Full wwPDB X-ray Structure Validation Report ⓘ

Jun 7, 2020 – 02:59 am BST

PDB ID	:	6HSG
Title	:	Crystal structure of Schistosoma mansoni HDAC8 H292M mutant complexed with NCC-149
Authors	:	Shaik, T.B.; Marek, M.; Romier, C.
Deposited on	:	2018-10-01
Resolution	:	1.85 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 ①) were used in the production of this report:

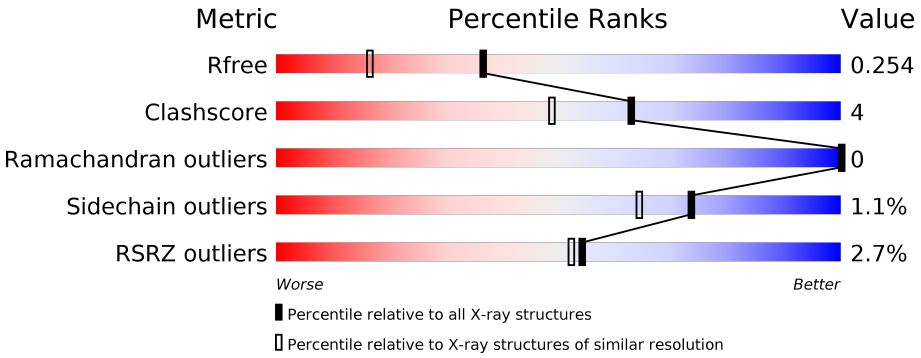
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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 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 <=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	3% 83% 6% 11%
1	B	447	% 85% 7% 8%
1	C	447	2% 84% 8% 8%
1	D	447	4% 78% 11% 11%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 14130 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	400	Total	C	N	O	S	0	1	0
			3204	2068	532	588	16			
1	B	412	Total	C	N	O	S	0	3	0
			3295	2123	548	606	18			
1	C	412	Total	C	N	O	S	0	3	0
			3298	2127	550	603	18			
1	D	398	Total	C	N	O	S	0	2	0
			3192	2061	529	586	16			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP A5H660
A	292	MET	HIS	engineered mutation	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	292	MET	HIS	engineered mutation	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	292	MET	HIS	engineered mutation	UNP A5H660
C	441	GLY	-	expression tag	UNP A5H660
C	442	SER	-	expression tag	UNP A5H660
C	443	LEU	-	expression tag	UNP A5H660

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Chain	Residue	Modelled	Actual	Comment	Reference
C	444	VAL	-	expression tag	UNP A5H660
C	445	PRO	-	expression tag	UNP A5H660
C	446	ARG	-	expression tag	UNP A5H660
D	0	HIS	-	expression tag	UNP A5H660
D	292	MET	HIS	engineered mutation	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

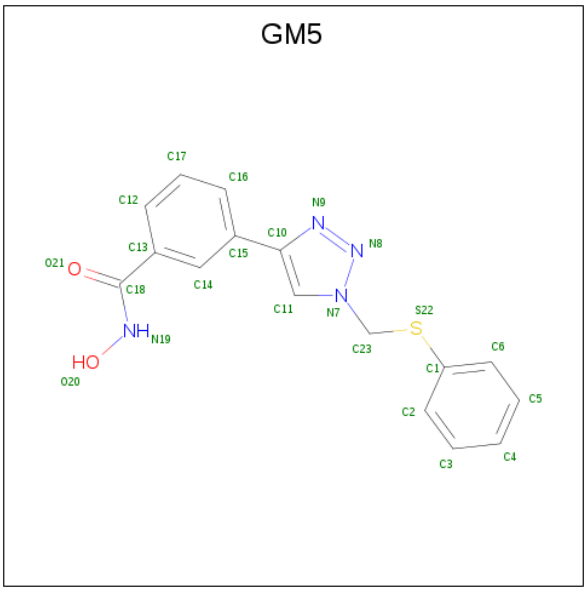
- Molecule 2 is ZINC ION (three-letter code: ZN) (formula: Zn).

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).

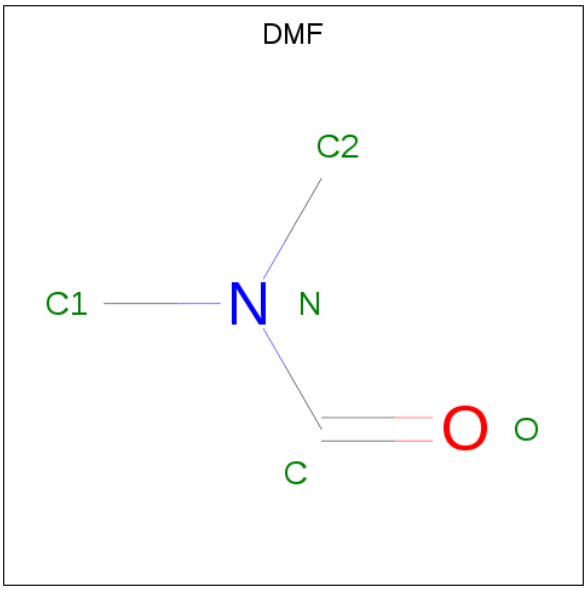
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	2	Total K 2 2	0	0
3	A	2	Total K 2 2	0	0
3	D	2	Total K 2 2	0	0
3	C	2	Total K 2 2	0	0

- Molecule 4 is {N}-oxidanyl-3-[1-(phenylsulfanylmethyl)-1,2,3-triazol-4-yl]benzamide (three-letter code: GM5) (formula: $C_{16}H_{14}N_4O_2S$).



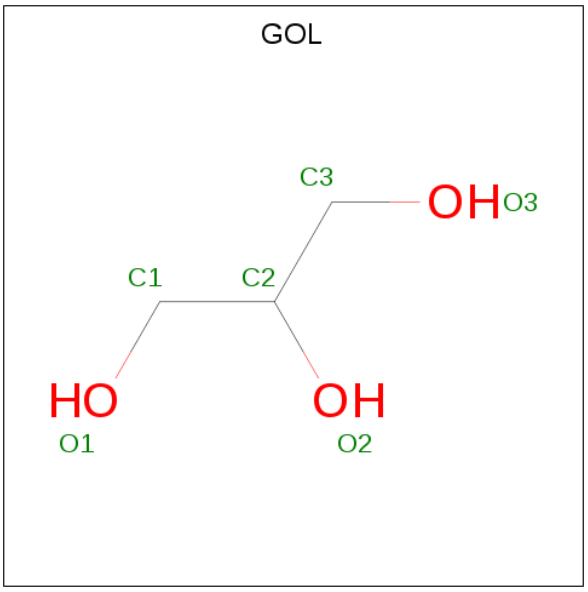
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			23	16	4	2	1		
4	B	1	Total	C	N	O	S	0	0
			23	16	4	2	1		
4	C	1	Total	C	N	O	S	0	0
			23	16	4	2	1		
4	D	1	Total	C	N	O	S	0	0
			23	16	4	2	1		

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



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

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



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

- Molecule 7 is water.

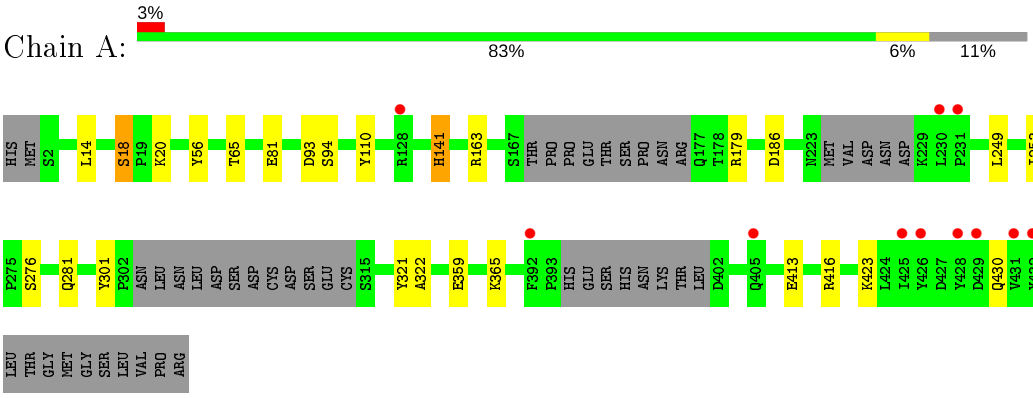
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	213	Total O 213 213	0	0
7	B	244	Total O 244 244	0	0
7	C	253	Total O 253 253	0	0
7	D	200	Total O 200 200	0	0

3 Residue-property plots (i)

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

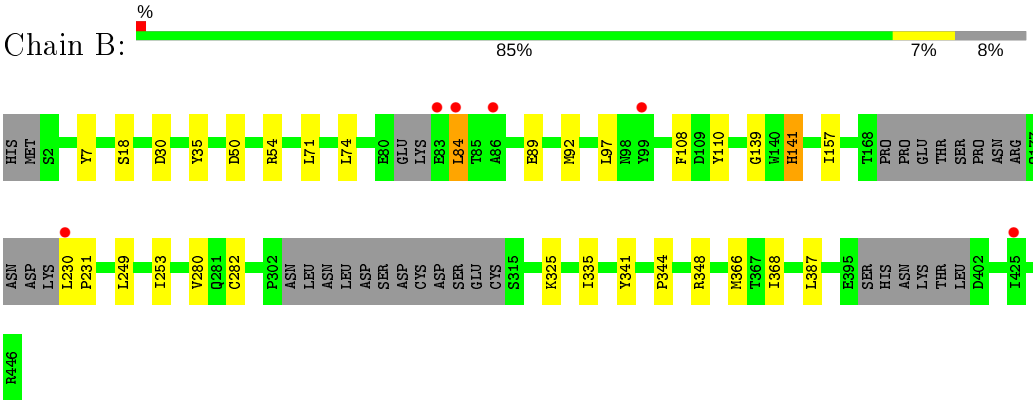
- Molecule 1: Histone deacetylase

Chain A:



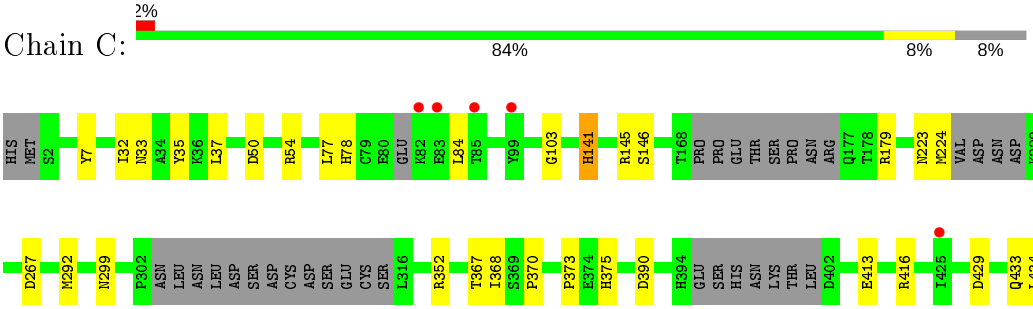
- Molecule 1: Histone deacetylase

Chain B:



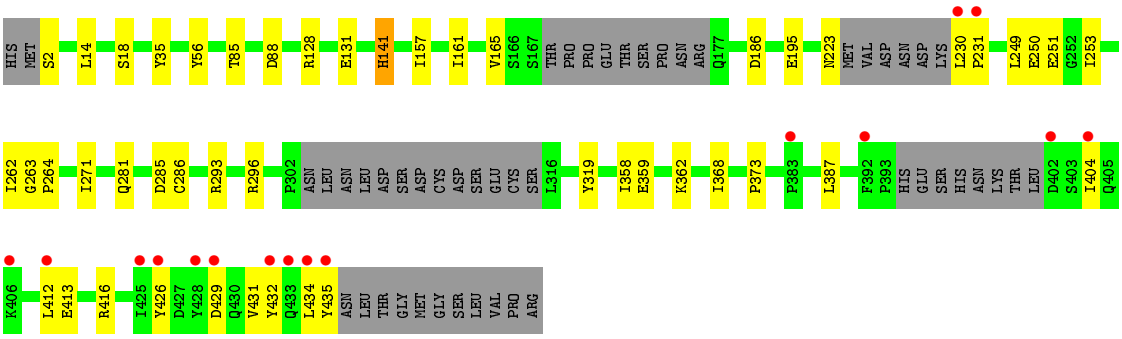
- Molecule 1: Histone deacetylase

Chain C:



• Molecule 1: Histone deacetylase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	70.80Å 70.83Å 98.35Å 78.31° 75.80° 85.98°	Depositor
Resolution (Å)	43.48 – 1.85 48.26 – 1.85	Depositor EDS
% Data completeness (in resolution range)	97.1 (43.48-1.85) 97.1 (48.26-1.85)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.07 (at 1.84Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.206 , 0.253 0.206 , 0.254	Depositor DCC
R_{free} test set	7575 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	21.3	Xtriage
Anisotropy	0.305	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 56.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.137 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	14130	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.07% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, GM5, K, DMF

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|>5$	RMSZ	#$\|Z\|>5$
1	A	0.39	0/3296	0.54	0/4481
1	B	0.42	0/3394	0.56	1/4615 (0.0%)
1	C	0.42	0/3397	0.56	0/4616
1	D	0.40	0/3287	0.54	0/4471
All	All	0.41	0/13374	0.55	1/18183 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	84	LEU	CB-CG-CD2	-5.18	102.19	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3204	0	3106	21	0
1	B	3295	0	3196	27	0
1	C	3298	0	3211	28	0
1	D	3192	0	3093	36	0
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	23	0	0	0	0
4	B	23	0	0	3	0
4	C	23	0	0	0	0
4	D	23	0	0	0	0
5	A	25	0	35	5	0
5	B	10	0	14	1	0
5	C	30	0	42	4	0
5	D	20	0	28	2	0
6	A	6	0	8	2	0
6	B	18	0	24	2	0
6	C	12	0	15	1	0
6	D	6	0	8	0	0
7	A	213	0	0	6	0
7	B	244	0	0	1	0
7	C	253	0	0	5	0
7	D	200	0	0	6	0
All	All	14130	0	12780	112	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (112) 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:C:416:ARG:NH1	7:C:601:HOH:O	2.11	0.83
1:B:50:ASP:OD1	1:B:54:ARG:HD3	1.86	0.74
1:A:274:GLN:NE2	7:A:603:HOH:O	2.21	0.72
1:A:93:ASP:O	5:A:508:DMF:H23	1.89	0.72
1:D:412:LEU:HD11	1:D:435:TYR:CZ	2.26	0.70
1:D:85:THR:HG23	1:D:88:ASP:H	1.57	0.70
1:C:223:ASN:HD22	1:C:234:LEU:HD11	1.58	0.68
1:B:74:LEU:HD13	1:B:92:MET:HE2	1.76	0.68
1:A:321:TYR:OH	7:A:601:HOH:O	2.11	0.67
1:A:94:SER:HA	5:A:508:DMF:H12	1.76	0.66
6:A:510:GOL:O1	7:A:602:HOH:O	2.12	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:368:ILE:HG21	1:D:387:LEU:HD22	1.78	0.65
1:D:250:GLU:OE1	7:D:601:HOH:O	2.15	0.65
1:B:35:TYR:CE1	1:B:368:ILE:HG23	2.33	0.64
1:A:14:LEU:HD12	5:A:506:DMF:HC	1.82	0.61
1:D:35:TYR:CE1	1:D:368:ILE:HG23	2.36	0.61
1:D:412:LEU:HD11	1:D:435:TYR:CE1	2.36	0.60
1:A:423:LYS:HE3	1:C:370:PRO:HG3	1.85	0.59
1:B:74:LEU:HB2	1:B:92:MET:CE	2.33	0.58
1:A:81:GLU:HG3	1:B:230:LEU:HD21	1.84	0.58
1:D:2:SER:N	1:D:131:GLU:OE1	2.39	0.56
1:C:50:ASP:OD1	1:C:54:ARG:HD2	2.06	0.55
1:D:426:TYR:HE2	1:D:431:VAL:HG11	1.71	0.55
1:B:341:TYR:HB3	4:B:504:GM5:C6	2.37	0.54
1:D:293:ARG:O	5:D:507:DMF:H13	2.07	0.54
1:A:186:ASP:HB2	1:A:281:GLN:OE1	2.07	0.54
1:A:179:ARG:HD2	7:A:774:HOH:O	2.08	0.54
1:A:359:GLU:HG3	1:A:365:LYS:HA	1.90	0.53
1:C:375:HIS:HB2	6:C:512:GOL:H32	1.91	0.53
1:B:139:GLY:HA2	1:B:157:ILE:HD11	1.91	0.52
1:D:186:ASP:HB2	1:D:281:GLN:OE1	2.09	0.52
1:D:18:SER:HB3	7:D:656:HOH:O	2.09	0.52
1:C:413:GLU:OE2	1:C:416:ARG:NH2	2.40	0.52
1:B:366:MET:O	5:B:505:DMF:H12	2.10	0.52
1:B:141:HIS:CD2	1:B:141:HIS:H	2.28	0.52
1:C:267:ASP:HB3	1:C:434:LEU:HD11	1.92	0.52
1:B:84:LEU:HD22	1:B:89:GLU:HG2	1.93	0.51
1:C:141:HIS:H	1:C:141:HIS:CD2	2.26	0.51
1:C:416:ARG:NH1	7:C:614:HOH:O	2.43	0.51
1:B:74:LEU:HB2	1:B:92:MET:HE1	1.93	0.50
1:A:56:TYR:OH	1:A:65:THR:HB	2.11	0.50
1:A:413:GLU:HG3	1:A:416:ARG:HH12	1.77	0.50
1:C:35:TYR:CE1	1:C:368:ILE:HG23	2.47	0.50
1:B:141:HIS:NE2	4:B:504:GM5:O20	2.31	0.49
1:D:128:ARG:NH2	7:D:610:HOH:O	2.45	0.49
1:A:18:SER:HB3	1:A:110:TYR:CE1	2.48	0.49
1:C:224:MET:HG3	1:C:231:PRO:HG3	1.95	0.49
1:C:77:LEU:HD13	1:C:84:LEU:HG	1.94	0.49
1:D:264:PRO:HB2	1:D:435:TYR:CE2	2.48	0.48
1:D:223:ASN:O	1:D:231:PRO:HB3	2.12	0.48
1:A:163:ARG:HH22	5:A:505:DMF:H23	1.79	0.48
1:B:71:LEU:HG	1:B:108:PHE:HD1	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:426:TYR:CE2	1:D:431:VAL:HG11	2.49	0.48
1:D:251:GLU:OE2	7:D:602:HOH:O	2.20	0.48
1:D:88:ASP:OD2	7:D:603:HOH:O	2.20	0.48
1:C:35:TYR:CD1	1:C:368:ILE:HG23	2.49	0.48
1:B:249:LEU:HD13	1:B:253:ILE:HD13	1.96	0.48
1:C:33:ASN:HB2	5:C:510:DMF:H23	1.96	0.47
1:D:141:HIS:HB3	1:D:157:ILE:HD12	1.96	0.47
1:C:78:HIS:CE1	1:C:103:GLY:HA3	2.49	0.47
1:D:195:GLU:HG3	5:D:506:DMF:HC	1.96	0.47
1:B:282[B]:CYS:SG	1:B:335:ILE:HG23	2.55	0.46
1:A:141:HIS:H	1:A:141:HIS:CD2	2.33	0.46
1:D:85:THR:CG2	1:D:88:ASP:H	2.28	0.46
1:C:367:THR:O	5:C:507:DMF:H12	2.16	0.46
1:B:224:MET:HG3	1:B:231:PRO:HB3	1.97	0.46
1:D:296:ARG:HA	1:D:296:ARG:HD3	1.77	0.46
1:D:358:ILE:HG23	1:D:362:LYS:HD3	1.98	0.46
1:D:413:GLU:HG3	1:D:416:ARG:NH2	2.30	0.46
1:C:179:ARG:HD2	7:C:622:HOH:O	2.16	0.45
1:D:249:LEU:HD13	1:D:253:ILE:HD13	1.97	0.45
1:B:325:LYS:NZ	7:B:601:HOH:O	2.17	0.45
1:D:230:LEU:HD23	1:D:231:PRO:O	2.17	0.45
1:D:271:ILE:HD12	1:D:434:LEU:HD11	1.98	0.45
1:B:18:SER:HB3	1:B:110:TYR:CE1	2.51	0.45
1:B:341:TYR:HB3	4:B:504:GM5:C5	2.47	0.45
1:B:7:TYR:CD2	6:B:507:GOL:H11	2.53	0.44
1:C:223:ASN:ND2	1:C:234:LEU:HD11	2.31	0.44
1:B:344:PRO:O	1:B:348:ARG:HG3	2.18	0.44
1:C:145:ARG:HE	5:C:509:DMF:H21	1.81	0.44
1:D:249:LEU:CD2	1:D:404:ILE:HD11	2.48	0.44
1:C:230:LEU:HG	1:C:231:PRO:HD2	2.00	0.44
1:C:32:ILE:HG23	1:C:37:LEU:HB2	1.99	0.44
1:B:74:LEU:HB2	1:B:92:MET:HE2	1.98	0.43
1:A:20:LYS:HD3	1:A:20:LYS:HA	1.78	0.43
1:B:30:ASP:OD1	6:B:507:GOL:O3	2.37	0.43
1:D:404:ILE:HA	1:D:404:ILE:HD13	1.65	0.43
1:B:84:LEU:CD2	1:B:89:GLU:HG2	2.48	0.43
1:D:128:ARG:HD2	7:D:626:HOH:O	2.19	0.43
1:B:368:ILE:HG21	1:B:387:LEU:CD2	2.49	0.43
1:C:7:TYR:CE2	5:C:510:DMF:H11	2.53	0.43
1:D:161:ILE:O	1:D:165:VAL:HG22	2.19	0.43
1:C:292:MET:HE2	1:C:292:MET:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:368:ILE:CG2	1:D:387:LEU:HD22	2.46	0.42
1:B:280:VAL:HG12	1:B:282[B]:CYS:SG	2.59	0.42
1:A:65:THR:HG23	7:A:752:HOH:O	2.19	0.42
1:D:35:TYR:CZ	1:D:373:PRO:HD3	2.55	0.42
1:A:262:ILE:HD11	1:A:322:ALA:HB2	2.01	0.42
5:A:509:DMF:HC	7:A:775:HOH:O	2.19	0.42
1:A:276:SER:O	6:A:510:GOL:H12	2.19	0.42
1:C:35:TYR:CZ	1:C:373:PRO:HD3	2.55	0.42
1:C:179:ARG:NH1	7:C:622:HOH:O	2.52	0.41
1:C:299:ASN:O	1:C:352:ARG:HD2	2.21	0.41
1:B:92:MET:HE3	1:B:97:LEU:CD1	2.50	0.41
1:C:390:ASP:HB3	7:C:617:HOH:O	2.19	0.41
1:D:262:ILE:HG13	1:D:263:GLY:N	2.36	0.41
1:D:14:LEU:HD23	1:D:14:LEU:HA	1.87	0.41
1:C:433:GLN:O	1:C:437:LEU:HD22	2.21	0.41
1:D:286:CYS:HB2	1:D:319:TYR:OH	2.21	0.41
1:D:429:ASP:O	1:D:432:TYR:N	2.54	0.41
1:A:430:GLN:O	1:A:433:GLN:HG3	2.21	0.40
1:A:249:LEU:HD13	1:A:253:ILE:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	391/447 (88%)	381 (97%)	10 (3%)	0	100	100
1	B	403/447 (90%)	394 (98%)	9 (2%)	0	100	100
1	C	403/447 (90%)	394 (98%)	9 (2%)	0	100	100
1	D	390/447 (87%)	379 (97%)	11 (3%)	0	100	100
All	All	1587/1788 (89%)	1548 (98%)	39 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	348/392 (89%)	345 (99%)	3 (1%)	78	71
1	B	360/392 (92%)	357 (99%)	3 (1%)	81	75
1	C	360/392 (92%)	355 (99%)	5 (1%)	67	55
1	D	347/392 (88%)	343 (99%)	4 (1%)	71	61
All	All	1415/1568 (90%)	1400 (99%)	15 (1%)	73	64

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

Mol	Chain	Res	Type
1	A	18	SER
1	A	141	HIS
1	A	301	TYR
1	B	141	HIS
1	B	430	GLN
1	B	438	THR
1	C	141	HIS
1	C	146	SER
1	C	429	ASP
1	C	437	LEU
1	C	438	THR
1	D	56	TYR
1	D	141	HIS
1	D	285	ASP
1	D	359	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	78	HIS
1	C	129	HIS

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Mol	Chain	Res	Type
1	D	260	ASN

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	$\#\|Z\| > 2$
5	DMF	C	510	-	4,4,4	0.35	0	4,4,4	0.36	0
5	DMF	C	506	-	4,4,4	0.32	0	4,4,4	0.49	0
6	GOL	B	509	-	5,5,5	0.37	0	5,5,5	0.11	0
5	DMF	D	507	-	4,4,4	0.32	0	4,4,4	0.45	0
6	GOL	C	511	-	5,5,5	0.37	0	5,5,5	0.89	0
5	DMF	A	509	-	4,4,4	0.27	0	4,4,4	0.43	0
5	DMF	B	505	-	4,4,4	0.32	0	4,4,4	0.61	0
5	DMF	D	505	-	4,4,4	0.34	0	4,4,4	0.17	0
6	GOL	B	508	-	5,5,5	0.34	0	5,5,5	0.77	0
6	GOL	A	510	-	5,5,5	0.35	0	5,5,5	0.35	0
5	DMF	A	505	-	4,4,4	0.35	0	4,4,4	0.30	0
4	GM5	D	504	2	24,25,25	0.44	0	27,33,33	0.46	0
5	DMF	A	506	-	4,4,4	0.33	0	4,4,4	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
6	GOL	C	512	-	5,5,5	0.55	0	5,5,5	0.56	0
4	GM5	A	504	2	24,25,25	0.45	0	27,33,33	0.43	0
5	DMF	C	509	-	4,4,4	0.31	0	4,4,4	0.20	0
4	GM5	C	504	2	24,25,25	0.44	0	27,33,33	0.54	0
5	DMF	C	507	-	4,4,4	0.38	0	4,4,4	0.51	0
5	DMF	A	507	-	4,4,4	0.34	0	4,4,4	0.54	0
5	DMF	C	505	-	4,4,4	0.32	0	4,4,4	0.42	0
5	DMF	D	506	-	4,4,4	0.29	0	4,4,4	0.40	0
5	DMF	D	508	-	4,4,4	0.27	0	4,4,4	0.27	0
6	GOL	B	507	-	5,5,5	0.40	0	5,5,5	0.29	0
5	DMF	A	508	-	4,4,4	0.27	0	4,4,4	0.63	0
4	GM5	B	504	2	24,25,25	0.46	0	27,33,33	0.40	0
5	DMF	C	508	-	4,4,4	0.23	0	4,4,4	0.30	0
6	GOL	D	509	-	5,5,5	0.37	0	5,5,5	0.37	0
5	DMF	B	506	-	4,4,4	0.32	0	4,4,4	0.39	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	510	-	-	2/2/2/2	-
5	DMF	C	506	-	-	2/2/2/2	-
6	GOL	B	509	-	-	4/4/4/4	-
5	DMF	D	507	-	-	2/2/2/2	-
6	GOL	C	511	-	-	3/4/4/4	-
5	DMF	A	509	-	-	0/2/2/2	-
5	DMF	B	505	-	-	0/2/2/2	-
5	DMF	D	505	-	-	2/2/2/2	-
6	GOL	B	508	-	-	2/4/4/4	-
6	GOL	A	510	-	-	4/4/4/4	-
5	DMF	A	505	-	-	2/2/2/2	-
4	GM5	D	504	2	-	0/13/15/15	0/3/3/3
5	DMF	A	506	-	-	2/2/2/2	-
6	GOL	C	512	-	-	3/4/4/4	-
4	GM5	A	504	2	-	0/13/15/15	0/3/3/3
5	DMF	C	509	-	-	0/2/2/2	-
4	GM5	C	504	2	-	0/13/15/15	0/3/3/3
5	DMF	C	507	-	-	2/2/2/2	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	DMF	A	507	-	-	2/2/2/2	-
5	DMF	C	505	-	-	2/2/2/2	-
5	DMF	D	506	-	-	0/2/2/2	-
5	DMF	D	508	-	-	2/2/2/2	-
6	GOL	B	507	-	-	2/4/4/4	-
5	DMF	A	508	-	-	0/2/2/2	-
4	GM5	B	504	2	-	0/13/15/15	0/3/3/3
5	DMF	C	508	-	-	2/2/2/2	-
6	GOL	D	509	-	-	2/4/4/4	-
5	DMF	B	506	-	-	0/2/2/2	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	C	511	GOL	O2-C2-C3-O3
6	A	510	GOL	O1-C1-C2-O2
6	A	510	GOL	O2-C2-C3-O3
6	B	507	GOL	O1-C1-C2-C3
6	D	509	GOL	C1-C2-C3-O3
5	A	505	DMF	O-C-N-C1
5	A	505	DMF	O-C-N-C2
5	A	507	DMF	O-C-N-C2
5	C	510	DMF	O-C-N-C1
5	C	506	DMF	O-C-N-C1
5	C	506	DMF	O-C-N-C2
5	A	507	DMF	O-C-N-C1
5	C	507	DMF	O-C-N-C1
5	C	508	DMF	O-C-N-C1
5	C	508	DMF	O-C-N-C2
5	D	505	DMF	O-C-N-C1
5	C	507	DMF	O-C-N-C2
5	C	510	DMF	O-C-N-C2
5	D	505	DMF	O-C-N-C2
5	D	508	DMF	O-C-N-C1
5	D	508	DMF	O-C-N-C2
5	C	505	DMF	O-C-N-C1

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Mol	Chain	Res	Type	Atoms
5	A	506	DMF	O-C-N-C1
6	B	509	GOL	O1-C1-C2-C3
6	B	509	GOL	C1-C2-C3-O3
6	C	511	GOL	C1-C2-C3-O3
6	B	508	GOL	O1-C1-C2-C3
6	A	510	GOL	O1-C1-C2-C3
6	A	510	GOL	C1-C2-C3-O3
6	C	512	GOL	O1-C1-C2-C3
5	D	507	DMF	O-C-N-C2
6	B	509	GOL	O2-C2-C3-O3
6	C	512	GOL	O1-C1-C2-O2
6	B	507	GOL	O1-C1-C2-O2
6	D	509	GOL	O2-C2-C3-O3
5	A	506	DMF	O-C-N-C2
5	C	505	DMF	O-C-N-C2
6	B	509	GOL	O1-C1-C2-O2
6	B	508	GOL	O1-C1-C2-O2
5	D	507	DMF	O-C-N-C1
6	C	511	GOL	O1-C1-C2-C3
6	C	512	GOL	C1-C2-C3-O3

There are no ring outliers.

14 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	510	DMF	2	0
5	D	507	DMF	1	0
5	A	509	DMF	1	0
5	B	505	DMF	1	0
6	A	510	GOL	2	0
5	A	505	DMF	1	0
5	A	506	DMF	1	0
6	C	512	GOL	1	0
5	C	509	DMF	1	0
5	C	507	DMF	1	0
5	D	506	DMF	1	0
6	B	507	GOL	2	0
5	A	508	DMF	2	0
4	B	504	GM5	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	400/447 (89%)	0.06	14 (3%) 44 40	14, 25, 62, 87	0
1	B	412/447 (92%)	-0.11	6 (1%) 73 73	11, 22, 45, 97	0
1	C	412/447 (92%)	-0.07	7 (1%) 70 69	11, 22, 45, 84	0
1	D	398/447 (89%)	0.02	16 (4%) 38 35	13, 24, 62, 108	0
All	All	1622/1788 (90%)	-0.03	43 (2%) 54 52	11, 23, 52, 108	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	428	TYR	11.9
1	A	432	TYR	7.5
1	D	426	TYR	7.3
1	A	434	LEU	7.2
1	D	435	TYR	7.0
1	A	230	LEU	6.9
1	D	432	TYR	6.8
1	A	425	ILE	6.3
1	A	428	TYR	6.0
1	A	435	TYR	5.4
1	A	426	TYR	5.2
1	B	83	GLU	5.0
1	D	392	PHE	5.0
1	D	425	ILE	4.8
1	D	434	LEU	4.5
1	C	99	TYR	4.4
1	C	425	ILE	3.9
1	D	429	ASP	3.8
1	A	433	GLN	3.6
1	A	392	PHE	3.5
1	C	82	LYS	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	431	VAL	3.2
1	B	84	LEU	3.1
1	C	230	LEU	3.1
1	D	433	GLN	3.1
1	A	429	ASP	3.1
1	A	128	ARG	2.9
1	D	404	ILE	2.8
1	C	438	THR	2.6
1	D	406	LYS	2.5
1	C	83	GLU	2.5
1	B	99	TYR	2.5
1	B	425	ILE	2.4
1	D	383	PRO	2.3
1	B	230	LEU	2.3
1	A	231	PRO	2.1
1	B	86	ALA	2.1
1	C	85	THR	2.1
1	D	412	LEU	2.1
1	D	402	ASP	2.1
1	D	231	PRO	2.1
1	D	230	LEU	2.1
1	A	405	GLN	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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	C	508	5/5	0.59	0.23	31,45,49,49	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMF	D	505	5/5	0.60	0.24	50,51,56,57	0
5	DMF	C	510	5/5	0.67	0.24	34,40,53,54	0
6	GOL	C	512	6/6	0.74	0.17	35,39,43,43	0
4	GM5	D	504	23/23	0.78	0.19	27,55,74,75	0
5	DMF	A	508	5/5	0.79	0.17	35,37,39,42	0
5	DMF	B	506	5/5	0.79	0.19	30,43,44,47	0
4	GM5	B	504	23/23	0.81	0.22	26,47,63,71	0
4	GM5	A	504	23/23	0.82	0.17	27,49,69,74	0
5	DMF	C	509	5/5	0.82	0.17	46,51,52,52	0
6	GOL	A	510	6/6	0.83	0.19	38,46,47,53	0
4	GM5	C	504	23/23	0.83	0.16	23,43,66,75	0
5	DMF	D	507	5/5	0.84	0.16	29,30,41,42	0
5	DMF	C	507	5/5	0.84	0.16	38,39,40,42	0
5	DMF	C	505	5/5	0.85	0.19	32,33,38,42	0
6	GOL	C	511	6/6	0.87	0.17	19,36,44,44	0
5	DMF	A	506	5/5	0.87	0.16	35,43,46,52	0
5	DMF	A	509	5/5	0.87	0.21	33,37,44,47	0
6	GOL	B	507	6/6	0.88	0.18	43,50,57,62	0
5	DMF	D	508	5/5	0.88	0.21	54,54,57,60	0
6	GOL	D	509	6/6	0.89	0.15	25,34,35,41	0
5	DMF	A	505	5/5	0.89	0.28	38,47,51,52	0
6	GOL	B	509	6/6	0.90	0.15	41,46,50,59	0
5	DMF	A	507	5/5	0.90	0.16	48,49,52,56	0
6	GOL	B	508	6/6	0.91	0.12	24,26,34,34	0
5	DMF	B	505	5/5	0.92	0.14	29,37,46,47	0
5	DMF	D	506	5/5	0.92	0.17	37,44,49,52	0
5	DMF	C	506	5/5	0.95	0.11	29,35,46,56	0
3	K	B	502	1/1	0.99	0.09	25,25,25,25	0
2	ZN	C	501	1/1	0.99	0.04	22,22,22,22	0
2	ZN	B	501	1/1	0.99	0.05	22,22,22,22	0
2	ZN	D	501	1/1	1.00	0.05	22,22,22,22	0
3	K	D	503	1/1	1.00	0.09	18,18,18,18	0
3	K	B	503	1/1	1.00	0.07	14,14,14,14	0
2	ZN	A	501	1/1	1.00	0.04	22,22,22,22	0
3	K	A	502	1/1	1.00	0.09	17,17,17,17	0
3	K	C	502	1/1	1.00	0.07	19,19,19,19	0
3	K	A	503	1/1	1.00	0.07	22,22,22,22	0
3	K	C	503	1/1	1.00	0.07	16,16,16,16	0
3	K	D	502	1/1	1.00	0.07	23,23,23,23	0

6.5 Other polymers (i)

There are no such residues in this entry.