



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:09 AM UTC

PDB ID : 2YXT / pdb_00002yxt
Title : Human Pyridoxal Kinase
Authors : Safo, M.K.; Musayev, F.N.; Ko, T.P.; Schirch, V.
Deposited on : 2007-04-27
Resolution : 2.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

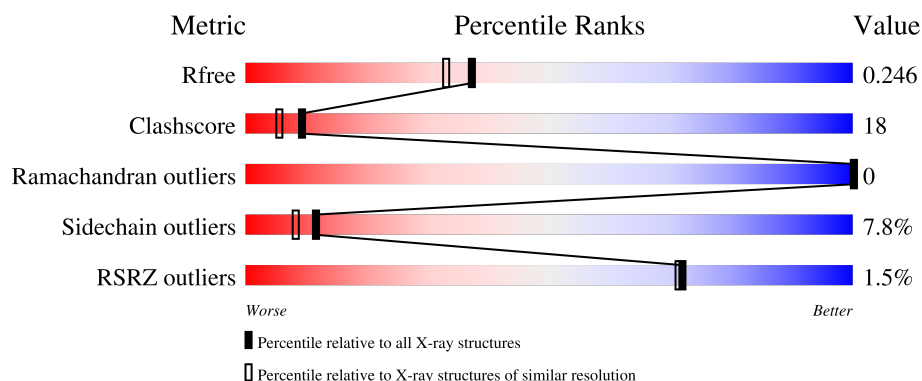
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	180053	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 $\leq 5\%$. 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	312	 62% 28% 6% . .
1	B	312	 65% 29% . .

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 5459 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 Pyridoxal kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	304	Total	C	N	O	S	0	0	0
			2392	1507	419	451	15			
1	B	304	Total	C	N	O	S	0	0	0
			2405	1517	421	452	15			

- Molecule 2 is SODIUM ION (CCD ID: NA) (formula: Na).

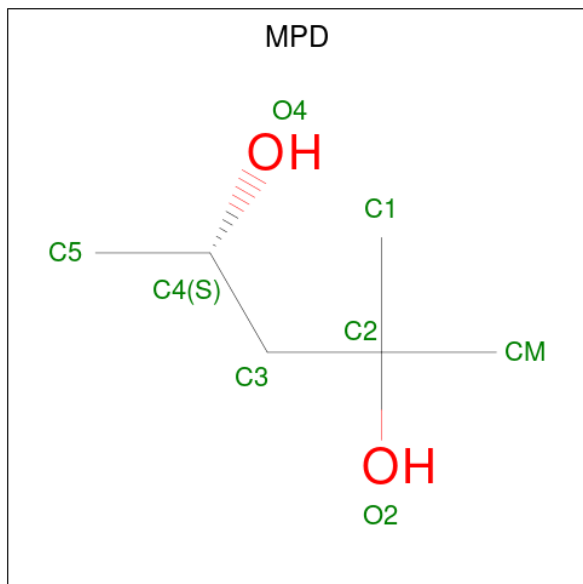
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Na	0	0
			1	1		
2	B	1	Total	Na	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).



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

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0
4	A	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0
4	B	1	Total C O 8 6 2	0	0

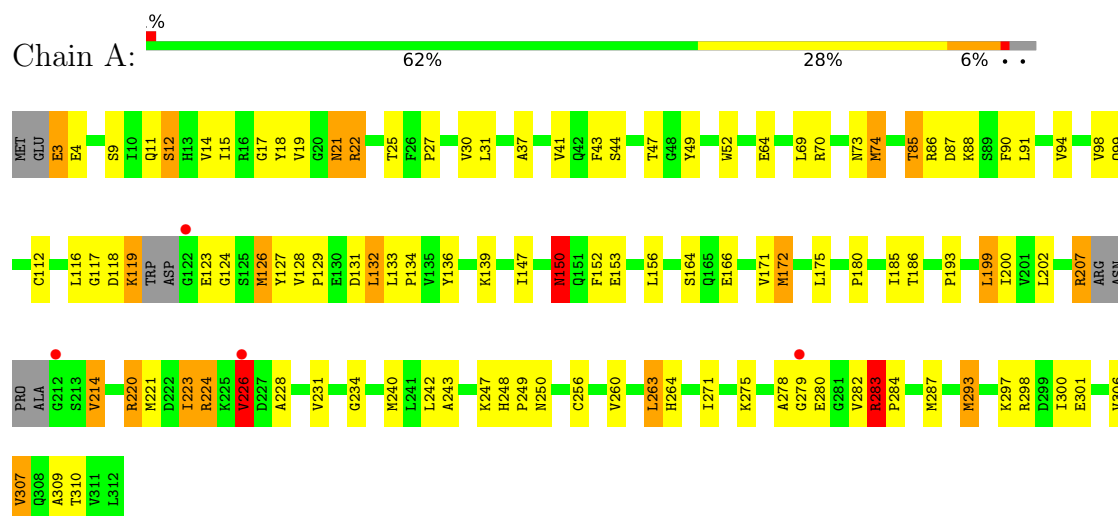
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	257	Total O 257 257	0	0
5	B	261	Total O 261 261	0	0

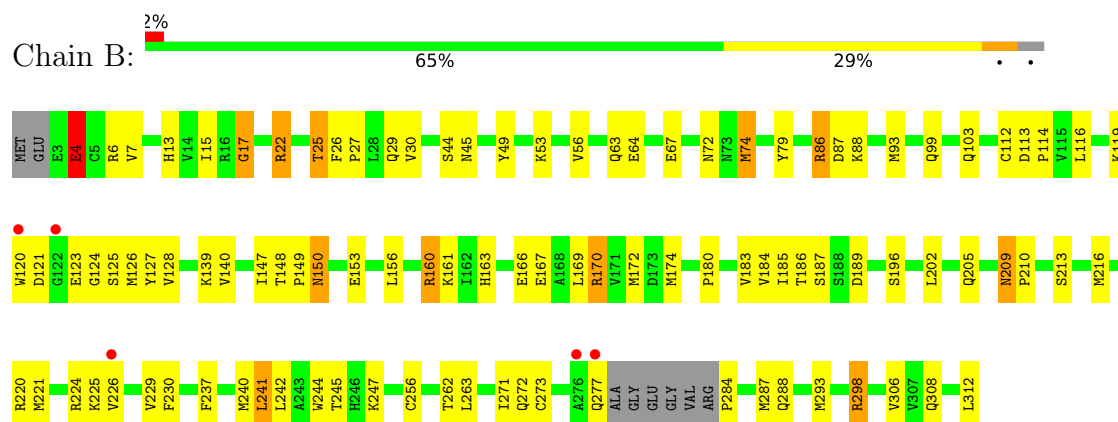
3 Residue-property plots [i](#)

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: Pyridoxal kinase



• Molecule 1: Pyridoxal kinase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	90.63Å 115.29Å 172.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.0 (30.00-2.00) 98.9 (30.00-2.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.46 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.206 , 0.245 0.207 , 0.246	Depositor DCC
R_{free} test set	3044 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	26.6	Xtriage
Anisotropy	0.235	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 79.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.35$, $\langle L^2 \rangle = 0.19$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	5459	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.71% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: NA, MPD, PO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.12	3/2433 (0.1%)	1.26	20/3293 (0.6%)
1	B	1.13	6/2450 (0.2%)	1.25	18/3320 (0.5%)
All	All	1.12	9/4883 (0.2%)	1.26	38/6613 (0.6%)

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	172	MET	SD-CE	-8.74	1.57	1.79
1	B	128	VAL	CA-CB	6.59	1.62	1.54
1	A	223	ILE	CA-CB	6.16	1.63	1.54
1	B	174	MET	SD-CE	6.06	1.94	1.79
1	B	183	VAL	CA-CB	5.98	1.62	1.54
1	B	15	ILE	CA-C	5.81	1.60	1.52
1	B	306	VAL	CA-CB	5.50	1.60	1.54
1	A	226	VAL	CA-CB	5.17	1.60	1.54
1	B	74	MET	SD-CE	-5.11	1.66	1.79

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	THR	N-CA-C	9.45	121.52	111.03
1	B	25	THR	N-CA-C	7.85	119.75	111.03
1	A	283	ARG	CA-C-N	7.70	127.71	119.78
1	A	283	ARG	C-N-CA	7.70	127.71	119.78
1	A	124	GLY	N-CA-C	7.46	124.88	113.02
1	A	280	GLU	N-CA-C	-7.43	98.46	110.20
1	B	4	GLU	N-CA-C	7.34	121.15	110.28
1	B	293	MET	N-CA-C	7.25	119.07	111.03
1	A	18	TYR	N-CA-C	6.60	121.49	107.70
1	A	180	PRO	N-CA-C	6.57	121.15	111.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	123	GLU	N-CA-C	6.55	118.81	108.79
1	A	293	MET	N-CA-C	6.45	118.00	110.97
1	B	185	ILE	N-CA-C	-6.29	97.42	106.55
1	A	85	THR	CB-CA-C	-6.21	96.77	109.38
1	B	180	PRO	N-CA-C	6.20	121.37	111.26
1	A	278	ALA	N-CA-C	-6.06	100.33	109.79
1	B	150	ASN	N-CA-C	-6.03	101.02	110.36
1	A	278	ALA	CA-C-N	-5.97	116.36	122.27
1	A	278	ALA	C-N-CA	-5.97	116.36	122.27
1	B	17	GLY	N-CA-C	5.88	120.40	112.17
1	A	248	HIS	CA-C-N	5.83	125.96	119.32
1	A	248	HIS	C-N-CA	5.83	125.96	119.32
1	A	150	ASN	N-CA-C	-5.75	101.45	110.36
1	B	241	LEU	N-CA-C	-5.75	105.02	111.28
1	A	12	SER	N-CA-C	5.71	117.91	110.43
1	B	229	VAL	N-CA-C	5.68	114.92	106.85
1	B	88	LYS	N-CA-C	5.53	116.98	111.07
1	B	140	VAL	N-CA-C	5.45	115.70	110.74
1	B	103	GLN	N-CA-C	-5.40	105.56	111.82
1	B	113	ASP	N-CA-C	-5.25	99.07	108.47
1	B	29	GLN	N-CA-C	-5.20	105.69	111.36
1	B	245	THR	N-CA-C	-5.20	106.45	112.89
1	A	186	THR	N-CA-C	5.19	118.87	112.54
1	B	225	LYS	CA-C-N	-5.12	116.84	123.19
1	B	225	LYS	C-N-CA	-5.12	116.84	123.19
1	A	249	PRO	N-CA-C	5.11	121.36	113.75
1	A	193	PRO	N-CA-C	-5.02	107.85	114.03
1	A	164	SER	N-CA-C	5.01	115.92	108.60

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	2392	0	2406	113	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2405	0	2414	65	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	0	0
3	B	25	0	0	1	0
4	A	40	0	70	9	0
4	B	72	0	126	5	0
5	A	257	0	0	7	2
5	B	261	0	0	9	2
All	All	5459	0	5016	180	5

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 18.

All (180) 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:A:172:MET:HE2	1:A:185:ILE:HD12	1.25	1.12
1:A:128:VAL:HG21	1:A:132:LEU:HD22	1.38	1.04
1:B:298:ARG:HG2	1:B:298:ARG:HH11	1.21	1.00
1:A:172:MET:HE2	1:A:185:ILE:CD1	1.93	0.98
1:A:19:VAL:HG12	1:A:231:VAL:HG12	1.51	0.89
1:A:200:ILE:HD12	1:A:220:ARG:HE	1.40	0.84
1:B:272:GLN:HG3	5:B:1479:HOH:O	1.79	0.82
1:A:172:MET:CE	1:A:185:ILE:HD12	2.07	0.82
1:A:85:THR:HG22	1:A:87:ASP:H	1.45	0.81
1:A:119:LYS:HG3	1:A:123:GLU:C	2.05	0.81
1:A:207:ARG:HH21	1:A:250:ASN:C	1.89	0.81
1:B:169:LEU:HD23	1:B:172:MET:HE3	1.61	0.80
1:A:200:ILE:HG23	1:A:220:ARG:HD2	1.62	0.80
1:B:224:ARG:O	4:B:1025:MPD:H11	1.83	0.78
1:A:126:MET:HE1	1:A:156:LEU:HD11	1.68	0.76
1:B:150:ASN:OD1	1:B:153:GLU:HG3	1.86	0.75
1:A:19:VAL:CG1	1:A:231:VAL:HG12	2.15	0.75
1:A:150:ASN:ND2	1:A:153:GLU:H	1.85	0.74
1:B:298:ARG:HG2	1:B:298:ARG:NH1	1.93	0.74
1:A:128:VAL:CG2	1:A:132:LEU:HD22	2.17	0.72
1:B:120:TRP:HZ2	1:B:127:TYR:HH	1.36	0.71
1:B:169:LEU:HD23	1:B:172:MET:CE	2.19	0.71
1:A:47:THR:HG23	4:A:1001:MPD:H13	1.72	0.70
1:B:49:TYR:OH	1:B:287:MET:HA	1.91	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:64:GLU:HG2	5:B:1522:HOH:O	1.92	0.69
1:A:297:LYS:O	1:A:301:GLU:HG3	1.93	0.68
1:B:242:LEU:HD23	1:B:242:LEU:C	2.18	0.68
1:A:166:GLU:O	5:A:1428:HOH:O	2.12	0.68
1:A:226:VAL:HG23	1:A:228:ALA:O	1.95	0.67
1:A:133:LEU:HB3	1:A:134:PRO:HD3	1.76	0.67
1:B:273:CYS:C	1:B:277:GLN:HE21	2.01	0.67
1:A:298:ARG:HH11	1:A:298:ARG:HG3	1.59	0.66
1:A:221:MET:HE1	1:A:260:VAL:HG21	1.76	0.66
1:A:243:ALA:O	1:A:247:LYS:HG2	1.95	0.66
1:B:209:ASN:ND2	1:B:213:SER:H	1.94	0.66
1:A:310:THR:HG22	5:A:1531:HOH:O	1.96	0.65
1:A:126:MET:HE1	1:A:156:LEU:CD1	2.26	0.65
1:A:150:ASN:HD22	1:A:150:ASN:C	2.03	0.65
1:A:172:MET:HE1	1:A:202:LEU:HB2	1.80	0.64
1:B:139:LYS:HA	1:B:139:LYS:HE2	1.80	0.64
1:A:224:ARG:HD3	4:A:1013:MPD:H31	1.78	0.64
1:A:199:LEU:HD12	1:A:199:LEU:C	2.24	0.63
1:A:86:ARG:O	1:A:86:ARG:HG2	2.00	0.62
1:A:19:VAL:CG1	1:A:231:VAL:CG1	2.77	0.62
1:B:209:ASN:HD21	1:B:213:SER:H	1.46	0.62
1:B:221:MET:HE1	1:B:256:CYS:HB3	1.82	0.61
1:A:200:ILE:HD12	1:A:220:ARG:NE	2.14	0.61
4:B:1031:MPD:HM2	4:B:1033:MPD:HM1	1.82	0.61
1:A:128:VAL:HG22	1:A:132:LEU:HD13	1.82	0.60
1:B:240:MET:HE2	1:B:262:THR:HG21	1.84	0.60
1:B:120:TRP:HZ2	1:B:127:TYR:OH	1.83	0.60
1:A:224:ARG:HD3	4:A:1013:MPD:C3	2.32	0.59
1:B:116:LEU:HB3	1:B:126:MET:HE3	1.83	0.59
1:A:85:THR:HG22	1:A:86:ARG:N	2.17	0.59
1:A:279:GLY:H	1:A:282:VAL:HB	1.67	0.58
1:A:117:GLY:HA2	1:A:127:TYR:CD2	2.39	0.58
1:A:119:LYS:HG3	1:A:123:GLU:CA	2.33	0.58
1:A:19:VAL:HG11	1:A:231:VAL:HG11	1.85	0.57
1:A:85:THR:HG23	5:A:1455:HOH:O	2.04	0.57
1:A:150:ASN:HD21	1:A:153:GLU:HG3	1.68	0.57
1:A:279:GLY:N	1:A:282:VAL:HB	2.20	0.57
1:A:9:SER:OG	1:A:21:ASN:ND2	2.38	0.56
1:A:17:GLY:O	1:A:22:ARG:HD3	2.04	0.56
4:B:1053:MPD:H52	5:B:1574:HOH:O	2.04	0.56
1:B:72:ASN:HB2	1:B:74:MET:HE2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:19:VAL:HG11	1:A:231:VAL:CG1	2.35	0.56
1:A:172:MET:HE1	1:A:202:LEU:CB	2.36	0.56
1:B:120:TRP:CZ2	1:B:127:TYR:OH	2.58	0.56
1:A:12:SER:HB2	1:A:41:VAL:HG22	1.89	0.55
1:A:223:ILE:HD12	1:A:223:ILE:O	2.05	0.55
1:A:223:ILE:HD12	1:A:223:ILE:C	2.32	0.55
1:A:207:ARG:HH21	1:A:250:ASN:CA	2.19	0.55
1:A:3:GLU:HA	1:A:3:GLU:OE1	2.07	0.55
1:A:15:ILE:HD12	1:A:44:SER:HA	1.89	0.54
1:A:150:ASN:HD21	1:A:153:GLU:H	1.53	0.54
1:A:207:ARG:NH2	1:A:250:ASN:C	2.64	0.54
1:A:207:ARG:HE	1:A:250:ASN:HB3	1.72	0.53
1:B:160:ARG:HH11	1:B:160:ARG:HG2	1.73	0.53
1:B:7:VAL:HG22	1:B:79:TYR:HB2	1.91	0.53
1:B:209:ASN:C	1:B:209:ASN:HD22	2.17	0.53
1:A:199:LEU:HD12	1:A:199:LEU:O	2.08	0.52
1:A:3:GLU:HG3	5:A:1448:HOH:O	2.10	0.52
1:A:263:LEU:HG	4:A:1003:MPD:HM2	1.90	0.52
1:A:112:CYS:O	1:A:147:ILE:HA	2.09	0.52
1:A:118:ASP:OD1	1:A:119:LYS:N	2.38	0.52
1:B:17:GLY:O	1:B:22:ARG:HD3	2.09	0.52
1:B:172:MET:HE1	1:B:202:LEU:HB3	1.92	0.52
1:B:209:ASN:HB3	5:B:1473:HOH:O	2.08	0.52
1:A:70:ARG:HD2	5:A:1460:HOH:O	2.09	0.51
1:A:87:ASP:OD2	1:A:90:PHE:N	2.39	0.51
1:B:119:LYS:HA	1:B:124:GLY:HA2	1.92	0.51
1:B:287:MET:HE2	1:B:288:GLN:HE22	1.74	0.51
1:B:284:PRO:N	5:B:1549:HOH:O	2.43	0.51
1:B:149:PRO:HD2	1:B:184:VAL:O	2.10	0.50
1:A:298:ARG:HG3	1:A:298:ARG:NH1	2.26	0.50
1:A:150:ASN:ND2	1:A:150:ASN:C	2.68	0.50
1:B:298:ARG:NH1	1:B:298:ARG:CG	2.71	0.50
1:A:199:LEU:C	1:A:199:LEU:CD1	2.85	0.50
4:B:1031:MPD:H51	5:B:1455:HOH:O	2.12	0.50
1:A:126:MET:HE3	1:A:152:PHE:CZ	2.47	0.50
3:B:1329:PO4:O3	5:B:1582:HOH:O	2.18	0.49
1:A:207:ARG:HG2	1:A:207:ARG:HH11	1.77	0.49
1:A:49:TYR:OH	1:A:287:MET:HA	2.13	0.49
1:A:256:CYS:O	1:A:260:VAL:HG23	2.12	0.49
1:B:161:LYS:HD3	1:B:163:HIS:NE2	2.27	0.49
1:B:226:VAL:HG21	1:B:271:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:MET:HG2	1:A:309:ALA:HA	1.95	0.49
1:B:26:PHE:HB3	1:B:27:PRO:HD3	1.94	0.49
1:B:169:LEU:HA	1:B:172:MET:HE3	1.96	0.48
1:A:200:ILE:CG2	1:A:220:ARG:HD2	2.38	0.48
1:A:207:ARG:HG2	1:A:207:ARG:NH1	2.28	0.48
1:A:242:LEU:C	1:A:242:LEU:HD23	2.39	0.48
1:A:126:MET:CE	1:A:156:LEU:HD11	2.41	0.48
1:A:69:LEU:HA	1:A:74:MET:HE2	1.96	0.48
1:A:133:LEU:HD11	1:A:156:LEU:HB3	1.96	0.48
1:A:37:ALA:O	1:B:13:HIS:HE1	1.97	0.47
1:B:221:MET:CE	1:B:256:CYS:HB3	2.43	0.47
1:A:150:ASN:ND2	1:A:153:GLU:HG3	2.28	0.47
1:A:307:VAL:HG12	4:A:1013:MPD:HM3	1.96	0.47
1:A:27:PRO:HB2	1:A:240:MET:HE3	1.95	0.47
1:A:119:LYS:HA	1:A:123:GLU:O	2.15	0.47
1:A:214:VAL:HG22	1:A:214:VAL:O	2.15	0.47
1:A:226:VAL:HG23	1:A:226:VAL:O	2.14	0.47
1:B:44:SER:OG	1:B:45:ASN:ND2	2.48	0.46
1:A:172:MET:HE2	1:A:185:ILE:CG1	2.45	0.46
1:B:63:GLN:HB2	1:B:93:MET:HE3	1.97	0.46
1:A:123:GLU:OE2	1:A:123:GLU:N	2.46	0.46
1:A:126:MET:HE3	1:A:152:PHE:CE2	2.50	0.46
1:A:224:ARG:CD	4:A:1013:MPD:H31	2.44	0.46
1:B:244:TRP:CZ3	1:B:247:LYS:HG3	2.50	0.46
1:A:126:MET:CE	1:A:152:PHE:CE2	2.99	0.46
1:A:221:MET:CE	1:A:260:VAL:HG21	2.43	0.46
1:A:264:HIS:CD2	1:A:306:VAL:HG21	2.51	0.45
1:B:166:GLU:HG3	1:B:167:GLU:N	2.31	0.45
1:A:47:THR:H	4:A:1001:MPD:H11	1.81	0.45
1:A:47:THR:HG22	1:A:52:TRP:CE2	2.52	0.45
1:A:64:GLU:HG2	1:B:53:LYS:HB3	1.98	0.45
1:B:226:VAL:HG21	1:B:230:PHE:HE2	1.82	0.45
1:B:148:THR:HB	1:B:186:THR:HG21	1.98	0.44
1:B:237:PHE:CD2	1:B:237:PHE:C	2.95	0.44
1:B:287:MET:HE2	1:B:288:GLN:NE2	2.32	0.44
1:A:226:VAL:HG12	4:A:1005:MPD:H52	2.00	0.44
1:A:171:VAL:O	1:A:175:LEU:HG	2.18	0.44
1:B:64:GLU:O	1:B:67:GLU:HB3	2.18	0.44
1:A:94:VAL:O	1:A:98:VAL:HG23	2.17	0.44
1:A:226:VAL:CG2	1:A:228:ALA:O	2.64	0.44
1:B:139:LYS:HE2	1:B:139:LYS:CA	2.46	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:ILE:HG22	1:A:275:LYS:HE2	1.98	0.43
1:A:14:VAL:HA	1:A:43:PHE:O	2.19	0.43
1:B:209:ASN:HB2	1:B:210:PRO:CD	2.49	0.43
1:A:226:VAL:O	1:A:226:VAL:CG2	2.67	0.43
1:B:244:TRP:CE3	1:B:247:LYS:HG3	2.54	0.43
1:B:25:THR:O	1:B:26:PHE:C	2.62	0.43
1:A:117:GLY:HA2	1:A:127:TYR:CG	2.54	0.43
1:A:126:MET:CE	1:A:152:PHE:HE2	2.32	0.43
1:B:220:ARG:HB2	1:B:312:LEU:HD11	2.01	0.42
1:B:242:LEU:C	1:B:242:LEU:CD2	2.88	0.42
1:A:293:MET:HE3	1:A:300:ILE:HD11	2.01	0.42
1:A:283:ARG:HA	1:A:284:PRO:HD3	1.77	0.42
1:A:297:LYS:NZ	1:B:30:VAL:O	2.51	0.42
1:A:31:LEU:HD23	1:A:31:LEU:HA	1.92	0.42
1:A:199:LEU:CD1	1:A:223:ILE:HG13	2.50	0.42
1:A:234:GLY:N	5:A:1392:HOH:O	2.51	0.42
1:B:112:CYS:O	1:B:147:ILE:HA	2.19	0.42
1:B:272:GLN:HA	1:B:272:GLN:OE1	2.19	0.42
4:B:1039:MPD:HM3	5:B:1496:HOH:O	2.20	0.42
1:A:221:MET:HB2	1:A:221:MET:HE3	1.80	0.41
1:B:4:GLU:OE2	1:B:6:ARG:NH2	2.51	0.41
1:B:241:LEU:HA	1:B:241:LEU:HD12	1.82	0.41
1:A:116:LEU:HD21	1:A:136:TYR:CD2	2.55	0.41
1:A:30:VAL:CG1	1:A:301:GLU:HG2	2.50	0.41
1:B:186:THR:O	1:B:187:SER:HB2	2.21	0.41
1:B:209:ASN:ND2	1:B:209:ASN:C	2.79	0.41
1:B:125:SER:HB3	5:B:1551:HOH:O	2.20	0.40
1:A:47:THR:HG22	1:A:52:TRP:CD2	2.56	0.40
1:A:70:ARG:CD	5:A:1460:HOH:O	2.68	0.40
1:B:86:ARG:H	1:B:86:ARG:HG3	1.73	0.40
1:B:205:GLN:O	1:B:216:MET:HA	2.22	0.40
1:A:247:LYS:HE3	4:A:1009:MPD:O2	2.22	0.40
1:B:156:LEU:HD23	1:B:156:LEU:HA	1.80	0.40

All (5) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1602:HOH:O	5:B:1602:HOH:O[2_555]	1.50	0.70
5:A:1568:HOH:O	5:A:1568:HOH:O[2_655]	1.59	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:1567:HOH:O	5:A:1567:HOH:O[2_655]	1.69	0.51
1:B:170:ARG:NH1	1:B:170:ARG:NH1[3_555]	1.75	0.45
5:B:1473:HOH:O	5:B:1473:HOH:O[3_555]	1.80	0.40

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	298/312 (96%)	290 (97%)	8 (3%)	0	100	100
1	B	300/312 (96%)	290 (97%)	10 (3%)	0	100	100
All	All	598/624 (96%)	580 (97%)	18 (3%)	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	268/275 (98%)	242 (90%)	26 (10%)	8	5
1	B	270/275 (98%)	254 (94%)	16 (6%)	18	14
All	All	538/550 (98%)	496 (92%)	42 (8%)	11	8

All (42) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	4	GLU
1	A	11	GLN
1	A	21	ASN
1	A	22	ARG
1	A	73	ASN
1	A	74	MET
1	A	88	LYS
1	A	91	LEU
1	A	99	GLN
1	A	119	LYS
1	A	126	MET
1	A	129	PRO
1	A	131	ASP
1	A	132	LEU
1	A	139	LYS
1	A	150	ASN
1	A	199	LEU
1	A	207	ARG
1	A	214	VAL
1	A	220	ARG
1	A	224	ARG
1	A	226	VAL
1	A	263	LEU
1	A	283	ARG
1	A	307	VAL
1	B	4	GLU
1	B	22	ARG
1	B	56	VAL
1	B	86	ARG
1	B	87	ASP
1	B	99	GLN
1	B	114	PRO
1	B	121	ASP
1	B	160	ARG
1	B	170	ARG
1	B	189	ASP
1	B	196	SER
1	B	209	ASN
1	B	263	LEU
1	B	298	ARG
1	B	308	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	21	ASN
1	A	39	ASN
1	A	45	ASN
1	A	51	HIS
1	A	103	GLN
1	A	150	ASN
1	A	264	HIS
1	A	277	GLN
1	B	13	HIS
1	B	29	GLN
1	B	45	ASN
1	B	209	ASN
1	B	268	GLN
1	B	277	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 22 ligands modelled in this entry, 2 are monoatomic - leaving 20 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	PO4	B	1349	-	4,4,4	1.50	0	6,6,6	0.48	0
4	MPD	B	1031	-	7,7,7	0.90	0	9,10,10	0.50	0
4	MPD	A	1009	-	7,7,7	0.49	0	9,10,10	0.39	0
4	MPD	A	1003	-	7,7,7	0.52	0	9,10,10	0.53	0
3	PO4	A	1319	-	4,4,4	1.36	0	6,6,6	0.44	0
4	MPD	B	1039	-	7,7,7	1.00	1 (14%)	9,10,10	0.56	0
4	MPD	B	1027	-	7,7,7	0.75	0	9,10,10	0.38	0
4	MPD	A	1013	-	7,7,7	0.52	0	9,10,10	0.56	0
4	MPD	A	1005	-	7,7,7	0.79	0	9,10,10	0.54	0
3	PO4	B	1347	-	4,4,4	1.60	0	6,6,6	0.42	0
4	MPD	B	1053	-	7,7,7	0.77	0	9,10,10	0.37	0
3	PO4	B	1329	-	4,4,4	1.46	0	6,6,6	0.52	0
3	PO4	B	1335	-	4,4,4	1.53	0	6,6,6	0.48	0
4	MPD	B	1041	-	7,7,7	0.90	0	9,10,10	0.54	0
4	MPD	A	1001	-	7,7,7	0.63	0	9,10,10	0.32	0
4	MPD	B	1033	-	7,7,7	0.76	0	9,10,10	0.59	0
4	MPD	B	1045	-	7,7,7	0.81	0	9,10,10	0.35	0
3	PO4	B	1337	-	4,4,4	1.38	0	6,6,6	0.45	0
4	MPD	B	1025	-	7,7,7	0.77	0	9,10,10	0.42	0
4	MPD	B	1023	-	7,7,7	0.43	0	9,10,10	0.51	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	MPD	B	1039	-	-	1/5/5/5	-
4	MPD	B	1025	-	-	1/5/5/5	-
4	MPD	B	1027	-	-	3/5/5/5	-
4	MPD	B	1041	-	-	3/5/5/5	-
4	MPD	B	1031	-	-	2/5/5/5	-
4	MPD	A	1013	-	-	1/5/5/5	-
4	MPD	A	1001	-	-	4/5/5/5	-
4	MPD	B	1033	-	-	4/5/5/5	-
4	MPD	A	1005	-	-	2/5/5/5	-
4	MPD	B	1045	-	-	3/5/5/5	-
4	MPD	A	1009	-	-	5/5/5/5	-
4	MPD	A	1003	-	-	2/5/5/5	-
4	MPD	B	1023	-	-	4/5/5/5	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPD	B	1053	-	-	2/5/5/5	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1039	MPD	C3-C2	2.05	1.60	1.54

There are no bond angle outliers.

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	MPD	C2-C3-C4-O4
4	A	1003	MPD	C2-C3-C4-O4
4	A	1003	MPD	C2-C3-C4-C5
4	A	1005	MPD	C2-C3-C4-O4
4	A	1005	MPD	C2-C3-C4-C5
4	A	1009	MPD	C2-C3-C4-O4
4	A	1009	MPD	C2-C3-C4-C5
4	B	1033	MPD	C2-C3-C4-O4
4	B	1041	MPD	C2-C3-C4-O4
4	B	1041	MPD	C2-C3-C4-C5
4	B	1053	MPD	C2-C3-C4-O4
4	A	1013	MPD	O2-C2-C3-C4
4	B	1039	MPD	O2-C2-C3-C4
4	B	1031	MPD	C2-C3-C4-O4
4	A	1001	MPD	C1-C2-C3-C4
4	A	1009	MPD	C1-C2-C3-C4
4	A	1009	MPD	CM-C2-C3-C4
4	B	1023	MPD	C1-C2-C3-C4
4	B	1023	MPD	CM-C2-C3-C4
4	B	1041	MPD	CM-C2-C3-C4
4	B	1045	MPD	C1-C2-C3-C4
4	A	1001	MPD	C2-C3-C4-C5
4	B	1025	MPD	C2-C3-C4-C5
4	B	1031	MPD	C2-C3-C4-C5
4	B	1033	MPD	C2-C3-C4-C5
4	B	1053	MPD	C2-C3-C4-C5
4	A	1009	MPD	O2-C2-C3-C4
4	B	1023	MPD	O2-C2-C3-C4
4	B	1027	MPD	O2-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
4	B	1033	MPD	O2-C2-C3-C4
4	B	1045	MPD	O2-C2-C3-C4
4	B	1023	MPD	C2-C3-C4-O4
4	A	1001	MPD	CM-C2-C3-C4
4	B	1027	MPD	C1-C2-C3-C4
4	B	1027	MPD	CM-C2-C3-C4
4	B	1033	MPD	C1-C2-C3-C4
4	B	1045	MPD	CM-C2-C3-C4

There are no ring outliers.

11 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1031	MPD	2	0
4	A	1009	MPD	1	0
4	A	1003	MPD	1	0
4	B	1039	MPD	1	0
4	A	1013	MPD	4	0
4	A	1005	MPD	1	0
4	B	1053	MPD	1	0
3	B	1329	PO4	1	0
4	A	1001	MPD	2	0
4	B	1033	MPD	1	0
4	B	1025	MPD	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	304/312 (97%)	-0.30	4 (1%) 75 74	21, 35, 75, 97	0
1	B	304/312 (97%)	-0.39	5 (1%) 70 70	20, 31, 67, 106	0
All	All	608/624 (97%)	-0.34	9 (1%) 72 71	20, 34, 71, 106	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	122	GLY	3.5
1	A	212	GLY	3.0
1	A	226	VAL	2.9
1	A	279	GLY	2.7
1	B	276	ALA	2.6
1	B	122	GLY	2.6
1	B	120	TRP	2.4
1	B	226	VAL	2.4
1	B	277	GLN	2.2

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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	PO4	B	1337	5/5	0.75	0.13	81,86,91,100	0
4	MPD	B	1041	8/8	0.81	0.18	65,73,77,83	0
3	PO4	B	1335	5/5	0.83	0.15	102,104,113,114	0
4	MPD	B	1025	8/8	0.86	0.20	81,83,86,87	0
3	PO4	A	1319	5/5	0.86	0.12	98,99,105,108	0
2	NA	B	1316	1/1	0.87	0.25	62,62,62,62	0
4	MPD	B	1045	8/8	0.87	0.13	100,102,104,104	0
4	MPD	A	1005	8/8	0.89	0.16	52,67,71,72	0
3	PO4	B	1329	5/5	0.89	0.11	73,78,84,86	0
4	MPD	B	1053	8/8	0.89	0.12	65,74,74,83	0
4	MPD	B	1023	8/8	0.90	0.13	57,58,65,66	0
4	MPD	A	1001	8/8	0.90	0.16	75,77,81,82	0
4	MPD	B	1033	8/8	0.90	0.15	60,67,72,76	0
4	MPD	A	1009	8/8	0.91	0.13	72,75,83,87	0
4	MPD	A	1013	8/8	0.91	0.13	61,68,78,78	0
3	PO4	B	1347	5/5	0.91	0.11	108,111,114,116	0
3	PO4	B	1349	5/5	0.91	0.11	85,87,95,98	0
4	MPD	B	1039	8/8	0.92	0.10	41,53,61,73	0
4	MPD	A	1003	8/8	0.92	0.12	54,60,71,72	0
4	MPD	B	1031	8/8	0.93	0.09	27,36,46,46	0
4	MPD	B	1027	8/8	0.93	0.11	45,55,64,69	0
2	NA	A	1314	1/1	0.99	0.05	61,61,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.