



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 04:28 am GMT

PDB ID : 4MM2
Title : Crystal structure of yeast primase catalytic subunit
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Deposited on : 2013-09-07
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

<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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

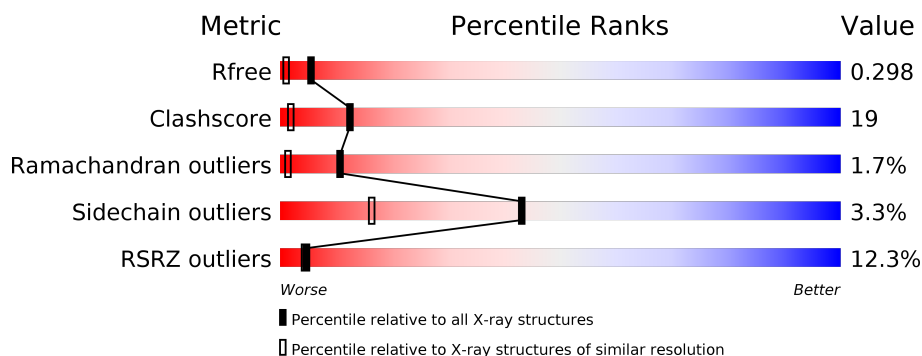
1 Overall quality at a glance

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}	100719	2696 (1.60-1.60)
Clashscore	112137	2967 (1.60-1.60)
Ramachandran outliers	110173	2887 (1.60-1.60)
Sidechain outliers	110143	2886 (1.60-1.60)
RSRZ outliers	101464	2714 (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. 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	414	<div> <div>10%</div> <div>73%</div> <div>18%</div> <div>• • •</div> </div>
1	B	414	<div> <div>13%</div> <div>73%</div> <div>19%</div> <div>• 5%</div> </div>

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	CIT	A	506	-	-	X	X
3	CIT	B	506	-	-	-	X

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6980 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 DNA primase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	396	Total	C	N	O	S	0	6	0
			3286	2094	568	608	16			
1	B	394	Total	C	N	O	S	0	3	0
			3263	2077	567	603	16			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-4	GLY	-	EXPRESSION TAG	UNP P10363
A	-3	ALA	-	EXPRESSION TAG	UNP P10363
A	-2	MET	-	EXPRESSION TAG	UNP P10363
A	-1	GLY	-	EXPRESSION TAG	UNP P10363
A	0	SER	-	EXPRESSION TAG	UNP P10363
B	-4	GLY	-	EXPRESSION TAG	UNP P10363
B	-3	ALA	-	EXPRESSION TAG	UNP P10363
B	-2	MET	-	EXPRESSION TAG	UNP P10363
B	-1	GLY	-	EXPRESSION TAG	UNP P10363
B	0	SER	-	EXPRESSION TAG	UNP P10363

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	5	Total	Cd	0	0
			5	5		
2	A	5	Total	Cd	0	0
			5	5		

- Molecule 3 is CITRIC ACID (three-letter code: CIT) (formula: C₆H₈O₇).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		

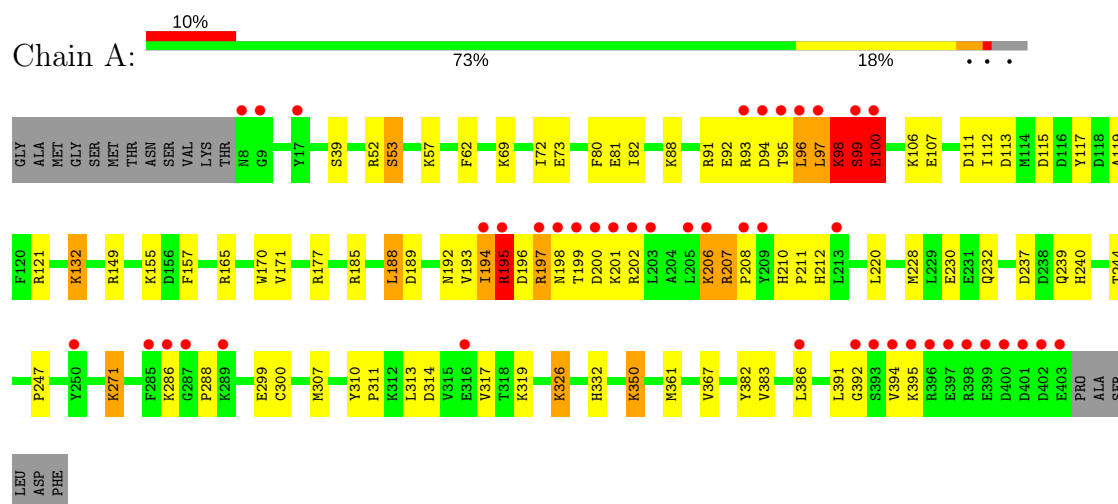
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	187	Total	O	0	0
			187	187		
4	B	208	Total	O	0	0
			208	208		

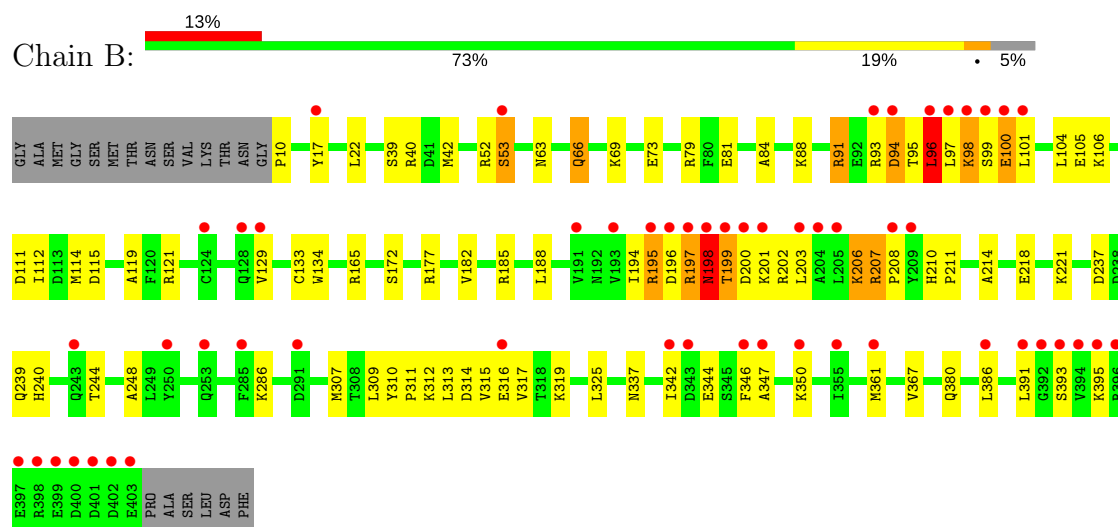
3 Residue-property plots [i](#)

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: DNA primase small subunit



• Molecule 1: DNA primase small subunit



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.37Å 196.04Å 53.96Å 90.00° 114.72° 90.00°	Depositor
Resolution (Å)	43.88 – 1.60 43.84 – 1.60	Depositor EDS
% Data completeness (in resolution range)	92.8 (43.88-1.60) 86.0 (43.84-1.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.27 (at 1.60Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.255 , 0.293 0.268 , 0.298	Depositor DCC
R_{free} test set	5568 reflections (5.28%)	DCC
Wilson B-factor (Å ²)	17.1	Xtriage
Anisotropy	0.212	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 32.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.169 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6980	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.61% 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

5.1 Standard geometry

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

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	0.56	1/3382 (0.0%)	0.81	7/4568 (0.2%)
1	B	0.51	0/3350	0.77	2/4523 (0.0%)
All	All	0.54	1/6732 (0.0%)	0.79	9/9091 (0.1%)

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	A	0	2
1	B	0	3
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	207	ARG	C-N	-7.18	1.20	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	207	ARG	NE-CZ-NH1	-7.75	116.42	120.30
1	B	207	ARG	NE-CZ-NH2	7.05	123.83	120.30
1	A	99	SER	N-CA-C	-6.88	92.41	111.00
1	A	207	ARG	O-C-N	6.47	133.38	121.10
1	A	113	ASP	CB-CG-OD1	-6.15	112.77	118.30
1	A	206	LYS	O-C-N	-5.78	113.45	122.70
1	A	188	LEU	CA-CB-CG	-5.31	103.10	115.30
1	A	97	LEU	CA-CB-CG	5.25	127.38	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	195	ARG	N-CA-C	5.10	124.77	111.00

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	98	LYS	Peptide
1	A	99	SER	Peptide
1	B	197	ARG	Peptide
1	B	198	ASN	Peptide
1	B	99	SER	Peptide

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	3286	0	3267	130	0
1	B	3263	0	3237	117	0
2	A	5	0	0	0	0
2	B	5	0	0	0	0
3	A	13	0	5	8	0
3	B	13	0	5	1	0
4	A	187	0	0	24	0
4	B	208	0	0	18	0
All	All	6980	0	6514	246	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 19.

All (246) 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:97:LEU:CD2	1:B:100:GLU:HB3	1.67	1.23
1:B:88:LYS:HD2	1:B:98:LYS:CD	1.69	1.20
1:B:97:LEU:HD23	1:B:100:GLU:CB	1.78	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:198:ASN:HB3	1:A:199:THR:HA	1.34	1.10
1:B:97:LEU:CD2	1:B:100:GLU:CB	2.31	1.09
1:B:88:LYS:HD2	1:B:98:LYS:HD3	1.37	1.06
1:A:199:THR:HB	1:A:200:ASP:HA	1.38	1.06
3:B:506:CIT:H41	4:B:645:HOH:O	1.57	1.04
1:B:97:LEU:HD23	1:B:100:GLU:HB2	1.36	1.02
1:B:97:LEU:HD22	1:B:100:GLU:HB3	1.36	1.01
1:B:199:THR:HB	1:B:200:ASP:HA	1.42	0.99
1:B:88:LYS:HD2	1:B:98:LYS:HD2	1.43	0.98
1:A:382:TYR:CE2	1:A:386:LEU:HD11	2.02	0.94
1:A:88:LYS:HD2	1:A:98:LYS:HD2	1.49	0.93
1:A:228:MET:SD	4:A:776:HOH:O	2.28	0.92
1:A:95:THR:HA	1:A:96:LEU:HB2	1.52	0.92
1:A:111:ASP:HB3	1:A:317[A]:VAL:HG21	1.53	0.90
1:A:97:LEU:HD23	1:A:100:GLU:HB3	1.50	0.90
1:B:88:LYS:CD	1:B:98:LYS:CD	2.50	0.90
1:A:207:ARG:HA	1:A:208:PRO:C	1.92	0.89
1:B:199:THR:CB	1:B:200:ASP:HA	2.03	0.88
1:B:198:ASN:HB2	1:B:307:MET:CE	2.03	0.88
1:A:81:GLU:CA	4:A:721:HOH:O	2.23	0.87
1:B:199:THR:HA	1:B:201:LYS:H	1.41	0.85
1:B:88:LYS:CD	1:B:98:LYS:HD3	2.06	0.85
1:A:326[B]:LYS:HE3	3:A:506:CIT:O5	1.76	0.85
1:A:96:LEU:CD1	1:A:97:LEU:HG	2.10	0.82
1:A:69:LYS:HE2	1:A:73:GLU:OE2	1.79	0.81
1:B:88:LYS:CD	1:B:98:LYS:HD2	2.10	0.80
1:B:198:ASN:HB2	1:B:307:MET:HE1	1.64	0.80
1:A:94:ASP:N	1:A:96:LEU:HD23	1.97	0.80
1:A:88:LYS:HD2	1:A:98:LYS:CD	2.12	0.79
1:B:100:GLU:HG2	1:B:101:LEU:H	1.48	0.78
1:B:42:MET:HB2	4:B:653:HOH:O	1.82	0.78
1:A:199:THR:HB	1:A:200:ASP:CA	2.13	0.77
1:A:326[B]:LYS:CE	3:A:506:CIT:O5	2.33	0.76
1:A:95:THR:CA	1:A:96:LEU:HB2	2.14	0.76
1:A:111:ASP:CB	1:A:317[A]:VAL:HG21	2.16	0.75
1:A:199:THR:CB	1:A:200:ASP:HA	2.15	0.75
1:A:107:GLU:HB3	4:A:644:HOH:O	1.87	0.74
1:A:314[B]:ASP:OD2	1:A:317[B]:VAL:CG2	2.36	0.73
1:A:332:HIS:CD2	3:A:506:CIT:O6	2.41	0.73
1:A:198:ASN:CB	1:A:199:THR:HA	2.15	0.73
1:A:81:GLU:HA	4:A:721:HOH:O	1.86	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:198:ASN:HB2	1:B:307:MET:HE3	1.70	0.72
1:A:88:LYS:NZ	1:A:96:LEU:O	2.23	0.72
1:B:111:ASP:HB2	4:B:683:HOH:O	1.88	0.72
1:B:40[A]:ARG:NH2	1:B:105:GLU:OE2	2.21	0.72
1:B:96:LEU:HD13	1:B:97:LEU:HB2	1.72	0.72
1:A:326[B]:LYS:NZ	3:A:506:CIT:O5	2.23	0.71
1:A:117:TYR:HB2	4:A:645:HOH:O	1.89	0.70
1:A:383:VAL:HA	1:A:386:LEU:HD12	1.74	0.70
1:B:198:ASN:CB	1:B:307:MET:HE3	2.21	0.69
1:A:197:ARG:NH1	4:A:725:HOH:O	2.25	0.68
1:B:69:LYS:HE2	1:B:73:GLU:OE1	1.94	0.68
1:A:132:LYS:NZ	1:A:132:LYS:HB3	2.08	0.68
1:A:198:ASN:HB3	1:A:199:THR:CA	2.18	0.68
1:A:314[B]:ASP:OD2	1:A:317[B]:VAL:HG21	1.95	0.67
1:A:94:ASP:H	1:A:96:LEU:HD23	1.57	0.66
1:A:94:ASP:C	1:A:96:LEU:HB2	2.14	0.66
1:A:200:ASP:O	1:A:247:PRO:HB3	1.96	0.66
1:B:81:GLU:HG3	4:B:731:HOH:O	1.94	0.66
1:B:88:LYS:HE3	1:B:98:LYS:HD2	1.78	0.66
1:A:185:ARG:CD	1:A:319:LYS:HD2	2.27	0.65
1:A:132:LYS:HZ2	1:A:132:LYS:HB3	1.60	0.64
1:B:325:LEU:HD11	4:B:683:HOH:O	1.96	0.64
1:A:97:LEU:HD23	1:A:100:GLU:CB	2.25	0.64
1:A:314[B]:ASP:CG	1:A:317[B]:VAL:HG23	2.18	0.64
1:A:96:LEU:HD13	1:A:97:LEU:HG	1.80	0.64
1:B:88:LYS:CE	1:B:98:LYS:HD2	2.28	0.64
1:A:200:ASP:O	1:A:247:PRO:CB	2.46	0.64
1:B:207:ARG:HA	1:B:208:PRO:C	2.17	0.64
1:A:94:ASP:O	1:A:96:LEU:HB2	1.98	0.63
1:B:93:ARG:O	1:B:94:ASP:HB2	1.97	0.62
1:A:196:ASP:HB2	1:A:198:ASN:HD21	1.65	0.62
1:A:88:LYS:CD	1:A:98:LYS:HD2	2.27	0.62
1:B:96:LEU:HD13	1:B:97:LEU:H	1.63	0.62
1:A:314[B]:ASP:OD2	1:A:317[B]:VAL:HG23	1.99	0.61
1:A:81:GLU:C	4:A:721:HOH:O	2.37	0.61
1:A:314[B]:ASP:OD1	1:A:317[B]:VAL:HG23	2.00	0.61
1:A:72:ILE:HG12	4:A:775:HOH:O	2.00	0.61
1:B:94:ASP:C	1:B:96:LEU:HB3	2.21	0.61
1:A:95:THR:HA	1:A:96:LEU:CB	2.28	0.61
1:A:94:ASP:CA	1:A:96:LEU:HD23	2.31	0.61
1:B:199:THR:HG21	1:B:244:THR:HA	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:199:THR:HB	1:B:200:ASP:CA	2.24	0.60
1:A:185:ARG:NH1	1:A:189:ASP:OD1	2.35	0.60
1:B:95:THR:N	1:B:96:LEU:HB3	2.16	0.60
1:A:93:ARG:O	1:A:94:ASP:HB2	2.02	0.59
1:B:88:LYS:CE	1:B:98:LYS:CD	2.79	0.59
1:A:121:ARG:CD	4:A:645:HOH:O	2.49	0.59
1:A:220:LEU:HD21	4:A:624:HOH:O	2.02	0.59
1:B:10:PRO:O	1:B:52:ARG:NH1	2.35	0.59
1:A:350:LYS:O	1:A:350:LYS:HG3	2.01	0.59
1:B:195:ARG:NH1	1:B:203:LEU:O	2.31	0.59
1:B:96:LEU:CD1	1:B:97:LEU:H	2.17	0.57
1:A:121:ARG:HD3	4:A:645:HOH:O	2.04	0.57
1:B:172[B]:SER:OG	1:B:386:LEU:HD21	2.06	0.56
1:A:193:VAL:HG23	1:A:194:ILE:CG2	2.36	0.56
1:A:39:SER:HA	1:B:39:SER:HA	1.87	0.56
1:B:198:ASN:CB	1:B:307:MET:CE	2.78	0.56
1:B:237:ASP:OD1	1:B:239:GLN:HG2	2.06	0.55
1:A:237:ASP:OD1	1:A:239:GLN:HG2	2.06	0.55
1:A:95:THR:N	1:A:96:LEU:HB2	2.20	0.55
1:B:79:ARG:HG3	4:B:731:HOH:O	2.06	0.55
1:A:391:LEU:O	1:A:394:VAL:HG22	2.07	0.55
1:A:198:ASN:HB2	1:A:307:MET:HE3	1.90	0.54
1:B:94:ASP:CA	1:B:96:LEU:HB3	2.38	0.54
1:A:52:ARG:O	1:A:53:SER:HB3	2.07	0.54
1:B:188:LEU:HD21	1:B:315:VAL:HB	1.90	0.54
1:A:394:VAL:HG23	1:B:391:LEU:HD21	1.90	0.54
1:A:326[B]:LYS:HZ1	3:A:506:CIT:C6	2.20	0.53
1:A:96:LEU:HD11	1:A:97:LEU:HG	1.90	0.53
1:B:188:LEU:HD22	1:B:319:LYS:HG3	1.90	0.53
1:B:200:ASP:O	1:B:201:LYS:HG3	2.07	0.53
1:B:96:LEU:HD13	1:B:97:LEU:N	2.23	0.53
1:B:194:ILE:HD11	1:B:312:LYS:HG2	1.90	0.53
1:A:157:PHE:HB3	1:A:171:VAL:HG22	1.91	0.53
1:B:52:ARG:O	1:B:53:SER:HB3	2.09	0.53
1:B:196:ASP:O	1:B:198:ASN:ND2	2.41	0.53
1:B:199:THR:HA	1:B:201:LYS:N	2.18	0.52
1:B:214:ALA:O	1:B:218:GLU:HG2	2.09	0.52
1:A:112:ILE:CD1	1:A:313:LEU:HD23	2.40	0.52
1:A:170:TRP:HA	4:A:644:HOH:O	2.08	0.51
1:B:95:THR:N	1:B:96:LEU:CA	2.74	0.51
1:A:185:ARG:HD2	1:A:319:LYS:HD2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:112:ILE:CD1	1:B:313:LEU:HD23	2.40	0.51
1:B:314:ASP:OD2	1:B:317:VAL:HG23	2.10	0.51
1:B:199:THR:CB	1:B:200:ASP:CA	2.81	0.51
1:B:194:ILE:HD12	1:B:197:ARG:NE	2.26	0.51
1:A:199:THR:HB	1:A:200:ASP:C	2.31	0.51
1:B:63:ASN:OD1	1:B:91:ARG:NH2	2.44	0.51
1:B:95:THR:N	1:B:96:LEU:CB	2.73	0.51
1:A:149:ARG:NH2	4:A:716:HOH:O	2.38	0.50
1:A:96:LEU:HD13	1:A:97:LEU:N	2.26	0.50
1:A:210:HIS:CD2	1:A:211:PRO:HD2	2.46	0.50
1:A:99:SER:O	1:A:100:GLU:HG2	2.10	0.50
1:A:193:VAL:HG23	1:A:194:ILE:HG22	1.93	0.50
3:A:506:CIT:O7	3:A:506:CIT:O3	2.21	0.50
1:A:52:ARG:NH2	4:A:783:HOH:O	2.44	0.50
1:B:347:ALA:HB3	1:B:350:LYS:HG2	1.92	0.50
1:B:17:TYR:OH	1:B:361:MET:SD	2.58	0.50
1:B:84:ALA:HB1	4:B:632:HOH:O	2.10	0.50
1:B:94:ASP:N	1:B:96:LEU:HB3	2.26	0.50
1:A:202:ARG:HD2	1:A:300:CYS:SG	2.52	0.50
1:B:66:GLN:CD	1:B:66:GLN:H	2.15	0.50
1:B:94:ASP:H	1:B:96:LEU:HB3	1.77	0.50
1:B:361:MET:HG3	1:B:367:VAL:HA	1.94	0.49
1:A:117:TYR:CB	4:A:645:HOH:O	2.56	0.49
1:B:115:ASP:OD1	1:B:165:ARG:HD2	2.12	0.49
1:B:133:CYS:C	4:B:634:HOH:O	2.51	0.49
1:A:332:HIS:NE2	3:A:506:CIT:O6	2.45	0.49
1:A:96:LEU:CD1	1:A:97:LEU:CG	2.88	0.49
1:B:22:LEU:HD11	1:B:361:MET:HE2	1.95	0.48
1:B:198:ASN:ND2	1:B:203:LEU:HD23	2.28	0.48
1:B:194:ILE:HD11	1:B:312:LYS:CG	2.42	0.48
1:A:199:THR:CB	1:A:200:ASP:CA	2.85	0.48
1:B:94:ASP:H	1:B:96:LEU:HA	1.79	0.48
1:B:182:VAL:HG22	1:B:185:ARG:NH2	2.29	0.48
1:A:314[B]:ASP:CG	1:A:317[B]:VAL:CG2	2.80	0.48
1:B:95:THR:H	1:B:96:LEU:HA	1.78	0.48
1:B:194:ILE:CD1	1:B:312:LYS:HG2	2.44	0.48
1:A:310:TYR:CG	1:A:311:PRO:HD2	2.49	0.47
1:B:344:GLU:O	4:B:762:HOH:O	2.20	0.47
1:A:80:PHE:C	4:A:721:HOH:O	2.53	0.47
1:A:210:HIS:CG	1:A:211:PRO:HD2	2.48	0.47
1:B:317:VAL:N	4:B:685:HOH:O	2.41	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:97:LEU:HD23	1:A:100:GLU:CG	2.45	0.47
1:A:207:ARG:CD	1:A:299:GLU:CD	2.83	0.47
1:A:106:LYS:O	1:A:177:ARG:HA	2.15	0.46
1:A:97:LEU:CD2	1:A:100:GLU:HG2	2.45	0.46
1:A:97:LEU:HD22	1:A:99:SER:O	2.15	0.46
1:A:92:GLU:OE1	1:B:91:ARG:NH1	2.48	0.46
1:B:88:LYS:HE3	1:B:98:LYS:CD	2.40	0.46
1:B:198:ASN:HB3	1:B:307:MET:HE3	1.95	0.46
1:A:237:ASP:C	1:A:237:ASP:OD1	2.54	0.46
1:A:82:ILE:N	4:A:721:HOH:O	2.46	0.46
1:A:115:ASP:OD1	1:A:165:ARG:HD2	2.16	0.45
1:B:63:ASN:HD21	1:B:91:ARG:HH12	1.65	0.45
1:A:193:VAL:CG2	1:A:194:ILE:HG23	2.45	0.45
1:A:112:ILE:HD11	1:A:313:LEU:HD23	1.99	0.45
1:A:232:GLN:HG3	4:A:776:HOH:O	2.16	0.45
1:B:199:THR:CA	1:B:201:LYS:H	2.20	0.45
1:B:342:ILE:HG23	1:B:346:PHE:HB2	1.99	0.44
1:A:96:LEU:HD13	1:A:97:LEU:CB	2.47	0.44
1:B:106:LYS:O	1:B:177:ARG:HA	2.18	0.44
1:A:96:LEU:HD13	1:A:97:LEU:CA	2.47	0.44
1:B:66:GLN:N	1:B:66:GLN:CD	2.69	0.44
1:A:230:GLU:CG	1:A:271:LYS:HE3	2.48	0.44
1:A:81:GLU:N	4:A:721:HOH:O	2.46	0.44
1:B:195:ARG:HD3	1:B:196:ASP:H	1.83	0.44
1:A:193:VAL:HG23	1:A:194:ILE:HG23	2.00	0.44
1:A:199:THR:HB	1:A:200:ASP:O	2.17	0.44
1:A:119:ALA:O	1:A:240:HIS:NE2	2.48	0.43
1:B:112:ILE:HD11	1:B:313:LEU:HD23	2.00	0.43
1:A:93:ARG:O	1:A:94:ASP:CB	2.65	0.43
1:B:22:LEU:HD11	1:B:361:MET:CE	2.48	0.43
1:B:111:ASP:CB	4:B:683:HOH:O	2.58	0.43
1:B:202:ARG:HG2	1:B:248:ALA:O	2.18	0.43
1:B:237:ASP:C	1:B:237:ASP:OD1	2.57	0.43
1:B:63:ASN:HD21	1:B:91:ARG:NH1	2.17	0.43
1:A:200:ASP:O	1:A:247:PRO:HB2	2.17	0.43
1:B:195:ARG:H	1:B:195:ARG:HG3	1.52	0.43
1:B:100:GLU:HG2	1:B:101:LEU:N	2.25	0.42
1:B:210:HIS:CG	1:B:211:PRO:HD2	2.54	0.42
1:B:221:LYS:HE3	1:B:221:LYS:HB2	1.94	0.42
1:B:310:TYR:CG	1:B:311:PRO:HD2	2.53	0.42
1:B:112:ILE:HD13	1:B:313:LEU:HD23	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:316:GLU:N	4:B:685:HOH:O	2.53	0.42
1:A:195:ARG:HB2	1:A:196:ASP:OD1	2.20	0.42
1:B:325:LEU:HD21	4:B:683:HOH:O	2.18	0.42
1:B:194:ILE:HD12	1:B:197:ARG:HE	1.84	0.42
1:A:332:HIS:HD2	3:A:506:CIT:O6	1.97	0.42
1:B:96:LEU:N	1:B:96:LEU:HD12	2.35	0.42
1:A:392:GLY:HA2	1:A:395:LYS:HB2	2.02	0.42
1:B:129:VAL:HG21	1:B:134:TRP:CE3	2.54	0.42
1:B:172[B]:SER:OG	1:B:386:LEU:CD2	2.68	0.42
1:B:206:LYS:O	1:B:206:LYS:CG	2.68	0.42
1:A:194:ILE:HD12	1:A:194:ILE:C	2.41	0.41
1:A:195:ARG:HG3	1:A:195:ARG:H	1.25	0.41
1:A:121:ARG:HG2	4:A:645:HOH:O	2.19	0.41
1:A:210:HIS:CG	1:A:211:PRO:CD	3.03	0.41
1:B:104:LEU:N	4:B:632:HOH:O	2.52	0.41
1:A:121:ARG:CG	4:A:645:HOH:O	2.68	0.41
1:A:82:ILE:HG13	4:A:721:HOH:O	2.20	0.41
1:B:121:ARG:O	4:B:610:HOH:O	2.22	0.41
1:B:380:GLN:NE2	4:B:699:HOH:O	2.52	0.41
1:B:314:ASP:OD2	1:B:317:VAL:CG2	2.69	0.41
1:A:192:ASN:OD1	1:A:197:ARG:NH2	2.51	0.41
1:B:114:MET:CE	4:B:634:HOH:O	2.68	0.41
1:A:210:HIS:CE1	1:A:212:HIS:H	2.37	0.41
1:A:232:GLN:CG	4:A:776:HOH:O	2.69	0.41
1:A:112:ILE:HD13	1:A:313:LEU:HD23	2.01	0.40
1:A:361:MET:CE	1:A:367:VAL:HG12	2.51	0.40
1:A:188:LEU:HG	1:A:188:LEU:O	2.18	0.40
1:B:195:ARG:HH12	1:B:203:LEU:C	2.21	0.40
1:A:199:THR:HG21	1:A:244:THR:HA	2.03	0.40
1:A:230:GLU:HG2	1:A:271:LYS:HE3	2.02	0.40
1:A:62:PHE:CE1	4:A:775:HOH:O	2.71	0.40
1:B:119:ALA:O	1:B:240:HIS:NE2	2.49	0.40
1:B:210:HIS:CD2	1:B:211:PRO:HD2	2.57	0.40
1:B:337:ASN:O	4:B:712:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	400/414 (97%)	383 (96%)	11 (3%)	6 (2%)	12	2
1	B	395/414 (95%)	373 (94%)	15 (4%)	7 (2%)	10	1
All	All	795/828 (96%)	756 (95%)	26 (3%)	13 (2%)	11	2

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	53	SER
1	A	96	LEU
1	A	98	LYS
1	B	53	SER
1	B	94	ASP
1	B	98	LYS
1	B	198	ASN
1	B	96	LEU
1	B	100	GLU
1	B	199	THR
1	A	100	GLU
1	A	197	ARG
1	A	288	PRO

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	367/375 (98%)	351 (96%)	16 (4%)	33	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	363/375 (97%)	354 (98%)	9 (2%)	53	25
All	All	730/750 (97%)	705 (97%)	25 (3%)	43	15

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	57	LYS
1	A	91	ARG
1	A	98	LYS
1	A	99	SER
1	A	100	GLU
1	A	132	LYS
1	A	155	LYS
1	A	194	ILE
1	A	195	ARG
1	A	201	LYS
1	A	206	LYS
1	A	271	LYS
1	A	286	LYS
1	A	326[A]	LYS
1	A	326[B]	LYS
1	A	350	LYS
1	B	66	GLN
1	B	91	ARG
1	B	96	LEU
1	B	195	ARG
1	B	206	LYS
1	B	286	LYS
1	B	309	LEU
1	B	393	SER
1	B	395	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	ASN
1	A	60	ASN
1	A	71	GLN
1	A	275	ASN
1	B	378	GLN
1	B	380	GLN

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Mol	Chain	Res	Type
1	B	389	ASN

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 12 ligands modelled in this entry, 10 are monoatomic - leaving 2 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$
3	CIT	A	506	-	3,12,12	1.53	1 (33%)	3,17,17	3.35	3 (100%)
3	CIT	B	506	2	3,12,12	0.56	0	3,17,17	4.06	2 (66%)

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
3	CIT	A	506	-	-	0/6/16/16	0/0/0/0
3	CIT	B	506	2	-	0/6/16/16	0/0/0/0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	506	CIT	O7-C3	2.47	1.47	1.43

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	506	CIT	C3-C4-C5	-4.42	108.04	114.95
3	A	506	CIT	C3-C2-C1	-2.98	110.29	114.95
3	A	506	CIT	C4-C3-C2	2.29	115.46	109.75
3	B	506	CIT	C3-C4-C5	3.69	120.72	114.95
3	B	506	CIT	C4-C3-C2	5.93	124.52	109.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	506	CIT	8	0
3	B	506	CIT	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

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	396/414 (95%)	0.94	43 (10%) 6 6	9, 22, 71, 150	0
1	B	394/414 (95%)	1.06	54 (13%) 3 3	10, 22, 72, 170	0
All	All	790/828 (95%)	1.00	97 (12%) 5 4	9, 22, 71, 170	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	400	ASP	24.9
1	B	398	ARG	12.6
1	A	394	VAL	12.5
1	A	401	ASP	11.8
1	A	398	ARG	11.7
1	B	396	ARG	11.5
1	B	200	ASP	11.4
1	B	99	SER	11.3
1	B	401	ASP	11.2
1	B	399	GLU	11.1
1	A	400	ASP	10.6
1	A	9	GLY	10.3
1	B	402	ASP	10.0
1	B	395	LYS	9.0
1	A	395	LYS	8.7
1	A	199	THR	8.2
1	B	403	GLU	7.7
1	A	402	ASP	7.4
1	A	99	SER	7.4
1	B	199	THR	6.8
1	A	399	GLU	6.2
1	A	396	ARG	6.0
1	A	97	LEU	5.8
1	A	198	ASN	5.8

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Mol	Chain	Res	Type	RSRZ
1	B	343	ASP	5.8
1	A	393	SER	5.5
1	A	287	GLY	5.4
1	B	397	GLU	5.3
1	B	394	VAL	5.1
1	B	250	TYR	5.0
1	A	403	GLU	4.8
1	B	198	ASN	4.8
1	B	204	ALA	4.7
1	B	393	SER	4.6
1	B	196	ASP	4.5
1	A	201	LYS	4.4
1	B	17	TYR	4.4
1	A	203	LEU	4.3
1	B	96	LEU	4.2
1	A	8	ASN	4.1
1	A	200	ASP	3.9
1	A	397	GLU	3.7
1	B	100	GLU	3.6
1	B	347	ALA	3.6
1	A	96	LEU	3.5
1	A	392	GLY	3.4
1	B	205	LEU	3.3
1	B	203	LEU	3.3
1	B	201	LYS	3.2
1	A	195	ARG	3.2
1	A	95	THR	3.2
1	B	191	VAL	3.0
1	A	17	TYR	3.0
1	B	386	LEU	2.9
1	A	250	TYR	2.9
1	B	98	LYS	2.8
1	A	285	PHE	2.8
1	A	386	LEU	2.8
1	A	205	LEU	2.8
1	B	94	ASP	2.8
1	B	342	ILE	2.7
1	B	208	PRO	2.7
1	B	128	GLN	2.7
1	B	195	ARG	2.6
1	A	202	ARG	2.6
1	B	53	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	94	ASP	2.5
1	B	124	CYS	2.5
1	A	208	PRO	2.5
1	B	355	ILE	2.5
1	B	97	LEU	2.5
1	B	93	ARG	2.4
1	A	197	ARG	2.4
1	A	194	ILE	2.4
1	B	101	LEU	2.4
1	B	197	ARG	2.3
1	A	286	LYS	2.3
1	B	350	LYS	2.3
1	B	316	GLU	2.2
1	A	316	GLU	2.2
1	B	285	PHE	2.2
1	A	289	LYS	2.2
1	A	213	LEU	2.2
1	A	206	LYS	2.1
1	A	209	TYR	2.1
1	B	253	GLN	2.1
1	B	391	LEU	2.1
1	B	346	PHE	2.1
1	B	129	VAL	2.1
1	A	100	GLU	2.1
1	B	209	TYR	2.1
1	A	93	ARG	2.0
1	B	243	GLN	2.0
1	B	392	GLY	2.0
1	B	291	ASP	2.0
1	B	361	MET	2.0
1	B	193	VAL	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, 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
3	CIT	B	506	13/13	0.72	0.18	3.17	16,30,37,39	0
3	CIT	A	506	13/13	0.84	0.19	2.12	8,21,31,40	0
2	CD	A	501	1/1	1.00	0.07	-2.07	17,17,17,17	0
2	CD	B	501	1/1	0.99	0.07	-2.61	21,21,21,21	0
2	CD	A	503	1/1	1.00	0.02	-3.52	18,18,18,18	0
2	CD	A	502	1/1	0.99	0.04	-4.78	15,15,15,15	0
2	CD	B	502	1/1	0.99	0.03	-5.38	23,23,23,23	0
2	CD	A	504	1/1	1.00	0.03	-	20,20,20,20	0
2	CD	B	504	1/1	1.00	0.02	-	23,23,23,23	0
2	CD	B	503	1/1	0.99	0.05	-	25,25,25,25	0
2	CD	A	505	1/1	0.90	0.07	-	58,58,58,58	0
2	CD	B	505	1/1	0.93	0.08	-	67,67,67,67	0

6.5 Other polymers [i](#)

There are no such residues in this entry.