Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 08:17 PM GMT

PDB ID	:	4RF8
Title	:	Crystal structure of double-domain arginine kinase from Anthopleura japonicas in complex with ADP
Authors	:	Wang, Z.; Qiao, Z.; Ye, S.; Zhang, R.
Deposited on	:	2014-09-25
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
http://wwpdb.org/validation/2016/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:

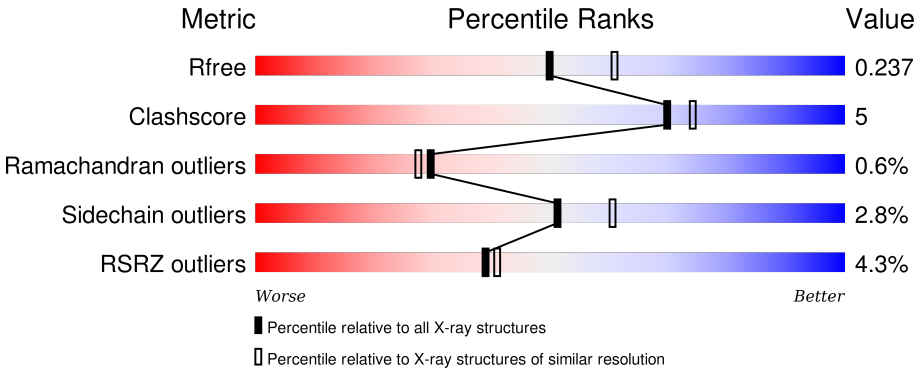
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance

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

The reported resolution of this entry is 2.17 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}	91344	5130 (2.20-2.16)
Clashscore	102246	5965 (2.20-2.16)
Ramachandran outliers	100387	5863 (2.20-2.16)
Sidechain outliers	100360	5864 (2.20-2.16)
RSRZ outliers	91569	5142 (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. 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	718	7% 83% 11%
1	B	718	% 86% 9%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ADP	A	1001	-	-	-	X
2	ADP	B	802	-	-	-	X
3	NO3	A	1002	-	X	-	-
3	NO3	A	1003	-	X	-	-
3	NO3	A	1004	-	X	-	X
3	NO3	A	1005	-	X	-	-
3	NO3	A	1006	-	X	-	-
3	NO3	A	1007	-	X	-	X
3	NO3	A	1008	-	X	-	-
3	NO3	A	1009	-	X	X	-
3	NO3	A	1010	-	X	-	-
3	NO3	B	801	-	X	-	-
3	NO3	B	803	-	X	-	-
3	NO3	B	804	-	X	-	-
3	NO3	B	805	-	X	-	-
3	NO3	B	806	-	X	-	-
3	NO3	B	807	-	X	-	X
3	NO3	B	808	-	X	-	-
3	NO3	B	809	-	X	-	X
3	NO3	B	810	-	X	-	-
3	NO3	B	811	-	X	-	-
3	NO3	B	812	-	X	-	X
4	EPE	B	813	-	-	-	X
4	EPE	B	814	-	-	-	X

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 11633 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.

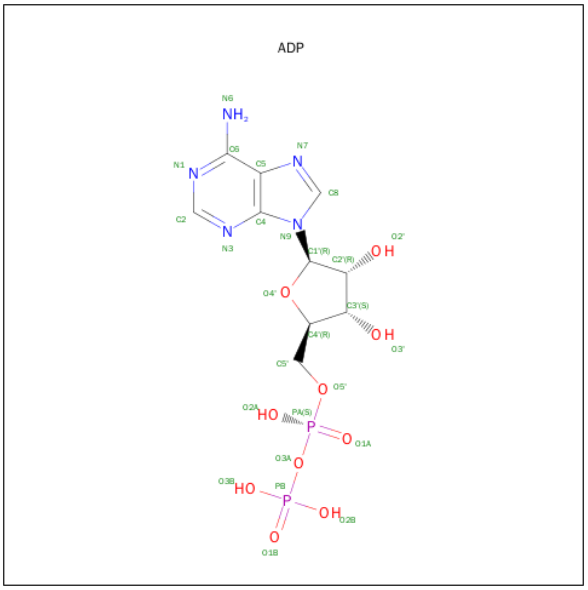
- Molecule 1 is a protein called Arginine kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	686	Total	C	N	O	S	0	1	0
			5431	3430	958	1019	24			
1	B	693	Total	C	N	O	S	0	3	0
			5490	3467	970	1029	24			

There are 6 discrepancies between the modelled and reference sequences:

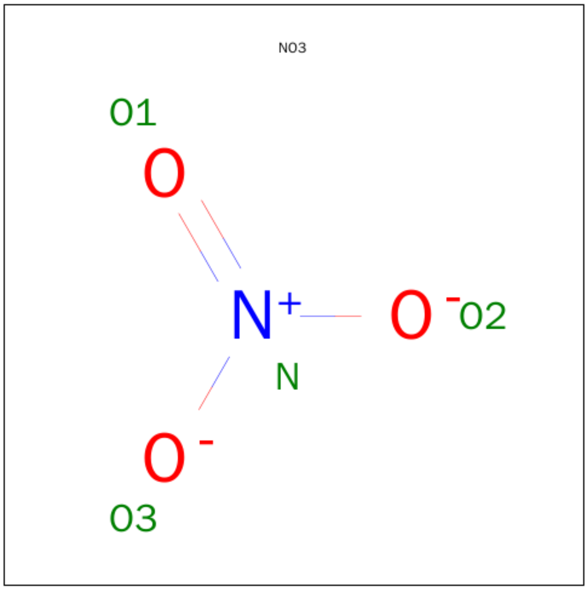
Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	EXPRESSION TAG	UNP O15992
A	-1	PRO	-	EXPRESSION TAG	UNP O15992
A	0	HIS	-	EXPRESSION TAG	UNP O15992
B	-2	GLY	-	EXPRESSION TAG	UNP O15992
B	-1	PRO	-	EXPRESSION TAG	UNP O15992
B	0	HIS	-	EXPRESSION TAG	UNP O15992

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 3 is NITRATE ION (three-letter code: NO3) (formula: NO_3).



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

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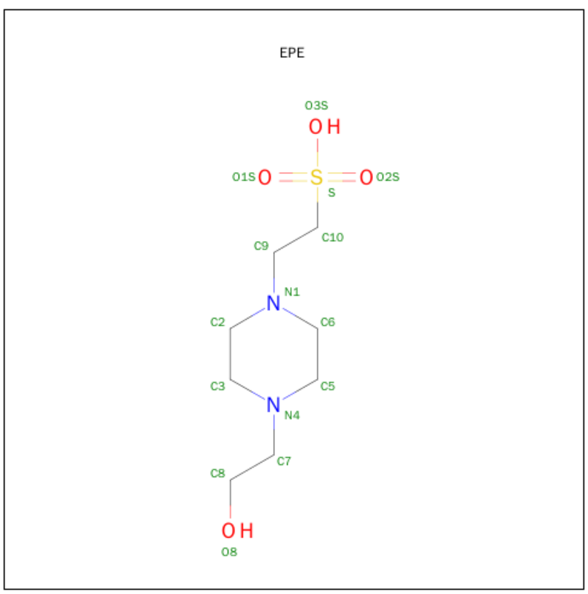
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total N O 4 1 3	0	0
3	B	1	Total N O 4 1 3	0	0
3	B	1	Total N O 4 1 3	0	0
3	B	1	Total N O 4 1 3	0	0
3	B	1	Total N O 4 1 3	0	0
3	B	1	Total N O 4 1 3	0	0
3	B	1	Total N O 4 1 3	0	0
3	B	1	Total N O 4 1 3	0	0
3	B	1	Total N O 4 1 3	0	0
3	B	1	Total N O 4 1 3	0	0

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O S 15 8 2 4 1	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	B	1	Total	C	N	O	S	0	0
			15	8	2	4	1		

- Molecule 5 is water.

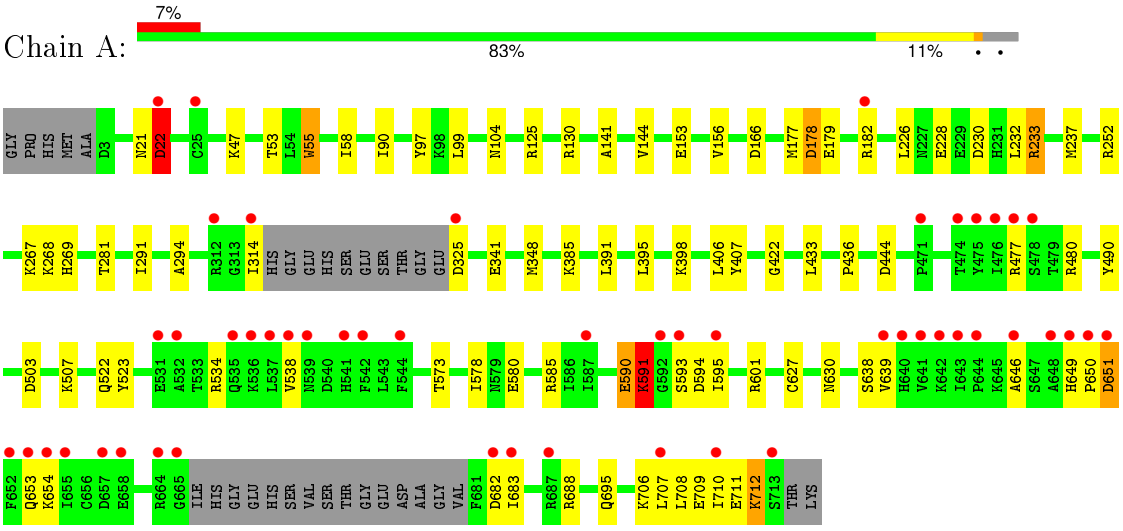
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	252	Total	O	0	0
			252	252		
5	B	296	Total	O	0	0
			296	296		

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

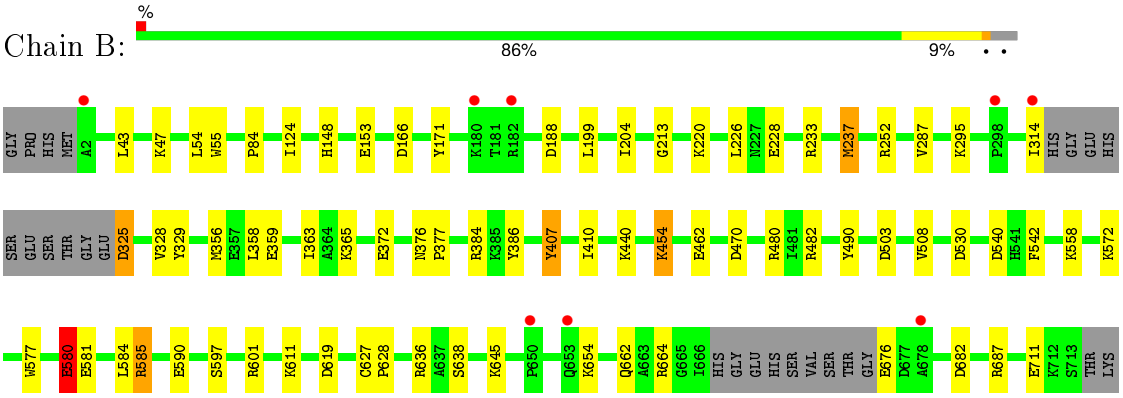
- Molecule 1: Arginine kinase

Chain A:



- Molecule 1: Arginine kinase

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	79.48Å 59.27Å 163.71Å 90.00° 90.75° 90.00°	Depositor
Resolution (Å)	47.51 – 2.17 47.51 – 2.17	Depositor EDS
% Data completeness (in resolution range)	98.4 (47.51-2.17) 92.3 (47.51-2.17)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 2.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.2_1309)	Depositor
R, R_{free}	0.192 , 0.239 0.190 , 0.237	Depositor DCC
R_{free} test set	3773 reflections (5.05%)	DCC
Wilson B-factor (Å^2)	39.5	Xtriage
Anisotropy	0.221	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.38 , 63.6	EDS
Estimated twinning fraction	0.016 for h,-k,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 79678 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11633	wwPDB-VP
Average B, all atoms (Å^2)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.00% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EPE, ADP, NO3

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	0.25	0/5543	0.43	0/7474
1	B	0.24	0/5611	0.42	0/7565
All	All	0.25	0/11154	0.42	0/15039

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5431	0	5422	51	0
1	B	5490	0	5491	48	0
2	A	27	0	12	1	0
2	B	27	0	12	0	0
3	A	36	0	0	2	0
3	B	44	0	0	1	0
4	B	30	0	34	7	0
5	A	252	0	0	7	0
5	B	296	0	0	8	0
All	All	11633	0	10971	100	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 5.

All (100) 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:462:GLU:HA	4:B:814:EPE:H91	1.66	0.76
1:A:125:ARG:NH1	1:A:325:ASP:OD2	2.16	0.73
1:B:558:LYS:NZ	3:B:809:NO3:O3	2.23	0.70
1:B:636:ARG:NH2	1:B:682:ASP:OD1	2.24	0.70
1:A:178:ASP:N	1:A:178:ASP:OD2	2.26	0.68
1:A:650:PRO:O	1:A:654:LYS:NZ	2.23	0.68
1:A:585:ARG:NH1	3:A:1009:NO3:O3	2.28	0.67
1:B:470:ASP:OD1	5:B:915:HOH:O	2.13	0.66
1:A:230:ASP:OD2	1:A:233:ARG:NH1	2.30	0.65
1:A:252:ARG:NH1	5:A:1219:HOH:O	2.30	0.65
1:B:148:HIS:ND1	5:B:1066:HOH:O	2.29	0.65
1:B:577:TRP:HB2	1:B:585[B]:ARG:HB2	1.77	0.65
1:A:166:ASP:OD1	1:A:252:ARG:NH2	2.29	0.64
1:A:153:GLU:HA	1:A:226:LEU:HD21	1.77	0.64
1:A:99:LEU:HD13	1:A:268:LYS:HE3	1.81	0.63
1:B:590:GLU:HG3	1:B:601:ARG:HH22	1.63	0.62
1:A:480:ARG:NH2	3:A:1009:NO3:O3	2.33	0.61
1:B:356:MET:SD	5:B:1136:HOH:O	2.57	0.61
1:A:695:GLN:HB3	4:B:813:EPE:H91	1.84	0.60
1:B:687:ARG:HH22	4:B:813:EPE:H101	1.68	0.59
1:A:591:LYS:NZ	1:A:591:LYS:H	2.00	0.59
1:A:590:GLU:OE1	1:A:601:ARG:NH2	2.28	0.59
1:B:47:LYS:NZ	5:B:1013:HOH:O	2.30	0.58
1:B:662:GLN:OE1	1:B:664:ARG:NH2	2.37	0.57
1:A:638:SER:OG	1:A:682:ASP:OD2	2.22	0.57
1:A:268:LYS:HE2	1:A:269:HIS:CE1	2.40	0.56
1:B:153:GLU:HA	1:B:226:LEU:HD21	1.87	0.55
1:B:508:VAL:HG11	1:B:584:LEU:HD21	1.89	0.55
1:A:22:ASP:OD2	1:A:22:ASP:N	2.34	0.55
1:B:480:ARG:NH1	5:B:1030:HOH:O	2.36	0.54
1:A:639:VAL:HB	1:A:683:ILE:HB	1.88	0.54
1:A:385:LYS:NZ	5:A:1344:HOH:O	2.40	0.54
1:A:490:TYR:OH	1:A:503:ASP:OD1	2.22	0.53
1:B:199:LEU:HD22	1:B:204:ILE:HD12	1.90	0.53
1:A:593:SER:O	1:A:595:ILE:N	2.42	0.53
1:A:398:LYS:NZ	5:A:1323:HOH:O	2.38	0.50
1:B:540:ASP:OD2	1:B:572:LYS:NZ	2.36	0.50
1:A:156:VAL:HG11	1:A:232:LEU:HD21	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ARG:NH1	2:A:1001:ADP:O3B	2.36	0.49
1:A:646:ALA:HB2	1:A:710:ILE:HB	1.94	0.49
1:B:188:ASP:OD2	1:B:220:LYS:NZ	2.29	0.48
1:B:295:LYS:HG3	1:B:329:TYR:CZ	2.49	0.48
1:A:706:LYS:NZ	5:A:1329:HOH:O	2.44	0.48
1:A:590:GLU:HB2	1:A:591:LYS:HD2	1.95	0.47
1:A:523:TYR:CE1	1:A:578:ILE:HD12	2.49	0.47
1:A:391:LEU:HD11	1:A:436:PRO:HB2	1.97	0.47
1:B:580:GLU:CD	1:B:581:GLU:H	2.18	0.47
1:B:325:ASP:OD1	1:B:325:ASP:N	2.47	0.47
1:B:558:LYS:NZ	5:B:923:HOH:O	2.42	0.47
1:B:490:TYR:OH	1:B:503:ASP:OD1	2.20	0.47
1:A:228:GLU:HB3	5:A:1226:HOH:O	2.14	0.47
1:B:386:TYR:CD1	1:B:440:LYS:HD3	2.50	0.46
1:A:422:GLY:N	5:A:1192:HOH:O	2.47	0.46
1:A:179:GLU:OE2	1:A:182:ARG:NE	2.49	0.46
1:A:281:THR:HB	1:A:341:GLU:HG3	1.98	0.45
1:B:611:LYS:NZ	5:B:1145:HOH:O	2.48	0.45
1:B:676:GLU:N	1:B:676:GLU:OE2	2.50	0.45
1:B:542:PHE:HZ	1:B:572:LYS:HB3	1.82	0.44
1:B:166:ASP:OD1	1:B:252:ARG:NH2	2.50	0.44
1:B:237:MET:N	1:B:237:MET:SD	2.90	0.44
1:B:124:ILE:HG23	1:B:287:VAL:HG13	1.99	0.44
1:A:649:HIS:ND1	1:A:651:ASP:HB2	2.33	0.44
1:B:314:ILE:HD12	1:B:328:VAL:HG12	2.00	0.44
1:B:359:GLU:O	1:B:363:ILE:HG12	2.17	0.44
1:B:228:GLU:HB3	5:B:1106:HOH:O	2.18	0.43
1:A:707:LEU:HD23	1:A:707:LEU:HA	1.87	0.43
1:B:627[B]:CYS:HA	1:B:628:PRO:HD3	1.89	0.43
1:A:706:LYS:HA	1:A:709:GLU:HB2	2.00	0.43
1:B:580:GLU:OE1	1:B:585[B]:ARG:HG3	2.19	0.43
1:A:630:ASN:OD1	1:A:688:ARG:NH1	2.52	0.43
1:A:593:SER:O	1:A:595:ILE:HG13	2.19	0.43
1:A:97:TYR:HE2	1:A:99:LEU:HD23	1.83	0.43
1:A:398:LYS:HD3	1:A:433:LEU:HD11	2.01	0.43
1:B:577:TRP:HB3	1:B:580:GLU:HG2	2.01	0.42
1:A:90:ILE:HG21	1:A:99:LEU:HD21	2.00	0.42
1:A:649:HIS:CG	1:A:650:PRO:HD2	2.54	0.42
1:B:590:GLU:HG3	1:B:601:ARG:NH2	2.33	0.42
1:A:47:LYS:HG2	1:A:53:THR:HG22	2.02	0.42
1:B:407:TYR:HA	1:B:410:ILE:HG12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:LEU:HB2	1:A:406:LEU:HD22	2.01	0.42
1:A:534:ARG:O	1:A:538:VAL:HG23	2.20	0.42
1:B:597:SER:N	4:B:814:EPE:H72	2.35	0.42
1:B:43:LEU:HD11	1:B:84:PRO:HG2	2.00	0.42
1:B:43:LEU:HB2	1:B:54:LEU:HD22	2.01	0.42
1:A:141:ALA:O	1:A:144:VAL:HG12	2.20	0.42
1:B:376:ASN:HA	1:B:377:PRO:HD3	1.87	0.41
1:B:171:TYR:OH	1:B:213:GLY:HA3	2.21	0.41
1:B:638:SER:HB2	1:B:682:ASP:OD2	2.21	0.41
1:B:480:ARG:HH22	1:B:482[B]:ARG:CZ	2.33	0.41
1:B:687:ARG:NH2	4:B:813:EPE:H101	2.34	0.41
1:A:444:ASP:OD1	5:A:1222:HOH:O	2.22	0.41
1:A:695:GLN:NE2	4:B:813:EPE:H21	2.36	0.41
1:A:490:TYR:OH	1:A:507:LYS:HE2	2.20	0.41
4:B:814:EPE:H102	4:B:814:EPE:H22	1.54	0.40
1:A:104:ASN:OD1	1:A:267:LYS:NZ	2.53	0.40
1:B:454:LYS:HG2	1:B:619:ASP:HB3	2.03	0.40
1:A:55:TRP:HA	1:A:58:ILE:HG12	2.02	0.40
1:B:645:LYS:NZ	1:B:711:GLU:O	2.54	0.40
1:B:482[B]:ARG:HH11	1:B:636:ARG:HD3	1.86	0.40
1:A:291:ILE:HB	1:A:294:ALA:HB3	2.02	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	681/718 (95%)	648 (95%)	26 (4%)	7 (1%)	19 15
1	B	690/718 (96%)	675 (98%)	14 (2%)	1 (0%)	56 63
All	All	1371/1436 (96%)	1323 (96%)	40 (3%)	8 (1%)	30 27

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	712	LYS
1	A	177	MET
1	A	594	ASP
1	A	21	ASN
1	A	580	GLU
1	A	591	LYS
1	A	22	ASP
1	B	580	GLU

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	593/616 (96%)	573 (97%)	20 (3%)	44 52
1	B	599/616 (97%)	584 (98%)	15 (2%)	55 65
All	All	1192/1232 (97%)	1157 (97%)	35 (3%)	51 59

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	22	ASP
1	A	55	TRP
1	A	178	ASP
1	A	233	ARG
1	A	237	MET
1	A	314	ILE
1	A	348	MET
1	A	407	TYR
1	A	477	ARG
1	A	522	GLN
1	A	573	THR
1	A	590	GLU
1	A	591	LYS
1	A	627[A]	CYS
1	A	627[B]	CYS

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Mol	Chain	Res	Type
1	A	651	ASP
1	A	653	GLN
1	A	708	LEU
1	A	711	GLU
1	A	712	LYS
1	B	55	TRP
1	B	233	ARG
1	B	237	MET
1	B	325	ASP
1	B	358	LEU
1	B	365	LYS
1	B	372	GLU
1	B	384	ARG
1	B	407	TYR
1	B	454	LYS
1	B	530	ASP
1	B	580	GLU
1	B	585[A]	ARG
1	B	585[B]	ARG
1	B	654	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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)

24 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	ADP	A	1001	-	22,29,29	1.01	1 (4%)	27,45,45	1.91	5 (18%)
3	NO3	A	1002	-	3,3,3	3.31	3 (100%)	3,3,3	0.14	0
3	NO3	A	1003	-	3,3,3	3.27	3 (100%)	3,3,3	0.16	0
3	NO3	A	1004	-	3,3,3	3.28	3 (100%)	3,3,3	0.06	0
3	NO3	A	1005	-	3,3,3	3.27	3 (100%)	3,3,3	0.14	0
3	NO3	A	1006	-	3,3,3	3.27	3 (100%)	3,3,3	0.14	0
3	NO3	A	1007	-	3,3,3	3.26	3 (100%)	3,3,3	0.15	0
3	NO3	A	1008	-	3,3,3	3.26	3 (100%)	3,3,3	0.11	0
3	NO3	A	1009	-	3,3,3	3.25	3 (100%)	3,3,3	0.15	0
3	NO3	A	1010	-	3,3,3	3.27	3 (100%)	3,3,3	0.14	0
3	NO3	B	801	-	3,3,3	3.32	3 (100%)	3,3,3	0.10	0
2	ADP	B	802	-	22,29,29	1.01	1 (4%)	27,45,45	1.88	4 (14%)
3	NO3	B	803	-	3,3,3	3.31	3 (100%)	3,3,3	0.07	0
3	NO3	B	804	-	3,3,3	3.32	3 (100%)	3,3,3	0.05	0
3	NO3	B	805	-	3,3,3	3.24	3 (100%)	3,3,3	0.19	0
3	NO3	B	806	-	3,3,3	3.27	3 (100%)	3,3,3	0.16	0
3	NO3	B	807	-	3,3,3	3.29	3 (100%)	3,3,3	0.10	0
3	NO3	B	808	-	3,3,3	3.31	3 (100%)	3,3,3	0.10	0
3	NO3	B	809	-	3,3,3	3.26	3 (100%)	3,3,3	0.10	0
3	NO3	B	810	-	3,3,3	3.27	3 (100%)	3,3,3	0.11	0
3	NO3	B	811	-	3,3,3	3.24	3 (100%)	3,3,3	0.16	0
3	NO3	B	812	-	3,3,3	3.26	3 (100%)	3,3,3	0.16	0
4	EPE	B	813	-	14,15,15	0.35	0	18,20,20	2.05	6 (33%)
4	EPE	B	814	-	14,15,15	0.44	0	18,20,20	2.29	6 (33%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	A	1001	-	-	0/12/32/32	0/3/3/3
3	NO3	A	1002	-	-	0/0/0/0	0/0/0/0
3	NO3	A	1003	-	-	0/0/0/0	0/0/0/0
3	NO3	A	1004	-	-	0/0/0/0	0/0/0/0
3	NO3	A	1005	-	-	0/0/0/0	0/0/0/0
3	NO3	A	1006	-	-	0/0/0/0	0/0/0/0
3	NO3	A	1007	-	-	0/0/0/0	0/0/0/0
3	NO3	A	1008	-	-	0/0/0/0	0/0/0/0
3	NO3	A	1009	-	-	0/0/0/0	0/0/0/0
3	NO3	A	1010	-	-	0/0/0/0	0/0/0/0
3	NO3	B	801	-	-	0/0/0/0	0/0/0/0
2	ADP	B	802	-	-	0/12/32/32	0/3/3/3
3	NO3	B	803	-	-	0/0/0/0	0/0/0/0
3	NO3	B	804	-	-	0/0/0/0	0/0/0/0
3	NO3	B	805	-	-	0/0/0/0	0/0/0/0
3	NO3	B	806	-	-	0/0/0/0	0/0/0/0
3	NO3	B	807	-	-	0/0/0/0	0/0/0/0
3	NO3	B	808	-	-	0/0/0/0	0/0/0/0
3	NO3	B	809	-	-	0/0/0/0	0/0/0/0
3	NO3	B	810	-	-	0/0/0/0	0/0/0/0
3	NO3	B	811	-	-	0/0/0/0	0/0/0/0
3	NO3	B	812	-	-	0/0/0/0	0/0/0/0
4	EPE	B	813	-	-	0/9/19/19	0/1/1/1
4	EPE	B	814	-	-	0/9/19/19	0/1/1/1

All (62) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	811	NO3	O3-N	2.83	1.40	1.25
3	B	812	NO3	O2-N	2.87	1.40	1.25
3	B	809	NO3	O3-N	2.87	1.40	1.25
3	B	810	NO3	O3-N	2.88	1.40	1.25
3	A	1004	NO3	O3-N	2.88	1.40	1.25
3	A	1002	NO3	O2-N	2.88	1.40	1.25
3	A	1004	NO3	O2-N	2.88	1.40	1.25
3	A	1008	NO3	O2-N	2.88	1.40	1.25
3	A	1005	NO3	O2-N	2.89	1.40	1.25
3	A	1007	NO3	O3-N	2.89	1.40	1.25
3	B	803	NO3	O2-N	2.89	1.40	1.25
3	A	1009	NO3	O3-N	2.89	1.40	1.25
3	B	807	NO3	O2-N	2.89	1.40	1.25
3	B	809	NO3	O2-N	2.90	1.40	1.25
3	B	806	NO3	O3-N	2.90	1.40	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	805	NO3	O2-N	2.90	1.40	1.25
3	A	1010	NO3	O3-N	2.90	1.40	1.25
3	B	804	NO3	O2-N	2.90	1.40	1.25
3	A	1005	NO3	O3-N	2.90	1.40	1.25
3	B	812	NO3	O3-N	2.91	1.40	1.25
3	A	1006	NO3	O3-N	2.91	1.40	1.25
3	A	1007	NO3	O2-N	2.91	1.40	1.25
3	B	810	NO3	O2-N	2.91	1.40	1.25
3	A	1008	NO3	O3-N	2.91	1.40	1.25
3	A	1009	NO3	O2-N	2.91	1.40	1.25
3	B	801	NO3	O2-N	2.92	1.40	1.25
3	B	807	NO3	O3-N	2.92	1.40	1.25
3	A	1010	NO3	O2-N	2.92	1.40	1.25
3	B	808	NO3	O2-N	2.92	1.40	1.25
3	A	1003	NO3	O2-N	2.92	1.40	1.25
3	B	806	NO3	O2-N	2.92	1.40	1.25
3	A	1003	NO3	O3-N	2.93	1.40	1.25
3	A	1006	NO3	O2-N	2.93	1.40	1.25
3	B	803	NO3	O3-N	2.93	1.40	1.25
3	B	811	NO3	O2-N	2.93	1.40	1.25
3	B	805	NO3	O3-N	2.93	1.40	1.25
3	B	804	NO3	O3-N	2.93	1.40	1.25
3	B	808	NO3	O3-N	2.94	1.40	1.25
3	B	801	NO3	O3-N	2.95	1.40	1.25
3	A	1002	NO3	O3-N	2.96	1.40	1.25
2	A	1001	ADP	C5-C4	3.13	1.47	1.40
2	B	802	ADP	C5-C4	3.16	1.47	1.40
3	B	805	NO3	O1-N	3.82	1.40	1.24
3	A	1009	NO3	O1-N	3.85	1.40	1.24
3	B	811	NO3	O1-N	3.87	1.40	1.24
3	A	1006	NO3	O1-N	3.87	1.40	1.24
3	A	1003	NO3	O1-N	3.88	1.40	1.24
3	A	1008	NO3	O1-N	3.88	1.40	1.24
3	A	1007	NO3	O1-N	3.89	1.40	1.24
3	B	806	NO3	O1-N	3.89	1.40	1.24
3	B	809	NO3	O1-N	3.90	1.40	1.24
3	A	1010	NO3	O1-N	3.90	1.40	1.24
3	B	812	NO3	O1-N	3.90	1.40	1.24
3	A	1005	NO3	O1-N	3.91	1.40	1.24
3	B	810	NO3	O1-N	3.92	1.40	1.24
3	B	807	NO3	O1-N	3.94	1.40	1.24
3	B	808	NO3	O1-N	3.95	1.40	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	1002	NO3	O1-N	3.97	1.40	1.24
3	A	1004	NO3	O1-N	3.97	1.40	1.24
3	B	801	NO3	O1-N	3.99	1.40	1.24
3	B	804	NO3	O1-N	4.00	1.40	1.24
3	B	803	NO3	O1-N	4.00	1.40	1.24

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1001	ADP	N3-C2-N1	-6.97	123.56	128.89
2	B	802	ADP	N3-C2-N1	-6.89	123.62	128.89
2	A	1001	ADP	C4-C5-N7	-3.33	106.41	109.48
2	B	802	ADP	C2'-C1'-N9	-3.21	109.39	114.29
2	B	802	ADP	C4-C5-N7	-3.01	106.71	109.48
2	B	802	ADP	PA-O3A-PB	-2.84	123.13	132.67
2	A	1001	ADP	PA-O3A-PB	-2.55	124.11	132.67
4	B	813	EPE	C5-C6-N1	-2.35	106.41	110.63
2	A	1001	ADP	C2'-C1'-N9	-2.26	110.84	114.29
4	B	813	EPE	C7-N4-C3	2.35	117.28	111.27
2	A	1001	ADP	O4'-C1'-N9	2.35	113.02	108.10
4	B	813	EPE	C7-N4-C5	2.68	118.15	111.27
4	B	814	EPE	O1S-S-C10	2.71	109.22	106.91
4	B	814	EPE	O2S-S-C10	3.13	109.57	106.91
4	B	813	EPE	O1S-S-C10	3.50	109.89	106.91
4	B	813	EPE	O2S-S-C10	3.55	109.94	106.91
4	B	814	EPE	C7-N4-C5	3.56	120.39	111.27
4	B	814	EPE	C7-N4-C3	3.81	121.03	111.27
4	B	814	EPE	C6-N1-C2	4.15	117.89	108.90
4	B	814	EPE	C5-N4-C3	4.47	118.57	108.90
4	B	813	EPE	C5-N4-C3	4.71	119.10	108.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	ADP	1	0
3	A	1009	NO3	2	0
3	B	809	NO3	1	0
4	B	813	EPE	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	814	EPE	3	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	686/718 (95%)	0.39	51 (7%) 17 19	29, 47, 100, 135	0
1	B	693/718 (96%)	0.17	8 (1%) 81 81	25, 41, 73, 114	0
All	All	1379/1436 (96%)	0.28	59 (4%) 39 41	25, 44, 88, 135	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	535	GLN	7.2
1	A	651	ASP	6.7
1	A	641	VAL	5.4
1	A	532	ALA	5.3
1	A	710	ILE	5.3
1	A	707	LEU	5.1
1	A	650	PRO	5.0
1	A	643	ILE	4.8
1	A	654	LYS	4.6
1	A	642	LYS	3.8
1	A	713	SER	3.5
1	A	653	GLN	3.4
1	A	537	LEU	3.3
1	A	471	PRO	3.2
1	B	2	ALA	3.2
1	B	314	ILE	3.2
1	A	539	ASN	3.2
1	A	476	ILE	3.2
1	B	298	PRO	3.1
1	A	542	PHE	3.1
1	A	657	ASP	3.1
1	A	544	PHE	3.1
1	A	646	ALA	3.0
1	A	314	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	474	THR	2.9
1	A	687	ARG	2.9
1	A	664	ARG	2.9
1	A	665	GLY	2.9
1	A	477	ARG	2.9
1	A	652	PHE	2.8
1	A	475	TYR	2.8
1	A	593	SER	2.7
1	A	538	VAL	2.7
1	A	312	ARG	2.7
1	A	325	ASP	2.7
1	A	25	CYS	2.6
1	A	595	ILE	2.6
1	A	22	ASP	2.5
1	A	182	ARG	2.5
1	A	655	ILE	2.4
1	A	658	GLU	2.4
1	A	649	HIS	2.4
1	A	478	SER	2.4
1	A	592	GLY	2.4
1	B	650	PRO	2.3
1	A	648	ALA	2.3
1	A	640	HIS	2.2
1	A	683	ILE	2.2
1	B	182	ARG	2.2
1	A	682	ASP	2.2
1	A	644	PRO	2.2
1	B	180	LYS	2.1
1	A	541	HIS	2.1
1	A	639	VAL	2.1
1	B	653	GLN	2.1
1	A	536	LYS	2.0
1	A	531	GLU	2.0
1	B	678	ALA	2.0
1	A	587	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 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, 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	LLDF	B-factors(Å^2)	Q<0.9
3	NO3	B	809	4/4	0.83	0.27	17.23	97,97,98,100	0
3	NO3	A	1004	4/4	0.83	0.27	9.93	63,69,69,73	0
2	ADP	A	1001	27/27	0.86	0.24	5.11	48,95,140,286	0
2	ADP	B	802	27/27	0.84	0.31	4.97	34,85,121,299	0
4	EPE	B	813	15/15	0.58	0.35	3.57	105,114,143,144	0
4	EPE	B	814	15/15	0.79	0.23	3.10	75,86,135,135	0
3	NO3	B	807	4/4	0.80	0.17	3.00	70,71,73,78	0
3	NO3	A	1007	4/4	0.89	0.15	2.35	56,69,71,72	0
3	NO3	B	812	4/4	0.85	0.16	2.02	64,69,71,71	0
3	NO3	B	808	4/4	0.83	0.16	1.98	51,55,60,60	0
3	NO3	B	804	4/4	0.76	0.17	1.97	47,52,62,63	0
3	NO3	B	811	4/4	0.91	0.14	0.03	57,72,74,74	0
3	NO3	B	810	4/4	0.83	0.12	-0.02	76,76,81,87	0
3	NO3	B	801	4/4	0.84	0.13	-0.14	39,47,60,61	0
3	NO3	A	1010	4/4	0.90	0.13	-0.33	66,71,73,74	0
3	NO3	A	1003	4/4	0.96	0.11	-0.34	48,54,60,64	0
3	NO3	A	1005	4/4	0.91	0.13	-0.41	63,66,67,73	0
3	NO3	B	805	4/4	0.91	0.12	-0.59	43,53,53,55	0
3	NO3	A	1008	4/4	0.93	0.17	-	84,84,85,85	0
3	NO3	B	803	4/4	0.76	0.15	-	42,54,58,65	0
3	NO3	A	1006	4/4	0.94	0.08	-	71,74,77,81	0
3	NO3	A	1009	4/4	0.74	0.23	-	88,88,91,98	0
3	NO3	A	1002	4/4	0.90	0.13	-	34,49,54,62	0
3	NO3	B	806	4/4	0.65	0.22	-	96,97,98,99	0

6.5 Other polymers (i)

There are no such residues in this entry.