



# wwPDB X-ray Structure Validation Summary Report ⓘ

Nov 22, 2018 – 08:51 AM EST

PDB ID : 6HSH  
Title : Crystal structure of Schistosoma mansoni HDAC8 complexed with Quisinostat  
Authors : Shaik, T.B.; Marek, M.; Romier, C.  
Deposited on : 2018-10-01  
Resolution : 1.54 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.

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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-20031633  
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-20031633

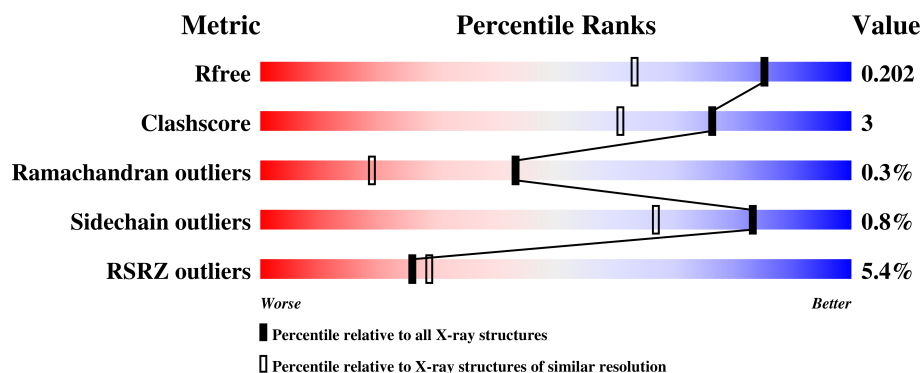
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.54 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	2055 (1.56-1.52)
Clashscore	122126	2124 (1.56-1.52)
Ramachandran outliers	120053	2083 (1.56-1.52)
Sidechain outliers	120020	2081 (1.56-1.52)
RSRZ outliers	108989	2027 (1.56-1.52)

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	<div> <div>6%</div> <div>85% 5% 10%</div> </div>
1	B	447	<div> <div>3%</div> <div>87% . 8%</div> </div>
1	C	447	<div> <div>4%</div> <div>85% 7% 7%</div> </div>
1	D	447	<div> <div>7%</div> <div>82% 9% 9%</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
5	DMF	A	510	-	-	X	-
5	DMF	C	507	-	-	X	-

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14595 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	404	Total	C	N	O	S	0	4	0
			3247	2089	542	599	17			
1	B	410	Total	C	N	O	S	0	6	0
			3300	2128	550	605	17			
1	C	415	Total	C	N	O	S	0	3	0
			3319	2139	553	610	17			
1	D	405	Total	C	N	O	S	0	5	0
			3258	2104	540	596	18			

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

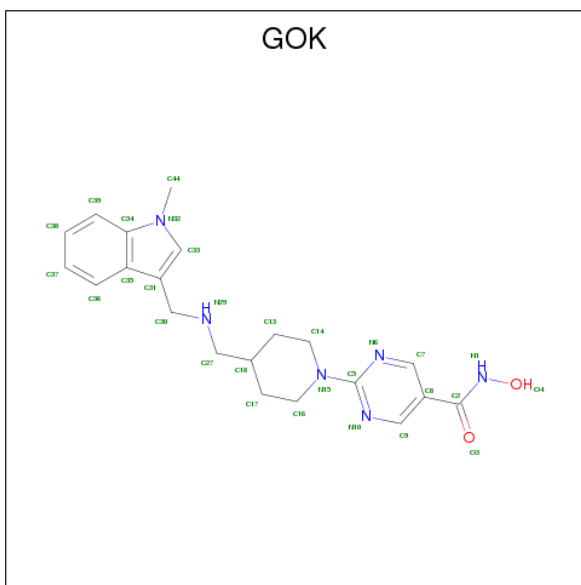
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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).

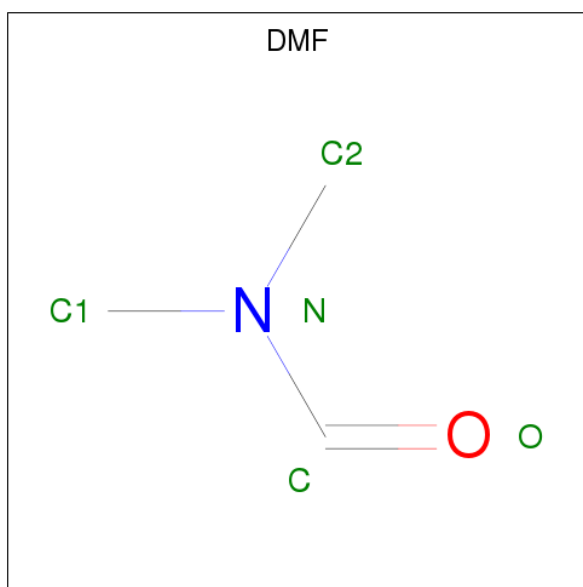
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total K 2 2	0	0
3	A	2	Total K 2 2	0	0
3	D	2	Total K 2 2	0	0
3	C	2	Total K 2 2	0	0

- Molecule 4 is 2-[4-[[[(1-methylindol-3-yl)methylamino]methyl]piperidin-1-yl]- {N}-oxidanyl-pyrimidine-5-carboxamide (three-letter code: GOK) (formula: C<sub>21</sub>H<sub>26</sub>N<sub>6</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			29	21	6	2		
4	B	1	Total	C	N	O	0	0
			29	21	6	2		
4	B	1	Total	C	N	O	0	0
			29	21	6	2		
4	C	1	Total	C	N	O	0	0
			29	21	6	2		
4	C	1	Total	C	N	O	0	0
			29	21	6	2		
4	D	1	Total	C	N	O	0	0
			29	21	6	2		

- 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	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		

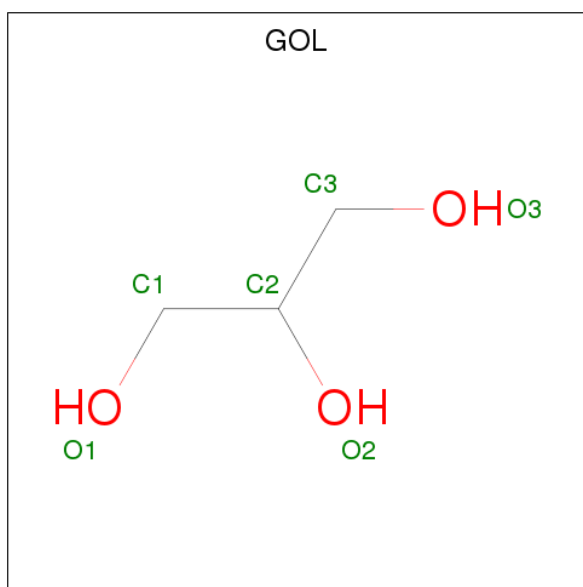
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	C	1	Total	C	N	O	0	0
			5	3	1	1		
5	C	1	Total	C	N	O	0	0
			5	3	1	1		
5	C	1	Total	C	N	O	0	0
			5	3	1	1		
5	C	1	Total	C	N	O	0	0
			5	3	1	1		
5	C	1	Total	C	N	O	0	0
			5	3	1	1		
5	C	1	Total	C	N	O	0	0
			5	3	1	1		
5	D	1	Total	C	N	O	0	0
			5	3	1	1		
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	C	1	Total	C	O	0	0
			6	3	3		
6	C	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		
6	D	1	Total	C	O	0	0
			6	3	3		

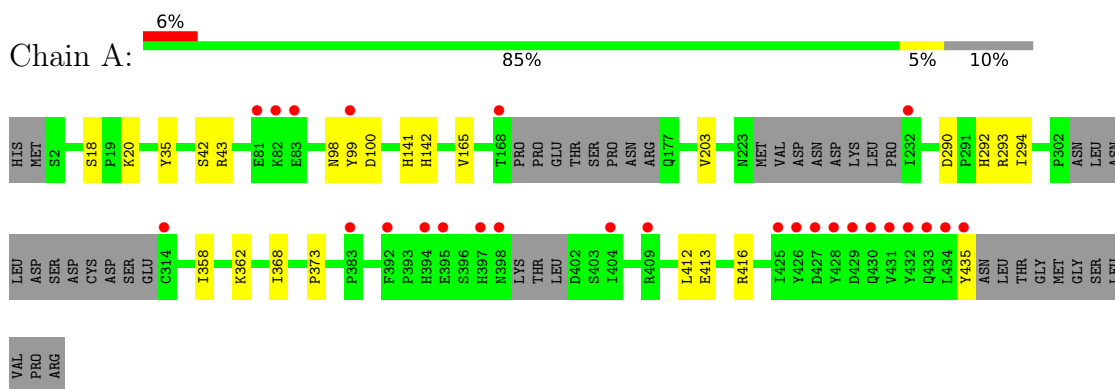
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	272	Total	O	0	0
			272	272		
7	B	304	Total	O	0	0
			304	304		
7	C	291	Total	O	0	0
			291	291		
7	D	235	Total	O	0	0
			235	235		

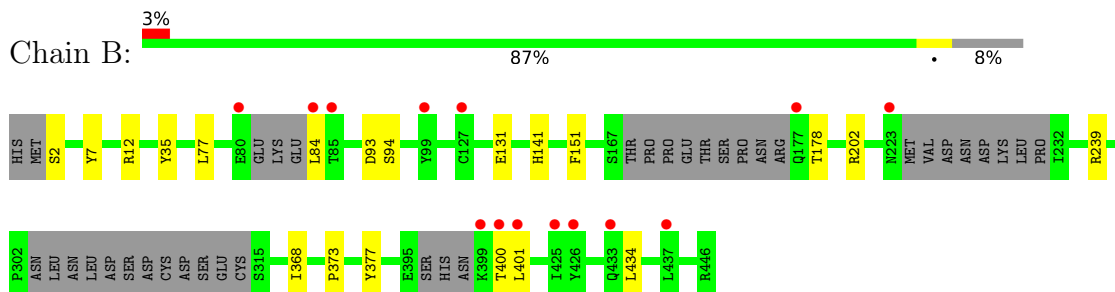
### 3 Residue-property plots [i](#)

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.

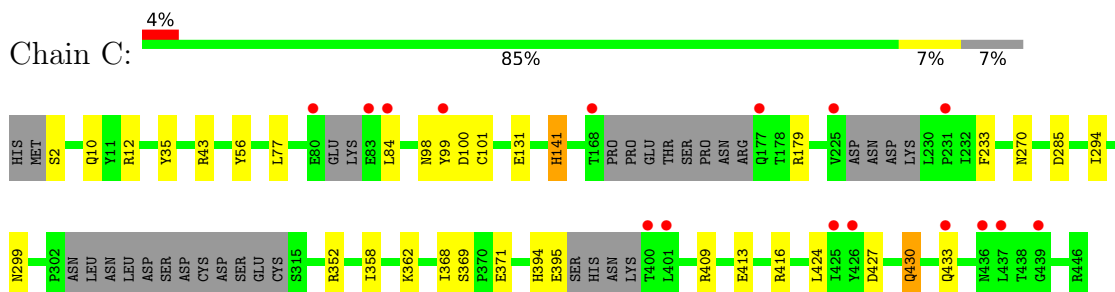
- Molecule 1: Histone deacetylase



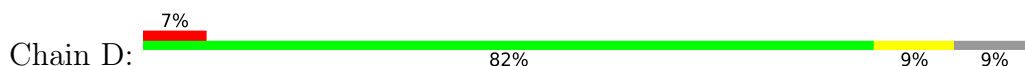
- Molecule 1: Histone deacetylase

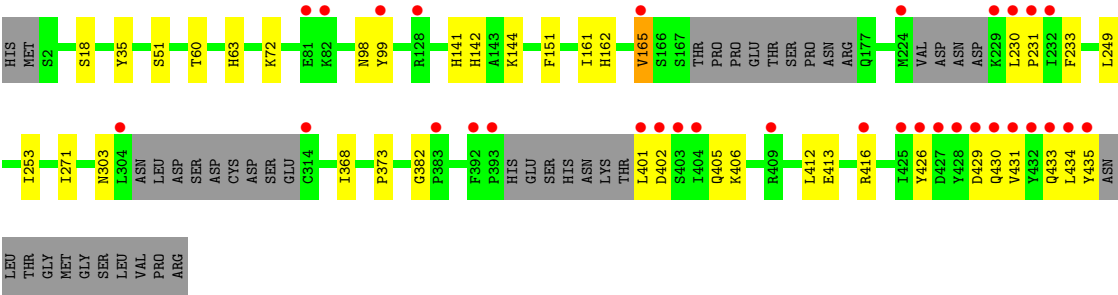


- Molecule 1: Histone deacetylase



- Molecule 1: Histone deacetylase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	70.75Å 70.80Å 97.82Å 78.03° 75.67° 85.74°	Depositor
Resolution (Å)	46.47 – 1.54 46.47 – 1.54	Depositor EDS
% Data completeness (in resolution range)	82.8 (46.47-1.54) 82.8 (46.47-1.54)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.17 (at 1.55Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, $R_{free}$	0.168 , 0.202 0.169 , 0.202	Depositor DCC
$R_{free}$ test set	10917 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	21.5	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 52.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.095 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	14595	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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: K, GOL, ZN, DMF, GOK

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	0/3350	0.54	0/4556
1	B	0.41	0/3406	0.58	1/4631 (0.0%)
1	C	0.40	0/3419	0.56	1/4651 (0.0%)
1	D	0.38	0/3363	0.54	0/4573
All	All	0.40	0/13538	0.55	2/18411 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	434	LEU	CA-CB-CG	6.43	130.09	115.30
1	C	285	ASP	CB-CG-OD1	5.12	122.91	118.30

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	3247	0	3131	16	0
1	B	3300	0	3203	18	0
1	C	3319	0	3221	29	0
1	D	3258	0	3172	25	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
4	A	29	0	0	2	0
4	B	58	0	0	1	0
4	C	58	0	0	1	0
4	D	29	0	0	1	0
5	A	30	0	42	5	0
5	B	30	0	40	2	0
5	C	45	0	63	8	0
5	D	30	0	42	2	0
6	A	6	0	8	0	0
6	B	12	0	15	3	0
6	C	18	0	24	3	0
6	D	12	0	16	0	0
7	A	272	0	0	1	0
7	B	304	0	0	1	0
7	C	291	0	0	2	1
7	D	235	0	0	4	1
All	All	14595	0	12977	87	1

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 87 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:12:ARG:HH21	6:B:513:GOL:H31	1.42	0.84
1:A:42:SER:HA	5:A:510:DMF:H13	1.61	0.82
1:C:43:ARG:HE	5:C:508:DMF:H12	1.49	0.77
1:D:429:ASP:OD1	1:D:430:GLN:N	2.21	0.74
1:A:98:ASN:OD1	7:A:601:HOH:O	2.10	0.69

All (1) 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:C:861:HOH:O	7:D:681:HOH:O[1_545]	2.18	0.02

## 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	398/447 (89%)	392 (98%)	5 (1%)	1 (0%)	43	19
1	B	404/447 (90%)	398 (98%)	6 (2%)	0	100	100
1	C	406/447 (91%)	402 (99%)	3 (1%)	1 (0%)	49	24
1	D	400/447 (90%)	395 (99%)	3 (1%)	2 (0%)	31	9
All	All	1608/1788 (90%)	1587 (99%)	17 (1%)	4 (0%)	43	24

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	99	TYR
1	A	99	TYR
1	D	99	TYR
1	D	303	ASN

### 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	355/392 (91%)	353 (99%)	2 (1%)	87	74
1	B	361/392 (92%)	359 (99%)	2 (1%)	87	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	363/392 (93%)	359 (99%)	4 (1%)	76	53
1	D	357/392 (91%)	353 (99%)	4 (1%)	76	53
All	All	1436/1568 (92%)	1424 (99%)	12 (1%)	83	67

5 of 12 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	141	HIS
1	C	233	PHE
1	D	151	PHE
1	C	56	TYR
1	D	141	HIS

Some 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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 53 ligands modelled in this entry, 12 are monoatomic - leaving 41 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	GOK	A	504	2	32,32,32	1.62	3 (9%)	38,44,44	1.39	4 (10%)
5	DMF	A	505	-	4,4,4	0.30	0	4,4,4	0.27	0
5	DMF	A	506	-	4,4,4	0.33	0	4,4,4	0.43	0
5	DMF	A	507	-	4,4,4	0.37	0	4,4,4	0.50	0
5	DMF	A	508	-	4,4,4	0.34	0	4,4,4	0.39	0
6	GOL	A	509	-	5,5,5	0.29	0	5,5,5	0.27	0
5	DMF	A	510	-	4,4,4	0.29	0	4,4,4	0.28	0
5	DMF	A	511	-	4,4,4	0.30	0	4,4,4	0.30	0
4	GOK	B	504	2	32,32,32	1.63	3 (9%)	38,44,44	1.40	4 (10%)
4	GOK	B	505	-	32,32,32	1.64	3 (9%)	38,44,44	1.42	5 (13%)
5	DMF	B	506	-	4,4,4	0.33	0	4,4,4	0.39	0
5	DMF	B	507	-	4,4,4	0.32	0	4,4,4	0.44	0
5	DMF	B	508	-	4,4,4	0.34	0	4,4,4	0.34	0
5	DMF	B	509	-	4,4,4	0.36	0	4,4,4	0.43	0
5	DMF	B	510	-	4,4,4	0.37	0	4,4,4	0.22	0
5	DMF	B	511	6	4,4,4	0.45	0	4,4,4	0.43	0
6	GOL	B	512	-	5,5,5	0.27	0	5,5,5	0.35	0
6	GOL	B	513	5	5,5,5	0.40	0	5,5,5	1.27	0
5	DMF	C	501	-	4,4,4	0.30	0	4,4,4	0.33	0
4	GOK	C	505	2	32,32,32	1.64	3 (9%)	38,44,44	1.41	4 (10%)
4	GOK	C	506	-	32,32,32	1.65	3 (9%)	38,44,44	1.45	5 (13%)
5	DMF	C	507	-	4,4,4	0.36	0	4,4,4	0.35	0
5	DMF	C	508	-	4,4,4	0.32	0	4,4,4	0.55	0
5	DMF	C	509	-	4,4,4	0.35	0	4,4,4	0.36	0
5	DMF	C	510	-	4,4,4	0.26	0	4,4,4	0.48	0
5	DMF	C	511	-	4,4,4	0.37	0	4,4,4	0.48	0
5	DMF	C	512	-	4,4,4	0.31	0	4,4,4	0.36	0
5	DMF	C	513	-	4,4,4	0.27	0	4,4,4	0.37	0
5	DMF	C	514	-	4,4,4	0.43	0	4,4,4	0.21	0
6	GOL	C	515	-	5,5,5	0.26	0	5,5,5	0.49	0
6	GOL	C	516	-	5,5,5	0.34	0	5,5,5	0.37	0
6	GOL	C	517	-	5,5,5	0.39	0	5,5,5	0.22	0
4	GOK	D	504	2	32,32,32	1.63	3 (9%)	38,44,44	1.41	4 (10%)
5	DMF	D	505	-	4,4,4	0.30	0	4,4,4	0.45	0
5	DMF	D	506	-	4,4,4	0.34	0	4,4,4	0.41	0
5	DMF	D	507	-	4,4,4	0.32	0	4,4,4	0.41	0
5	DMF	D	508	-	4,4,4	0.34	0	4,4,4	0.39	0
5	DMF	D	509	-	4,4,4	0.33	0	4,4,4	0.42	0
5	DMF	D	510	-	4,4,4	0.29	0	4,4,4	0.40	0
6	GOL	D	511	-	5,5,5	0.37	0	5,5,5	0.30	0
6	GOL	D	512	-	5,5,5	0.30	0	5,5,5	0.50	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	GOK	A	504	2	-	0/16/38/38	0/4/4/4
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
6	GOL	A	509	-	-	0/4/4/4	0/0/0/0
5	DMF	A	510	-	-	0/2/2/2	0/0/0/0
5	DMF	A	511	-	-	0/2/2/2	0/0/0/0
4	GOK	B	504	2	-	0/16/38/38	0/4/4/4
4	GOK	B	505	-	-	0/16/38/38	0/4/4/4
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
5	DMF	B	511	6	-	0/2/2/2	0/0/0/0
6	GOL	B	512	-	-	0/4/4/4	0/0/0/0
6	GOL	B	513	5	-	0/4/4/4	0/0/0/0
5	DMF	C	501	-	-	0/2/2/2	0/0/0/0
4	GOK	C	505	2	-	0/16/38/38	0/4/4/4
4	GOK	C	506	-	-	0/16/38/38	0/4/4/4
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
5	DMF	C	514	-	-	0/2/2/2	0/0/0/0
6	GOL	C	515	-	-	0/4/4/4	0/0/0/0
6	GOL	C	516	-	-	0/4/4/4	0/0/0/0
6	GOL	C	517	-	-	0/4/4/4	0/0/0/0
4	GOK	D	504	2	-	0/16/38/38	0/4/4/4
5	DMF	D	505	-	-	0/2/2/2	0/0/0/0
5	DMF	D	506	-	-	0/2/2/2	0/0/0/0
5	DMF	D	507	-	-	0/2/2/2	0/0/0/0
5	DMF	D	508	-	-	0/2/2/2	0/0/0/0
5	DMF	D	509	-	-	0/2/2/2	0/0/0/0
5	DMF	D	510	-	-	0/2/2/2	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	D	511	-	-	0/4/4/4	0/0/0/0
6	GOL	D	512	-	-	0/4/4/4	0/0/0/0

The worst 5 of 18 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	506	GOK	C33-C31	-7.92	1.36	1.53
4	B	505	GOK	C33-C31	-7.91	1.36	1.53
4	C	505	GOK	C33-C31	-7.89	1.36	1.53
4	D	504	GOK	C33-C31	-7.87	1.36	1.53
4	B	504	GOK	C33-C31	-7.85	1.36	1.53

The worst 5 of 26 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	504	GOK	C35-C34-N32	-4.53	107.76	110.99
4	C	506	GOK	C35-C34-N32	-4.51	107.77	110.99
4	B	505	GOK	C35-C34-N32	-4.51	107.77	110.99
4	A	504	GOK	C35-C34-N32	-4.46	107.80	110.99
4	C	505	GOK	C35-C34-N32	-4.43	107.82	110.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

15 monomers are involved in 28 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	504	GOK	2	0
5	A	506	DMF	1	0
5	A	510	DMF	4	0
4	B	505	GOK	1	0
5	B	507	DMF	2	0
6	B	513	GOL	3	0
4	C	505	GOK	1	0
5	C	507	DMF	4	0
5	C	508	DMF	3	0
5	C	511	DMF	1	0
6	C	515	GOL	2	0
6	C	516	GOL	1	0
4	D	504	GOK	1	0
5	D	505	DMF	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	D	510	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	404/447 (90%)	0.07	26 (6%)	19 21	17, 25, 59, 95	0
1	B	410/447 (91%)	-0.05	14 (3%)	45 51	16, 22, 42, 83	0
1	C	415/447 (92%)	-0.01	16 (3%)	39 44	16, 23, 45, 90	0
1	D	405/447 (90%)	0.14	32 (7%)	12 14	18, 25, 60, 97	0
All	All	1634/1788 (91%)	0.04	88 (5%)	26 28	16, 24, 51, 97	0

The worst 5 of 88 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	432	TYR	11.7
1	D	401	LEU	11.3
1	A	432	TYR	11.1
1	D	426	TYR	8.5
1	D	425	ILE	8.1

### 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 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
6	GOL	B	513	6/6	0.55	0.19	53,56,58,68	0
5	DMF	B	509	5/5	0.66	0.18	48,56,62,63	0
5	DMF	D	506	5/5	0.67	0.16	62,63,68,71	0
5	DMF	B	508	5/5	0.75	0.19	44,55,55,56	0
5	DMF	A	510	5/5	0.77	0.20	43,48,56,61	0
5	DMF	B	511	5/5	0.79	0.23	61,63,66,68	0
5	DMF	D	505	5/5	0.81	0.17	32,32,36,40	0
6	GOL	C	515	6/6	0.82	0.12	38,41,45,48	0
6	GOL	C	516	6/6	0.83	0.22	34,42,49,59	0
5	DMF	C	501	5/5	0.83	0.13	35,37,44,44	0
5	DMF	C	507	5/5	0.83	0.16	48,55,57,61	0
5	DMF	D	508	5/5	0.83	0.14	63,65,69,69	0
4	GOK	C	506	29/29	0.84	0.16	35,45,61,64	0
5	DMF	C	514	5/5	0.84	0.13	33,40,43,47	0
5	DMF	C	508	5/5	0.85	0.11	33,33,44,45	0
5	DMF	A	505	5/5	0.86	0.13	60,62,63,65	0
4	GOK	B	505	29/29	0.86	0.24	29,64,75,78	0
5	DMF	C	511	5/5	0.87	0.20	46,52,56,59	0
5	DMF	A	506	5/5	0.87	0.14	35,40,43,45	0
5	DMF	D	510	5/5	0.88	0.12	49,50,52,53	0
5	DMF	C	513	5/5	0.88	0.15	48,49,50,55	0
6	GOL	D	512	6/6	0.89	0.14	41,46,53,56	0
5	DMF	C	509	5/5	0.89	0.13	63,64,65,70	0
5	DMF	A	511	5/5	0.89	0.11	32,39,46,49	0
4	GOK	C	505	29/29	0.90	0.12	24,35,48,51	0
5	DMF	C	512	5/5	0.91	0.13	34,40,44,48	0
6	GOL	B	512	6/6	0.91	0.08	28,28,32,33	0
5	DMF	B	506	5/5	0.91	0.10	31,32,45,49	0
5	DMF	A	508	5/5	0.91	0.09	41,44,47,48	0
4	GOK	D	504	29/29	0.91	0.10	27,36,46,47	0
4	GOK	A	504	29/29	0.92	0.11	24,31,50,50	0
6	GOL	A	509	6/6	0.93	0.09	24,29,31,33	0
5	DMF	B	510	5/5	0.93	0.12	29,31,38,39	0
6	GOL	D	511	6/6	0.93	0.07	28,32,32,35	0
5	DMF	B	507	5/5	0.93	0.11	42,44,47,53	0
4	GOK	B	504	29/29	0.93	0.11	24,33,43,43	0
5	DMF	A	507	5/5	0.93	0.10	39,40,48,54	0
6	GOL	C	517	6/6	0.93	0.07	25,29,30,32	0
5	DMF	D	507	5/5	0.94	0.12	42,47,49,56	0
5	DMF	C	510	5/5	0.95	0.07	33,36,41,42	0
5	DMF	D	509	5/5	0.97	0.08	46,47,54,58	0
3	K	C	504	1/1	1.00	0.09	17,17,17,17	0
2	ZN	B	501	1/1	1.00	0.07	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	K	A	503	1/1	1.00	0.09	18,18,18,18	0
3	K	D	502	1/1	1.00	0.08	22,22,22,22	0
2	ZN	A	501	1/1	1.00	0.06	33,33,33,33	0
3	K	D	503	1/1	1.00	0.09	18,18,18,18	0
2	ZN	D	501	1/1	1.00	0.07	34,34,34,34	0
3	K	C	503	1/1	1.00	0.06	23,23,23,23	0
3	K	B	503	1/1	1.00	0.10	17,17,17,17	0
2	ZN	C	502	1/1	1.00	0.08	33,33,33,33	0
3	K	A	502	1/1	1.00	0.08	22,22,22,22	0
3	K	B	502	1/1	1.00	0.08	20,20,20,20	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.