



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 15, 2024 – 09:12 pm GMT

PDB ID : 6HRQ  
Title : Crystal structure of Schistosoma mansoni HDAC8 complexed with NCC-149  
Authors : Shaik, T.B.; Marek, M.; Romier, C.  
Deposited on : 2018-09-28  
Resolution : 1.84 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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.

The types of validation reports are described at

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

---

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

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.36  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.36

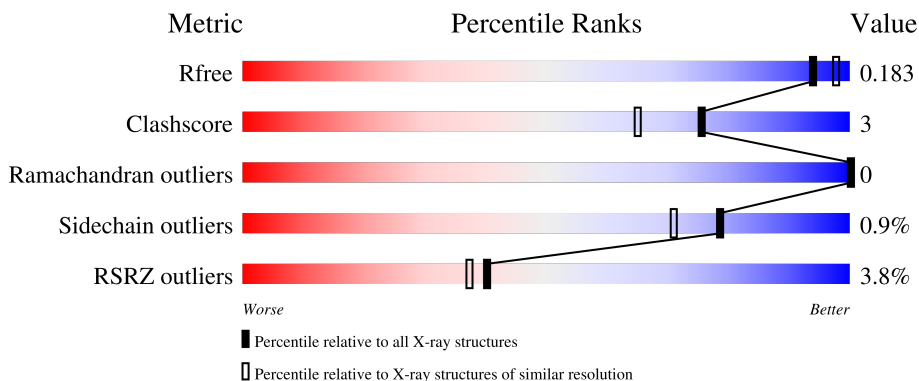
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.84 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	4003 (1.86-1.82)
Clashscore	141614	4233 (1.86-1.82)
Ramachandran outliers	138981	4185 (1.86-1.82)
Sidechain outliers	138945	4186 (1.86-1.82)
RSRZ outliers	127900	3957 (1.86-1.82)

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  $\geq 3$ , 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  $\leq 5\%$ . 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% 85% 5% 10%
1	B	447	 2% 88% 5% 7%
1	C	447	 3% 90% 6% . 6%
1	D	447	 5% 83% 6% 11%

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:

<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
5	DMF	A	505	-	-	X	-
6	GOL	D	515	-	-	X	-

## 2 Entry composition i

There are 7 unique types of molecules in this entry. The entry contains 14601 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
			Total	C	N	O	S			
1	A	401	3223	2080	537	591	15	0	3	0
1	B	416	3332	2147	559	609	17	0	2	0
1	C	419	3355	2158	560	621	16	0	3	0
1	D	400	3209	2071	534	589	15	0	2	0

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

*Continued on next page...*

*Continued from previous page...*

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

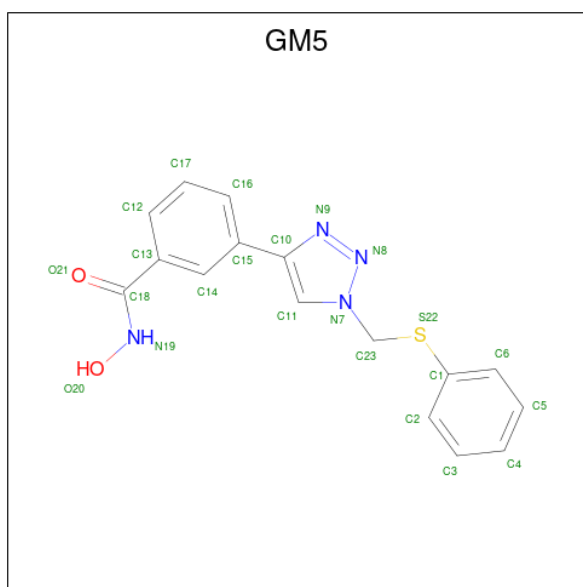
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

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

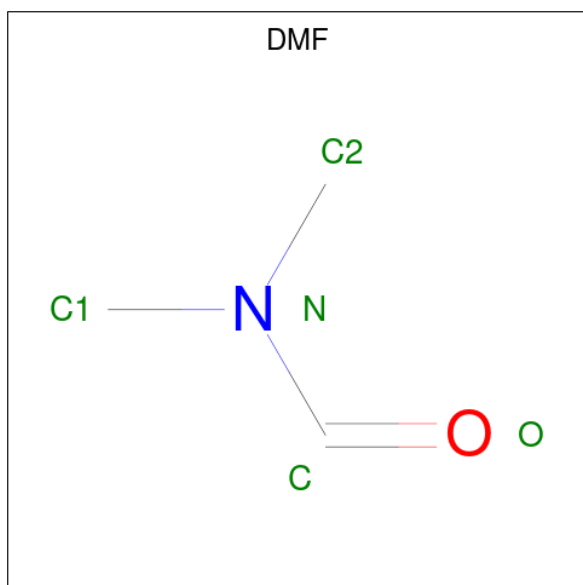
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total K 2 2	0	0
3	B	2	Total K 2 2	0	0
3	C	2	Total K 2 2	0	0
3	D	2	Total K 2 2	0	0

- Molecule 4 is {N}-oxidanyl-3-[1-(phenylsulfanylmethyl)-1,2,3-triazol-4-yl]benzamide (three-letter code: GM5) (formula: C<sub>16</sub>H<sub>14</sub>N<sub>4</sub>O<sub>2</sub>S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	A	1	Total	C	N	O	S	0	0
			23	16	4	2	1		
4	B	1	Total	C	N	O	S	0	0
			23	16	4	2	1		
4	C	1	Total	C	N	O	S	0	0
			23	16	4	2	1		
4	D	1	Total	C	N	O	S	0	0
			23	16	4	2	1		

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



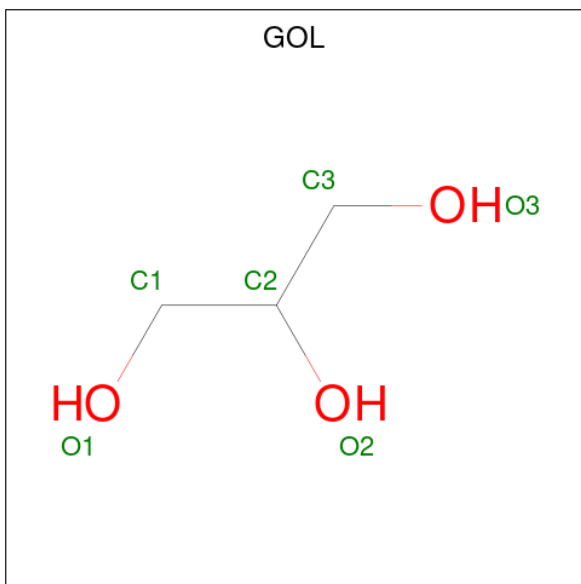
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			5	3	1	1		
5	A	1	Total	C	N	O	0	0
			5	3	1	1		
5	A	1	Total	C	N	O	0	0
			5	3	1	1		
5	A	1	Total	C	N	O	0	0
			5	3	1	1		
5	A	1	Total	C	N	O	0	0
			5	3	1	1		
5	B	1	Total	C	N	O	0	0
			5	3	1	1		
5	B	1	Total	C	N	O	0	0
			5	3	1	1		
5	B	1	Total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

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
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		
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<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		
6	B	1	Total	C	O	0	0
			6	3	3		

Continued on next page...



*Continued from previous page...*

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

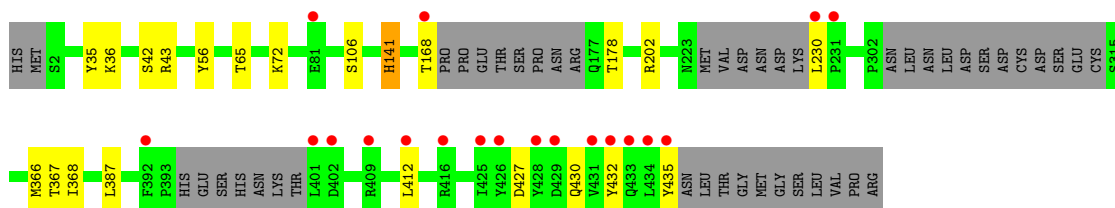
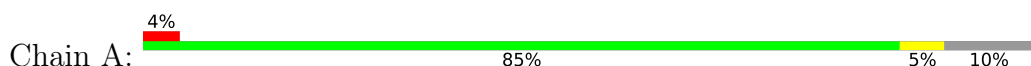
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	266	Total O 266 266	0	0
7	B	314	Total O 314 314	0	0
7	C	317	Total O 317 317	0	0
7	D	263	Total O 263 263	0	0

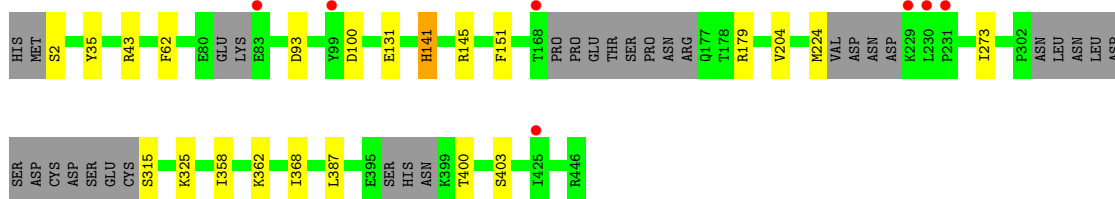
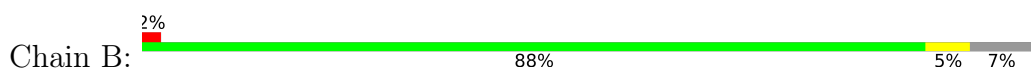
### 3 Residue-property plots [i](#)

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

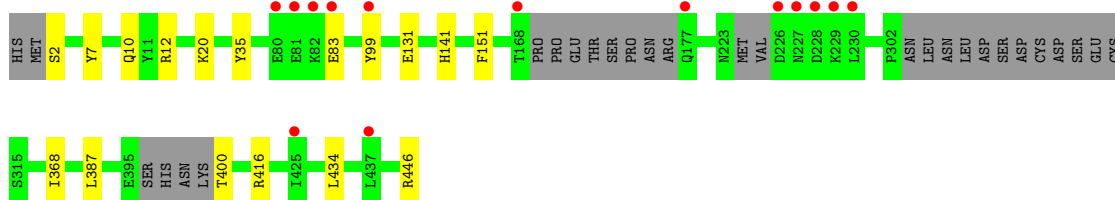
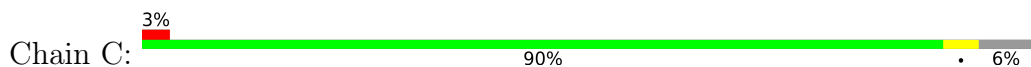
- Molecule 1: Histone deacetylase



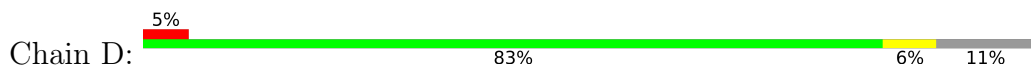
- Molecule 1: Histone deacetylase

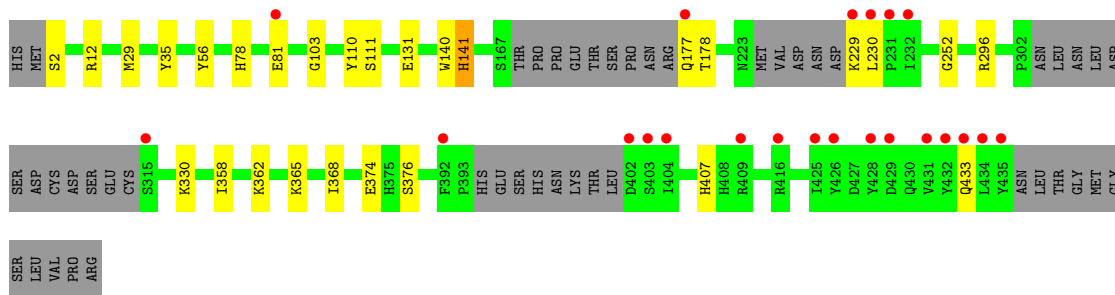


- Molecule 1: Histone deacetylase



- Molecule 1: Histone deacetylase





## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	71.43Å 71.48Å 99.26Å 78.11° 75.54° 85.37°	Depositor
Resolution (Å)	47.16 – 1.84 48.42 – 1.84	Depositor EDS
% Data completeness (in resolution range)	95.0 (47.16-1.84) 95.0 (48.42-1.84)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 1.84Å)	Xtrriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.150 , 0.183 0.150 , 0.183	Depositor DCC
$R_{free}$ test set	7607 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	25.1	Xtrriage
Anisotropy	0.182	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 59.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	0.080 for -k,-h,-l	Xtrriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	14601	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	30.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.32% 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: DMF, GOL, K, GM5, ZN

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	0.40	0/3322	0.52	0/4518
1	B	0.42	0/3429	0.53	0/4660
1	C	0.41	0/3456	0.53	1/4700 (0.0%)
1	D	0.40	0/3305	0.52	0/4495
All	All	0.41	0/13512	0.53	1/18373 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	434	LEU	CA-CB-CG	5.57	128.10	115.30

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	3223	0	3127	21	0
1	B	3332	0	3241	18	0
1	C	3355	0	3250	12	0
1	D	3209	0	3109	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0

*Continued on next page...*

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	23	0	0	0	0
4	B	23	0	0	0	0
4	C	23	0	0	0	0
4	D	23	0	0	0	0
5	A	30	0	42	7	0
5	B	50	0	70	6	0
5	C	35	0	49	2	0
5	D	25	0	35	4	0
6	A	6	0	8	0	0
6	B	24	0	32	3	0
6	C	12	0	16	2	0
6	D	36	0	48	12	0
7	A	266	0	0	5	2
7	B	314	0	0	4	2
7	C	317	0	0	2	0
7	D	263	0	0	4	0
All	All	14601	0	13027	81	2

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 3.

The worst 5 of 81 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:D:103:GLY:H	6:D:512:GOL:H11	1.30	0.95
1:B:43:ARG:HE	5:B:512:DMF:H13	1.34	0.90
1:A:43:ARG:H	5:A:505:DMF:H22	1.42	0.85
1:D:140:TRP:O	7:D:601:HOH:O	1.95	0.83
1:A:42[B]:SER:HA	5:A:505:DMF:H13	1.67	0.76

All (2) 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)
7:A:634:HOH:O	7:B:844:HOH:O[1_455]	2.14	0.06
7:A:810:HOH:O	7:B:844:HOH:O[1_455]	2.17	0.03

### 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	394/447 (88%)	390 (99%)	4 (1%)	0	100	100
1	B	406/447 (91%)	401 (99%)	5 (1%)	0	100	100
1	C	412/447 (92%)	408 (99%)	4 (1%)	0	100	100
1	D	392/447 (88%)	388 (99%)	4 (1%)	0	100	100
All	All	1604/1788 (90%)	1587 (99%)	17 (1%)	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	351/392 (90%)	348 (99%)	3 (1%)	78	71
1	B	363/392 (93%)	360 (99%)	3 (1%)	81	75
1	C	367/392 (94%)	364 (99%)	3 (1%)	81	75
1	D	349/392 (89%)	345 (99%)	4 (1%)	73	64
All	All	1430/1568 (91%)	1417 (99%)	13 (1%)	78	71

5 of 13 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	141	HIS
1	C	400	THR
1	D	433	GLN
1	D	81	GLU
1	D	141	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 57 ligands modelled in this entry, 12 are monoatomic - leaving 45 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	$\# Z  > 2$
5	DMF	C	507	-	4,4,4	0.29	0	4,4,4	0.30	0
5	DMF	B	512	-	4,4,4	0.26	0	4,4,4	0.39	0
5	DMF	D	507	-	4,4,4	0.26	0	4,4,4	0.29	0
6	GOL	A	510	-	5,5,5	0.39	0	5,5,5	0.15	0
6	GOL	D	513	-	5,5,5	0.36	0	5,5,5	0.30	0



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	GM5	D	504	2	24,25,25	0.45	0	27,33,33	0.36	0
5	DMF	A	509	-	4,4,4	0.27	0	4,4,4	0.33	0
6	GOL	B	515	-	5,5,5	0.31	0	5,5,5	0.31	0
5	DMF	D	506	-	4,4,4	0.30	0	4,4,4	0.51	0
5	DMF	A	506	-	4,4,4	0.32	0	4,4,4	0.41	0
5	DMF	C	508	-	4,4,4	0.34	0	4,4,4	0.47	0
5	DMF	B	507	-	4,4,4	0.15	0	4,4,4	0.63	0
5	DMF	B	505	-	4,4,4	0.28	0	4,4,4	0.40	0
5	DMF	C	511	-	4,4,4	0.36	0	4,4,4	0.65	0
5	DMF	A	507	-	4,4,4	0.35	0	4,4,4	0.44	0
5	DMF	B	514	-	4,4,4	0.36	0	4,4,4	0.38	0
5	DMF	B	506	-	4,4,4	0.33	0	4,4,4	0.40	0
6	GOL	B	518	-	5,5,5	0.34	0	5,5,5	0.84	0
5	DMF	C	510	-	4,4,4	0.35	0	4,4,4	0.50	0
5	DMF	A	511	-	4,4,4	0.27	0	4,4,4	0.26	0
5	DMF	C	509	-	4,4,4	0.36	0	4,4,4	0.41	0
6	GOL	B	517	-	5,5,5	0.33	0	5,5,5	0.34	0
5	DMF	D	509	-	4,4,4	0.28	0	4,4,4	0.50	0
5	DMF	D	505	-	4,4,4	0.32	0	4,4,4	0.47	0
6	GOL	C	513	-	5,5,5	0.26	0	5,5,5	0.52	0
4	GM5	A	504	2	24,25,25	0.44	0	27,33,33	0.41	0
5	DMF	A	505	-	4,4,4	0.27	0	4,4,4	0.34	0
5	DMF	B	511	-	4,4,4	0.30	0	4,4,4	0.41	0
5	DMF	B	510	-	4,4,4	0.31	0	4,4,4	0.49	0
6	GOL	D	510	-	5,5,5	0.37	0	5,5,5	0.41	0
6	GOL	D	512	-	5,5,5	0.43	0	5,5,5	0.41	0
5	DMF	C	506	-	4,4,4	0.38	0	4,4,4	0.22	0
4	GM5	C	504	2	24,25,25	0.42	0	27,33,33	0.38	0
6	GOL	C	512	-	5,5,5	0.37	0	5,5,5	0.37	0
6	GOL	D	514	-	5,5,5	0.39	0	5,5,5	0.26	0
5	DMF	D	508	-	4,4,4	0.35	0	4,4,4	0.34	0
5	DMF	B	509	-	4,4,4	0.36	0	4,4,4	0.35	0
5	DMF	A	508	-	4,4,4	0.34	0	4,4,4	0.45	0
5	DMF	B	513	-	4,4,4	0.30	0	4,4,4	0.28	0
6	GOL	B	516	-	5,5,5	0.35	0	5,5,5	0.35	0
6	GOL	D	511	-	5,5,5	0.30	0	5,5,5	0.32	0
6	GOL	D	515	-	5,5,5	0.46	0	5,5,5	1.19	0
5	DMF	B	508	-	4,4,4	0.31	0	4,4,4	0.25	0
4	GM5	B	504	2	24,25,25	0.40	0	27,33,33	0.35	0
5	DMF	C	505	-	4,4,4	0.30	0	4,4,4	0.47	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
5	DMF	C	507	-	-	2/2/2/2	-
5	DMF	B	512	-	-	0/2/2/2	-
5	DMF	D	507	-	-	2/2/2/2	-
6	GOL	A	510	-	-	0/4/4/4	-
6	GOL	D	513	-	-	4/4/4/4	-
4	GM5	D	504	2	-	0/13/15/15	0/3/3/3
5	DMF	A	509	-	-	2/2/2/2	-
6	GOL	B	515	-	-	0/4/4/4	-
5	DMF	D	506	-	-	2/2/2/2	-
5	DMF	A	506	-	-	2/2/2/2	-
5	DMF	C	508	-	-	2/2/2/2	-
5	DMF	B	507	-	-	0/2/2/2	-
5	DMF	B	505	-	-	1/2/2/2	-
5	DMF	C	511	-	-	0/2/2/2	-
5	DMF	A	507	-	-	0/2/2/2	-
5	DMF	B	514	-	-	2/2/2/2	-
5	DMF	B	506	-	-	2/2/2/2	-
6	GOL	B	518	-	-	4/4/4/4	-
5	DMF	C	510	-	-	2/2/2/2	-
5	DMF	A	511	-	-	0/2/2/2	-
5	DMF	C	509	-	-	0/2/2/2	-
6	GOL	B	517	-	-	2/4/4/4	-
5	DMF	D	509	-	-	0/2/2/2	-
5	DMF	D	505	-	-	2/2/2/2	-
6	GOL	C	513	-	-	2/4/4/4	-
4	GM5	A	504	2	-	0/13/15/15	0/3/3/3
5	DMF	A	505	-	-	2/2/2/2	-
5	DMF	B	511	-	-	0/2/2/2	-
5	DMF	B	510	-	-	1/2/2/2	-
6	GOL	D	510	-	-	0/4/4/4	-
6	GOL	D	512	-	-	2/4/4/4	-
5	DMF	C	506	-	-	0/2/2/2	-
4	GM5	C	504	2	-	0/13/15/15	0/3/3/3
6	GOL	C	512	-	-	2/4/4/4	-
6	GOL	D	514	-	-	0/4/4/4	-
5	DMF	D	508	-	-	2/2/2/2	-

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMF	B	509	-	-	2/2/2/2	-
5	DMF	A	508	-	-	0/2/2/2	-
5	DMF	B	513	-	-	2/2/2/2	-
6	GOL	B	516	-	-	2/4/4/4	-
6	GOL	D	511	-	-	1/4/4/4	-
6	GOL	D	515	-	-	0/4/4/4	-
5	DMF	B	508	-	-	2/2/2/2	-
4	GM5	B	504	2	-	0/13/15/15	0/3/3/3
5	DMF	C	505	-	-	2/2/2/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 53 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	518	GOL	O1-C1-C2-C3
6	B	518	GOL	C1-C2-C3-O3
6	B	518	GOL	O2-C2-C3-O3
6	C	512	GOL	O1-C1-C2-C3
6	D	513	GOL	O1-C1-C2-C3

There are no ring outliers.

19 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	507	DMF	1	0
5	B	512	DMF	3	0
5	D	507	DMF	1	0
6	D	513	GOL	3	0
5	A	509	DMF	1	0
5	D	506	DMF	1	0
5	A	506	DMF	1	0
5	B	506	DMF	1	0
6	B	518	GOL	2	0
6	B	517	GOL	1	0
5	D	509	DMF	2	0
6	C	513	GOL	2	0
5	A	505	DMF	5	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	511	DMF	1	0
6	D	512	GOL	3	0
5	B	513	DMF	1	0
6	D	511	GOL	1	0
6	D	515	GOL	5	0
5	C	505	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 [i](#)

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

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	401/447 (89%)	-0.15	19 (4%) 31 28	18, 26, 62, 96	0
1	B	416/447 (93%)	-0.18	7 (1%) 70 69	17, 24, 47, 90	0
1	C	419/447 (93%)	-0.10	14 (3%) 46 43	16, 25, 50, 112	0
1	D	400/447 (89%)	-0.19	22 (5%) 25 22	18, 26, 61, 92	0
All	All	1636/1788 (91%)	-0.15	62 (3%) 40 37	16, 25, 52, 112	0

The worst 5 of 62 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	432	TYR	11.0
1	C	228	ASP	7.6
1	A	428	TYR	7.3
1	D	432	TYR	7.0
1	C	81	GLU	6.9

### 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 monosaccharides in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 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	D	509	5/5	0.77	0.21	46,58,66,69	0
6	GOL	D	512	6/6	0.82	0.29	45,51,53,61	0
6	GOL	C	513	6/6	0.83	0.15	37,45,46,48	0
5	DMF	C	508	5/5	0.83	0.36	64,68,77,81	0
6	GOL	D	513	6/6	0.84	0.19	51,60,64,66	0
5	DMF	D	507	5/5	0.85	0.14	51,55,72,77	0
6	GOL	C	512	6/6	0.87	0.11	29,32,35,36	0
5	DMF	C	506	5/5	0.87	0.14	34,42,46,47	0
5	DMF	A	507	5/5	0.87	0.17	38,45,46,48	0
6	GOL	B	516	6/6	0.87	0.34	59,64,65,66	0
5	DMF	D	506	5/5	0.88	0.12	39,50,53,59	0
5	DMF	B	505	5/5	0.88	0.23	39,43,51,58	0
5	DMF	B	509	5/5	0.89	0.13	56,57,61,62	0
4	GM5	C	504	23/23	0.89	0.17	25,37,46,52	0
4	GM5	D	504	23/23	0.89	0.13	27,35,45,53	0
5	DMF	C	509	5/5	0.89	0.22	37,41,45,50	0
4	GM5	A	504	23/23	0.89	0.12	25,39,46,48	0
4	GM5	B	504	23/23	0.89	0.21	27,38,49,51	0
6	GOL	D	515	6/6	0.89	0.32	29,38,48,53	0
5	DMF	A	505	5/5	0.90	0.16	26,45,50,54	0
5	DMF	B	511	5/5	0.90	0.21	49,56,62,66	0
5	DMF	B	512	5/5	0.90	0.17	38,44,50,59	0
6	GOL	D	514	6/6	0.90	0.12	59,62,62,68	0
5	DMF	B	514	5/5	0.90	0.20	31,39,45,45	0
5	DMF	B	506	5/5	0.91	0.15	61,62,63,65	0
5	DMF	C	510	5/5	0.91	0.14	48,50,53,53	0
5	DMF	A	506	5/5	0.91	0.15	38,44,48,55	0
5	DMF	B	513	5/5	0.91	0.14	48,49,55,56	0
6	GOL	D	510	6/6	0.92	0.13	25,32,33,35	0
5	DMF	B	510	5/5	0.92	0.11	40,59,62,64	0
6	GOL	B	518	6/6	0.92	0.14	32,47,56,64	0
5	DMF	A	511	5/5	0.92	0.26	42,54,60,64	0
5	DMF	A	508	5/5	0.92	0.10	58,59,63,65	0
5	DMF	C	505	5/5	0.93	0.19	43,45,52,59	0
5	DMF	D	505	5/5	0.93	0.16	47,52,57,58	0
5	DMF	A	509	5/5	0.93	0.11	45,46,50,52	0
5	DMF	C	507	5/5	0.93	0.15	67,69,70,70	0
6	GOL	D	511	6/6	0.93	0.20	41,46,48,48	0
5	DMF	B	507	5/5	0.93	0.19	37,39,49,51	0
6	GOL	A	510	6/6	0.93	0.10	26,33,38,39	0
5	DMF	B	508	5/5	0.93	0.11	33,37,43,48	0
6	GOL	B	517	6/6	0.93	0.18	38,49,57,62	0
6	GOL	B	515	6/6	0.95	0.08	25,31,33,33	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
5	DMF	C	511	5/5	0.95	0.12	35,37,39,46	0
5	DMF	D	508	5/5	0.95	0.10	31,40,50,54	0
2	ZN	A	501	1/1	0.99	0.03	30,30,30,30	0
2	ZN	C	501	1/1	1.00	0.04	30,30,30,30	0
2	ZN	D	501	1/1	1.00	0.04	31,31,31,31	0
3	K	A	502	1/1	1.00	0.10	19,19,19,19	0
3	K	A	503	1/1	1.00	0.09	22,22,22,22	0
3	K	B	502	1/1	1.00	0.09	22,22,22,22	0
3	K	B	503	1/1	1.00	0.10	18,18,18,18	0
3	K	C	502	1/1	1.00	0.07	22,22,22,22	0
3	K	C	503	1/1	1.00	0.11	18,18,18,18	0
3	K	D	502	1/1	1.00	0.10	22,22,22,22	0
3	K	D	503	1/1	1.00	0.11	18,18,18,18	0
2	ZN	B	501	1/1	1.00	0.04	30,30,30,30	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.