



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:53 AM UTC

PDB ID : 6HRQ / pdb_00006hrq
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 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 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

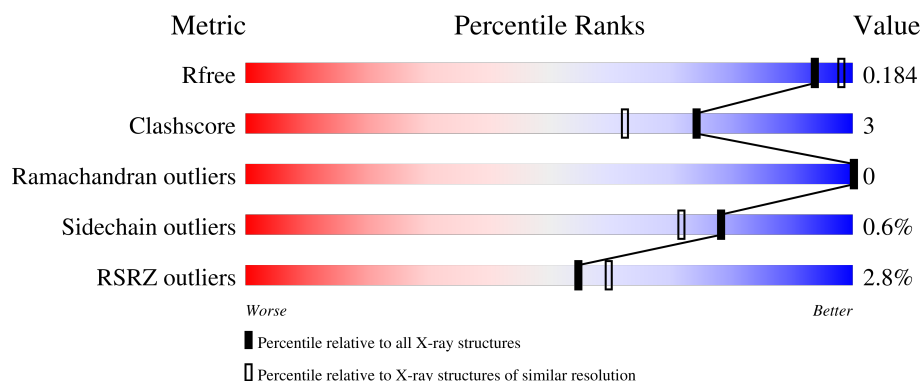
1 Overall quality at a glance

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}	180053	1296 (1.84-1.84)
Clashscore	190562	1329 (1.84-1.84)
Ramachandran outliers	187476	1318 (1.84-1.84)
Sidechain outliers	187428	1318 (1.84-1.84)
RSRZ outliers	180081	1296 (1.84-1.84)

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 ≥ 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% 10%
1	B	447	2% 88% 5% 7%
1	C	447	% 90% 6%
1	D	447	4% 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:

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

2 Entry composition

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
1	A	401	Total	C	N	O	S	0	3	0
			3223	2080	537	591	15			
1	B	416	Total	C	N	O	S	0	2	0
			3332	2147	559	609	17			
1	C	419	Total	C	N	O	S	0	3	0
			3355	2158	560	621	16			
1	D	400	Total	C	N	O	S	0	2	0
			3209	2071	534	589	15			

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

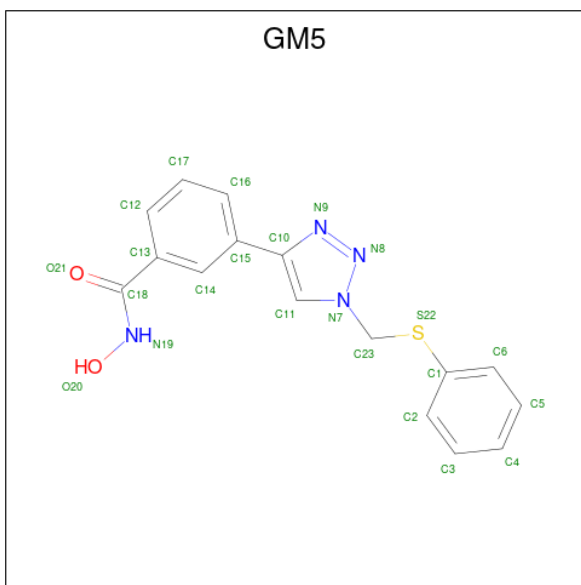
- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

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 (CCD ID: K) (formula: K).

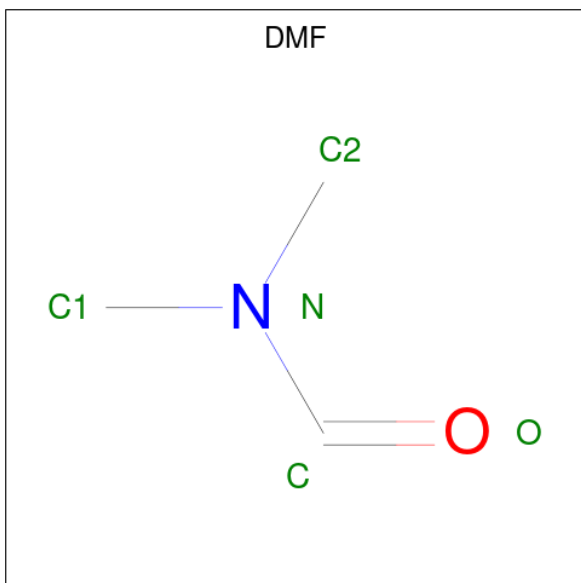
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	2	Total K 2 2	0	0
3	B	2	Total K 2 2	0	0
3	C	2	Total K 2 2	0	0
3	D	2	Total K 2 2	0	0

- Molecule 4 is {N}-oxidanyl-3-[1-(phenylsulfanylmethyl)-1,2,3-triazol-4-yl]benzamide (CCD ID: GM5) (formula: C₁₆H₁₄N₄O₂S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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 (CCD ID: DMF) (formula: C_3H_7NO).



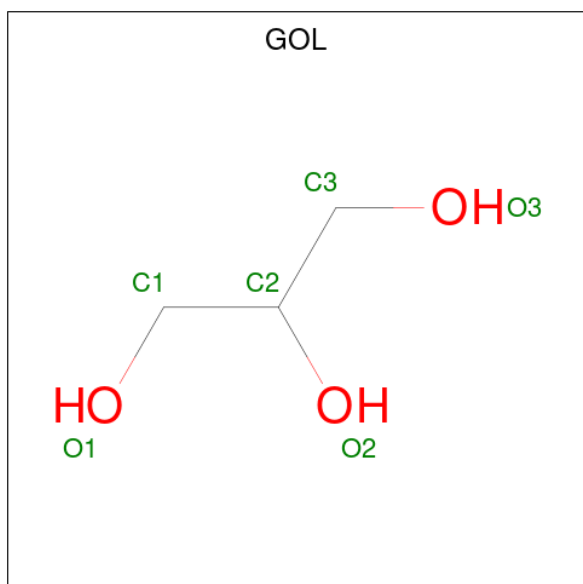
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			5	3	1	1		
5	A	1	Total	C	N	O	0	0
			5	3	1	1		
5	A	1	Total	C	N	O	0	0
			5	3	1	1		
5	A	1	Total	C	N	O	0	0
			5	3	1	1		
5	A	1	Total	C	N	O	0	0
			5	3	1	1		
5	B	1	Total	C	N	O	0	0
			5	3	1	1		
5	B	1	Total	C	N	O	0	0
			5	3	1	1		
5	B	1	Total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

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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 (CCD ID: 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	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		

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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

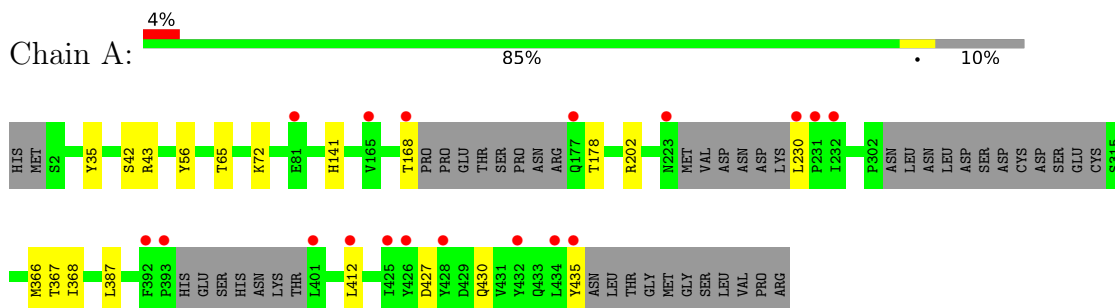
- Molecule 7 is water.

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

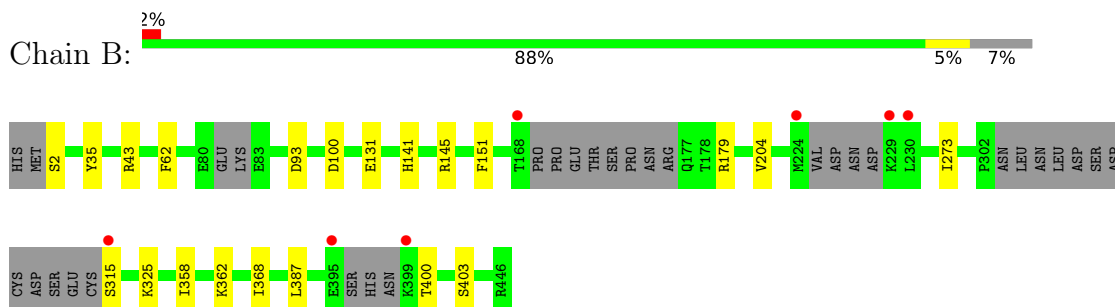
3 Residue-property plots [i](#)

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.

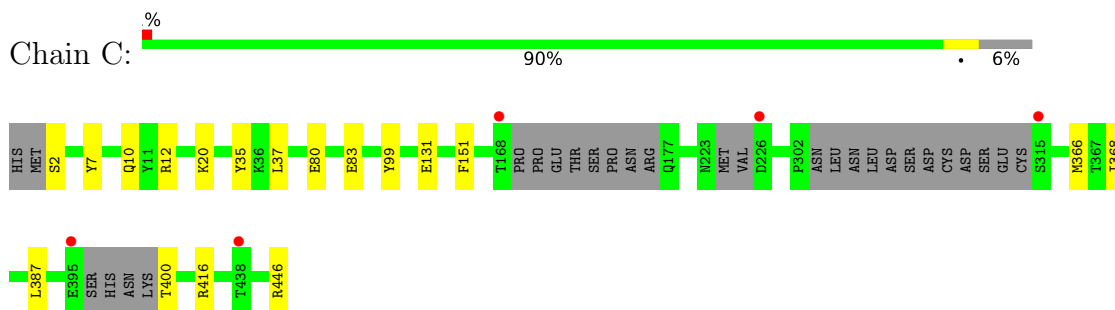
- Molecule 1: Histone deacetylase



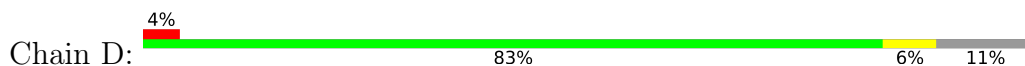
- Molecule 1: Histone deacetylase

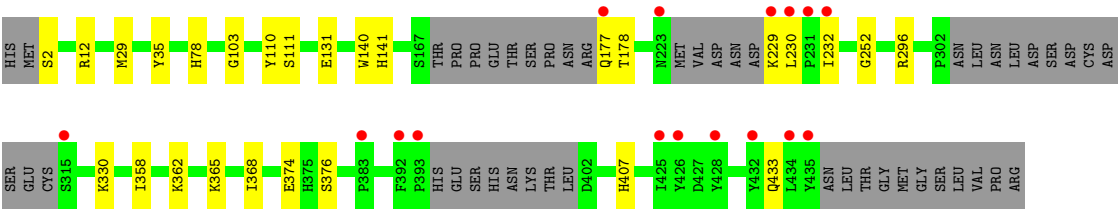


- Molecule 1: Histone deacetylase



- Molecule 1: Histone deacetylase





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	71.43Å 71.48Å 99.26Å 78.11° 75.54° 85.37°	Depositor
Resolution (Å)	47.16 – 1.84 47.16 – 1.84	Depositor EDS
% Data completeness (in resolution range)	95.0 (47.16-1.84) 95.0 (47.16-1.84)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.29 (at 1.84Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.150 , 0.183 0.152 , 0.184	Depositor DCC
R_{free} test set	7607 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	25.1	Xtriage
Anisotropy	0.182	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 53.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.080 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	14601	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage'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.*

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: DMF, GM5, ZN, K, GOL

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	0.34	0/3322	0.48	0/4518
1	B	0.38	0/3429	0.50	0/4660
1	C	0.36	0/3456	0.49	0/4700
1	D	0.35	0/3305	0.49	0/4495
All	All	0.36	0/13512	0.49	0/18373

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	3223	0	3127	19	0
1	B	3332	0	3241	17	0
1	C	3355	0	3250	14	0
1	D	3209	0	3109	26	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	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	4	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.

All (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
1:C:99:TYR:OH	7:C:601:HOH:O	2.03	0.75
1:A:42[A]:SER:HA	5:A:505:DMF:H13	1.69	0.74
1:D:407:HIS:HE2	5:D:509:DMF:H13	1.53	0.74
1:C:2:SER:N	1:C:131:GLU:OE1	2.24	0.69
1:A:168:THR:OG1	1:A:178:THR:OG1	2.11	0.68
1:B:35:TYR:CE1	1:B:368:ILE:HG23	2.29	0.68
1:C:35:TYR:CE1	1:C:368:ILE:HG23	2.28	0.67
1:D:252:GLY:O	1:D:296:ARG:NH1	2.28	0.66
1:B:403:SER:HA	5:B:513:DMF:H22	1.75	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:110:TYR:CE2	6:D:515:GOL:H32	2.33	0.64
1:D:35:TYR:CE1	1:D:368:ILE:HG23	2.33	0.63
6:D:511:GOL:O1	7:D:602:HOH:O	2.15	0.63
1:D:140:TRP:CD1	6:D:515:GOL:H2	2.35	0.62
1:B:2:SER:N	1:B:131:GLU:OE1	2.34	0.61
1:A:412:LEU:HD21	1:A:435:TYR:CE1	2.37	0.60
6:B:517:GOL:H32	7:B:714:HOH:O	2.01	0.60
1:A:35:TYR:CE1	1:A:368:ILE:HG23	2.36	0.60
1:D:374:GLU:OE2	7:D:603:HOH:O	2.16	0.59
1:A:43:ARG:N	5:A:505:DMF:H22	2.15	0.59
5:A:505:DMF:H12	1:B:93:ASP:HB2	1.83	0.59
1:C:416:ARG:NE	1:C:446:ARG:O	2.37	0.58
1:C:10:GLN:HB2	6:C:513:GOL:H12	1.86	0.57
6:C:513:GOL:O3	7:C:602:HOH:O	2.17	0.56
5:B:506:DMF:HC	7:B:605:HOH:O	2.05	0.56
1:D:110:TYR:HE2	6:D:515:GOL:H32	1.71	0.55
1:B:43:ARG:HE	5:B:512:DMF:C1	2.14	0.54
1:D:29:MET:HB3	6:D:513:GOL:H2	1.91	0.53
1:A:368:ILE:HD12	5:A:506:DMF:H12	1.91	0.52
1:D:111:SER:HA	6:D:515:GOL:H12	1.91	0.52
1:A:427:ASP:HB3	1:A:430:GLN:HB3	1.92	0.51
1:C:368:ILE:HG21	1:C:387:LEU:HD22	1.92	0.51
1:D:2:SER:N	1:D:131:GLU:OE1	2.44	0.51
5:B:512:DMF:HC	7:B:798:HOH:O	2.11	0.50
1:D:140:TRP:CG	6:D:515:GOL:H2	2.46	0.50
1:A:412:LEU:HD11	1:A:435:TYR:CD1	2.46	0.50
1:D:78:HIS:CE1	6:D:512:GOL:H12	2.47	0.50
1:D:407:HIS:NE2	5:D:509:DMF:H13	2.25	0.49
1:D:12:ARG:HH11	6:D:513:GOL:H32	1.76	0.49
1:C:37:LEU:HD22	1:C:366:MET:HE2	1.94	0.49
1:B:358:ILE:HG23	1:B:362:LYS:HD2	1.95	0.49
1:B:325:LYS:HG3	5:B:511:DMF:H22	1.95	0.49
1:D:365:LYS:NZ	7:D:613:HOH:O	2.43	0.48
1:A:202:ARG:NE	7:A:614:HOH:O	2.46	0.48
1:B:368:ILE:HG21	1:B:387:LEU:HD22	1.95	0.47
1:A:72:LYS:NZ	7:A:616:HOH:O	2.47	0.47
1:B:204:VAL:HG21	1:B:273:ILE:HD12	1.97	0.47
1:D:330:LYS:HA	5:D:506:DMF:HC	1.96	0.47
1:B:179[A]:ARG:NE	7:B:603:HOH:O	2.34	0.47
1:D:229:LYS:HG3	1:D:230:LEU:HD12	1.97	0.47
1:A:56:TYR:OH	1:A:65:THR:HB	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:376:SER:HB2	5:D:507:DMF:H22	1.98	0.46
1:B:62:PHE:O	6:B:518:GOL:H11	2.17	0.45
1:A:366:MET:SD	5:A:509:DMF:HC	2.57	0.44
1:B:145:ARG:HE	6:B:518:GOL:H12	1.81	0.44
1:C:35:TYR:CD1	1:C:368:ILE:HG23	2.51	0.44
1:C:7:TYR:CD1	5:C:505:DMF:H13	2.52	0.44
1:D:141:HIS:H	1:D:141:HIS:CD2	2.35	0.44
1:C:12:ARG:HG2	5:C:507:DMF:H12	1.98	0.44
1:B:368:ILE:CG2	1:B:387:LEU:HD22	2.48	0.44
1:D:35:TYR:CD1	1:D:368:ILE:HG23	2.52	0.44
1:A:141:HIS:H	1:A:141:HIS:CD2	2.35	0.43
1:D:103:GLY:N	6:D:512:GOL:H11	2.14	0.43
1:A:202:ARG:NH1	7:A:612:HOH:O	2.52	0.43
1:A:367:THR:HG23	7:A:654:HOH:O	2.19	0.42
1:C:366:MET:HE3	1:C:366:MET:HB3	1.70	0.42
1:D:12:ARG:NH1	6:D:513:GOL:H32	2.34	0.42
1:A:412:LEU:HD23	1:A:412:LEU:HA	1.68	0.42
1:B:35:TYR:CD1	1:B:368:ILE:HG23	2.54	0.42
1:C:368:ILE:CG2	1:C:387:LEU:HD22	2.50	0.42
1:B:141:HIS:H	1:B:141:HIS:CD2	2.37	0.41
1:C:20:LYS:HE2	1:C:151:PHE:CE2	2.56	0.41
1:B:100:ASP:HB3	1:B:151:PHE:CE1	2.56	0.41
1:C:368:ILE:HG21	1:C:387:LEU:CD2	2.50	0.41
1:D:177:GLN:OE1	1:D:178:THR:N	2.53	0.41
1:A:368:ILE:HG21	1:A:387:LEU:HD22	2.03	0.41
1:D:358:ILE:HG23	1:D:362:LYS:HD3	2.03	0.40

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

5.3.1 Protein backbone

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 ⓘ

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%)	350 (100%)	1 (0%)	86	81
1	B	363/392 (93%)	361 (99%)	2 (1%)	78	72
1	C	367/392 (94%)	364 (99%)	3 (1%)	73	65
1	D	349/392 (89%)	347 (99%)	2 (1%)	78	72
All	All	1430/1568 (91%)	1422 (99%)	8 (1%)	78	72

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	230	LEU
1	B	315	SER
1	B	400	THR
1	C	80	GLU
1	C	83	GLU
1	C	400	THR
1	D	232	ILE
1	D	433	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	48	GLN
1	B	10	GLN
1	B	33	ASN
1	B	422	ASN
1	C	33	ASN
1	C	48	GLN
1	C	129	HIS
1	D	33	ASN

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 oligosaccharides 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	$\# Z > 2$
4	GM5	B	504	2	24,25,25	0.15	0	30,33,33	0.18	0
5	DMF	C	505	-	4,4,4	0.31	0	4,4,4	0.49	0
6	GOL	B	518	-	5,5,5	0.34	0	5,5,5	0.90	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	GOL	D	511	-	5,5,5	0.30	0	5,5,5	0.36	0
5	DMF	C	508	-	4,4,4	0.35	0	4,4,4	0.49	0
6	GOL	B	516	-	5,5,5	0.36	0	5,5,5	0.39	0
5	DMF	A	505	-	4,4,4	0.28	0	4,4,4	0.36	0
6	GOL	C	512	-	5,5,5	0.38	0	5,5,5	0.39	0
5	DMF	A	509	-	4,4,4	0.28	0	4,4,4	0.35	0
5	DMF	D	508	-	4,4,4	0.37	0	4,4,4	0.36	0
5	DMF	B	514	-	4,4,4	0.38	0	4,4,4	0.40	0
6	GOL	D	515	-	5,5,5	0.46	0	5,5,5	1.27	1 (20%)
5	DMF	A	506	-	4,4,4	0.33	0	4,4,4	0.43	0
5	DMF	B	507	-	4,4,4	0.15	0	4,4,4	0.66	0
4	GM5	A	504	2	24,25,25	0.20	0	30,33,33	0.32	0
5	DMF	B	505	-	4,4,4	0.29	0	4,4,4	0.43	0
6	GOL	B	517	-	5,5,5	0.34	0	5,5,5	0.37	0
5	DMF	A	511	-	4,4,4	0.28	0	4,4,4	0.28	0
5	DMF	B	508	-	4,4,4	0.32	0	4,4,4	0.27	0
5	DMF	C	509	-	4,4,4	0.37	0	4,4,4	0.43	0
5	DMF	A	508	-	4,4,4	0.35	0	4,4,4	0.47	0
6	GOL	D	510	-	5,5,5	0.37	0	5,5,5	0.47	0
5	DMF	B	511	-	4,4,4	0.31	0	4,4,4	0.43	0
5	DMF	D	507	-	4,4,4	0.26	0	4,4,4	0.31	0
5	DMF	C	507	-	4,4,4	0.30	0	4,4,4	0.32	0
5	DMF	D	509	-	4,4,4	0.29	0	4,4,4	0.53	0
5	DMF	C	506	-	4,4,4	0.39	0	4,4,4	0.24	0
5	DMF	B	506	-	4,4,4	0.34	0	4,4,4	0.42	0
5	DMF	B	509	-	4,4,4	0.38	0	4,4,4	0.37	0
5	DMF	B	512	-	4,4,4	0.26	0	4,4,4	0.41	0
5	DMF	D	506	-	4,4,4	0.31	0	4,4,4	0.53	0
6	GOL	A	510	-	5,5,5	0.40	0	5,5,5	0.16	0
5	DMF	C	510	-	4,4,4	0.36	0	4,4,4	0.52	0
5	DMF	C	511	-	4,4,4	0.37	0	4,4,4	0.68	0
5	DMF	B	510	-	4,4,4	0.32	0	4,4,4	0.51	0
6	GOL	D	512	-	5,5,5	0.43	0	5,5,5	0.44	0
5	DMF	D	505	-	4,4,4	0.33	0	4,4,4	0.49	0
6	GOL	C	513	-	5,5,5	0.26	0	5,5,5	0.56	0
5	DMF	A	507	-	4,4,4	0.36	0	4,4,4	0.46	0
6	GOL	D	514	-	5,5,5	0.40	0	5,5,5	0.29	0
6	GOL	D	513	-	5,5,5	0.36	0	5,5,5	0.33	0
5	DMF	B	513	-	4,4,4	0.31	0	4,4,4	0.30	0
4	GM5	C	504	2	24,25,25	0.17	0	30,33,33	0.24	0
6	GOL	B	515	-	5,5,5	0.32	0	5,5,5	0.34	0
4	GM5	D	504	2	24,25,25	0.23	0	30,33,33	0.22	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	GM5	B	504	2	-	0/15/15/15	0/3/3/3
5	DMF	C	505	-	-	2/2/2/2	-
6	GOL	B	518	-	-	4/4/4/4	-
6	GOL	D	511	-	-	2/4/4/4	-
5	DMF	C	508	-	-	2/2/2/2	-
6	GOL	B	516	-	-	2/4/4/4	-
5	DMF	A	505	-	-	2/2/2/2	-
6	GOL	C	512	-	-	2/4/4/4	-
5	DMF	A	509	-	-	2/2/2/2	-
5	DMF	D	508	-	-	2/2/2/2	-
5	DMF	B	514	-	-	2/2/2/2	-
6	GOL	D	515	-	-	0/4/4/4	-
5	DMF	A	506	-	-	2/2/2/2	-
5	DMF	B	507	-	-	0/2/2/2	-
4	GM5	A	504	2	-	0/15/15/15	0/3/3/3
5	DMF	B	505	-	-	1/2/2/2	-
6	GOL	B	517	-	-	1/4/4/4	-
5	DMF	A	511	-	-	0/2/2/2	-
5	DMF	B	508	-	-	2/2/2/2	-
5	DMF	C	509	-	-	0/2/2/2	-
5	DMF	A	508	-	-	0/2/2/2	-
6	GOL	D	510	-	-	0/4/4/4	-
5	DMF	B	511	-	-	0/2/2/2	-
5	DMF	D	507	-	-	2/2/2/2	-
5	DMF	C	507	-	-	2/2/2/2	-
5	DMF	D	509	-	-	0/2/2/2	-
5	DMF	C	506	-	-	0/2/2/2	-
5	DMF	B	506	-	-	2/2/2/2	-
5	DMF	B	509	-	-	2/2/2/2	-
5	DMF	B	512	-	-	0/2/2/2	-
5	DMF	D	506	-	-	2/2/2/2	-
6	GOL	A	510	-	-	0/4/4/4	-
5	DMF	C	510	-	-	2/2/2/2	-
5	DMF	C	511	-	-	0/2/2/2	-
5	DMF	B	510	-	-	1/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GOL	D	512	-	-	2/4/4/4	-
5	DMF	D	505	-	-	2/2/2/2	-
6	GOL	C	513	-	-	2/4/4/4	-
5	DMF	A	507	-	-	0/2/2/2	-
6	GOL	D	514	-	-	0/4/4/4	-
6	GOL	D	513	-	-	4/4/4/4	-
5	DMF	B	513	-	-	2/2/2/2	-
4	GM5	C	504	2	-	0/15/15/15	0/3/3/3
6	GOL	B	515	-	-	0/4/4/4	-
4	GM5	D	504	2	-	0/15/15/15	0/3/3/3

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	515	GOL	C3-C2-C1	-2.14	103.94	111.80

There are no chirality outliers.

All (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
5	A	509	DMF	O-C-N-C2
5	C	507	DMF	O-C-N-C1
5	C	507	DMF	O-C-N-C2
5	A	509	DMF	O-C-N-C1
5	D	506	DMF	O-C-N-C2
5	D	506	DMF	O-C-N-C1
5	C	508	DMF	O-C-N-C2
5	C	508	DMF	O-C-N-C1
5	D	507	DMF	O-C-N-C1
6	D	513	GOL	O1-C1-C2-O2
5	D	507	DMF	O-C-N-C2
5	B	509	DMF	O-C-N-C1
5	D	505	DMF	O-C-N-C2
5	B	513	DMF	O-C-N-C1

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Mol	Chain	Res	Type	Atoms
6	B	516	GOL	O1-C1-C2-C3
6	C	513	GOL	C1-C2-C3-O3
6	D	511	GOL	O1-C1-C2-C3
6	D	512	GOL	O1-C1-C2-C3
6	D	513	GOL	C1-C2-C3-O3
6	B	516	GOL	O1-C1-C2-O2
6	D	512	GOL	O1-C1-C2-O2
5	C	505	DMF	O-C-N-C1
5	D	505	DMF	O-C-N-C1
5	B	509	DMF	O-C-N-C2
5	B	513	DMF	O-C-N-C2
5	C	505	DMF	O-C-N-C2
5	B	514	DMF	O-C-N-C2
5	A	505	DMF	O-C-N-C1
6	B	517	GOL	O1-C1-C2-O2
6	B	518	GOL	O1-C1-C2-O2
5	B	514	DMF	O-C-N-C1
5	B	508	DMF	O-C-N-C2
6	C	513	GOL	O2-C2-C3-O3
5	C	510	DMF	O-C-N-C1
5	B	508	DMF	O-C-N-C1
5	A	505	DMF	O-C-N-C2
5	A	506	DMF	O-C-N-C1
5	D	508	DMF	O-C-N-C2
5	B	506	DMF	O-C-N-C1
5	D	508	DMF	O-C-N-C1
5	C	510	DMF	O-C-N-C2
5	A	506	DMF	O-C-N-C2
6	C	512	GOL	O1-C1-C2-O2
6	D	513	GOL	O2-C2-C3-O3
5	B	506	DMF	O-C-N-C2
5	B	510	DMF	O-C-N-C1
5	B	505	DMF	O-C-N-C1
6	D	511	GOL	O1-C1-C2-O2

There are no ring outliers.

19 monomers are involved in 36 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	505	DMF	1	0
6	B	518	GOL	2	0
6	D	511	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	505	DMF	5	0
5	A	509	DMF	1	0
6	D	515	GOL	5	0
5	A	506	DMF	1	0
6	B	517	GOL	1	0
5	B	511	DMF	1	0
5	D	507	DMF	1	0
5	C	507	DMF	1	0
5	D	509	DMF	2	0
5	B	506	DMF	1	0
5	B	512	DMF	3	0
5	D	506	DMF	1	0
6	D	512	GOL	3	0
6	C	513	GOL	2	0
6	D	513	GOL	3	0
5	B	513	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%)	-0.16	18 (4%)	38 40	15, 26, 62, 96	3 (0%)
1	B	416/447 (93%)	-0.36	7 (1%)	69 77	14, 24, 47, 90	2 (0%)
1	C	419/447 (93%)	-0.30	5 (1%)	76 82	13, 24, 50, 112	3 (0%)
1	D	400/447 (89%)	-0.23	16 (4%)	42 45	14, 26, 61, 92	2 (0%)
All	All	1636/1788 (91%)	-0.26	46 (2%)	55 60	13, 25, 52, 112	10 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	401	LEU	5.0
1	D	230	LEU	4.8
1	A	230	LEU	4.7
1	A	168	THR	4.3
1	A	432	TYR	4.2
1	D	428	TYR	3.8
1	D	315	SER	3.8
1	A	435	TYR	3.7
1	B	168	THR	3.6
1	A	428	TYR	3.4
1	D	426	TYR	3.4
1	D	231	PRO	3.4
1	C	168	THR	3.4
1	A	426	TYR	3.3
1	A	392	PHE	3.2
1	C	438	THR	3.2
1	D	223	ASN	3.2
1	D	229	LYS	3.1
1	C	315	SER	3.1
1	B	315	SER	3.0
1	D	434	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	393	PRO	3.0
1	A	425	ILE	3.0
1	B	399	LYS	2.9
1	A	231	PRO	2.8
1	B	224	MET	2.8
1	D	392	PHE	2.8
1	D	232	ILE	2.8
1	D	425	ILE	2.8
1	A	434	LEU	2.6
1	B	395	GLU	2.6
1	D	432	TYR	2.5
1	A	177	GLN	2.5
1	A	223	ASN	2.5
1	B	229	LYS	2.5
1	A	165	VAL	2.3
1	C	226	ASP	2.3
1	D	435	TYR	2.2
1	A	232	ILE	2.2
1	D	383	PRO	2.2
1	D	393	PRO	2.2
1	D	177	GLN	2.2
1	A	81	GLU	2.1
1	C	395	GLU	2.1
1	B	230	LEU	2.1
1	A	412	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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($\text{\AA}^2$)	Q<0.9
5	DMF	C	508	5/5	0.79	0.17	64,68,77,81	0
5	DMF	B	512	5/5	0.81	0.18	38,44,50,59	0
6	GOL	B	516	6/6	0.82	0.16	59,64,65,66	0
5	DMF	D	509	5/5	0.83	0.20	46,58,66,69	0
5	DMF	B	509	5/5	0.83	0.17	56,57,61,62	0
5	DMF	C	505	5/5	0.84	0.17	43,45,52,59	0
5	DMF	A	506	5/5	0.84	0.18	38,44,48,55	0
6	GOL	D	513	6/6	0.84	0.17	51,60,64,66	0
5	DMF	C	510	5/5	0.85	0.17	48,50,53,53	0
5	DMF	D	506	5/5	0.85	0.18	39,50,53,59	0
5	DMF	B	510	5/5	0.85	0.19	40,59,62,64	0
5	DMF	C	507	5/5	0.85	0.21	67,69,70,70	0
5	DMF	A	507	5/5	0.85	0.13	38,45,46,48	0
5	DMF	D	505	5/5	0.86	0.20	47,52,57,58	0
6	GOL	D	514	6/6	0.86	0.16	59,62,62,68	0
6	GOL	B	517	6/6	0.87	0.14	38,49,57,62	0
6	GOL	C	513	6/6	0.87	0.13	37,45,46,48	0
5	DMF	B	511	5/5	0.87	0.16	49,56,62,66	0
5	DMF	B	505	5/5	0.87	0.17	39,43,51,58	0
5	DMF	A	508	5/5	0.88	0.15	58,59,63,65	0
5	DMF	A	505	5/5	0.88	0.13	26,45,50,54	0
5	DMF	D	507	5/5	0.88	0.17	51,55,72,77	0
5	DMF	B	513	5/5	0.89	0.16	48,49,55,56	0
5	DMF	C	509	5/5	0.89	0.12	37,41,45,50	0
6	GOL	D	512	6/6	0.89	0.12	45,51,53,61	0
5	DMF	B	506	5/5	0.89	0.17	61,62,63,65	0
5	DMF	B	507	5/5	0.89	0.17	37,39,49,51	0
5	DMF	B	514	5/5	0.90	0.11	31,39,45,45	0
5	DMF	C	511	5/5	0.90	0.12	35,37,39,46	0
5	DMF	A	511	5/5	0.90	0.16	42,54,60,64	0
5	DMF	C	506	5/5	0.90	0.12	34,42,46,47	0
4	GM5	D	504	23/23	0.91	0.10	27,35,45,53	0
5	DMF	D	508	5/5	0.91	0.12	31,40,50,54	0
4	GM5	B	504	23/23	0.91	0.11	27,38,49,51	0
6	GOL	D	515	6/6	0.91	0.14	29,38,48,53	0
4	GM5	C	504	23/23	0.92	0.10	25,37,46,52	0
5	DMF	A	509	5/5	0.92	0.12	45,46,50,52	0
6	GOL	B	518	6/6	0.92	0.11	32,47,56,64	0
5	DMF	B	508	5/5	0.92	0.11	33,37,43,48	0
6	GOL	C	512	6/6	0.93	0.09	29,32,35,36	0
4	GM5	A	504	23/23	0.93	0.09	25,39,46,48	0
6	GOL	D	510	6/6	0.94	0.09	25,32,33,35	0
6	GOL	D	511	6/6	0.94	0.10	41,46,48,48	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	GOL	A	510	6/6	0.94	0.09	26,33,38,39	0
6	GOL	B	515	6/6	0.96	0.07	25,31,33,33	0
3	K	C	502	1/1	0.99	0.03	22,22,22,22	0
2	ZN	C	501	1/1	1.00	0.06	30,30,30,30	0
2	ZN	D	501	1/1	1.00	0.06	31,31,31,31	0
3	K	A	502	1/1	1.00	0.01	19,19,19,19	0
3	K	A	503	1/1	1.00	0.01	22,22,22,22	0
3	K	B	502	1/1	1.00	0.02	22,22,22,22	0
3	K	B	503	1/1	1.00	0.02	18,18,18,18	0
2	ZN	A	501	1/1	1.00	0.07	30,30,30,30	0
3	K	C	503	1/1	1.00	0.02	18,18,18,18	0
3	K	D	502	1/1	1.00	0.01	22,22,22,22	0
3	K	D	503	1/1	1.00	0.01	18,18,18,18	0
2	ZN	B	501	1/1	1.00	0.06	30,30,30,30	0

6.5 Other polymers [i](#)

There are no such residues in this entry.