



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 30, 2020 – 01:43 PM BST

PDB ID : 1XXX  
Title : Crystal structure of Dihydrodipicolinate Synthase (DapA, Rv2753c) from Mycobacterium tuberculosis  
Authors : Kefala, G.; Panjikar, S.; Janowski, R.; Weiss, M.S.; TB Structural Genomics Consortium (TBSGC)  
Deposited on : 2004-11-09  
Resolution : 2.28 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](mailto: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.

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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	:	<b>FAILED</b>
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13

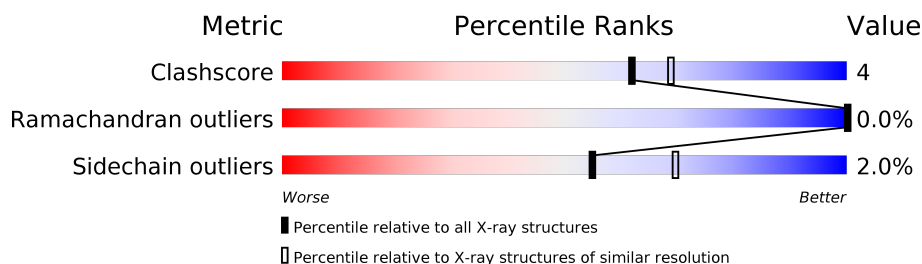
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.28 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))
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)

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  $\geq 3$ , 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  $\leq 5\%$ .

Note EDS failed to run properly.

Mol	Chain	Length	Quality of chain
1	A	303	
1	B	303	
1	C	303	
1	D	303	
1	E	303	
1	F	303	
1	G	303	
1	H	303	

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 18739 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 Dihydrodipicolinate synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	296	Total	C	N	O	S	0	0	0
			2136	1335	379	413	9			
1	B	295	Total	C	N	O	S	0	0	0
			2132	1333	378	412	9			
1	C	296	Total	C	N	O	S	0	0	0
			2136	1335	379	413	9			
1	D	295	Total	C	N	O	S	0	0	0
			2132	1333	378	412	9			
1	E	295	Total	C	N	O	S	0	0	0
			2132	1333	378	412	9			
1	F	296	Total	C	N	O	S	0	0	0
			2136	1335	379	413	9			
1	G	295	Total	C	N	O	S	0	0	0
			2132	1333	378	412	9			
1	H	296	Total	C	N	O	S	0	0	0
			2136	1335	379	413	9			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	cloning artifact	UNP P63945
A	-1	ALA	-	cloning artifact	UNP P63945
A	0	MET	-	cloning artifact	UNP P63945
A	1	VAL	MET	see remark 999	UNP P63945
B	-2	GLY	-	cloning artifact	UNP P63945
B	-1	ALA	-	cloning artifact	UNP P63945
B	0	MET	-	cloning artifact	UNP P63945
B	1	VAL	MET	see remark 999	UNP P63945
C	-2	GLY	-	cloning artifact	UNP P63945
C	-1	ALA	-	cloning artifact	UNP P63945
C	0	MET	-	cloning artifact	UNP P63945
C	1	VAL	MET	see remark 999	UNP P63945
D	-2	GLY	-	cloning artifact	UNP P63945

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-1	ALA	-	cloning artifact	UNP P63945
D	0	MET	-	cloning artifact	UNP P63945
D	1	VAL	MET	see remark 999	UNP P63945
E	-2	GLY	-	cloning artifact	UNP P63945
E	-1	ALA	-	cloning artifact	UNP P63945
E	0	MET	-	cloning artifact	UNP P63945
E	1	VAL	MET	see remark 999	UNP P63945
F	-2	GLY	-	cloning artifact	UNP P63945
F	-1	ALA	-	cloning artifact	UNP P63945
F	0	MET	-	cloning artifact	UNP P63945
F	1	VAL	MET	see remark 999	UNP P63945
G	-2	GLY	-	cloning artifact	UNP P63945
G	-1	ALA	-	cloning artifact	UNP P63945
G	0	MET	-	cloning artifact	UNP P63945
G	1	VAL	MET	see remark 999	UNP P63945
H	-2	GLY	-	cloning artifact	UNP P63945
H	-1	ALA	-	cloning artifact	UNP P63945
H	0	MET	-	cloning artifact	UNP P63945
H	1	VAL	MET	see remark 999	UNP P63945

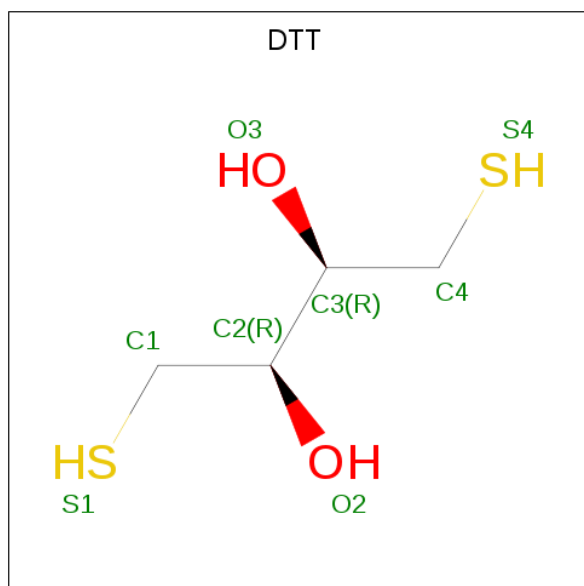
- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	G	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	A	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	G	1	Total Cl 1 1	0	0
3	D	1	Total Cl 1 1	0	0
3	E	1	Total Cl 1 1	0	0
3	H	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0
3	A	1	Total Cl 1 1	0	0
3	F	1	Total Cl 1 1	0	0

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



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O S 8 4 2 2	0	0
4	B	1	Total C O S 8 4 2 2	0	0
4	C	1	Total C O S 8 4 2 2	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	D	1	Total	C	O	S	0	0
			8	4	2	2		
4	E	1	Total	C	O	S	0	0
			8	4	2	2		
4	F	1	Total	C	O	S	0	0
			8	4	2	2		
4	G	1	Total	C	O	S	0	0
			8	4	2	2		
4	H	1	Total	C	O	S	0	0
			8	4	2	2		

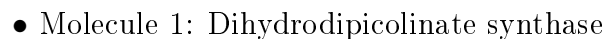
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	236	Total	O	0	0
			236	236		
5	B	236	Total	O	0	0
			236	236		
5	C	213	Total	O	0	0
			213	213		
5	D	241	Total	O	0	0
			241	241		
5	E	139	Total	O	0	0
			139	139		
5	F	106	Total	O	0	0
			106	106		
5	G	222	Total	O	0	0
			222	222		
5	H	194	Total	O	0	0
			194	194		

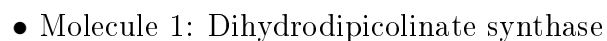



Note EDS failed to run properly.

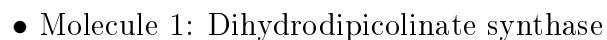
- Chain A:  88% 9% .



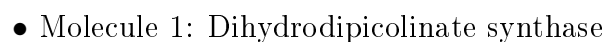
Chain B:  88% 9% .



Chain C:  89% 9%



Chain D:  87% 10% .



Chain E: 

89%

8%

• •



• Molecule 1: Dihydrodipicolinate synthase

Chain F: 

88%

9%

•



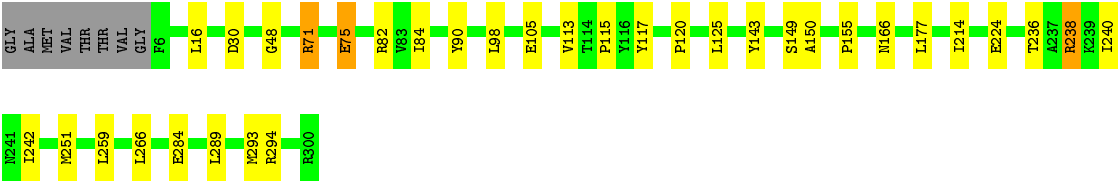
• Molecule 1: Dihydrodipicolinate synthase

Chain G: 

86%

10%

• •



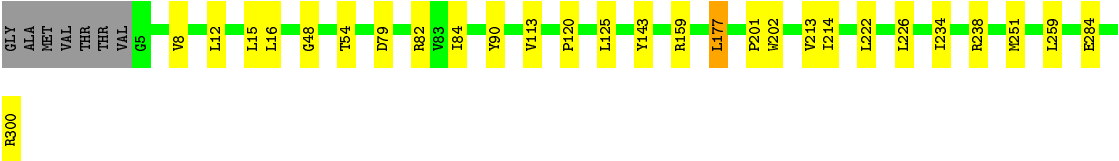
• Molecule 1: Dihydrodipicolinate synthase

Chain H: 

88%

9%

•



R300

## 4 Data and refinement statistics

EDS failed to run properly - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	94.79Å 87.37Å 139.85Å 90.00° 107.78° 90.00°	Depositor
Resolution (Å)	30.00 – 2.28	Depositor
% Data completeness (in resolution range)	100.0 (30.00-2.28)	Depositor
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	9.22 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.148 , 0.215	Depositor
Wilson B-factor (Å <sup>2</sup> )	24.6	Xtriage
Anisotropy	0.473	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
Total number of atoms	18739	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.59% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, CL, 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	0.88	1/2170 (0.0%)	0.81	0/2956
1	B	0.91	1/2166 (0.0%)	0.87	1/2951 (0.0%)
1	C	0.89	1/2170 (0.0%)	0.81	1/2956 (0.0%)
1	D	0.91	1/2166 (0.0%)	0.86	6/2951 (0.2%)
1	E	0.78	1/2166 (0.0%)	0.77	1/2951 (0.0%)
1	F	0.76	1/2170 (0.0%)	0.72	3/2956 (0.1%)
1	G	0.88	2/2166 (0.1%)	0.88	5/2951 (0.2%)
1	H	0.84	2/2170 (0.1%)	0.82	1/2956 (0.0%)
All	All	0.86	10/17344 (0.1%)	0.82	18/23628 (0.1%)

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 (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	75	GLU	CD-OE1	12.05	1.39	1.25
1	D	224	GLU	CG-CD	7.84	1.63	1.51
1	E	224	GLU	CG-CD	6.78	1.62	1.51
1	G	224	GLU	CG-CD	5.99	1.60	1.51
1	H	284	GLU	CG-CD	5.93	1.60	1.51
1	G	284	GLU	CG-CD	5.18	1.59	1.51
1	C	68	GLU	CG-CD	5.15	1.59	1.51
1	A	284	GLU	CG-CD	5.12	1.59	1.51
1	B	224	GLU	CG-CD	5.01	1.59	1.51
1	H	213	VAL	CB-CG2	5.01	1.63	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	294	ARG	NE-CZ-NH2	-8.35	116.13	120.30
1	G	238	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	D	294	ARG	CG-CD-NE	-6.29	98.59	111.80
1	G	238	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	G	98	LEU	CA-CB-CG	5.76	128.55	115.30
1	B	98	LEU	CA-CB-CG	5.66	128.31	115.30
1	F	238	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	C	294	ARG	CG-CD-NE	-5.56	100.12	111.80
1	D	159	ARG	NE-CZ-NH1	-5.55	117.52	120.30
1	H	159	ARG	NE-CZ-NH1	-5.45	117.58	120.30
1	E	36	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	D	97	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	D	148	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	F	80	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	G	30	ASP	CB-CG-OD2	5.17	122.96	118.30
1	D	223	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	D	159	ARG	NE-CZ-NH2	5.06	122.83	120.30
1	F	91	ASP	CB-CG-OD1	-5.00	113.80	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	5	GLY	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	2136	0	2158	29	0
1	B	2132	0	2155	25	0
1	C	2136	0	2158	15	0
1	D	2132	0	2155	15	0
1	E	2132	0	2155	18	0
1	F	2136	0	2158	24	0
1	G	2132	0	2155	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	H	2136	0	2158	18	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
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	8	0	9	0	0
4	B	8	0	9	1	0
4	C	8	0	9	2	0
4	D	8	0	9	0	0
4	E	8	0	9	1	0
4	F	8	0	9	1	0
4	G	8	0	9	0	0
4	H	8	0	9	0	0
5	A	236	0	0	0	0
5	B	236	0	0	1	0
5	C	213	0	0	0	0
5	D	241	0	0	1	0
5	E	139	0	0	1	0
5	F	106	0	0	1	0
5	G	222	0	0	2	0
5	H	194	0	0	1	0
All	All	18739	0	17324	153	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 4.

All (153) 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:289:LEU:HG	1:A:293:MET:HE2	1.25	1.18
1:A:289:LEU:HG	1:A:293:MET:CE	1.78	1.12
1:G:266:LEU:HD13	1:G:293:MET:CE	1.90	1.02
1:A:289:LEU:CG	1:A:293:MET:HE2	1.89	1.02
1:D:284:GLU:HG3	5:D:3097:HOH:O	1.62	0.99
1:A:266:LEU:HD12	1:A:293:MET:HE1	1.40	0.99
1:B:266:LEU:HD13	1:B:293:MET:CE	1.96	0.96
1:G:266:LEU:CD1	1:G:293:MET:HE1	1.95	0.94
1:G:266:LEU:HD13	1:G:293:MET:HE3	1.46	0.94
1:B:6:PHE:HE2	1:B:8:VAL:HG22	1.35	0.92
1:G:266:LEU:HD12	1:G:293:MET:HE1	1.55	0.89
1:F:289:LEU:HG	1:F:293:MET:CE	2.05	0.86
1:G:266:LEU:CD1	1:G:293:MET:CE	2.53	0.84
1:B:266:LEU:HD13	1:B:293:MET:HE1	1.59	0.82
1:F:266:LEU:HD12	1:F:293:MET:HE1	1.62	0.81
1:F:289:LEU:HG	1:F:293:MET:HE2	1.63	0.80
1:F:266:LEU:HD13	1:F:293:MET:HE3	1.64	0.79
1:B:6:PHE:CE2	1:B:8:VAL:HG22	2.16	0.78
1:B:266:LEU:HD13	1:B:293:MET:HE2	1.64	0.78
1:G:289:LEU:HG	1:G:293:MET:CE	2.16	0.76
1:E:204:ALA:O	1:H:238:ARG:HD3	1.88	0.72
1:E:214:ILE:HG23	1:E:251:MET:CE	2.21	0.71
1:A:238:ARG:HD3	1:D:204:ALA:O	1.90	0.70
1:C:252:SER:OG	4:C:3003:DTT:H12	1.91	0.70
1:C:113:VAL:HA	1:C:143:TYR:HB3	1.74	0.70
1:A:266:LEU:CD1	1:A:293:MET:HE1	2.19	0.69
1:G:113:VAL:HA	1:G:143:TYR:HB3	1.73	0.69
1:A:289:LEU:HG	1:A:293:MET:HE3	1.71	0.69
1:A:113:VAL:HA	1:A:143:TYR:HB3	1.74	0.69
1:B:290:ALA:HA	1:B:293:MET:HE3	1.73	0.69
1:F:289:LEU:HG	1:F:293:MET:HE1	1.73	0.68
1:A:266:LEU:HD12	1:A:293:MET:CE	2.20	0.67
1:F:294:ARG:HG2	1:F:300:ARG:HB3	1.77	0.66
1:F:266:LEU:CD1	1:F:293:MET:CE	2.73	0.66
1:F:294:ARG:HE	1:F:300:ARG:HD3	1.61	0.66
1:B:113:VAL:HA	1:B:143:TYR:HB3	1.79	0.65
1:A:6:PHE:CE2	1:A:8:VAL:HG22	2.32	0.64
1:F:214:ILE:HG23	1:F:251:MET:CE	2.27	0.64
1:G:289:LEU:HG	1:G:293:MET:HE1	1.77	0.64
1:E:300:ARG:HD2	5:E:3053:HOH:O	1.96	0.64
1:B:266:LEU:CD1	1:B:293:MET:CE	2.75	0.63
1:B:195:ASP:OD1	4:B:3002:DTT:O3	2.17	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:266:LEU:CD1	1:F:293:MET:HE1	2.27	0.63
1:B:214:ILE:HG23	1:B:251:MET:CE	2.28	0.62
1:G:214:ILE:HG23	1:G:251:MET:CE	2.30	0.61
1:E:113:VAL:HA	1:E:143:TYR:HB3	1.83	0.61
1:F:266:LEU:HD13	1:F:293:MET:CE	2.31	0.61
1:B:290:ALA:HA	1:B:293:MET:CE	2.29	0.61
1:F:252:SER:HA	4:F:3006:DTT:H12	1.83	0.61
1:E:6:PHE:O	1:E:7:ASP:HB2	2.02	0.60
1:H:79:ASP:HB2	5:H:3081:HOH:O	2.00	0.60
1:A:67:ILE:O	1:A:71:ARG:HG3	2.02	0.59
1:C:214:ILE:HG23	1:C:251:MET:CE	2.33	0.59
1:G:75:GLU:HB2	5:G:3186:HOH:O	2.00	0.59
1:B:151:VAL:HG12	5:B:3110:HOH:O	2.01	0.59
1:B:266:LEU:CD1	1:B:293:MET:HE2	2.32	0.58
1:F:113:VAL:HA	1:F:143:TYR:HB3	1.85	0.58
1:A:6:PHE:HE2	1:A:8:VAL:HG22	1.67	0.57
1:F:39:ASN:OD1	1:F:80:ARG:NH2	2.35	0.57
1:G:236:THR:O	1:G:240:ILE:HG13	2.04	0.57
1:H:234:ILE:N	1:H:234:ILE:HD13	2.18	0.57
1:H:214:ILE:HG23	1:H:251:MET:CE	2.35	0.56
1:H:177:LEU:HD13	1:H:202:TRP:CD2	2.42	0.55
1:A:289:LEU:CD2	1:A:293:MET:HE2	2.36	0.55
1:E:214:ILE:HG23	1:E:251:MET:HE2	1.89	0.54
1:D:113:VAL:HA	1:D:143:TYR:HB3	1.88	0.54
1:H:113:VAL:HA	1:H:143:TYR:HB3	1.89	0.54
1:B:266:LEU:CD1	1:B:293:MET:HE1	2.36	0.53
1:A:266:LEU:CD1	1:A:293:MET:CE	2.83	0.53
1:A:204:ALA:O	1:D:238:ARG:HD3	2.09	0.53
1:A:214:ILE:HG23	1:A:251:MET:CE	2.39	0.52
1:G:71:ARG:HG3	1:G:105:GLU:OE2	2.09	0.52
1:D:43:ASP:OD2	1:D:80:ARG:NH1	2.40	0.52
1:B:204:ALA:O	1:C:238:ARG:HD3	2.09	0.52
1:H:15:LEU:HB2	1:H:226:LEU:CD1	2.40	0.51
1:C:282:THR:HB	1:C:283:PRO:HD2	1.91	0.51
1:G:289:LEU:HG	1:G:293:MET:HE2	1.90	0.51
1:B:229:PHE:CE1	1:B:234:ILE:HD12	2.46	0.51
1:E:90:TYR:HA	1:E:115:PRO:HB3	1.93	0.51
1:D:214:ILE:HG23	1:D:251:MET:CE	2.41	0.50
1:F:214:ILE:HG23	1:F:251:MET:HE2	1.93	0.50
1:A:204:ALA:HB2	1:D:204:ALA:HB2	1.95	0.49
1:E:195:ASP:OD1	4:E:3005:DTT:O3	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:214:ILE:CG2	1:F:251:MET:HE2	2.43	0.48
1:A:16:LEU:HA	1:A:48:GLY:O	2.14	0.48
1:B:299:LEU:HG	1:B:300:ARG:HD2	1.94	0.48
1:D:16:LEU:HA	1:D:48:GLY:O	2.14	0.48
1:F:21:THR:HG23	1:F:69:LEU:HD22	1.96	0.47
1:G:16:LEU:HA	1:G:48:GLY:O	2.14	0.47
1:F:16:LEU:HA	1:F:48:GLY:O	2.14	0.47
1:H:48:GLY:HA2	1:H:82:ARG:O	2.14	0.47
1:A:238:ARG:CD	1:D:204:ALA:O	2.59	0.47
1:F:284:GLU:HB2	5:F:3073:HOH:O	2.15	0.47
1:G:149:SER:O	1:G:150:ALA:HB3	2.15	0.46
1:D:96:ILE:HD11	1:D:131:ALA:HB1	1.97	0.46
1:E:31:THR:HG21	1:E:68:GLU:HG2	1.96	0.46
1:G:120:PRO:HG2	1:G:125:LEU:CD2	2.45	0.46
1:E:16:LEU:HA	1:E:48:GLY:O	2.16	0.46
1:F:70:LEU:HD21	1:F:107:ALA:HB2	1.98	0.46
1:F:266:LEU:HD12	1:F:293:MET:CE	2.33	0.46
1:H:177:LEU:HD13	1:H:202:TRP:CE3	2.51	0.46
1:G:214:ILE:CG2	1:G:251:MET:CE	2.94	0.46
1:F:204:ALA:O	1:G:238:ARG:HD3	2.16	0.45
1:H:177:LEU:HD22	1:H:202:TRP:CZ2	2.51	0.45
1:A:199:ASN:HB3	1:A:210:PHE:CZ	2.52	0.45
1:H:214:ILE:CG2	1:H:251:MET:CE	2.94	0.45
1:A:263:GLY:HA2	1:A:293:MET:HE1	1.99	0.45
1:E:214:ILE:CG2	1:E:251:MET:CE	2.93	0.45
1:C:251:MET:HB3	4:C:3003:DTT:H41	1.99	0.45
1:A:289:LEU:CD1	1:A:293:MET:HE2	2.44	0.44
1:G:166:ASN:ND2	5:G:3161:HOH:O	2.45	0.44
1:H:120:PRO:HG2	1:H:125:LEU:CD2	2.48	0.44
1:E:96:ILE:HD11	1:E:131:ALA:HB1	1.98	0.44
1:F:214:ILE:CG2	1:F:251:MET:CE	2.94	0.44
1:B:204:ALA:HB2	1:C:204:ALA:HB2	1.99	0.44
1:A:289:LEU:CG	1:A:293:MET:CE	2.63	0.44
1:D:200:LEU:HB3	1:D:201:PRO:HD3	1.99	0.44
1:E:201:PRO:HB3	1:H:201:PRO:HB3	2.00	0.44
1:C:58:SER:N	1:C:59:PRO:CD	2.81	0.44
1:D:58:SER:N	1:D:59:PRO:CD	2.81	0.44
1:A:199:ASN:HB3	1:A:210:PHE:CE2	2.53	0.43
1:G:242:ILE:HD13	1:G:242:ILE:HA	1.84	0.43
1:G:48:GLY:HA2	1:G:82:ARG:O	2.17	0.43
1:B:16:LEU:HA	1:B:48:GLY:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:197:ALA:HB1	1:C:178:HIS:HB2	2.01	0.43
1:B:238:ARG:HD3	1:C:204:ALA:O	2.19	0.43
1:B:294:ARG:HE	1:B:300:ARG:HE	1.65	0.43
1:A:120:PRO:HG2	1:A:125:LEU:CD2	2.49	0.43
1:A:282:THR:OG1	1:A:285:GLN:HG3	2.19	0.42
1:D:149:SER:O	1:D:150:ALA:HB3	2.18	0.42
1:H:120:PRO:HG2	1:H:125:LEU:HD21	2.01	0.42
1:E:184:MET:HG2	1:E:189:LEU:O	2.20	0.42
1:E:214:ILE:CG2	1:E:251:MET:HE2	2.48	0.42
1:B:8:VAL:HG13	1:B:12:LEU:HD12	2.01	0.42
1:B:289:LEU:HG	1:B:293:MET:HE2	2.02	0.42
1:D:6:PHE:CE2	1:D:8:VAL:HG22	2.55	0.42
1:C:245:ALA:N	1:C:246:PRO:CD	2.83	0.41
1:C:24:SER:HB2	1:C:26:ASP:OD1	2.20	0.41
1:C:120:PRO:HG2	1:C:125:LEU:HD21	2.02	0.41
1:H:8:VAL:HG13	1:H:12:LEU:HD12	2.02	0.41
1:E:90:TYR:N	1:E:90:TYR:CD2	2.85	0.41
1:A:6:PHE:CD2	1:A:8:VAL:HG22	2.55	0.41
1:G:117:TYR:HH	1:H:54:THR:HG1	1.66	0.41
1:A:58:SER:N	1:A:59:PRO:CD	2.84	0.41
1:G:120:PRO:HG2	1:G:125:LEU:HD21	2.03	0.41
1:H:222:LEU:HD23	1:H:222:LEU:HA	1.92	0.41
1:H:16:LEU:HA	1:H:48:GLY:O	2.21	0.41
1:B:293:MET:HE3	1:B:293:MET:HB2	1.69	0.40
1:C:14:THR:O	1:C:209:GLY:HA3	2.20	0.40
1:C:214:ILE:CG2	1:C:251:MET:HE2	2.51	0.40
1:E:203:LEU:HD11	1:E:226:LEU:HD23	2.03	0.40
1:E:90:TYR:HH	1:F:116:TYR:HH	1.66	0.40
1:A:234:ILE:HG13	1:D:234:ILE:HD11	2.03	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	294/303 (97%)	289 (98%)	5 (2%)	0	100	100
1	B	293/303 (97%)	289 (99%)	4 (1%)	0	100	100
1	C	294/303 (97%)	288 (98%)	6 (2%)	0	100	100
1	D	293/303 (97%)	286 (98%)	7 (2%)	0	100	100
1	E	293/303 (97%)	285 (97%)	7 (2%)	1 (0%)	41	49
1	F	294/303 (97%)	287 (98%)	7 (2%)	0	100	100
1	G	293/303 (97%)	287 (98%)	6 (2%)	0	100	100
1	H	294/303 (97%)	287 (98%)	7 (2%)	0	100	100
All	All	2348/2424 (97%)	2298 (98%)	49 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	7	ASP

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	216/221 (98%)	212 (98%)	4 (2%)	57	71
1	B	216/221 (98%)	210 (97%)	6 (3%)	43	57
1	C	216/221 (98%)	213 (99%)	3 (1%)	67	79
1	D	216/221 (98%)	213 (99%)	3 (1%)	67	79
1	E	216/221 (98%)	214 (99%)	2 (1%)	78	88
1	F	216/221 (98%)	212 (98%)	4 (2%)	57	71
1	G	216/221 (98%)	208 (96%)	8 (4%)	34	45
1	H	216/221 (98%)	211 (98%)	5 (2%)	50	65
All	All	1728/1768 (98%)	1693 (98%)	35 (2%)	55	70

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	90	TYR
1	A	259	LEU
1	A	284	GLU
1	A	300	ARG
1	B	71	ARG
1	B	84	ILE
1	B	90	TYR
1	B	98	LEU
1	B	259	LEU
1	B	300	ARG
1	C	90	TYR
1	C	259	LEU
1	C	287	ASP
1	D	90	TYR
1	D	115	PRO
1	D	177	LEU
1	E	84	ILE
1	E	90	TYR
1	F	84	ILE
1	F	90	TYR
1	F	126	GLN
1	F	259	LEU
1	G	71	ARG
1	G	75	GLU
1	G	84	ILE
1	G	90	TYR
1	G	115	PRO
1	G	155	PRO
1	G	177	LEU
1	G	259	LEU
1	H	84	ILE
1	H	90	TYR
1	H	177	LEU
1	H	259	LEU
1	H	300	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	44	GLN
1	F	278	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

Of 24 ligands modelled in this entry, 16 are monoatomic - leaving 8 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$
4	DTT	G	3007	1	7,7,7	1.25	1 (14%)	4,8,8	1.99	1 (25%)
4	DTT	C	3003	1	7,7,7	0.93	0	4,8,8	3.13	3 (75%)
4	DTT	B	3002	1	7,7,7	1.35	1 (14%)	4,8,8	2.08	1 (25%)
4	DTT	F	3006	1	7,7,7	0.72	0	4,8,8	2.28	2 (50%)
4	DTT	A	3001	1	7,7,7	1.64	1 (14%)	4,8,8	1.48	1 (25%)
4	DTT	E	3005	1	7,7,7	1.02	0	4,8,8	1.24	1 (25%)
4	DTT	H	3008	1	7,7,7	0.90	1 (14%)	4,8,8	2.23	1 (25%)
4	DTT	D	3004	1	7,7,7	1.32	2 (28%)	4,8,8	1.72	1 (25%)

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
4	DTT	G	3007	1	-	5/8/8/8	-
4	DTT	C	3003	1	-	3/8/8/8	-
4	DTT	B	3002	1	-	1/8/8/8	-
4	DTT	F	3006	1	-	7/8/8/8	-
4	DTT	A	3001	1	-	3/8/8/8	-
4	DTT	E	3005	1	-	1/8/8/8	-
4	DTT	H	3008	1	-	6/8/8/8	-
4	DTT	D	3004	1	-	0/8/8/8	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3007	DTT	O3-C3	-2.95	1.37	1.43
4	B	3002	DTT	O3-C3	-2.91	1.37	1.43
4	A	3001	DTT	O3-C3	-2.47	1.38	1.43
4	D	3004	DTT	O2-C2	-2.41	1.38	1.43
4	H	3008	DTT	O3-C3	-2.12	1.38	1.43
4	D	3004	DTT	O3-C3	-2.11	1.38	1.43

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3003	DTT	O2-C2-C3	5.07	120.15	109.72
4	H	3008	DTT	O3-C3-C2	-3.85	101.81	109.72
4	F	3006	DTT	C2-C1-S1	-3.56	104.11	114.47
4	B	3002	DTT	O2-C2-C3	-3.50	102.53	109.72
4	G	3007	DTT	O3-C3-C2	-3.16	103.23	109.72
4	C	3003	DTT	O3-C3-C2	2.65	115.17	109.72
4	D	3004	DTT	O3-C3-C2	-2.52	104.55	109.72
4	F	3006	DTT	C3-C4-S4	2.45	121.58	114.47
4	A	3001	DTT	C3-C4-S4	2.20	120.87	114.47
4	E	3005	DTT	O3-C3-C2	-2.14	105.34	109.72
4	C	3003	DTT	C2-C1-S1	2.02	120.35	114.47

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	3003	DTT	S1-C1-C2-O2
4	C	3003	DTT	S1-C1-C2-C3
4	B	3002	DTT	O3-C3-C4-S4

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Mol	Chain	Res	Type	Atoms
4	H	3008	DTT	C1-C2-C3-O3
4	H	3008	DTT	C1-C2-C3-C4
4	H	3008	DTT	O2-C2-C3-O3
4	H	3008	DTT	O2-C2-C3-C4
4	H	3008	DTT	O3-C3-C4-S4
4	A	3001	DTT	S1-C1-C2-O2
4	A	3001	DTT	S1-C1-C2-C3
4	A	3001	DTT	O3-C3-C4-S4
4	F	3006	DTT	S1-C1-C2-O2
4	F	3006	DTT	C1-C2-C3-O3
4	F	3006	DTT	C1-C2-C3-C4
4	F	3006	DTT	O2-C2-C3-O3
4	F	3006	DTT	O2-C2-C3-C4
4	F	3006	DTT	C2-C3-C4-S4
4	F	3006	DTT	O3-C3-C4-S4
4	E	3005	DTT	S1-C1-C2-O2
4	G	3007	DTT	C1-C2-C3-O3
4	G	3007	DTT	C1-C2-C3-C4
4	G	3007	DTT	O2-C2-C3-O3
4	G	3007	DTT	O2-C2-C3-C4
4	G	3007	DTT	O3-C3-C4-S4
4	C	3003	DTT	C1-C2-C3-C4
4	H	3008	DTT	C2-C3-C4-S4

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	3003	DTT	2	0
4	B	3002	DTT	1	0
4	F	3006	DTT	1	0
4	E	3005	DTT	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data [i](#)

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

EDS failed to run properly - this section is therefore empty.

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

EDS failed to run properly - this section is therefore empty.

### 6.3 Carbohydrates [i](#)

EDS failed to run properly - this section is therefore empty.

### 6.4 Ligands [i](#)

EDS failed to run properly - this section is therefore empty.

### 6.5 Other polymers [i](#)

EDS failed to run properly - this section is therefore empty.