



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 05:56 am BST

PDB ID : 4COG
Title : Crystal structure of kynurenine formamidase from Burkholderia cenocepacia
Authors : Diaz-Saez, L.; Srikannathasan, V.; Zoltner, M.; Hunter, W.N.
Deposited on : 2014-01-28
Resolution : 1.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

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

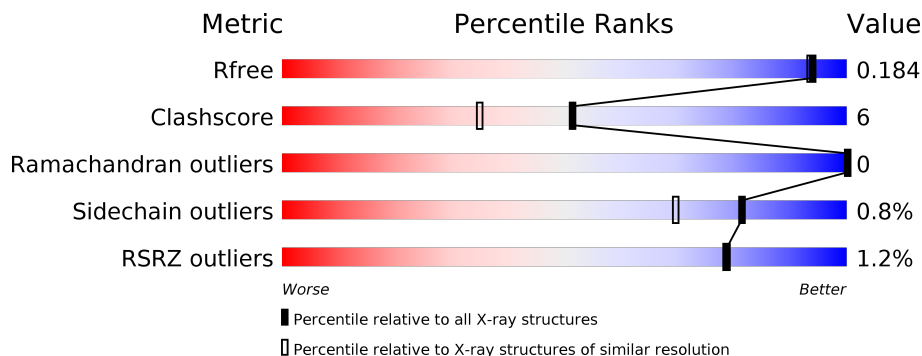
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	130704	3398 (1.60-1.60)
Clashscore	141614	3665 (1.60-1.60)
Ramachandran outliers	138981	3564 (1.60-1.60)
Sidechain outliers	138945	3563 (1.60-1.60)
RSRZ outliers	127900	3321 (1.60-1.60)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	215	
1	B	215	
1	C	215	
1	D	215	

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	MG	D	1210	-	-	X	-
7	PEG	C	1215	-	-	X	-

2 Entry composition i

There are 8 unique types of molecules in this entry. The entry contains 7700 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 KYNURENINE FORMAMIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	207	Total 1638	C 1050	N 290	O 289	S 9	0	19	0
1	B	207	Total 1617	C 1035	N 286	O 287	S 9	0	13	0
1	C	207	Total 1624	C 1039	N 285	O 291	S 9	0	15	0
1	D	207	Total 1622	C 1039	N 286	O 288	S 9	0	14	0

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP B4E9I9
A	0	HIS	-	expression tag	UNP B4E9I9
B	-1	GLY	-	expression tag	UNP B4E9I9
B	0	HIS	-	expression tag	UNP B4E9I9
C	-1	GLY	-	expression tag	UNP B4E9I9
C	0	HIS	-	expression tag	UNP B4E9I9
D	-1	GLY	-	expression tag	UNP B4E9I9
D	0	HIS	-	expression tag	UNP B4E9I9

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

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

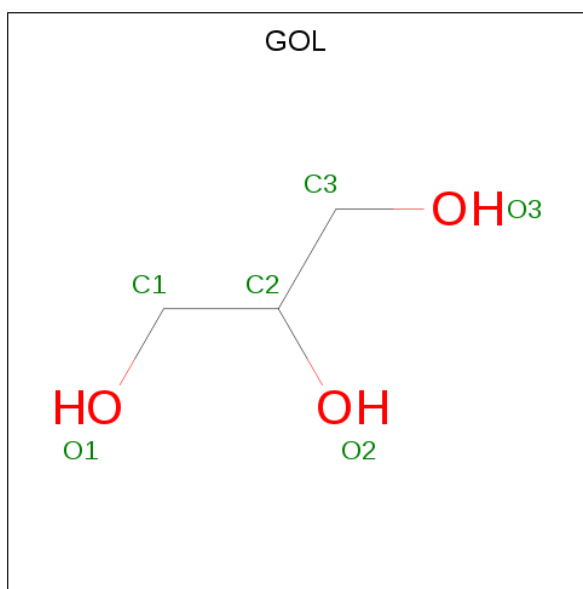
- Molecule 3 is CADMIUM ION (three-letter code: CD) (formula: Cd).

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

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

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

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



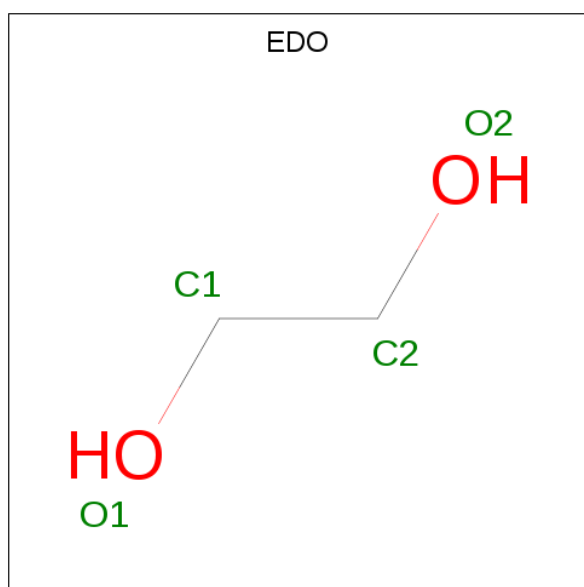
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			6	3	3		

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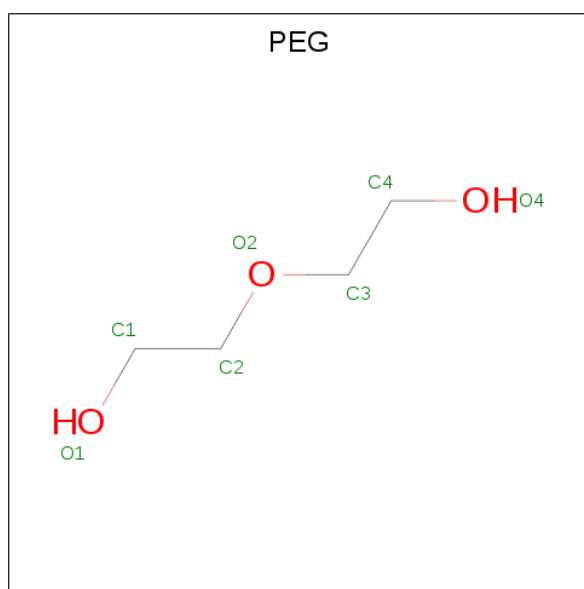
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 6 3 3	0	0
5	A	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	B	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	C	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0
5	D	1	Total C O 6 3 3	0	0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

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	A	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	B	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0
6	D	1	Total C O 4 2 2	0	0

- Molecule 7 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	1	Total C O 7 4 3	0	0

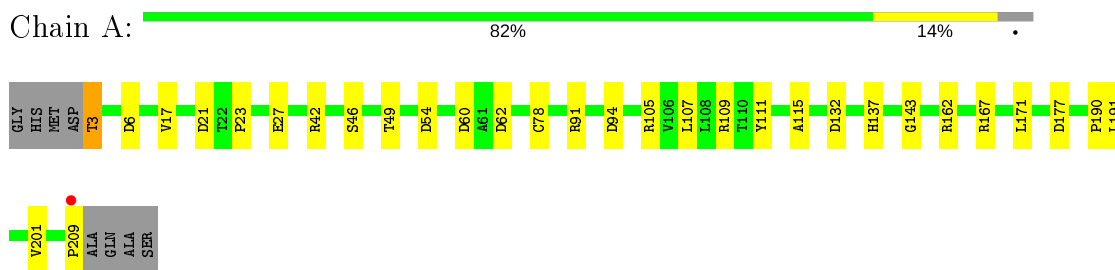
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	281	Total 281	O 281	0	0
8	B	268	Total 268	O 268	0	0
8	C	280	Total 280	O 280	0	0
8	D	239	Total 239	O 239	0	0

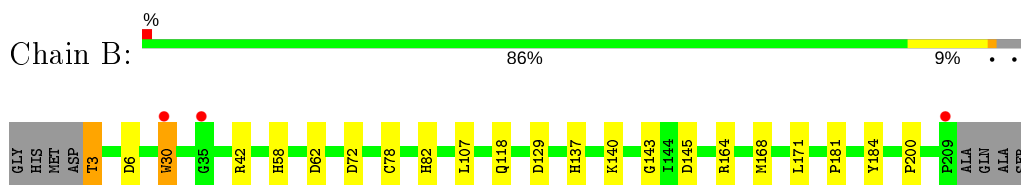
3 Residue-property plots [i](#)

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

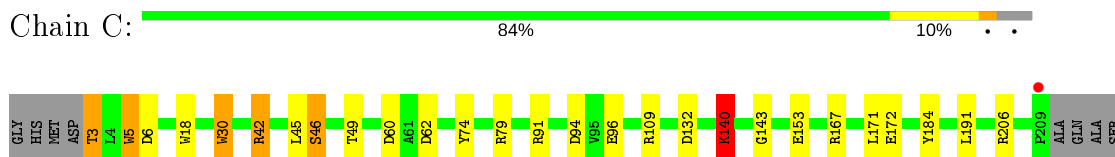
- Molecule 1: KYNURENINE FORMAMIDASE



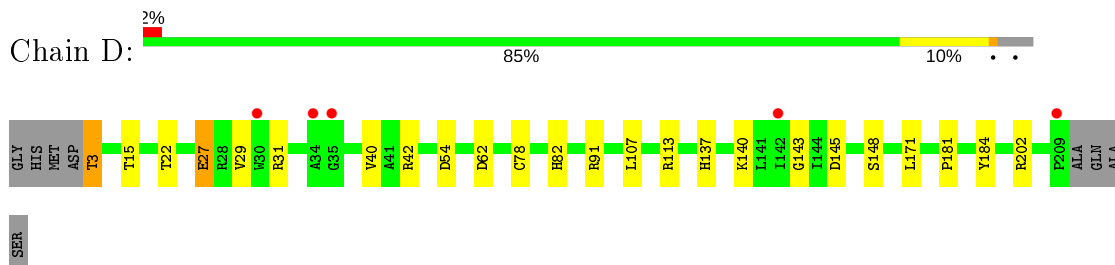
- Molecule 1: KYNURENINE FORMAMIDASE



- Molecule 1: KYNURENINE FORMAMIDASE



- Molecule 1: KYNURENINE FORMAMIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	76.86Å 50.12Å 135.20Å 90.00° 94.15° 90.00°	Depositor
Resolution (Å)	134.84 – 1.60 28.18 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.2 (134.84-1.60) 99.2 (28.18-1.60)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 1.60Å)	Xtrriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.149 , 0.184 0.148 , 0.184	Depositor DCC
R_{free} test set	6778 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	13.9	Xtrriage
Anisotropy	0.185	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	7700	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.72% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, MG, EDO, CD, PEG

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	1.20	0/1757	1.27	17/2417 (0.7%)
1	B	1.16	2/1715 (0.1%)	1.23	14/2360 (0.6%)
1	C	1.22	4/1730 (0.2%)	1.30	22/2382 (0.9%)
1	D	1.14	1/1724 (0.1%)	1.26	13/2372 (0.5%)
All	All	1.18	7/6926 (0.1%)	1.27	66/9531 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	1	0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	74	TYR	CG-CD2	6.10	1.47	1.39
1	B	30[A]	TRP	CB-CG	5.38	1.59	1.50
1	B	30[C]	TRP	CB-CG	5.38	1.59	1.50
1	C	5	TRP	CZ3-CH2	5.25	1.48	1.40
1	C	46	SER	CB-OG	5.11	1.48	1.42
1	D	148	SER	CA-CB	5.11	1.60	1.52
1	C	184	TYR	CE2-CZ	5.08	1.45	1.38

All (66) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	62	ASP	CB-CG-OD1	12.79	129.81	118.30
1	A	54	ASP	CB-CG-OD2	-9.57	109.69	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	191	LEU	CB-CG-CD2	-9.16	95.42	111.00
1	C	167	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	A	132	ASP	CB-CG-OD1	8.34	125.81	118.30
1	D	42	ARG	NE-CZ-NH1	7.88	124.24	120.30
1	C	6	ASP	CB-CG-OD2	-7.26	111.76	118.30
1	A	6	ASP	CB-CG-OD2	-7.15	111.87	118.30
1	A	167	ARG	NE-CZ-NH1	7.14	123.87	120.30
1	C	140[A]	LYS	CB-CG-CD	7.04	129.91	111.60
1	C	140[B]	LYS	CB-CG-CD	7.04	129.91	111.60
1	C	62	ASP	CB-CG-OD1	7.01	124.61	118.30
1	A	105	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	D	3	THR	N-CA-CB	6.94	123.49	110.30
1	A	105	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	D	184	TYR	CB-CG-CD2	-6.88	116.87	121.00
1	B	3	THR	N-CA-CB	6.86	123.33	110.30
1	C	206	ARG	NE-CZ-NH1	-6.85	116.88	120.30
1	D	54	ASP	CB-CG-OD2	-6.85	112.14	118.30
1	A	167	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	C	79	ARG	NE-CZ-NH1	-6.80	116.90	120.30
1	A	62	ASP	CB-CG-OD1	6.66	124.30	118.30
1	A	177	ASP	CB-CG-OD1	6.37	124.03	118.30
1	B	145	ASP	CB-CG-OD2	-6.28	112.64	118.30
1	A	94	ASP	CB-CG-OD2	6.18	123.86	118.30
1	D	62	ASP	CB-CG-OD1	6.10	123.79	118.30
1	A	109	ARG	NE-CZ-NH1	6.03	123.31	120.30
1	D	145	ASP	CB-CG-OD2	-6.03	112.88	118.30
1	B	62	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	B	6	ASP	CB-CG-OD2	-5.93	112.96	118.30
1	D	42	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	B	42	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	D	184	TYR	CZ-CE2-CD2	-5.79	114.59	119.80
1	A	3	THR	N-CA-CB	5.76	121.25	110.30
1	C	167	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	A	3	THR	CA-CB-CG2	5.74	120.43	112.40
1	B	3	THR	CA-CB-CG2	5.74	120.43	112.40
1	C	94	ASP	CB-CG-OD2	5.73	123.45	118.30
1	D	3	THR	CA-CB-CG2	5.71	120.40	112.40
1	B	184	TYR	CB-CG-CD2	-5.64	117.61	121.00
1	C	172	GLU	OE1-CD-OE2	-5.64	116.53	123.30
1	D	202	ARG	NE-CZ-NH2	-5.60	117.50	120.30
1	C	3	THR	N-CA-CB	5.57	120.88	110.30
1	A	109	ARG	NE-CZ-NH2	-5.56	117.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	72	ASP	CB-CG-OD1	5.51	123.26	118.30
1	C	140[A]	LYS	CD-CE-NZ	5.36	124.04	111.70
1	C	140[B]	LYS	CD-CE-NZ	5.36	124.04	111.70
1	C	30[B]	TRP	CB-CA-C	5.36	121.11	110.40
1	C	30[C]	TRP	CB-CA-C	5.36	121.11	110.40
1	B	184	TYR	CZ-CE2-CD2	-5.33	115.01	119.80
1	D	140[A]	LYS	CD-CE-NZ	-5.30	99.52	111.70
1	D	140[B]	LYS	CD-CE-NZ	-5.30	99.52	111.70
1	C	109	ARG	NE-CZ-NH2	-5.27	117.67	120.30
1	C	45	LEU	CB-CG-CD1	-5.24	102.09	111.00
1	A	162	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	B	129	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	C	3	THR	CA-CB-CG2	5.17	119.63	112.40
1	A	21	ASP	CB-CG-OD2	-5.16	113.66	118.30
1	A	6	ASP	CB-CG-OD1	5.14	122.93	118.30
1	C	132	ASP	CB-CG-OD1	5.13	122.91	118.30
1	B	164[A]	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	B	164[B]	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	D	27	GLU	OE1-CD-OE2	-5.07	117.21	123.30
1	B	42	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	C	42[A]	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	C	42[B]	ARG	NE-CZ-NH1	5.03	122.81	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	B	3	THR	CA

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	1638	0	1672	21	0
1	B	1617	0	1629	14	0
1	C	1624	0	1634	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1622	0	1636	14	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	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
4	A	2	0	0	2	0
4	B	2	0	0	2	0
4	C	2	0	0	2	0
4	D	2	0	0	3	0
5	A	18	0	22	0	0
5	B	18	0	22	1	0
5	C	18	0	22	5	0
5	D	18	0	22	2	0
6	A	12	0	18	4	0
6	B	12	0	18	1	0
6	D	12	0	18	3	0
7	C	7	0	10	4	0
8	A	281	0	0	13	0
8	B	268	0	0	7	0
8	C	280	0	0	11	0
8	D	239	0	0	6	1
All	All	7700	0	6723	75	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 6.

All (75) 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)
4:D:1211:MG:MG	8:D:2181:HOH:O	0.85	1.17
4:B:1211:MG:MG	8:B:2206:HOH:O	0.89	1.16
5:C:1214:GOL:H12	8:C:2186:HOH:O	1.47	1.12
4:D:1210:MG:MG	8:D:2083:HOH:O	0.98	1.06
4:C:1211:MG:MG	8:C:2116:HOH:O	0.95	1.06
4:B:1210:MG:MG	8:B:2107:HOH:O	1.01	1.04
1:A:27:GLU:HG3	1:D:27:GLU:OE2	1.60	1.00
4:A:1211:MG:MG	8:A:2131:HOH:O	1.05	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:1210:MG:MG	8:A:2225:HOH:O	1.13	0.92
8:A:2010:HOH:O	1:B:30[C]:TRP:CH2	2.22	0.90
1:C:5:TRP:HE1	7:C:1215:PEG:H31	1.38	0.87
8:A:2010:HOH:O	1:B:30[C]:TRP:CZ3	2.32	0.80
1:D:137:HIS:NE2	8:D:2181:HOH:O	2.17	0.76
1:C:49[B]:THR:HG23	8:C:2051:HOH:O	1.84	0.76
1:C:5:TRP:HE1	7:C:1215:PEG:C3	1.99	0.76
6:D:1216:EDO:H12	8:D:2019:HOH:O	1.85	0.76
1:C:60:ASP:OD1	8:C:2116:HOH:O	2.03	0.74
1:C:91[B]:ARG:NH2	8:C:2158:HOH:O	2.21	0.74
1:A:137:HIS:NE2	8:A:2225:HOH:O	2.20	0.74
1:B:137:HIS:NE2	8:B:2206:HOH:O	2.19	0.74
6:A:1217:EDO:O2	8:A:2278:HOH:O	2.08	0.72
6:A:1217:EDO:H21	8:A:2192:HOH:O	1.89	0.71
1:C:5:TRP:NE1	7:C:1215:PEG:H31	2.04	0.71
4:C:1210:MG:MG	8:C:2216:HOH:O	1.35	0.69
4:D:1210:MG:MG	8:D:2082:HOH:O	1.36	0.68
1:D:15:THR:OG1	6:D:1216:EDO:H22	1.95	0.67
1:A:60:ASP:OD1	8:A:2131:HOH:O	2.13	0.66
1:D:91[B]:ARG:NE	8:D:2124:HOH:O	2.29	0.65
1:A:42[B]:ARG:CZ	8:A:2107:HOH:O	2.45	0.63
1:A:91[B]:ARG:NH1	8:A:2176:HOH:O	2.32	0.62
1:A:27:GLU:CG	1:D:27:GLU:OE2	2.46	0.58
5:C:1212:GOL:H2	1:D:40:VAL:HG21	1.86	0.57
1:A:17[B]:VAL:HG12	1:A:49[B]:THR:CG2	2.35	0.56
1:D:82:HIS:CE1	1:D:181:PRO:HD3	2.41	0.56
1:C:30[B]:TRP:HZ3	5:D:1212:GOL:H11	1.71	0.56
1:B:58:HIS:NE2	5:B:1213:GOL:O1	2.32	0.56
1:D:113:ARG:O	6:D:1217:EDO:H12	2.05	0.56
1:A:191[A]:LEU:HD23	1:B:200:PRO:HB2	1.89	0.54
1:B:82:HIS:CE1	1:B:181:PRO:HD3	2.43	0.54
1:A:78[B]:CYS:SG	1:A:107:LEU:HG	2.48	0.54
8:B:2083:HOH:O	1:D:29:VAL:HG11	2.07	0.54
1:B:143:GLY:HA2	1:B:171:LEU:O	2.10	0.52
1:B:78[B]:CYS:SG	1:B:107:LEU:HG	2.50	0.52
1:D:143:GLY:HA2	1:D:171:LEU:O	2.10	0.52
1:A:17[B]:VAL:HG12	1:A:49[B]:THR:HG21	1.93	0.51
1:A:111:TYR:HA	6:A:1217:EDO:H11	1.92	0.51
5:C:1214:GOL:C1	8:C:2186:HOH:O	2.24	0.50
1:C:46:SER:O	1:C:49[B]:THR:OG1	2.26	0.50
1:C:140[A]:LYS:HG2	8:C:2222:HOH:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:PRO:HG2	1:D:31[B]:ARG:HH12	1.77	0.50
1:C:153[B]:GLU:HG3	8:C:2232:HOH:O	2.11	0.49
1:C:30[B]:TRP:HZ3	5:D:1212:GOL:C1	2.24	0.49
1:B:118[B]:GLN:HG3	8:B:2183:HOH:O	2.13	0.49
1:A:46:SER:HB3	1:A:49[B]:THR:HG23	1.96	0.48
1:C:143:GLY:HA2	1:C:171:LEU:O	2.13	0.48
1:D:78[B]:CYS:SG	1:D:107:LEU:HG	2.53	0.48
1:A:191[A]:LEU:CD2	1:B:200:PRO:HB2	2.44	0.47
1:A:143:GLY:HA2	1:A:171:LEU:O	2.14	0.47
8:A:2010:HOH:O	1:B:30[C]:TRP:HH2	1.75	0.46
1:C:5:TRP:HE1	7:C:1215:PEG:C4	2.29	0.46
1:A:115:ALA:HB2	6:A:1215:EDO:H11	1.98	0.45
1:C:18:TRP:CG	5:C:1212:GOL:H11	2.52	0.45
1:B:140[B]:LYS:HD3	1:B:168:MET:HA	2.00	0.44
1:A:23:PRO:CG	1:D:31[B]:ARG:HH12	2.30	0.44
6:B:1217:EDO:C2	8:B:2141:HOH:O	2.65	0.44
5:C:1214:GOL:C2	8:C:2186:HOH:O	2.58	0.43
1:C:42[A]:ARG:HG3	1:D:22:THR:HG21	1.99	0.43
1:C:96[B]:GLU:HG3	8:C:2163:HOH:O	2.19	0.43
1:B:140[A]:LYS:HD2	8:B:2211:HOH:O	2.20	0.41
1:A:190:PRO:HA	1:A:201:VAL:HG12	2.02	0.41
1:A:209:PRO:HD3	8:A:2147:HOH:O	2.20	0.41
1:A:17[B]:VAL:HG12	1:A:49[B]:THR:HG22	2.02	0.41
1:A:209:PRO:CD	8:A:2147:HOH:O	2.69	0.41
1:C:91[A]:ARG:HB2	1:C:91[A]:ARG:HE	1.63	0.40

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)
8:D:2113:HOH:O	8:D:2182:HOH:O[2_647]	1.67	0.53

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	224/215 (104%)	215 (96%)	9 (4%)	0	100	100
1	B	218/215 (101%)	210 (96%)	8 (4%)	0	100	100
1	C	220/215 (102%)	210 (96%)	10 (4%)	0	100	100
1	D	219/215 (102%)	210 (96%)	9 (4%)	0	100	100
All	All	881/860 (102%)	845 (96%)	36 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	185/171 (108%)	184 (100%)	1 (0%)	88	80
1	B	179/171 (105%)	178 (99%)	1 (1%)	86	77
1	C	181/171 (106%)	178 (98%)	3 (2%)	60	38
1	D	180/171 (105%)	179 (99%)	1 (1%)	86	77
All	All	725/684 (106%)	719 (99%)	6 (1%)	81	70

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	THR
1	B	3	THR
1	C	3	THR
1	C	140[A]	LYS
1	C	140[B]	LYS
1	D	3	THR

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

Mol	Chain	Res	Type
1	A	122	ASN
1	D	122	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 38 ligands modelled in this entry, 16 are monoatomic - leaving 22 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
7	PEG	C	1215	-	6,6,6	0.37	0	5,5,5	1.20	0
5	GOL	A	1214	-	5,5,5	1.24	0	5,5,5	1.90	1 (20%)
6	EDO	B	1216	-	3,3,3	0.74	0	2,2,2	0.52	0
5	GOL	D	1212	-	5,5,5	0.39	0	5,5,5	1.06	0
6	EDO	D	1216	-	3,3,3	0.67	0	2,2,2	0.80	0
5	GOL	C	1214	-	5,5,5	0.83	0	5,5,5	1.62	1 (20%)
5	GOL	D	1214	3,2	5,5,5	0.80	0	5,5,5	0.69	0
5	GOL	B	1214	-	5,5,5	1.00	0	5,5,5	1.40	1 (20%)
6	EDO	D	1217	-	3,3,3	0.35	0	2,2,2	1.08	0
5	GOL	A	1213	3,2	5,5,5	0.68	0	5,5,5	0.88	0
5	GOL	C	1213	3,2	5,5,5	1.23	0	5,5,5	0.81	0
6	EDO	B	1215	-	3,3,3	0.37	0	2,2,2	0.89	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	EDO	D	1215	-	3,3,3	0.38	0	2,2,2	0.42	0
5	GOL	B	1213	3,2	5,5,5	1.06	0	5,5,5	1.21	0
5	GOL	D	1213	-	5,5,5	1.21	0	5,5,5	1.71	2 (40%)
6	EDO	B	1217	-	3,3,3	0.41	0	2,2,2	2.35	1 (50%)
6	EDO	A	1217	-	3,3,3	0.70	0	2,2,2	1.29	0
6	EDO	A	1215	-	3,3,3	0.46	0	2,2,2	0.35	0
6	EDO	A	1216	-	3,3,3	0.20	0	2,2,2	0.73	0
5	GOL	A	1212	-	5,5,5	0.24	0	5,5,5	1.12	1 (20%)
5	GOL	C	1212	-	5,5,5	0.36	0	5,5,5	0.82	0
5	GOL	B	1212	-	5,5,5	0.56	0	5,5,5	1.28	1 (20%)

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
7	PEG	C	1215	-	-	3/4/4/4	-
5	GOL	A	1214	-	-	2/4/4/4	-
6	EDO	B	1216	-	-	1/1/1/1	-
5	GOL	D	1212	-	-	0/4/4/4	-
6	EDO	D	1216	-	-	0/1/1/1	-
5	GOL	C	1214	-	-	0/4/4/4	-
5	GOL	D	1214	3,2	-	0/4/4/4	-
5	GOL	B	1214	-	-	2/4/4/4	-
6	EDO	D	1217	-	-	1/1/1/1	-
5	GOL	A	1213	3,2	-	0/4/4/4	-
5	GOL	C	1213	3,2	-	0/4/4/4	-
6	EDO	B	1215	-	-	1/1/1/1	-
6	EDO	D	1215	-	-	0/1/1/1	-
5	GOL	B	1213	3,2	-	0/4/4/4	-
5	GOL	D	1213	-	-	2/4/4/4	-
6	EDO	B	1217	-	-	1/1/1/1	-
6	EDO	A	1217	-	-	1/1/1/1	-
6	EDO	A	1215	-	-	1/1/1/1	-
6	EDO	A	1216	-	-	0/1/1/1	-
5	GOL	A	1212	-	-	0/4/4/4	-
5	GOL	C	1212	-	-	4/4/4/4	-
5	GOL	B	1212	-	-	0/4/4/4	-

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1214	GOL	O3-C3-C2	3.78	128.31	110.20
6	B	1217	EDO	O1-C1-C2	3.02	133.64	111.91
5	B	1214	GOL	O1-C1-C2	2.64	122.85	110.20
5	D	1213	GOL	O1-C1-C2	2.55	122.44	110.20
5	C	1214	GOL	O3-C3-C2	2.55	122.42	110.20
5	B	1212	GOL	O3-C3-C2	-2.13	99.97	110.20
5	D	1213	GOL	O2-C2-C1	2.10	118.38	109.12
5	A	1212	GOL	O1-C1-C2	-2.07	100.27	110.20

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1214	GOL	C1-C2-C3-O3
5	D	1213	GOL	O1-C1-C2-O2
5	D	1213	GOL	O1-C1-C2-C3
5	C	1212	GOL	O1-C1-C2-C3
5	C	1212	GOL	C1-C2-C3-O3
7	C	1215	PEG	O2-C3-C4-O4
5	C	1212	GOL	O2-C2-C3-O3
7	C	1215	PEG	O1-C1-C2-O2
6	A	1215	EDO	O1-C1-C2-O2
5	B	1214	GOL	O1-C1-C2-C3
5	A	1214	GOL	O2-C2-C3-O3
5	C	1212	GOL	O1-C1-C2-O2
6	D	1217	EDO	O1-C1-C2-O2
6	B	1217	EDO	O1-C1-C2-O2
5	B	1214	GOL	O1-C1-C2-O2
6	B	1216	EDO	O1-C1-C2-O2
6	B	1215	EDO	O1-C1-C2-O2
7	C	1215	PEG	C1-C2-O2-C3
6	A	1217	EDO	O1-C1-C2-O2

There are no ring outliers.

10 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1215	PEG	4	0
5	D	1212	GOL	2	0
6	D	1216	EDO	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	1214	GOL	3	0
6	D	1217	EDO	1	0
5	B	1213	GOL	1	0
6	B	1217	EDO	1	0
6	A	1217	EDO	3	0
6	A	1215	EDO	1	0
5	C	1212	GOL	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	207/215 (96%)	-0.27	1 (0%) 91 90	9, 15, 28, 52	6 (2%)
1	B	207/215 (96%)	-0.33	3 (1%) 75 75	8, 14, 28, 44	5 (2%)
1	C	207/215 (96%)	-0.33	1 (0%) 91 90	8, 14, 27, 48	6 (2%)
1	D	207/215 (96%)	-0.32	5 (2%) 59 56	8, 14, 27, 47	9 (4%)
All	All	828/860 (96%)	-0.31	10 (1%) 79 78	8, 14, 28, 52	26 (3%)

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	209	PRO	5.7
1	C	209	PRO	4.5
1	D	209	PRO	4.4
1	B	30[A]	TRP	4.0
1	B	35	GLY	3.9
1	D	30[A]	TRP	2.7
1	D	35	GLY	2.7
1	B	209	PRO	2.7
1	D	142[A]	ILE	2.4
1	D	34	ALA	2.2

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands i

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	EDO	B	1216	4/4	0.84	0.23	39,39,47,48	0
7	PEG	C	1215	7/7	0.85	0.33	35,41,45,46	0
6	EDO	B	1215	4/4	0.87	0.10	39,39,42,49	0
6	EDO	D	1217	4/4	0.88	0.17	34,43,45,45	0
6	EDO	A	1216	4/4	0.91	0.14	30,42,44,48	0
6	EDO	A	1217	4/4	0.93	0.21	20,27,32,38	0
5	GOL	C	1212	6/6	0.93	0.12	34,35,44,45	0
6	EDO	D	1215	4/4	0.94	0.07	37,38,39,46	0
5	GOL	D	1213	6/6	0.94	0.09	21,23,28,29	0
6	EDO	A	1215	4/4	0.94	0.16	38,39,40,46	0
6	EDO	D	1216	4/4	0.94	0.17	32,33,35,41	0
5	GOL	A	1212	6/6	0.94	0.10	35,39,42,43	0
5	GOL	B	1214	6/6	0.94	0.13	22,27,30,30	0
5	GOL	B	1212	6/6	0.94	0.08	25,26,29,30	0
5	GOL	A	1214	6/6	0.95	0.10	23,24,30,33	0
5	GOL	D	1212	6/6	0.95	0.07	24,27,29,30	0
5	GOL	C	1214	6/6	0.95	0.11	21,26,37,50	0
4	MG	C	1210	1/1	0.95	0.06	18,18,18,18	0
6	EDO	B	1217	4/4	0.95	0.17	23,25,34,35	0
4	MG	A	1210	1/1	0.95	0.07	24,24,24,24	0
5	GOL	B	1213	6/6	0.97	0.12	11,13,16,18	0
5	GOL	A	1213	6/6	0.97	0.10	14,17,18,20	0
5	GOL	C	1213	6/6	0.97	0.09	10,13,16,17	0
5	GOL	D	1214	6/6	0.98	0.11	11,14,15,18	0
4	MG	A	1211	1/1	0.99	0.04	14,14,14,14	0
4	MG	C	1211	1/1	0.99	0.04	14,14,14,14	0
4	MG	B	1210	1/1	0.99	0.03	12,12,12,12	0
4	MG	D	1210	1/1	0.99	0.04	13,13,13,13	0
4	MG	D	1211	1/1	1.00	0.04	10,10,10,10	0
4	MG	B	1211	1/1	1.00	0.04	9,9,9,9	0
2	ZN	D	401	1/1	1.00	0.06	9,9,9,9	0
3	CD	B	402	1/1	1.00	0.04	10,10,10,10	0
3	CD	C	402	1/1	1.00	0.03	11,11,11,11	0
2	ZN	C	401	1/1	1.00	0.06	9,9,9,9	0
3	CD	A	402	1/1	1.00	0.04	13,13,13,13	0
3	CD	D	402	1/1	1.00	0.04	10,10,10,10	0
2	ZN	A	401	1/1	1.00	0.06	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ZN	B	401	1/1	1.00	0.07	9,9,9,9	0

6.5 Other polymers [i](#)

There are no such residues in this entry.