



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:22 PM GMT

PDB ID : 4EN4
Title : Crystal Structure of the Ternary Human PL Kinase-Ginkgotoxin-MgATP Complex
Authors : Safo, M.K.; Musayev, F.N.; Gandhi, A.K.
Deposited on : 2012-04-12
Resolution : 2.15 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 (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

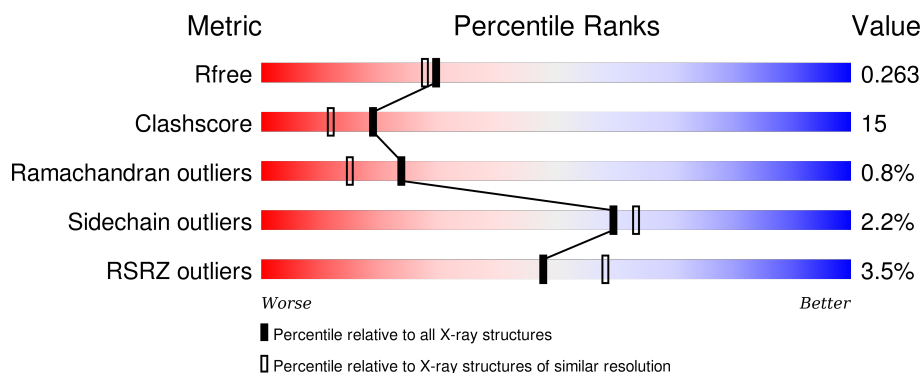
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.15 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	1045 (2.16-2.16)
Clashscore	102246	1152 (2.16-2.16)
Ramachandran outliers	100387	1131 (2.16-2.16)
Sidechain outliers	100360	1131 (2.16-2.16)
RSRZ outliers	91569	1050 (2.16-2.16)

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 $\leq 5\%$. 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	<div> <div>4%</div> <div>70%</div> <div>28%</div> <div>..</div> </div>
1	B	312	<div> <div>3%</div> <div>75%</div> <div>22%</div> <div>..</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
5	GT0	B	414[A]	-	-	-	X
6	MPD	B	408	-	-	-	X
6	MPD	B	410	-	-	-	X
7	SO4	A	409	-	-	-	X
8	GT1	A	410[B]	-	-	-	X
8	GT1	B	405[B]	-	-	X	X

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 5364 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	310	Total	C	N	O	S	0	0	0
			2445	1540	430	460	15			
1	B	310	Total	C	N	O	S	0	0	0
			2445	1540	430	460	15			

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

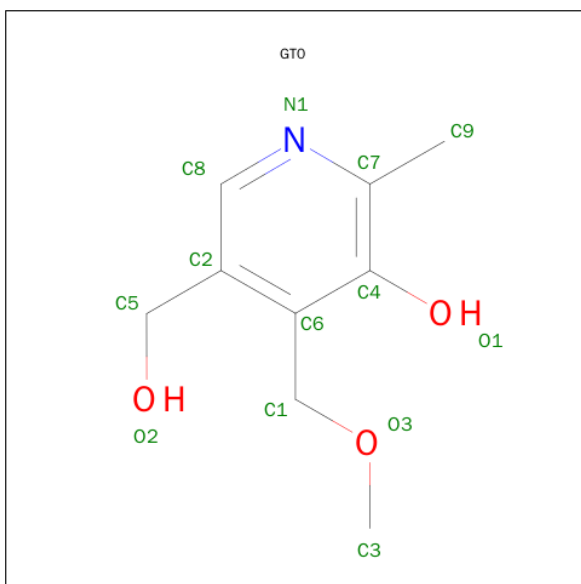
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Na	0	0
			1	1		
3	A	1	Total	Na	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: C₁₀H₁₆N₅O₁₃P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 10	N 5	O 13	P 3	0	0
4	B	1	Total 31	C 10	N 5	O 13	P 3	0	0

- Molecule 5 is 5-(HYDROXYMETHYL)-4-(METHOXYMETHYL)-2-METHYLPYRIDIN-3-OL (three-letter code: GT0) (formula: $C_9H_{13}NO_3$).



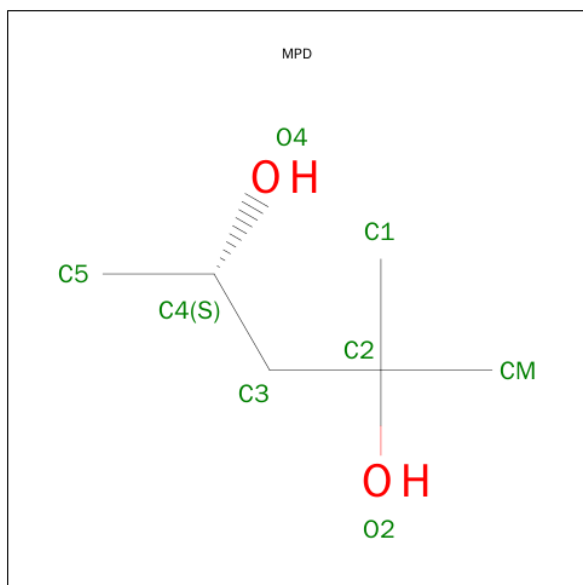
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	1
			13	9	1	3		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	N	O	0	1
			13	9	1	3		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



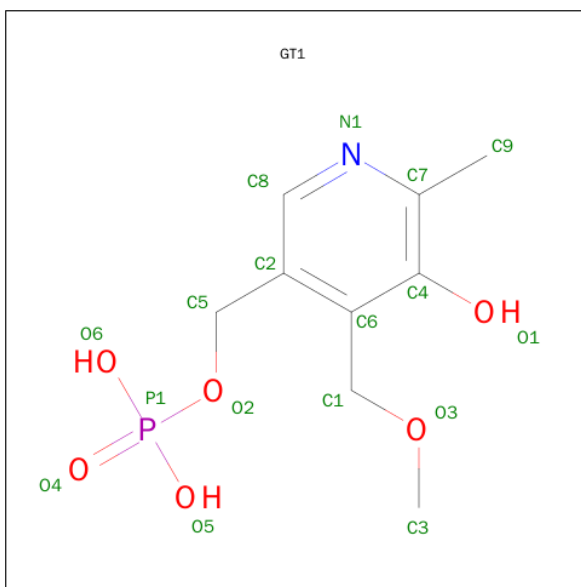
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 8 is [5-HYDROXY-4-(METHOXYMETHYL)-6-METHYLPYRIDIN-3-YL]METHYL DIHYDROGEN PHOSPHATE (three-letter code: GT1) (formula: C₉H₁₄NO₆P).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	N	O	P	0	1
			17	9	1	6	1		
8	B	1	Total	C	N	O	P	0	1
			17	9	1	6	1		

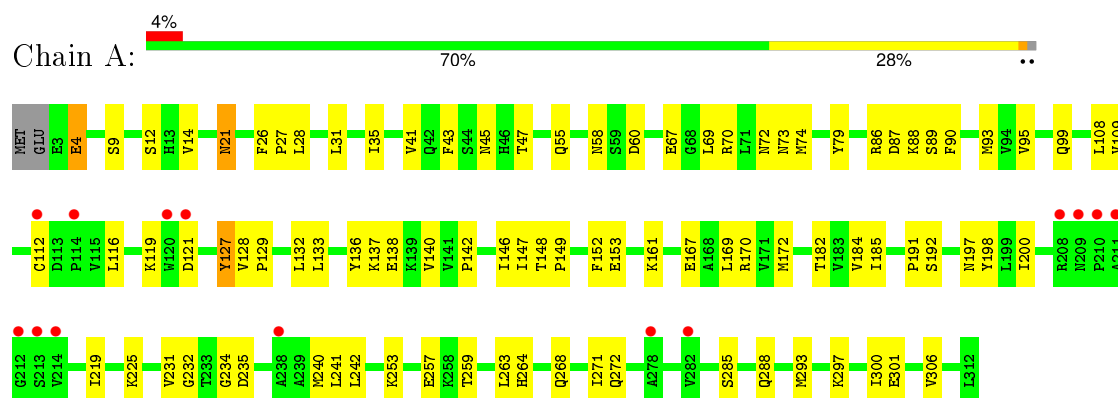
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	120	Total	O	0	0
			120	120		
9	B	148	Total	O	0	0
			148	148		

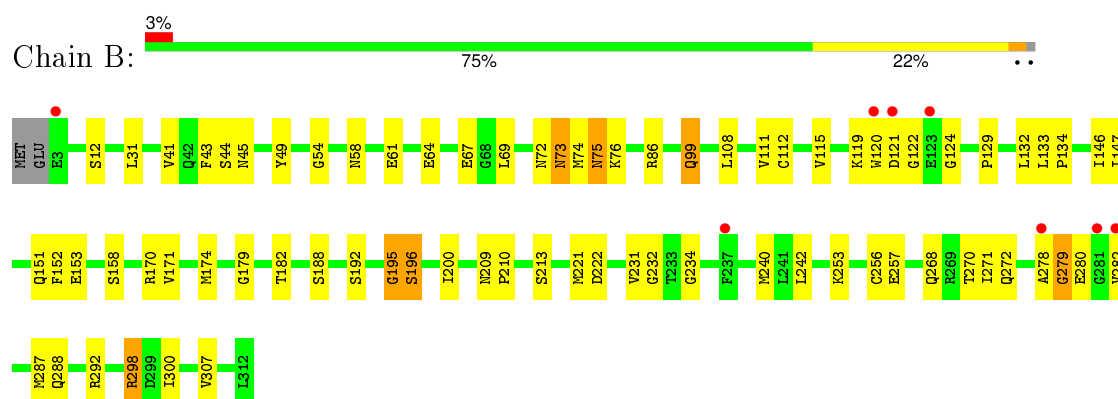
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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	92.75Å 115.22Å 169.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	28.81 – 2.15 28.81 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.5 (28.81-2.15) 92.5 (28.81-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.17 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.219 , 0.262 0.219 , 0.263	Depositor DCC
R_{free} test set	2312 reflections (5.03%)	DCC
Wilson B-factor (Å ²)	29.9	Xtriage
Anisotropy	0.406	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 70.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 49278 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	5364	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.61% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MG, NA, MPD, GT0, GT1, SO4, ATP

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	0.49	0/2491	0.73	1/3377 (0.0%)
1	B	0.48	0/2491	0.70	1/3377 (0.0%)
All	All	0.48	0/4982	0.72	2/6754 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	4	GLU	N-CA-C	6.50	128.55	111.00
1	B	279	GLY	N-CA-C	6.44	129.21	113.10

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2445	0	2453	73	0
1	B	2445	0	2452	74	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	31	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	31	0	12	1	0
5	A	13	0	13	1	0
5	B	13	0	13	0	0
6	A	8	0	13	3	0
6	B	40	0	70	11	0
7	A	15	0	0	0	0
7	B	15	0	0	0	0
8	A	17	0	12	6	0
8	B	17	0	11	7	0
9	A	120	0	0	4	0
9	B	148	0	0	11	0
All	All	5364	0	5061	155	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 15.

All (155) 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)
6:B:408:MPD:H52	6:B:408:MPD:H12	1.34	1.09
1:B:278:ALA:HB2	1:B:288:GLN:HE22	1.15	1.07
1:A:47:THR:HG23	5:A:405[A]:GT0:H10	1.41	1.02
6:B:406:MPD:H53	6:B:406:MPD:HM1	1.44	0.99
6:B:410:MPD:HM3	9:B:528:HOH:O	1.72	0.90
1:B:278:ALA:HB2	1:B:288:GLN:NE2	1.89	0.88
1:A:129:PRO:HB2	1:A:132:LEU:HD13	1.55	0.86
6:A:406:MPD:O2	6:A:406:MPD:H52	1.80	0.81
1:A:74:MET:HG2	1:B:287:MET:CE	2.11	0.81
1:B:232:GLY:N	8:B:405[B]:GT1:O6	2.17	0.78
1:B:278:ALA:O	1:B:282:VAL:HB	1.84	0.77
1:B:268:GLN:O	1:B:272:GLN:HG2	1.85	0.77
1:A:234:GLY:HA3	8:A:410[B]:GT1:O6	1.86	0.76
1:B:69:LEU:HA	1:B:74:MET:HE3	1.70	0.73
1:B:195:GLY:O	1:B:196:SER:HB3	1.89	0.72
6:B:406:MPD:H53	6:B:406:MPD:CM	2.20	0.71
6:B:408:MPD:H52	6:B:408:MPD:C1	2.17	0.70
1:A:232:GLY:N	8:A:410[B]:GT1:O4	2.23	0.70
6:B:410:MPD:H52	6:B:410:MPD:O2	1.90	0.70
1:A:234:GLY:CA	8:A:410[B]:GT1:O6	2.41	0.69
1:A:234:GLY:N	8:A:410[B]:GT1:O6	2.27	0.68
1:B:234:GLY:N	8:B:405[B]:GT1:O4	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:75:ASN:H	1:B:75:ASN:HD22	1.44	0.66
1:B:196:SER:HA	9:B:563:HOH:O	1.97	0.65
1:B:69:LEU:HA	1:B:74:MET:CE	2.28	0.64
1:A:169:LEU:HD23	1:A:172:MET:CE	2.28	0.63
1:A:67:GLU:HG3	9:A:601:HOH:O	1.98	0.63
1:A:74:MET:HG2	1:B:287:MET:HE2	1.80	0.63
6:B:408:MPD:C5	6:B:408:MPD:H12	2.20	0.62
1:A:72:ASN:O	1:A:73:ASN:HB2	2.00	0.61
1:A:268:GLN:O	1:A:272:GLN:HG3	2.01	0.61
1:B:75:ASN:ND2	1:B:75:ASN:H	1.98	0.61
1:B:307:VAL:HG13	9:B:639:HOH:O	1.99	0.61
1:A:253:LYS:O	1:A:257:GLU:HG3	2.00	0.61
1:B:221:MET:CE	1:B:256:CYS:HB3	2.30	0.60
1:B:209:ASN:ND2	1:B:213:SER:HB2	2.16	0.59
1:B:292:ARG:HD3	9:B:571:HOH:O	2.01	0.59
1:A:146:ILE:HG12	1:A:182:THR:HB	1.84	0.59
1:A:74:MET:HG2	1:B:287:MET:HE3	1.84	0.59
1:A:87:ASP:OD2	1:A:90:PHE:N	2.36	0.59
1:A:264:HIS:CD2	1:A:306:VAL:HG21	2.38	0.59
1:A:88:LYS:HB3	1:A:88:LYS:NZ	2.18	0.58
1:B:253:LYS:O	1:B:257:GLU:HG3	2.03	0.58
1:B:75:ASN:N	1:B:75:ASN:HD22	2.01	0.57
1:B:73:ASN:OD1	1:B:76:LYS:NZ	2.32	0.57
1:A:169:LEU:HD23	1:A:172:MET:HE1	1.85	0.57
1:B:192:SER:HB2	1:B:200:ILE:HD11	1.85	0.57
1:B:119:LYS:HG3	1:B:152:PHE:HB2	1.87	0.57
1:A:172:MET:HE2	1:A:185:ILE:HD12	1.86	0.57
1:B:234:GLY:HA3	8:B:405[B]:GT1:O4	2.04	0.56
1:B:234:GLY:CA	8:B:405[B]:GT1:O4	2.53	0.56
6:A:406:MPD:O2	6:A:406:MPD:C5	2.53	0.56
1:B:179:GLY:O	6:B:410:MPD:HM2	2.05	0.56
1:B:129:PRO:O	1:B:132:LEU:HB2	2.06	0.56
1:A:293:MET:CE	1:A:300:ILE:HD11	2.36	0.55
1:A:72:ASN:HD22	1:A:74:MET:HE1	1.72	0.55
4:B:404:ATP:PG	9:B:626:HOH:O	2.64	0.55
1:B:298:ARG:HG2	9:B:640:HOH:O	2.06	0.55
1:A:138:GLU:O	1:A:142:PRO:HG2	2.07	0.54
1:A:235:ASP:OD2	8:A:410[B]:GT1:H9	2.06	0.54
1:B:221:MET:HE1	1:B:256:CYS:HB3	1.88	0.54
1:A:79:TYR:CD2	1:A:109:VAL:HB	2.43	0.54
1:A:297:LYS:O	1:A:301:GLU:HG3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ASP:OD2	1:A:89:SER:HB3	2.08	0.53
1:B:240:MET:HE3	9:B:573:HOH:O	2.09	0.53
1:B:231:VAL:HG13	8:B:405[B]:GT1:H3	1.89	0.53
1:B:270:THR:HA	1:B:292:ARG:HG2	1.91	0.52
4:A:404:ATP:PG	9:A:596:HOH:O	2.67	0.52
6:A:406:MPD:H32	9:A:589:HOH:O	2.09	0.52
1:A:240:MET:HE2	1:A:300:ILE:HG23	1.91	0.52
1:B:240:MET:CE	1:B:300:ILE:HG23	2.40	0.52
1:B:209:ASN:HD21	1:B:213:SER:HB2	1.73	0.52
1:A:88:LYS:HZ3	1:A:88:LYS:HB3	1.74	0.52
1:B:115:VAL:HG13	9:B:626:HOH:O	2.10	0.52
1:B:209:ASN:HB2	1:B:210:PRO:HD2	1.92	0.51
1:B:231:VAL:CG1	8:B:405[B]:GT1:H3	2.40	0.51
1:B:115:VAL:HA	1:B:153:GLU:OE2	2.10	0.51
1:B:86:ARG:NH1	9:B:555:HOH:O	2.44	0.51
1:B:112:CYS:O	1:B:147:ILE:HA	2.09	0.51
1:B:69:LEU:HD23	1:B:74:MET:HE1	1.93	0.51
1:A:259:THR:O	1:A:263:LEU:HD23	2.11	0.50
1:B:75:ASN:ND2	1:B:75:ASN:N	2.60	0.50
1:B:43:PHE:CD1	1:B:54:GLY:HA3	2.47	0.50
1:B:49:TYR:OH	1:B:287:MET:HA	2.12	0.49
1:B:170:ARG:HD3	9:B:614:HOH:O	2.12	0.49
1:B:111:VAL:HG22	1:B:146:ILE:HD12	1.95	0.49
1:B:151:GLN:OE1	1:B:188:SER:HB2	2.12	0.49
1:A:86:ARG:O	1:A:129:PRO:HG2	2.13	0.49
1:A:293:MET:HE3	1:A:300:ILE:HD11	1.94	0.49
1:A:191:PRO:HG2	9:A:568:HOH:O	2.11	0.49
6:B:408:MPD:C5	6:B:408:MPD:C1	2.87	0.48
1:A:74:MET:HE1	1:B:45:ASN:ND2	2.29	0.48
1:B:12:SER:HB2	8:B:405[B]:GT1:H10	1.94	0.48
1:B:72:ASN:HB2	1:B:74:MET:HE2	1.96	0.48
1:A:242:LEU:C	1:A:242:LEU:HD23	2.34	0.47
1:A:12:SER:HB3	1:A:41:VAL:HG22	1.97	0.47
1:A:149:PRO:HB2	1:A:153:GLU:HB2	1.96	0.47
1:A:45:ASN:ND2	1:B:72:ASN:HD22	2.12	0.47
1:B:146:ILE:HG12	1:B:182:THR:HB	1.96	0.47
1:B:58:ASN:OD1	1:B:61:GLU:HG3	2.15	0.47
1:A:192:SER:HB2	1:A:200:ILE:HD11	1.95	0.47
1:B:307:VAL:HA	9:B:622:HOH:O	2.15	0.46
1:A:108:LEU:HD23	1:A:108:LEU:C	2.36	0.46
1:A:198:TYR:N	1:A:225:LYS:NZ	2.63	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:231:VAL:HG13	8:A:410[B]:GT1:H3	1.96	0.46
1:A:93:MET:HE3	1:A:93:MET:O	2.16	0.46
1:A:167:GLU:HG2	1:A:170:ARG:HH21	1.81	0.46
1:A:169:LEU:HD23	1:A:172:MET:HE3	1.96	0.46
1:A:31:LEU:HD11	1:A:240:MET:HE1	1.98	0.45
1:B:240:MET:HE2	1:B:300:ILE:HG23	1.98	0.45
1:A:95:VAL:O	1:A:99:GLN:HG3	2.16	0.45
1:B:99:GLN:HB2	1:B:99:GLN:HE21	1.43	0.45
1:B:209:ASN:HB2	1:B:210:PRO:CD	2.47	0.45
1:A:9:SER:OG	1:A:21:ASN:ND2	2.49	0.45
1:A:58:ASN:OD1	1:A:60:ASP:HB2	2.16	0.45
6:B:406:MPD:CM	6:B:406:MPD:C5	2.90	0.45
1:B:74:MET:HB2	1:B:74:MET:HE3	1.70	0.45
1:B:170:ARG:O	1:B:174:MET:HG3	2.17	0.45
1:A:14:VAL:HA	1:A:43:PHE:O	2.17	0.45
1:B:242:LEU:HD23	1:B:242:LEU:C	2.37	0.45
1:B:158:SER:CB	1:B:171:VAL:HG13	2.47	0.45
1:B:31:LEU:HD11	1:B:240:MET:HE1	1.98	0.45
1:A:72:ASN:ND2	1:A:74:MET:HE1	2.30	0.44
1:A:219:ILE:C	1:A:219:ILE:HD12	2.37	0.44
1:B:271:ILE:HD12	1:B:271:ILE:HA	1.89	0.44
1:A:108:LEU:HD23	1:A:109:VAL:N	2.32	0.44
1:A:136:TYR:HA	1:A:140:VAL:HB	1.99	0.44
1:A:26:PHE:HB3	1:A:27:PRO:CD	2.48	0.43
1:A:70:ARG:HG3	1:A:70:ARG:HH11	1.84	0.43
1:A:116:LEU:HB2	1:A:153:GLU:HG2	2.00	0.43
1:A:197:ASN:C	1:A:198:TYR:CD1	2.92	0.43
1:B:133:LEU:HB3	1:B:134:PRO:HD3	2.01	0.43
1:A:148:THR:HA	1:A:184:VAL:O	2.19	0.43
1:A:45:ASN:ND2	1:B:72:ASN:ND2	2.67	0.43
1:B:278:ALA:CB	1:B:288:GLN:HE22	2.06	0.42
1:A:119:LYS:HE2	1:A:152:PHE:HB2	2.00	0.42
6:B:406:MPD:HM3	6:B:410:MPD:O4	2.20	0.42
1:A:26:PHE:N	1:A:27:PRO:HD2	2.34	0.42
1:A:285:SER:OG	1:A:288:GLN:HG3	2.20	0.42
1:A:69:LEU:HA	1:A:74:MET:HE2	2.02	0.42
1:B:69:LEU:HD23	1:B:74:MET:CE	2.49	0.42
1:A:148:THR:HG21	1:A:241:LEU:HD23	2.01	0.41
1:A:119:LYS:HG3	1:A:152:PHE:HB2	2.01	0.41
1:A:271:ILE:HD12	1:A:271:ILE:HA	1.90	0.41
1:B:108:LEU:HD23	1:B:108:LEU:C	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:CYS:O	1:A:147:ILE:HA	2.21	0.41
1:A:74:MET:CE	1:B:45:ASN:ND2	2.83	0.41
1:A:21:ASN:HD22	1:A:21:ASN:HA	1.69	0.41
1:B:64:GLU:O	1:B:67:GLU:HB3	2.21	0.41
1:B:44:SER:OG	1:B:45:ASN:ND2	2.54	0.41
1:B:120:TRP:O	1:B:121:ASP:HB2	2.20	0.41
1:A:133:LEU:HG	1:A:137:LYS:HE3	2.03	0.40
1:A:127:TYR:O	1:A:128:VAL:HG12	2.20	0.40
1:B:119:LYS:HA	1:B:124:GLY:HA2	2.03	0.40
1:A:28:LEU:HD13	1:A:35:ILE:HD12	2.04	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	308/312 (99%)	288 (94%)	19 (6%)	1 (0%)	46	42
1	B	308/312 (99%)	292 (95%)	12 (4%)	4 (1%)	15	8
All	All	616/624 (99%)	580 (94%)	31 (5%)	5 (1%)	24	15

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	196	SER
1	B	279	GLY
1	A	121	ASP
1	B	122	GLY
1	B	195	GLY

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	273 / 275 (99%)	268 (98%)	5 (2%)	66	71
1	B	273 / 275 (99%)	266 (97%)	7 (3%)	54	55
All	All	546 / 550 (99%)	534 (98%)	12 (2%)	60	63

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	21	ASN
1	A	55	GLN
1	A	127	TYR
1	A	161	LYS
1	B	41	VAL
1	B	73	ASN
1	B	75	ASN
1	B	99	GLN
1	B	222	ASP
1	B	280	GLU
1	B	298	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	21	ASN
1	A	39	ASN
1	A	45	ASN
1	A	72	ASN
1	A	73	ASN
1	A	104	GLN
1	A	264	HIS
1	B	45	ASN
1	B	72	ASN
1	B	75	ASN

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Mol	Chain	Res	Type
1	B	99	GLN
1	B	264	HIS

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](#)

Of 24 ligands modelled in this entry, 6 are monoatomic - leaving 18 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	ATP	A	404	3,2	24,33,33	1.07	1 (4%)	31,52,52	2.32	11 (35%)
5	GT0	A	405[A]	-	13,13,13	2.04	6 (46%)	17,17,17	1.02	2 (11%)
6	MPD	A	406	2	6,7,7	0.35	0	7,10,10	0.57	0
7	SO4	A	407	-	4,4,4	0.25	0	6,6,6	0.11	0
7	SO4	A	408	-	4,4,4	0.24	0	6,6,6	0.07	0
7	SO4	A	409	-	4,4,4	0.20	0	6,6,6	0.11	0
8	GT1	A	410[B]	2	17,17,17	3.18	4 (23%)	23,24,24	2.95	8 (34%)
4	ATP	B	404	3,2	24,33,33	1.20	3 (12%)	31,52,52	2.34	10 (32%)
8	GT1	B	405[B]	2	17,17,17	3.12	4 (23%)	23,24,24	1.60	5 (21%)
6	MPD	B	406	-	6,7,7	0.34	0	7,10,10	0.48	0
6	MPD	B	407	2	6,7,7	0.36	0	7,10,10	0.53	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MPD	B	408	-	6,7,7	0.35	0	7,10,10	0.52	0
6	MPD	B	409	-	6,7,7	0.35	0	7,10,10	0.59	0
6	MPD	B	410	-	6,7,7	0.37	0	7,10,10	0.57	0
7	SO4	B	411	-	4,4,4	0.24	0	6,6,6	0.12	0
7	SO4	B	412	-	4,4,4	0.21	0	6,6,6	0.08	0
7	SO4	B	413	-	4,4,4	0.20	0	6,6,6	0.12	0
5	GT0	B	414[A]	-	13,13,13	1.84	4 (30%)	17,17,17	0.97	1 (5%)

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	ATP	A	404	3,2	-	0/18/38/38	0/3/3/3
5	GT0	A	405[A]	-	-	0/5/5/5	0/1/1/1
6	MPD	A	406	2	-	0/5/5/5	0/0/0/0
7	SO4	A	407	-	-	0/0/0/0	0/0/0/0
7	SO4	A	408	-	-	0/0/0/0	0/0/0/0
7	SO4	A	409	-	-	0/0/0/0	0/0/0/0
8	GT1	A	410[B]	2	-	0/9/9/9	0/1/1/1
4	ATP	B	404	3,2	-	0/18/38/38	0/3/3/3
8	GT1	B	405[B]	2	-	0/9/9/9	0/1/1/1
6	MPD	B	406	-	-	0/5/5/5	0/0/0/0
6	MPD	B	407	2	-	0/5/5/5	0/0/0/0
6	MPD	B	408	-	-	0/5/5/5	0/0/0/0
6	MPD	B	409	-	-	0/5/5/5	0/0/0/0
6	MPD	B	410	-	-	0/5/5/5	0/0/0/0
7	SO4	B	411	-	-	0/0/0/0	0/0/0/0
7	SO4	B	412	-	-	0/0/0/0	0/0/0/0
7	SO4	B	413	-	-	0/0/0/0	0/0/0/0
5	GT0	B	414[A]	-	-	0/5/5/5	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	410[B]	GT1	C4-C7	-7.95	1.35	1.40
8	A	410[B]	GT1	C1-C6	-7.88	1.35	1.51
8	B	405[B]	GT1	C4-C7	-7.66	1.35	1.40
8	B	405[B]	GT1	C1-C6	-5.57	1.40	1.51
8	B	405[B]	GT1	C4-C6	-2.20	1.36	1.40
5	B	414[A]	GT0	C8-C2	2.08	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	410[B]	GT1	O3-C1	2.10	1.50	1.41
5	A	405[A]	GT0	C1-C6	2.14	1.55	1.51
4	B	404	ATP	PG-O2G	2.15	1.62	1.54
5	B	414[A]	GT0	C2-C6	2.25	1.43	1.40
5	A	405[A]	GT0	C4-C6	2.32	1.43	1.40
5	A	405[A]	GT0	C4-C7	2.50	1.42	1.40
4	B	404	ATP	O4'-C1'	2.56	1.44	1.41
4	A	404	ATP	O4'-C1'	2.59	1.44	1.41
5	A	405[A]	GT0	C2-C6	2.90	1.44	1.40
4	B	404	ATP	PG-O1G	2.90	1.60	1.51
5	A	405[A]	GT0	C7-N1	3.01	1.40	1.34
5	B	414[A]	GT0	C7-N1	3.39	1.41	1.34
5	A	405[A]	GT0	C8-N1	3.42	1.41	1.34
5	B	414[A]	GT0	C8-N1	3.55	1.42	1.34
8	A	410[B]	GT1	C2-C6	4.94	1.47	1.40
8	B	405[B]	GT1	C2-C6	7.72	1.51	1.40

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	404	ATP	N3-C2-N1	-9.00	122.00	128.89
4	A	404	ATP	N3-C2-N1	-8.86	122.11	128.89
8	A	410[B]	GT1	O3-C1-C6	-6.88	99.50	108.17
8	A	410[B]	GT1	C8-C2-C6	-4.63	114.64	118.09
8	A	410[B]	GT1	C1-C6-C2	-3.78	115.73	120.00
4	B	404	ATP	O5'-PA-O1A	-3.42	96.35	109.62
4	A	404	ATP	O3A-PA-O5'	-3.41	93.89	102.94
4	A	404	ATP	O5'-PA-O1A	-3.23	97.06	109.62
4	B	404	ATP	PA-O3A-PB	-3.03	124.21	132.73
4	B	404	ATP	O3A-PA-O5'	-2.97	95.05	102.94
8	B	405[B]	GT1	O3-C1-C6	-2.88	104.55	108.17
4	A	404	ATP	PB-O3B-PG	-2.68	123.67	132.67
4	A	404	ATP	PA-O3A-PB	-2.64	125.30	132.73
8	A	410[B]	GT1	C5-C2-C6	-2.62	116.83	121.89
8	B	405[B]	GT1	C8-C2-C6	-2.56	116.18	118.09
4	B	404	ATP	C4-C5-N7	-2.44	107.24	109.48
4	A	404	ATP	C4-C5-N7	-2.38	107.29	109.48
4	A	404	ATP	O2A-PA-O5'	-2.38	96.45	108.46
4	B	404	ATP	PB-O3B-PG	-2.24	125.17	132.67
8	A	410[B]	GT1	O6-P1-O4	-2.22	103.44	110.58
5	B	414[A]	GT0	C2-C8-N1	-2.21	120.02	123.86
4	B	404	ATP	O2A-PA-O5'	-2.15	97.62	108.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	405[B]	GT1	O6-P1-O4	-2.14	103.69	110.58
5	A	405[A]	GT0	C2-C8-N1	-2.02	120.36	123.86
5	A	405[A]	GT0	O3-C1-C6	2.13	110.86	108.17
4	B	404	ATP	O2B-PB-O1B	2.15	124.19	112.53
4	A	404	ATP	O2A-PA-O1A	2.16	124.21	112.53
4	B	404	ATP	O2A-PA-O1A	2.23	124.63	112.53
4	A	404	ATP	O2B-PB-O1B	2.28	124.89	112.53
8	B	405[B]	GT1	C4-C7-N1	2.62	124.24	120.61
4	A	404	ATP	O2B-PB-O3B	2.63	117.04	105.09
4	B	404	ATP	O2B-PB-O3B	2.67	117.21	105.09
8	A	410[B]	GT1	C4-C6-C2	2.98	121.95	118.82
4	A	404	ATP	O2A-PA-O3A	2.99	118.67	105.09
8	B	405[B]	GT1	O2-C5-C2	3.89	115.42	108.99
8	A	410[B]	GT1	C5-C2-C8	4.90	128.53	119.28
8	A	410[B]	GT1	O2-C5-C2	7.12	120.76	108.99

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 30 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	ATP	1	0
5	A	405[A]	GT0	1	0
6	A	406	MPD	3	0
8	A	410[B]	GT1	6	0
4	B	404	ATP	1	0
8	B	405[B]	GT1	7	0
6	B	406	MPD	4	0
6	B	408	MPD	4	0
6	B	410	MPD	4	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	310/312 (99%)	-0.01	14 (4%) 37 48	24, 40, 69, 100	0
1	B	310/312 (99%)	-0.14	8 (2%) 59 68	23, 36, 65, 85	0
All	All	620/624 (99%)	-0.08	22 (3%) 48 58	23, 38, 67, 100	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	211	ALA	6.1
1	A	212	GLY	5.9
1	A	120	TRP	5.6
1	A	210	PRO	5.4
1	B	120	TRP	4.9
1	A	208	ARG	4.4
1	B	282	VAL	3.6
1	A	214	VAL	3.6
1	A	282	VAL	3.2
1	A	278	ALA	3.1
1	B	121	ASP	3.0
1	A	209	ASN	2.9
1	A	121	ASP	2.6
1	B	281	GLY	2.4
1	B	123	GLU	2.4
1	A	114	PRO	2.3
1	B	278	ALA	2.3
1	B	3	GLU	2.3
1	A	112	CYS	2.2
1	A	213	SER	2.2
1	B	237	PHE	2.1
1	A	238	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
6	MPD	B	410	8/8	0.72	0.28	20.16	70,74,78,80	0
7	SO4	A	409	5/5	0.93	0.23	10.27	60,61,62,63	5
5	GT0	B	414[A]	13/13	0.76	0.35	6.43	56,68,84,84	13
8	GT1	B	405[B]	17/17	0.87	0.29	4.98	19,52,62,65	17
6	MPD	B	408	8/8	0.73	0.28	4.49	89,90,92,94	0
8	GT1	A	410[B]	17/17	0.82	0.28	3.98	42,65,73,74	17
5	GT0	A	405[A]	13/13	0.84	0.21	1.92	46,56,64,68	13
3	NA	B	402	1/1	0.97	0.19	1.51	35,35,35,35	0
7	SO4	B	412	5/5	0.95	0.14	1.09	52,54,59,60	5
7	SO4	A	407	5/5	0.95	0.11	1.06	54,56,58,59	5
6	MPD	A	406	8/8	0.87	0.19	0.53	70,71,76,79	0
7	SO4	B	413	5/5	0.94	0.15	0.26	53,58,61,62	5
3	NA	A	402	1/1	0.90	0.16	-0.40	38,38,38,38	0
4	ATP	B	404	31/31	0.97	0.10	-0.43	22,30,48,61	0
4	ATP	A	404	31/31	0.96	0.11	-0.45	26,32,59,68	0
6	MPD	B	407	8/8	0.96	0.10	-0.47	44,47,53,57	0
7	SO4	B	411	5/5	0.95	0.11	-	46,50,55,58	5
2	MG	A	403	1/1	0.97	0.61	-	27,27,27,27	1
6	MPD	B	409	8/8	0.78	0.34	-	87,91,95,97	0
6	MPD	B	406	8/8	0.89	0.15	-	49,53,63,65	0
7	SO4	A	408	5/5	0.91	0.13	-	57,60,61,65	5
2	MG	B	403	1/1	0.93	0.43	-	18,18,18,18	1
2	MG	B	401	1/1	0.66	0.20	-	44,44,44,44	0
2	MG	A	401	1/1	0.91	0.17	-	34,34,34,34	0

6.5 Other polymers

There are no such residues in this entry.