



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:54 AM GMT

PDB ID : 2V8T  
Title : CRYSTAL STRUCTURE OF MN CATALASE FROM THERMUS THERMOPHILUS COMPLEXED WITH CHLORIDE  
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Deposited on : 2007-08-14  
Resolution : 0.98 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

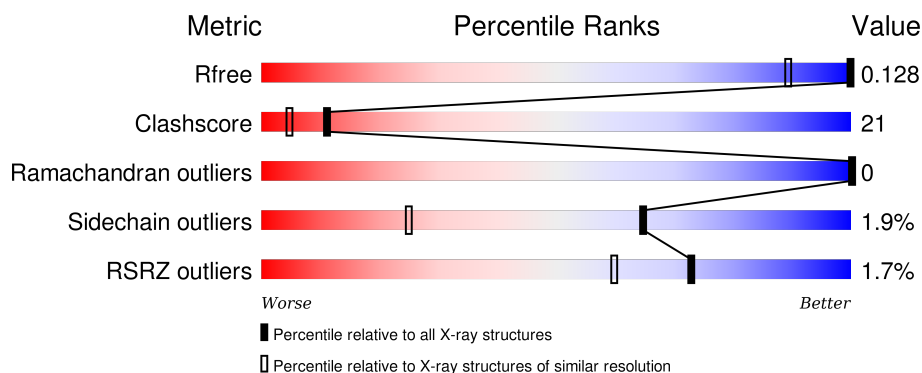
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 0.98 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))
$R_{free}$	91344	1291 (1.10-0.86)
Clashscore	102246	1390 (1.10-0.86)
Ramachandran outliers	100387	1301 (1.10-0.86)
Sidechain outliers	100360	1300 (1.10-0.86)
RSRZ outliers	91569	1295 (1.10-0.86)

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. 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	302	<div> <div></div> <div>79%17%•</div> </div>
1	B	302	<div> <div>2%</div> <div>82%16%•</div> </div>

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
4	SO4	A	1307	-	-	X	X
4	SO4	A	1310	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6073 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 MANGANESE-CONTAINING PSEUDOCATALASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	3	37	0
			2519	1618	418	467	16			
1	B	302	Total	C	N	O	S	5	35	0
			2516	1623	421	458	14			

- Molecule 2 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mn	0	0
			2	2		
2	A	2	Total	Mn	0	0
			2	2		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total	Cl	0	0
			2	2		
3	A	2	Total	Cl	0	0
			2	2		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		
4	B	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is LITHIUM ION (three-letter code: LI) (formula: Li).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Li	0	0
			1	1		

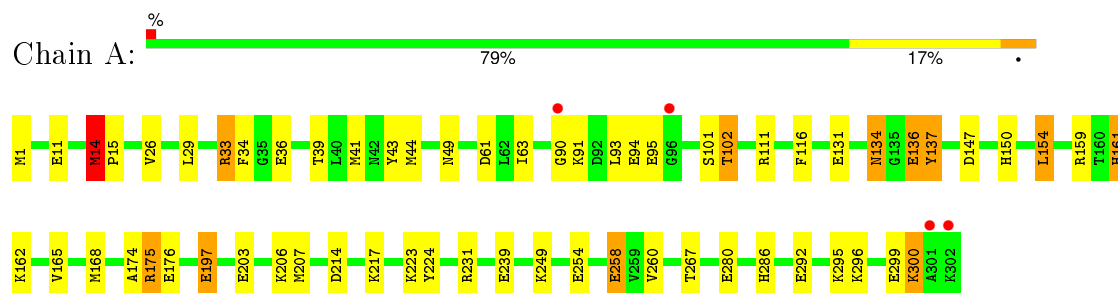
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	517	Total	O	0	0
			517	517		
6	B	482	Total	O	0	0
			482	482		

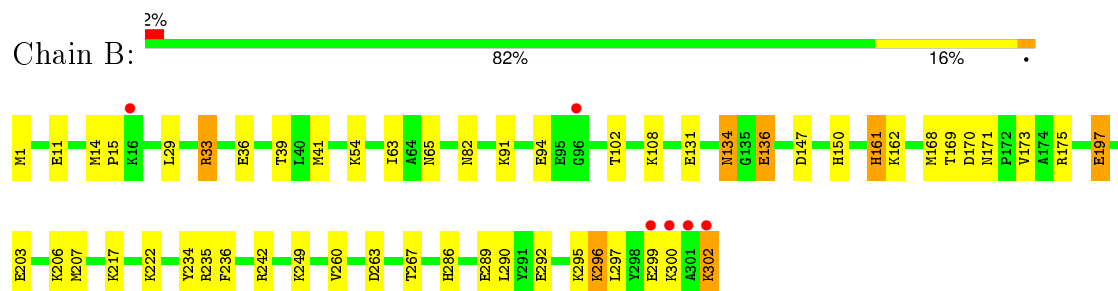
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: MANGANESE-CONTAINING PSEUDOCATALASE



#### • Molecule 1: MANGANESE-CONTAINING PSEUDOCATALASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	132.07Å 132.07Å 132.07Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 0.98 28.16 – 0.98	Depositor EDS
% Data completeness (in resolution range)	97.9 (30.00-0.98) 97.9 (28.16-0.98)	Depositor EDS
$R_{merge}$	0.04	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.38 (at 0.98Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.101 , 0.117 0.113 , 0.128	Depositor DCC
$R_{free}$ test set	866 reflections (0.20%)	DCC
Wilson B-factor (Å <sup>2</sup> )	9.4	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.4	EDS
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Outliers	0 of 425226 reflections	Xtriage
$F_o, F_c$ correlation	0.99	EDS
Total number of atoms	6073	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.63% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: CL, MN, SO4, LI

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	0.97	11/2722 (0.4%)	1.15	19/3674 (0.5%)
1	B	4.56	10/2712 (0.4%)	1.10	26/3659 (0.7%)
All	All	3.29	21/5434 (0.4%)	1.13	45/7333 (0.6%)

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	197[A]	GLU	CD-OE1	164.43	3.06	1.25
1	B	197[B]	GLU	CD-OE1	164.43	3.06	1.25
1	A	33[A]	ARG	CZ-NH1	-8.12	1.22	1.33
1	A	33[B]	ARG	CZ-NH1	-8.12	1.22	1.33
1	B	94	GLU	CG-CD	8.07	1.64	1.51
1	A	136	GLU	CD-OE1	-8.01	1.16	1.25
1	A	101	SER	CB-OG	7.54	1.52	1.42
1	B	136	GLU	CD-OE1	-7.00	1.18	1.25
1	A	136	GLU	CB-CG	6.58	1.64	1.52
1	B	295[A]	LYS	CD-CE	-6.45	1.35	1.51
1	B	295[B]	LYS	CD-CE	-6.45	1.35	1.51
1	A	207	MET	CA-CB	6.43	1.68	1.53
1	B	234	TYR	CD1-CE1	6.37	1.49	1.39
1	A	258	GLU	CD-OE1	6.20	1.32	1.25
1	B	207	MET	CA-CB	6.06	1.67	1.53
1	B	136	GLU	CB-CG	5.93	1.63	1.52
1	A	94	GLU	CG-CD	5.60	1.60	1.51
1	A	44	MET	SD-CE	-5.51	1.47	1.77
1	A	197[A]	GLU	CD-OE1	5.36	1.31	1.25
1	A	197[B]	GLU	CD-OE1	5.36	1.31	1.25
1	B	168	MET	SD-CE	-5.35	1.47	1.77

All (45) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175[A]	ARG	NE-CZ-NH2	-14.65	112.97	120.30
1	A	175[B]	ARG	NE-CZ-NH2	-14.65	112.97	120.30
1	A	33[A]	ARG	NE-CZ-NH1	-13.73	113.44	120.30
1	A	33[B]	ARG	NE-CZ-NH1	-13.73	113.44	120.30
1	B	33[A]	ARG	NE-CZ-NH1	-13.26	113.67	120.30
1	B	33[B]	ARG	NE-CZ-NH1	-13.26	113.67	120.30
1	A	175[A]	ARG	NE-CZ-NH1	13.20	126.90	120.30
1	A	175[B]	ARG	NE-CZ-NH1	13.20	126.90	120.30
1	B	15[A]	PRO	C-N-CA	8.86	143.85	121.70
1	B	15[B]	PRO	C-N-CA	8.86	143.85	121.70
1	B	263	ASP	CB-CG-OD1	7.24	124.81	118.30
1	B	136	GLU	CA-CB-CG	-7.13	97.70	113.40
1	B	175	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	A	147	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	B	197[A]	GLU	OE1-CD-OE2	6.69	131.33	123.30
1	B	197[B]	GLU	OE1-CD-OE2	6.69	131.33	123.30
1	B	197[A]	GLU	CG-CD-OE1	-6.62	105.05	118.30
1	B	197[B]	GLU	CG-CD-OE1	-6.62	105.05	118.30
1	A	33[A]	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	A	33[B]	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	A	137	TYR	CB-CG-CD1	6.36	124.81	121.00
1	A	136	GLU	CA-CB-CG	-6.34	99.46	113.40
1	B	235[A]	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	B	235[B]	ARG	NE-CZ-NH2	-6.01	117.30	120.30
1	B	267[A]	THR	N-CA-CB	-5.98	98.94	110.30
1	B	267[B]	THR	N-CA-CB	-5.98	98.94	110.30
1	A	175[A]	ARG	CD-NE-CZ	5.89	131.85	123.60
1	A	175[B]	ARG	CD-NE-CZ	5.89	131.85	123.60
1	A	134[A]	ASN	N-CA-CB	5.85	121.13	110.60
1	A	134[B]	ASN	N-CA-CB	5.85	121.13	110.60
1	A	43	TYR	CB-CG-CD1	5.65	124.39	121.00
1	B	15[A]	PRO	N-CA-C	5.62	126.70	112.10
1	B	15[B]	PRO	N-CA-C	5.62	126.70	112.10
1	A	111	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	15[A]	PRO	O-C-N	-5.54	113.84	122.70
1	B	15[B]	PRO	O-C-N	-5.54	113.84	122.70
1	B	147	ASP	CB-CG-OD2	-5.53	113.33	118.30
1	B	136	GLU	OE1-CD-OE2	-5.42	116.79	123.30
1	A	14[A]	MET	CG-SD-CE	5.31	108.70	100.20
1	A	14[B]	MET	CG-SD-CE	5.31	108.70	100.20
1	B	170	ASP	CB-CG-OD1	5.18	122.97	118.30
1	B	134[A]	ASN	N-CA-CB	5.16	119.88	110.60
1	B	134[B]	ASN	N-CA-CB	5.16	119.88	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	295[A]	LYS	CD-CE-NZ	5.08	123.37	111.70
1	B	295[B]	LYS	CD-CE-NZ	5.08	123.37	111.70

There are no chirality outliers.

There are no planarity outliers.

## 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	2519	0	2478	126	2
1	B	2516	0	2504	94	1
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	2	0	0	1	0
3	B	2	0	0	1	0
4	A	15	0	0	3	0
4	B	15	0	0	1	0
5	A	1	0	0	0	0
6	A	517	0	0	75	3
6	B	482	0	0	69	0
All	All	6073	0	4982	212	3

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 21.

All (212) 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:B:197[B]:GLU:CB	1:B:197[B]:GLU:CA	1.76	1.54
1:A:14[B]:MET:CA	1:A:14[B]:MET:CB	1.89	1.48
1:A:286[B]:HIS:CD2	6:A:2471:HOH:O	1.82	1.31
1:A:286[A]:HIS:CD2	6:A:2468:HOH:O	1.82	1.28
1:A:26:VAL:HG21	6:A:2300:HOH:O	1.32	1.27
1:A:175[B]:ARG:NH2	6:A:2304:HOH:O	1.66	1.27
1:A:14[A]:MET:HE2	1:A:15:PRO:CD	1.65	1.25

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134[B]:ASN:ND2	6:A:2264:HOH:O	1.65	1.23
1:A:33[A]:ARG:NE	6:A:2073:HOH:O	1.65	1.22
1:A:11[B]:GLU:CD	6:A:2020:HOH:O	1.77	1.20
1:A:90[B]:GLY:HA2	6:A:2168:HOH:O	1.39	1.18
1:B:203[B]:GLU:HG3	6:B:2313:HOH:O	1.42	1.17
1:A:14[A]:MET:CE	1:A:15:PRO:HD2	1.72	1.17
1:A:11[A]:GLU:OE2	6:A:2025:HOH:O	1.60	1.16
1:B:162[B]:LYS:CE	6:B:2273:HOH:O	1.91	1.15
1:A:292[A]:GLU:OE2	6:A:2489:HOH:O	1.62	1.14
1:A:14[A]:MET:HA	1:A:14[A]:MET:HE3	1.16	1.13
1:B:286[A]:HIS:CD2	6:B:2448:HOH:O	1.98	1.13
1:A:292[A]:GLU:CD	6:A:2489:HOH:O	1.86	1.13
1:A:41[A]:MET:HE3	1:B:41[A]:MET:CE	1.78	1.12
1:A:90[B]:GLY:O	6:A:2171:HOH:O	1.67	1.10
1:A:162[B]:LYS:NZ	6:A:2286:HOH:O	1.85	1.10
1:A:63[A]:ILE:CD1	6:A:2112:HOH:O	2.02	1.07
1:B:169:THR:OG1	1:B:171[B]:ASN:OD1	1.70	1.07
1:B:197[A]:GLU:HG2	6:B:2300:HOH:O	1.54	1.05
1:B:33[B]:ARG:NH2	6:B:2080:HOH:O	1.88	1.05
1:A:286[A]:HIS:HD2	6:A:2468:HOH:O	1.23	1.04
1:A:90[A]:GLY:HA2	6:A:2168:HOH:O	1.57	1.04
1:A:41[A]:MET:CE	1:B:41[A]:MET:CE	2.36	1.03
1:B:63[A]:ILE:CD1	6:B:2117:HOH:O	2.04	1.03
1:A:286[B]:HIS:HD2	6:A:2471:HOH:O	1.26	1.02
1:A:14[A]:MET:HA	1:A:14[A]:MET:CE	1.90	1.01
1:A:41[A]:MET:HE3	1:B:41[A]:MET:HE3	1.42	1.01
1:B:296[A]:LYS:NZ	1:B:299:GLU:CD	2.15	1.01
1:A:95:GLU:OE1	6:A:2201:HOH:O	1.78	1.00
1:A:254[B]:GLU:OE1	6:A:2422:HOH:O	1.80	0.99
1:B:171[A]:ASN:ND2	6:B:2284:HOH:O	1.94	0.98
1:B:286[B]:HIS:CD2	6:B:2447:HOH:O	2.17	0.97
1:A:14[A]:MET:CE	1:A:15:PRO:CD	2.36	0.97
1:A:214[B]:ASP:OD2	6:A:2353:HOH:O	1.83	0.96
1:B:91[B]:LYS:HD3	6:B:2184:HOH:O	1.66	0.95
1:A:197[B]:GLU:CD	1:A:203[B]:GLU:OE2	2.04	0.94
1:B:91[B]:LYS:CD	6:B:2184:HOH:O	2.14	0.94
1:A:91:LYS:HA	6:A:2167:HOH:O	1.66	0.94
1:A:197[B]:GLU:OE1	1:A:203[B]:GLU:OE2	1.84	0.94
1:A:286[B]:HIS:CD2	6:A:2475:HOH:O	2.21	0.93
1:B:33[A]:ARG:NH1	6:B:2079:HOH:O	1.81	0.92
1:B:290:LEU:HD21	6:B:2455:HOH:O	1.70	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33[B]:ARG:CZ	6:B:2080:HOH:O	2.13	0.92
1:B:296[A]:LYS:HZ2	1:B:299:GLU:CD	1.73	0.92
1:A:33[A]:ARG:NH1	6:A:2072:HOH:O	1.82	0.91
1:A:90[A]:GLY:CA	6:A:2168:HOH:O	2.17	0.91
4:B:1303:SO4:O1	6:B:2479:HOH:O	1.86	0.91
1:B:286[A]:HIS:HD2	6:B:2448:HOH:O	1.40	0.91
1:A:176[A]:GLU:OE1	6:A:2366:HOH:O	1.89	0.90
1:A:11[A]:GLU:OE1	6:A:2024:HOH:O	1.90	0.89
1:A:14[A]:MET:HE2	1:A:15:PRO:HD2	0.89	0.88
1:A:292[B]:GLU:OE2	6:A:2488:HOH:O	1.93	0.87
1:A:41[A]:MET:HE3	1:B:41[A]:MET:HE2	1.57	0.86
1:B:290:LEU:CD2	6:B:2455:HOH:O	2.24	0.86
1:A:33[B]:ARG:NE	6:B:2074:HOH:O	1.91	0.86
1:B:289[B]:GLU:CD	6:B:2454:HOH:O	2.12	0.85
1:B:217:LYS:HE2	6:B:2327:HOH:O	1.75	0.85
1:A:197[B]:GLU:HG2	6:A:2320:HOH:O	1.76	0.84
1:B:289[B]:GLU:OE2	6:B:2455:HOH:O	1.93	0.84
1:A:90[A]:GLY:O	6:A:2167:HOH:O	1.94	0.84
1:B:91[B]:LYS:CE	6:B:2184:HOH:O	2.26	0.83
1:B:222:LYS:NZ	6:B:2340:HOH:O	2.09	0.83
1:B:286[A]:HIS:NE2	6:B:2449:HOH:O	2.11	0.82
1:A:300:LYS:HE2	6:A:2496:HOH:O	1.78	0.82
1:B:63[A]:ILE:HD11	6:B:2117:HOH:O	1.72	0.82
1:B:197[A]:GLU:HG2	6:B:2299:HOH:O	1.78	0.82
1:A:150[B]:HIS:NE2	6:A:2277:HOH:O	2.12	0.81
1:B:65:ASN:HD21	1:B:236:PHE:H	1.28	0.81
1:B:297:LEU:O	1:B:300:LYS:HD2	1.81	0.81
1:A:176[B]:GLU:HG2	6:A:2022:HOH:O	1.80	0.80
1:A:63[A]:ILE:HD11	6:A:2112:HOH:O	1.69	0.80
1:A:254[B]:GLU:OE2	6:A:2422:HOH:O	1.99	0.79
1:B:302:LYS:CE	6:B:2473:HOH:O	2.32	0.78
1:A:254[B]:GLU:CD	6:A:2422:HOH:O	2.18	0.77
1:B:162[B]:LYS:CD	6:B:2273:HOH:O	2.24	0.77
1:A:49:ASN:HD22	1:B:82:ASN:HD21	1.30	0.77
1:A:33[A]:ARG:CD	6:A:2073:HOH:O	2.17	0.76
1:B:14:MET:HE2	6:B:2189:HOH:O	1.83	0.76
1:B:203[B]:GLU:CG	6:B:2313:HOH:O	2.11	0.76
1:B:302:LYS:NZ	6:B:2473:HOH:O	2.16	0.75
1:B:134[B]:ASN:HD22	1:B:136:GLU:H	1.33	0.75
1:B:150[B]:HIS:NE2	6:B:2262:HOH:O	2.19	0.74
1:B:197[B]:GLU:HB3	6:B:2300:HOH:O	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292[A]:GLU:OE2	1:A:296:LYS:HE3	1.88	0.73
1:B:300:LYS:HB2	6:B:2470:HOH:O	1.87	0.73
1:B:197[A]:GLU:OE2	6:B:2296:HOH:O	2.05	0.73
1:B:197[B]:GLU:CG	1:B:197[B]:GLU:CA	2.66	0.73
1:B:162[B]:LYS:HE2	6:B:2273:HOH:O	1.67	0.73
1:A:90[A]:GLY:C	6:A:2167:HOH:O	2.27	0.73
1:A:41[A]:MET:CE	1:B:41[A]:MET:HE2	2.14	0.73
1:B:108[B]:LYS:NZ	6:B:2216:HOH:O	2.20	0.73
1:A:95:GLU:CD	6:A:2201:HOH:O	2.25	0.71
1:A:150[B]:HIS:CE1	6:A:2277:HOH:O	2.44	0.71
1:B:296[A]:LYS:HZ1	1:B:299:GLU:CD	1.85	0.70
1:A:134[B]:ASN:ND2	6:A:2262:HOH:O	2.21	0.70
1:B:91[B]:LYS:HE3	6:B:2184:HOH:O	1.85	0.70
1:A:286[B]:HIS:CD2	6:A:2469:HOH:O	2.43	0.70
1:A:36[B]:GLU:OE2	6:A:2084:HOH:O	2.09	0.70
1:A:11[B]:GLU:OE2	6:A:2020:HOH:O	1.92	0.70
1:A:159:ARG:HA	1:A:162[B]:LYS:HE3	1.72	0.70
1:A:296:LYS:HE3	6:A:2489:HOH:O	1.93	0.69
1:A:249:LYS:NZ	6:A:2409:HOH:O	2.26	0.69
1:A:231[B]:ARG:NH2	4:A:1310:SO4:O4	2.26	0.68
1:A:176[B]:GLU:OE2	1:A:224:TYR:OH	2.08	0.68
1:A:33[A]:ARG:CZ	6:A:2073:HOH:O	2.21	0.68
1:B:131:GLU:HG2	6:B:2069:HOH:O	1.95	0.67
1:A:203[B]:GLU:HG3	1:A:206[B]:LYS:HG3	1.75	0.67
1:B:296[A]:LYS:NZ	1:B:299:GLU:OE2	2.15	0.66
6:A:2017:HOH:O	1:B:1:MET:HG2	1.94	0.66
1:A:33[B]:ARG:NH2	6:B:2074:HOH:O	2.27	0.66
1:B:260[A]:VAL:HG12	6:B:2412:HOH:O	1.95	0.66
1:A:296:LYS:HD2	1:A:299:GLU:OE1	1.96	0.66
1:A:41[A]:MET:CE	1:B:41[A]:MET:HE3	2.12	0.65
1:A:131:GLU:HG2	6:A:2066:HOH:O	1.97	0.65
1:B:300:LYS:HD3	6:B:2474:HOH:O	1.97	0.65
1:B:292[A]:GLU:OE2	1:B:296[A]:LYS:HD3	1.96	0.65
1:A:258:GLU:OE1	6:A:2438:HOH:O	2.14	0.65
1:A:197[B]:GLU:OE2	1:A:203[B]:GLU:OE2	2.15	0.64
1:B:242[A]:ARG:CZ	6:B:2365:HOH:O	2.46	0.64
1:A:14[A]:MET:CA	1:A:14[A]:MET:CE	2.72	0.63
1:B:150[B]:HIS:CE1	6:B:2262:HOH:O	2.50	0.63
1:B:63[A]:ILE:HG13	6:B:2117:HOH:O	1.97	0.63
1:A:175[B]:ARG:NH1	6:A:2301:HOH:O	2.31	0.62
1:A:295[A]:LYS:CE	6:A:2488:HOH:O	2.46	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175[B]:ARG:HG2	6:A:2293:HOH:O	1.98	0.62
1:A:14[B]:MET:CA	1:A:14[B]:MET:CG	2.75	0.61
1:B:162[B]:LYS:HD2	6:B:2273:HOH:O	1.93	0.61
1:B:296[A]:LYS:NZ	1:B:299:GLU:OE1	2.30	0.60
1:A:217:LYS:HE2	6:A:2356:HOH:O	2.01	0.60
1:A:203[B]:GLU:CG	1:A:206[B]:LYS:HG3	2.30	0.60
1:A:165:VAL:HA	1:A:168[B]:MET:CE	2.31	0.59
1:A:33[B]:ARG:CZ	6:B:2074:HOH:O	2.36	0.59
1:B:249[B]:LYS:NZ	6:B:2383:HOH:O	2.36	0.59
1:B:33[B]:ARG:NE	6:B:2080:HOH:O	2.32	0.59
1:A:165:VAL:HA	1:A:168[B]:MET:HE3	1.83	0.58
1:B:203[A]:GLU:HG2	6:B:2296:HOH:O	2.03	0.58
1:A:11[B]:GLU:CG	6:A:2020:HOH:O	2.41	0.58
1:B:289[B]:GLU:CG	6:B:2454:HOH:O	2.50	0.58
1:B:173[A]:VAL:HG23	6:B:2281:HOH:O	2.03	0.57
1:A:49:ASN:ND2	1:B:82:ASN:HD21	2.00	0.57
1:B:242[A]:ARG:CZ	6:B:2366:HOH:O	2.53	0.56
1:A:91:LYS:CA	6:A:2167:HOH:O	2.39	0.56
1:A:136:GLU:CG	6:A:2269:HOH:O	2.54	0.56
1:A:63[A]:ILE:CG1	6:A:2112:HOH:O	2.47	0.55
1:A:267[A]:THR:HG22	4:A:1307:SO4:S	2.48	0.54
1:A:14[A]:MET:CA	1:A:14[A]:MET:HE3	2.11	0.54
1:A:63[A]:ILE:HG13	6:A:2112:HOH:O	2.07	0.53
1:A:14[A]:MET:HE3	1:A:15:PRO:CD	2.36	0.52
1:A:34:PHE:HD1	1:A:154[A]:LEU:HD23	1.74	0.52
1:A:41[A]:MET:HE1	1:B:41[A]:MET:CE	2.37	0.51
1:A:239[B]:GLU:OE2	6:A:2385:HOH:O	2.19	0.51
1:B:65:ASN:ND2	1:B:236:PHE:H	2.03	0.51
1:A:14[A]:MET:CE	1:A:15:PRO:HD3	2.34	0.50
1:B:297:LEU:O	1:B:300:LYS:CD	2.56	0.50
1:A:223[A]:LYS:NZ	6:A:2365:HOH:O	2.20	0.50
1:A:165:VAL:HG22	1:A:168[B]:MET:CE	2.43	0.49
1:B:36[B]:GLU:OE2	6:B:2090:HOH:O	2.17	0.49
1:B:197[A]:GLU:CD	6:B:2296:HOH:O	2.48	0.49
1:A:174:ALA:HB2	6:A:2300:HOH:O	2.13	0.48
1:B:162[B]:LYS:NZ	6:B:2273:HOH:O	2.06	0.48
1:B:300:LYS:HD2	6:B:2470:HOH:O	2.14	0.48
1:B:63[A]:ILE:CG1	6:B:2117:HOH:O	2.41	0.48
1:A:102[B]:THR:HG23	6:A:2219:HOH:O	2.14	0.47
1:A:1:MET:HG2	6:B:2020:HOH:O	2.13	0.47
1:B:302:LYS:HE2	6:B:2473:HOH:O	2.07	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:LEU:O	1:B:36[B]:GLU:HG2	2.13	0.47
1:B:54:LYS:NZ	6:B:2107:HOH:O	2.47	0.46
1:A:296:LYS:HD2	1:A:299:GLU:CD	2.35	0.46
1:A:11[B]:GLU:HG3	6:A:2020:HOH:O	2.12	0.46
1:B:197[A]:GLU:HG3	6:B:2296:HOH:O	2.15	0.46
1:A:33[B]:ARG:HG3	1:A:137:TYR:CD1	2.51	0.46
1:B:63[A]:ILE:HD12	6:B:2117:HOH:O	1.96	0.46
1:A:260[B]:VAL:HG11	6:A:2375:HOH:O	2.15	0.46
1:A:29:LEU:O	1:A:36[B]:GLU:HG2	2.16	0.45
1:A:33[A]:ARG:HD2	6:A:2073:HOH:O	2.03	0.45
1:A:176[A]:GLU:OE2	6:A:2309:HOH:O	2.21	0.45
1:B:206[A]:LYS:NZ	6:B:2313:HOH:O	2.50	0.45
1:A:63[A]:ILE:HD12	6:A:2112:HOH:O	1.92	0.45
1:B:197[A]:GLU:CG	6:B:2296:HOH:O	2.66	0.44
1:A:197[B]:GLU:OE2	1:A:203[B]:GLU:CD	2.56	0.44
1:A:267[A]:THR:HG22	4:A:1307:SO4:O3	2.18	0.44
1:A:39:THR:HG21	3:A:1306:CL:CL	2.55	0.43
1:B:203[A]:GLU:CG	6:B:2296:HOH:O	2.63	0.43
1:A:197[B]:GLU:CG	6:A:2320:HOH:O	2.52	0.43
1:B:134[B]:ASN:ND2	1:B:136:GLU:H	2.08	0.43
1:A:93:LEU:HD11	6:A:2475:HOH:O	2.18	0.42
1:A:116:PHE:HD1	1:A:280[B]:GLU:OE2	2.01	0.42
1:B:39:THR:HG21	3:B:1308:CL:CL	2.56	0.42
1:A:14[A]:MET:SD	6:A:2060:HOH:O	2.62	0.42
1:B:286[A]:HIS:NE2	6:B:2448:HOH:O	2.35	0.42
1:A:165:VAL:HA	1:A:168[B]:MET:HE2	2.02	0.42
1:A:260[B]:VAL:CG1	6:A:2375:HOH:O	2.67	0.42
1:B:197[A]:GLU:CG	6:B:2300:HOH:O	2.32	0.41
1:A:90[A]:GLY:C	6:A:2168:HOH:O	2.49	0.41
1:B:161:HIS:HD2	6:B:2065:HOH:O	2.03	0.41
1:B:11:GLU:HA	6:B:2426:HOH:O	2.20	0.41
1:A:34:PHE:CD1	1:A:154[A]:LEU:HD23	2.54	0.41
1:A:161:HIS:HD2	6:A:2059:HOH:O	2.03	0.40
1:A:90[B]:GLY:CA	6:A:2168:HOH:O	2.24	0.40
1:A:14[A]:MET:HE2	1:A:15:PRO:N	2.29	0.40
1:A:61[B]:ASP:OD1	6:A:2116:HOH:O	2.22	0.40
1:A:39:THR:HG22	1:A:154[A]:LEU:HD13	2.03	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168[A]:MET:SD	6:A:2243:HOH:O[5_555]	1.28	0.92
1:B:206[B]:LYS:CE	6:A:2331:HOH:O[9_555]	1.64	0.56
1:A:168[B]:MET:SD	6:A:2243:HOH:O[5_555]	1.94	0.26

## 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	337/302 (112%)	330 (98%)	7 (2%)	0	100	100
1	B	335/302 (111%)	328 (98%)	7 (2%)	0	100	100
All	All	672/604 (111%)	658 (98%)	14 (2%)	0	100	100

There are no Ramachandran outliers to report.

### 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	277/241 (115%)	269 (97%)	8 (3%)	50	12
1	B	276/241 (114%)	271 (98%)	5 (2%)	66	27
All	All	553/482 (115%)	540 (98%)	13 (2%)	65	16

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14[A]	MET

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Mol	Chain	Res	Type
1	A	14[B]	MET
1	A	102[A]	THR
1	A	102[B]	THR
1	A	154[A]	LEU
1	A	154[B]	LEU
1	A	161	HIS
1	A	300	LYS
1	B	102	THR
1	B	161	HIS
1	B	296[A]	LYS
1	B	296[B]	LYS
1	B	302	LYS

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

Mol	Chain	Res	Type
1	A	49	ASN
1	A	122	ASN
1	A	161	HIS
1	B	65	ASN
1	B	122	ASN
1	B	161	HIS

### 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 9 are monoatomic - leaving 6 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	SO4	A	1307	-	4,4,4	2.21	2 (50%)	6,6,6	0.84	0
4	SO4	A	1308	-	4,4,4	0.24	0	6,6,6	0.16	0
4	SO4	A	1310	-	4,4,4	0.68	0	6,6,6	0.64	0
4	SO4	B	1303	-	4,4,4	1.05	0	6,6,6	0.52	0
4	SO4	B	1304	-	4,4,4	0.08	0	6,6,6	0.08	0
4	SO4	B	1309	-	4,4,4	1.32	1 (25%)	6,6,6	1.28	1 (16%)

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	SO4	A	1307	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1308	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1310	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1303	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1304	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1309	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1307	SO4	O4-S	-2.93	1.36	1.47
4	B	1309	SO4	O1-S	-2.60	1.38	1.47
4	A	1307	SO4	O3-S	2.95	1.58	1.47

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1309	SO4	O2-S-O1	-2.80	100.61	109.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1307	SO4	2	0
4	A	1310	SO4	1	0
4	B	1303	SO4	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	302/302 (100%)	-0.43	4 (1%) 79 68	6, 9, 16, 42	10 (3%)
1	B	302/302 (100%)	-0.32	6 (1%) 68 55	7, 9, 18, 53	11 (3%)
All	All	604/604 (100%)	-0.37	10 (1%) 73 60	6, 9, 17, 53	21 (3%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	301	ALA	20.8
1	B	302	LYS	18.8
1	A	302	LYS	9.3
1	B	16	LYS	4.5
1	B	299	GLU	4.4
1	A	301	ALA	3.9
1	A	90[A]	GLY	3.9
1	B	300	LYS	3.8
1	B	96	GLY	3.6
1	A	96	GLY	2.1

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

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

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	SO4	A	1307	5/5	0.99	0.12	3.29	12,13,16,17	0
4	SO4	A	1310	5/5	0.94	0.11	3.20	20,21,22,27	5
4	SO4	B	1303	5/5	0.94	0.09	1.23	14,18,20,23	5
4	SO4	B	1309	5/5	0.97	0.10	0.63	13,13,16,18	4
4	SO4	A	1308	5/5	0.99	0.10	0.24	10,10,12,13	0
3	CL	A	1305	1/1	1.00	0.05	-0.26	7,7,7,7	1
3	CL	B	1308	1/1	1.00	0.04	-1.16	9,9,9,9	1
3	CL	A	1306	1/1	1.00	0.04	-1.41	8,8,8,8	1
3	CL	B	1307	1/1	1.00	0.02	-1.90	9,9,9,9	0
2	MN	B	1306	1/1	1.00	0.02	-2.30	7,7,7,7	0
2	MN	B	1305	1/1	1.00	0.02	-2.59	7,7,7,7	0
2	MN	A	1303	1/1	1.00	0.02	-3.68	7,7,7,7	0
2	MN	A	1304	1/1	1.00	0.02	-3.93	7,7,7,7	0
5	LI	A	1309	1/1	0.97	0.26	-	14,14,14,14	0
4	SO4	B	1304	5/5	0.94	0.17	-	22,22,23,28	5

## 6.5 Other polymers [i](#)

There are no such residues in this entry.