	B	1404	MES	C8-S	-6.36	1.68	1.77
4	D	1403	MES	C8-S	-5.54	1.69	1.77
4	B	1403	MES	C8-S	-5.02	1.70	1.77

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1403	MES	O3S-S-C8	5.93	115.35	105.77
4	B	1404	MES	O3S-S-C8	4.89	113.67	105.77
4	A	1401	MES	O2S-S-C8	4.12	111.87	106.92
4	B	1403	MES	C6-C5-N4	3.51	115.42	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	1403	MES	O2S-S-C8	3.24	110.81	106.92
4	B	1403	MES	O3S-S-C8	3.09	110.76	105.77
4	A	1401	MES	O1-C2-C3	3.06	118.54	111.80
4	A	1401	MES	C6-O1-C2	2.93	119.66	109.89
4	B	1403	MES	O1S-S-C8	2.87	110.37	106.92
4	B	1403	MES	O2S-S-O1S	-2.70	104.61	113.95
3	A	1400	DTT	C2-C1-S1	-2.67	106.71	114.47
4	A	1401	MES	O2S-S-O1S	-2.38	105.72	113.95
4	B	1404	MES	O3S-S-O1S	-2.09	106.18	111.27
4	A	1401	MES	C7-N4-C3	2.04	116.45	111.23

There are no chirality outliers.

All (20) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1400	DTT	C1-C2-C3-O3
3	A	1400	DTT	C1-C2-C3-C4
3	A	1400	DTT	O2-C2-C3-O3
3	A	1400	DTT	O2-C2-C3-C4
4	A	1401	MES	C8-C7-N4-C3
4	B	1403	MES	C7-C8-S-O1S
4	B	1403	MES	C7-C8-S-O2S
4	B	1403	MES	C7-C8-S-O3S
2	C	1400	EDO	O1-C1-C2-O2
4	B	1403	MES	N4-C7-C8-S
4	A	1401	MES	C8-C7-N4-C5
2	C	1401	EDO	O1-C1-C2-O2
2	C	1404	EDO	O1-C1-C2-O2
2	B	1399	EDO	O1-C1-C2-O2
2	C	1398	EDO	O1-C1-C2-O2
2	C	1399	EDO	O1-C1-C2-O2
2	B	1401	EDO	O1-C1-C2-O2
2	C	1402	EDO	O1-C1-C2-O2
2	A	1397	EDO	O1-C1-C2-O2
2	B	1398	EDO	O1-C1-C2-O2

There are no ring outliers.

7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1400	EDO	2	0

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Full wwPDB X-ray Structure Validation Report

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1403	EDO	2	0
2	B	1400	EDO	1	0
3	A	1400	DTT	3	0
4	B	1403	MES	1	0
2	C	1402	EDO	1	0
2	A	1397	EDO	1	0

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(Å²)	Q<0.9
1	A	395/417 (94%)	-0.23	5 (1%)	77	76	12, 20, 37, 64	0
1	B	395/417 (94%)	-0.05	5 (1%)	77	76	13, 22, 39, 56	0
1	C	394/417 (94%)	-0.29	2 (0%)	91	90	12, 20, 37, 58	0
1	D	399/417 (95%)	-0.25	3 (0%)	86	85	14, 23, 40, 66	0
All	All	1583/1668 (94%)	-0.20	15 (0%)	84	83	12, 21, 38, 66	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	210	THR	4.6
1	B	338	ILE	3.9
1	C	397	ALA	3.8
1	A	211	LYS	3.6
1	D	211	LYS	3.2
1	D	242	ASP	2.7
1	B	233	GLN	2.6
1	B	1	MET	2.6
1	B	242	ASP	2.5
1	A	88	ILE	2.4
1	A	141	ASP	2.3
1	B	234	LYS	2.3
1	D	212	LYS	2.1
1	A	226	GLN	2.1
1	A	3	LEU	2.1

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 carbohydrates 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	EDO	B	1401	4/4	0.71	0.18	37,38,39,46	0
3	DTT	A	1400	8/8	0.78	0.39	46,53,61,66	0
2	EDO	B	1402	4/4	0.83	0.16	40,41,42,45	0
2	EDO	C	1402	4/4	0.85	0.20	41,44,47,47	0
2	EDO	C	1404	4/4	0.86	0.28	33,39,40,45	0
4	MES	D	1403	12/12	0.88	0.26	33,43,51,51	0
2	EDO	D	1402	4/4	0.90	0.17	43,44,47,49	0
2	EDO	C	1401	4/4	0.91	0.22	24,28,32,35	0
4	MES	B	1404	12/12	0.91	0.17	32,41,47,55	0
2	EDO	D	1401	4/4	0.91	0.15	35,41,41,42	0
2	EDO	C	1399	4/4	0.91	0.13	34,37,42,47	0
2	EDO	C	1400	4/4	0.93	0.24	27,29,29,30	0
2	EDO	C	1403	4/4	0.93	0.14	37,37,38,44	0
4	MES	A	1401	12/12	0.93	0.24	33,37,42,44	0
2	EDO	D	1398	4/4	0.93	0.17	29,33,34,34	0
4	MES	B	1403	12/12	0.93	0.18	36,40,46,54	0
2	EDO	D	1400	4/4	0.93	0.15	30,33,34,34	0
2	EDO	B	1400	4/4	0.93	0.13	28,32,34,35	0
2	EDO	A	1397	4/4	0.93	0.14	21,22,23,23	0
2	EDO	B	1398	4/4	0.94	0.08	27,31,32,34	0
2	EDO	B	1399	4/4	0.95	0.15	30,32,33,34	0
2	EDO	D	1399	4/4	0.96	0.12	25,31,34,39	0
2	EDO	A	1399	4/4	0.96	0.14	28,30,30,32	0
2	EDO	C	1398	4/4	0.96	0.09	24,25,26,29	0
2	EDO	A	1398	4/4	0.97	0.06	28,28,30,30	0
2	EDO	D	1397	4/4	0.97	0.11	25,25,27,28	0

6.5 Other polymers (i)

There are no such residues in this entry.