



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 11:08 pm BST

PDB ID : 3FMF
Title : Crystal structure of Mycobacterium tuberculosis dethiobiotin synthetase complexed with 7,8 diaminopelargonic acid carbamate
Authors : Dey, S.; Sacchettini, J.C.
Deposited on : 2008-12-21
Resolution : 2.05 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

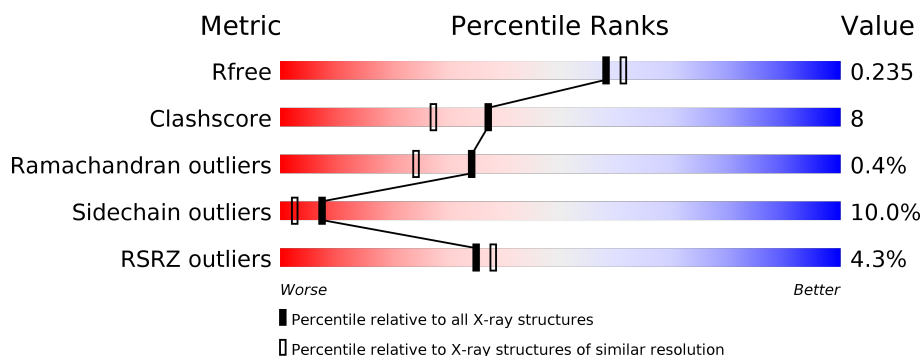
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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 $\leq 5\%$. 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	251	<div> <div>3%</div> <div> <div></div> <div>79%</div> <div>10%</div> <div>•</div> <div>8%</div> </div> </div>
1	B	251	<div> <div>4%</div> <div> <div></div> <div>78%</div> <div>10%</div> <div>•</div> <div>9%</div> </div> </div>
1	C	251	<div> <div>2%</div> <div> <div></div> <div>78%</div> <div>9%</div> <div>•</div> <div>8%</div> </div> </div>
1	D	251	<div> <div>6%</div> <div> <div></div> <div>69%</div> <div>14%</div> <div>5%</div> <div>12%</div> </div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6748 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 Dethiobiotin synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	1	0
			1614	1007	294	305	8			
1	B	228	Total	C	N	O	S	0	2	0
			1600	997	289	305	9			
1	C	230	Total	C	N	O	S	0	0	0
			1609	1005	291	305	8			
1	D	220	Total	C	N	O	S	0	1	0
			1538	962	278	291	7			

There are 100 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-24	MET	-	EXPRESSION TAG	UNP O06620
A	-23	GLY	-	EXPRESSION TAG	UNP O06620
A	-22	SER	-	EXPRESSION TAG	UNP O06620
A	-21	SER	-	EXPRESSION TAG	UNP O06620
A	-20	HIS	-	EXPRESSION TAG	UNP O06620
A	-19	HIS	-	EXPRESSION TAG	UNP O06620
A	-18	HIS	-	EXPRESSION TAG	UNP O06620
A	-17	HIS	-	EXPRESSION TAG	UNP O06620
A	-16	HIS	-	EXPRESSION TAG	UNP O06620
A	-15	HIS	-	EXPRESSION TAG	UNP O06620
A	-14	SER	-	EXPRESSION TAG	UNP O06620
A	-13	SER	-	EXPRESSION TAG	UNP O06620
A	-12	GLY	-	EXPRESSION TAG	UNP O06620
A	-11	LEU	-	EXPRESSION TAG	UNP O06620
A	-10	GLN	-	EXPRESSION TAG	UNP O06620
A	-9	GLY	-	EXPRESSION TAG	UNP O06620
A	-8	THR	-	EXPRESSION TAG	UNP O06620
A	-7	GLU	-	EXPRESSION TAG	UNP O06620
A	-6	ASN	-	EXPRESSION TAG	UNP O06620
A	-5	LEU	-	EXPRESSION TAG	UNP O06620
A	-4	TYR	-	EXPRESSION TAG	UNP O06620

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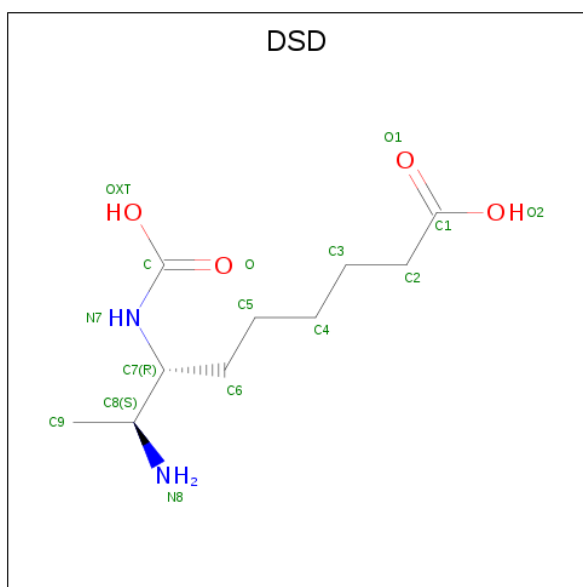
Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	PHE	-	EXPRESSION TAG	UNP O06620
A	-2	GLN	-	EXPRESSION TAG	UNP O06620
A	-1	SER	-	EXPRESSION TAG	UNP O06620
A	0	HIS	-	EXPRESSION TAG	UNP O06620
B	-24	MET	-	EXPRESSION TAG	UNP O06620
B	-23	GLY	-	EXPRESSION TAG	UNP O06620
B	-22	SER	-	EXPRESSION TAG	UNP O06620
B	-21	SER	-	EXPRESSION TAG	UNP O06620
B	-20	HIS	-	EXPRESSION TAG	UNP O06620
B	-19	HIS	-	EXPRESSION TAG	UNP O06620
B	-18	HIS	-	EXPRESSION TAG	UNP O06620
B	-17	HIS	-	EXPRESSION TAG	UNP O06620
B	-16	HIS	-	EXPRESSION TAG	UNP O06620
B	-15	HIS	-	EXPRESSION TAG	UNP O06620
B	-14	SER	-	EXPRESSION TAG	UNP O06620
B	-13	SER	-	EXPRESSION TAG	UNP O06620
B	-12	GLY	-	EXPRESSION TAG	UNP O06620
B	-11	LEU	-	EXPRESSION TAG	UNP O06620
B	-10	GLN	-	EXPRESSION TAG	UNP O06620
B	-9	GLY	-	EXPRESSION TAG	UNP O06620
B	-8	THR	-	EXPRESSION TAG	UNP O06620
B	-7	GLU	-	EXPRESSION TAG	UNP O06620
B	-6	ASN	-	EXPRESSION TAG	UNP O06620
B	-5	LEU	-	EXPRESSION TAG	UNP O06620
B	-4	TYR	-	EXPRESSION TAG	UNP O06620
B	-3	PHE	-	EXPRESSION TAG	UNP O06620
B	-2	GLN	-	EXPRESSION TAG	UNP O06620
B	-1	SER	-	EXPRESSION TAG	UNP O06620
B	0	HIS	-	EXPRESSION TAG	UNP O06620
C	-24	MET	-	EXPRESSION TAG	UNP O06620
C	-23	GLY	-	EXPRESSION TAG	UNP O06620
C	-22	SER	-	EXPRESSION TAG	UNP O06620
C	-21	SER	-	EXPRESSION TAG	UNP O06620
C	-20	HIS	-	EXPRESSION TAG	UNP O06620
C	-19	HIS	-	EXPRESSION TAG	UNP O06620
C	-18	HIS	-	EXPRESSION TAG	UNP O06620
C	-17	HIS	-	EXPRESSION TAG	UNP O06620
C	-16	HIS	-	EXPRESSION TAG	UNP O06620
C	-15	HIS	-	EXPRESSION TAG	UNP O06620
C	-14	SER	-	EXPRESSION TAG	UNP O06620
C	-13	SER	-	EXPRESSION TAG	UNP O06620
C	-12	GLY	-	EXPRESSION TAG	UNP O06620

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	LEU	-	EXPRESSION TAG	UNP O06620
C	-10	GLN	-	EXPRESSION TAG	UNP O06620
C	-9	GLY	-	EXPRESSION TAG	UNP O06620
C	-8	THR	-	EXPRESSION TAG	UNP O06620
C	-7	GLU	-	EXPRESSION TAG	UNP O06620
C	-6	ASN	-	EXPRESSION TAG	UNP O06620
C	-5	LEU	-	EXPRESSION TAG	UNP O06620
C	-4	TYR	-	EXPRESSION TAG	UNP O06620
C	-3	PHE	-	EXPRESSION TAG	UNP O06620
C	-2	GLN	-	EXPRESSION TAG	UNP O06620
C	-1	SER	-	EXPRESSION TAG	UNP O06620
C	0	HIS	-	EXPRESSION TAG	UNP O06620
D	-24	MET	-	EXPRESSION TAG	UNP O06620
D	-23	GLY	-	EXPRESSION TAG	UNP O06620
D	-22	SER	-	EXPRESSION TAG	UNP O06620
D	-21	SER	-	EXPRESSION TAG	UNP O06620
D	-20	HIS	-	EXPRESSION TAG	UNP O06620
D	-19	HIS	-	EXPRESSION TAG	UNP O06620
D	-18	HIS	-	EXPRESSION TAG	UNP O06620
D	-17	HIS	-	EXPRESSION TAG	UNP O06620
D	-16	HIS	-	EXPRESSION TAG	UNP O06620
D	-15	HIS	-	EXPRESSION TAG	UNP O06620
D	-14	SER	-	EXPRESSION TAG	UNP O06620
D	-13	SER	-	EXPRESSION TAG	UNP O06620
D	-12	GLY	-	EXPRESSION TAG	UNP O06620
D	-11	LEU	-	EXPRESSION TAG	UNP O06620
D	-10	GLN	-	EXPRESSION TAG	UNP O06620
D	-9	GLY	-	EXPRESSION TAG	UNP O06620
D	-8	THR	-	EXPRESSION TAG	UNP O06620
D	-7	GLU	-	EXPRESSION TAG	UNP O06620
D	-6	ASN	-	EXPRESSION TAG	UNP O06620
D	-5	LEU	-	EXPRESSION TAG	UNP O06620
D	-4	TYR	-	EXPRESSION TAG	UNP O06620
D	-3	PHE	-	EXPRESSION TAG	UNP O06620
D	-2	GLN	-	EXPRESSION TAG	UNP O06620
D	-1	SER	-	EXPRESSION TAG	UNP O06620
D	0	HIS	-	EXPRESSION TAG	UNP O06620

- Molecule 2 is 7-(CARBOXYAMINO)-8-AMINO-NONANOIC ACID (three-letter code: DSD) (formula: C₁₀H₂₀N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			16	10	2	4		
2	B	1	Total	C	N	O	0	0
			16	10	2	4		
2	C	1	Total	C	N	O	0	0
			16	10	2	4		
2	D	1	Total	C	N	O	0	0
			16	10	2	4		

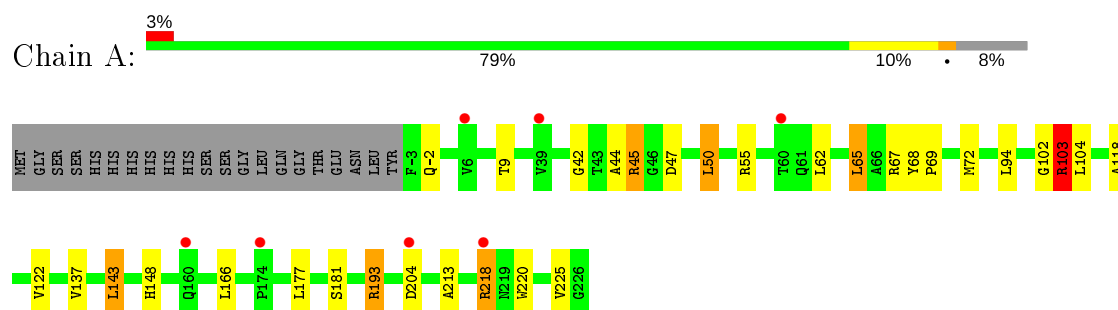
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	98	Total	O	0	0
			98	98		
3	B	76	Total	O	0	0
			76	76		
3	C	93	Total	O	0	0
			93	93		
3	D	56	Total	O	0	0
			56	56		

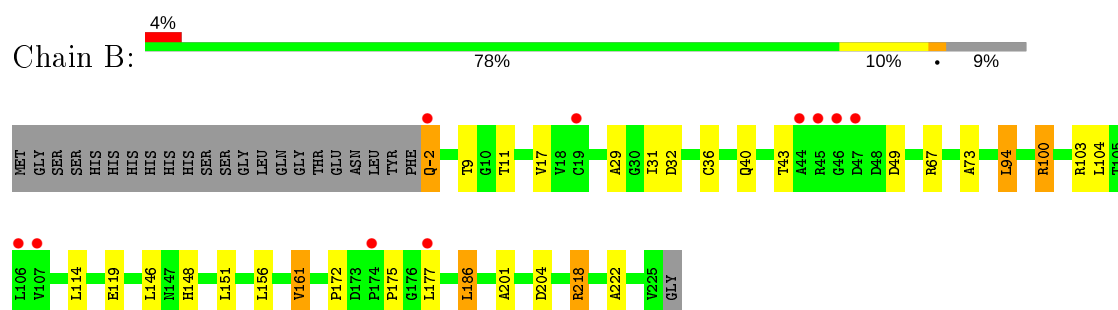
3 Residue-property plots [i](#)

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.

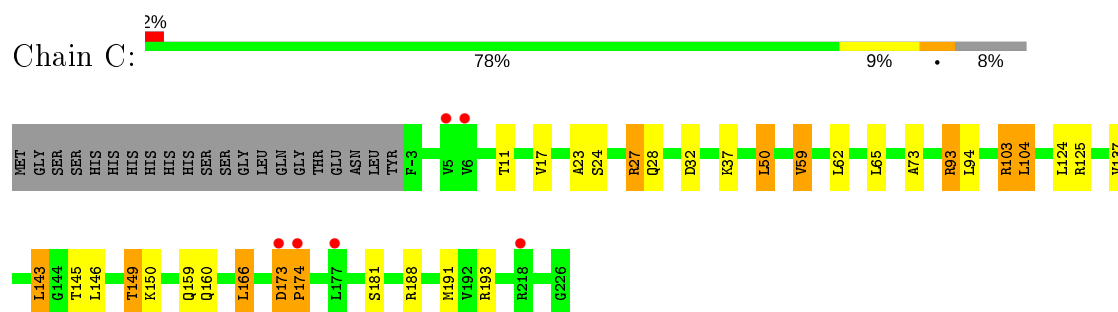
- Molecule 1: Dethiobiotin synthetase



- Molecule 1: Dethiobiotin synthetase

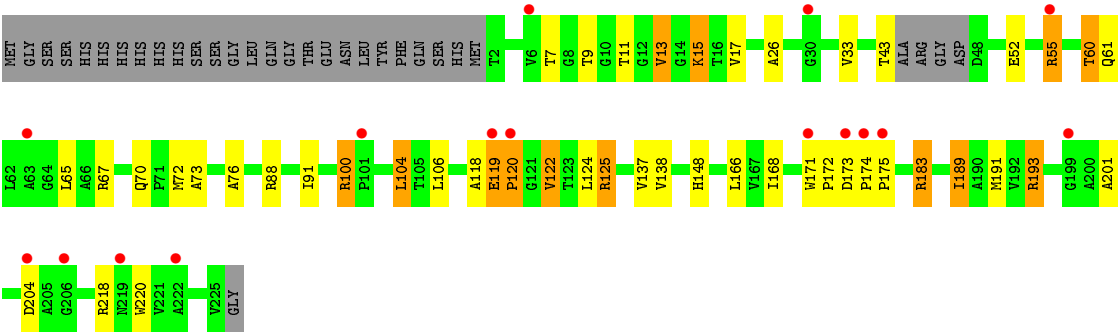


- Molecule 1: Dethiobiotin synthetase



- Molecule 1: Dethiobiotin synthetase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	55.31Å 103.75Å 151.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.07 – 2.05 29.08 – 2.05	Depositor EDS
% Data completeness (in resolution range)	91.6 (29.07-2.05) 91.6 (29.08-2.05)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.20 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.195 , 0.237 0.197 , 0.235	Depositor DCC
R_{free} test set	2554 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	24.4	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 45.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6748	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.42	0/1633	0.63	1/2230 (0.0%)
1	B	0.42	0/1620	0.61	0/2214
1	C	0.42	0/1622	0.63	0/2216
1	D	0.42	0/1554	0.68	2/2124 (0.1%)
All	All	0.42	0/6429	0.64	3/8784 (0.0%)

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.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	D	125	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	D	125	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	A	103	ARG	NE-CZ-NH2	-5.35	117.62	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	173	ASP	Peptide

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	1614	0	1659	20	0
1	B	1600	0	1643	22	0
1	C	1609	0	1654	22	0
1	D	1538	0	1589	38	0
2	A	16	0	18	2	0
2	B	16	0	18	0	0
2	C	16	0	18	2	0
2	D	16	0	18	2	0
3	A	98	0	0	1	0
3	B	76	0	0	1	0
3	C	93	0	0	2	0
3	D	56	0	0	1	0
All	All	6748	0	6617	102	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 8.

All (102) 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:D:88[B]:ARG:HH11	1:D:88[B]:ARG:HG2	1.00	1.10
1:B:40:GLN:NE2	1:B:49:ASP:H	1.51	1.08
1:D:100:ARG:HH11	1:D:100:ARG:HG3	1.23	1.02
1:B:100:ARG:HH11	1:B:100:ARG:HG3	1.23	0.97
1:B:40:GLN:HE22	1:B:49:ASP:N	1.64	0.95
1:B:40:GLN:HE22	1:B:49:ASP:H	0.90	0.89
1:D:88[B]:ARG:NH1	1:D:88[B]:ARG:HG2	1.79	0.89
1:D:100:ARG:HH11	1:D:100:ARG:CG	1.86	0.89
1:B:100:ARG:HH11	1:B:100:ARG:CG	1.85	0.88
1:A:225:VAL:HG12	1:A:225:VAL:O	1.76	0.82
1:D:13:VAL:HG13	1:D:138:VAL:HG12	1.62	0.81
1:B:-2:GLN:HE21	1:B:-2:GLN:HA	1.44	0.80
1:C:23:ALA:O	1:C:27:ARG:HG2	1.84	0.76
1:B:100:ARG:HG3	1:B:100:ARG:NH1	1.96	0.76
1:A:218:ARG:HE	1:A:218:ARG:HA	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:MET:CE	1:D:76:ALA:HB1	2.19	0.72
1:A:225:VAL:CG1	1:A:225:VAL:O	2.36	0.72
1:A:42:GLY:O	1:A:45:ARG:HG3	1.90	0.70
1:B:17:VAL:HG21	1:B:201:ALA:HB2	1.73	0.70
1:D:26:ALA:HB3	1:D:33:VAL:HG21	1.75	0.68
1:C:103:ARG:HG3	1:C:104:LEU:N	2.12	0.64
1:B:156:LEU:HD22	1:B:161:VAL:HG22	1.80	0.64
1:A:102:GLY:O	1:A:225:VAL:HG11	1.98	0.64
1:A:218:ARG:NE	1:A:218:ARG:HA	2.11	0.63
1:D:100:ARG:HG3	1:D:100:ARG:NH1	2.04	0.63
1:D:104:LEU:HD11	1:D:106:LEU:HD21	1.80	0.63
1:D:60:THR:HG23	1:D:61:GLN:OE1	1.98	0.62
1:D:43:THR:HG21	1:D:67:ARG:HB3	1.79	0.62
1:C:145:THR:O	1:C:149:THR:CG2	2.47	0.61
1:A:45:ARG:HD2	1:A:47:ASP:OD1	2.02	0.59
1:D:61:GLN:NE2	3:D:280:HOH:O	2.35	0.59
1:C:32:ASP:OD1	1:C:103:ARG:HD3	2.04	0.58
1:D:17:VAL:HG21	1:D:201:ALA:HB2	1.86	0.57
1:A:9:THR:HB	1:A:148:HIS:HB3	1.86	0.57
1:D:193:ARG:HG2	1:D:220:TRP:CH2	2.39	0.57
1:D:72:MET:CE	1:D:76:ALA:CB	2.82	0.57
1:D:52:GLU:HA	1:D:55:ARG:HD3	1.88	0.56
1:B:43:THR:HG21	1:B:67:ARG:HB3	1.88	0.56
1:C:143:LEU:HD22	2:C:250:DSD:H32	1.89	0.55
1:D:60:THR:CG2	1:D:61:GLN:OE1	2.55	0.55
1:D:72:MET:HE3	1:D:76:ALA:HB1	1.87	0.55
1:D:13:VAL:CG1	1:D:138:VAL:HG12	2.35	0.54
1:B:40:GLN:NE2	1:B:49:ASP:N	2.35	0.54
1:C:125:ARG:HD2	1:C:159:GLN:HG3	1.89	0.54
1:C:188:ARG:NH2	3:C:270:HOH:O	2.41	0.53
1:C:145:THR:O	1:C:149:THR:HG23	2.07	0.53
1:A:50:LEU:HG	1:A:62:LEU:HB3	1.91	0.53
1:C:145:THR:O	1:C:149:THR:HG22	2.08	0.53
1:D:91:ILE:HD12	1:D:118:ALA:HB2	1.91	0.52
1:A:44:ALA:HB2	1:A:69:PRO:HB3	1.90	0.52
1:C:37:LYS:HB3	1:C:50:LEU:CD2	2.40	0.52
1:D:100:ARG:NH1	1:D:100:ARG:CG	2.55	0.51
1:D:9:THR:HB	1:D:148:HIS:HB3	1.93	0.51
1:D:118:ALA:HB3	1:D:122:VAL:HG13	1.92	0.51
1:D:104:LEU:CD1	1:D:106:LEU:HD21	2.41	0.51
1:A:102:GLY:HA2	1:A:225:VAL:HG13	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:65:LEU:HB2	1:A:94:LEU:HD22	1.92	0.50
1:C:146:LEU:O	1:C:150:LYS:HD3	2.11	0.50
1:D:72:MET:HE2	1:D:76:ALA:CB	2.43	0.49
1:C:37:LYS:HB3	1:C:50:LEU:HD22	1.94	0.49
1:B:9:THR:HB	1:B:148:HIS:HB3	1.94	0.49
1:B:119:GLU:HA	1:B:119:GLU:OE2	2.12	0.49
1:A:193:ARG:HG2	1:A:220:TRP:CH2	2.48	0.49
3:A:312:HOH:O	1:B:11:THR:HG23	2.12	0.48
1:D:168:ILE:CD1	1:D:183:ARG:HG2	2.43	0.48
1:B:36:CYS:SG	1:B:94:LEU:HD13	2.54	0.47
1:C:73:ALA:HB2	2:D:250:DSD:H21	1.97	0.47
1:A:218:ARG:HE	1:A:218:ARG:CA	2.25	0.47
1:A:213:ALA:HA	1:A:218:ARG:HH22	1.80	0.47
1:C:59:VAL:HG22	1:C:62:LEU:HD21	1.97	0.47
1:B:172:PRO:HG2	1:B:175:PRO:HA	1.97	0.46
1:C:191:MET:HG2	1:C:193:ARG:NH2	2.31	0.45
1:B:31:ILE:HD11	1:B:222:ALA:HA	1.98	0.45
1:D:70:GLN:HB3	1:D:72:MET:HG3	1.99	0.45
1:D:171:TRP:HA	1:D:172:PRO:HD3	1.83	0.44
1:A:68:TYR:HA	1:A:69:PRO:HD3	1.87	0.43
1:D:26:ALA:HB3	1:D:33:VAL:CG2	2.44	0.43
1:A:118:ALA:HB3	1:A:122:VAL:HB	2.00	0.43
1:C:73:ALA:HA	2:D:250:DSD:H41	1.99	0.43
1:A:103:ARG:HG3	1:A:104:LEU:N	2.34	0.43
1:C:11:THR:HG22	3:C:245:HOH:O	2.19	0.42
2:C:250:DSD:H41	1:D:73:ALA:HA	2.00	0.42
1:C:93:ARG:HB2	1:C:93:ARG:NH2	2.35	0.42
1:C:65:LEU:HB2	1:C:94:LEU:HD22	2.02	0.42
1:C:125:ARG:CD	1:C:159:GLN:HG3	2.48	0.42
1:D:119:GLU:HA	1:D:120:PRO:HA	1.81	0.42
1:C:24:SER:O	1:C:28:GLN:HG3	2.20	0.42
1:A:143:LEU:HD22	2:A:250:DSD:H32	2.01	0.42
1:B:17:VAL:HG23	3:B:286:HOH:O	2.20	0.41
1:B:29:ALA:HA	1:B:218:ARG:NH1	2.35	0.41
1:D:7:THR:C	1:D:15:LYS:HD2	2.40	0.41
1:B:100:ARG:CG	1:B:100:ARG:NH1	2.57	0.41
1:B:146:LEU:HD23	1:B:186:LEU:HD13	2.01	0.41
1:C:137:VAL:HB	1:C:166:LEU:HD12	2.03	0.41
1:D:173:ASP:HA	1:D:174:PRO:HA	1.83	0.41
1:D:218:ARG:HG3	1:D:218:ARG:O	2.20	0.41
1:D:189:ILE:HG12	1:D:189:ILE:H	1.81	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:250:DSD:H41	1:B:73:ALA:HA	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	228/251 (91%)	222 (97%)	6 (3%)	0	100	100
1	B	227/251 (90%)	221 (97%)	6 (3%)	0	100	100
1	C	227/251 (90%)	222 (98%)	4 (2%)	1 (0%)	34	24
1	D	216/251 (86%)	209 (97%)	4 (2%)	3 (1%)	11	3
All	All	898/1004 (89%)	874 (97%)	20 (2%)	4 (0%)	34	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	174	PRO
1	D	204	ASP
1	D	175	PRO
1	D	120	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	156/173 (90%)	141 (90%)	15 (10%)	8	3
1	B	156/173 (90%)	143 (92%)	13 (8%)	11	5
1	C	155/173 (90%)	140 (90%)	15 (10%)	8	3
1	D	149/173 (86%)	131 (88%)	18 (12%)	5	1
All	All	616/692 (89%)	555 (90%)	61 (10%)	7	3

All (61) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	-2	GLN
1	A	45	ARG
1	A	50	LEU
1	A	65	LEU
1	A	67	ARG
1	A	72	MET
1	A	103	ARG
1	A	137	VAL
1	A	143	LEU
1	A	166	LEU
1	A	177	LEU
1	A	181	SER
1	A	193	ARG
1	A	204	ASP
1	A	218	ARG
1	B	-2	GLN
1	B	32	ASP
1	B	94	LEU
1	B	100	ARG
1	B	103	ARG
1	B	104	LEU
1	B	114	LEU
1	B	151	LEU
1	B	161	VAL
1	B	177	LEU
1	B	186	LEU
1	B	204	ASP
1	B	218	ARG
1	C	17	VAL
1	C	27	ARG
1	C	50	LEU
1	C	59	VAL
1	C	93	ARG

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Mol	Chain	Res	Type
1	C	103	ARG
1	C	104	LEU
1	C	124	LEU
1	C	143	LEU
1	C	149	THR
1	C	160	GLN
1	C	166	LEU
1	C	173	ASP
1	C	174	PRO
1	C	181	SER
1	D	11	THR
1	D	13	VAL
1	D	15	LYS
1	D	55	ARG
1	D	60	THR
1	D	65	LEU
1	D	100	ARG
1	D	104	LEU
1	D	119	GLU
1	D	122	VAL
1	D	124	LEU
1	D	125	ARG
1	D	137	VAL
1	D	166	LEU
1	D	183	ARG
1	D	189	ILE
1	D	191	MET
1	D	193	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	HIS
1	B	-2	GLN
1	B	40	GLN
1	C	28	GLN
1	D	80	HIS

5.3.3 RNA ⓘ

There are no RNA molecules 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	CSX	C	163	1	3,6,7	1.96	1 (33%)	1,6,8	1.84	0
1	CSX	B	163	1	3,6,7	3.61	1 (33%)	1,6,8	2.99	1 (100%)
1	CSX	D	163	1	3,6,7	0.94	0	1,6,8	1.29	0
1	CSX	A	163	1	3,6,7	0.95	0	1,6,8	0.04	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	CSX	C	163	1	-	0/1/5/7	-
1	CSX	B	163	1	-	0/1/5/7	-
1	CSX	D	163	1	-	0/1/5/7	-
1	CSX	A	163	1	-	0/1/5/7	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	163	CSX	O-C	6.15	1.44	1.19
1	C	163	CSX	O-C	3.27	1.33	1.19

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	163	CSX	CA-CB-SG	-2.99	106.83	113.36

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

4 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	DSD	C	250	-	9,15,15	0.63	0	5,18,18	1.58	1 (20%)
2	DSD	D	250	-	9,15,15	0.62	0	5,18,18	1.70	1 (20%)
2	DSD	A	250	-	9,15,15	0.51	0	5,18,18	1.76	1 (20%)
2	DSD	B	250	-	9,15,15	0.34	0	5,18,18	2.58	1 (20%)

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	DSD	C	250	-	-	2/11/16/16	-
2	DSD	D	250	-	-	2/11/16/16	-
2	DSD	A	250	-	-	2/11/16/16	-
2	DSD	B	250	-	-	2/11/16/16	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	250	DSD	C6-C7-N7	-5.34	103.15	110.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	250	DSD	C6-C7-N7	-3.69	105.34	110.25
2	C	250	DSD	C6-C7-N7	-3.49	105.61	110.25
2	D	250	DSD	C6-C7-N7	-3.47	105.63	110.25

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	250	DSD	C5-C6-C7-C8
2	B	250	DSD	C5-C6-C7-C8
2	C	250	DSD	C5-C6-C7-N7
2	D	250	DSD	C5-C6-C7-N7
2	A	250	DSD	C5-C6-C7-N7
2	B	250	DSD	C5-C6-C7-N7
2	C	250	DSD	C5-C6-C7-C8
2	D	250	DSD	C5-C6-C7-C8

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	250	DSD	2	0
2	D	250	DSD	2	0
2	A	250	DSD	2	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 ⓘ

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	229/251 (91%)	0.10	7 (3%) 49 53	11, 19, 32, 46	1 (0%)
1	B	227/251 (90%)	0.15	10 (4%) 34 37	12, 21, 37, 71	0
1	C	229/251 (91%)	0.06	6 (2%) 56 60	14, 21, 33, 54	1 (0%)
1	D	219/251 (87%)	0.27	16 (7%) 15 16	14, 24, 40, 55	0
All	All	904/1004 (90%)	0.15	39 (4%) 35 38	11, 21, 37, 71	2 (0%)

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	44	ALA	5.5
1	C	174	PRO	5.3
1	C	177	LEU	4.2
1	B	46	GLY	3.8
1	C	173	ASP	3.6
1	B	47	ASP	3.6
1	B	177	LEU	3.5
1	A	218	ARG	3.3
1	C	6	VAL	3.2
1	A	6	VAL	3.0
1	D	120	PRO	3.0
1	D	101	PRO	3.0
1	B	45	ARG	3.0
1	D	204	ASP	2.9
1	D	219	ASN	2.9
1	D	119	GLU	2.8
1	D	173	ASP	2.7
1	D	175	PRO	2.6
1	D	171	TRP	2.6
1	D	206	GLY	2.6
1	D	174	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	-2	GLN	2.5
1	C	5	VAL	2.3
1	A	174	PRO	2.3
1	B	174	PRO	2.3
1	B	19[A]	CYS	2.3
1	A	60	THR	2.2
1	A	204	ASP	2.2
1	B	106	LEU	2.2
1	B	107	VAL	2.2
1	D	222	ALA	2.2
1	A	160	GLN	2.2
1	D	55	ARG	2.2
1	D	199	GLY	2.1
1	D	6	VAL	2.1
1	A	39	VAL	2.1
1	D	30	GLY	2.0
1	C	218	ARG	2.0
1	D	63	ALA	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	CSX	B	163	7/8	0.87	0.21	15,25,27,40	0
1	CSX	D	163	7/8	0.91	0.13	18,26,27,35	0
1	CSX	C	163	7/8	0.92	0.11	15,19,21,27	0
1	CSX	A	163	7/8	0.93	0.12	19,20,23,25	0

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	DSD	D	250	16/16	0.95	0.15	17,22,27,28	0
2	DSD	A	250	16/16	0.96	0.10	12,23,29,31	0
2	DSD	C	250	16/16	0.97	0.10	18,21,29,31	0
2	DSD	B	250	16/16	0.97	0.12	14,20,24,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.