



wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 1, 2016 – 10:30 AM GMT

PDB ID : 3LY2
Title : Catalytic Domain of Human Phosphodiesterase 4B in Complex with A
Coumarin-Based Inhibitor
Authors : Shiau, A.K.; Coyle, A.R.; Hsien, J.H.; Staszewski, L.M.
Deposited on : 2010-02-26
Resolution : 2.60 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at 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.

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

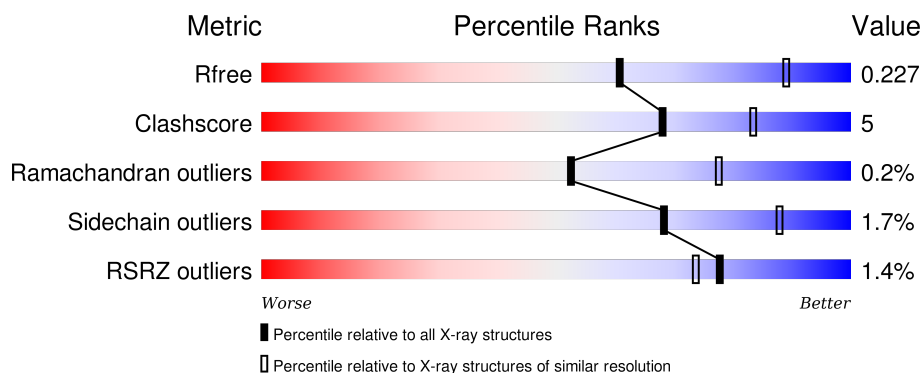
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

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. 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	357	<div> <div></div> <div>82%15%•</div> </div>
1	B	357	<div> <div></div> <div>84%13%•</div> </div>
1	C	357	<div> <div>%</div> <div>81%12%•7%</div> </div>
1	D	357	<div> <div>%</div> <div>80%11%8%</div> </div>
1	E	357	<div> <div>2%</div> <div>81%11%•8%</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	357	
1	G	357	
1	H	357	

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
2	Z72	A	1000	-	-	-	X
2	Z72	B	1000	-	-	-	X
2	Z72	C	1000	-	-	-	X
2	Z72	D	1000	-	-	-	X
2	Z72	F	1000	-	-	-	X
2	Z72	G	1000	-	-	-	X
2	Z72	H	1000	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22265 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 cAMP-specific 3',5'-cyclic phosphodiesterase 4B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	345	Total	C	N	O	S	0	0	0
			2761	1742	470	529	20			
1	B	345	Total	C	N	O	S	0	0	0
			2764	1742	469	533	20			
1	C	332	Total	C	N	O	S	0	0	0
			2671	1684	453	515	19			
1	D	328	Total	C	N	O	S	0	0	0
			2648	1671	448	510	19			
1	E	329	Total	C	N	O	S	0	0	0
			2652	1673	449	511	19			
1	F	329	Total	C	N	O	S	0	0	0
			2655	1675	450	511	19			
1	G	332	Total	C	N	O	S	0	0	0
			2687	1695	456	517	19			
1	H	332	Total	C	N	O	S	0	0	0
			2683	1693	456	515	19			

There are 168 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	131	MET	-	EXPRESSION TAG	UNP Q07343
A	132	GLY	-	EXPRESSION TAG	UNP Q07343
A	133	SER	-	EXPRESSION TAG	UNP Q07343
A	134	SER	-	EXPRESSION TAG	UNP Q07343
A	135	HIS	-	EXPRESSION TAG	UNP Q07343
A	136	HIS	-	EXPRESSION TAG	UNP Q07343
A	137	HIS	-	EXPRESSION TAG	UNP Q07343
A	138	HIS	-	EXPRESSION TAG	UNP Q07343
A	139	HIS	-	EXPRESSION TAG	UNP Q07343
A	140	HIS	-	EXPRESSION TAG	UNP Q07343
A	141	SER	-	EXPRESSION TAG	UNP Q07343
A	142	SER	-	EXPRESSION TAG	UNP Q07343
A	143	GLY	-	EXPRESSION TAG	UNP Q07343

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Chain	Residue	Modelled	Actual	Comment	Reference
A	144	LEU	-	EXPRESSION TAG	UNP Q07343
A	145	VAL	-	EXPRESSION TAG	UNP Q07343
A	146	PRO	-	EXPRESSION TAG	UNP Q07343
A	147	ARG	-	EXPRESSION TAG	UNP Q07343
A	148	GLY	-	EXPRESSION TAG	UNP Q07343
A	149	SER	-	EXPRESSION TAG	UNP Q07343
A	150	HIS	-	EXPRESSION TAG	UNP Q07343
A	151	MET	-	EXPRESSION TAG	UNP Q07343
B	131	MET	-	EXPRESSION TAG	UNP Q07343
B	132	GLY	-	EXPRESSION TAG	UNP Q07343
B	133	SER	-	EXPRESSION TAG	UNP Q07343
B	134	SER	-	EXPRESSION TAG	UNP Q07343
B	135	HIS	-	EXPRESSION TAG	UNP Q07343
B	136	HIS	-	EXPRESSION TAG	UNP Q07343
B	137	HIS	-	EXPRESSION TAG	UNP Q07343
B	138	HIS	-	EXPRESSION TAG	UNP Q07343
B	139	HIS	-	EXPRESSION TAG	UNP Q07343
B	140	HIS	-	EXPRESSION TAG	UNP Q07343
B	141	SER	-	EXPRESSION TAG	UNP Q07343
B	142	SER	-	EXPRESSION TAG	UNP Q07343
B	143	GLY	-	EXPRESSION TAG	UNP Q07343
B	144	LEU	-	EXPRESSION TAG	UNP Q07343
B	145	VAL	-	EXPRESSION TAG	UNP Q07343
B	146	PRO	-	EXPRESSION TAG	UNP Q07343
B	147	ARG	-	EXPRESSION TAG	UNP Q07343
B	148	GLY	-	EXPRESSION TAG	UNP Q07343
B	149	SER	-	EXPRESSION TAG	UNP Q07343
B	150	HIS	-	EXPRESSION TAG	UNP Q07343
B	151	MET	-	EXPRESSION TAG	UNP Q07343
C	131	MET	-	EXPRESSION TAG	UNP Q07343
C	132	GLY	-	EXPRESSION TAG	UNP Q07343
C	133	SER	-	EXPRESSION TAG	UNP Q07343
C	134	SER	-	EXPRESSION TAG	UNP Q07343
C	135	HIS	-	EXPRESSION TAG	UNP Q07343
C	136	HIS	-	EXPRESSION TAG	UNP Q07343
C	137	HIS	-	EXPRESSION TAG	UNP Q07343
C	138	HIS	-	EXPRESSION TAG	UNP Q07343
C	139	HIS	-	EXPRESSION TAG	UNP Q07343
C	140	HIS	-	EXPRESSION TAG	UNP Q07343
C	141	SER	-	EXPRESSION TAG	UNP Q07343
C	142	SER	-	EXPRESSION TAG	UNP Q07343
C	143	GLY	-	EXPRESSION TAG	UNP Q07343

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Chain	Residue	Modelled	Actual	Comment	Reference
C	144	LEU	-	EXPRESSION TAG	UNP Q07343
C	145	VAL	-	EXPRESSION TAG	UNP Q07343
C	146	PRO	-	EXPRESSION TAG	UNP Q07343
C	147	ARG	-	EXPRESSION TAG	UNP Q07343
C	148	GLY	-	EXPRESSION TAG	UNP Q07343
C	149	SER	-	EXPRESSION TAG	UNP Q07343
C	150	HIS	-	EXPRESSION TAG	UNP Q07343
C	151	MET	-	EXPRESSION TAG	UNP Q07343
D	131	MET	-	EXPRESSION TAG	UNP Q07343
D	132	GLY	-	EXPRESSION TAG	UNP Q07343
D	133	SER	-	EXPRESSION TAG	UNP Q07343
D	134	SER	-	EXPRESSION TAG	UNP Q07343
D	135	HIS	-	EXPRESSION TAG	UNP Q07343
D	136	HIS	-	EXPRESSION TAG	UNP Q07343
D	137	HIS	-	EXPRESSION TAG	UNP Q07343
D	138	HIS	-	EXPRESSION TAG	UNP Q07343
D	139	HIS	-	EXPRESSION TAG	UNP Q07343
D	140	HIS	-	EXPRESSION TAG	UNP Q07343
D	141	SER	-	EXPRESSION TAG	UNP Q07343
D	142	SER	-	EXPRESSION TAG	UNP Q07343
D	143	GLY	-	EXPRESSION TAG	UNP Q07343
D	144	LEU	-	EXPRESSION TAG	UNP Q07343
D	145	VAL	-	EXPRESSION TAG	UNP Q07343
D	146	PRO	-	EXPRESSION TAG	UNP Q07343
D	147	ARG	-	EXPRESSION TAG	UNP Q07343
D	148	GLY	-	EXPRESSION TAG	UNP Q07343
D	149	SER	-	EXPRESSION TAG	UNP Q07343
D	150	HIS	-	EXPRESSION TAG	UNP Q07343
D	151	MET	-	EXPRESSION TAG	UNP Q07343
E	131	MET	-	EXPRESSION TAG	UNP Q07343
E	132	GLY	-	EXPRESSION TAG	UNP Q07343
E	133	SER	-	EXPRESSION TAG	UNP Q07343
E	134	SER	-	EXPRESSION TAG	UNP Q07343
E	135	HIS	-	EXPRESSION TAG	UNP Q07343
E	136	HIS	-	EXPRESSION TAG	UNP Q07343
E	137	HIS	-	EXPRESSION TAG	UNP Q07343
E	138	HIS	-	EXPRESSION TAG	UNP Q07343
E	139	HIS	-	EXPRESSION TAG	UNP Q07343
E	140	HIS	-	EXPRESSION TAG	UNP Q07343
E	141	SER	-	EXPRESSION TAG	UNP Q07343
E	142	SER	-	EXPRESSION TAG	UNP Q07343
E	143	GLY	-	EXPRESSION TAG	UNP Q07343

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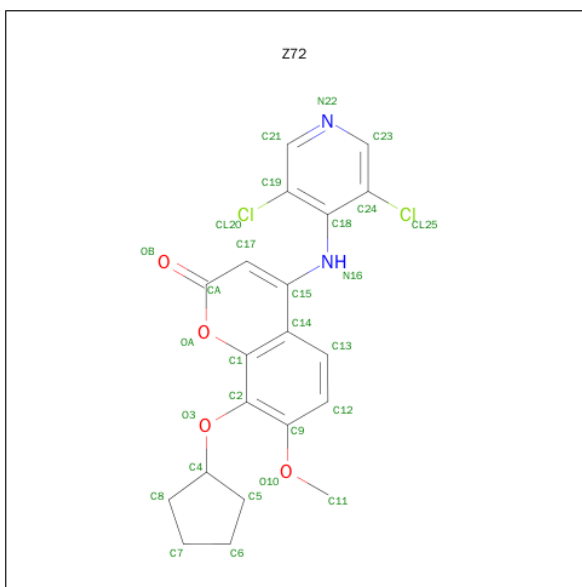
Chain	Residue	Modelled	Actual	Comment	Reference
E	144	LEU	-	EXPRESSION TAG	UNP Q07343
E	145	VAL	-	EXPRESSION TAG	UNP Q07343
E	146	PRO	-	EXPRESSION TAG	UNP Q07343
E	147	ARG	-	EXPRESSION TAG	UNP Q07343
E	148	GLY	-	EXPRESSION TAG	UNP Q07343
E	149	SER	-	EXPRESSION TAG	UNP Q07343
E	150	HIS	-	EXPRESSION TAG	UNP Q07343
E	151	MET	-	EXPRESSION TAG	UNP Q07343
F	131	MET	-	EXPRESSION TAG	UNP Q07343
F	132	GLY	-	EXPRESSION TAG	UNP Q07343
F	133	SER	-	EXPRESSION TAG	UNP Q07343
F	134	SER	-	EXPRESSION TAG	UNP Q07343
F	135	HIS	-	EXPRESSION TAG	UNP Q07343
F	136	HIS	-	EXPRESSION TAG	UNP Q07343
F	137	HIS	-	EXPRESSION TAG	UNP Q07343
F	138	HIS	-	EXPRESSION TAG	UNP Q07343
F	139	HIS	-	EXPRESSION TAG	UNP Q07343
F	140	HIS	-	EXPRESSION TAG	UNP Q07343
F	141	SER	-	EXPRESSION TAG	UNP Q07343
F	142	SER	-	EXPRESSION TAG	UNP Q07343
F	143	GLY	-	EXPRESSION TAG	UNP Q07343
F	144	LEU	-	EXPRESSION TAG	UNP Q07343
F	145	VAL	-	EXPRESSION TAG	UNP Q07343
F	146	PRO	-	EXPRESSION TAG	UNP Q07343
F	147	ARG	-	EXPRESSION TAG	UNP Q07343
F	148	GLY	-	EXPRESSION TAG	UNP Q07343
F	149	SER	-	EXPRESSION TAG	UNP Q07343
F	150	HIS	-	EXPRESSION TAG	UNP Q07343
F	151	MET	-	EXPRESSION TAG	UNP Q07343
G	131	MET	-	EXPRESSION TAG	UNP Q07343
G	132	GLY	-	EXPRESSION TAG	UNP Q07343
G	133	SER	-	EXPRESSION TAG	UNP Q07343
G	134	SER	-	EXPRESSION TAG	UNP Q07343
G	135	HIS	-	EXPRESSION TAG	UNP Q07343
G	136	HIS	-	EXPRESSION TAG	UNP Q07343
G	137	HIS	-	EXPRESSION TAG	UNP Q07343
G	138	HIS	-	EXPRESSION TAG	UNP Q07343
G	139	HIS	-	EXPRESSION TAG	UNP Q07343
G	140	HIS	-	EXPRESSION TAG	UNP Q07343
G	141	SER	-	EXPRESSION TAG	UNP Q07343
G	142	SER	-	EXPRESSION TAG	UNP Q07343
G	143	GLY	-	EXPRESSION TAG	UNP Q07343

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Chain	Residue	Modelled	Actual	Comment	Reference
G	144	LEU	-	EXPRESSION TAG	UNP Q07343
G	145	VAL	-	EXPRESSION TAG	UNP Q07343
G	146	PRO	-	EXPRESSION TAG	UNP Q07343
G	147	ARG	-	EXPRESSION TAG	UNP Q07343
G	148	GLY	-	EXPRESSION TAG	UNP Q07343
G	149	SER	-	EXPRESSION TAG	UNP Q07343
G	150	HIS	-	EXPRESSION TAG	UNP Q07343
G	151	MET	-	EXPRESSION TAG	UNP Q07343
H	131	MET	-	EXPRESSION TAG	UNP Q07343
H	132	GLY	-	EXPRESSION TAG	UNP Q07343
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H	135	HIS	-	EXPRESSION TAG	UNP Q07343
H	136	HIS	-	EXPRESSION TAG	UNP Q07343
H	137	HIS	-	EXPRESSION TAG	UNP Q07343
H	138	HIS	-	EXPRESSION TAG	UNP Q07343
H	139	HIS	-	EXPRESSION TAG	UNP Q07343
H	140	HIS	-	EXPRESSION TAG	UNP Q07343
H	141	SER	-	EXPRESSION TAG	UNP Q07343
H	142	SER	-	EXPRESSION TAG	UNP Q07343
H	143	GLY	-	EXPRESSION TAG	UNP Q07343
H	144	LEU	-	EXPRESSION TAG	UNP Q07343
H	145	VAL	-	EXPRESSION TAG	UNP Q07343
H	146	PRO	-	EXPRESSION TAG	UNP Q07343
H	147	ARG	-	EXPRESSION TAG	UNP Q07343
H	148	GLY	-	EXPRESSION TAG	UNP Q07343
H	149	SER	-	EXPRESSION TAG	UNP Q07343
H	150	HIS	-	EXPRESSION TAG	UNP Q07343
H	151	MET	-	EXPRESSION TAG	UNP Q07343

- Molecule 2 is 8-(CYCLOPENTYLOXY)-4-[(3,5-DICHLOROPYRIDIN-4-YL)AMINO]-7-METHOXY-2H-CHROMEN-2-ONE (three-letter code: Z72) (formula: C₂₀H₁₈Cl₂N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	
			28	20	2	2	4	0
2	B	1	Total	C	Cl	N	O	
			28	20	2	2	4	0
2	C	1	Total	C	Cl	N	O	
			28	20	2	2	4	0
2	D	1	Total	C	Cl	N	O	
			28	20	2	2	4	0
2	E	1	Total	C	Cl	N	O	
			28	20	2	2	4	0
2	F	1	Total	C	Cl	N	O	
			28	20	2	2	4	0
2	G	1	Total	C	Cl	N	O	
			28	20	2	2	4	0
2	H	1	Total	C	Cl	N	O	
			28	20	2	2	4	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	G	1	Total	Zn		
			1	1	0	0
3	D	1	Total	Zn		
			1	1	0	0
3	E	1	Total	Zn		
			1	1	0	0
3	H	1	Total	Zn		
			1	1	0	0

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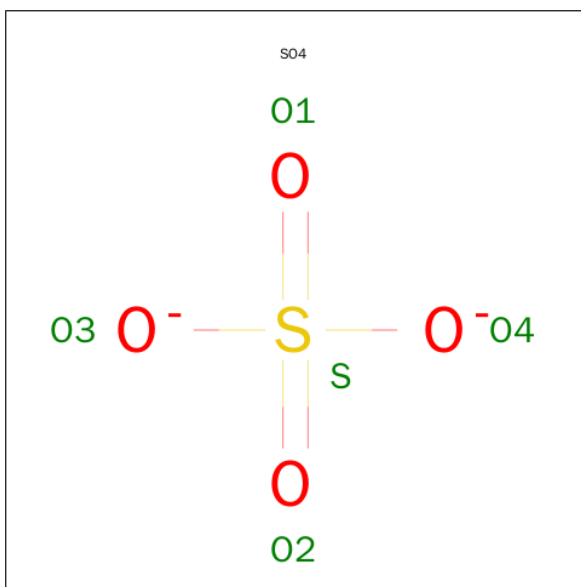
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Zn 1	0	0
3	C	1	Total 1	Zn 1	0	0
3	A	1	Total 1	Zn 1	0	0
3	F	1	Total 1	Zn 1	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	1	Total 1	Mg 1	0	0
4	D	1	Total 1	Mg 1	0	0
4	E	1	Total 1	Mg 1	0	0
4	H	1	Total 1	Mg 1	0	0
4	B	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0
4	A	1	Total 1	Mg 1	0	0
4	F	1	Total 1	Mg 1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	B	1	Total	O	S	0	0
			5	4	1		

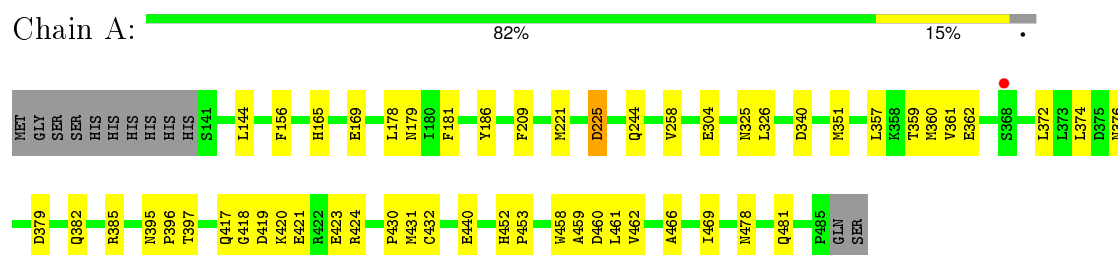
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	81	Total	O	0	0
			81	81		
6	B	91	Total	O	0	0
			91	91		
6	C	46	Total	O	0	0
			46	46		
6	D	100	Total	O	0	0
			100	100		
6	E	39	Total	O	0	0
			39	39		
6	F	27	Total	O	0	0
			27	27		
6	G	53	Total	O	0	0
			53	53		
6	H	57	Total	O	0	0
			57	57		

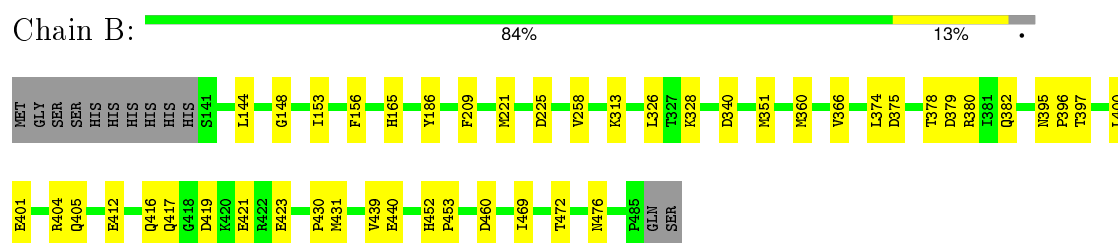
3 Residue-property plots

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.

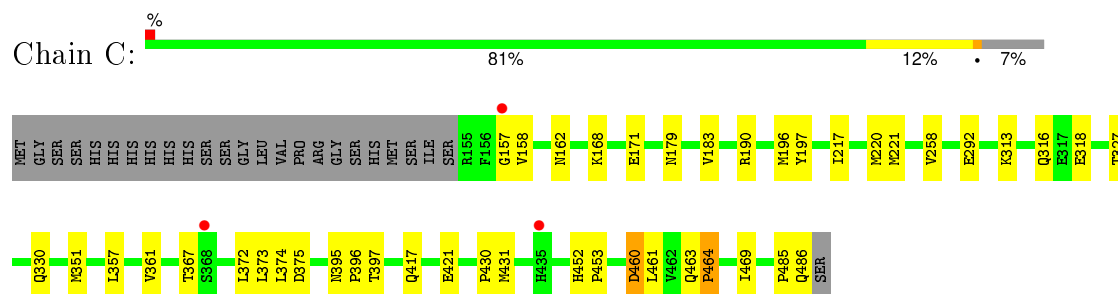
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4B



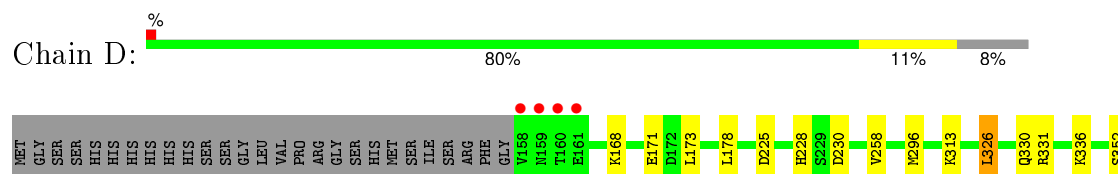
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4B



- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4B

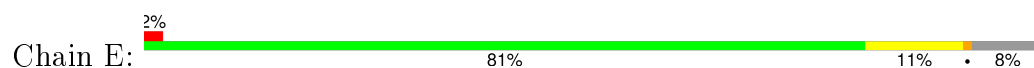


- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4B

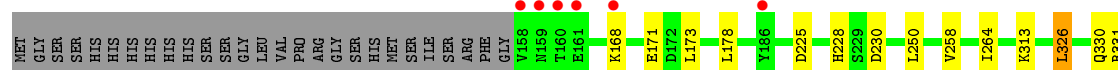
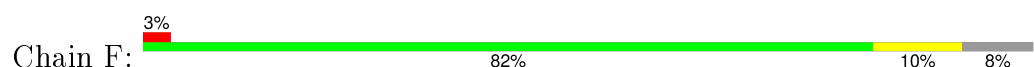




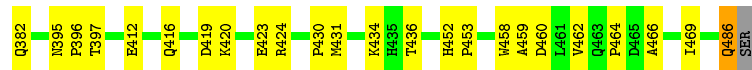
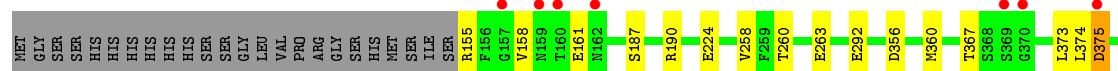
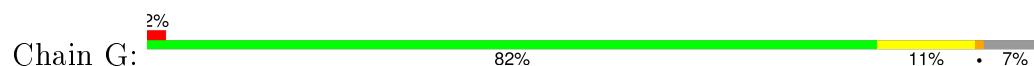
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4B



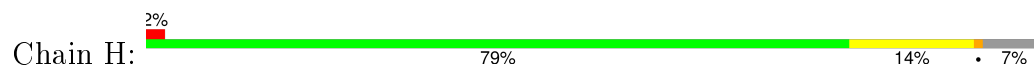
- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4B



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- Molecule 1: cAMP-specific 3',5'-cyclic phosphodiesterase 4B



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	214.80Å 233.96Å 165.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.84 – 2.60 49.84 – 2.59	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.84-2.60) 99.5 (49.84-2.59)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.99 (at 2.58Å)	Xtriage
Refinement program	CNX	Depositor
R, R_{free}	0.205 , 0.233 0.202 , 0.227	Depositor DCC
R_{free} test set	6407 reflections (5.30%)	DCC
Wilson B-factor (Å ²)	35.6	Xtriage
Anisotropy	0.209	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	5 of 127964 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	22265	wwPDB-VP
Average B, all atoms (Å ²)	38.0	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 20.18 % 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 9.1946e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical 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: MG, Z72, ZN, SO4

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	0/2819	0.59	0/3824
1	B	0.40	0/2822	0.59	0/3829
1	C	0.36	0/2726	0.54	0/3699
1	D	0.35	0/2703	0.54	0/3668
1	E	0.36	0/2707	0.54	0/3673
1	F	0.37	0/2710	0.54	0/3677
1	G	0.39	2/2743 (0.1%)	0.55	0/3720
1	H	0.39	2/2739 (0.1%)	0.54	0/3715
All	All	0.38	4/21969 (0.0%)	0.56	0/29805

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	486	GLN	CD-NE2	-6.30	1.17	1.32
1	H	486	GLN	CD-NE2	-6.30	1.17	1.32
1	H	486	GLN	CD-OE1	-6.26	1.10	1.24
1	G	486	GLN	CD-OE1	-6.13	1.10	1.24

There are no bond angle outliers.

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	2761	0	2681	31	0
1	B	2764	0	2676	24	0
1	C	2671	0	2589	32	0
1	D	2648	0	2574	26	1
1	E	2652	0	2577	28	0
1	F	2655	0	2577	20	0
1	G	2687	0	2611	22	0
1	H	2683	0	2607	31	0
2	A	28	0	18	3	0
2	B	28	0	18	3	0
2	C	28	0	18	1	0
2	D	28	0	18	4	0
2	E	28	0	18	1	0
2	F	28	0	18	3	0
2	G	28	0	18	0	0
2	H	28	0	18	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	1	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	81	0	0	1	0
6	B	91	0	0	1	0
6	C	46	0	0	0	0
6	D	100	0	0	4	0
6	E	39	0	0	0	0
6	F	27	0	0	0	0
6	G	53	0	0	0	0
6	H	57	0	0	1	0
All	All	22265	0	21036	203	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

The worst 5 of 203 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:156:PHE:HA	1:B:221:MET:HE1	1.38	1.06
1:A:156:PHE:HA	1:A:221:MET:HE1	1.47	0.93
1:E:221:MET:SD	1:F:423:GLU:HG2	2.26	0.75
1:F:422:ARG:HB2	1:F:428:ILE:HD11	1.72	0.69
1:D:422:ARG:HB2	1:D:428:ILE:HD11	1.75	0.69

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:456:GLU:OE2	1:D:456:GLU:OE2[4_555]	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	343/357 (96%)	335 (98%)	8 (2%)	0	100	100
1	B	343/357 (96%)	335 (98%)	7 (2%)	1 (0%)	46	72
1	C	330/357 (92%)	316 (96%)	13 (4%)	1 (0%)	46	72
1	D	326/357 (91%)	313 (96%)	13 (4%)	0	100	100
1	E	327/357 (92%)	314 (96%)	13 (4%)	0	100	100
1	F	327/357 (92%)	313 (96%)	14 (4%)	0	100	100
1	G	330/357 (92%)	323 (98%)	6 (2%)	1 (0%)	46	72
1	H	330/357 (92%)	323 (98%)	6 (2%)	1 (0%)	46	72
All	All	2656/2856 (93%)	2572 (97%)	80 (3%)	4 (0%)	52	77

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	375	ASP
1	H	375	ASP
1	C	485	PRO
1	B	439	VAL

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	308/323 (95%)	303 (98%)	5 (2%)	70	89
1	B	309/323 (96%)	301 (97%)	8 (3%)	54	80
1	C	298/323 (92%)	294 (99%)	4 (1%)	76	91
1	D	297/323 (92%)	291 (98%)	6 (2%)	63	85
1	E	297/323 (92%)	293 (99%)	4 (1%)	76	91
1	F	297/323 (92%)	291 (98%)	6 (2%)	63	85
1	G	301/323 (93%)	297 (99%)	4 (1%)	76	91
1	H	300/323 (93%)	295 (98%)	5 (2%)	68	88
All	All	2407/2584 (93%)	2365 (98%)	42 (2%)	68	88

5 of 42 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	326	LEU
1	E	162	ASN
1	H	360	MET
1	D	360	MET
1	D	460	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	481	GLN

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Mol	Chain	Res	Type
1	E	481	GLN

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 26 ligands modelled in this entry, 16 are monoatomic - leaving 10 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	Z72	A	1000	-	29,31,31	2.03	12 (41%)	37,44,44	1.27	5 (13%)
5	SO4	A	1003	-	4,4,4	0.20	0	6,6,6	0.24	0
2	Z72	B	1000	-	29,31,31	1.80	11 (37%)	37,44,44	1.20	5 (13%)
5	SO4	B	1003	-	4,4,4	0.16	0	6,6,6	0.11	0
2	Z72	C	1000	-	29,31,31	1.77	12 (41%)	37,44,44	1.19	4 (10%)
2	Z72	D	1000	-	29,31,31	1.70	7 (24%)	37,44,44	1.23	5 (13%)
2	Z72	E	1000	-	29,31,31	1.86	10 (34%)	37,44,44	1.22	5 (13%)
2	Z72	F	1000	-	29,31,31	1.74	7 (24%)	37,44,44	1.24	5 (13%)
2	Z72	G	1000	-	29,31,31	1.73	8 (27%)	37,44,44	1.27	5 (13%)
2	Z72	H	1000	-	29,31,31	1.74	9 (31%)	37,44,44	1.28	5 (13%)

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	Z72	A	1000	-	-	0/10/17/17	0/4/4/4
5	SO4	A	1003	-	-	0/0/0/0	0/0/0/0
2	Z72	B	1000	-	-	0/10/17/17	0/4/4/4
5	SO4	B	1003	-	-	0/0/0/0	0/0/0/0
2	Z72	C	1000	-	-	0/10/17/17	0/4/4/4
2	Z72	D	1000	-	-	0/10/17/17	0/4/4/4
2	Z72	E	1000	-	-	0/10/17/17	0/4/4/4
2	Z72	F	1000	-	-	0/10/17/17	0/4/4/4
2	Z72	G	1000	-	-	0/10/17/17	0/4/4/4
2	Z72	H	1000	-	-	0/10/17/17	0/4/4/4

The worst 5 of 76 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1000	Z72	C18-C19	-3.32	1.34	1.40
2	F	1000	Z72	C18-C19	-3.30	1.34	1.40
2	G	1000	Z72	C18-C19	-3.27	1.34	1.40
2	A	1000	Z72	C18-C19	-2.84	1.35	1.40
2	D	1000	Z72	C18-C19	-2.76	1.35	1.40

The worst 5 of 39 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	Z72	O10-C9-C12	-2.77	119.69	124.35
2	D	1000	Z72	O10-C9-C12	-2.74	119.74	124.35
2	H	1000	Z72	C24-C23-N22	-2.72	120.69	123.03
2	F	1000	Z72	O10-C9-C12	-2.71	119.78	124.35
2	H	1000	Z72	O10-C9-C12	-2.67	119.86	124.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000	Z72	3	0
2	B	1000	Z72	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1000	Z72	1	0
2	D	1000	Z72	4	0
2	E	1000	Z72	1	0
2	F	1000	Z72	3	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	345/357 (96%)	-0.48	1 (0%) 94 93	17, 30, 51, 66	0
1	B	345/357 (96%)	-0.49	0 100 100	16, 29, 52, 67	0
1	C	332/357 (92%)	-0.20	3 (0%) 85 83	21, 38, 66, 86	0
1	D	328/357 (91%)	-0.20	4 (1%) 81 77	21, 34, 64, 92	0
1	E	329/357 (92%)	-0.20	6 (1%) 71 66	21, 39, 64, 86	0
1	F	329/357 (92%)	-0.12	9 (2%) 58 51	24, 39, 66, 93	0
1	G	332/357 (92%)	-0.11	7 (2%) 67 61	20, 39, 72, 88	0
1	H	332/357 (92%)	-0.14	7 (2%) 67 61	18, 41, 72, 89	0
All	All	2672/2856 (93%)	-0.25	37 (1%) 78 74	16, 36, 64, 93	0

The worst 5 of 37 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	158	VAL	4.7
1	D	160	THR	4.1
1	F	369	SER	3.5
1	D	159	ASN	3.4
1	G	369	SER	3.4

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 carbohydrates 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. 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, 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	LLDF	B-factors(Å ²)	Q<0.9
2	Z72	G	1000	28/28	0.91	0.22	4.04	48,56,69,71	0
2	Z72	A	1000	28/28	0.88	0.23	3.94	53,59,69,71	0
2	Z72	H	1000	28/28	0.90	0.20	3.53	50,57,69,71	0
2	Z72	D	1000	28/28	0.92	0.21	3.52	52,56,65,68	0
2	Z72	F	1000	28/28	0.84	0.28	3.40	57,60,69,73	0
2	Z72	B	1000	28/28	0.93	0.20	3.33	44,53,58,60	0
2	Z72	C	1000	28/28	0.91	0.20	2.71	47,54,60,61	0
2	Z72	E	1000	28/28	0.93	0.18	1.73	48,55,60,62	0
5	SO4	B	1003	5/5	0.99	0.13	1.07	33,33,33,34	0
5	SO4	A	1003	5/5	0.99	0.12	0.13	29,29,31,32	0
3	ZN	D	1001	1/1	1.00	0.07	-2.76	27,27,27,27	0
4	MG	D	1002	1/1	0.97	0.04	-3.16	24,24,24,24	0
3	ZN	H	1001	1/1	1.00	0.07	-3.65	31,31,31,31	0
3	ZN	G	1001	1/1	0.98	0.06	-3.79	32,32,32,32	0
3	ZN	E	1001	1/1	0.99	0.08	-3.80	35,35,35,35	0
3	ZN	C	1001	1/1	0.99	0.08	-3.91	33,33,33,33	0
4	MG	A	1002	1/1	0.93	0.06	-4.17	24,24,24,24	0
3	ZN	A	1001	1/1	0.99	0.07	-4.53	27,27,27,27	0
4	MG	F	1002	1/1	0.94	0.06	-4.72	29,29,29,29	0
3	ZN	B	1001	1/1	0.99	0.07	-5.58	27,27,27,27	0
4	MG	H	1002	1/1	0.98	0.06	-5.62	26,26,26,26	0
4	MG	E	1002	1/1	0.93	0.05	-6.16	28,28,28,28	0
4	MG	G	1002	1/1	0.96	0.03	-6.35	27,27,27,27	0
4	MG	C	1002	1/1	0.98	0.08	-6.50	24,24,24,24	0
3	ZN	F	1001	1/1	0.99	0.05	-6.71	36,36,36,36	0
4	MG	B	1002	1/1	0.97	0.06	-8.18	20,20,20,20	0

6.5 Other polymers ⓘ

There are no such residues in this entry.