



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 27, 2023 – 01:10 AM EDT

PDB ID : 3FPA
Title : Crystal structure of Mycobacterium tuberculosis dethiobiotin synthetase complexed with dethiobiotin and phosphate
Authors : Dey, S.; Sacchettini, J.C.
Deposited on : 2009-01-04
Resolution : 2.30 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.35
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) : 2.35

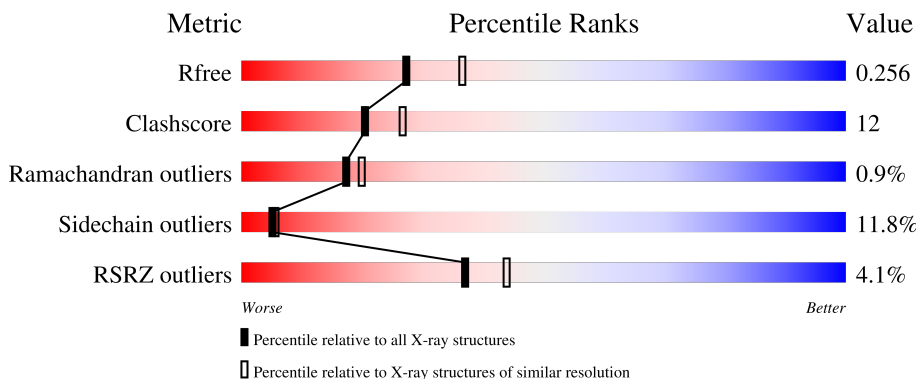
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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	251	 3% 73% 15% 8%
1	B	251	 % 70% 16% 10%
1	C	251	 2% 73% 14% 9%
1	D	251	 9% 60% 25% 10%

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
2	PO4	B	5257	-	-	X	-
3	DTB	A	803	-	-	X	-

2 Entry composition i

There are 5 unique types of molecules in this entry. The entry contains 6626 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
			Total	C	N	O	S			
1	A	230	1614	1007	294	305	8	0	1	0
1	B	226	1579	986	286	299	8	0	0	0
1	C	228	1589	991	288	302	8	0	0	0
1	D	225	1569	980	283	298	8	0	0	0

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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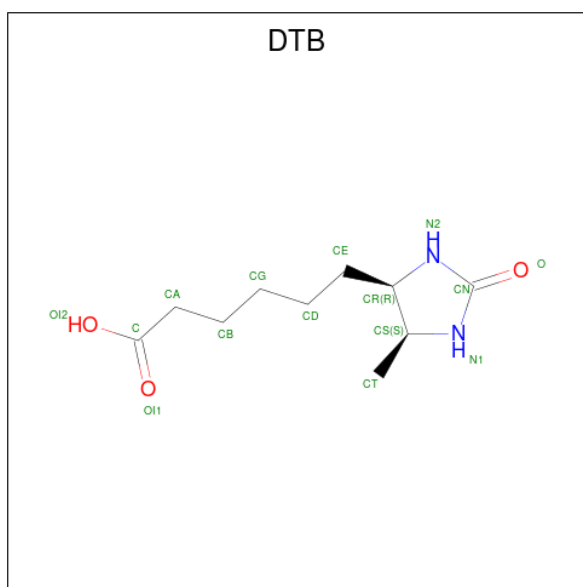
Chain	Residue	Modelled	Actual	Comment	Reference
C	-11	LEU	-	expression tag	UNP O06620
C	-10	GLN	-	expression tag	UNP O06620
C	-9	GLY	-	expression tag	UNP O06620
C	-8	THR	-	expression tag	UNP O06620
C	-7	GLU	-	expression tag	UNP O06620
C	-6	ASN	-	expression tag	UNP O06620
C	-5	LEU	-	expression tag	UNP 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 PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		

- Molecule 3 is 6-(5-METHYL-2-OXO-IMIDAZOLIDIN-4-YL)-HEXANOIC ACID (three-letter code: DTB) (formula: C₁₀H₁₈N₂O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	
3	A	1	Total	C	N	O	0	0
			15	10	2	3		
3	B	1	Total	C	N	O	0	0
			15	10	2	3		
3	C	1	Total	C	N	O	0	0
			15	10	2	3		

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		
4	C	1	Total	Mg	0	0
			1	1		
4	D	1	Total	Mg	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	51	Total	O	0	0
			51	51		
5	B	44	Total	O	0	0
			44	44		

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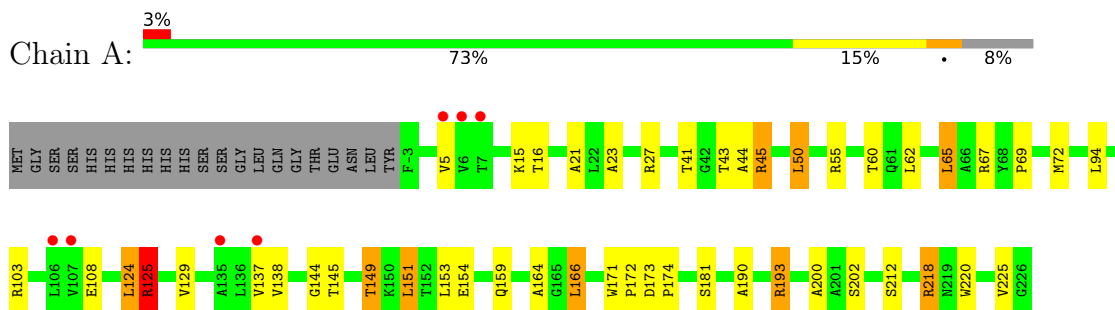
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	54	Total	O	0	0
			54	54		
5	D	37	Total	O	0	0
			37	37		

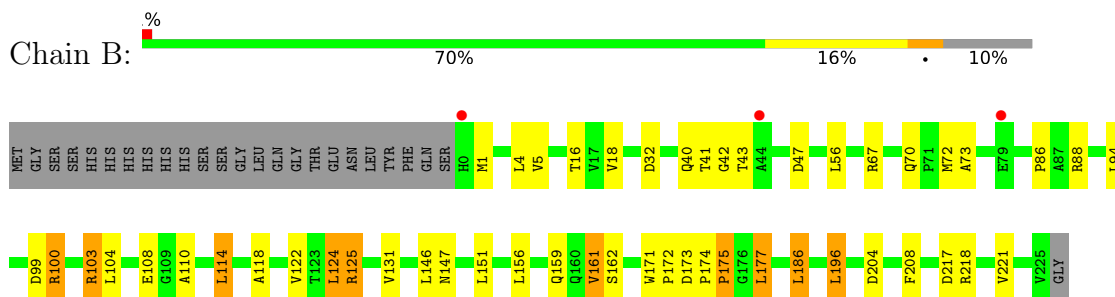
3 Residue-property plots i

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.

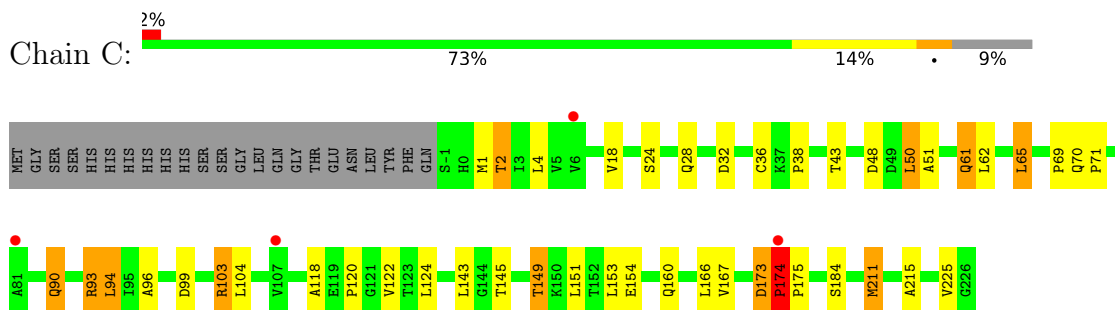
- Molecule 1: Dethiobiotin synthetase



- Molecule 1: Dethiobiotin synthetase

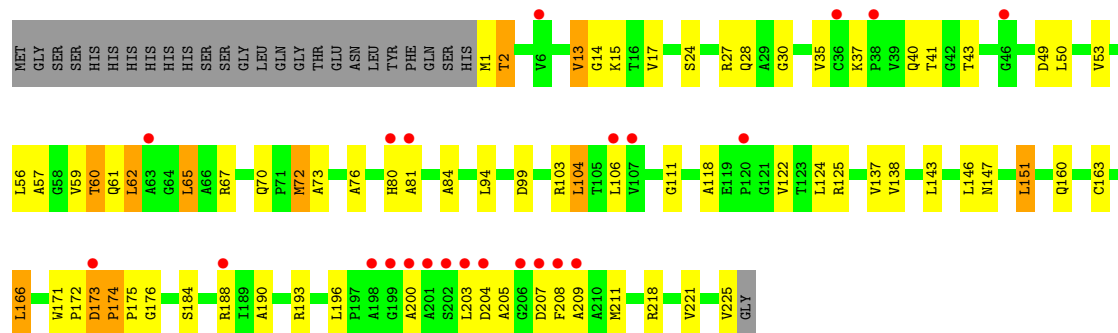


- Molecule 1: Dethiobiotin synthetase



- 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	55.13Å 104.45Å 151.13Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	35.00 – 2.30 31.62 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.8 (35.00-2.30) 99.8 (31.62-2.30)	Depositor EDS
R_{merge}	0.21	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.53 (at 2.31Å)	Xtrriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.205 , 0.260 0.201 , 0.256	Depositor DCC
R_{free} test set	1980 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	39.7	Xtrriage
Anisotropy	0.554	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6626	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.27% 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: DTB, MG, CSX, PO4

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	0.56	0/1633	0.72	1/2230 (0.0%)
1	B	0.54	0/1591	0.71	0/2175
1	C	0.57	1/1601 (0.1%)	0.69	0/2188
1	D	0.51	0/1580	0.72	1/2160 (0.0%)
All	All	0.54	1/6405 (0.0%)	0.71	2/8753 (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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	174	PRO	CB-CG	6.20	1.80	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	125	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	D	151	LEU	CA-CB-CG	5.37	127.65	115.30

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 [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	1614	0	1658	32	0
1	B	1579	0	1628	37	0
1	C	1589	0	1636	39	0
1	D	1569	0	1622	50	0
2	A	10	0	0	0	0
2	B	10	0	0	3	0
2	C	10	0	0	1	0
2	D	10	0	0	1	0
3	A	15	0	17	12	0
3	B	15	0	17	2	0
3	C	15	0	17	5	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
5	A	51	0	0	2	0
5	B	44	0	0	3	0
5	C	54	0	0	1	0
5	D	37	0	0	1	0
All	All	6626	0	6595	162	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 12.

All (162) 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:C:174:PRO:CB	1:C:174:PRO:CG	1.80	1.50
1:C:173:ASP:OD2	1:C:174:PRO:HD2	1.20	1.34
1:B:100:ARG:HH11	1:B:100:ARG:HG2	0.99	1.10
1:D:65:LEU:HD13	1:D:94:LEU:HD22	1.35	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:173:ASP:OD2	1:C:174:PRO:CD	2.02	1.07
1:C:93:ARG:HH21	1:C:93:ARG:HG3	1.21	1.01
3:A:803:DTB:HCT1	5:B:264:HOH:O	1.59	1.01
3:C:803:DTB:HCS	1:D:41:THR:OG1	1.63	0.98
1:B:204:ASP:HB2	5:B:233:HOH:O	1.66	0.95
3:A:803:DTB:HCS	1:B:41:THR:OG1	1.70	0.91
1:B:100:ARG:HG2	1:B:100:ARG:NH1	1.78	0.91
1:A:151:LEU:HD13	1:B:114:LEU:HD22	1.56	0.87
1:D:225:VAL:HG23	1:D:225:VAL:O	1.75	0.86
1:C:61:GLN:HA	1:C:61:GLN:HE21	1.39	0.86
1:C:211:MET:CE	1:C:215:ALA:HB2	2.06	0.85
1:C:93:ARG:HG3	1:C:93:ARG:NH2	1.84	0.85
1:A:145:THR:O	1:A:149:THR:HG23	1.78	0.83
1:A:145:THR:O	1:A:149:THR:CG2	2.28	0.81
1:C:2:THR:HG21	1:C:225:VAL:HA	1.62	0.81
3:A:803:DTB:HCB2	1:B:73:ALA:HB2	1.62	0.80
1:C:32:ASP:OD2	1:C:103:ARG:HD3	1.82	0.80
1:D:65:LEU:CD1	1:D:94:LEU:HD22	2.15	0.76
1:D:70:GLN:HG3	1:D:80:HIS:CD2	2.21	0.75
1:C:93:ARG:HH21	1:C:93:ARG:CG	2.00	0.74
1:C:211:MET:HE1	1:C:215:ALA:HB2	1.69	0.73
1:D:173:ASP:HB2	1:D:174:PRO:HD3	1.68	0.73
1:C:1:MET:HG3	1:C:99:ASP:OD2	1.88	0.71
1:C:145:THR:O	1:C:149:THR:HG23	1.91	0.70
1:C:24:SER:O	1:C:28:GLN:HG3	1.92	0.69
3:A:803:DTB:HCT3	2:B:5257:PO4:P	2.33	0.69
1:D:173:ASP:CB	1:D:174:PRO:HD3	2.24	0.68
1:D:59:VAL:HG22	1:D:62:LEU:HD11	1.73	0.68
1:B:1:MET:SD	1:B:99:ASP:OD2	2.51	0.68
3:C:803:DTB:HCS	1:D:41:THR:HG1	1.57	0.65
3:A:803:DTB:HCT3	2:B:5257:PO4:O2	1.96	0.65
3:C:803:DTB:CS	1:D:41:THR:OG1	2.42	0.63
1:D:59:VAL:HG22	1:D:62:LEU:CD1	2.28	0.63
1:B:100:ARG:HH11	1:B:100:ARG:CG	1.91	0.63
3:A:803:DTB:HCB2	1:B:73:ALA:CB	2.29	0.63
1:D:56:LEU:HD22	1:D:208:PHE:CD1	2.33	0.62
1:C:50:LEU:HG	1:C:62:LEU:HB3	1.81	0.62
1:A:23:ALA:O	1:A:27:ARG:HG3	1.99	0.62
3:A:803:DTB:HCT2	1:B:110:ALA:HB1	1.80	0.62
1:C:1:MET:SD	1:C:99:ASP:HA	2.40	0.62
1:C:173:ASP:CG	1:C:174:PRO:HD2	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:GLY:N	2:D:5259:PO4:O1	2.30	0.62
1:A:41:THR:OG1	3:B:803:DTB:HCS	2.00	0.61
1:D:59:VAL:CG2	1:D:62:LEU:CD1	2.79	0.60
1:B:88:ARG:HB2	1:B:122:VAL:HG21	1.82	0.60
1:A:144:GLY:H	3:A:803:DTB:HCA2	1.66	0.60
1:A:154:GLU:OE2	1:B:125:ARG:NH2	2.34	0.60
1:D:225:VAL:O	1:D:225:VAL:CG2	2.47	0.60
1:D:2:THR:HG21	1:D:225:VAL:HA	1.84	0.59
1:D:104:LEU:CD1	1:D:106:LEU:HD21	2.34	0.58
1:C:145:THR:O	1:C:149:THR:CG2	2.52	0.57
1:A:44:ALA:HB2	1:A:69:PRO:HB3	1.86	0.57
1:A:145:THR:O	1:A:149:THR:HG22	2.03	0.57
1:C:65:LEU:HD11	1:C:90:GLN:HG2	1.86	0.57
1:D:1:MET:HA	1:D:99:ASP:OD1	2.04	0.57
1:A:125:ARG:HD3	1:A:159:GLN:HG3	1.87	0.57
1:D:184:SER:O	1:D:188:ARG:HG3	2.04	0.56
1:C:61:GLN:HA	1:C:61:GLN:NE2	2.13	0.56
1:A:164:ALA:O	1:A:193:ARG:HD3	2.06	0.56
1:C:61:GLN:HE21	1:C:61:GLN:CA	2.15	0.55
1:B:118:ALA:HB3	1:B:122:VAL:HB	1.88	0.55
1:A:218:ARG:HD3	1:A:218:ARG:H	1.70	0.54
1:C:96:ALA:O	1:C:99:ASP:HB2	2.08	0.54
1:B:156:LEU:HD22	1:B:161:VAL:HG22	1.90	0.54
1:D:13:VAL:HG13	1:D:138:VAL:HG12	1.88	0.54
1:A:5:VAL:HG13	1:A:124:LEU:HD13	1.89	0.53
1:D:59:VAL:CG2	1:D:62:LEU:HD13	2.39	0.53
1:D:28:GLN:NE2	1:D:209:ALA:HB1	2.23	0.53
1:D:104:LEU:HD13	1:D:106:LEU:HD21	1.89	0.53
1:B:147:ASN:O	1:B:151:LEU:HB2	2.08	0.52
3:C:803:DTB:CT	1:D:41:THR:OG1	2.58	0.52
1:A:50:LEU:HG	1:A:62:LEU:HB3	1.92	0.51
1:D:173:ASP:N	1:D:173:ASP:OD1	2.42	0.51
3:A:803:DTB:CB	1:B:73:ALA:HB2	2.37	0.51
1:D:173:ASP:CB	1:D:174:PRO:CD	2.88	0.51
1:A:21:ALA:O	1:A:212:SER:HB3	2.11	0.51
1:B:146:LEU:HD23	1:B:186:LEU:HD13	1.93	0.51
1:C:211:MET:HE1	1:C:215:ALA:CB	2.38	0.51
1:D:15:LYS:HE3	1:D:111:GLY:O	2.11	0.51
1:A:225:VAL:HG23	1:A:225:VAL:O	2.10	0.50
1:B:43:THR:HG21	1:B:67:ARG:HB3	1.93	0.50
1:C:211:MET:HE2	1:C:215:ALA:HB2	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:193:ARG:HG2	1:A:220:TRP:CH2	2.47	0.49
1:B:32:ASP:OD1	1:B:103:ARG:HD3	2.12	0.49
1:B:217:ASP:O	1:B:221:VAL:HG23	2.12	0.49
1:D:27:ARG:O	1:D:30:GLY:N	2.33	0.49
1:C:38:PRO:HD2	5:C:266:HOH:O	2.12	0.49
1:C:1:MET:HG3	1:C:99:ASP:HA	1.93	0.49
1:A:16:THR:OG1	1:A:108:GLU:OE1	2.31	0.49
1:D:147:ASN:O	1:D:151:LEU:HB2	2.12	0.49
1:A:200:ALA:C	1:A:202:SER:H	2.15	0.48
1:D:35:VAL:HG21	1:D:53:VAL:HG11	1.96	0.48
1:A:166:LEU:HD22	1:A:190:ALA:HB3	1.94	0.47
1:B:125:ARG:HD3	1:B:159:GLN:HG3	1.96	0.47
1:B:172:PRO:HB2	1:B:175:PRO:HA	1.95	0.47
1:A:5:VAL:HG13	1:A:124:LEU:CD1	2.44	0.47
1:D:104:LEU:HD13	1:D:106:LEU:CD2	2.44	0.47
1:A:173:ASP:HA	1:A:174:PRO:HA	1.53	0.47
1:B:171:TRP:HA	1:B:172:PRO:HD3	1.74	0.47
1:C:43:THR:OG1	1:C:69:PRO:HA	2.14	0.47
1:D:166:LEU:HD22	1:D:190:ALA:HB3	1.97	0.47
1:D:72:MET:CE	1:D:76:ALA:HB1	2.45	0.47
1:C:1:MET:CG	1:C:99:ASP:HA	2.44	0.47
1:C:118:ALA:HB3	1:C:122:VAL:HB	1.97	0.46
1:B:100:ARG:NH1	1:B:100:ARG:CG	2.61	0.46
1:D:59:VAL:HG23	1:D:62:LEU:HD13	1.98	0.46
1:D:200:ALA:HB1	1:D:211:MET:CE	2.46	0.46
1:B:5:VAL:HG13	1:B:124:LEU:CD1	2.46	0.46
1:D:28:GLN:NE2	1:D:209:ALA:O	2.43	0.45
1:C:153:LEU:HD23	1:C:153:LEU:HA	1.73	0.45
1:D:173:ASP:O	1:D:175:PRO:HD3	2.17	0.45
1:C:65:LEU:HD11	1:C:90:GLN:CG	2.46	0.45
1:D:70:GLN:HG3	1:D:80:HIS:HD2	1.78	0.45
1:D:172:PRO:HB2	1:D:175:PRO:HA	1.97	0.45
1:B:204:ASP:CB	5:B:233:HOH:O	2.45	0.45
1:D:171:TRP:HA	1:D:172:PRO:HD3	1.82	0.45
1:B:5:VAL:CG1	1:B:124:LEU:HD13	2.47	0.44
1:D:24:SER:HB2	1:D:57:ALA:HA	1.99	0.44
1:A:43:THR:HG21	1:A:67:ARG:HB3	1.99	0.44
1:D:60:THR:CG2	1:D:61:GLN:OE1	2.65	0.44
1:A:144:GLY:H	3:A:803:DTB:CA	2.28	0.44
1:A:15:LYS:HA	1:A:138:VAL:HG21	2.00	0.43
1:A:144:GLY:H	3:A:803:DTB:C	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:2:THR:CG2	1:C:225:VAL:HA	2.41	0.43
5:A:264:HOH:O	3:B:803:DTB:HCT2	2.18	0.43
1:C:70:GLN:HA	1:C:71:PRO:HD3	1.94	0.43
1:D:17:VAL:HG23	5:D:253:HOH:O	2.18	0.43
3:C:803:DTB:HCA2	1:D:73:ALA:HB2	1.98	0.43
1:B:42:GLY:O	1:B:47:ASP:HB2	2.19	0.43
1:B:177:LEU:HD23	1:B:177:LEU:HA	1.72	0.43
1:B:16:THR:OG1	1:B:108:GLU:OE1	2.37	0.43
1:C:225:VAL:HG12	1:C:225:VAL:O	2.18	0.43
1:D:37:LYS:HD3	1:D:49:ASP:HB2	2.01	0.43
1:D:173:ASP:HB2	1:D:174:PRO:CD	2.43	0.42
1:C:18:VAL:HG22	1:C:167:VAL:HG11	2.01	0.42
1:D:203:LEU:HD13	1:D:207:ASP:HB3	2.01	0.42
2:C:5261:PO4:O2	2:C:5262:PO4:O1	2.37	0.42
1:B:56:LEU:HD22	1:B:208:PHE:CD1	2.54	0.42
1:A:218:ARG:H	1:A:218:ARG:CD	2.31	0.41
3:A:803:DTB:CT	2:B:5257:PO4:O2	2.66	0.41
1:B:18:VAL:HG22	1:B:196:LEU:HD22	2.03	0.41
1:B:70:GLN:HB3	1:B:72:MET:HG3	2.03	0.41
1:D:40:GLN:O	1:D:67:ARG:HA	2.21	0.41
1:B:125:ARG:CD	1:B:159:GLN:HG3	2.49	0.41
1:C:174:PRO:HA	1:C:175:PRO:HD2	1.67	0.41
1:B:40:GLN:O	1:B:67:ARG:HA	2.21	0.41
1:A:65:LEU:HB2	1:A:94:LEU:HD22	2.03	0.41
1:A:171:TRP:HA	1:A:172:PRO:HD3	1.74	0.41
1:B:5:VAL:HG13	1:B:124:LEU:HD11	2.03	0.41
1:A:125:ARG:O	1:A:129:VAL:HG23	2.21	0.41
1:C:4:LEU:HA	1:C:4:LEU:HD23	1.84	0.41
1:C:36:CYS:SG	1:C:94:LEU:HD13	2.61	0.41
1:D:43:THR:HG21	1:D:67:ARG:HB3	2.02	0.41
1:C:48:ASP:HB3	1:C:51:ALA:HB3	2.03	0.41
1:B:173:ASP:HA	1:B:174:PRO:HA	1.91	0.40
1:A:55[B]:ARG:NH1	5:A:272:HOH:O	2.53	0.40
1:D:118:ALA:HB3	1:D:122:VAL:HB	2.03	0.40
1:A:45:ARG:HE	1:A:45:ARG:HB3	1.56	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%)	224 (98%)	4 (2%)	0	100	100
1	B	223/251 (89%)	217 (97%)	4 (2%)	2 (1%)	17	20
1	C	225/251 (90%)	220 (98%)	3 (1%)	2 (1%)	17	20
1	D	222/251 (88%)	206 (93%)	12 (5%)	4 (2%)	8	7
All	All	898/1004 (89%)	867 (96%)	23 (3%)	8 (1%)	17	20

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	174	PRO
1	D	81	ALA
1	D	84	ALA
1	D	176	GLY
1	D	205	ALA
1	B	86	PRO
1	B	175	PRO
1	C	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%)	140 (90%)	16 (10%)	7	8
1	B	152/173 (88%)	137 (90%)	15 (10%)	8	9

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	153/173 (88%)	135 (88%)	18 (12%)	5	5
1	D	151/173 (87%)	128 (85%)	23 (15%)	3	2
All	All	612/692 (88%)	540 (88%)	72 (12%)	5	5

All (72) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	ARG
1	A	50	LEU
1	A	60	THR
1	A	65	LEU
1	A	72	MET
1	A	103	ARG
1	A	124	LEU
1	A	125	ARG
1	A	137	VAL
1	A	149	THR
1	A	151	LEU
1	A	153	LEU
1	A	166	LEU
1	A	181	SER
1	A	193	ARG
1	A	218	ARG
1	B	4	LEU
1	B	94	LEU
1	B	100	ARG
1	B	103	ARG
1	B	104	LEU
1	B	114	LEU
1	B	124	LEU
1	B	125	ARG
1	B	131	VAL
1	B	161	VAL
1	B	162	SER
1	B	177	LEU
1	B	186	LEU
1	B	196	LEU
1	B	218	ARG
1	C	2	THR
1	C	50	LEU
1	C	61	GLN

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Mol	Chain	Res	Type
1	C	65	LEU
1	C	90	GLN
1	C	93	ARG
1	C	94	LEU
1	C	103	ARG
1	C	104	LEU
1	C	124	LEU
1	C	143	LEU
1	C	149	THR
1	C	151	LEU
1	C	154	GLU
1	C	160	GLN
1	C	166	LEU
1	C	184	SER
1	C	211	MET
1	D	2	THR
1	D	13	VAL
1	D	50	LEU
1	D	60	THR
1	D	62	LEU
1	D	65	LEU
1	D	72	MET
1	D	103	ARG
1	D	104	LEU
1	D	124	LEU
1	D	125	ARG
1	D	137	VAL
1	D	143	LEU
1	D	146	LEU
1	D	160	GLN
1	D	166	LEU
1	D	173	ASP
1	D	174	PRO
1	D	193	ARG
1	D	196	LEU
1	D	204	ASP
1	D	218	ARG
1	D	221	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	159	GLN
1	C	61	GLN
1	D	80	HIS
1	D	160	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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	D	163	1	3,6,7	1.88	1 (33%)	1,6,8	0.50	0
1	CSX	A	163	1	3,6,7	0.97	0	1,6,8	0.26	0
1	CSX	C	163	1	3,6,7	0.69	0	1,6,8	1.63	0
1	CSX	B	163	1	3,6,7	1.15	0	1,6,8	0.05	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	D	163	1	-	0/1/5/7	-
1	CSX	A	163	1	-	0/1/5/7	-
1	CSX	C	163	1	-	0/1/5/7	-
1	CSX	B	163	1	-	0/1/5/7	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	163	CSX	CB-CA	2.94	1.60	1.53

There are no bond angle outliers.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 4 are monoatomic - leaving 11 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	DTB	B	803	-	15,15,15	0.97	0	16,19,19	1.35	1 (6%)
2	PO4	D	5260	4	4,4,4	0.90	0	6,6,6	0.82	0
2	PO4	C	5261	4	4,4,4	0.92	0	6,6,6	0.64	0
2	PO4	D	5259	4	4,4,4	1.15	0	6,6,6	1.14	0
2	PO4	C	5262	4	4,4,4	0.92	0	6,6,6	0.62	0
2	PO4	B	5255	4	4,4,4	1.18	0	6,6,6	0.40	0
2	PO4	B	5257	4	4,4,4	1.22	0	6,6,6	0.63	0
3	DTB	C	803	-	15,15,15	0.75	0	16,19,19	1.02	1 (6%)
2	PO4	A	5256	4	4,4,4	1.22	0	6,6,6	0.56	0
3	DTB	A	803	-	15,15,15	0.86	0	16,19,19	1.18	2 (12%)
2	PO4	A	5254	4	4,4,4	0.80	0	6,6,6	0.71	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	DTB	B	803	-	-	3/8/20/20	0/1/1/1
3	DTB	A	803	-	-	7/8/20/20	0/1/1/1
3	DTB	C	803	-	-	3/8/20/20	0/1/1/1

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	803	DTB	CT-CS-N1	-3.36	107.69	111.70
3	A	803	DTB	CB-CA-C	-2.10	109.19	114.47
3	C	803	DTB	OI2-C-CA	2.09	120.73	114.03
3	A	803	DTB	CS-N1-CN	-2.01	110.20	112.42

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	803	DTB	CD-CE-CR-N2
3	A	803	DTB	CD-CE-CR-CS
3	A	803	DTB	C-CA-CB-CG
3	B	803	DTB	CG-CD-CE-CR
3	A	803	DTB	CG-CD-CE-CR
3	C	803	DTB	CG-CD-CE-CR
3	B	803	DTB	OI2-C-CA-CB
3	B	803	DTB	OI1-C-CA-CB
3	C	803	DTB	OI1-C-CA-CB
3	C	803	DTB	OI2-C-CA-CB
3	A	803	DTB	OI2-C-CA-CB
3	A	803	DTB	CE-CD-CG-CB
3	A	803	DTB	OI1-C-CA-CB

There are no ring outliers.

7 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	803	DTB	2	0
2	C	5261	PO4	1	0
2	D	5259	PO4	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	5262	PO4	1	0
2	B	5257	PO4	3	0
3	C	803	DTB	5	0
3	A	803	DTB	12	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%)	-0.03	7 (3%) 49 56	18, 30, 46, 64	3 (1%)
1	B	225/251 (89%)	-0.08	3 (1%) 77 81	22, 33, 52, 65	4 (1%)
1	C	227/251 (90%)	-0.13	4 (1%) 68 74	22, 35, 52, 72	3 (1%)
1	D	224/251 (89%)	0.43	23 (10%) 6 9	25, 41, 65, 82	3 (1%)
All	All	905/1004 (90%)	0.05	37 (4%) 37 44	18, 34, 57, 82	13 (1%)

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	202	SER	4.6
1	D	203	LEU	4.5
1	D	107	VAL	4.0
1	A	6	VAL	3.5
1	D	6	VAL	3.4
1	D	80	HIS	3.4
1	D	198	ALA	3.2
1	C	174	PRO	3.1
1	D	120	PRO	3.1
1	D	204	ASP	3.0
1	A	5	VAL	3.0
1	D	200	ALA	2.9
1	D	46	GLY	2.8
1	B	44	ALA	2.8
1	D	38	PRO	2.7
1	D	208	PHE	2.7
1	D	207	ASP	2.7
1	D	106	LEU	2.7
1	D	81	ALA	2.7
1	D	209	ALA	2.6
1	A	106	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	36	CYS	2.5
1	D	173	ASP	2.5
1	B	79	GLU	2.5
1	A	7	THR	2.4
1	A	137	VAL	2.4
1	D	201	ALA	2.3
1	B	0	HIS	2.3
1	D	199	GLY	2.2
1	D	63	ALA	2.2
1	D	206	GLY	2.2
1	C	81	ALA	2.1
1	C	107	VAL	2.1
1	A	107	VAL	2.1
1	D	188	ARG	2.1
1	C	6	VAL	2.1
1	A	135	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	D	163	7/8	0.87	0.11	30,35,40,59	0
1	CSX	B	163	7/8	0.94	0.12	27,31,34,38	0
1	CSX	A	163	7/8	0.94	0.13	28,34,37,38	0
1	CSX	C	163	7/8	0.96	0.07	32,36,37,40	0

6.3 Carbohydrates [i](#)

There are no monosaccharides 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
3	DTB	C	803	15/15	0.77	0.28	25,43,67,74	15
4	MG	B	901	1/1	0.80	0.13	46,46,46,46	0
3	DTB	B	803	15/15	0.82	0.23	21,33,48,49	0
3	DTB	A	803	15/15	0.84	0.22	27,35,57,58	15
4	MG	D	901	1/1	0.87	0.09	44,44,44,44	0
4	MG	A	901	1/1	0.95	0.14	32,32,32,32	0
2	PO4	B	5257	5/5	0.98	0.11	32,32,37,43	0
2	PO4	D	5259	5/5	0.98	0.12	33,39,49,56	0
2	PO4	D	5260	5/5	0.98	0.11	34,37,39,43	0
2	PO4	C	5261	5/5	0.99	0.12	21,27,29,30	0
2	PO4	C	5262	5/5	0.99	0.16	26,32,34,37	0
2	PO4	A	5256	5/5	0.99	0.14	25,26,30,38	0
2	PO4	A	5254	5/5	0.99	0.08	22,22,27,32	0
4	MG	C	901	1/1	0.99	0.10	29,29,29,29	0
2	PO4	B	5255	5/5	0.99	0.12	25,27,31,35	0

6.5 Other polymers [i](#)

There are no such residues in this entry.