



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2018 – 09:09 AM EDT

PDB ID : 6GXU  
Title : Crystal structure of Schistosoma mansoni HDAC8 complexed with an hydroxamate 3  
Authors : Shaik, T.B.; Marek, M.; Romier, C.  
Deposited on : 2018-06-27  
Resolution : 1.92 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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031172  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031172

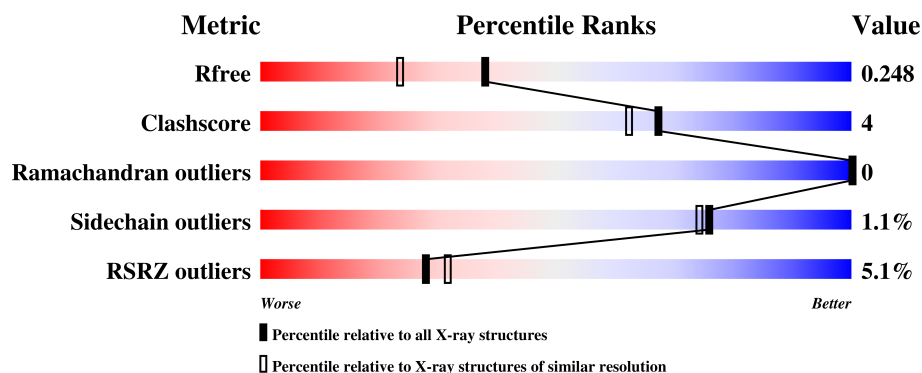
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.92 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))
$R_{free}$	111664	6904 (1.94-1.90)
Clashscore	122126	7577 (1.94-1.90)
Ramachandran outliers	120053	7491 (1.94-1.90)
Sidechain outliers	120020	7491 (1.94-1.90)
RSRZ outliers	108989	6759 (1.94-1.90)

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	447	 4% 78% 9% 13%
1	B	447	 4% 83% 9% 8%
1	C	447	 4% 82% 10% 8%
1	D	447	 6% 82% 7% 11%

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13661 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 Histone deacetylase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	391	Total	C	N	O	S	0	2	0
			3129	2018	523	573	15			
1	B	410	Total	C	N	O	S	0	2	0
			3280	2113	549	602	16			
1	C	411	Total	C	N	O	S	0	1	0
			3283	2115	549	603	16			
1	D	397	Total	C	N	O	S	0	2	0
			3188	2057	530	585	16			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP A5H660
A	441	GLY	-	expression tag	UNP A5H660
A	442	SER	-	expression tag	UNP A5H660
A	443	LEU	-	expression tag	UNP A5H660
A	444	VAL	-	expression tag	UNP A5H660
A	445	PRO	-	expression tag	UNP A5H660
A	446	ARG	-	expression tag	UNP A5H660
B	0	HIS	-	expression tag	UNP A5H660
B	441	GLY	-	expression tag	UNP A5H660
B	442	SER	-	expression tag	UNP A5H660
B	443	LEU	-	expression tag	UNP A5H660
B	444	VAL	-	expression tag	UNP A5H660
B	445	PRO	-	expression tag	UNP A5H660
B	446	ARG	-	expression tag	UNP A5H660
C	0	HIS	-	expression tag	UNP A5H660
C	441	GLY	-	expression tag	UNP A5H660
C	442	SER	-	expression tag	UNP A5H660
C	443	LEU	-	expression tag	UNP A5H660
C	444	VAL	-	expression tag	UNP A5H660
C	445	PRO	-	expression tag	UNP A5H660
C	446	ARG	-	expression tag	UNP A5H660

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP A5H660
D	441	GLY	-	expression tag	UNP A5H660
D	442	SER	-	expression tag	UNP A5H660
D	443	LEU	-	expression tag	UNP A5H660
D	444	VAL	-	expression tag	UNP A5H660
D	445	PRO	-	expression tag	UNP A5H660
D	446	ARG	-	expression tag	UNP A5H660

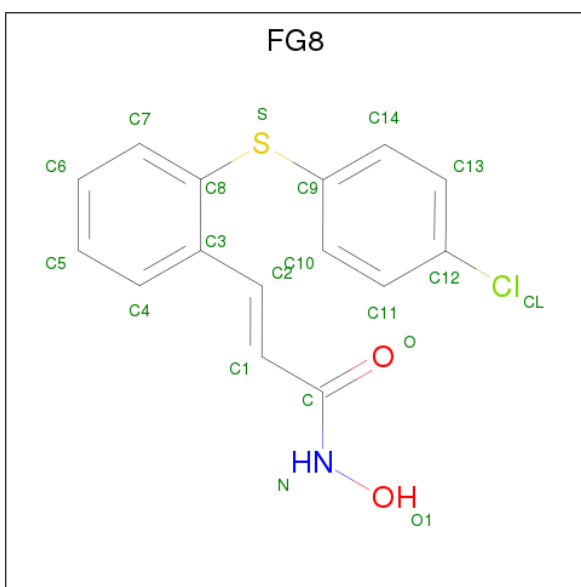
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Zn 1 1	0	0
2	A	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0

- Molecule 3 is POTASSIUM ION (three-letter code: K) (formula: K).

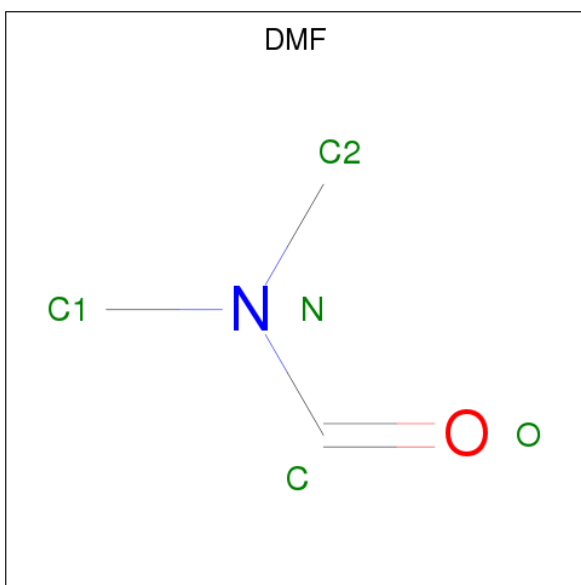
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total K 2 2	0	0
3	A	2	Total K 2 2	0	0
3	D	2	Total K 2 2	0	0
3	C	2	Total K 2 2	0	0

- Molecule 4 is ( {E} )-3-[2-(4-chlorophenyl)sulfanylphenyl]- {N}-oxidanyl-prop-2-enamide (three-letter code: FG8) (formula: C<sub>15</sub>H<sub>12</sub>ClNO<sub>2</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total 20	C 15	Cl 1	N 1	O 2	S 1	0	0
4	B	1	Total 20	C 15	Cl 1	N 1	O 2	S 1	0	0
4	C	1	Total 20	C 15	Cl 1	N 1	O 2	S 1	0	0
4	D	1	Total 20	C 15	Cl 1	N 1	O 2	S 1	0	0

- Molecule 5 is DIMETHYLFORMAMIDE (three-letter code: DMF) (formula:  $C_3H_7NO$ ).



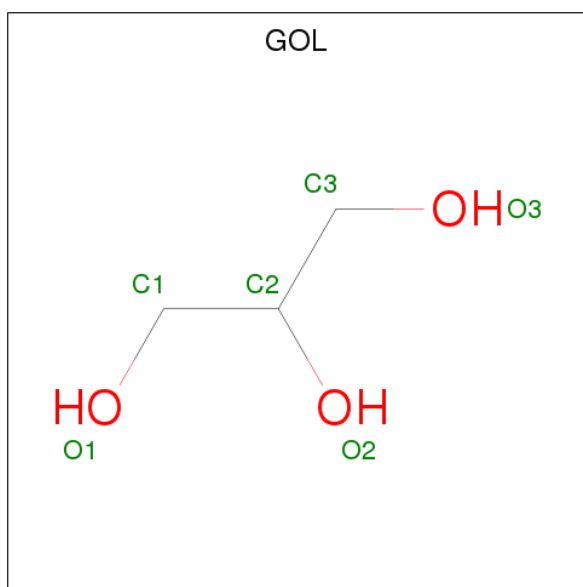
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			5	3	1	1		
5	A	1	Total	C	N	O	0	0
			5	3	1	1		
5	A	1	Total	C	N	O	0	0
			5	3	1	1		
5	A	1	Total	C	N	O	0	0
			5	3	1	1		
5	B	1	Total	C	N	O	0	0
			5	3	1	1		
5	B	1	Total	C	N	O	0	0
			5	3	1	1		
5	B	1	Total	C	N	O	0	0
			5	3	1	1		
5	B	1	Total	C	N	O	0	0
			5	3	1	1		
5	B	1	Total	C	N	O	0	0
			5	3	1	1		
5	B	1	Total	C	N	O	0	0
			5	3	1	1		
5	C	1	Total	C	N	O	0	0
			5	3	1	1		
5	C	1	Total	C	N	O	0	0
			5	3	1	1		
5	C	1	Total	C	N	O	0	0
			5	3	1	1		
5	C	1	Total	C	N	O	0	0
			5	3	1	1		
5	C	1	Total	C	N	O	0	0
			5	3	1	1		
5	C	1	Total	C	N	O	0	0
			5	3	1	1		
5	C	1	Total	C	N	O	0	0
			5	3	1	1		
5	D	1	Total	C	N	O	0	0
			5	3	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			5	3	1	1		
5	D	1	Total	C	N	O	0	0
			5	3	1	1		
5	D	1	Total	C	N	O	0	0
			5	3	1	1		

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	C	1	Total	C	O	0	0
			6	3	3		
6	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	126	Total	O	0	0
			126	126		
7	B	137	Total	O	0	0
			137	137		

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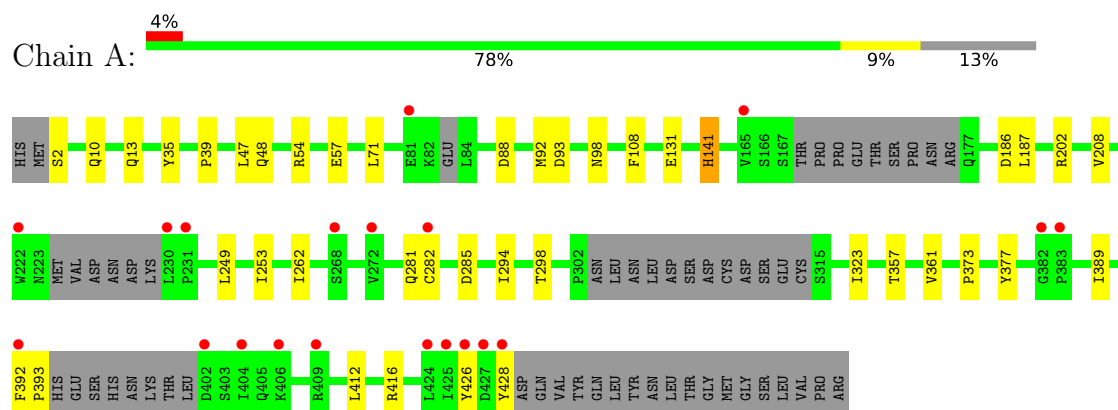
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	156	Total 156	O 156	0	0
7	D	121	Total 121	O 121	0	0



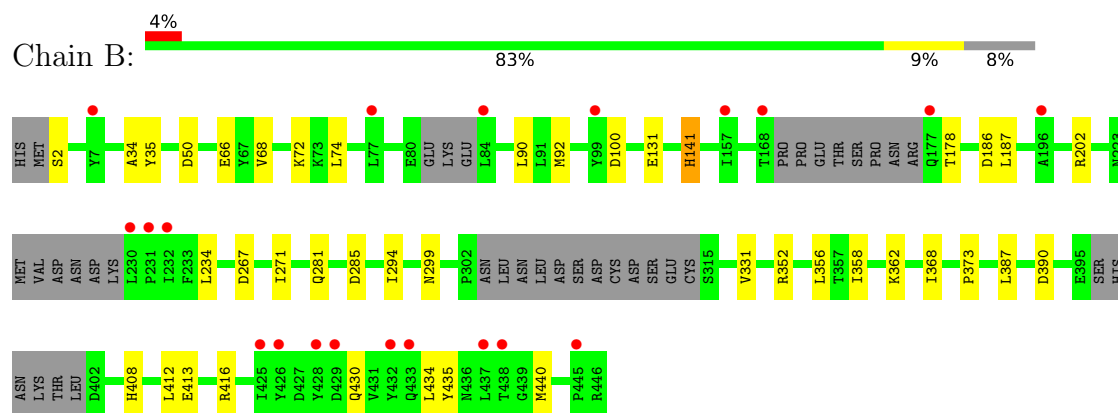
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

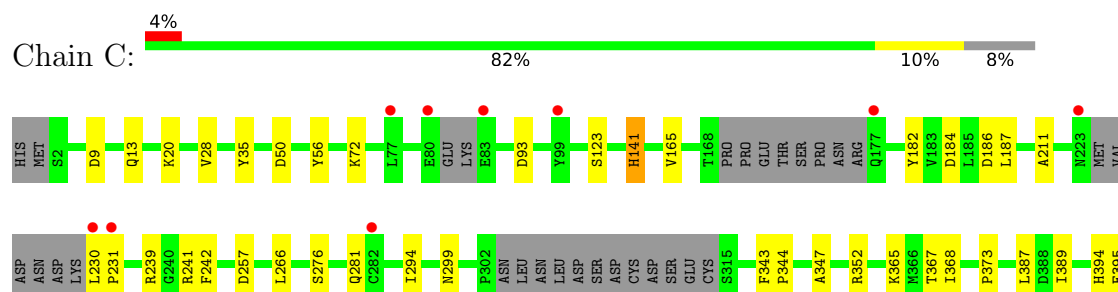
#### • Molecule 1: Histone deacetylase



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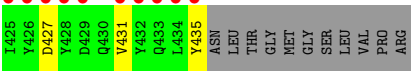
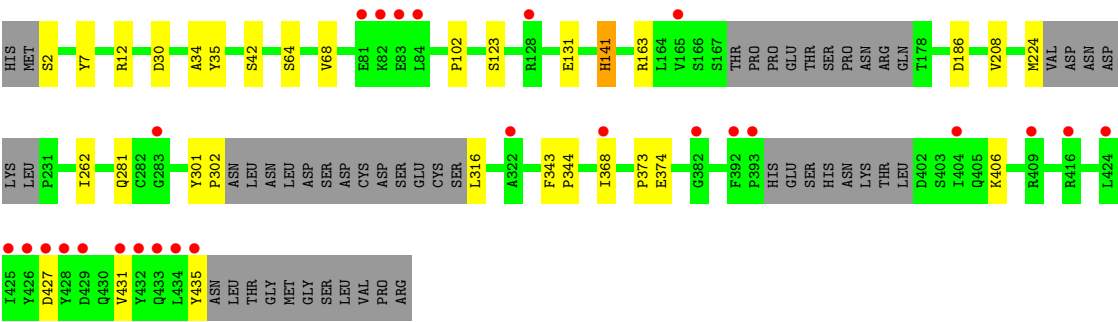
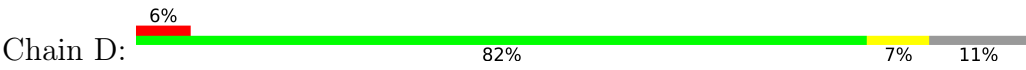


#### • Molecule 1: Histone deacetylase





● Molecule 1: Histone deacetylase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.42Å 70.46Å 97.91Å 77.96° 75.94° 85.97°	Depositor
Resolution (Å)	46.55 – 1.92 46.55 – 1.92	Depositor EDS
% Data completeness (in resolution range)	86.7 (46.55-1.92) 86.7 (46.55-1.92)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.19 (at 1.92Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.201 , 0.248 0.201 , 0.248	Depositor DCC
$R_{free}$ test set	5940 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.5	Xtriage
Anisotropy	0.090	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 56.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.190 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	13661	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% 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, 0.333 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: GOL, ZN, FG8, K, DMF

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	0.38	0/3219	0.53	0/4377
1	B	0.39	0/3374	0.55	0/4589
1	C	0.40	0/3377	0.56	0/4593
1	D	0.38	0/3281	0.54	0/4461
All	All	0.39	0/13251	0.55	0/18020

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 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	3129	0	3031	22	0
1	B	3280	0	3173	32	0
1	C	3283	0	3176	33	0
1	D	3188	0	3081	20	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
3	A	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	20	0	0	0	0
4	B	20	0	0	0	0
4	C	20	0	0	0	0
4	D	20	0	0	0	0
5	A	25	0	35	4	0
5	B	35	0	49	7	0
5	C	45	0	63	4	0
5	D	20	0	28	6	0
6	A	6	0	8	0	0
6	B	6	0	8	1	0
6	C	6	0	8	0	0
6	D	6	0	8	0	0
7	A	126	0	0	0	0
7	B	137	0	0	1	0
7	C	156	0	0	7	0
7	D	121	0	0	1	0
All	All	13661	0	12668	107	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 (107) 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:74:LEU:HB2	1:B:92:MET:HE2	1.55	0.85
1:C:13:GLN:NE2	7:C:601:HOH:O	2.12	0.81
1:D:12:ARG:HH11	5:D:505:DMF:HC	1.54	0.73
1:C:56:TYR:HE1	1:C:72:LYS:HZ1	1.38	0.72
1:B:408:HIS:NE2	5:B:508:DMF:O	2.24	0.70
1:D:302:PRO:HD2	1:D:316:LEU:HD12	1.75	0.68
1:B:413:GLU:OE2	1:B:416:ARG:NH2	2.23	0.66
1:D:2:SER:N	1:D:131:GLU:OE1	2.28	0.66
1:C:35:TYR:CE1	1:C:368:ILE:HG23	2.31	0.66
1:C:230:LEU:HD12	1:C:231:PRO:HD2	1.78	0.65
5:A:506:DMF:H13	1:B:90:LEU:O	1.98	0.63
1:B:187:LEU:HD21	1:B:294:ILE:HD12	1.81	0.62
1:D:301:TYR:CE2	5:D:507:DMF:HC	2.34	0.62
1:B:35:TYR:CE1	1:B:368:ILE:HG23	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:416:ARG:NH1	7:C:604:HOH:O	2.33	0.61
1:C:72:LYS:NZ	7:C:605:HOH:O	2.33	0.60
1:A:377:TYR:OH	5:A:505:DMF:O	2.18	0.60
1:B:234:LEU:HB2	6:B:511:GOL:H31	1.83	0.60
1:A:10:GLN:HA	1:A:13:GLN:HG2	1.84	0.58
1:C:239:ARG:NH2	7:C:606:HOH:O	2.37	0.57
1:C:367:THR:H	5:C:509:DMF:H23	1.70	0.56
1:B:178:THR:HB	1:B:202:ARG:HH21	1.70	0.56
1:D:435:TYR:HA	7:D:710:HOH:O	2.05	0.56
1:C:430:GLN:O	1:C:433:GLN:HG3	2.06	0.56
1:C:211:ALA:O	5:C:506:DMF:H21	2.05	0.56
1:A:361:VAL:HG22	5:A:509:DMF:H22	1.87	0.55
1:D:35:TYR:CE1	1:D:368:ILE:HG23	2.41	0.55
1:D:208:VAL:HG11	1:D:262:ILE:HD12	1.88	0.54
1:B:368:ILE:HG21	1:B:387:LEU:HD22	1.89	0.54
1:C:93:ASP:OD2	1:D:42:SER:OG	2.21	0.54
1:C:241:ARG:HG2	1:C:242:PHE:CE2	2.43	0.53
1:B:34:ALA:HB1	1:B:373:PRO:HG2	1.90	0.53
1:B:2:SER:N	1:B:131:GLU:OE2	2.41	0.53
1:C:187:LEU:HD21	1:C:294:ILE:HD12	1.91	0.53
1:C:9:ASP:O	1:C:13:GLN:HG2	2.09	0.52
5:C:505:DMF:H13	7:C:614:HOH:O	2.08	0.52
1:C:424:LEU:O	7:C:602:HOH:O	2.19	0.52
1:D:12:ARG:NH1	5:D:505:DMF:HC	2.22	0.51
1:B:358:ILE:HG23	1:B:362:LYS:HD3	1.91	0.51
1:A:2:SER:N	1:A:131:GLU:OE2	2.45	0.49
1:B:271:ILE:HD13	1:B:430:GLN:HG2	1.94	0.49
1:C:141:HIS:H	1:C:141:HIS:CD2	2.30	0.49
1:B:100:ASP:OD2	7:B:601:HOH:O	2.19	0.48
1:A:35:TYR:CZ	1:A:373:PRO:HD3	2.48	0.48
1:B:66:GLU:CD	1:B:66:GLU:H	2.16	0.48
1:D:186:ASP:HB2	1:D:281:GLN:OE1	2.14	0.48
1:A:249:LEU:HD13	1:A:253:ILE:HD13	1.96	0.47
1:D:141:HIS:CD2	1:D:141:HIS:H	2.32	0.47
1:A:186:ASP:HB2	1:A:281:GLN:OE1	2.13	0.47
1:C:368:ILE:HG21	1:C:387:LEU:HD22	1.96	0.47
1:A:282[B]:CYS:SG	1:A:323:ILE:HD11	2.53	0.47
1:B:412:LEU:HD11	1:B:435:TYR:CZ	2.50	0.47
1:A:54:ARG:NH1	1:A:57:GLU:OE1	2.40	0.47
1:A:93:ASP:HA	1:A:98:ASN:ND2	2.30	0.46
1:A:412:LEU:O	1:A:416:ARG:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:390:ASP:OD1	5:B:509:DMF:H13	2.16	0.46
1:C:299:ASN:OD1	1:C:389:ILE:HG23	2.16	0.45
1:D:64:SER:O	1:D:68:VAL:HG23	2.16	0.45
1:D:34:ALA:HB1	1:D:373:PRO:HG2	1.98	0.45
1:B:331:VAL:C	5:B:501:DMF:H12	2.38	0.44
1:B:356:LEU:HB2	5:B:507:DMF:H13	1.99	0.44
1:B:74:LEU:HB2	1:B:92:MET:CE	2.38	0.44
1:B:267:ASP:HB3	1:B:434:LEU:HD11	2.00	0.44
1:A:208:VAL:HG11	1:A:262:ILE:HD12	1.99	0.44
1:B:440:MET:SD	5:B:508:DMF:H22	2.58	0.44
1:C:257:ASP:OD2	7:C:603:HOH:O	2.21	0.44
1:C:35:TYR:CD1	1:C:368:ILE:HG23	2.51	0.44
1:C:394:HIS:O	1:C:395:GLU:HB2	2.18	0.43
1:A:141:HIS:H	1:A:141:HIS:CD2	2.35	0.43
1:C:56:TYR:HE1	1:C:72:LYS:NZ	2.13	0.43
1:A:187:LEU:HD21	1:A:294:ILE:HD12	2.01	0.43
1:D:427:ASP:O	1:D:431:VAL:HG12	2.19	0.43
1:B:299:ASN:O	1:B:352:ARG:HD2	2.19	0.43
1:B:271:ILE:HD12	1:B:434:LEU:HD12	2.00	0.43
1:C:186:ASP:HB2	1:C:281:GLN:OE1	2.18	0.43
1:D:102:PRO:HB2	5:D:506:DMF:H12	2.01	0.43
1:D:12:ARG:HH22	1:D:30:ASP:CG	2.21	0.43
1:B:141:HIS:CD2	1:B:141:HIS:H	2.36	0.43
1:C:299:ASN:O	1:C:352:ARG:HD2	2.19	0.43
1:A:39:PRO:HA	5:A:506:DMF:H23	2.01	0.42
1:C:365:LYS:HE3	1:C:367:THR:OG1	2.19	0.42
1:A:71:LEU:HG	1:A:108:PHE:HD1	1.84	0.42
1:B:285:ASP:N	1:B:285:ASP:OD1	2.53	0.42
1:B:131:GLU:HB3	5:B:501:DMF:H13	2.02	0.42
1:C:50:ASP:HB2	5:C:511:DMF:H23	2.00	0.42
1:C:343:PHE:HB2	1:C:344:PRO:HD3	2.02	0.42
1:B:368:ILE:HG21	1:B:387:LEU:CD2	2.50	0.41
1:B:368:ILE:CG2	1:B:387:LEU:HD22	2.50	0.41
1:B:68:VAL:O	1:B:72:LYS:HG3	2.20	0.41
1:D:123:SER:OG	1:D:163:ARG:NH1	2.50	0.41
1:B:186:ASP:HB2	1:B:281:GLN:OE1	2.20	0.41
1:A:47:LEU:HD23	1:A:48:GLN:N	2.34	0.41
1:C:430:GLN:HG3	1:C:433:GLN:HE21	1.86	0.41
1:A:392:PHE:HA	1:A:393:PRO:HD3	1.88	0.41
1:C:182:TYR:CE2	1:C:184:ASP:HB2	2.55	0.41
1:A:416:ARG:HD2	1:A:426:TYR:OH	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:THR:O	1:A:361:VAL:HG23	2.21	0.41
1:B:390:ASP:HA	5:B:509:DMF:H22	2.02	0.41
1:C:266:LEU:HD23	1:C:266:LEU:HA	1.85	0.41
1:A:298:THR:HA	1:A:389:ILE:HD11	2.02	0.41
1:C:28:VAL:HG22	1:C:347:ALA:HA	2.03	0.41
1:C:368:ILE:CG2	1:C:387:LEU:HD22	2.51	0.41
1:D:7:TYR:CD2	5:D:505:DMF:H21	2.56	0.40
1:D:102:PRO:HA	5:D:506:DMF:H23	2.03	0.40
1:D:343:PHE:HB2	1:D:344:PRO:HD3	2.03	0.40
1:A:88:ASP:O	1:A:92:MET:HG2	2.21	0.40
1:C:35:TYR:CZ	1:C:373:PRO:HD3	2.57	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	381/447 (85%)	371 (97%)	10 (3%)	0	100	100
1	B	400/447 (90%)	394 (98%)	6 (2%)	0	100	100
1	C	400/447 (90%)	394 (98%)	6 (2%)	0	100	100
1	D	389/447 (87%)	379 (97%)	10 (3%)	0	100	100
All	All	1570/1788 (88%)	1538 (98%)	32 (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	340/392 (87%)	336 (99%)	4 (1%)	74	71
1	B	357/392 (91%)	355 (99%)	2 (1%)	87	88
1	C	357/392 (91%)	352 (99%)	5 (1%)	69	66
1	D	346/392 (88%)	342 (99%)	4 (1%)	74	71
All	All	1400/1568 (89%)	1385 (99%)	15 (1%)	76	74

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	HIS
1	A	202	ARG
1	A	285	ASP
1	A	428	TYR
1	B	50	ASP
1	B	141	HIS
1	C	20	LYS
1	C	123	SER
1	C	141	HIS
1	C	165	VAL
1	C	276	SER
1	D	141	HIS
1	D	224	MET
1	D	374	GLU
1	D	406	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	10	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 45 ligands modelled in this entry, 12 are monoatomic - leaving 33 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	FG8	A	504	2	21,21,21	0.13	0	25,27,27	0.38	0
5	DMF	A	505	-	4,4,4	0.28	0	4,4,4	0.36	0
5	DMF	A	506	-	4,4,4	0.31	0	4,4,4	0.73	0
5	DMF	A	507	-	4,4,4	0.37	0	4,4,4	0.39	0
5	DMF	A	508	-	4,4,4	0.26	0	4,4,4	0.54	0
5	DMF	A	509	-	4,4,4	0.32	0	4,4,4	0.35	0
6	GOL	A	510	-	5,5,5	0.29	0	5,5,5	0.41	0
5	DMF	B	501	-	4,4,4	0.28	0	4,4,4	0.45	0
4	FG8	B	505	2	21,21,21	0.13	0	25,27,27	0.38	0
5	DMF	B	506	-	4,4,4	0.35	0	4,4,4	0.35	0
5	DMF	B	507	-	4,4,4	0.30	0	4,4,4	0.31	0
5	DMF	B	508	-	4,4,4	0.37	0	4,4,4	0.38	0
5	DMF	B	509	-	4,4,4	0.31	0	4,4,4	0.51	0
5	DMF	B	510	-	4,4,4	0.36	0	4,4,4	0.42	0
6	GOL	B	511	-	5,5,5	0.24	0	5,5,5	0.28	0
5	DMF	B	512	-	4,4,4	0.29	0	4,4,4	0.38	0
4	FG8	C	504	2	21,21,21	0.15	0	25,27,27	0.42	0
5	DMF	C	505	-	4,4,4	0.36	0	4,4,4	0.33	0
5	DMF	C	506	-	4,4,4	0.37	0	4,4,4	0.27	0
5	DMF	C	507	-	4,4,4	0.33	0	4,4,4	0.42	0
5	DMF	C	508	-	4,4,4	0.30	0	4,4,4	0.25	0
5	DMF	C	509	-	4,4,4	0.27	0	4,4,4	0.43	0
5	DMF	C	510	-	4,4,4	0.33	0	4,4,4	0.36	0
5	DMF	C	511	-	4,4,4	0.32	0	4,4,4	0.29	0
5	DMF	C	512	-	4,4,4	0.33	0	4,4,4	0.41	0
5	DMF	C	513	-	4,4,4	0.31	0	4,4,4	0.30	0
6	GOL	C	514	-	5,5,5	0.26	0	5,5,5	0.51	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	FG8	D	504	2	21,21,21	0.15	0	25,27,27	0.42	0
5	DMF	D	505	-	4,4,4	0.31	0	4,4,4	0.20	0
5	DMF	D	506	-	4,4,4	0.34	0	4,4,4	0.40	0
5	DMF	D	507	-	4,4,4	0.33	0	4,4,4	0.41	0
5	DMF	D	508	-	4,4,4	0.27	0	4,4,4	0.36	0
6	GOL	D	509	-	5,5,5	0.31	0	5,5,5	0.19	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
4	FG8	A	504	2	-	0/11/11/11	0/2/2/2
5	DMF	A	505	-	-	0/2/2/2	0/0/0/0
5	DMF	A	506	-	-	0/2/2/2	0/0/0/0
5	DMF	A	507	-	-	0/2/2/2	0/0/0/0
5	DMF	A	508	-	-	0/2/2/2	0/0/0/0
5	DMF	A	509	-	-	0/2/2/2	0/0/0/0
6	GOL	A	510	-	-	0/4/4/4	0/0/0/0
5	DMF	B	501	-	-	0/2/2/2	0/0/0/0
4	FG8	B	505	2	-	0/11/11/11	0/2/2/2
5	DMF	B	506	-	-	0/2/2/2	0/0/0/0
5	DMF	B	507	-	-	0/2/2/2	0/0/0/0
5	DMF	B	508	-	-	0/2/2/2	0/0/0/0
5	DMF	B	509	-	-	0/2/2/2	0/0/0/0
5	DMF	B	510	-	-	0/2/2/2	0/0/0/0
6	GOL	B	511	-	-	0/4/4/4	0/0/0/0
5	DMF	B	512	-	-	0/2/2/2	0/0/0/0
4	FG8	C	504	2	-	0/11/11/11	0/2/2/2
5	DMF	C	505	-	-	0/2/2/2	0/0/0/0
5	DMF	C	506	-	-	0/2/2/2	0/0/0/0
5	DMF	C	507	-	-	0/2/2/2	0/0/0/0
5	DMF	C	508	-	-	0/2/2/2	0/0/0/0
5	DMF	C	509	-	-	0/2/2/2	0/0/0/0
5	DMF	C	510	-	-	0/2/2/2	0/0/0/0
5	DMF	C	511	-	-	0/2/2/2	0/0/0/0
5	DMF	C	512	-	-	0/2/2/2	0/0/0/0
5	DMF	C	513	-	-	0/2/2/2	0/0/0/0
6	GOL	C	514	-	-	0/4/4/4	0/0/0/0
4	FG8	D	504	2	-	0/11/11/11	0/2/2/2
5	DMF	D	505	-	-	0/2/2/2	0/0/0/0
5	DMF	D	506	-	-	0/2/2/2	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMF	D	507	-	-	0/2/2/2	0/0/0/0
5	DMF	D	508	-	-	0/2/2/2	0/0/0/0
6	GOL	D	509	-	-	0/4/4/4	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	505	DMF	1	0
5	A	506	DMF	2	0
5	A	509	DMF	1	0
5	B	501	DMF	2	0
5	B	507	DMF	1	0
5	B	508	DMF	2	0
5	B	509	DMF	2	0
6	B	511	GOL	1	0
5	C	505	DMF	1	0
5	C	506	DMF	1	0
5	C	509	DMF	1	0
5	C	511	DMF	1	0
5	D	505	DMF	3	0
5	D	506	DMF	2	0
5	D	507	DMF	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	391/447 (87%)	0.38	20 (5%) 28 32	18, 29, 55, 105	0
1	B	410/447 (91%)	0.29	20 (4%) 29 33	17, 28, 50, 79	0
1	C	411/447 (91%)	0.30	16 (3%) 39 43	18, 28, 49, 81	0
1	D	397/447 (88%)	0.43	26 (6%) 19 22	20, 30, 60, 111	0
All	All	1609/1788 (89%)	0.35	82 (5%) 28 32	17, 29, 53, 111	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	425	ILE	9.8
1	A	428	TYR	9.4
1	D	434	LEU	8.4
1	D	432	TYR	7.7
1	C	230	LEU	7.3
1	D	426	TYR	7.1
1	D	435	TYR	6.4
1	D	429	ASP	6.4
1	D	428	TYR	6.0
1	D	433	GLN	5.9
1	D	425	ILE	5.8
1	A	426	TYR	5.8
1	B	425	ILE	5.6
1	D	81	GLU	5.2
1	A	231	PRO	5.0
1	A	81	GLU	4.9
1	C	425	ILE	4.6
1	A	392	PHE	4.5
1	B	438	THR	4.2
1	C	426	TYR	4.2
1	B	230	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	231	PRO	4.2
1	B	232	ILE	4.1
1	A	230	LEU	4.0
1	A	409	ARG	3.7
1	D	128	ARG	3.5
1	B	437	LEU	3.4
1	D	382	GLY	3.4
1	A	404	ILE	3.3
1	D	431	VAL	3.3
1	A	427	ASP	3.1
1	B	99	TYR	3.1
1	C	429	ASP	3.0
1	B	428	TYR	3.0
1	C	282[A]	CYS	3.0
1	C	438	THR	3.0
1	C	445	PRO	2.9
1	C	231	PRO	2.9
1	D	82	LYS	2.9
1	C	83	GLU	2.8
1	A	282[A]	CYS	2.8
1	D	165	VAL	2.8
1	A	382	GLY	2.7
1	B	426	TYR	2.7
1	B	77	LEU	2.7
1	B	84	LEU	2.7
1	B	168	THR	2.7
1	A	402	ASP	2.6
1	A	222	TRP	2.5
1	B	433	GLN	2.5
1	A	424	LEU	2.5
1	D	409	ARG	2.5
1	B	429	ASP	2.4
1	D	424	LEU	2.4
1	B	157	ILE	2.4
1	C	443	LEU	2.4
1	D	84	LEU	2.4
1	A	406	LYS	2.3
1	C	177	GLN	2.3
1	A	383	PRO	2.3
1	D	392	PHE	2.3
1	A	165	VAL	2.3
1	A	268	SER	2.3

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Mol	Chain	Res	Type	RSRZ
1	D	404	ILE	2.2
1	C	99	TYR	2.2
1	D	393	PRO	2.2
1	D	283	GLY	2.2
1	C	223	ASN	2.2
1	B	432	TYR	2.2
1	D	427	ASP	2.2
1	B	445	PRO	2.1
1	D	368	ILE	2.1
1	D	416	ARG	2.1
1	B	196	ALA	2.1
1	C	80	GLU	2.1
1	C	423	LYS	2.1
1	D	322	ALA	2.1
1	A	272	VAL	2.1
1	B	7	TYR	2.0
1	B	177	GLN	2.0
1	C	77	LEU	2.0
1	D	83	GLU	2.0

## 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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	B-factors( $\text{\AA}^2$ )	Q<0.9
5	DMF	C	505	5/5	0.67	0.22	35,47,62,70	0
5	DMF	C	506	5/5	0.71	0.19	47,52,57,59	0
5	DMF	B	506	5/5	0.79	0.21	54,54,63,64	0
5	DMF	B	508	5/5	0.80	0.27	48,52,56,56	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
5	DMF	B	512	5/5	0.81	0.27	60,62,71,73	0
5	DMF	C	508	5/5	0.82	0.18	52,59,64,66	0
5	DMF	B	509	5/5	0.83	0.13	46,57,61,61	0
6	GOL	C	514	6/6	0.83	0.14	29,33,42,42	0
5	DMF	A	505	5/5	0.83	0.18	59,59,63,66	0
5	DMF	B	501	5/5	0.84	0.18	45,46,53,56	0
5	DMF	D	505	5/5	0.84	0.23	48,53,67,74	0
4	FG8	D	504	20/20	0.85	0.15	32,46,51,52	0
5	DMF	A	507	5/5	0.85	0.21	44,45,53,54	0
6	GOL	A	510	6/6	0.86	0.19	30,34,35,36	0
4	FG8	A	504	20/20	0.88	0.13	25,39,49,55	0
5	DMF	C	509	5/5	0.88	0.17	39,44,53,58	0
5	DMF	C	511	5/5	0.89	0.17	52,56,59,62	0
4	FG8	B	505	20/20	0.89	0.15	27,38,46,49	0
5	DMF	C	510	5/5	0.90	0.14	67,71,73,73	0
5	DMF	A	506	5/5	0.90	0.16	43,43,49,49	0
6	GOL	B	511	6/6	0.91	0.17	32,40,41,47	0
5	DMF	C	513	5/5	0.91	0.20	39,45,52,61	0
5	DMF	A	509	5/5	0.92	0.22	51,53,53,56	0
5	DMF	A	508	5/5	0.92	0.19	37,38,41,46	0
5	DMF	C	507	5/5	0.92	0.20	45,48,53,59	0
5	DMF	B	510	5/5	0.92	0.14	35,42,46,47	0
5	DMF	D	508	5/5	0.93	0.13	37,47,52,56	0
4	FG8	C	504	20/20	0.93	0.15	27,35,42,43	0
5	DMF	D	506	5/5	0.93	0.25	58,58,61,61	0
5	DMF	C	512	5/5	0.94	0.15	40,45,47,50	0
5	DMF	B	507	5/5	0.94	0.12	37,40,44,48	0
6	GOL	D	509	6/6	0.94	0.11	31,35,42,42	0
5	DMF	D	507	5/5	0.95	0.22	47,48,48,50	0
3	K	A	503	1/1	0.96	0.11	31,31,31,31	0
3	K	B	504	1/1	0.99	0.11	26,26,26,26	0
3	K	B	503	1/1	0.99	0.10	26,26,26,26	0
3	K	C	502	1/1	0.99	0.10	23,23,23,23	0
3	K	A	502	1/1	0.99	0.12	25,25,25,25	0
3	K	D	502	1/1	0.99	0.11	26,26,26,26	0
3	K	D	503	1/1	0.99	0.09	31,31,31,31	0
2	ZN	D	501	1/1	1.00	0.06	32,32,32,32	0
2	ZN	C	501	1/1	1.00	0.07	30,30,30,30	0
2	ZN	A	501	1/1	1.00	0.07	29,29,29,29	0
2	ZN	B	502	1/1	1.00	0.08	28,28,28,28	0
3	K	C	503	1/1	1.00	0.07	27,27,27,27	0



## 6.5 Other polymers [i](#)

There are no such residues in this entry.