Full wwPDB X-ray Structure Validation Report (i)

Feb 18, 2024 – 07:23 AM EST

PDB ID	:	4DZI
Title	:	Crystal structure of amidohydrolase map2389c (target EFI-500390) from Mycobacterium avium subsp. paratuberculosis K-10
Authors	:	Patskovsky, Y.; Toro, R.; Bhosle, R.; Hillerich, B.; Seidel, R.D.; Washington, E.; Scott Glenn, A.; Chowdhury, S.; Evans, B.; Hammonds, J.; Zencheck, W.D.; Imker, H.J.; Gerlt, J.A.; Raushel, F.M.; Almo, S.C.; Enzyme Function Initiative (EFI)
Deposited on	:	2012-03-01
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 (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

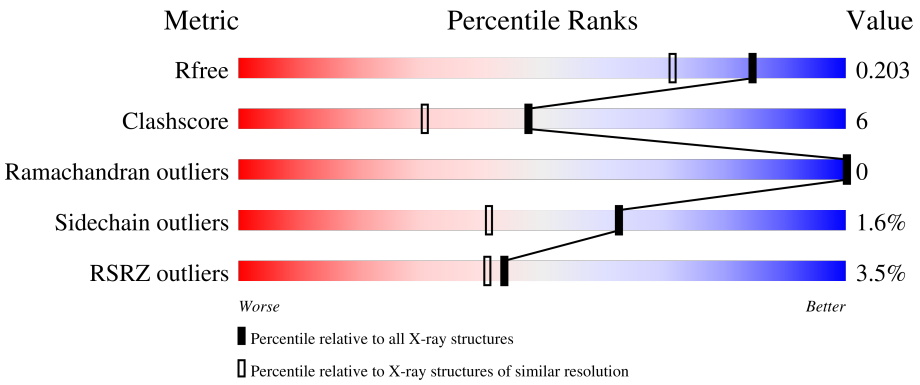
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 1.60 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 of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	423	3% 79% 11% 9%
1	B	423	2% 79% 10% • 10%
1	C	423	4% 85% 6% 8%
1	D	423	4% 80% 9% • 10%

Validation Pipeline (wwPDB-VP) : 2.36

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
3	CL	A	507	-	-	X	-

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 14003 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 Putative TIM-barrel metal-dependent hydrolase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	384	3070	1962	543	555	10	0	4	0
1	B	382	3077	1974	539	554	10	0	7	0
1	C	388	3092	1976	542	564	10	0	4	0
1	D	382	3070	1965	538	557	10	0	7	0

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	expression tag	UNP F7P4T2
A	1	VAL	-	expression tag	UNP F7P4T2
A	401	ALA	-	expression tag	UNP F7P4T2
A	402	GLU	-	expression tag	UNP F7P4T2
A	403	ASN	-	expression tag	UNP F7P4T2
A	404	LEU	-	expression tag	UNP F7P4T2
A	405	TYR	-	expression tag	UNP F7P4T2
A	406	PHE	-	expression tag	UNP F7P4T2
A	407	GLN	-	expression tag	UNP F7P4T2
A	408	SER	-	expression tag	UNP F7P4T2
A	409	HIS	-	expression tag	UNP F7P4T2
A	410	HIS	-	expression tag	UNP F7P4T2
A	411	HIS	-	expression tag	UNP F7P4T2
A	412	HIS	-	expression tag	UNP F7P4T2
A	413	HIS	-	expression tag	UNP F7P4T2
A	414	HIS	-	expression tag	UNP F7P4T2
A	415	TRP	-	expression tag	UNP F7P4T2
A	416	SER	-	expression tag	UNP F7P4T2
A	417	HIS	-	expression tag	UNP F7P4T2
A	418	PRO	-	expression tag	UNP F7P4T2
A	419	GLN	-	expression tag	UNP F7P4T2

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Chain	Residue	Modelled	Actual	Comment	Reference
A	420	PHE	-	expression tag	UNP F7P4T2
A	421	GLU	-	expression tag	UNP F7P4T2
A	422	LYS	-	expression tag	UNP F7P4T2
B	0	MET	-	expression tag	UNP F7P4T2
B	1	VAL	-	expression tag	UNP F7P4T2
B	401	ALA	-	expression tag	UNP F7P4T2
B	402	GLU	-	expression tag	UNP F7P4T2
B	403	ASN	-	expression tag	UNP F7P4T2
B	404	LEU	-	expression tag	UNP F7P4T2
B	405	TYR	-	expression tag	UNP F7P4T2
B	406	PHE	-	expression tag	UNP F7P4T2
B	407	GLN	-	expression tag	UNP F7P4T2
B	408	SER	-	expression tag	UNP F7P4T2
B	409	HIS	-	expression tag	UNP F7P4T2
B	410	HIS	-	expression tag	UNP F7P4T2
B	411	HIS	-	expression tag	UNP F7P4T2
B	412	HIS	-	expression tag	UNP F7P4T2
B	413	HIS	-	expression tag	UNP F7P4T2
B	414	HIS	-	expression tag	UNP F7P4T2
B	415	TRP	-	expression tag	UNP F7P4T2
B	416	SER	-	expression tag	UNP F7P4T2
B	417	HIS	-	expression tag	UNP F7P4T2
B	418	PRO	-	expression tag	UNP F7P4T2
B	419	GLN	-	expression tag	UNP F7P4T2
B	420	PHE	-	expression tag	UNP F7P4T2
B	421	GLU	-	expression tag	UNP F7P4T2
B	422	LYS	-	expression tag	UNP F7P4T2
C	0	MET	-	expression tag	UNP F7P4T2
C	1	VAL	-	expression tag	UNP F7P4T2
C	401	ALA	-	expression tag	UNP F7P4T2
C	402	GLU	-	expression tag	UNP F7P4T2
C	403	ASN	-	expression tag	UNP F7P4T2
C	404	LEU	-	expression tag	UNP F7P4T2
C	405	TYR	-	expression tag	UNP F7P4T2
C	406	PHE	-	expression tag	UNP F7P4T2
C	407	GLN	-	expression tag	UNP F7P4T2
C	408	SER	-	expression tag	UNP F7P4T2
C	409	HIS	-	expression tag	UNP F7P4T2
C	410	HIS	-	expression tag	UNP F7P4T2
C	411	HIS	-	expression tag	UNP F7P4T2
C	412	HIS	-	expression tag	UNP F7P4T2
C	413	HIS	-	expression tag	UNP F7P4T2

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Chain	Residue	Modelled	Actual	Comment	Reference
C	414	HIS	-	expression tag	UNP F7P4T2
C	415	TRP	-	expression tag	UNP F7P4T2
C	416	SER	-	expression tag	UNP F7P4T2
C	417	HIS	-	expression tag	UNP F7P4T2
C	418	PRO	-	expression tag	UNP F7P4T2
C	419	GLN	-	expression tag	UNP F7P4T2
C	420	PHE	-	expression tag	UNP F7P4T2
C	421	GLU	-	expression tag	UNP F7P4T2
C	422	LYS	-	expression tag	UNP F7P4T2
D	0	MET	-	expression tag	UNP F7P4T2
D	1	VAL	-	expression tag	UNP F7P4T2
D	401	ALA	-	expression tag	UNP F7P4T2
D	402	GLU	-	expression tag	UNP F7P4T2
D	403	ASN	-	expression tag	UNP F7P4T2
D	404	LEU	-	expression tag	UNP F7P4T2
D	405	TYR	-	expression tag	UNP F7P4T2
D	406	PHE	-	expression tag	UNP F7P4T2
D	407	GLN	-	expression tag	UNP F7P4T2
D	408	SER	-	expression tag	UNP F7P4T2
D	409	HIS	-	expression tag	UNP F7P4T2
D	410	HIS	-	expression tag	UNP F7P4T2
D	411	HIS	-	expression tag	UNP F7P4T2
D	412	HIS	-	expression tag	UNP F7P4T2
D	413	HIS	-	expression tag	UNP F7P4T2
D	414	HIS	-	expression tag	UNP F7P4T2
D	415	TRP	-	expression tag	UNP F7P4T2
D	416	SER	-	expression tag	UNP F7P4T2
D	417	HIS	-	expression tag	UNP F7P4T2
D	418	PRO	-	expression tag	UNP F7P4T2
D	419	GLN	-	expression tag	UNP F7P4T2
D	420	PHE	-	expression tag	UNP F7P4T2
D	421	GLU	-	expression tag	UNP F7P4T2
D	422	LYS	-	expression tag	UNP F7P4T2

- Molecule 2 is CADMIUM ION (three-letter code: CD) (formula: Cd).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
2	A	2	2	2	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cd		
2	D	2	2	2	0	0

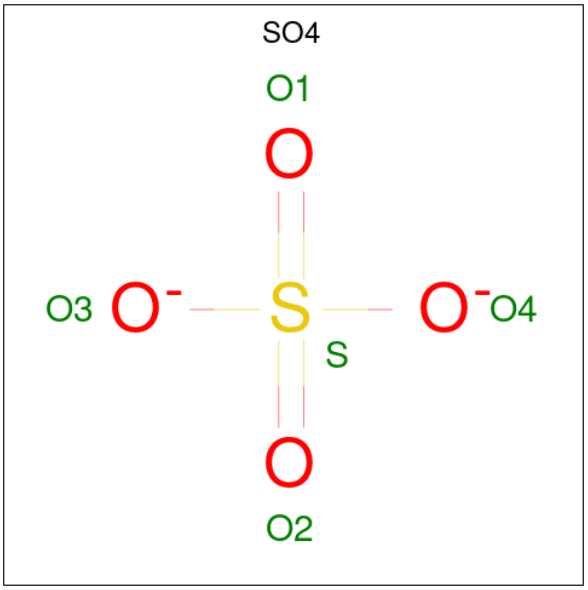
- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
4	A	1	1	1	0	0

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	B	1	10	8	2	0	1

- Molecule 6 is water.

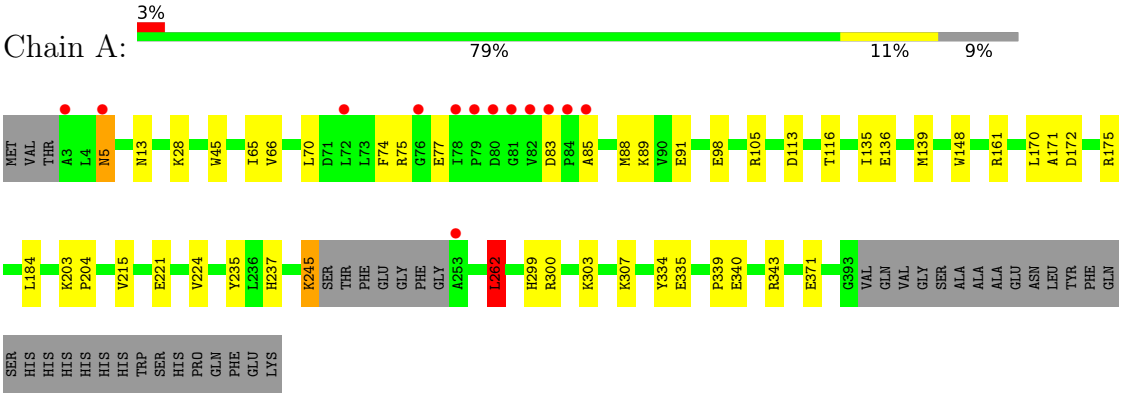
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	438	438	438	0	0
			Total	O		
6	B	448	448	448	0	0
			Total	O		
6	C	415	415	415	0	0
			Total	O		
6	D	363	363	363	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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.

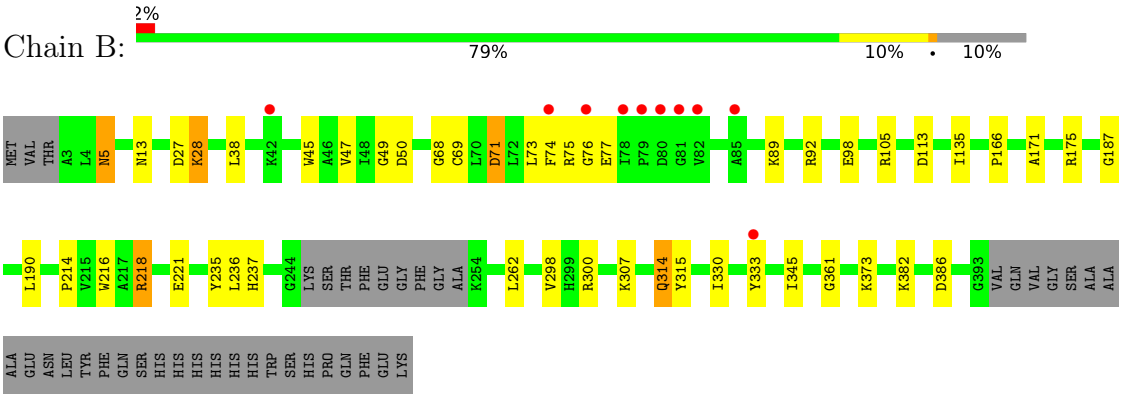
• Molecule 1: Putative TIM-barrel metal-dependent hydrolase

Chain A:



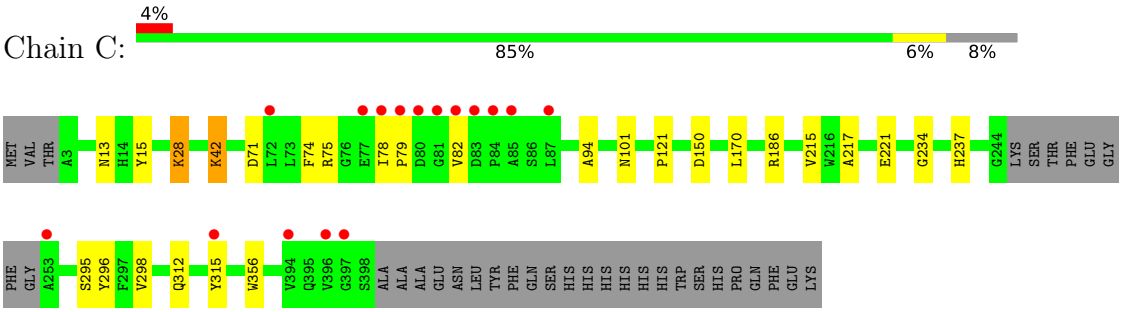
• Molecule 1: Putative TIM-barrel metal-dependent hydrolase

Chain B:



• Molecule 1: Putative TIM-barrel metal-dependent hydrolase

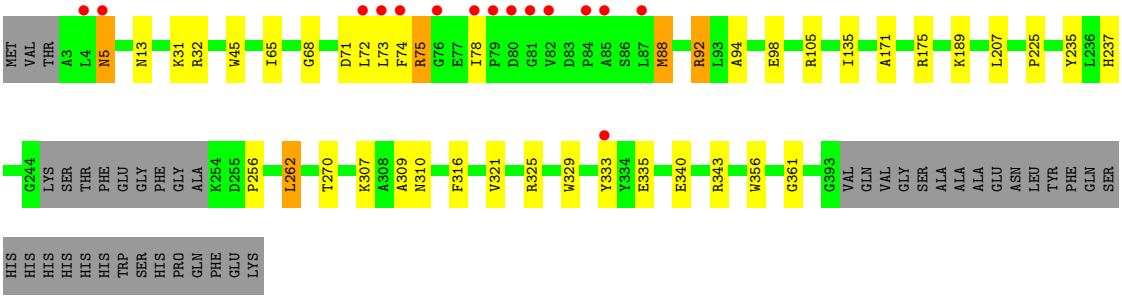
Chain C:



• Molecule 1: Putative TIM-barrel metal-dependent hydrolase

Chain D:

4%
80%
9%
10%


MET VAL THR A3 L4 N5 N13 K31 R32 W45 I65 G68 D71 L72 L73 F74 R75 G76 E77 I78 P79 D80 G81 V82 D83 P84 A85 S86 L87 M88 R92 L93 A94 E98 R105 I135 A171 R175 K189 L207 P225 Y235 L236 H237
G244 LYS SER THR PHE GLU GLY PHE GLY ALA K254 D255 P256 L262 T270 K307 A308 A309 N310 F316 V321 R325 W329 Y333 Y334 E335 E340 R343 W356 G361 G393 VAL GLN VAL GLY SER ALA ALA ALA GLU ASN LEU TYR PHE GLN SER
HIS HIS HIS HIS HIS HIS TRP SER HIS PRO GLN PHE GLU LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	75.11Å 136.13Å 93.23Å 90.00° 113.09° 90.00°	Depositor
Resolution (Å)	50.00 – 1.60 40.11 – 1.60	Depositor EDS
% Data completeness (in resolution range)	93.2 (50.00-1.60) 93.2 (40.11-1.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [1]	1.38 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.166 , 0.203 0.167 , 0.203	Depositor DCC
R_{free} test set	6300 reflections (3.00%)	wwPDB-VP
Wilson B-factor (Å^2)	16.8	Xtriage
Anisotropy	0.176	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 42.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	14003	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.55% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

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

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CD, SO4, MG, CL

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	0.66	2/3162 (0.1%)	0.73	1/4295 (0.0%)
1	B	0.70	2/3180 (0.1%)	0.74	2/4322 (0.0%)
1	C	0.64	1/3185 (0.0%)	0.71	0/4332
1	D	0.65	3/3172 (0.1%)	0.69	0/4312
All	All	0.67	8/12699 (0.1%)	0.72	3/17261 (0.0%)

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	45	TRP	CD2-CE2	5.44	1.47	1.41
1	A	148	TRP	CD2-CE2	5.41	1.47	1.41
1	B	216	TRP	CD2-CE2	5.23	1.47	1.41
1	A	45	TRP	CD2-CE2	5.14	1.47	1.41
1	B	45	TRP	CD2-CE2	5.12	1.47	1.41
1	D	329	TRP	CD2-CE2	5.11	1.47	1.41
1	C	356	TRP	CD2-CE2	5.02	1.47	1.41
1	D	356	TRP	CD2-CE2	5.00	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	262	LEU	CA-CB-CG	5.55	128.07	115.30
1	B	218[A]	ARG	NE-CZ-NH2	5.20	122.90	120.30
1	B	218[B]	ARG	NE-CZ-NH2	5.20	122.90	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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	3070	0	3047	54	0
1	B	3077	0	3056	42	0
1	C	3092	0	3051	19	0
1	D	3070	0	3035	40	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
3	A	3	0	0	2	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	1	0	0	0	0
5	A	5	0	0	0	0
5	B	10	0	0	1	0
6	A	438	0	0	11	0
6	B	448	0	0	8	0
6	C	415	0	0	5	0
6	D	363	0	0	3	0
All	All	14003	0	12189	150	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 6.

All (150) 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:71:ASP:HB3	6:B:1020:HOH:O	1.46	1.14
1:A:136:GLU:HG2	1:A:175[B]:ARG:HH22	1.21	1.05
1:D:75:ARG:HG3	1:D:335:GLU:HG3	1.41	0.98
1:B:69:CYS:HB2	1:B:89:LYS:HE2	1.48	0.93
1:A:307:LYS:HE2	1:C:74:PHE:O	1.70	0.92
1:D:65:ILE:CD1	1:D:88:MET:HE1	2.00	0.91
1:D:65:ILE:HD12	1:D:88:MET:HE1	1.52	0.90
1:B:237:HIS:HB3	6:B:964:HOH:O	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ARG:NH2	1:A:334:TYR:CD1	2.40	0.89
1:D:73:LEU:CD1	1:D:78:ILE:HD11	2.06	0.85
1:D:75:ARG:CG	1:D:335:GLU:HG3	2.09	0.82
1:D:65:ILE:CD1	1:D:88:MET:CE	2.58	0.82
1:B:221:GLU:HG3	6:B:1000:HOH:O	1.79	0.80
1:A:335:GLU:HB2	3:A:507:CL:CL	2.19	0.79
1:D:5:ASN:C	1:D:5:ASN:HD22	1.85	0.79
1:D:73:LEU:HD12	1:D:78:ILE:HD11	1.62	0.78
1:D:65:ILE:HD12	1:D:88:MET:CE	2.17	0.75
1:D:75:ARG:HG3	1:D:335:GLU:CG	2.16	0.73
1:B:235:TYR:HB3	1:B:262:LEU:HD13	1.70	0.73
1:D:340:GLU:OE2	1:D:343:ARG:NH2	2.22	0.73
1:B:76:GLY:C	1:D:310:ASN:OD1	2.28	0.72
1:B:175:ARG:NH1	6:B:844:HOH:O	2.22	0.72
1:A:75:ARG:HG2	3:A:507:CL:CL	2.28	0.71
1:C:150:ASP:OD2	1:C:186:ARG:HD2	1.92	0.70
1:B:69:CYS:CB	1:B:89:LYS:HE2	2.24	0.67
1:B:5:ASN:HD22	1:B:5:ASN:C	1.99	0.66
1:A:300:ARG:CG	6:A:912:HOH:O	2.43	0.66
1:A:299:HIS:NE2	6:A:912:HOH:O	2.28	0.65
1:D:73:LEU:HD13	1:D:78:ILE:HD11	1.77	0.65
1:B:74[B]:PHE:HE1	6:B:880:HOH:O	1.79	0.65
1:B:235:TYR:HB3	1:B:262:LEU:CD1	2.27	0.65
1:D:237:HIS:NE2	6:D:863:HOH:O	2.30	0.65
1:A:74:PHE:HE1	6:A:921:HOH:O	1.79	0.65
1:A:300:ARG:HD2	6:A:912:HOH:O	1.97	0.65
1:A:221:GLU:HG3	6:A:810:HOH:O	1.98	0.64
1:A:75:ARG:NH2	1:A:334:TYR:HD1	1.92	0.64
1:D:75:ARG:CG	1:D:335:GLU:CG	2.75	0.63
1:A:172:ASP:CG	1:A:175[B]:ARG:HD2	2.20	0.62
1:A:172:ASP:OD2	1:A:175[B]:ARG:HD2	1.99	0.61
1:A:136:GLU:HG2	1:A:175[B]:ARG:NH2	2.03	0.61
1:A:340:GLU:OE1	1:A:343[B]:ARG:NH1	2.34	0.60
1:A:334:TYR:CZ	1:A:371:GLU:OE2	2.55	0.59
1:A:75:ARG:NH2	1:A:334:TYR:CE1	2.70	0.59
1:A:83:ASP:OD1	1:A:83:ASP:C	2.42	0.58
1:C:28:LYS:HG3	6:C:925:HOH:O	2.03	0.58
1:D:235:TYR:HB3	1:D:262:LEU:HD22	1.85	0.58
1:B:73:LEU:HD23	1:B:73:LEU:C	2.23	0.58
1:C:234:GLY:O	1:C:237:HIS:HD2	1.87	0.58
1:D:333[B]:TYR:CE2	1:D:335:GLU:HB2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:217:ALA:O	1:C:221:GLU:HG2	2.04	0.57
1:B:300:ARG:NE	5:B:504[B]:SO4:O4	2.38	0.57
1:D:65:ILE:HD11	1:D:88:MET:CE	2.34	0.57
1:B:69:CYS:HB2	1:B:89:LYS:CE	2.29	0.57
1:A:334:TYR:CE2	1:A:371:GLU:HG2	2.39	0.57
1:D:65:ILE:CG1	1:D:88:MET:HE1	2.34	0.57
1:B:235:TYR:CB	1:B:262:LEU:CD1	2.83	0.56
1:A:75:ARG:HD3	1:A:335:GLU:HG3	1.88	0.56
1:C:94:ALA:HA	6:C:921:HOH:O	2.05	0.56
1:D:5:ASN:C	1:D:5:ASN:ND2	2.59	0.56
1:B:235:TYR:CB	1:B:262:LEU:HD13	2.36	0.55
1:B:69:CYS:CB	1:B:89:LYS:CE	2.83	0.55
1:A:85:ALA:HA	6:A:1038:HOH:O	2.05	0.55
1:A:300:ARG:CD	6:A:912:HOH:O	2.53	0.55
1:A:136:GLU:CG	1:A:175[B]:ARG:HH22	2.09	0.55
1:D:75:ARG:HD2	1:D:333[B]:TYR:OH	2.06	0.55
1:A:75:ARG:HD3	1:A:335:GLU:CG	2.38	0.54
1:B:27:ASP:HB2	6:B:831:HOH:O	2.07	0.54
1:A:5:ASN:C	1:A:5:ASN:HD22	2.12	0.53
1:A:300:ARG:HG3	6:A:912:HOH:O	2.07	0.53
1:D:74[A]:PHE:HZ	1:D:333[A]:TYR:CZ	2.28	0.52
1:A:77:GLU:OE1	1:A:335:GLU:OE2	2.28	0.51
1:A:235:TYR:HB3	1:A:262:LEU:HD13	1.92	0.51
1:B:314:GLN:O	1:B:314:GLN:HG2	2.06	0.51
1:B:382[B]:LYS:HA	1:B:386:ASP:HB2	1.92	0.50
1:B:382[A]:LYS:HA	1:B:386:ASP:HB2	1.92	0.50
1:A:334:TYR:CE1	1:A:371:GLU:OE2	2.65	0.50
1:A:5:ASN:C	1:A:5:ASN:ND2	2.64	0.49
1:A:65:ILE:HD11	1:A:70:LEU:CD1	2.42	0.49
1:D:92:ARG:C	1:D:94:ALA:N	2.64	0.49
1:A:75:ARG:CZ	1:A:334:TYR:CD1	2.96	0.49
1:D:68:GLY:O	1:D:71:ASP:HB2	2.13	0.49
1:C:42:LYS:CD	1:C:42:LYS:N	2.76	0.48
1:B:38:LEU:HD12	1:B:47:VAL:HG21	1.96	0.48
1:B:298:VAL:CG2	1:B:330[B]:ILE:HD13	2.44	0.48
1:A:65:ILE:HD11	1:A:70:LEU:HD11	1.94	0.48
1:C:170:LEU:HD21	1:C:215:VAL:HG11	1.96	0.48
1:A:65:ILE:CD1	1:A:70:LEU:HD11	2.44	0.48
1:B:373:LYS:HB2	6:B:692:HOH:O	2.13	0.48
1:B:28:LYS:N	1:B:28:LYS:HD3	2.29	0.48
1:A:245:LYS:HB3	1:A:245:LYS:NZ	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:309:ALA:HA	1:D:316:PHE:CD1	2.49	0.47
1:B:75:ARG:HG3	1:B:333[B]:TYR:OH	2.15	0.47
1:D:31:LYS:HE3	1:D:32:ARG:CZ	2.44	0.47
1:D:135:ILE:HD12	1:D:171:ALA:HB1	1.97	0.47
1:B:298:VAL:HG21	1:B:330[B]:ILE:HD13	1.96	0.47
1:A:66:VAL:HG22	1:A:91:GLU:HG3	1.97	0.47
1:A:139:MET:HG3	1:A:175[B]:ARG:HD3	1.97	0.46
1:A:98:GLU:HB2	1:A:105:ARG:HA	1.96	0.46
1:A:113:ASP:OD2	6:A:860:HOH:O	2.20	0.46
1:C:312:GLN:HB3	1:C:315:TYR:HD2	1.80	0.46
1:D:65:ILE:HG13	1:D:88:MET:HE1	1.96	0.46
1:A:303[A]:LYS:HD3	1:C:296:TYR:CZ	2.51	0.46
1:A:303[A]:LYS:HD3	1:C:296:TYR:CE2	2.51	0.45
1:B:135:ILE:HD12	1:B:171:ALA:HB1	1.99	0.45
1:C:295:SER:O	1:C:298[B]:VAL:HG22	2.17	0.45
1:B:214:PRO:O	1:B:218[B]:ARG:HG2	2.16	0.45
1:A:334:TYR:CE2	1:A:371:GLU:CG	2.99	0.45
1:C:298[B]:VAL:CG2	6:C:752:HOH:O	2.64	0.45
1:B:330[B]:ILE:HD12	1:B:345:ILE:HD13	1.99	0.45
1:C:71:ASP:O	1:C:75:ARG:HG3	2.17	0.44
1:B:73:LEU:HD23	1:B:73:LEU:O	2.18	0.44
1:D:207:LEU:CD1	1:D:270:THR:HG23	2.47	0.44
1:A:75:ARG:CB	1:A:77:GLU:HG2	2.48	0.43
1:B:92[B]:ARG:HD3	1:B:92[B]:ARG:HA	1.62	0.43
1:A:339:PRO:O	1:A:343[A]:ARG:HG3	2.18	0.43
1:C:42:LYS:N	1:C:42:LYS:HD3	2.33	0.43
1:C:298[B]:VAL:HG22	6:C:752:HOH:O	2.17	0.43
1:A:237:HIS:NE2	6:A:927:HOH:O	2.33	0.43
1:C:101:ASN:HB2	6:C:769:HOH:O	2.18	0.43
1:A:116:THR:HA	1:A:161:ARG:O	2.18	0.43
1:B:68:GLY:HA2	1:B:361:GLY:O	2.19	0.42
1:D:189:LYS:O	1:D:225:PRO:HD2	2.19	0.42
1:A:235:TYR:CB	1:A:262:LEU:HD13	2.49	0.42
1:A:184:LEU:CD2	1:A:224:VAL:HG21	2.49	0.42
1:B:236:LEU:HD23	1:B:236:LEU:HA	1.79	0.42
1:A:28:LYS:HE2	6:A:1024:HOH:O	2.20	0.42
1:A:203:LYS:HB2	1:A:204:PRO:HD2	2.01	0.41
1:B:315:TYR:CG	1:D:256:PRO:HG3	2.55	0.41
1:A:135:ILE:HD12	1:A:171:ALA:HB1	2.02	0.41
1:B:166:PRO:HD2	1:B:190:LEU:O	2.21	0.41
1:B:187:GLY:HA3	6:B:943:HOH:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:TYR:CE1	1:C:121:PRO:HA	2.55	0.41
1:A:170:LEU:HD21	1:A:215:VAL:HG11	2.02	0.41
1:B:69:CYS:HB3	1:B:89:LYS:CE	2.49	0.41
1:D:68:GLY:HA2	1:D:361:GLY:O	2.21	0.41
1:D:321:VAL:O	1:D:325[A]:ARG:HG3	2.21	0.41
1:B:49:GLY:O	1:B:50:ASP:HB2	2.21	0.41
1:D:72:LEU:HG	6:D:740:HOH:O	2.21	0.41
1:D:98:GLU:HB2	1:D:105:ARG:HA	2.02	0.41
1:A:88:MET:O	1:A:89:LYS:HD3	2.21	0.40
1:B:98:GLU:HB2	1:B:105:ARG:HA	2.03	0.40
1:D:92:ARG:C	1:D:94:ALA:H	2.24	0.40
1:A:65:ILE:HD11	1:A:70:LEU:HG	2.04	0.40
1:B:74[A]:PHE:HZ	1:B:333[A]:TYR:CE2	2.40	0.40
1:C:79:PRO:HG2	1:C:82:VAL:HG21	2.02	0.40
1:D:94:ALA:HA	6:D:944:HOH:O	2.21	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	384/423 (91%)	373 (97%)	11 (3%)	0	100	100
1	B	385/423 (91%)	377 (98%)	8 (2%)	0	100	100
1	C	388/423 (92%)	379 (98%)	9 (2%)	0	100	100
1	D	385/423 (91%)	374 (97%)	11 (3%)	0	100	100
All	All	1542/1692 (91%)	1503 (98%)	39 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	328/357 (92%)	324 (99%)	4 (1%)	71	54
1	B	330/357 (92%)	323 (98%)	7 (2%)	53	29
1	C	331/357 (93%)	327 (99%)	4 (1%)	71	54
1	D	329/357 (92%)	323 (98%)	6 (2%)	59	36
All	All	1318/1428 (92%)	1297 (98%)	21 (2%)	62	41

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	A	13	ASN
1	A	245	LYS
1	A	262	LEU
1	B	5	ASN
1	B	13	ASN
1	B	28	LYS
1	B	71	ASP
1	B	77	GLU
1	B	113	ASP
1	B	314	GLN
1	C	13	ASN
1	C	28	LYS
1	C	42	LYS
1	C	78	ILE
1	D	5	ASN
1	D	13	ASN
1	D	75	ARG
1	D	88	MET
1	D	92	ARG
1	D	262	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	ASN
1	B	5	ASN
1	C	259	GLN
1	D	5	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 monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 18 ligands modelled in this entry, 15 are monoatomic - leaving 3 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	SO4	B	504[B]	-	4,4,4	0.31	0	6,6,6	0.29	0
5	SO4	B	504[A]	-	4,4,4	0.48	0	6,6,6	0.17	0
5	SO4	A	506	-	4,4,4	0.35	0	6,6,6	1.49	1 (16%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	506	SO4	O4-S-O1	2.34	121.52	109.31

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	504[B]	SO4	1	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	384/423 (90%)	-0.23	13 (3%)	45	42	10, 20, 53, 102	0
1	B	382/423 (90%)	-0.34	10 (2%)	56	53	10, 19, 45, 73	0
1	C	388/423 (91%)	-0.30	16 (4%)	37	34	11, 19, 50, 126	0
1	D	382/423 (90%)	-0.20	15 (3%)	39	36	12, 21, 54, 111	0
All	All	1536/1692 (90%)	-0.27	54 (3%)	44	41	10, 20, 51, 126	0

All (54) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	76	GLY	7.6
1	A	80	ASP	6.7
1	C	80	ASP	6.1
1	A	253	ALA	6.0
1	D	80	ASP	5.8
1	C	81	GLY	5.7
1	D	74[A]	PHE	5.6
1	C	79	PRO	5.4
1	A	81	GLY	5.1
1	D	82	VAL	5.0
1	A	82	VAL	5.0
1	D	78	ILE	4.6
1	C	82	VAL	4.4
1	A	83	ASP	4.0
1	C	394	VAL	3.9
1	B	82	VAL	3.9
1	C	78	ILE	3.8
1	D	79	PRO	3.7
1	B	85	ALA	3.5
1	C	253	ALA	3.3
1	C	84	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	79	PRO	3.1
1	D	72	LEU	3.1
1	A	85	ALA	3.0
1	D	85	ALA	3.0
1	C	83	ASP	3.0
1	C	77	GLU	2.8
1	A	78	ILE	2.8
1	A	84	PRO	2.8
1	B	79	PRO	2.8
1	A	76	GLY	2.7
1	C	315	TYR	2.6
1	D	81	GLY	2.6
1	B	81	GLY	2.6
1	A	72	LEU	2.6
1	D	73	LEU	2.5
1	D	87	LEU	2.5
1	B	333[A]	TYR	2.5
1	D	84	PRO	2.5
1	B	76	GLY	2.4
1	C	72	LEU	2.4
1	B	80	ASP	2.3
1	A	3	ALA	2.3
1	C	396	VAL	2.3
1	B	78	ILE	2.3
1	C	397	GLY	2.3
1	B	42	LYS	2.3
1	C	85	ALA	2.3
1	B	74[A]	PHE	2.3
1	D	5	ASN	2.2
1	D	4	LEU	2.1
1	D	333[A]	TYR	2.0
1	A	5	ASN	2.0
1	C	87	LEU	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 monosaccharides 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
3	CL	C	503	1/1	0.96	0.04	26,26,26,26	0
3	CL	A	507	1/1	0.97	0.05	52,52,52,52	0
3	CL	D	503	1/1	0.97	0.04	25,25,25,25	0
5	SO4	A	506	5/5	0.98	0.06	21,24,24,55	0
3	CL	B	503	1/1	0.99	0.03	23,23,23,23	0
4	MG	A	504	1/1	0.99	0.18	30,30,30,30	0
3	CL	A	503	1/1	0.99	0.04	25,25,25,25	0
5	SO4	B	504[A]	5/5	0.99	0.10	19,21,33,37	5
5	SO4	B	504[B]	5/5	0.99	0.10	16,17,20,35	5
3	CL	A	505	1/1	1.00	0.03	21,21,21,21	0
2	CD	A	502	1/1	1.00	0.06	13,13,13,13	0
2	CD	B	501	1/1	1.00	0.04	14,14,14,14	0
2	CD	B	502	1/1	1.00	0.04	12,12,12,12	0
2	CD	C	501	1/1	1.00	0.04	14,14,14,14	0
2	CD	C	502	1/1	1.00	0.05	12,12,12,12	0
2	CD	D	501	1/1	1.00	0.05	16,16,16,16	0
2	CD	D	502	1/1	1.00	0.05	14,14,14,14	0
2	CD	A	501	1/1	1.00	0.05	16,16,16,16	0

6.5 Other polymers (i)

There are no such residues in this entry.