



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 08:30 AM GMT

PDB ID : 3EWF  
Title : Crystal Structure Analysis of human HDAC8 H143A variant complexed with substrate.  
Authors : Dowling, D.P.; Gantt, S.L.; Gattis, S.G.; Fierke, C.A.; Christianon, D.W.  
Deposited on : 2008-10-14  
Resolution : 2.50 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

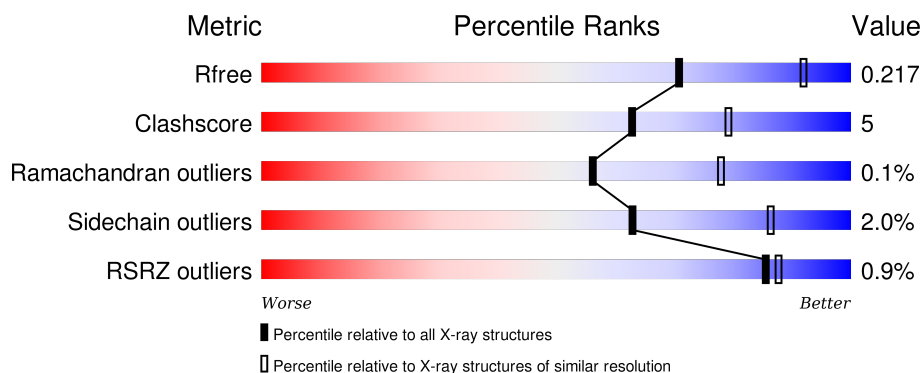
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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	388	<div> <div>82%</div> <div>12%</div> <div>6%</div> </div>
1	B	388	<div> <div>81%</div> <div>12%</div> <div>6%</div> </div>
1	C	388	<div> <div>79%</div> <div>14%</div> <div>6%</div> </div>
1	D	388	<div> <div>81%</div> <div>12%</div> <div>6%</div> </div>
2	I	5	<div> <div>80%</div> <div>20%</div> </div>

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Mol	Chain	Length	Quality of chain
2	J	5	<div><div></div><div>80%</div><div>20%</div></div>
2	K	5	<div><div></div><div>40%</div><div>60%</div></div>
2	L	5	<div><div></div><div>20%</div><div>80%</div><div>20%</div></div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 11893 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 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	364	Total	C	N	O	S	0	0	0
			2834	1816	470	529	19			
1	B	364	Total	C	N	O	S	6	0	0
			2834	1816	470	529	19			
1	C	364	Total	C	N	O	S	5	0	0
			2834	1816	470	529	19			
1	D	364	Total	C	N	O	S	1	0	0
			2834	1816	470	529	19			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	143	ALA	HIS	ENGINEERED	UNP Q9BY41
A	378	ILE	-	EXPRESSION TAG	UNP Q9BY41
A	379	GLU	-	EXPRESSION TAG	UNP Q9BY41
A	380	GLY	-	EXPRESSION TAG	UNP Q9BY41
A	381	ARG	-	EXPRESSION TAG	UNP Q9BY41
A	382	SER	-	EXPRESSION TAG	UNP Q9BY41
A	383	HIS	-	EXPRESSION TAG	UNP Q9BY41
A	384	HIS	-	EXPRESSION TAG	UNP Q9BY41
A	385	HIS	-	EXPRESSION TAG	UNP Q9BY41
A	386	HIS	-	EXPRESSION TAG	UNP Q9BY41
A	387	HIS	-	EXPRESSION TAG	UNP Q9BY41
A	388	HIS	-	EXPRESSION TAG	UNP Q9BY41
B	143	ALA	HIS	ENGINEERED	UNP Q9BY41
B	378	ILE	-	EXPRESSION TAG	UNP Q9BY41
B	379	GLU	-	EXPRESSION TAG	UNP Q9BY41
B	380	GLY	-	EXPRESSION TAG	UNP Q9BY41
B	381	ARG	-	EXPRESSION TAG	UNP Q9BY41
B	382	SER	-	EXPRESSION TAG	UNP Q9BY41
B	383	HIS	-	EXPRESSION TAG	UNP Q9BY41
B	384	HIS	-	EXPRESSION TAG	UNP Q9BY41
B	385	HIS	-	EXPRESSION TAG	UNP Q9BY41

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Chain	Residue	Modelled	Actual	Comment	Reference
B	386	HIS	-	EXPRESSION TAG	UNP Q9BY41
B	387	HIS	-	EXPRESSION TAG	UNP Q9BY41
B	388	HIS	-	EXPRESSION TAG	UNP Q9BY41
C	143	ALA	HIS	ENGINEERED	UNP Q9BY41
C	378	ILE	-	EXPRESSION TAG	UNP Q9BY41
C	379	GLU	-	EXPRESSION TAG	UNP Q9BY41
C	380	GLY	-	EXPRESSION TAG	UNP Q9BY41
C	381	ARG	-	EXPRESSION TAG	UNP Q9BY41
C	382	SER	-	EXPRESSION TAG	UNP Q9BY41
C	383	HIS	-	EXPRESSION TAG	UNP Q9BY41
C	384	HIS	-	EXPRESSION TAG	UNP Q9BY41
C	385	HIS	-	EXPRESSION TAG	UNP Q9BY41
C	386	HIS	-	EXPRESSION TAG	UNP Q9BY41
C	387	HIS	-	EXPRESSION TAG	UNP Q9BY41
C	388	HIS	-	EXPRESSION TAG	UNP Q9BY41
D	143	ALA	HIS	ENGINEERED	UNP Q9BY41
D	378	ILE	-	EXPRESSION TAG	UNP Q9BY41
D	379	GLU	-	EXPRESSION TAG	UNP Q9BY41
D	380	GLY	-	EXPRESSION TAG	UNP Q9BY41
D	381	ARG	-	EXPRESSION TAG	UNP Q9BY41
D	382	SER	-	EXPRESSION TAG	UNP Q9BY41
D	383	HIS	-	EXPRESSION TAG	UNP Q9BY41
D	384	HIS	-	EXPRESSION TAG	UNP Q9BY41
D	385	HIS	-	EXPRESSION TAG	UNP Q9BY41
D	386	HIS	-	EXPRESSION TAG	UNP Q9BY41
D	387	HIS	-	EXPRESSION TAG	UNP Q9BY41
D	388	HIS	-	EXPRESSION TAG	UNP Q9BY41

- Molecule 2 is a protein called PEPTIDIC SUBSTRATE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	I	5	Total	C	N	O	0	0	0
			48	30	11	7			
2	J	5	Total	C	N	O	0	0	0
			48	30	11	7			
2	K	5	Total	C	N	O	0	0	0
			48	30	11	7			
2	L	5	Total	C	N	O	0	0	0
			48	30	11	7			

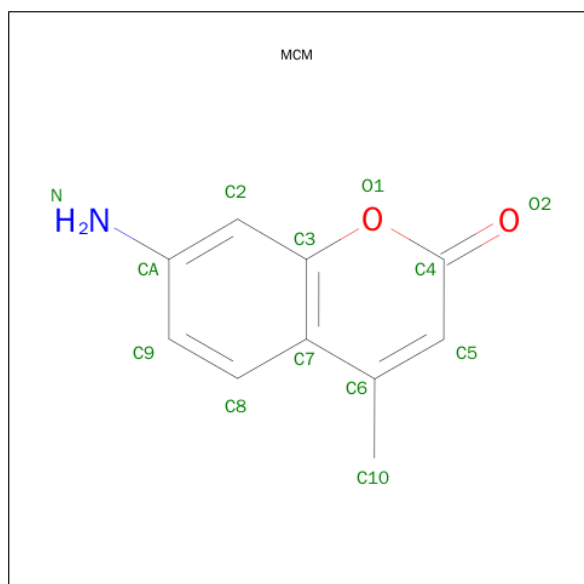
- Molecule 3 is ZINC ION (three-letter code: ZN) (formula: Zn).

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

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

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

- Molecule 5 is 7-AMINO-4-METHYL-CHROMEN-2-ONE (three-letter code: MCM) (formula: C<sub>10</sub>H<sub>9</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	I	1	Total	C	N	O	0	0
			13	10	1	2		

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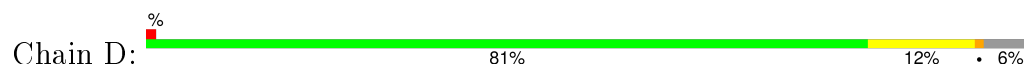
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	J	1	Total	C	N	O	0	0
			13	10	1	2		
5	K	1	Total	C	N	O	0	0
			13	10	1	2		
5	L	1	Total	C	N	O	0	0
			13	10	1	2		

- Molecule 6 is water.

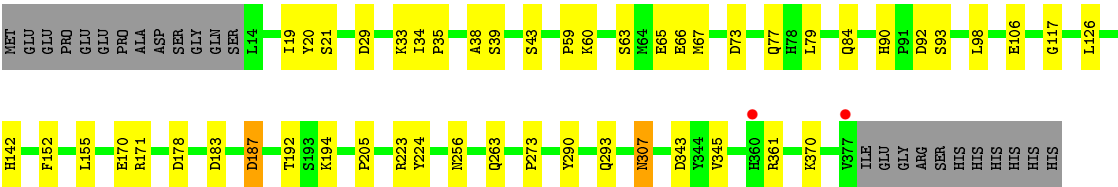
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	85	Total	O	0	0
			85	85		
6	B	82	Total	O	0	0
			82	82		
6	C	65	Total	O	0	0
			65	65		
6	D	58	Total	O	0	0
			58	58		
6	I	4	Total	O	0	0
			4	4		
6	J	3	Total	O	0	0
			3	3		
6	K	1	Total	O	0	0
			1	1		
6	L	1	Total	O	0	0
			1	1		



- Molecule 1: Histone deacetylase 8



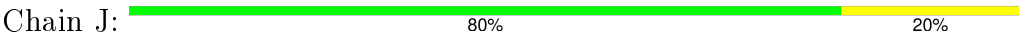




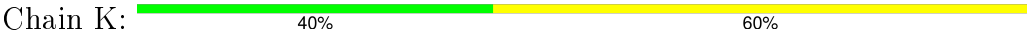
● Molecule 2: PEPTIDIC SUBSTRATE



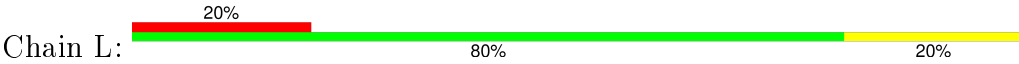
● Molecule 2: PEPTIDIC SUBSTRATE



● Molecule 2: PEPTIDIC SUBSTRATE



● Molecule 2: PEPTIDIC SUBSTRATE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.90Å 91.84Å 196.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.15 – 2.50 49.14 – 2.49	Depositor EDS
% Data completeness (in resolution range)	93.6 (49.15-2.50) 99.0 (49.14-2.49)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.69 (at 2.48Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, $R_{free}$	0.198 , 0.229 0.206 , 0.217	Depositor DCC
$R_{free}$ test set	2667 reflections (5.09%)	DCC
Wilson B-factor (Å <sup>2</sup> )	29.0	Xtriage
Anisotropy	0.595	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 43.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 52706 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11893	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 2.95% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ZN, MCM, K, ACE, ALY

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	0/2904	0.65	3/3941 (0.1%)
1	B	0.40	1/2904 (0.0%)	0.71	6/3941 (0.2%)
1	C	0.46	4/2904 (0.1%)	0.70	6/3941 (0.2%)
1	D	0.41	1/2904 (0.0%)	0.63	3/3941 (0.1%)
2	I	0.32	0/22	0.60	0/28
2	J	0.22	0/22	0.51	0/28
2	K	0.31	0/22	0.55	0/28
2	L	0.23	0/22	0.41	0/28
All	All	0.41	6/11704 (0.1%)	0.68	18/15876 (0.1%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	363	GLN	CG-CD	-7.12	1.34	1.51
1	C	363	GLN	CD-OE1	-6.80	1.08	1.24
1	C	367	ASN	CB-CG	-6.01	1.37	1.51
1	D	65	GLU	CG-CD	-5.39	1.43	1.51
1	B	65	GLU	CG-CD	-5.28	1.44	1.51
1	C	95	GLU	CB-CG	-5.11	1.42	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	164	ARG	NE-CZ-NH2	-15.24	112.68	120.30
1	B	164	ARG	NE-CZ-NH1	13.68	127.14	120.30
1	C	356	ARG	NE-CZ-NH1	11.68	126.14	120.30
1	C	356	ARG	NE-CZ-NH2	-11.55	114.52	120.30
1	C	361	ARG	NE-CZ-NH1	8.69	124.64	120.30
1	A	361	ARG	NE-CZ-NH1	8.53	124.57	120.30
1	A	361	ARG	NE-CZ-NH2	-8.50	116.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	361	ARG	NE-CZ-NH1	-8.19	116.21	120.30
1	B	361	ARG	NE-CZ-NH1	-7.93	116.34	120.30
1	C	361	ARG	NE-CZ-NH2	-7.82	116.39	120.30
1	D	361	ARG	NE-CZ-NH2	7.67	124.13	120.30
1	B	361	ARG	NE-CZ-NH2	6.82	123.71	120.30
1	B	164	ARG	CD-NE-CZ	6.03	132.04	123.60
1	D	307	ASN	N-CA-C	-5.78	95.39	111.00
1	B	307	ASN	N-CA-C	-5.72	95.56	111.00
1	C	307	ASN	N-CA-C	-5.51	96.11	111.00
1	A	307	ASN	N-CA-C	-5.51	96.13	111.00
1	C	164	ARG	NE-CZ-NH1	-5.16	117.72	120.30

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	2834	0	2786	32	0
1	B	2834	0	2785	28	0
1	C	2834	0	2786	34	0
1	D	2834	0	2784	32	0
2	I	48	0	50	1	0
2	J	48	0	50	1	0
2	K	48	0	50	4	0
2	L	48	0	50	1	0
3	A	2	0	0	0	0
3	B	1	0	0	0	0
3	C	2	0	0	0	0
3	D	1	0	0	0	0
4	A	2	0	0	0	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
4	D	2	0	0	0	0
5	I	13	0	7	1	0
5	J	13	0	7	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	K	13	0	7	2	0
5	L	13	0	7	2	0
6	A	85	0	0	2	0
6	B	82	0	0	1	0
6	C	65	0	0	1	0
6	D	58	0	0	2	0
6	I	4	0	0	0	0
6	J	3	0	0	0	0
6	K	1	0	0	1	0
6	L	1	0	0	0	0
All	All	11893	0	11369	122	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 5.

All (122) 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:192:THR:HG22	1:B:194:LYS:H	1.45	0.80
1:D:192:THR:HG22	1:D:194:LYS:H	1.47	0.80
1:C:334:HIS:H	1:C:337:PHE:HB2	1.45	0.79
1:A:33:LYS:HG3	5:J:6:MCM:H5	1.66	0.78
1:A:192:THR:HG22	1:A:194:LYS:H	1.54	0.73
1:C:192:THR:HG22	1:C:194:LYS:H	1.54	0.73
1:C:333:ASP:HA	1:C:337:PHE:CD2	2.27	0.70
1:B:73:ASP:O	1:B:77:GLN:HG2	1.92	0.69
1:B:33:LYS:HG3	5:I:6:MCM:H5	1.75	0.68
1:C:170:GLU:OE2	1:C:170:GLU:HA	1.93	0.67
1:A:73:ASP:O	1:A:77:GLN:HG2	1.95	0.66
1:C:33:LYS:HG3	5:L:6:MCM:H5	1.79	0.63
1:A:221:LYS:HB3	2:K:1:ACE:H3	1.81	0.63
1:D:73:ASP:O	1:D:77:GLN:HG2	1.99	0.63
1:C:73:ASP:O	1:C:77:GLN:HG2	2.00	0.61
1:D:90:HIS:HD2	1:D:92:ASP:H	1.49	0.60
1:C:343:ASP:O	1:C:344:TYR:HB2	2.01	0.60
1:C:90:HIS:HD2	1:C:92:ASP:H	1.49	0.59
6:C:885:HOH:O	2:K:2:ARG:HG2	2.03	0.58
1:D:92:ASP:HA	6:D:1023:HOH:O	2.03	0.58
1:D:90:HIS:CD2	1:D:92:ASP:H	2.21	0.58
1:B:90:HIS:HD2	1:B:92:ASP:H	1.51	0.58
1:A:90:HIS:HD2	1:A:92:ASP:H	1.51	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:GLN:NE2	1:A:84:GLN:HA	2.19	0.57
1:C:67:MET:SD	1:C:155:LEU:HD21	2.44	0.57
1:A:90:HIS:CD2	1:A:92:ASP:H	2.23	0.57
1:D:290:TYR:O	1:D:293:GLN:HG3	2.04	0.57
1:B:67:MET:SD	1:B:155:LEU:HD21	2.45	0.57
1:C:205:PRO:HA	6:K:994:HOH:O	2.04	0.57
1:B:90:HIS:CD2	1:B:92:ASP:H	2.23	0.56
1:D:273:PRO:HB2	5:K:6:MCM:H9	1.87	0.56
1:D:67:MET:SD	1:D:155:LEU:HD21	2.45	0.56
1:C:90:HIS:CD2	1:C:92:ASP:H	2.23	0.56
1:D:171:ARG:NH1	1:D:256:ASN:O	2.39	0.56
1:C:290:TYR:O	1:C:293:GLN:HG3	2.06	0.55
1:A:290:TYR:O	1:A:293:GLN:HG3	2.07	0.55
1:D:170:GLU:HA	1:D:170:GLU:OE2	2.07	0.55
1:B:290:TYR:O	1:B:293:GLN:HG3	2.06	0.55
1:A:170:GLU:HA	1:A:170:GLU:OE2	2.06	0.55
1:C:178:ASP:HB2	1:C:263:GLN:OE1	2.07	0.54
1:A:93:SER:HB3	1:A:98:LEU:HB2	1.89	0.54
1:D:93:SER:HB3	1:D:98:LEU:HB2	1.90	0.53
1:C:352:CYS:O	1:D:205:PRO:HG2	2.08	0.53
1:D:33:LYS:HG3	5:K:6:MCM:H5	1.91	0.53
1:D:223:ARG:O	1:D:224:TYR:HB2	2.09	0.53
1:D:84:GLN:HA	1:D:84:GLN:NE2	2.24	0.52
1:A:370:LYS:NZ	1:A:370:LYS:HB2	2.25	0.52
1:A:342:PRO:HD2	6:A:912:HOH:O	2.09	0.52
1:B:170:GLU:OE2	1:B:170:GLU:HA	2.08	0.52
1:B:84:GLN:HA	1:B:84:GLN:NE2	2.24	0.52
1:B:343:ASP:OD1	1:C:192:THR:HG23	2.10	0.52
1:A:171:ARG:NH1	1:A:256:ASN:O	2.42	0.51
1:B:178:ASP:HB2	1:B:263:GLN:OE1	2.10	0.51
1:B:214:VAL:HG22	1:B:368:TYR:HD2	1.76	0.51
1:C:93:SER:HB3	1:C:98:LEU:HB2	1.93	0.51
1:B:93:SER:HB3	1:B:98:LEU:HB2	1.93	0.51
1:C:84:GLN:NE2	1:C:84:GLN:HA	2.26	0.51
1:A:223:ARG:O	1:A:224:TYR:HB2	2.09	0.51
1:A:67:MET:SD	1:A:155:LEU:HD21	2.51	0.50
1:A:341:GLY:C	2:J:1:ACE:H3	2.32	0.50
1:B:223:ARG:O	1:B:224:TYR:HB2	2.11	0.50
1:A:14:LEU:N	1:A:14:LEU:HD13	2.27	0.50
1:C:171:ARG:NH1	1:C:256:ASN:O	2.45	0.49
1:A:34:ILE:N	1:A:35:PRO:HD3	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:GLU:CA	1:C:170:GLU:OE2	2.58	0.49
1:D:29:ASP:OD2	1:D:38:ALA:HB3	2.13	0.49
1:D:152:PHE:CE1	2:L:5:ALY:HD2	2.47	0.49
1:B:370:LYS:HB2	1:B:370:LYS:NZ	2.27	0.49
1:C:223:ARG:O	1:C:224:TYR:HB2	2.12	0.48
1:D:370:LYS:NZ	1:D:370:LYS:HB2	2.28	0.48
1:C:221:LYS:HB3	2:I:1:ACE:H3	1.94	0.48
1:A:192:THR:HG23	1:D:343:ASP:OD1	2.14	0.47
1:D:34:ILE:N	1:D:35:PRO:HD3	2.29	0.47
1:B:34:ILE:N	1:B:35:PRO:HD3	2.30	0.47
1:C:183:ASP:O	1:C:187:ASP:HB2	2.14	0.47
1:D:178:ASP:HB2	1:D:263:GLN:OE1	2.14	0.47
1:A:178:ASP:HB2	1:A:263:GLN:OE1	2.15	0.47
1:D:39:SER:O	1:D:43:SER:HB2	2.15	0.47
1:A:183:ASP:O	1:A:187:ASP:HB2	2.15	0.47
1:C:273:PRO:HB2	5:L:6:MCM:H9	1.97	0.46
1:C:34:ILE:N	1:C:35:PRO:HD3	2.29	0.46
1:C:20:TYR:CG	1:C:21:SER:N	2.83	0.46
1:A:39:SER:O	1:A:43:SER:HB2	2.15	0.46
1:D:307:ASN:HA	2:K:4:ALY:HD3	1.97	0.46
1:C:370:LYS:HB2	1:C:370:LYS:NZ	2.30	0.46
1:B:345:VAL:HG11	1:C:194:LYS:HE2	1.97	0.46
1:B:183:ASP:O	1:B:187:ASP:HB2	2.16	0.46
1:B:171:ARG:NH1	1:B:256:ASN:O	2.48	0.46
1:D:20:TYR:CG	1:D:21:SER:N	2.85	0.45
1:C:19:ILE:CG2	1:C:59:PRO:HB3	2.47	0.45
1:A:194:LYS:HE2	1:D:345:VAL:HG11	1.99	0.45
1:B:20:TYR:CG	1:B:21:SER:N	2.85	0.45
1:D:183:ASP:O	1:D:187:ASP:HB2	2.18	0.44
1:B:15:VAL:HA	1:B:16:PRO:HD3	1.90	0.44
1:C:39:SER:O	1:C:43:SER:HB2	2.17	0.44
6:D:917:HOH:O	2:K:4:ALY:HH33	2.18	0.43
1:D:192:THR:HG22	1:D:194:LYS:N	2.26	0.43
1:C:334:HIS:O	1:C:337:PHE:HB2	2.17	0.43
1:D:19:ILE:CG2	1:D:59:PRO:HB3	2.49	0.43
1:B:39:SER:O	1:B:43:SER:HB2	2.18	0.43
1:D:63:SER:OG	1:D:66:GLU:HG3	2.19	0.43
1:A:20:TYR:CG	1:A:21:SER:N	2.86	0.43
1:C:353:ARG:HD3	1:D:205:PRO:O	2.19	0.42
1:B:192:THR:HG22	1:B:194:LYS:N	2.24	0.42
1:A:19:ILE:CG2	1:A:59:PRO:HB3	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:337:PHE:O	1:C:344:TYR:HE1	2.03	0.42
1:A:145:LYS:NZ	6:A:924:HOH:O	2.53	0.42
1:A:84:GLN:HA	1:A:84:GLN:HE21	1.84	0.42
1:B:88:ASP:HA	6:B:834:HOH:O	2.19	0.42
1:B:19:ILE:CG2	1:B:59:PRO:HB3	2.49	0.42
1:A:273:PRO:HB2	5:J:6:MCM:H9	2.02	0.42
1:D:60:LYS:O	1:D:117:GLY:HA3	2.20	0.42
1:B:164:ARG:HD2	1:B:167:ARG:HD2	2.02	0.42
1:C:156:ASN:OD1	1:C:159:VAL:HG23	2.20	0.41
1:B:169:PHE:HB2	1:B:172:ILE:HD11	2.03	0.41
1:D:152:PHE:CD2	1:D:152:PHE:N	2.89	0.41
1:A:63:SER:OG	1:A:66:GLU:HG3	2.21	0.41
1:A:171:ARG:NH1	1:A:256:ASN:HB3	2.36	0.41
1:C:122:ALA:HB1	1:C:299:LEU:HD13	2.03	0.41
1:B:152:PHE:CD2	1:B:152:PHE:N	2.88	0.41
1:A:152:PHE:N	1:A:152:PHE:CD2	2.88	0.40
1:A:84:GLN:CA	1:A:84:GLN:HE21	2.33	0.40

There are no symmetry-related clashes.

## 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	362/388 (93%)	350 (97%)	12 (3%)	0	100	100
1	B	362/388 (93%)	351 (97%)	11 (3%)	0	100	100
1	C	362/388 (93%)	348 (96%)	13 (4%)	1 (0%)	46	68
1	D	362/388 (93%)	349 (96%)	13 (4%)	0	100	100
2	I	2/5 (40%)	2 (100%)	0	0	100	100
2	J	2/5 (40%)	2 (100%)	0	0	100	100
2	K	2/5 (40%)	2 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	2/5 (40%)	2 (100%)	0	0	100	100
All	All	1456/1572 (93%)	1406 (97%)	49 (3%)	1 (0%)	56	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	344	TYR

### 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	304/325 (94%)	298 (98%)	6 (2%)	63	86
1	B	304/325 (94%)	297 (98%)	7 (2%)	58	83
1	C	304/325 (94%)	298 (98%)	6 (2%)	63	86
1	D	304/325 (94%)	299 (98%)	5 (2%)	70	90
2	I	2/2 (100%)	2 (100%)	0	100	100
2	J	2/2 (100%)	2 (100%)	0	100	100
2	K	2/2 (100%)	2 (100%)	0	100	100
2	L	2/2 (100%)	2 (100%)	0	100	100
All	All	1224/1308 (94%)	1200 (98%)	24 (2%)	63	86

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	LEU
1	A	79	LEU
1	A	106	GLU
1	A	126	LEU
1	A	142	HIS
1	A	187	ASP
1	B	65	GLU

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Mol	Chain	Res	Type
1	B	79	LEU
1	B	106	GLU
1	B	126	LEU
1	B	142	HIS
1	B	164	ARG
1	B	187	ASP
1	C	79	LEU
1	C	106	GLU
1	C	126	LEU
1	C	142	HIS
1	C	187	ASP
1	C	356	ARG
1	D	79	LEU
1	D	106	GLU
1	D	126	LEU
1	D	142	HIS
1	D	187	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	84	GLN
1	A	90	HIS
1	A	242	GLN
1	A	256	ASN
1	B	84	GLN
1	B	90	HIS
1	B	256	ASN
1	C	84	GLN
1	C	90	HIS
1	C	256	ASN
1	D	84	GLN
1	D	90	HIS
1	D	256	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

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$
2	ALY	I	4	2	10,11,12	0.35	0	10,12,14	0.97	1 (10%)
2	ALY	I	5	3,2,5	10,11,12	0.40	0	10,12,14	0.81	0
2	ALY	J	4	2	10,11,12	0.40	0	10,12,14	0.83	1 (10%)
2	ALY	J	5	3,2,5	10,11,12	0.38	0	10,12,14	0.80	0
2	ALY	K	4	2	10,11,12	0.42	0	10,12,14	0.99	1 (10%)
2	ALY	K	5	3,2,5	10,11,12	0.43	0	10,12,14	0.87	0
2	ALY	L	4	2	10,11,12	0.37	0	10,12,14	0.95	1 (10%)
2	ALY	L	5	3,2,5	10,11,12	0.43	0	10,12,14	0.78	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
2	ALY	I	4	2	-	0/8/10/12	0/0/0/0
2	ALY	I	5	3,2,5	-	0/8/10/12	0/0/0/0
2	ALY	J	4	2	-	0/8/10/12	0/0/0/0
2	ALY	J	5	3,2,5	-	0/8/10/12	0/0/0/0
2	ALY	K	4	2	-	0/8/10/12	0/0/0/0
2	ALY	K	5	3,2,5	-	0/8/10/12	0/0/0/0
2	ALY	L	4	2	-	0/8/10/12	0/0/0/0
2	ALY	L	5	3,2,5	-	0/8/10/12	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	4	ALY	O-C-CA	-2.28	119.55	125.49
2	J	4	ALY	O-C-CA	-2.10	120.01	125.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	4	ALY	O-C-CA	-2.08	120.07	125.49
2	L	4	ALY	O-C-CA	-2.02	120.24	125.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	K	4	ALY	2	0
2	L	5	ALY	1	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 18 ligands modelled in this entry, 14 are monoatomic - leaving 4 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	MCM	I	6	2	13,14,14	2.57	5 (38%)	13,20,20	1.60	3 (23%)
5	MCM	J	6	2	13,14,14	2.62	5 (38%)	13,20,20	1.52	4 (30%)
5	MCM	K	6	2	13,14,14	2.55	4 (30%)	13,20,20	1.61	3 (23%)
5	MCM	L	6	2	13,14,14	2.62	4 (30%)	13,20,20	1.57	4 (30%)

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	MCM	I	6	2	-	0/0/0/0	0/2/2/2
5	MCM	J	6	2	-	0/0/0/0	0/2/2/2
5	MCM	K	6	2	-	0/0/0/0	0/2/2/2
5	MCM	L	6	2	-	0/0/0/0	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	6	MCM	C2-C3	2.15	1.42	1.37
5	I	6	MCM	C2-C3	2.31	1.42	1.37
5	J	6	MCM	C8-C9	2.47	1.41	1.36
5	L	6	MCM	C8-C9	2.54	1.41	1.36
5	K	6	MCM	C8-C9	2.56	1.42	1.36
5	I	6	MCM	C8-C9	2.57	1.42	1.36
5	K	6	MCM	C7-C3	2.87	1.45	1.41
5	I	6	MCM	C7-C3	3.22	1.45	1.41
5	L	6	MCM	C7-C3	3.27	1.45	1.41
5	J	6	MCM	C7-C3	3.36	1.45	1.41
5	J	6	MCM	C6-C7	3.57	1.49	1.42
5	I	6	MCM	C6-C7	3.72	1.50	1.42
5	L	6	MCM	C6-C7	3.86	1.50	1.42
5	K	6	MCM	C6-C7	4.13	1.50	1.42
5	I	6	MCM	C5-C4	6.29	1.50	1.37
5	K	6	MCM	C5-C4	6.42	1.50	1.37
5	J	6	MCM	C5-C4	6.72	1.51	1.37
5	L	6	MCM	C5-C4	6.74	1.51	1.37

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	6	MCM	C4-O1-C3	-3.19	118.25	122.37
5	L	6	MCM	C4-O1-C3	-3.17	118.28	122.37
5	K	6	MCM	C4-O1-C3	-3.11	118.35	122.37
5	J	6	MCM	C4-O1-C3	-3.10	118.36	122.37
5	I	6	MCM	C9-CA-N	-2.79	115.29	120.90
5	K	6	MCM	C9-CA-N	-2.42	116.05	120.90
5	J	6	MCM	C9-CA-N	-2.39	116.10	120.90
5	L	6	MCM	C9-CA-N	-2.39	116.10	120.90
5	L	6	MCM	O1-C3-C7	2.06	123.39	121.21
5	J	6	MCM	O1-C3-C7	2.06	123.39	121.21
5	J	6	MCM	O1-C4-C5	2.21	121.88	119.40
5	L	6	MCM	O1-C4-C5	2.38	122.07	119.40
5	I	6	MCM	O1-C4-C5	2.46	122.16	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	K	6	MCM	O1-C4-C5	2.72	122.45	119.40

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	I	6	MCM	1	0
5	J	6	MCM	2	0
5	K	6	MCM	2	0
5	L	6	MCM	2	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, 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	364/388 (93%)	-0.08	4 (1%) 82 84	14, 27, 45, 64	5 (1%)
1	B	364/388 (93%)	-0.13	2 (0%) 91 92	14, 27, 45, 64	3 (0%)
1	C	364/388 (93%)	0.02	4 (1%) 82 84	14, 29, 46, 64	5 (1%)
1	D	364/388 (93%)	-0.07	2 (0%) 91 92	16, 29, 46, 63	5 (1%)
2	I	2/5 (40%)	0.34	0 100 100	29, 29, 29, 44	0
2	J	2/5 (40%)	0.59	0 100 100	37, 37, 37, 50	0
2	K	2/5 (40%)	0.33	0 100 100	31, 31, 31, 39	0
2	L	2/5 (40%)	1.30	1 (50%) 0 0	39, 39, 39, 56	0
All	All	1464/1572 (93%)	-0.06	13 (0%) 85 88	14, 28, 46, 64	18 (1%)

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	14	LEU	3.7
1	C	334	HIS	3.2
1	D	377	VAL	3.1
1	A	377	VAL	2.8
1	B	377	VAL	2.4
2	L	2	ARG	2.4
1	C	20	TYR	2.3
1	A	170	GLU	2.2
1	C	377	VAL	2.2
1	A	89	ASP	2.2
1	B	375	HIS	2.1
1	D	360	HIS	2.1
1	C	331	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	ALY	I	4	12/13	0.91	0.23	-	20,35,54,55	0
2	ALY	K	4	12/13	0.90	0.20	-	20,33,49,50	0
2	ALY	L	5	12/13	0.96	0.16	-	20,23,29,30	0
2	ALY	L	4	12/13	0.93	0.18	-	23,31,42,43	0
2	ALY	J	4	12/13	0.94	0.16	-	21,28,33,33	0
2	ALY	I	5	12/13	0.95	0.17	-	13,19,24,25	0
2	ALY	J	5	12/13	0.97	0.15	-	16,19,21,21	0
2	ALY	K	5	12/13	0.94	0.17	-	9,15,19,20	0

## 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
5	MCM	K	6	13/13	0.96	0.16	0.69	18,23,26,30	0
4	K	A	401	1/1	0.99	0.13	-0.15	16,16,16,16	0
5	MCM	I	6	13/13	0.96	0.14	-0.37	17,21,21,24	0
5	MCM	L	6	13/13	0.96	0.12	-0.50	23,25,28,28	0
4	K	B	404	1/1	0.98	0.11	-0.69	21,21,21,21	0
4	K	D	410	1/1	0.98	0.10	-0.87	23,23,23,23	0
5	MCM	J	6	13/13	0.97	0.13	-1.28	16,18,19,21	0
3	ZN	A	400	1/1	1.00	0.11	-1.39	14,14,14,14	0
4	K	C	407	1/1	1.00	0.11	-2.04	20,20,20,20	0
4	K	A	402	1/1	0.99	0.09	-2.06	20,20,20,20	0
4	K	D	411	1/1	0.98	0.07	-2.12	28,28,28,28	0

*Continued on next page...*



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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	C	406	1/1	1.00	0.10	-2.18	16,16,16,16	0
4	K	C	408	1/1	0.98	0.11	-2.22	23,23,23,23	0
3	ZN	B	403	1/1	1.00	0.10	-2.86	14,14,14,14	0
3	ZN	D	409	1/1	1.00	0.07	-3.26	17,17,17,17	0
4	K	B	405	1/1	0.98	0.04	-3.58	24,24,24,24	0
3	ZN	C	412	1/1	0.98	0.12	-	46,46,46,46	0
3	ZN	A	413	1/1	0.98	0.05	-	49,49,49,49	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.