



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 12:35 PM UTC

PDB ID : 3HPY / pdb_00003hpy
Title : Crystal Structure Analysis of the 2,3-dioxygenase LapB from Pseudomonas in the complex with 4-methylcatechol
Authors : Cho, J.-H.; Rhee, S.
Deposited on : 2009-06-05
Resolution : 1.94 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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
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

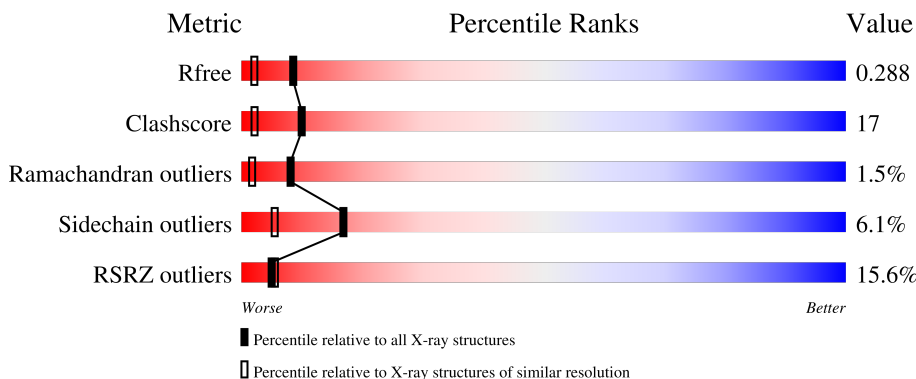
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.94 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	1452 (1.94-1.94)
Clashscore	190562	1494 (1.94-1.94)
Ramachandran outliers	187476	1479 (1.94-1.94)
Sidechain outliers	187428	1479 (1.94-1.94)
RSRZ outliers	180081	1453 (1.94-1.94)

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	309	 11% 60% 29% 7%
1	B	309	 11% 61% 27% 5% 7%
1	C	309	 21% 58% 34% 5% 5%
1	D	309	 16% 57% 33% 5% 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MCT	A	311	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9706 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.

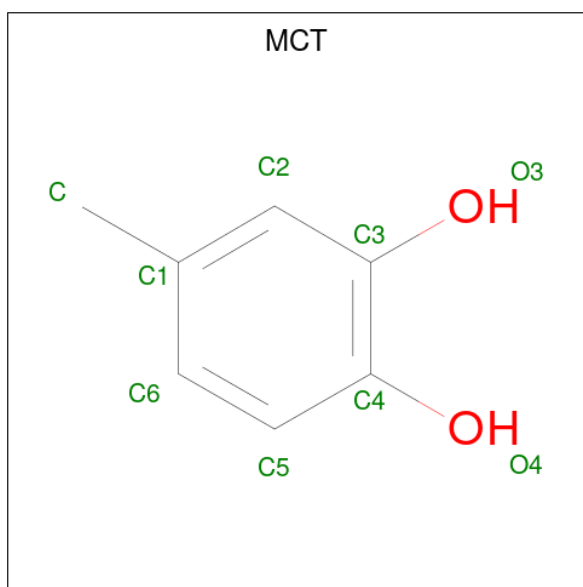
- Molecule 1 is a protein called Catechol 2,3-dioxygenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	288	2300	1464	392	431	13	0	0	0
1	B	288	2300	1464	392	431	13	0	0	0
1	C	296	2362	1503	402	444	13	0	0	0
1	D	296	2362	1503	402	444	13	0	0	0

- Molecule 2 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Fe 1 1	0	0
2	B	1	Total Fe 1 1	0	0
2	C	1	Total Fe 1 1	0	0
2	D	1	Total Fe 1 1	0	0

- Molecule 3 is 4-METHYLCATECHOL (CCD ID: MCT) (formula: C₇H₈O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 9 7 2	0	0
3	B	1	Total C O 9 7 2	0	0
3	C	1	Total C O 9 7 2	0	0

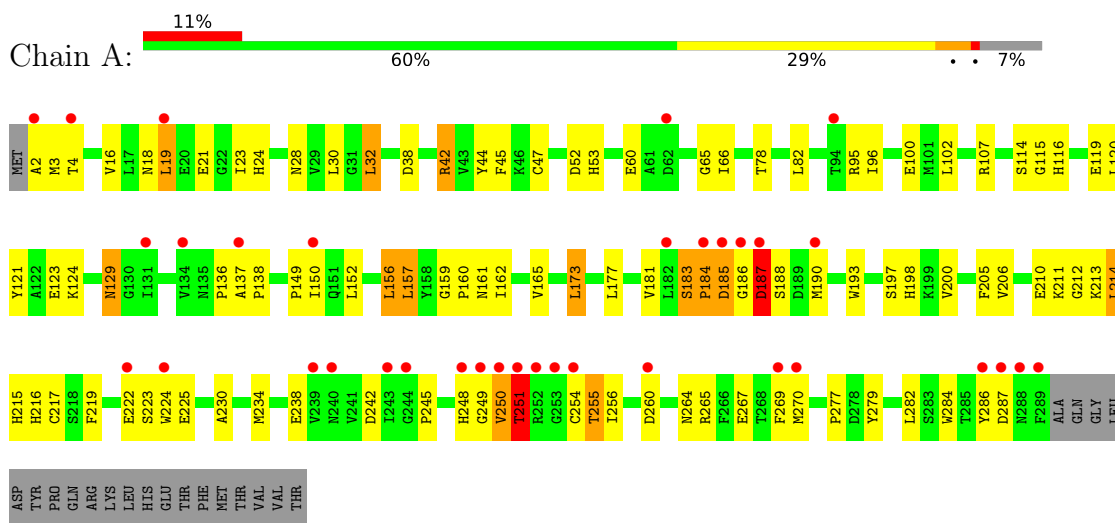
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	95	Total O 95 95	0	0
4	B	102	Total O 102 102	0	0
4	C	80	Total O 80 80	0	0
4	D	74	Total O 74 74	0	0

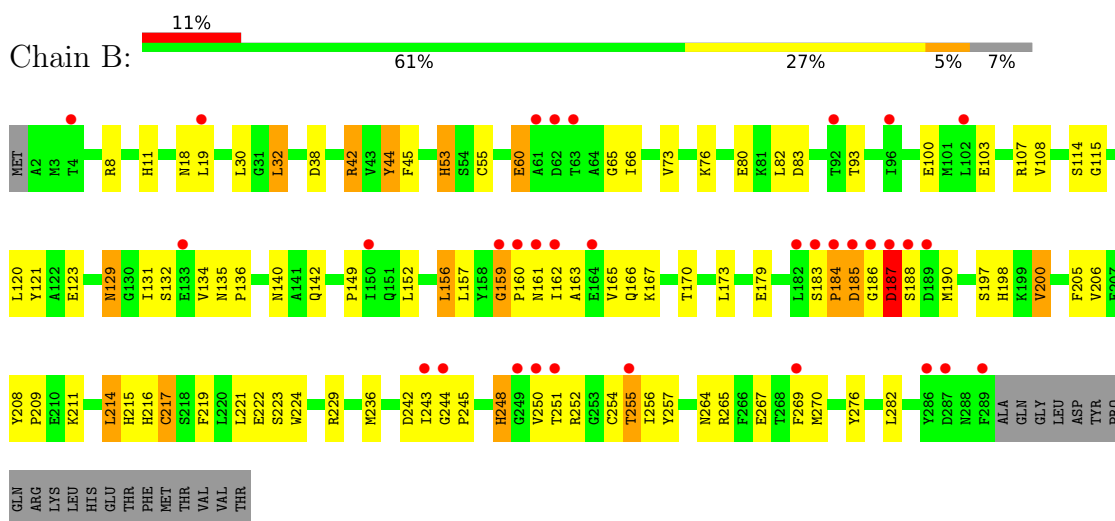
3 Residue-property plots [i](#)

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

- Molecule 1: Catechol 2,3-dioxygenase

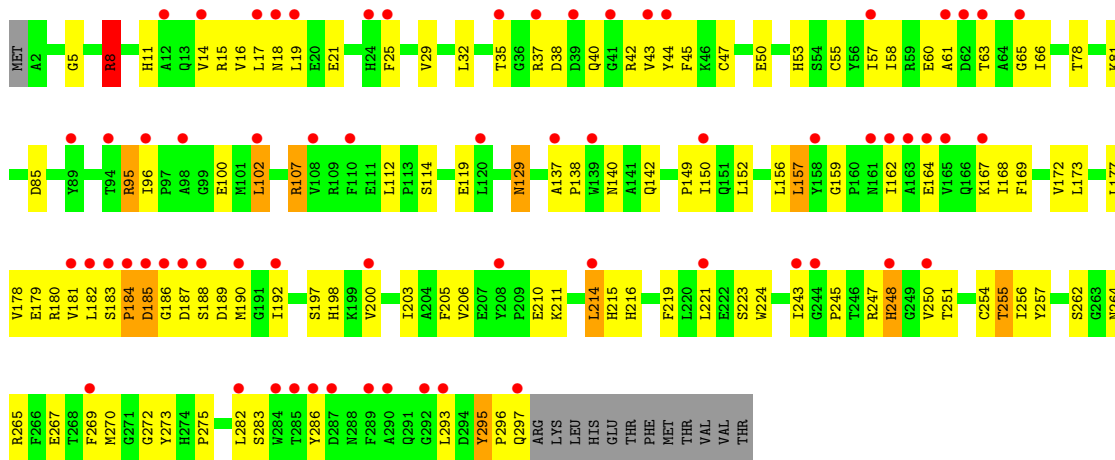


- Molecule 1: Catechol 2,3-dioxygenase

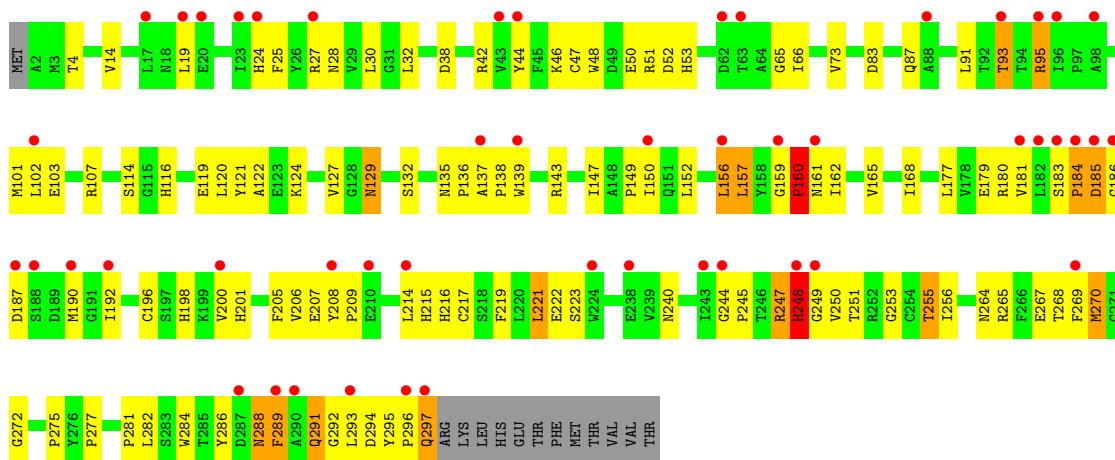


- Molecule 1: Catechol 2,3-dioxygenase





• Molecule 1: Catechol 2,3-dioxygenase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	96.10Å 97.60Å 133.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.94 50.00 – 1.94	Depositor EDS
% Data completeness (in resolution range)	78.4 (50.00-1.94) 94.6 (50.00-1.94)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 1.94Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.244 , 0.278 0.255 , 0.288	Depositor DCC
R_{free} test set	9350 reflections (9.98%)	wwPDB-VP
Wilson B-factor (Å ²)	27.7	Xtrriage
Anisotropy	0.028	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 36.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	0.025 for k,h,-l	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9706	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.18 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 9.8029e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: MCT, FE

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	0.52	0/2363	1.10	12/3210 (0.4%)
1	B	0.50	0/2363	1.06	15/3210 (0.5%)
1	C	0.46	0/2427	1.02	10/3298 (0.3%)
1	D	0.58	2/2427 (0.1%)	1.04	12/3298 (0.4%)
All	All	0.51	2/9580 (0.0%)	1.06	49/13016 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	288	ASN	C-N	-6.92	1.24	1.33
1	D	248	HIS	CA-C	-5.06	1.48	1.53

The worst 5 of 49 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	187	ASP	CA-CB-CG	-10.36	102.24	112.60
1	A	188	SER	N-CA-C	-9.04	97.06	108.45
1	A	183	SER	CA-C-N	8.76	130.79	119.84
1	A	183	SER	C-N-CA	8.76	130.79	119.84
1	C	187	ASP	N-CA-C	8.02	121.57	110.35

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2300	0	2193	87	0
1	B	2300	0	2193	76	0
1	C	2362	0	2248	86	0
1	D	2362	0	2248	94	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
3	A	9	0	6	12	0
3	B	9	0	7	0	0
3	C	9	0	6	1	0
4	A	95	0	0	3	0
4	B	102	0	0	1	0
4	C	80	0	0	0	0
4	D	74	0	0	3	0
All	All	9706	0	8901	318	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 17.

The worst 5 of 318 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:250:VAL:HG23	3:A:311:MCT:H6	1.28	1.07
1:D:150:ILE:HD11	1:D:222:GLU:HG2	1.46	0.95
1:A:193:TRP:HZ2	3:A:311:MCT:C	1.82	0.93
1:D:247:ARG:HG3	1:D:248:HIS:N	1.82	0.92
1:C:215:HIS:HD2	1:C:216:HIS:HD1	1.18	0.90

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	286/309 (93%)	271 (95%)	9 (3%)	6 (2%)	5 1
1	B	286/309 (93%)	270 (94%)	12 (4%)	4 (1%)	9 2
1	C	294/309 (95%)	271 (92%)	21 (7%)	2 (1%)	18 9
1	D	294/309 (95%)	273 (93%)	16 (5%)	5 (2%)	7 1
All	All	1160/1236 (94%)	1085 (94%)	58 (5%)	17 (2%)	8 2

5 of 17 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	184	PRO
1	B	185	ASP
1	B	187	ASP
1	B	244	GLY
1	D	187	ASP

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	245/264 (93%)	227 (93%)	18 (7%)	13 3
1	B	245/264 (93%)	230 (94%)	15 (6%)	17 5
1	C	251/264 (95%)	239 (95%)	12 (5%)	23 10
1	D	251/264 (95%)	235 (94%)	16 (6%)	16 5
All	All	992/1056 (94%)	931 (94%)	61 (6%)	17 5

5 of 61 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	173	LEU
1	D	221	LEU
1	C	95	ARG
1	D	192	ILE

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Mol	Chain	Res	Type
1	D	293	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 37 such sidechains are listed below:

Mol	Chain	Res	Type
1	D	129	ASN
1	D	288	ASN
1	D	166	GLN
1	D	237	ASN
1	B	240	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 7 ligands modelled in this entry, 4 are monoatomic - leaving 3 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	$\# Z > 2$
3	MCT	C	311	2	9,9,9	1.46	2 (22%)	12,12,12	1.07	1 (8%)
3	MCT	B	311	2	9,9,9	1.64	3 (33%)	12,12,12	0.93	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MCT	A	311	2	9,9,9	1.38	1 (11%)	12,12,12	1.10	1 (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
3	MCT	C	311	2	-	-	0/1/1/1
3	MCT	B	311	2	-	-	0/1/1/1
3	MCT	A	311	2	-	-	0/1/1/1

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	311	MCT	C4-C3	2.53	1.44	1.40
3	B	311	MCT	C2-C3	2.21	1.42	1.38
3	B	311	MCT	C5-C4	2.16	1.43	1.39
3	B	311	MCT	C6-C5	2.13	1.42	1.38
3	C	311	MCT	C6-C5	2.12	1.42	1.38

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	311	MCT	C3-C2-C1	-2.19	119.17	121.03
3	A	311	MCT	C3-C2-C1	-2.03	119.30	121.03

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	311	MCT	1	0
3	A	311	MCT	12	0

5.7 Other polymers [i](#)

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	288/309 (93%)	0.79	35 (12%) 8 9	15, 26, 44, 59	0
1	B	288/309 (93%)	0.83	33 (11%) 9 10	16, 27, 39, 58	0
1	C	296/309 (95%)	1.34	65 (21%) 2 2	21, 33, 48, 63	0
1	D	296/309 (95%)	1.08	49 (16%) 4 4	19, 30, 44, 62	0
All	All	1168/1236 (94%)	1.01	182 (15%) 5 5	15, 29, 45, 63	0

The worst 5 of 182 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	244	GLY	8.3
1	A	289	PHE	7.1
1	D	244	GLY	6.5
1	A	2	ALA	6.4
1	A	250	VAL	5.8

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(\AA^2)	Q<0.9
2	FE	D	310	1/1	0.55	0.24	59,59,59,59	0
3	MCT	A	311	9/9	0.74	0.19	51,51,53,53	0
3	MCT	B	311	9/9	0.86	0.16	42,44,47,48	0
3	MCT	C	311	9/9	0.88	0.18	49,50,50,51	0
2	FE	C	310	1/1	0.96	0.05	31,31,31,31	0
2	FE	A	310	1/1	0.97	0.05	33,33,33,33	0
2	FE	B	310	1/1	0.99	0.03	29,29,29,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.