



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 10:27 pm BST

PDB ID : 6HU2
Title : Crystal structure of Schistosoma mansoni HDAC8 complexed with a benzohydroxamate inhibitor 11
Authors : Shaik, T.B.; Marek, M.; Romier, C.
Deposited on : 2018-10-05
Resolution : 1.99 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
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)	:	2.11

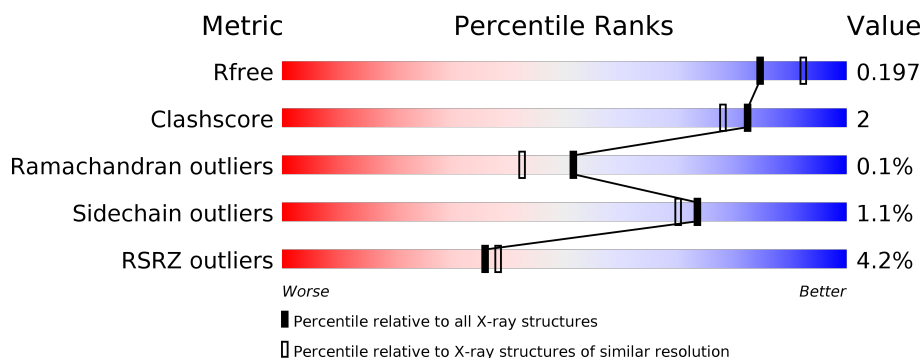
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	11647 (2.00-1.96)
Clashscore	141614	1014 (1.98-1.98)
Ramachandran outliers	138981	1006 (1.98-1.98)
Sidechain outliers	138945	1006 (1.98-1.98)
RSRZ outliers	127900	11410 (2.00-1.96)

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 ≥ 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	<div> <div>5%</div> <div> <div></div> <div>85%</div> <div>5%</div> <div>10%</div> </div> </div>
1	B	447	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>5%</div> <div>7%</div> </div> </div>
1	C	447	<div> <div>2%</div> <div> <div></div> <div>87%</div> <div>5%</div> <div>7%</div> </div> </div>
1	D	447	<div> <div>5%</div> <div> <div></div> <div>86%</div> <div>• •</div> <div>10%</div> </div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14138 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	401	Total	C	N	O	S	0	2	0
			3218	2075	537	590	16			
1	B	414	Total	C	N	O	S	0	4	0
			3334	2150	557	610	17			
1	C	414	Total	C	N	O	S	0	4	0
			3336	2149	559	611	17			
1	D	403	Total	C	N	O	S	0	4	0
			3243	2091	542	593	17			

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

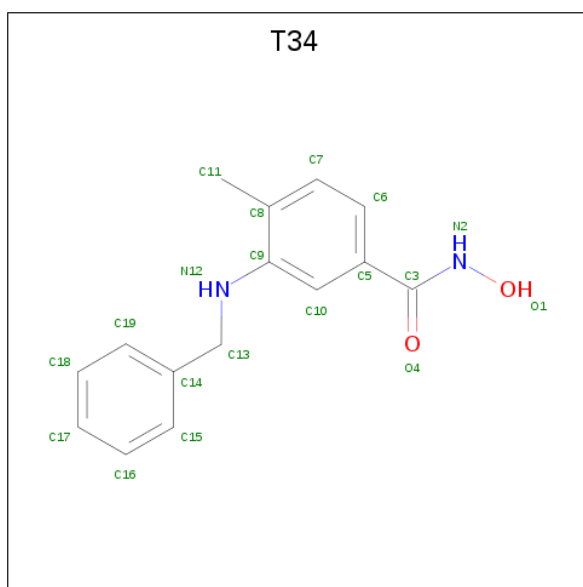
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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).

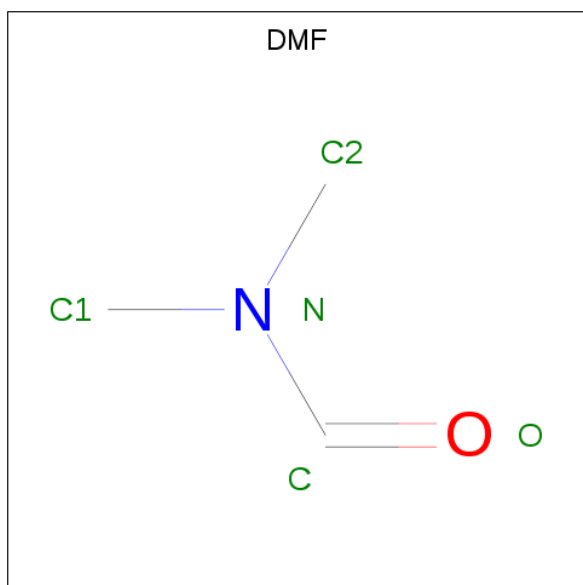
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total K 2 2	0	0
3	A	2	Total K 2 2	0	0
3	D	2	Total K 2 2	0	0
3	C	2	Total K 2 2	0	0

- Molecule 4 is 4-methyl- {N}-oxidanyl-3-[(phenylmethyl)amino]benzamide (three-letter code: T34) (formula: C₁₅H₁₆N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			19	15	2	2		
4	B	1	Total	C	N	O	0	0
			19	15	2	2		
4	C	1	Total	C	N	O	0	0
			19	15	2	2		
4	D	1	Total	C	N	O	0	0
			19	15	2	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	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	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: C₃H₈O₃).



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	D	1	Total	C	O	0	0
			6	3	3		

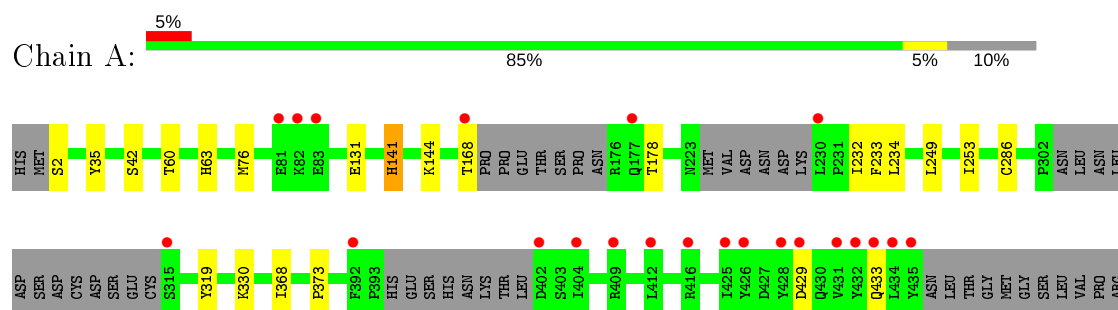
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	181	Total	O	0	0
			181	181		
7	B	220	Total	O	0	0
			220	220		
7	C	208	Total	O	0	0
			208	208		
7	D	185	Total	O	0	0
			185	185		

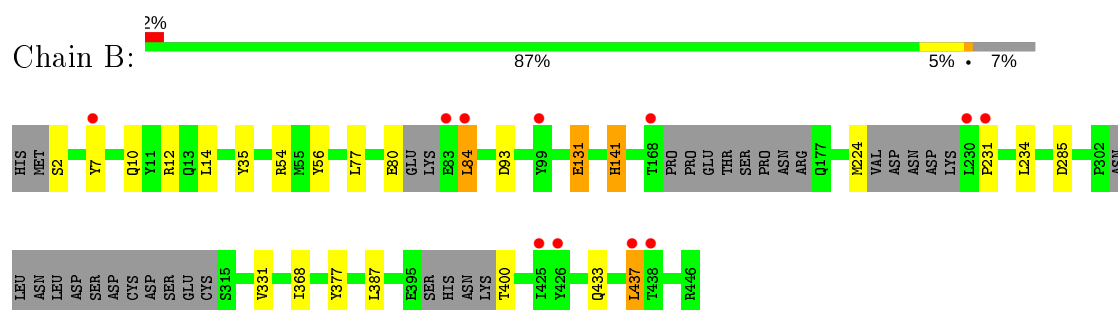
3 Residue-property plots [i](#)

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.

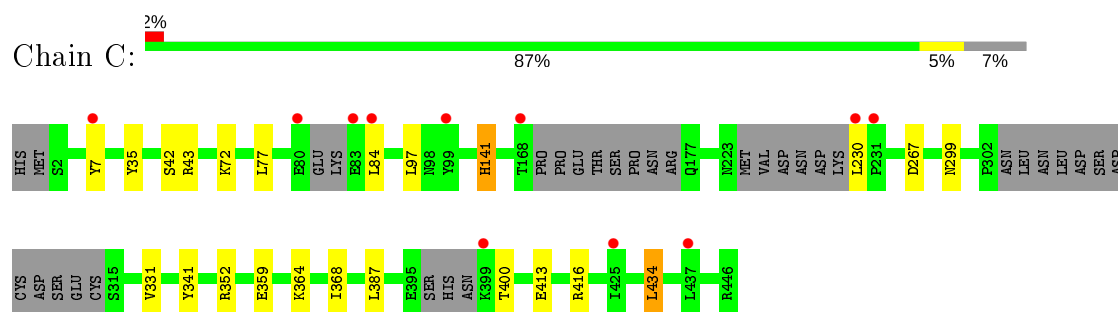
• Molecule 1: Histone deacetylase



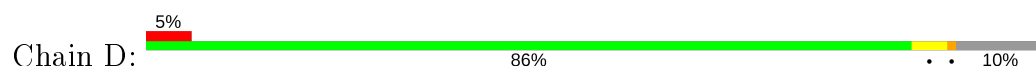
• Molecule 1: Histone deacetylase

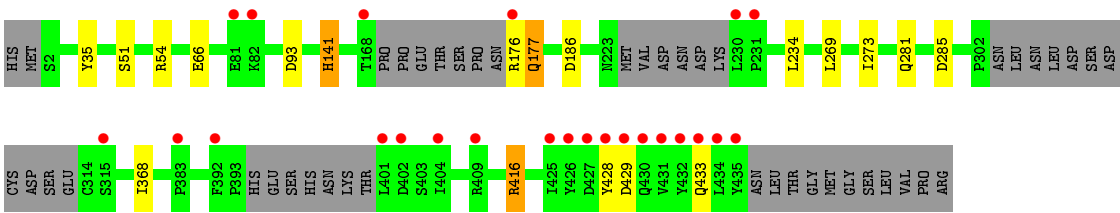


• Molecule 1: Histone deacetylase



• Molecule 1: Histone deacetylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.29Å 71.33Å 99.08Å 75.72° 78.17° 85.61°	Depositor
Resolution (Å)	48.43 – 1.99 48.43 – 1.99	Depositor EDS
% Data completeness (in resolution range)	95.7 (48.43-1.99) 95.8 (48.43-1.99)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.39 (at 1.98Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.156 , 0.197 0.156 , 0.197	Depositor DCC
R_{free} test set	6114 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.096 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14138	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.91% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, K, DMF, T34

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	0/3314	0.52	0/4507
1	B	0.43	0/3432	0.53	0/4667
1	C	0.43	0/3431	0.55	1/4665 (0.0%)
1	D	0.40	0/3345	0.52	0/4549
All	All	0.42	0/13522	0.53	1/18388 (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	5.50	127.94	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	3218	0	3116	16	0
1	B	3334	0	3233	20	0
1	C	3336	0	3230	18	1
1	D	3243	0	3150	11	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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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	19	0	0	0	0
4	B	19	0	0	0	0
4	C	19	0	0	1	0
4	D	19	0	0	0	0
5	A	20	0	28	1	0
5	B	30	0	42	8	0
5	C	35	0	49	5	0
5	D	10	0	14	0	0
6	A	6	0	8	1	0
6	B	12	0	16	4	0
6	C	6	0	8	0	0
6	D	6	0	8	1	0
7	A	181	0	0	2	0
7	B	220	0	0	1	0
7	C	208	0	0	1	0
7	D	185	0	0	0	0
All	All	14138	0	12902	65	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 2.

All (65) 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:HE	5:B:506:DMF:H12	1.47	0.80
1:C:72:LYS:NZ	7:C:601:HOH:O	2.18	0.75
1:C:352[B]:ARG:NH1	5:C:508:DMF:O	2.27	0.67
1:A:234:LEU:HB2	6:A:509:GOL:H32	1.82	0.62
1:B:35:TYR:CE1	1:B:368:ILE:HG23	2.36	0.60
1:B:433:GLN:O	1:B:437:LEU:HD12	2.03	0.59
1:C:35:TYR:CE1	1:C:368:ILE:HG23	2.38	0.59
1:A:429:ASP:O	1:A:433:GLN:HG2	2.05	0.56
1:A:42:SER:OG	1:B:93:ASP:OD2	2.19	0.56
1:B:14:LEU:HD12	6:B:512:GOL:H11	1.87	0.56
1:C:331:VAL:O	5:C:511:DMF:H12	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:224:MET:HG3	1:B:231:PRO:HB3	1.87	0.55
1:D:176:ARG:O	1:D:177:GLN:HB2	2.07	0.55
1:B:234:LEU:HB2	6:B:511:GOL:H32	1.89	0.55
1:D:429:ASP:O	1:D:433:GLN:HG2	2.06	0.55
1:B:331:VAL:O	5:B:508:DMF:H12	2.07	0.54
1:D:416:ARG:HD2	1:D:428:TYR:HE2	1.72	0.54
1:C:77:LEU:HD13	1:C:84:LEU:HD22	1.89	0.53
1:D:234:LEU:HB2	6:D:507:GOL:H32	1.92	0.52
1:C:368:ILE:HG21	1:C:387:LEU:HD22	1.92	0.51
1:A:232:ILE:HG12	1:A:233:PHE:N	2.25	0.51
1:A:2:SER:N	1:A:131:GLU:OE1	2.44	0.51
6:B:512:GOL:O2	7:B:601:HOH:O	2.20	0.50
1:A:286:CYS:HB2	1:A:319:TYR:OH	2.11	0.50
1:C:413:GLU:OE1	1:C:416:ARG:NH2	2.30	0.50
1:D:141:HIS:CD2	1:D:141:HIS:H	2.30	0.49
1:A:330:LYS:HD2	5:A:506:DMF:H13	1.93	0.49
1:B:12:ARG:HH21	5:B:506:DMF:H23	1.77	0.49
1:C:352[B]:ARG:HG3	5:C:508:DMF:H21	1.94	0.49
1:B:2:SER:N	1:B:131:GLU:OE1	2.47	0.48
1:B:368:ILE:HG21	1:B:387:LEU:HD22	1.95	0.48
1:C:267:ASP:HB3	1:C:434:LEU:HD11	1.95	0.48
1:C:43:ARG:HE	5:C:506:DMF:C	2.27	0.47
1:B:77:LEU:HD13	1:B:84:LEU:HD22	1.97	0.46
1:A:35:TYR:CZ	1:A:373:PRO:HD3	2.51	0.45
1:A:232:ILE:HG12	1:A:233:PHE:H	1.81	0.45
1:D:51:SER:OG	1:D:54:ARG:HG2	2.17	0.45
1:B:141:HIS:CD2	1:B:141:HIS:H	2.35	0.45
1:B:7[A]:TYR:CD2	5:B:507:DMF:H23	2.51	0.45
1:A:144:LYS:NZ	7:A:604:HOH:O	2.50	0.45
1:A:60:THR:HA	1:A:63:HIS:O	2.17	0.45
1:A:76:MET:HB2	7:A:769:HOH:O	2.17	0.44
1:B:368:ILE:HG21	1:B:387:LEU:CD2	2.48	0.44
1:A:35:TYR:CD1	1:A:368:ILE:HG23	2.53	0.43
1:C:368:ILE:CG2	1:C:387:LEU:HD22	2.48	0.43
1:C:7[B]:TYR:CE1	5:C:505:DMF:H12	2.52	0.43
1:B:12:ARG:NE	5:B:506:DMF:H12	2.22	0.43
1:A:168:THR:HB	1:A:178:THR:OG1	2.19	0.43
1:B:10:GLN:HG2	6:B:512:GOL:H2	2.01	0.43
1:C:368:ILE:HG21	1:C:387:LEU:CD2	2.49	0.42
1:D:269:LEU:O	1:D:273:ILE:HG12	2.18	0.42
1:B:7[B]:TYR:CD2	5:B:507:DMF:H23	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:299:ASN:O	1:C:352[A]:ARG:HD2	2.20	0.42
1:C:97:LEU:HA	1:C:97:LEU:HD23	1.93	0.42
1:D:35:TYR:CE1	1:D:368:ILE:HG23	2.55	0.42
1:A:141:HIS:CD2	1:A:141:HIS:H	2.37	0.42
1:B:368:ILE:HD12	5:B:509:DMF:H23	2.03	0.41
1:C:359:GLU:HG2	1:C:364:LYS:O	2.20	0.41
1:D:186:ASP:HB2	1:D:281:GLN:OE1	2.21	0.41
1:D:176:ARG:HB3	1:D:177:GLN:H	1.63	0.41
1:A:249:LEU:HD13	1:A:253:ILE:HD13	2.03	0.41
1:C:341:TYR:OH	4:C:504:T34:O4	2.33	0.41
1:D:66:GLU:H	1:D:66:GLU:CD	2.24	0.41
1:B:377:TYR:CE1	5:B:510:DMF:HC	2.56	0.40
1:C:141:HIS:H	1:C:141:HIS:CD2	2.40	0.40

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)
1:C:42:SER:OG	1:D:93:ASP:OD2[1_545]	2.19	0.01

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	393/447 (88%)	387 (98%)	6 (2%)	0	100	100
1	B	406/447 (91%)	400 (98%)	6 (2%)	0	100	100
1	C	406/447 (91%)	401 (99%)	5 (1%)	0	100	100
1	D	397/447 (89%)	390 (98%)	6 (2%)	1 (0%)	41	29
All	All	1602/1788 (90%)	1578 (98%)	23 (1%)	1 (0%)	51	42

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	177	GLN

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	350/392 (89%)	349 (100%)	1 (0%)	92	92
1	B	363/392 (93%)	354 (98%)	9 (2%)	47	39
1	C	363/392 (93%)	360 (99%)	3 (1%)	81	80
1	D	354/392 (90%)	351 (99%)	3 (1%)	81	80
All	All	1430/1568 (91%)	1414 (99%)	16 (1%)	73	70

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	141	HIS
1	B	54	ARG
1	B	56	TYR
1	B	80	GLU
1	B	84	LEU
1	B	131	GLU
1	B	141	HIS
1	B	285	ASP
1	B	400	THR
1	B	437	LEU
1	C	141	HIS
1	C	230	LEU
1	C	400	THR
1	D	141	HIS
1	D	285	ASP
1	D	416	ARG

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

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 40 ligands modelled in this entry, 12 are monoatomic - leaving 28 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	$\# Z > 2$
6	GOL	A	509	-	5,5,5	0.50	0	5,5,5	1.01	0
6	GOL	B	512	-	5,5,5	0.36	0	5,5,5	0.32	0
5	DMF	B	506	-	4,4,4	0.29	0	4,4,4	0.30	0
6	GOL	C	512	-	5,5,5	0.37	0	5,5,5	0.30	0
5	DMF	A	508	-	4,4,4	0.30	0	4,4,4	0.44	0
4	T34	D	504	2	20,20,20	0.27	0	26,26,26	0.32	0
4	T34	B	504	2	20,20,20	0.22	0	26,26,26	0.28	0
4	T34	C	504	2	20,20,20	0.23	0	26,26,26	0.27	0
6	GOL	B	511	-	5,5,5	0.36	0	5,5,5	0.51	0
5	DMF	C	510	-	4,4,4	0.38	0	4,4,4	0.48	0
5	DMF	B	508	-	4,4,4	0.31	0	4,4,4	0.41	0
5	DMF	C	511	-	4,4,4	0.32	0	4,4,4	0.42	0
5	DMF	C	505	-	4,4,4	0.29	0	4,4,4	0.44	0
5	DMF	A	505	-	4,4,4	0.33	0	4,4,4	0.33	0
5	DMF	D	505	-	4,4,4	0.33	0	4,4,4	0.50	0
5	DMF	B	507	-	4,4,4	0.32	0	4,4,4	0.42	0
6	GOL	D	507	-	5,5,5	0.41	0	5,5,5	0.78	0
5	DMF	A	507	-	4,4,4	0.33	0	4,4,4	0.36	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	DMF	B	505	-	4,4,4	0.33	0	4,4,4	0.54	0
5	DMF	B	509	-	4,4,4	0.33	0	4,4,4	0.56	0
5	DMF	D	506	-	4,4,4	0.33	0	4,4,4	0.27	0
4	T34	A	504	2	20,20,20	0.22	0	26,26,26	0.32	0
5	DMF	C	507	-	4,4,4	0.29	0	4,4,4	0.58	0
5	DMF	A	506	-	4,4,4	0.34	0	4,4,4	0.39	0
5	DMF	C	506	-	4,4,4	0.32	0	4,4,4	0.34	0
5	DMF	C	508	-	4,4,4	0.29	0	4,4,4	0.50	0
5	DMF	C	509	-	4,4,4	0.34	0	4,4,4	0.40	0
5	DMF	B	510	-	4,4,4	0.34	0	4,4,4	0.37	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
6	GOL	A	509	-	-	4/4/4/4	-
6	GOL	B	512	-	-	3/4/4/4	-
5	DMF	B	506	-	-	0/2/2/2	-
6	GOL	C	512	-	-	0/4/4/4	-
5	DMF	A	508	-	-	2/2/2/2	-
4	T34	D	504	2	-	0/11/11/11	0/2/2/2
4	T34	B	504	2	-	0/11/11/11	0/2/2/2
4	T34	C	504	2	-	0/11/11/11	0/2/2/2
6	GOL	B	511	-	-	3/4/4/4	-
5	DMF	C	510	-	-	2/2/2/2	-
5	DMF	B	508	-	-	2/2/2/2	-
5	DMF	C	511	-	-	2/2/2/2	-
5	DMF	C	505	-	-	2/2/2/2	-
5	DMF	A	505	-	-	2/2/2/2	-
5	DMF	D	505	-	-	0/2/2/2	-
5	DMF	B	507	-	-	2/2/2/2	-
6	GOL	D	507	-	-	2/4/4/4	-
5	DMF	A	507	-	-	0/2/2/2	-
5	DMF	B	505	-	-	2/2/2/2	-
5	DMF	B	509	-	-	0/2/2/2	-
5	DMF	D	506	-	-	0/2/2/2	-
4	T34	A	504	2	-	0/11/11/11	0/2/2/2
5	DMF	C	507	-	-	2/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMF	A	506	-	-	0/2/2/2	-
5	DMF	C	506	-	-	0/2/2/2	-
5	DMF	C	508	-	-	0/2/2/2	-
5	DMF	C	509	-	-	0/2/2/2	-
5	DMF	B	510	-	-	2/2/2/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	512	GOL	O1-C1-C2-C3
6	B	511	GOL	O1-C1-C2-O2
6	B	511	GOL	O1-C1-C2-C3
6	D	507	GOL	O1-C1-C2-C3
6	A	509	GOL	O1-C1-C2-O2
6	A	509	GOL	O1-C1-C2-C3
5	B	510	DMF	O-C-N-C2
5	B	510	DMF	O-C-N-C1
5	C	507	DMF	O-C-N-C1
5	C	507	DMF	O-C-N-C2
5	A	508	DMF	O-C-N-C2
5	C	511	DMF	O-C-N-C1
5	A	508	DMF	O-C-N-C1
5	C	505	DMF	O-C-N-C1
5	C	511	DMF	O-C-N-C2
6	B	512	GOL	C1-C2-C3-O3
5	C	505	DMF	O-C-N-C2
6	B	512	GOL	O1-C1-C2-O2
6	D	507	GOL	O1-C1-C2-O2
5	B	508	DMF	O-C-N-C1
5	B	508	DMF	O-C-N-C2
5	A	505	DMF	O-C-N-C2
6	B	511	GOL	O2-C2-C3-O3
6	A	509	GOL	O2-C2-C3-O3
5	C	510	DMF	O-C-N-C2
5	B	505	DMF	O-C-N-C1
5	A	505	DMF	O-C-N-C1
5	C	510	DMF	O-C-N-C1
5	B	505	DMF	O-C-N-C2

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Mol	Chain	Res	Type	Atoms
5	B	507	DMF	O-C-N-C2
5	B	507	DMF	O-C-N-C1
6	A	509	GOL	C1-C2-C3-O3

There are no ring outliers.

15 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	509	GOL	1	0
6	B	512	GOL	3	0
5	B	506	DMF	3	0
4	C	504	T34	1	0
6	B	511	GOL	1	0
5	B	508	DMF	1	0
5	C	511	DMF	1	0
5	C	505	DMF	1	0
5	B	507	DMF	2	0
6	D	507	GOL	1	0
5	B	509	DMF	1	0
5	A	506	DMF	1	0
5	C	506	DMF	1	0
5	C	508	DMF	2	0
5	B	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

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	401/447 (89%)	-0.03	22 (5%) 25 27	19, 29, 61, 102	0
1	B	414/447 (92%)	-0.02	11 (2%) 54 56	17, 27, 52, 89	0
1	C	414/447 (92%)	-0.05	11 (2%) 54 56	16, 26, 50, 85	0
1	D	403/447 (90%)	0.03	24 (5%) 21 23	20, 29, 69, 106	0
All	All	1632/1788 (91%)	-0.02	68 (4%) 36 38	16, 28, 57, 106	0

All (68) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	432	TYR	10.4
1	D	428	TYR	9.5
1	A	432	TYR	9.0
1	D	401	LEU	7.6
1	D	434	LEU	7.2
1	D	429	ASP	6.0
1	D	435	TYR	5.9
1	D	426	TYR	5.7
1	D	230	LEU	5.7
1	D	425	ILE	5.7
1	A	428	TYR	5.4
1	A	434	LEU	5.4
1	A	426	TYR	5.2
1	A	435	TYR	5.2
1	C	230	LEU	5.1
1	D	433	GLN	5.0
1	B	425	ILE	4.5
1	C	83	GLU	4.4
1	A	433	GLN	4.2
1	B	230	LEU	4.1
1	A	429	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	168	THR	3.8
1	A	425	ILE	3.7
1	B	437	LEU	3.6
1	A	230	LEU	3.4
1	A	82	LYS	3.3
1	C	425	ILE	3.2
1	A	404	ILE	3.2
1	A	409	ARG	3.0
1	D	176	ARG	3.0
1	D	383	PRO	2.8
1	D	81	GLU	2.8
1	D	392	PHE	2.8
1	D	82	LYS	2.7
1	B	99	TYR	2.7
1	B	438	THR	2.7
1	D	409	ARG	2.7
1	D	231	PRO	2.6
1	C	231	PRO	2.5
1	B	168	THR	2.5
1	D	168	THR	2.5
1	A	315	SER	2.5
1	B	426	TYR	2.5
1	C	168	THR	2.5
1	B	83	GLU	2.5
1	A	402	ASP	2.4
1	A	412	LEU	2.4
1	D	404	ILE	2.4
1	B	7[A]	TYR	2.4
1	C	80	GLU	2.4
1	C	437	LEU	2.4
1	B	231	PRO	2.4
1	A	416	ARG	2.3
1	D	431	VAL	2.3
1	A	83	GLU	2.3
1	A	431	VAL	2.2
1	C	399	LYS	2.2
1	D	430	GLN	2.2
1	C	7[A]	TYR	2.1
1	B	84	LEU	2.1
1	D	402	ASP	2.1
1	A	392	PHE	2.1
1	C	84	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	81	GLU	2.0
1	A	177	GLN	2.0
1	D	315	SER	2.0
1	C	99	TYR	2.0
1	D	427	ASP	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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	DMF	B	506	5/5	0.82	0.18	60,63,70,71	0
5	DMF	D	506	5/5	0.85	0.20	55,55,63,64	0
4	T34	D	504	19/19	0.86	0.17	30,41,60,61	0
4	T34	A	504	19/19	0.86	0.14	35,41,56,58	0
5	DMF	B	508	5/5	0.88	0.22	35,42,49,51	0
5	DMF	A	507	5/5	0.88	0.13	44,50,61,62	0
5	DMF	C	509	5/5	0.88	0.16	56,59,66,67	0
5	DMF	B	510	5/5	0.88	0.16	61,63,64,66	0
5	DMF	C	507	5/5	0.89	0.17	58,63,67,67	0
5	DMF	B	507	5/5	0.89	0.21	52,54,59,59	0
5	DMF	C	511	5/5	0.89	0.24	38,47,47,52	0
5	DMF	C	506	5/5	0.90	0.14	43,46,55,57	0
4	T34	C	504	19/19	0.90	0.20	33,45,59,63	0
5	DMF	A	506	5/5	0.90	0.13	50,51,54,55	0
5	DMF	A	505	5/5	0.91	0.12	45,45,47,51	0
6	GOL	B	511	6/6	0.92	0.11	30,40,45,50	0
6	GOL	D	507	6/6	0.92	0.12	28,42,47,48	0
6	GOL	A	509	6/6	0.92	0.11	30,37,39,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	GOL	B	512	6/6	0.92	0.15	45,52,54,59	0
5	DMF	B	505	5/5	0.92	0.13	45,52,58,63	0
5	DMF	B	509	5/5	0.92	0.14	39,40,41,46	0
4	T34	B	504	19/19	0.92	0.18	27,42,60,61	0
5	DMF	C	505	5/5	0.94	0.17	43,47,58,65	0
5	DMF	C	510	5/5	0.94	0.12	45,48,49,49	0
5	DMF	C	508	5/5	0.95	0.11	35,36,45,52	0
6	GOL	C	512	6/6	0.95	0.08	31,33,36,39	0
5	DMF	D	505	5/5	0.95	0.15	50,54,57,61	0
5	DMF	A	508	5/5	0.96	0.13	48,50,53,60	0
2	ZN	B	501	1/1	1.00	0.06	34,34,34,34	0
3	K	C	502	1/1	1.00	0.13	20,20,20,20	0
3	K	A	502	1/1	1.00	0.12	22,22,22,22	0
3	K	D	502	1/1	1.00	0.11	22,22,22,22	0
3	K	B	502	1/1	1.00	0.12	19,19,19,19	0
2	ZN	C	501	1/1	1.00	0.05	34,34,34,34	0
2	ZN	D	501	1/1	1.00	0.05	35,35,35,35	0
3	K	A	503	1/1	1.00	0.11	25,25,25,25	0
2	ZN	A	501	1/1	1.00	0.06	36,36,36,36	0
3	K	C	503	1/1	1.00	0.09	25,25,25,25	0
3	K	B	503	1/1	1.00	0.07	26,26,26,26	0
3	K	D	503	1/1	1.00	0.11	24,24,24,24	0

6.5 Other polymers ⓘ

There are no such residues in this entry.