Full wwPDB X-ray Structure Validation Report (i)

Aug 22, 2020 – 02:26 PM BST

PDB ID	:	4BUC
Title	:	CRYSTAL STRUCTURE OF MURD LIGASE FROM THERMOTOGA MARITIMA IN APO FORM
Authors	:	Favini-Stabile, S.; Contreras-Martel, C.; Thielens, N.; Dessen, A.
Deposited on	:	2013-06-20
Resolution	:	2.17 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 following versions of software and data (see references (1)) were used in the production of this report:

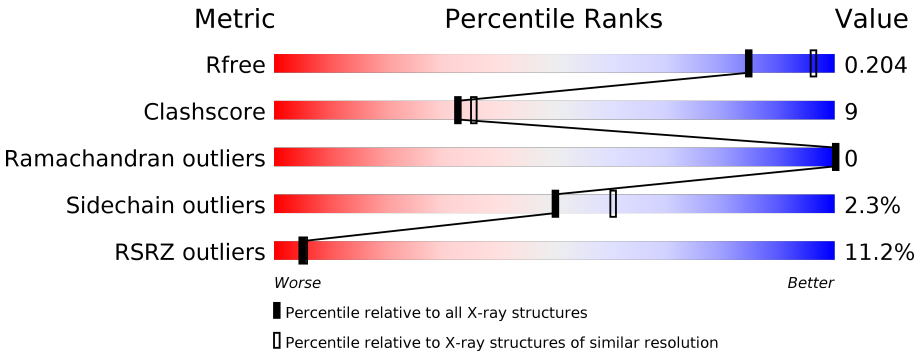
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

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 2.17 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	6864 (2.20-2.16)
Clashscore	141614	7689 (2.20-2.16)
Ramachandran outliers	138981	7564 (2.20-2.16)
Sidechain outliers	138945	7564 (2.20-2.16)
RSRZ outliers	127900	6738 (2.20-2.16)

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 <=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	450	10% 81% 13% • 5%
1	B	450	11% 80% 14% • 5%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	B	1202	-	-	X	-

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 7253 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 UDP-N-ACETYLMURAMOYLALANINE--D-GLUTAMATE LIGASE.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	427	Total	C	N	O	S	Se	0	0	0
			3433	2212	569	638	2	12			
1	B	427	Total	C	N	O	S	Se	0	0	0
			3433	2212	569	638	2	12			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	-	expression tag	UNP Q9WY76
A	2	GLY	-	expression tag	UNP Q9WY76
A	3	SER	-	expression tag	UNP Q9WY76
A	4	SER	-	expression tag	UNP Q9WY76
A	5	HIS	-	expression tag	UNP Q9WY76
A	6	HIS	-	expression tag	UNP Q9WY76
A	7	HIS	-	expression tag	UNP Q9WY76
A	8	HIS	-	expression tag	UNP Q9WY76
A	9	HIS	-	expression tag	UNP Q9WY76
A	10	HIS	-	expression tag	UNP Q9WY76
A	11	SER	-	expression tag	UNP Q9WY76
A	12	SER	-	expression tag	UNP Q9WY76
A	13	GLY	-	expression tag	UNP Q9WY76
A	14	LEU	-	expression tag	UNP Q9WY76
A	15	VAL	-	expression tag	UNP Q9WY76
A	16	PRO	-	expression tag	UNP Q9WY76
A	17	ARG	-	expression tag	UNP Q9WY76
A	18	GLY	-	expression tag	UNP Q9WY76
A	19	SER	-	expression tag	UNP Q9WY76
A	20	HIS	-	expression tag	UNP Q9WY76
B	1	MSE	-	expression tag	UNP Q9WY76
B	2	GLY	-	expression tag	UNP Q9WY76
B	3	SER	-	expression tag	UNP Q9WY76
B	4	SER	-	expression tag	UNP Q9WY76

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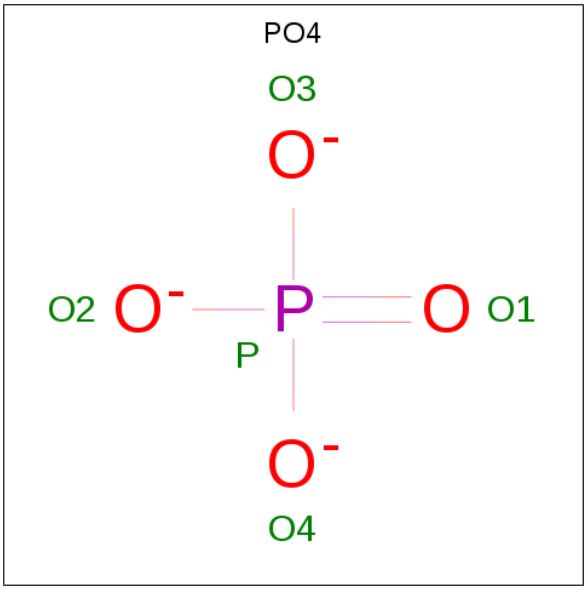
Chain	Residue	Modelled	Actual	Comment	Reference
B	5	HIS	-	expression tag	UNP Q9WY76
B	6	HIS	-	expression tag	UNP Q9WY76
B	7	HIS	-	expression tag	UNP Q9WY76
B	8	HIS	-	expression tag	UNP Q9WY76
B	9	HIS	-	expression tag	UNP Q9WY76
B	10	HIS	-	expression tag	UNP Q9WY76
B	11	SER	-	expression tag	UNP Q9WY76
B	12	SER	-	expression tag	UNP Q9WY76
B	13	GLY	-	expression tag	UNP Q9WY76
B	14	LEU	-	expression tag	UNP Q9WY76
B	15	VAL	-	expression tag	UNP Q9WY76
B	16	PRO	-	expression tag	UNP Q9WY76
B	17	ARG	-	expression tag	UNP Q9WY76
B	18	GLY	-	expression tag	UNP Q9WY76
B	19	SER	-	expression tag	UNP Q9WY76
B	20	HIS	-	expression tag	UNP Q9WY76

- Molecule 2 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

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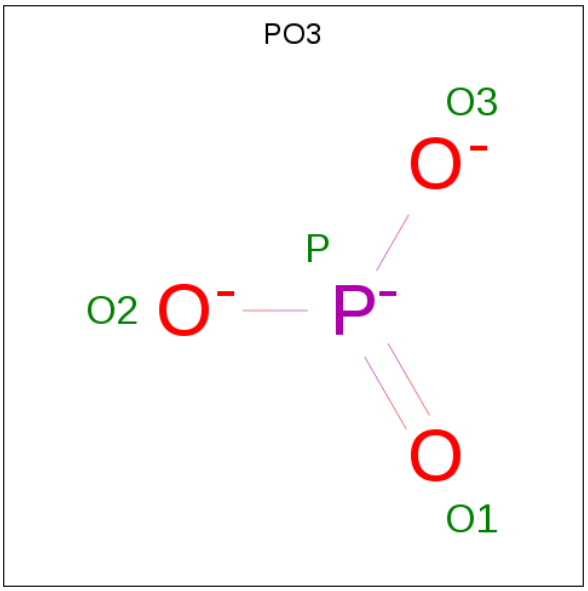
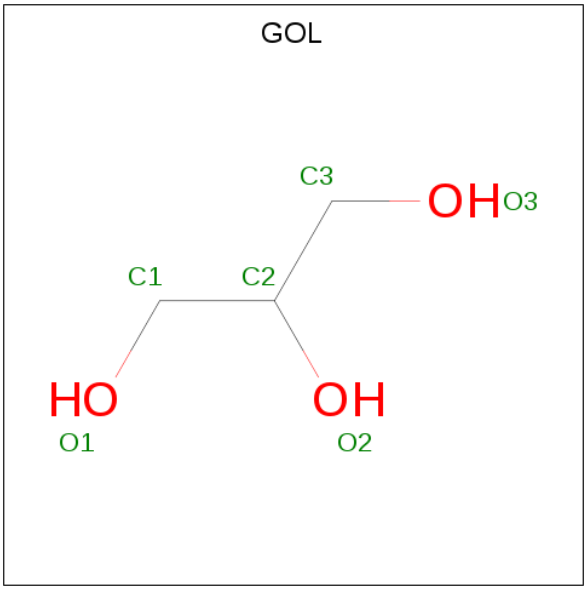
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	A	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0
2	B	1	Total O P 5 4 1	0	0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

- Molecule 3 is PHOSPHITE ION (three-letter code: PO3) (formula: O_3P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 4 3 1	0	0
3	B	1	Total O P 4 3 1	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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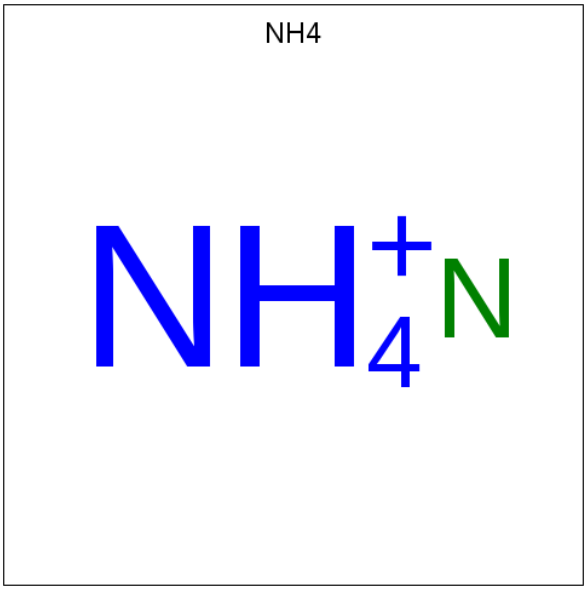
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0
4	B	1	Total C O 6 3 3	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	3	Total Cl 3 3	0	0
5	A	3	Total Cl 3 3	0	0

- Molecule 6 is AMMONIUM ION (three-letter code: NH4) (formula: H_4N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total N 1 1	0	0
6	B	1	Total N 1 1	0	0

- Molecule 7 is water.

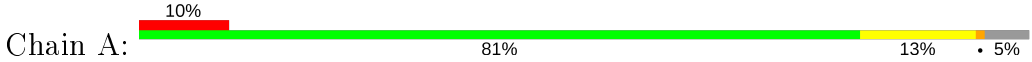
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	169	Total O 169 169	0	0
7	B	86	Total O 86 86	0	0

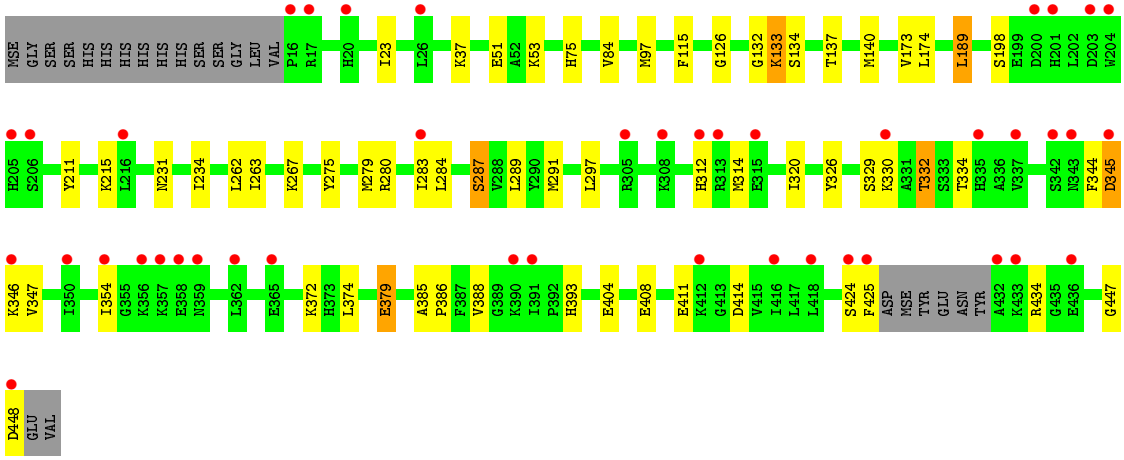
3 Residue-property plots (i)

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: UDP-N-ACETYLMURAMOYLALANINE--D-GLUTAMATE LIGASE

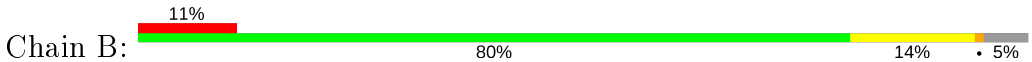
Chain A:

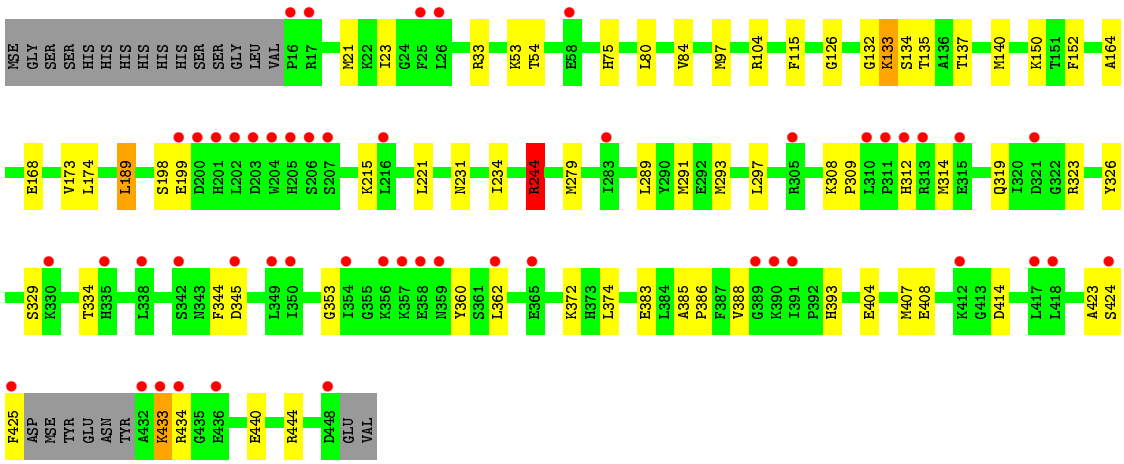




• Molecule 1: UDP-N-ACETYLMURAMOYLALANINE--D-GLUTAMATE LIGASE

Chain B:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	56.17Å 135.84Å 67.27Å 90.00° 98.17° 90.00°	Depositor
Resolution (Å)	19.78 – 2.17 19.77 – 2.17	Depositor EDS
% Data completeness (in resolution range)	99.3 (19.78-2.17) 99.5 (19.77-2.17)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.87 (at 2.17Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.163 , 0.197 0.173 , 0.204	Depositor DCC
R_{free} test set	2664 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å^2)	34.0	Xtriage
Anisotropy	0.074	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 49.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	7253	wwPDB-VP
Average B, all atoms (Å^2)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.62% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, PO4, NH4, PO3, 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	0.57	1/3503 (0.0%)	0.70	1/4691 (0.0%)
1	B	0.56	0/3503	0.73	3/4691 (0.1%)
All	All	0.57	1/7006 (0.0%)	0.72	4/9382 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	287	SER	CB-OG	-6.36	1.33	1.42

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	244	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	B	21	MSE	CA-CB-CG	-8.86	98.24	113.30
1	A	287	SER	CB-CA-C	-5.24	100.15	110.10
1	B	244	ARG	NE-CZ-NH2	-5.11	117.75	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3433	0	3396	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	3433	0	3396	67	0
2	A	40	0	0	1	0
2	B	40	0	0	2	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
4	A	18	0	24	4	0
4	B	18	0	24	6	0
5	A	3	0	0	0	0
5	B	3	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	169	0	0	4	0
7	B	86	0	0	2	0
All	All	7253	0	6840	121	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 9.

All (121) 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:134:SER:HB3	4:B:1202:GOL:H11	1.44	1.00
1:A:134:SER:HB3	4:A:1202:GOL:H11	1.45	0.98
1:A:314:MSE:HE1	1:A:344:PHE:CZ	2.01	0.95
1:B:291:MSE:HE3	7:B:2068:HOH:O	1.75	0.87
1:A:140:MSE:CE	1:A:289:LEU:HD23	2.05	0.85
1:B:314:MSE:HE1	1:B:344:PHE:CZ	2.13	0.83
1:A:291:MSE:HE3	7:A:2115:HOH:O	1.79	0.82
1:A:75:HIS:HB3	1:A:97:MSE:HE3	1.63	0.81
1:A:140:MSE:HE1	1:A:289:LEU:HD23	1.61	0.81
1:B:75:HIS:HB3	1:B:97:MSE:HE3	1.63	0.80
1:B:134:SER:H	4:B:1202:GOL:H12	1.49	0.77
1:A:314:MSE:CE	1:A:344:PHE:HZ	2.00	0.75
1:B:140:MSE:CE	1:B:289:LEU:HD13	2.18	0.74
1:B:289:LEU:CD2	1:B:293:MSE:SE	2.89	0.71
1:A:314:MSE:CE	1:A:344:PHE:CZ	2.72	0.70
1:B:134:SER:HB3	4:B:1202:GOL:C1	2.21	0.68
1:A:51:GLU:OE2	1:A:53:LYS:HE2	1.94	0.67
1:B:314:MSE:CE	1:B:344:PHE:CZ	2.78	0.67
1:B:140:MSE:HE1	1:B:289:LEU:HD13	1.77	0.67
1:A:75:HIS:CB	1:A:97:MSE:HE3	2.25	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:TYR:O	1:A:280:ARG:NH1	2.27	0.66
1:B:199:GLU:HB3	7:B:2049:HOH:O	1.96	0.66
1:B:75:HIS:CB	1:B:97:MSE:HE3	2.24	0.66
1:B:244:ARG:HG3	1:B:244:ARG:HH11	1.62	0.65
1:B:323:ARG:HD3	1:B:407:MSE:SE	2.46	0.65
1:A:140:MSE:HE3	1:A:289:LEU:HD23	1.78	0.65
1:A:314:MSE:HE1	1:A:344:PHE:CE2	2.32	0.64
1:B:291:MSE:HE2	1:B:297:LEU:HG	1.79	0.64
1:B:53:LYS:HG3	1:B:54:THR:H	1.63	0.63
1:A:291:MSE:HE2	1:A:297:LEU:HG	1.80	0.63
1:A:388:VAL:O	1:A:388:VAL:CG1	2.48	0.62
1:A:332:THR:CG2	1:A:332:THR:O	2.47	0.62
1:B:314:MSE:HE1	1:B:344:PHE:CE2	2.34	0.61
1:B:126:GLY:HA3	1:B:189:LEU:HD22	1.83	0.61
1:B:314:MSE:CE	1:B:344:PHE:HZ	2.13	0.60
1:B:53:LYS:CG	1:B:54:THR:H	2.15	0.60
1:A:134:SER:CB	4:A:1202:GOL:H11	2.26	0.59
1:B:388:VAL:O	1:B:388:VAL:CG1	2.50	0.59
1:A:284:LEU:O	1:A:287:SER:HB2	2.02	0.59
1:B:80:LEU:HD13	1:B:104:ARG:HD2	1.84	0.59
1:B:134:SER:CB	4:B:1202:GOL:H11	2.25	0.59
1:A:126:GLY:HA3	1:A:189:LEU:HD22	1.84	0.59
1:A:411:GLU:OE2	1:B:372:LYS:NZ	2.30	0.58
1:B:53:LYS:CG	1:B:54:THR:N	2.67	0.58
1:A:314:MSE:HE3	1:A:326:TYR:CD2	2.39	0.56
1:B:115:PHE:CE2	1:B:174:LEU:HD11	2.41	0.56
1:B:289:LEU:HD22	1:B:293:MSE:SE	2.54	0.56
1:A:332:THR:HG21	7:A:2147:HOH:O	2.07	0.55
1:A:434:ARG:NE	7:A:2161:HOH:O	2.40	0.55
1:B:132:GLY:H	4:B:1202:GOL:H31	1.71	0.55
1:A:345:ASP:OD2	1:B:345:ASP:HB2	2.06	0.54
1:A:37:LYS:HE3	4:A:1201:GOL:O1	2.08	0.54
1:A:115:PHE:CE2	1:A:174:LEU:HD11	2.43	0.54
1:B:312:HIS:CD2	1:B:314:MSE:HB3	2.42	0.53
1:B:140:MSE:HE3	1:B:289:LEU:HD13	1.88	0.52
1:A:279:MSE:HE3	1:A:283:ILE:HG13	1.92	0.52
1:A:312:HIS:CG	1:A:330:LYS:HB2	2.44	0.52
1:B:104:ARG:HH11	1:B:104:ARG:HG3	1.76	0.51
1:B:314:MSE:HE3	1:B:344:PHE:HZ	1.76	0.50
1:B:244:ARG:CG	1:B:244:ARG:HH11	2.25	0.49
1:A:332:THR:HG23	1:A:332:THR:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:THR:HG23	1:B:173:VAL:HG12	1.96	0.48
1:B:80:LEU:HD13	1:B:104:ARG:CD	2.43	0.48
1:B:404:GLU:O	1:B:408:GLU:HG3	2.13	0.48
1:B:133:LYS:HG3	1:B:133:LYS:H	1.48	0.48
1:A:385:ALA:N	1:A:386:PRO:CD	2.77	0.48
1:A:51:GLU:OE2	1:A:53:LYS:HG2	2.14	0.47
1:B:244:ARG:NH1	1:B:244:ARG:HG3	2.29	0.47
1:B:289:LEU:HD23	1:B:289:LEU:O	2.15	0.47
1:A:354:ILE:HA	1:A:379:GLU:HG3	1.97	0.47
1:B:440:GLU:O	1:B:444:ARG:HG2	2.14	0.47
1:B:385:ALA:N	1:B:386:PRO:CD	2.77	0.47
1:A:262:LEU:HD21	1:A:287:SER:OG	2.14	0.47
1:A:314:MSE:HE3	1:A:344:PHE:HZ	1.79	0.47
1:B:374:LEU:O	1:B:393:HIS:HA	2.15	0.47
1:A:132:GLY:HA2	2:A:1001:PO4:O4	2.16	0.46
1:A:23:ILE:HD12	1:A:84:VAL:CG1	2.46	0.46
1:B:433:LYS:HG3	1:B:434:ARG:H	1.79	0.46
1:B:423:ALA:O	1:B:434:ARG:NH2	2.49	0.46
1:A:448:ASP:OD1	1:A:448:ASP:C	2.53	0.45
1:B:385:ALA:HB3	1:B:386:PRO:HD3	1.97	0.45
1:A:385:ALA:HB3	1:A:386:PRO:HD3	1.97	0.45
1:B:23:ILE:HD12	1:B:84:VAL:CG1	2.47	0.45
1:A:374:LEU:O	1:A:393:HIS:HA	2.17	0.44
1:B:231:ASN:O	1:B:234:ILE:HG12	2.17	0.44
1:A:133:LYS:HG3	1:A:133:LYS:H	1.50	0.44
1:A:137:THR:HG23	1:A:173:VAL:HG12	1.99	0.44
1:A:372:LYS:NZ	1:A:414:ASP:OD2	2.49	0.44
1:A:231:ASN:O	1:A:234:ILE:HG12	2.17	0.44
1:A:320:ILE:HG12	1:A:447:GLY:HA2	1.98	0.44
1:A:404:GLU:O	1:A:408:GLU:HG3	2.17	0.44
1:B:289:LEU:HD21	1:B:293:MSE:SE	2.67	0.43
1:B:135:THR:HG21	1:B:279:MSE:HE1	1.99	0.43
1:B:132:GLY:HA2	2:B:1001:PO4:O4	2.18	0.43
1:A:75:HIS:C	1:A:97:MSE:HE3	2.38	0.43
1:B:308:LYS:O	1:B:309:PRO:C	2.57	0.43
1:A:388:VAL:O	1:A:388:VAL:HG12	2.17	0.43
1:B:314:MSE:HE3	1:B:326:TYR:CD2	2.54	0.43
1:B:319:GLN:HA	1:B:323:ARG:O	2.19	0.43
1:A:75:HIS:C	1:A:97:MSE:CE	2.88	0.42
1:A:314:MSE:HE3	1:A:326:TYR:CG	2.54	0.42
1:B:104:ARG:NH1	1:B:104:ARG:HG3	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:424:SER:O	1:B:425:PHE:C	2.58	0.42
1:B:33:ARG:NH1	4:B:1201:GOL:O2	2.53	0.41
1:B:353:GLY:HA3	1:B:434:ARG:NH2	2.34	0.41
1:B:215:LYS:NZ	2:B:1000:PO4:O2	2.51	0.41
1:A:424:SER:O	1:A:425:PHE:C	2.59	0.41
1:B:360:TYR:CE1	1:B:383:GLU:HB3	2.55	0.41
1:B:425:PHE:O	1:B:425:PHE:CD2	2.73	0.41
1:B:388:VAL:O	1:B:388:VAL:HG12	2.19	0.41
1:A:346:LYS:O	1:A:347:VAL:HG23	2.20	0.41
1:B:150:LYS:HE2	1:B:168:GLU:O	2.21	0.41
1:A:291:MSE:CE	7:A:2115:HOH:O	2.52	0.41
1:A:263:ILE:HA	1:A:267:LYS:O	2.21	0.41
1:B:23:ILE:HD12	1:B:84:VAL:HG12	2.03	0.40
1:A:23:ILE:HD12	1:A:84:VAL:HG12	2.03	0.40
1:B:152:PHE:CD1	1:B:164:ALA:HB2	2.57	0.40
1:A:134:SER:H	4:A:1202:GOL:H12	1.86	0.40
1:A:211:TYR:CZ	1:A:215:LYS:HD2	2.57	0.40
1:B:372:LYS:NZ	1:B:414:ASP:OD2	2.48	0.40
1:B:75:HIS:C	1:B:97:MSE:HE3	2.42	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	423/450 (94%)	409 (97%)	14 (3%)	0	100	100
1	B	423/450 (94%)	406 (96%)	17 (4%)	0	100	100
All	All	846/900 (94%)	815 (96%)	31 (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	374/381 (98%)	366 (98%)	8 (2%)	53 64
1	B	374/381 (98%)	365 (98%)	9 (2%)	49 59
All	All	748/762 (98%)	731 (98%)	17 (2%)	50 60

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	133	LYS
1	A	189	LEU
1	A	198	SER
1	A	329	SER
1	A	332	THR
1	A	334	THR
1	A	345	ASP
1	A	379	GLU
1	B	133	LYS
1	B	189	LEU
1	B	198	SER
1	B	221	LEU
1	B	244	ARG
1	B	329	SER
1	B	334	THR
1	B	362	LEU
1	B	433	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	205	HIS
1	A	295	ASN
1	A	343	ASN
1	B	205	HIS
1	B	274	ASN

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Mol	Chain	Res	Type
1	B	343	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 monosaccharides in this entry.

5.6 Ligand geometry

Of 32 ligands modelled in this entry, 2 are modelled with single atom and 6 are monoatomic - leaving 24 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	$\#\|Z\| > 2$
4	GOL	A	1202	-	5,5,5	0.28	0	5,5,5	1.55	1 (20%)
2	PO4	B	1007	-	4,4,4	0.67	0	6,6,6	0.99	0
2	PO4	A	1003	-	4,4,4	1.20	0	6,6,6	1.02	0
2	PO4	B	1004	-	4,4,4	0.84	0	6,6,6	0.87	0
2	PO4	B	1001	-	4,4,4	0.74	0	6,6,6	0.65	0
2	PO4	B	1002	-	4,4,4	1.08	0	6,6,6	1.13	0
2	PO4	A	1005	-	4,4,4	0.55	0	6,6,6	0.83	0
4	GOL	B	1202	-	5,5,5	0.31	0	5,5,5	1.16	0
2	PO4	A	1006	-	4,4,4	0.72	0	6,6,6	0.77	0
4	GOL	B	1200	-	5,5,5	0.50	0	5,5,5	0.86	0
4	GOL	B	1201	-	5,5,5	0.31	0	5,5,5	0.56	0
3	PO3	B	1008	-	0,3,3	0.00	-	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	PO4	B	1003	-	4,4,4	1.52	1 (25%)	6,6,6	1.28	1 (16%)
3	PO3	A	1008	-	0,3,3	0.00	-	0,3,3	0.00	-
2	PO4	A	1004	-	4,4,4	1.03	0	6,6,6	0.91	0
4	GOL	A	1201	-	5,5,5	0.26	0	5,5,5	0.53	0
2	PO4	A	1002	-	4,4,4	0.90	0	6,6,6	0.71	0
2	PO4	B	1000	-	4,4,4	1.29	0	6,6,6	0.83	0
2	PO4	A	1001	-	4,4,4	0.79	0	6,6,6	0.57	0
4	GOL	A	1200	-	5,5,5	0.55	0	5,5,5	0.46	0
2	PO4	A	1000	-	4,4,4	1.33	1 (25%)	6,6,6	0.85	0
2	PO4	B	1005	-	4,4,4	0.56	0	6,6,6	0.59	0
2	PO4	A	1007	-	4,4,4	0.91	0	6,6,6	0.74	0
2	PO4	B	1006	-	4,4,4	0.65	0	6,6,6	0.93	0

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
4	GOL	A	1202	-	-	0/4/4/4	-
4	GOL	B	1202	-	-	0/4/4/4	-
4	GOL	B	1201	-	-	4/4/4/4	-
4	GOL	A	1200	-	-	2/4/4/4	-
4	GOL	B	1200	-	-	0/4/4/4	-
4	GOL	A	1201	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	PO4	P-O3	-2.02	1.48	1.54
2	B	1003	PO4	P-O4	-2.01	1.48	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	1202	GOL	C3-C2-C1	-3.03	99.93	111.70
2	B	1003	PO4	O3-P-O2	2.40	115.68	107.97

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1201	GOL	O1-C1-C2-C3
4	B	1201	GOL	C1-C2-C3-O3
4	A	1200	GOL	C1-C2-C3-O3
4	A	1200	GOL	O2-C2-C3-O3
4	B	1201	GOL	O1-C1-C2-O2
4	B	1201	GOL	O2-C2-C3-O3

There are no ring outliers.

7 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1202	GOL	3	0
2	B	1001	PO4	1	0
4	B	1202	GOL	5	0
4	B	1201	GOL	1	0
4	A	1201	GOL	1	0
2	B	1000	PO4	1	0
2	A	1001	PO4	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, 95^{th} 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	415/450 (92%)	0.44	43 (10%)	6	6	20, 37, 92, 123	0
1	B	415/450 (92%)	0.57	50 (12%)	4	4	22, 39, 100, 153	0
All	All	830/900 (92%)	0.50	93 (11%)	5	5	20, 38, 96, 153	0

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	362	LEU	11.0
1	A	425	PHE	8.9
1	B	425	PHE	8.7
1	B	201	HIS	8.3
1	A	201	HIS	7.9
1	B	310	LEU	7.9
1	B	313	ARG	7.1
1	A	362	LEU	7.0
1	B	311	PRO	6.8
1	B	357	LYS	6.6
1	A	432	ALA	6.5
1	B	205	HIS	6.4
1	A	205	HIS	6.1
1	B	312	HIS	6.0
1	A	206	SER	6.0
1	B	356	LYS	5.6
1	A	357	LYS	5.5
1	B	432	ALA	5.4
1	B	206	SER	5.3
1	A	16	PRO	5.0
1	A	356	LYS	4.9
1	A	424	SER	4.9
1	B	16	PRO	4.6
1	B	203	ASP	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	350	ILE	4.3
1	B	390	LYS	4.3
1	B	350	ILE	4.1
1	A	335	HIS	4.0
1	B	200	ASP	4.0
1	B	345	ASP	4.0
1	A	345	ASP	3.9
1	B	359	ASN	3.9
1	B	199	GLU	3.7
1	A	359	ASN	3.5
1	A	391	ILE	3.5
1	B	17	ARG	3.5
1	A	200	ASP	3.5
1	B	330	LYS	3.4
1	A	203	ASP	3.4
1	A	390	LYS	3.4
1	A	204	TRP	3.3
1	A	313	ARG	3.3
1	A	342	SER	3.3
1	A	412	LYS	3.2
1	B	315	GLU	3.2
1	A	448	ASP	3.2
1	B	335	HIS	3.1
1	B	412	LYS	3.1
1	B	433	LYS	3.1
1	B	424	SER	3.1
1	A	343	ASN	3.0
1	B	358	GLU	3.0
1	B	202	LEU	3.0
1	B	342	SER	3.0
1	B	349	LEU	2.9
1	A	354	ILE	2.8
1	A	358	GLU	2.8
1	A	305	ARG	2.8
1	A	433	LYS	2.8
1	B	389	GLY	2.7
1	B	26	LEU	2.7
1	B	305	ARG	2.7
1	A	315	GLU	2.7
1	A	418	LEU	2.7
1	A	365	GLU	2.6
1	A	216	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	337	VAL	2.6
1	B	58	GLU	2.6
1	A	346	LYS	2.5
1	B	417	LEU	2.4
1	B	436	GLU	2.4
1	A	20	HIS	2.4
1	A	312	HIS	2.4
1	A	416	ILE	2.4
1	B	204	TRP	2.4
1	B	354	ILE	2.4
1	A	436	GLU	2.3
1	A	283	ILE	2.3
1	A	308	LYS	2.3
1	B	283	ILE	2.3
1	A	17	ARG	2.3
1	B	448	ASP	2.3
1	A	26	LEU	2.2
1	B	321	ASP	2.2
1	B	207	SER	2.2
1	B	418	LEU	2.2
1	A	330	LYS	2.1
1	B	216	LEU	2.1
1	B	338	LEU	2.1
1	B	434	ARG	2.1
1	B	365	GLU	2.1
1	B	25	PHE	2.1
1	B	391	ILE	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, 95^{th} 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
4	GOL	B	1202	6/6	0.82	0.16	44,55,69,73	0
4	GOL	A	1200	6/6	0.84	0.19	51,63,67,69	0
4	GOL	B	1200	6/6	0.89	0.14	50,60,63,63	0
4	GOL	A	1201	6/6	0.89	0.17	66,71,74,87	0
4	GOL	A	1202	6/6	0.89	0.17	41,48,67,69	0
5	CL	B	1402	1/1	0.90	0.12	55,55,55,55	0
2	PO4	B	1001	5/5	0.90	0.34	59,63,77,78	0
5	CL	A	1402	1/1	0.91	0.11	54,54,54,54	0
5	CL	A	1401	1/1	0.92	0.09	65,65,65,65	0
6	NH4	A	1501	1/1	0.92	0.39	34,34,34,34	0
6	NH4	B	1501	1/1	0.94	0.30	38,38,38,38	0
4	GOL	B	1201	6/6	0.95	0.16	62,64,71,82	0
2	PO4	A	1005	5/5	0.95	0.14	42,49,58,69	0
3	PO3	B	1008	4/4	0.96	0.16	31,43,53,55	0
2	PO4	B	1005	5/5	0.96	0.14	48,52,66,75	0
2	PO4	B	1006	5/5	0.96	0.19	48,49,52,61	0
2	PO4	B	1007	5/5	0.97	0.09	42,47,56,57	0
3	PO3	A	1008	4/4	0.97	0.14	32,41,49,56	0
2	PO4	A	1004	5/5	0.97	0.12	44,47,51,70	0
5	CL	B	1401	1/1	0.97	0.09	63,63,63,63	0
2	PO4	A	1007	5/5	0.97	0.11	43,47,53,55	0
2	PO4	A	1006	5/5	0.97	0.22	41,49,53,60	0
2	PO4	B	1004	5/5	0.98	0.15	44,45,54,67	0
2	PO4	A	1003	5/5	0.98	0.10	32,35,35,37	0
2	PO4	A	1001	5/5	0.98	0.26	39,46,54,56	0
2	PO4	B	1003	5/5	0.98	0.07	30,32,37,37	0
5	CL	B	1400	1/1	0.99	0.04	33,33,33,33	0
2	PO4	A	1002	5/5	0.99	0.09	30,30,32,38	0
2	PO4	A	1000	5/5	0.99	0.06	29,31,34,37	0
2	PO4	B	1002	5/5	0.99	0.11	33,34,42,47	0
2	PO4	B	1000	5/5	0.99	0.07	31,32,35,38	0
5	CL	A	1400	1/1	0.99	0.04	32,32,32,32	0

6.5 Other polymers (i)

There are no such residues in this entry.