



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 03:36 PM UTC

PDB ID : 1XXX / pdb_00001xxx
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

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:

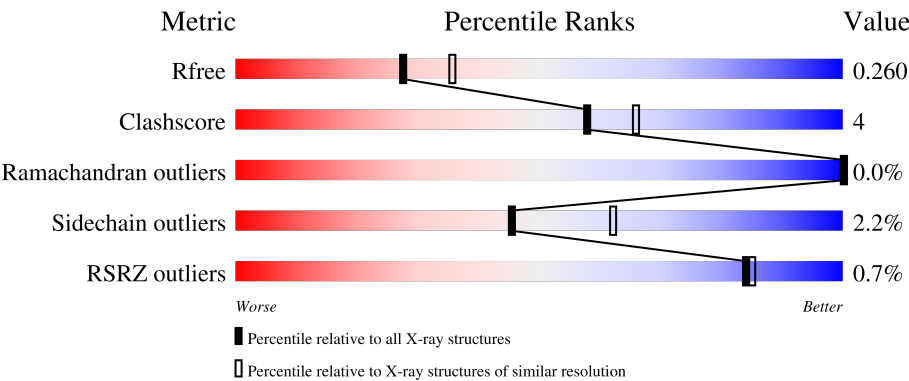
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

1 Overall quality at a glance i

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))
R _{free}	180053	9078 (2.30-2.26)
Clashscore	190562	9802 (2.30-2.26)
Ramachandran outliers	187476	9690 (2.30-2.26)
Sidechain outliers	187428	9691 (2.30-2.26)
RSRZ outliers	180081	9085 (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 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	303	86%11%.
1	B	303	% 86%11%.
1	C	303	86%12%.
1	D	303	87%10%.
1	E	303	89%8%..

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Mol	Chain	Length	Quality of chain
1	F	303	4% 89% 9%
1	G	303	87% 10%
1	H	303	89% 8%

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

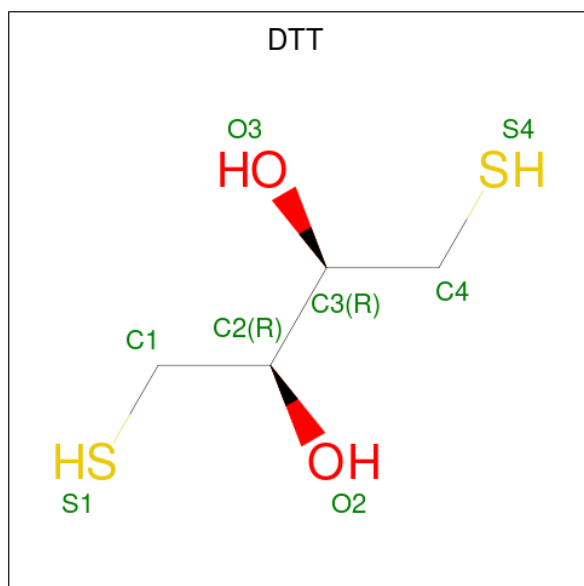
- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is 2,3-DIHYDROXY-1,4-DITHIOBUTANE (CCD ID: 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		

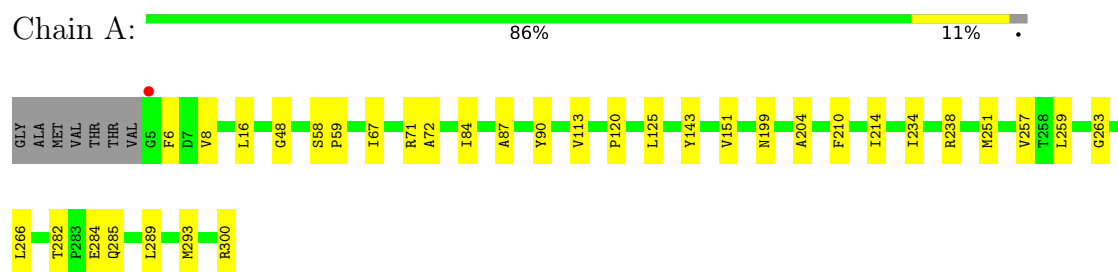
- Molecule 5 is water.

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		

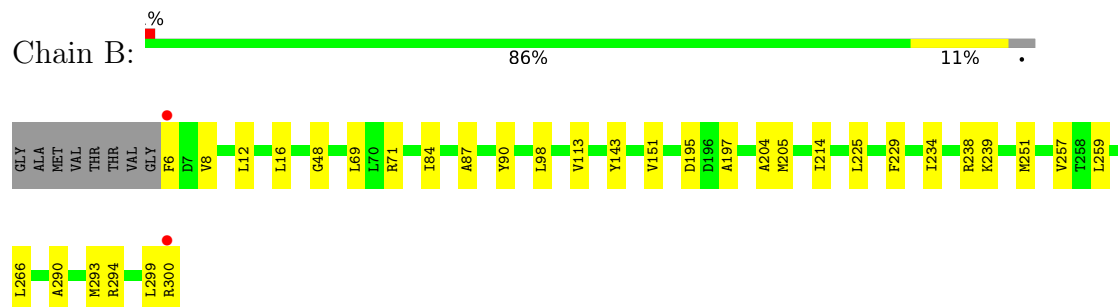
3 Residue-property plots

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.

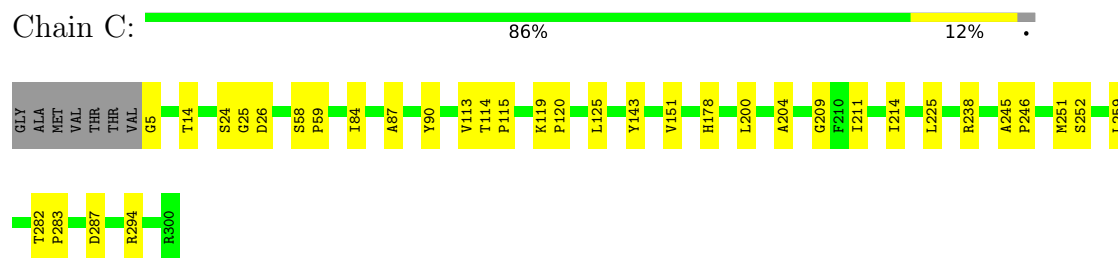
• Molecule 1: Dihydrodipicolinate synthase



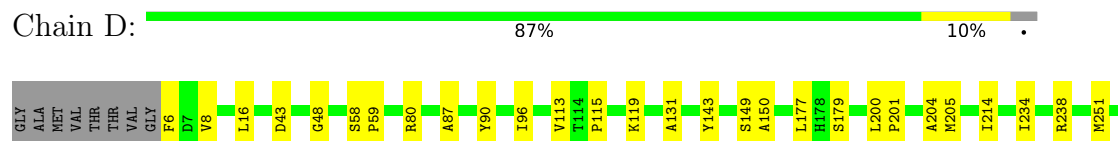
• Molecule 1: Dihydrodipicolinate synthase



• Molecule 1: Dihydrodipicolinate synthase



• Molecule 1: Dihydrodipicolinate synthase





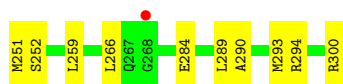
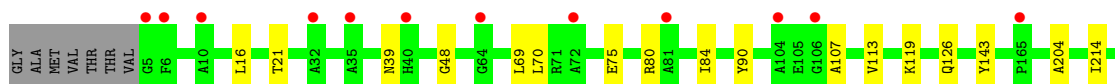
- Molecule 1: Dihydrodipicolinate synthase

Chain E:  89% 8% ..



- Molecule 1: Dihydrodipicolinate synthase

Chain F:  4% 89% 9% .



- Molecule 1: Dihydrodipicolinate synthase

Chain G:  87% 10% ..



- Molecule 1: Dihydrodipicolinate synthase

Chain H:  89% 8% .



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	94.79Å 87.37Å 139.85Å 90.00° 107.78° 90.00°	Depositor
Resolution (Å)	30.00 – 2.28 30.00 – 2.28	Depositor EDS
% Data completeness (in resolution range)	100.0 (30.00-2.28) 99.9 (30.00-2.28)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.22 (at 2.29Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.148 , 0.215 (Not available) , 0.260	Depositor DCC
R_{free} test set	1987 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.473	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 31.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18739	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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: 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	1.11	2/2170 (0.1%)	1.07	3/2956 (0.1%)
1	B	1.11	1/2166 (0.0%)	1.10	2/2951 (0.1%)
1	C	1.12	3/2170 (0.1%)	1.09	7/2956 (0.2%)
1	D	1.14	2/2166 (0.1%)	1.07	5/2951 (0.2%)
1	E	0.97	2/2166 (0.1%)	0.95	0/2951
1	F	0.91	2/2170 (0.1%)	0.96	0/2956
1	G	1.11	1/2166 (0.0%)	1.07	2/2951 (0.1%)
1	H	1.02	0/2170	1.04	3/2956 (0.1%)
All	All	1.07	13/17344 (0.1%)	1.05	22/23628 (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 (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	75	GLU	CD-OE1	7.13	1.39	1.25
1	A	151	VAL	CA-CB	6.11	1.62	1.54
1	D	179	SER	C-O	-6.01	1.17	1.24
1	E	298	VAL	CA-CB	5.76	1.60	1.54
1	A	257	VAL	CA-CB	5.51	1.60	1.54
1	B	257	VAL	CA-CB	5.48	1.60	1.54
1	C	211	ILE	CA-CB	5.35	1.60	1.53
1	F	119	LYS	C-O	-5.34	1.21	1.23
1	C	200	LEU	CA-C	5.34	1.58	1.52
1	C	151	VAL	CA-CB	5.15	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	281	ALA	CA-CB	5.11	1.62	1.53
1	E	20	VAL	CA-CB	5.08	1.59	1.54
1	G	99	ALA	CA-CB	5.03	1.61	1.53

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	87	ALA	CA-C-N	-10.93	111.95	122.66
1	C	87	ALA	C-N-CA	-10.93	111.95	122.66
1	B	87	ALA	CA-C-N	-9.38	115.71	122.18
1	B	87	ALA	C-N-CA	-9.38	115.71	122.18
1	H	87	ALA	CA-C-N	-9.00	115.97	122.18
1	H	87	ALA	C-N-CA	-9.00	115.97	122.18
1	A	87	ALA	CA-C-N	-8.20	114.84	122.80
1	A	87	ALA	C-N-CA	-8.20	114.84	122.80
1	G	87	ALA	CA-C-N	-6.92	116.09	122.80
1	G	87	ALA	C-N-CA	-6.92	116.09	122.80
1	C	25	GLY	N-CA-C	-6.13	105.39	112.50
1	D	294	ARG	CG-CD-NE	-6.10	98.59	112.00
1	H	93	ALA	N-CA-C	-6.06	104.76	111.36
1	C	225	LEU	N-CA-C	-5.90	104.76	111.07
1	D	87	ALA	CA-C-N	-5.82	117.15	122.80
1	D	87	ALA	C-N-CA	-5.82	117.15	122.80
1	C	294	ARG	CG-CD-NE	-5.40	100.12	112.00
1	C	119	LYS	CA-C-N	-5.10	115.12	120.38
1	C	119	LYS	C-N-CA	-5.10	115.12	120.38
1	A	72	ALA	N-CA-C	-5.07	105.84	111.36
1	D	119	LYS	CA-C-N	-5.04	115.19	120.38
1	D	119	LYS	C-N-CA	-5.04	115.19	120.38

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

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	30	0
1	B	2132	0	2155	26	0
1	C	2136	0	2158	17	0
1	D	2132	0	2155	16	0
1	E	2132	0	2155	17	0
1	F	2136	0	2158	23	0
1	G	2132	0	2155	22	0
1	H	2136	0	2158	17	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	2	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	154	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 (154) 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:G:266:LEU:CD1	1:G:293:MET:HE1	1.65	1.25
1:B:266:LEU:HD13	1:B:293:MET:HE1	1.22	1.18
1:G:266:LEU:HD13	1:G:293:MET:HE1	1.24	1.14
1:F:289:LEU:HG	1:F:293:MET:HE2	1.20	1.13
1:A:289:LEU:HG	1:A:293:MET:CE	1.78	1.12
1:A:289:LEU:HG	1:A:293:MET:HE2	1.19	1.11
1:G:289:LEU:HG	1:G:293:MET:HE2	1.28	1.08
1:F:266:LEU:CD1	1:F:293:MET:HE1	1.85	1.07
1:A:289:LEU:CG	1:A:293:MET:HE2	1.87	1.05
1:G:266:LEU:HD13	1:G:293:MET:CE	1.90	1.02
1:F:266:LEU:HD12	1:F:293:MET:HE1	1.37	1.02
1:D:284:GLU:HG3	5:D:3097:HOH:O	1.62	0.99
1:B:266:LEU:CD1	1:B:293:MET:HE1	1.94	0.97
1:G:266:LEU:HD12	1:G:293:MET:HE1	1.46	0.96
1:B:266:LEU:HD13	1:B:293:MET:CE	1.96	0.96
1:A:266:LEU:HD12	1:A:293:MET:HE1	1.45	0.95
1:B:6:PHE:HE2	1:B:8:VAL:HG22	1.35	0.92
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	0.80
1:B:6:PHE:CE2	1:B:8:VAL:HG22	2.16	0.78
1:F:266:LEU:HD13	1:F:293:MET:HE1	1.65	0.76
1:F:289:LEU:CG	1:F:293:MET:HE2	2.11	0.73
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:G:113:VAL:HA	1:G:143:TYR:HB3	1.73	0.69
1:G:290:ALA:HA	1:G:293:MET:HE3	1.74	0.69
1:A:113:VAL:HA	1:A:143:TYR:HB3	1.74	0.69
1:B:293:MET:HE3	1:B:299:LEU:HD22	1.76	0.68
1:A:266:LEU:HD12	1:A:293:MET:CE	2.20	0.67
1:G:289:LEU:HG	1:G:293:MET:CE	2.16	0.67
1:F:294:ARG:HG2	1:F:300:ARG:HB3	1.77	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:214:ILE:HG23	1:F:251:MET:CE	2.27	0.64
1:E:300:ARG:HD2	5:E:3053:HOH:O	1.96	0.64
1:B:195:ASP:OD1	4:B:3002:DTT:O3	2.17	0.63
1:B:214:ILE:HG23	1:B:251:MET:CE	2.28	0.62
1:B:290:ALA:HA	1:B:293:MET:CE	2.29	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:A:289:LEU:HG	1:A:293:MET:HE3	1.77	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:F:113:VAL:HA	1:F:143:TYR:HB3	1.85	0.58
1:A:266:LEU:CD1	1:A:293:MET:HE1	2.27	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:A:266:LEU:CD1	1:A:293:MET:CE	2.83	0.57
1:F:266:LEU:CD1	1:F:293:MET:CE	2.73	0.56
1:H:214:ILE:HG23	1:H:251:MET:CE	2.35	0.56
1:E:214:ILE:HG23	1:E:251:MET:HE2	1.89	0.55
1:H:177:LEU:HD13	1:H:202:TRP:CD2	2.42	0.55
1:D:113:VAL:HA	1:D:143:TYR:HB3	1.88	0.54
1:F:290:ALA:HA	1:F:293:MET:HE3	1.90	0.54
1:H:113:VAL:HA	1:H:143:TYR:HB3	1.89	0.54
1:A:204:ALA:O	1:D:238:ARG:HD3	2.09	0.53
1:F:214:ILE:HG23	1:F:251:MET:HE2	1.90	0.52
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:B:290:ALA:HA	1:B:293:MET:HE2	1.91	0.51
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:A:263:GLY:HA2	1:A:293:MET:HE1	1.92	0.51
1:B:229:PHE:CE1	1:B:234:ILE:HD12	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:204:ALA:HB2	1:D:204:ALA:HB2	1.95	0.49
1:A:289:LEU:CD2	1:A:293:MET:HE2	2.40	0.49
1:E:195:ASP:OD1	4:E:3005:DTT:O3	2.31	0.49
1:F:214:ILE:CG2	1:F:251:MET:HE2	2.44	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:B:266:LEU:CD1	1:B:293:MET:CE	2.75	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:A:289:LEU:CD1	1:A:293:MET:HE2	2.41	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: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: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: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:A:238:ARG:HD2	1:D:205:MET:C	2.43	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:B:290:ALA:HA	1:B:293:MET:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:48:GLY:HA2	1:G:82:ARG:O	2.17	0.43
1:G:242:ILE:HD13	1:G:242:ILE:HA	1.84	0.43
1:B:16:LEU:HA	1:B:48:GLY:O	2.19	0.43
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:B:225:LEU:C	1:B:225:LEU:HD23	2.44	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:C:214:ILE:HG23	1:C:251:MET:HE2	2.01	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:C:114:THR:O	1:C:115:PRO:C	2.60	0.42
1:E:184:MET:HG2	1:E:189:LEU:O	2.20	0.42
1:B:8:VAL:HG13	1:B:12:LEU:HD12	2.01	0.42
1:D:6:PHE:CE2	1:D:8:VAL:HG22	2.55	0.42
1:E:214:ILE:CG2	1:E:251:MET:HE2	2.49	0.42
1:B:239:LYS:NZ	5:B:3166:HOH:O	2.53	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:B:205:MET:C	1:C:238:ARG:HD2	2.45	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: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:C:14:THR:O	1:C:209:GLY:HA3	2.20	0.40
1:E:203:LEU:HD11	1:E:226:LEU:HD23	2.03	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%)	36	44
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%)	211 (98%)	5 (2%)	44	60
1	B	216/221 (98%)	210 (97%)	6 (3%)	38	53
1	C	216/221 (98%)	212 (98%)	4 (2%)	50	66
1	D	216/221 (98%)	213 (99%)	3 (1%)	59	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	216/221 (98%)	213 (99%)	3 (1%)	59	74
1	F	216/221 (98%)	212 (98%)	4 (2%)	50	66
1	G	216/221 (98%)	208 (96%)	8 (4%)	30	43
1	H	216/221 (98%)	211 (98%)	5 (2%)	44	60
All	All	1728/1768 (98%)	1690 (98%)	38 (2%)	45	62

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	ILE
1	A	90	TYR
1	A	259	LEU
1	A	284	GLU
1	A	300	ARG
1	B	69	LEU
1	B	71	ARG
1	B	84	ILE
1	B	90	TYR
1	B	98	LEU
1	B	259	LEU
1	C	84	ILE
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	E	239	LYS
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	98	LEU
1	G	115	PRO
1	G	177	LEU

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Mol	Chain	Res	Type
1	G	259	LEU
1	H	84	ILE
1	H	90	TYR
1	H	177	LEU
1	H	259	LEU
1	H	300	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	126	GLN
1	A	166	ASN
1	B	44	GLN
1	B	267	GLN
1	D	166	ASN
1	F	126	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](#)

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 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	D	3004	1	7,7,7	1.33	2 (28%)	4,8,8	1.66	1 (25%)
4	DTT	F	3006	1	7,7,7	0.74	0	4,8,8	2.35	2 (50%)
4	DTT	B	3002	1	7,7,7	1.36	1 (14%)	4,8,8	2.00	1 (25%)
4	DTT	C	3003	1	7,7,7	0.95	0	4,8,8	3.14	3 (75%)
4	DTT	G	3007	1	7,7,7	1.26	1 (14%)	4,8,8	1.93	1 (25%)
4	DTT	H	3008	1	7,7,7	0.91	1 (14%)	4,8,8	2.17	2 (50%)
4	DTT	A	3001	1	7,7,7	1.67	2 (28%)	4,8,8	1.49	1 (25%)
4	DTT	E	3005	1	7,7,7	1.03	0	4,8,8	1.18	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	D	3004	1	-	0/8/8/8	-
4	DTT	F	3006	1	-	7/8/8/8	-
4	DTT	B	3002	1	-	1/8/8/8	-
4	DTT	C	3003	1	-	3/8/8/8	-
4	DTT	G	3007	1	-	5/8/8/8	-
4	DTT	H	3008	1	-	6/8/8/8	-
4	DTT	A	3001	1	-	3/8/8/8	-
4	DTT	E	3005	1	-	1/8/8/8	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	3007	DTT	O3-C3	-2.98	1.37	1.43
4	B	3002	DTT	O3-C3	-2.93	1.37	1.43
4	A	3001	DTT	O3-C3	-2.49	1.38	1.43
4	D	3004	DTT	O2-C2	-2.43	1.38	1.43
4	H	3008	DTT	O3-C3	-2.14	1.38	1.43
4	D	3004	DTT	O3-C3	-2.13	1.38	1.43
4	A	3001	DTT	C1-S1	2.01	1.85	1.81

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	3003	DTT	O2-C2-C3	5.03	120.15	109.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	3008	DTT	O3-C3-C2	-3.69	101.81	109.57
4	F	3006	DTT	C2-C1-S1	-3.69	104.11	114.43
4	B	3002	DTT	O2-C2-C3	-3.35	102.53	109.57
4	G	3007	DTT	O3-C3-C2	-3.02	103.23	109.57
4	C	3003	DTT	O3-C3-C2	2.66	115.17	109.57
4	F	3006	DTT	C3-C4-S4	2.56	121.58	114.43
4	D	3004	DTT	O3-C3-C2	-2.39	104.55	109.57
4	A	3001	DTT	C3-C4-S4	2.30	120.87	114.43
4	C	3003	DTT	C2-C1-S1	2.12	120.35	114.43
4	H	3008	DTT	C2-C1-S1	-2.02	108.78	114.43
4	E	3005	DTT	O3-C3-C2	-2.02	105.34	109.57

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
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	B	3002	DTT	O3-C3-C4-S4
4	C	3003	DTT	S1-C1-C2-O2
4	C	3003	DTT	S1-C1-C2-C3
4	E	3005	DTT	S1-C1-C2-O2
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	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	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	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	F	3006	DTT	1	0
4	B	3002	DTT	1	0
4	C	3003	DTT	2	0
4	E	3005	DTT	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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	296/303 (97%)	0.08	1 (0%) 90 90	25, 28, 35, 54	0
1	B	295/303 (97%)	-0.30	2 (0%) 84 85	23, 28, 35, 53	0
1	C	296/303 (97%)	0.07	0 100 100	25, 28, 36, 55	0
1	D	295/303 (97%)	-0.32	0 100 100	25, 28, 35, 49	0
1	E	295/303 (97%)	0.34	1 (0%) 90 90	25, 28, 36, 60	0
1	F	296/303 (97%)	0.87	13 (4%) 39 40	25, 29, 35, 48	0
1	G	295/303 (97%)	0.05	0 100 100	24, 28, 35, 57	0
1	H	296/303 (97%)	-0.12	0 100 100	24, 28, 36, 54	0
All	All	2364/2424 (97%)	0.08	17 (0%) 84 85	23, 28, 36, 60	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	6	PHE	4.7
1	A	5	GLY	3.6
1	F	5	GLY	3.3
1	F	32	ALA	2.8
1	B	300	ARG	2.6
1	F	6	PHE	2.5
1	F	64	GLY	2.5
1	F	268	GLY	2.5
1	F	81	ALA	2.4
1	F	72	ALA	2.3
1	F	104	ALA	2.3
1	F	106	GLY	2.3
1	B	6	PHE	2.2
1	F	165	PRO	2.2
1	F	40	HIS	2.1
1	F	10	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	F	35	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no 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($\text{\AA}^2$)	Q<0.9
2	MG	D	2004	1/1	0.73	0.12	38,38,38,38	0
2	MG	F	2006	1/1	0.83	0.11	52,52,52,52	0
2	MG	H	2008	1/1	0.85	0.07	34,34,34,34	0
4	DTT	C	3003	8/8	0.85	0.14	32,43,56,70	0
4	DTT	F	3006	8/8	0.87	0.15	35,53,56,59	0
4	DTT	E	3005	8/8	0.88	0.13	35,46,58,59	0
2	MG	A	2001	1/1	0.88	0.07	31,31,31,31	0
4	DTT	A	3001	8/8	0.89	0.14	32,41,53,56	0
4	DTT	D	3004	8/8	0.89	0.13	27,37,47,47	0
2	MG	C	2003	1/1	0.90	0.07	28,28,28,28	0
4	DTT	B	3002	8/8	0.90	0.12	26,37,46,52	0
2	MG	E	2005	1/1	0.90	0.10	41,41,41,41	0
2	MG	G	2007	1/1	0.91	0.10	32,32,32,32	0
4	DTT	G	3007	8/8	0.91	0.11	31,39,51,54	0
4	DTT	H	3008	8/8	0.91	0.12	35,48,56,59	0
2	MG	B	2002	1/1	0.94	0.07	34,34,34,34	0
3	CL	E	2013	1/1	0.96	0.11	42,42,42,42	0
3	CL	G	2015	1/1	0.97	0.14	39,39,39,39	0
3	CL	H	2016	1/1	0.97	0.13	42,42,42,42	0
3	CL	C	2011	1/1	0.98	0.07	30,30,30,30	0
3	CL	B	2010	1/1	0.98	0.12	36,36,36,36	0
3	CL	A	2009	1/1	0.99	0.11	26,26,26,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CL	F	2014	1/1	0.99	0.09	37,37,37,37	0
3	CL	D	2012	1/1	0.99	0.06	31,31,31,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.