



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:28 PM GMT

PDB ID : 4CBY  
Title : Design, synthesis, and biological evaluation of potent and selective Class IIa HDAC inhibitors as a potential therapy for Huntingtons disease  
Authors : Burli, R.W.; Luckhurst, C.A.; Aziz, O.; Matthews, K.L.; Yates, D.; Lyons, K.A.; Beconi, M.; McAllister, G.; Breccia, P.; Stott, A.J.; Penrose, S.D.; Wall, M.; Lamers, M.; Leonard, P.; Mueller, I.; Richardson, C.M.; Jarvis, R.; Stones, L.; Hughes, S.; Wishart, G.; Haughan, A.F.; OConnell, C.; Mead, T.; McNeil, H.; Vann, J.; Mangette, J.; Maillard, M.; Beaumont, V.; Munoz-Sanjuan, I.; Dominguez, C.  
Deposited on : 2013-10-17  
Resolution : 2.72 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

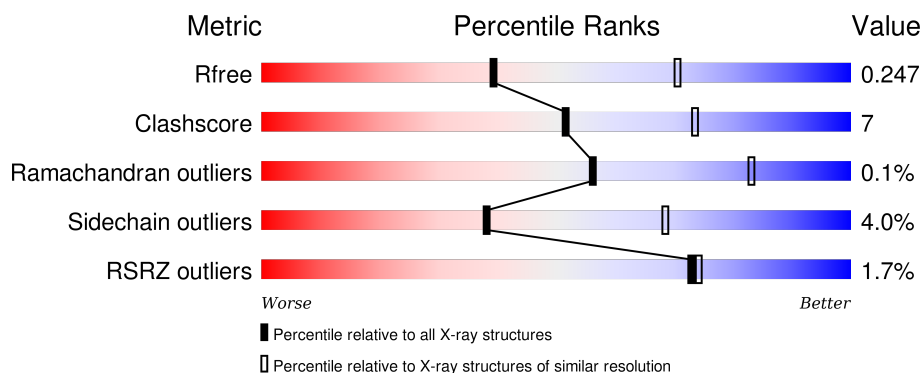
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.72 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	2439 (2.74-2.70)
Clashscore	102246	2771 (2.74-2.70)
Ramachandran outliers	100387	2726 (2.74-2.70)
Sidechain outliers	100360	2727 (2.74-2.70)
RSRZ outliers	91569	2443 (2.74-2.70)

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	395	 2% 82% 13% . .
1	B	395	 % 84% 12% . .
1	C	395	 2% 81% 15% . .
1	D	395	 3% 85% 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
4	NA	B	2035	-	-	-	X

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 11435 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 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	380	Total	C	N	O	S	0	0	0
			2823	1782	494	527	20			
1	B	380	Total	C	N	O	S	0	0	0
			2795	1767	483	525	20			
1	C	380	Total	C	N	O	S	0	0	0
			2802	1764	488	530	20			
1	D	383	Total	C	N	O	S	0	0	0
			2812	1772	492	528	20			

There are 40 discrepancies between the modelled and reference sequences:

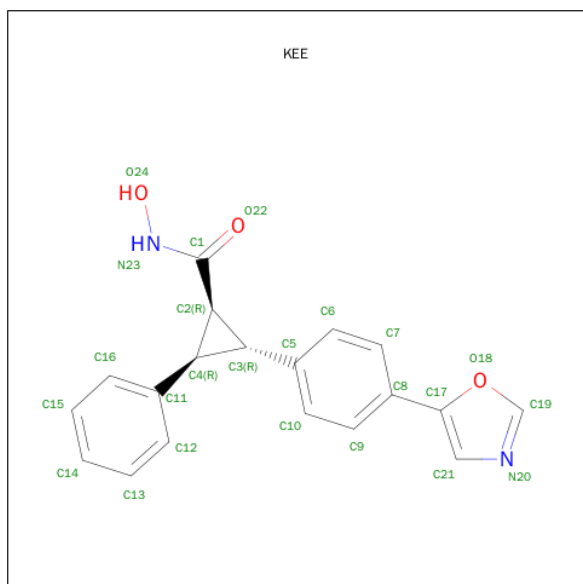
Chain	Residue	Modelled	Actual	Comment	Reference
A	645	MET	-	EXPRESSION TAG	UNP P56524
A	646	GLY	-	EXPRESSION TAG	UNP P56524
A	647	SER	-	EXPRESSION TAG	UNP P56524
A	728	ALA	LEU	ENGINEERED MUTATION	UNP P56524
A	1034	HIS	-	EXPRESSION TAG	UNP P56524
A	1035	HIS	-	EXPRESSION TAG	UNP P56524
A	1036	HIS	-	EXPRESSION TAG	UNP P56524
A	1037	HIS	-	EXPRESSION TAG	UNP P56524
A	1038	HIS	-	EXPRESSION TAG	UNP P56524
A	1039	HIS	-	EXPRESSION TAG	UNP P56524
B	645	MET	-	EXPRESSION TAG	UNP P56524
B	646	GLY	-	EXPRESSION TAG	UNP P56524
B	647	SER	-	EXPRESSION TAG	UNP P56524
B	728	ALA	LEU	ENGINEERED MUTATION	UNP P56524
B	1034	HIS	-	EXPRESSION TAG	UNP P56524
B	1035	HIS	-	EXPRESSION TAG	UNP P56524
B	1036	HIS	-	EXPRESSION TAG	UNP P56524
B	1037	HIS	-	EXPRESSION TAG	UNP P56524
B	1038	HIS	-	EXPRESSION TAG	UNP P56524
B	1039	HIS	-	EXPRESSION TAG	UNP P56524
C	645	MET	-	EXPRESSION TAG	UNP P56524

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Chain	Residue	Modelled	Actual	Comment	Reference
C	646	GLY	-	EXPRESSION TAG	UNP P56524
C	647	SER	-	EXPRESSION TAG	UNP P56524
C	728	ALA	LEU	ENGINEERED MUTATION	UNP P56524
C	1034	HIS	-	EXPRESSION TAG	UNP P56524
C	1035	HIS	-	EXPRESSION TAG	UNP P56524
C	1036	HIS	-	EXPRESSION TAG	UNP P56524
C	1037	HIS	-	EXPRESSION TAG	UNP P56524
C	1038	HIS	-	EXPRESSION TAG	UNP P56524
C	1039	HIS	-	EXPRESSION TAG	UNP P56524
D	645	MET	-	EXPRESSION TAG	UNP P56524
D	646	GLY	-	EXPRESSION TAG	UNP P56524
D	647	SER	-	EXPRESSION TAG	UNP P56524
D	728	ALA	LEU	ENGINEERED MUTATION	UNP P56524
D	1034	HIS	-	EXPRESSION TAG	UNP P56524
D	1035	HIS	-	EXPRESSION TAG	UNP P56524
D	1036	HIS	-	EXPRESSION TAG	UNP P56524
D	1037	HIS	-	EXPRESSION TAG	UNP P56524
D	1038	HIS	-	EXPRESSION TAG	UNP P56524
D	1039	HIS	-	EXPRESSION TAG	UNP P56524

- Molecule 2 is (1R,2R,3R)-2-[4-(1,3-OXAZOL-5-YL)PHENYL]-N-OXIDANYL-3-PHENYL-CYCLOPROPANE-1-CARBOXAMIDE (three-letter code: KEE) (formula: C<sub>19</sub>H<sub>16</sub>N<sub>2</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			24	19	2	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			24	19	2	3		
2	C	1	Total	C	N	O	0	0
			24	19	2	3		
2	D	1	Total	C	N	O	0	0
			24	19	2	3		

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

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

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

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

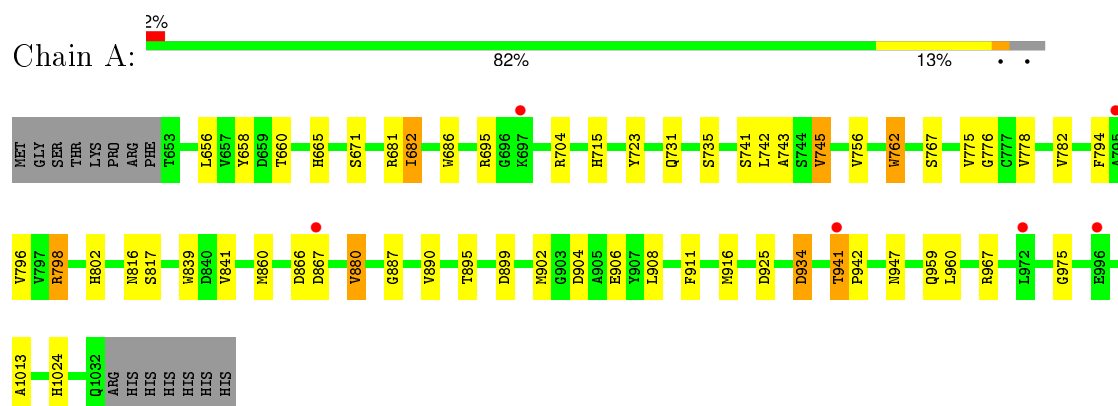
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	22	Total	O	0	0
			22	22		
5	B	23	Total	O	0	0
			23	23		
5	C	24	Total	O	0	0
			24	24		
5	D	22	Total	O	0	0
			22	22		

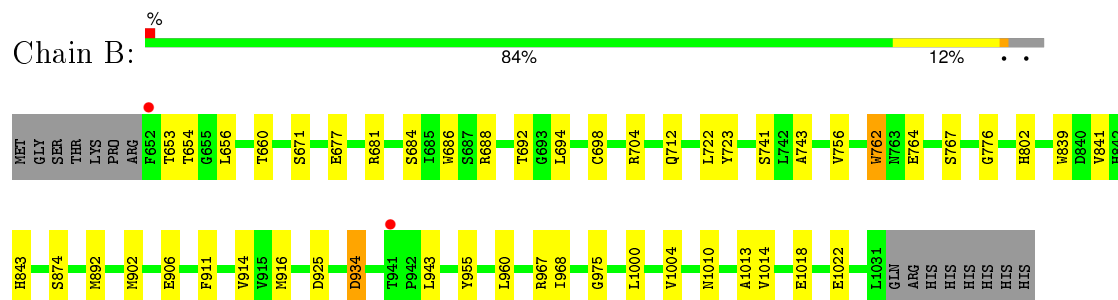
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

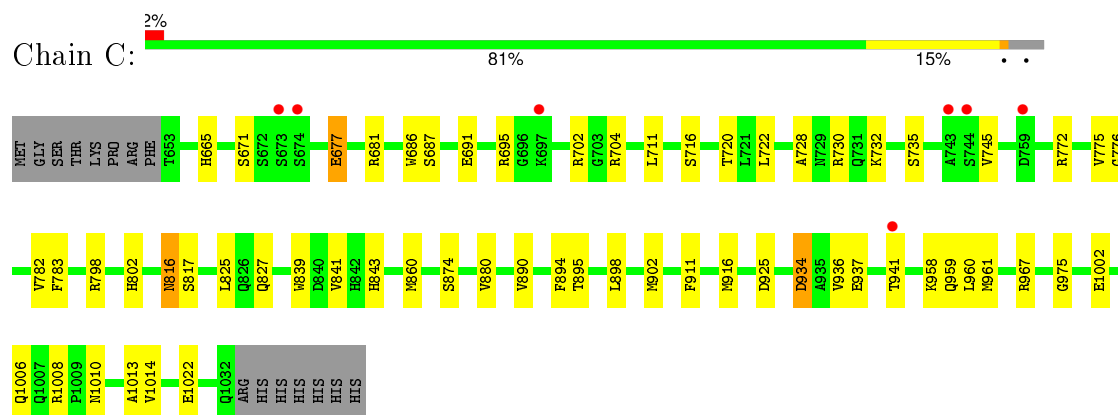
#### • Molecule 1: HISTONE DEACETYLASE 4



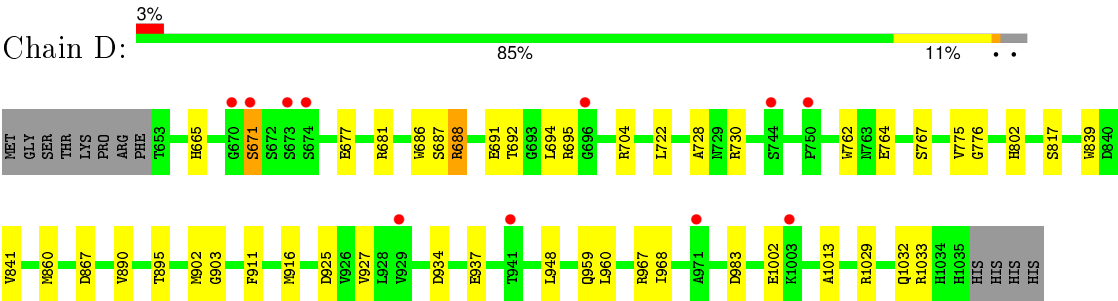
#### • Molecule 1: HISTONE DEACETYLASE 4



#### • Molecule 1: HISTONE DEACETYLASE 4



#### • Molecule 1: HISTONE DEACETYLASE 4





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.15Å 161.82Å 83.73Å 90.00° 97.03° 90.00°	Depositor
Resolution (Å)	83.10 – 2.72 29.37 – 2.72	Depositor EDS
% Data completeness (in resolution range)	98.3 (83.10-2.72) 98.5 (29.37-2.72)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 2.72Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, $R_{free}$	0.209 , 0.246 0.212 , 0.247	Depositor DCC
$R_{free}$ test set	1886 reflections (5.27%)	DCC
Wilson B-factor (Å <sup>2</sup> )	37.7	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 38.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	2 of 37669 reflections (0.005%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	11435	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 37.36 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 4.3423e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NA, ZN, KEE

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	0.58	1/2887 (0.0%)	0.68	2/3924 (0.1%)
1	B	0.60	3/2860 (0.1%)	0.65	0/3894
1	C	0.58	1/2865 (0.0%)	0.68	0/3899
1	D	0.57	0/2876	0.70	3/3912 (0.1%)
All	All	0.58	5/11488 (0.0%)	0.68	5/15629 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	712	GLN	CD-NE2	-5.42	1.19	1.32
1	C	816	ASN	CG-OD1	5.21	1.35	1.24
1	B	686	TRP	CD2-CE2	5.15	1.47	1.41
1	B	762	TRP	CD2-CE2	5.09	1.47	1.41
1	A	762	TRP	CD2-CE2	5.03	1.47	1.41

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	688	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	D	688	ARG	NE-CZ-NH2	-7.80	116.40	120.30
1	D	681	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	682	ILE	CB-CA-C	-5.32	100.96	111.60
1	A	798	ARG	NE-CZ-NH2	-5.25	117.67	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	2823	0	2753	44	0
1	B	2795	0	2683	42	0
1	C	2802	0	2693	38	0
1	D	2812	0	2701	35	0
2	A	24	0	13	0	0
2	B	24	0	12	0	0
2	C	24	0	13	0	0
2	D	24	0	13	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	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	A	22	0	0	1	0
5	B	23	0	0	2	0
5	C	24	0	0	1	0
5	D	22	0	0	4	0
All	All	11435	0	10881	152	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 7.

All (152) 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:688:ARG:NH2	1:D:983:ASP:OD1	1.96	0.98
1:D:937:GLU:CB	5:D:2017:HOH:O	2.16	0.94
1:D:902:MET:HE3	1:D:1013:ALA:HB2	1.46	0.94
1:A:682:ILE:HG23	1:A:796:VAL:HG12	1.52	0.92
1:B:968:ILE:HB	5:B:2019:HOH:O	1.76	0.86
1:A:916:MET:HE3	1:A:959:GLN:HB3	1.59	0.84
1:B:916:MET:CE	1:B:960:LEU:HD23	2.08	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:916:MET:HE1	1:B:960:LEU:HD23	1.62	0.81
1:C:902:MET:HE3	1:C:1013:ALA:HB2	1.63	0.80
1:B:660:THR:CG2	1:D:867:ASP:HB3	2.11	0.80
1:A:902:MET:HE3	1:A:1013:ALA:HB2	1.63	0.79
1:A:682:ILE:CG2	1:A:796:VAL:HG12	2.13	0.78
1:A:715:HIS:HE1	1:A:816:ASN:H	1.28	0.78
1:A:682:ILE:HD11	1:A:798:ARG:HB2	1.66	0.78
1:B:955:TYR:CE1	1:B:1000:LEU:HD12	2.19	0.78
1:C:665:HIS:O	1:C:798:ARG:NH2	2.17	0.77
1:B:902:MET:HE3	1:B:1013:ALA:HB2	1.65	0.77
1:A:902:MET:HE3	1:A:906:GLU:HG2	1.65	0.77
1:C:677:GLU:OE2	1:C:798:ARG:NH1	2.18	0.76
1:A:941:THR:HG23	1:A:942:PRO:HD3	1.67	0.75
1:A:860:MET:HE2	1:A:890:VAL:HG11	1.67	0.74
1:A:916:MET:CE	1:A:960:LEU:HD23	2.18	0.73
1:B:660:THR:HG21	1:D:867:ASP:HB3	1.69	0.72
1:C:958:LYS:HA	1:C:961:MET:HE2	1.73	0.70
1:B:955:TYR:CE1	1:B:1000:LEU:CD1	2.75	0.69
1:B:902:MET:HE3	1:B:906:GLU:HG2	1.73	0.68
1:A:916:MET:HE1	1:A:960:LEU:HD23	1.76	0.67
1:D:916:MET:CE	1:D:960:LEU:HD23	2.25	0.66
1:D:916:MET:HE1	1:D:960:LEU:HD23	1.76	0.66
1:D:902:MET:HE3	1:D:1013:ALA:CB	2.25	0.65
1:A:880:VAL:HG22	1:A:1024:HIS:CE1	2.32	0.65
1:B:741:SER:OG	1:B:743:ALA:HB3	1.97	0.64
1:C:916:MET:CE	1:C:960:LEU:HD23	2.29	0.62
1:B:892:MET:CE	1:B:914:VAL:HG11	2.29	0.61
1:B:955:TYR:CZ	1:B:1000:LEU:CD1	2.83	0.61
1:A:904:ASP:O	1:A:908:LEU:HD12	2.01	0.61
1:B:916:MET:HE2	1:B:960:LEU:HD23	1.82	0.59
1:B:660:THR:HG21	1:D:867:ASP:CB	2.31	0.59
1:C:843:HIS:HD2	1:C:874:SER:OG	1.84	0.59
1:A:916:MET:HE1	1:A:960:LEU:HA	1.84	0.59
1:C:916:MET:HE1	1:C:960:LEU:HD23	1.85	0.58
1:D:860:MET:CE	1:D:890:VAL:HG11	2.34	0.57
1:A:916:MET:HE2	1:A:960:LEU:HD23	1.85	0.57
1:B:902:MET:CE	1:B:1013:ALA:HB2	2.34	0.57
1:C:677:GLU:CD	1:C:798:ARG:NH1	2.57	0.57
1:A:902:MET:HE3	1:A:906:GLU:CG	2.33	0.56
1:A:742:LEU:HA	1:A:745:VAL:HG13	1.88	0.56
1:B:660:THR:CG2	1:D:867:ASP:CB	2.83	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:902:MET:CE	1:A:1013:ALA:HB2	2.35	0.56
1:C:1010:ASN:O	1:C:1014:VAL:HG23	2.05	0.56
1:A:665:HIS:HD2	1:A:767:SER:OG	1.88	0.56
1:A:841:VAL:HG12	1:A:934:ASP:CG	2.25	0.56
1:A:682:ILE:N	1:A:682:ILE:HD13	2.21	0.55
1:A:941:THR:CG2	1:A:942:PRO:HD3	2.36	0.55
1:C:860:MET:HE3	1:C:890:VAL:HG11	1.88	0.55
1:B:843:HIS:HD2	1:B:874:SER:OG	1.90	0.55
1:A:860:MET:HE2	1:A:890:VAL:CG1	2.37	0.55
1:B:892:MET:CE	1:B:914:VAL:HG21	2.37	0.54
5:B:2006:HOH:O	1:C:1008:ARG:HD3	2.07	0.54
1:C:860:MET:CE	1:C:890:VAL:HG11	2.38	0.54
1:D:665:HIS:HD2	1:D:767:SER:OG	1.89	0.54
1:B:841:VAL:HG12	1:B:934:ASP:CG	2.27	0.54
1:C:898:LEU:HD11	1:C:941:THR:HG23	1.88	0.54
1:B:955:TYR:CZ	1:B:1000:LEU:HD12	2.42	0.54
1:B:943:LEU:O	1:B:943:LEU:HD23	2.07	0.54
1:C:860:MET:HE3	1:C:890:VAL:CG1	2.38	0.53
1:B:653:THR:OG1	1:B:654:THR:N	2.38	0.53
1:D:692:THR:HG23	1:D:694:LEU:H	1.75	0.52
1:C:916:MET:HE1	1:C:960:LEU:HA	1.92	0.52
1:B:692:THR:HG23	1:B:694:LEU:H	1.75	0.51
1:A:741:SER:OG	1:A:743:ALA:HB3	2.11	0.51
1:A:794:PHE:CE2	1:A:796:VAL:HG22	2.46	0.51
1:B:660:THR:HG23	1:D:867:ASP:HB3	1.92	0.50
1:D:916:MET:HE1	1:D:960:LEU:HA	1.93	0.50
1:D:1002:GLU:CB	5:D:2019:HOH:O	2.59	0.50
1:B:902:MET:HE3	1:B:906:GLU:CG	2.40	0.49
1:B:660:THR:HG21	1:D:867:ASP:CG	2.32	0.49
1:B:892:MET:HE1	1:B:914:VAL:HG11	1.93	0.49
1:B:892:MET:HE1	1:B:914:VAL:HG21	1.93	0.49
1:B:1010:ASN:O	1:B:1014:VAL:HG23	2.13	0.49
1:C:681:ARG:NH1	1:C:975:GLY:O	2.41	0.49
1:D:775:VAL:HG22	1:D:817:SER:HA	1.95	0.49
1:B:1018:GLU:O	1:B:1022:GLU:HG3	2.13	0.48
1:A:681:ARG:NH1	1:A:975:GLY:O	2.44	0.48
1:A:860:MET:HE3	1:A:890:VAL:HG21	1.94	0.48
1:B:684:SER:HB3	1:C:1008:ARG:HD2	1.96	0.48
1:B:723:TYR:OH	1:B:756:VAL:HG11	2.13	0.48
1:B:681:ARG:NH1	1:B:975:GLY:O	2.44	0.47
1:D:687:SER:O	1:D:691:GLU:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:778:VAL:O	1:A:782:VAL:HG23	2.14	0.47
1:C:775:VAL:HG22	1:C:817:SER:HA	1.95	0.47
1:A:775:VAL:HG22	1:A:817:SER:HA	1.96	0.47
1:A:723:TYR:OH	1:A:756:VAL:HG11	2.15	0.47
1:C:936:VAL:CG1	1:C:937:GLU:N	2.78	0.47
1:C:841:VAL:HG12	1:C:934:ASP:CG	2.35	0.46
1:C:687:SER:O	1:C:691:GLU:HG3	2.15	0.46
1:C:916:MET:HE2	1:C:960:LEU:HD23	1.96	0.46
1:D:860:MET:HE3	1:D:890:VAL:HG11	1.96	0.46
1:C:686:TRP:CZ2	1:C:695:ARG:HD2	2.51	0.46
1:C:677:GLU:CD	1:C:798:ARG:HH11	2.19	0.46
1:C:902:MET:HE3	1:C:1013:ALA:CB	2.38	0.46
1:A:715:HIS:CE1	1:A:816:ASN:H	2.19	0.46
1:B:688:ARG:O	1:B:692:THR:HG22	2.16	0.45
1:A:660:THR:HG21	5:A:2001:HOH:O	2.16	0.45
1:C:716:SER:O	1:C:720:THR:HG23	2.17	0.45
1:C:936:VAL:HG12	1:C:937:GLU:N	2.31	0.45
1:D:860:MET:HE2	1:D:890:VAL:CG1	2.47	0.45
1:B:892:MET:HE2	1:B:914:VAL:HG11	1.99	0.45
1:D:860:MET:HE2	1:D:890:VAL:HG11	1.99	0.44
1:D:927:VAL:HG13	1:D:968:ILE:HA	2.00	0.44
1:C:925:ASP:O	1:C:967:ARG:NH1	2.50	0.44
1:D:925:ASP:O	1:D:967:ARG:NH1	2.51	0.44
1:A:902:MET:CE	1:A:906:GLU:HG2	2.43	0.44
1:A:686:TRP:CZ2	1:A:695:ARG:HD2	2.53	0.44
1:A:925:ASP:O	1:A:967:ARG:NH1	2.50	0.44
1:A:665:HIS:CD2	1:A:767:SER:OG	2.71	0.44
1:D:722:LEU:O	1:D:730:ARG:NH1	2.51	0.44
1:D:903:GLY:HA2	1:D:948:LEU:HD12	2.00	0.43
1:D:686:TRP:CZ2	1:D:695:ARG:HD2	2.53	0.43
1:B:925:ASP:O	1:B:967:ARG:NH1	2.51	0.43
1:A:658:TYR:CE1	1:A:682:ILE:HG22	2.53	0.43
1:D:916:MET:HE2	1:D:960:LEU:HD23	1.98	0.43
1:B:955:TYR:CZ	1:B:1000:LEU:HD13	2.53	0.43
1:A:880:VAL:HG13	1:A:887:GLY:H	1.83	0.43
1:B:656:LEU:HD12	1:B:698:CYS:HB2	2.00	0.43
1:D:916:MET:HE3	1:D:959:GLN:HB3	2.01	0.43
1:B:892:MET:CE	1:B:914:VAL:CB	2.96	0.43
1:D:692:THR:HG21	1:D:694:LEU:HD12	2.01	0.43
1:C:704:ARG:O	1:C:776:GLY:HA3	2.19	0.43
1:A:658:TYR:HE1	1:A:682:ILE:CG2	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:711:LEU:HD11	1:C:772:ARG:HG2	2.01	0.42
1:D:704:ARG:O	1:D:776:GLY:HA3	2.19	0.42
1:D:841:VAL:HA	5:D:2012:HOH:O	2.20	0.42
1:C:722:LEU:O	1:C:730:ARG:NH1	2.53	0.42
1:C:843:HIS:CD2	1:C:874:SER:OG	2.67	0.42
1:A:704:ARG:O	1:A:776:GLY:HA3	2.19	0.42
1:B:762:TRP:CZ3	1:B:767:SER:HB3	2.55	0.42
1:C:783:PHE:CE1	1:C:825:LEU:HD23	2.55	0.42
1:A:656:LEU:HD23	1:A:794:PHE:HB3	2.00	0.41
1:D:728:ALA:HB3	5:D:2006:HOH:O	2.20	0.41
1:C:782:VAL:CG1	1:C:825:LEU:HD11	2.50	0.41
1:D:1029:ARG:O	1:D:1032:GLN:HG3	2.19	0.41
1:B:704:ARG:O	1:B:776:GLY:HA3	2.21	0.41
1:A:762:TRP:CZ3	1:A:767:SER:HB3	2.56	0.41
1:A:866:ASP:O	1:A:867:ASP:CB	2.65	0.41
1:C:728:ALA:HB3	5:C:2010:HOH:O	2.19	0.41
1:A:866:ASP:O	1:A:867:ASP:HB3	2.21	0.41
1:C:894:PHE:CD1	1:C:902:MET:CE	3.04	0.40
1:D:762:TRP:CZ3	1:D:767:SER:HB3	2.57	0.40
1:C:894:PHE:CD1	1:C:902:MET:HE1	2.57	0.40
1:C:916:MET:HE3	1:C:959:GLN:HB3	2.03	0.40
1:B:892:MET:CE	1:B:914:VAL:CG1	2.99	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	378/395 (96%)	363 (96%)	15 (4%)	0	100	100
1	B	378/395 (96%)	361 (96%)	17 (4%)	0	100	100
1	C	378/395 (96%)	364 (96%)	13 (3%)	1 (0%)	46	74

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	381/395 (96%)	365 (96%)	15 (4%)	1 (0%)	46 74
All	All	1515/1580 (96%)	1453 (96%)	60 (4%)	2 (0%)	56 83

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	671	SER
1	D	671	SER

### 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	297/321 (92%)	284 (96%)	13 (4%)	35 64
1	B	290/321 (90%)	281 (97%)	9 (3%)	47 77
1	C	292/321 (91%)	276 (94%)	16 (6%)	27 54
1	D	291/321 (91%)	282 (97%)	9 (3%)	47 77
All	All	1170/1284 (91%)	1123 (96%)	47 (4%)	38 68

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	671	SER
1	A	731	GLN
1	A	735	SER
1	A	745	VAL
1	A	802	HIS
1	A	839	TRP
1	A	880	VAL
1	A	895	THR
1	A	899	ASP
1	A	911	PHE
1	A	934	ASP
1	A	941	THR

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Mol	Chain	Res	Type
1	A	947	ASN
1	B	671	SER
1	B	677	GLU
1	B	722	LEU
1	B	764	GLU
1	B	802	HIS
1	B	839	TRP
1	B	911	PHE
1	B	934	ASP
1	B	1004	VAL
1	C	677	GLU
1	C	702	ARG
1	C	732	LYS
1	C	735	SER
1	C	745	VAL
1	C	802	HIS
1	C	816	ASN
1	C	827	GLN
1	C	839	TRP
1	C	880	VAL
1	C	895	THR
1	C	911	PHE
1	C	934	ASP
1	C	1002	GLU
1	C	1006	GLN
1	C	1022	GLU
1	D	671	SER
1	D	677	GLU
1	D	764	GLU
1	D	802	HIS
1	D	839	TRP
1	D	895	THR
1	D	911	PHE
1	D	934	ASP
1	D	1033	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	665	HIS
1	A	678	HIS
1	A	712	GLN

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Mol	Chain	Res	Type
1	A	715	HIS
1	A	729	ASN
1	A	869	ASN
1	A	947	ASN
1	A	1012	ASN
1	A	1024	HIS
1	B	666	GLN
1	B	712	GLN
1	B	729	ASN
1	B	843	HIS
1	B	995	ASN
1	C	678	HIS
1	C	731	GLN
1	C	816	ASN
1	C	827	GLN
1	C	843	HIS
1	C	995	ASN
1	D	665	HIS
1	D	666	GLN
1	D	683	GLN
1	D	729	ASN
1	D	731	GLN
1	D	766	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

### 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 5.6 Ligand geometry [i](#)

Of 20 ligands modelled in this entry, 16 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
2	KEE	A	2033	3	23,27,27	0.93	1 (4%)	28,38,38	1.83	7 (25%)
2	KEE	B	2032	3	23,27,27	1.17	1 (4%)	28,38,38	1.12	3 (10%)
2	KEE	C	2033	3	23,27,27	1.02	2 (8%)	28,38,38	1.35	3 (10%)
2	KEE	D	2036	3	23,27,27	0.82	0	28,38,38	1.50	3 (10%)

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	KEE	A	2033	3	-	0/16/27/27	0/2/4/4
2	KEE	B	2032	3	-	0/16/27/27	0/2/4/4
2	KEE	C	2033	3	-	0/16/27/27	0/2/4/4
2	KEE	D	2036	3	-	0/16/27/27	0/2/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2033	KEE	C8-C17	2.12	1.48	1.46
2	C	2033	KEE	C2-C3	2.31	1.55	1.52
2	A	2033	KEE	C8-C17	2.62	1.49	1.46
2	B	2032	KEE	C8-C17	3.52	1.50	1.46

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2033	KEE	C5-C3-C2	-4.57	112.38	122.07
2	D	2036	KEE	C5-C3-C2	-4.24	113.08	122.07
2	A	2033	KEE	C7-C8-C17	-3.97	116.61	120.45
2	D	2036	KEE	C11-C4-C3	-3.61	113.45	122.00
2	A	2033	KEE	C11-C4-C3	-3.50	113.69	122.00
2	B	2032	KEE	C11-C4-C3	-3.40	113.94	122.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2036	KEE	C9-C8-C17	-2.92	117.63	120.45
2	C	2033	KEE	C5-C3-C2	-2.87	115.99	122.07
2	B	2032	KEE	C5-C3-C2	-2.30	117.20	122.07
2	A	2033	KEE	C2-C1-N23	-2.19	109.62	114.62
2	A	2033	KEE	C6-C5-C3	-2.05	115.76	121.13
2	A	2033	KEE	C21-N20-C19	2.08	108.99	105.71
2	B	2032	KEE	O22-C1-C2	2.15	128.29	122.55
2	C	2033	KEE	C21-N20-C19	2.17	109.14	105.71
2	C	2033	KEE	O24-N23-C1	2.99	124.09	119.86
2	A	2033	KEE	C9-C8-C17	3.44	123.78	120.45

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	380/395 (96%)	-0.06	6 (1%) 74 75	15, 29, 45, 57	0
1	B	380/395 (96%)	-0.10	2 (0%) 91 93	16, 28, 45, 57	0
1	C	380/395 (96%)	-0.06	7 (1%) 71 72	18, 29, 54, 79	0
1	D	383/395 (96%)	0.03	11 (2%) 55 56	20, 31, 55, 78	0
All	All	1523/1580 (96%)	-0.05	26 (1%) 73 74	15, 29, 50, 79	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	673	SER	5.4
1	A	972	LEU	3.5
1	B	941	THR	3.4
1	A	941	THR	2.9
1	D	696	GLY	2.9
1	D	673	SER	2.8
1	D	1003	LYS	2.7
1	C	743	ALA	2.7
1	A	697	LYS	2.6
1	D	674	SER	2.6
1	D	929	VAL	2.5
1	A	795	ALA	2.4
1	D	941	THR	2.4
1	D	744	SER	2.4
1	C	744	SER	2.3
1	A	867	ASP	2.3
1	D	750	PRO	2.3
1	C	697	LYS	2.3
1	A	996	GLU	2.2
1	D	670	GLY	2.1
1	D	971	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	941	THR	2.1
1	C	759	ASP	2.0
1	D	671	SER	2.0
1	C	674	SER	2.0
1	B	652	PHE	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. 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
4	NA	B	2035	1/1	0.75	0.34	4.36	28,28,28,28	0
4	NA	A	2036	1/1	0.79	0.21	0.91	28,28,28,28	0
4	NA	D	2039	1/1	0.89	0.19	0.81	23,23,23,23	0
4	NA	C	2036	1/1	0.84	0.18	0.46	25,25,25,25	0
4	NA	B	2036	1/1	0.90	0.16	0.45	23,23,23,23	0
2	KEE	C	2033	24/24	0.93	0.20	0.40	26,29,37,38	0
4	NA	D	2040	1/1	0.86	0.13	0.05	24,24,24,24	0
2	KEE	B	2032	24/24	0.94	0.17	-0.07	23,26,35,36	0
2	KEE	A	2033	24/24	0.93	0.17	-0.16	24,28,37,38	0
4	NA	C	2037	1/1	0.77	0.13	-0.24	22,22,22,22	0
4	NA	A	2037	1/1	0.91	0.13	-0.30	20,20,20,20	0
2	KEE	D	2036	24/24	0.95	0.16	-0.48	28,33,41,43	0
3	ZN	A	2034	1/1	0.99	0.08	-2.00	19,19,19,19	0
3	ZN	A	2035	1/1	0.99	0.04	-2.22	25,25,25,25	0
3	ZN	C	2035	1/1	0.95	0.04	-2.28	46,46,46,46	0
3	ZN	D	2038	1/1	0.98	0.04	-2.28	45,45,45,45	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	ZN	C	2034	1/1	0.99	0.07	-2.73	25,25,25,25	0
3	ZN	B	2034	1/1	0.99	0.03	-3.84	28,28,28,28	0
3	ZN	D	2037	1/1	0.99	0.06	-4.68	25,25,25,25	0
3	ZN	B	2033	1/1	0.99	0.05	-5.29	23,23,23,23	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.