



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 04:23 PM GMT

PDB ID : 4EOH  
Title : Crystal Structure of Human PL Kinase with bound Theophylline  
Authors : Safo, M.K.; Gandhi, A.K.; Musayev, F.N.  
Deposited on : 2012-04-14  
Resolution : 2.10 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](mailto: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.

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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

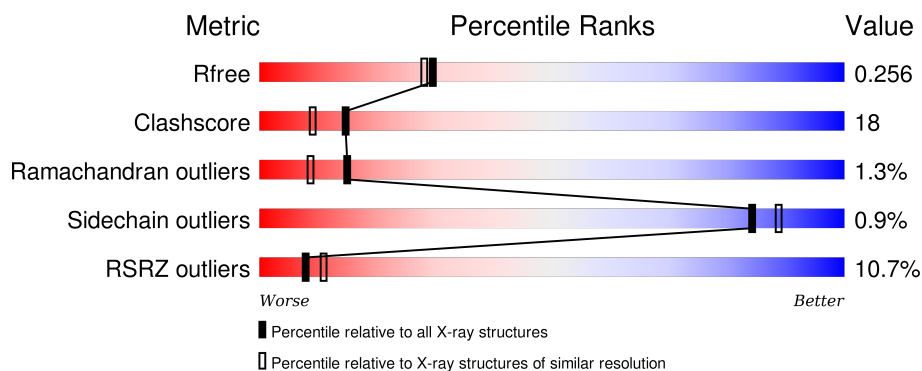
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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  $\geq 3$ , 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>12%</div> <div>73%</div> <div>23%</div> <div>..</div> </div>
1	B	312	<div> <div>9%</div> <div>72%</div> <div>25%</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
3	TEP	B	402[A]	-	-	X	X
4	MPD	A	404	-	-	-	X
4	MPD	A	406	-	-	X	-
4	MPD	A	407	-	-	-	X
4	MPD	B	403[B]	-	-	X	-
4	MPD	B	405	-	-	X	-
4	MPD	B	406	-	-	-	X
4	MPD	B	407	-	-	-	X
4	MPD	B	408	-	-	-	X
4	MPD	B	409	-	-	X	X
4	MPD	B	410	-	-	X	X
4	MPD	B	411	-	-	-	X
5	SO4	B	413	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 5348 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.

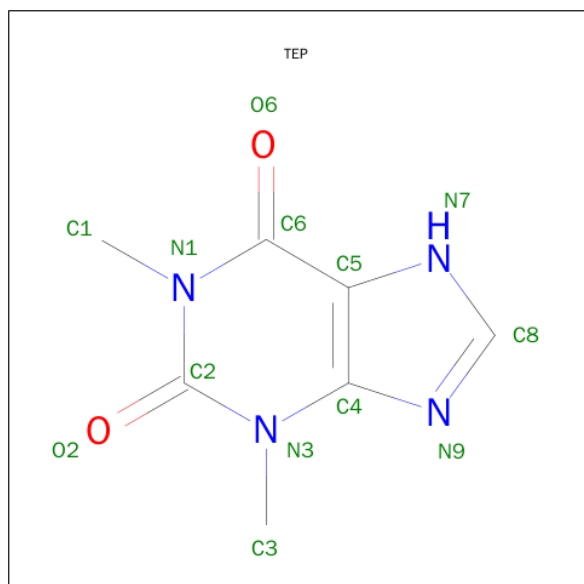
- Molecule 1 is a protein called Pyridoxal Kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2395	1512	419	449	15			
1	B	307	Total	C	N	O	S	0	0	0
			2423	1528	427	453	15			

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

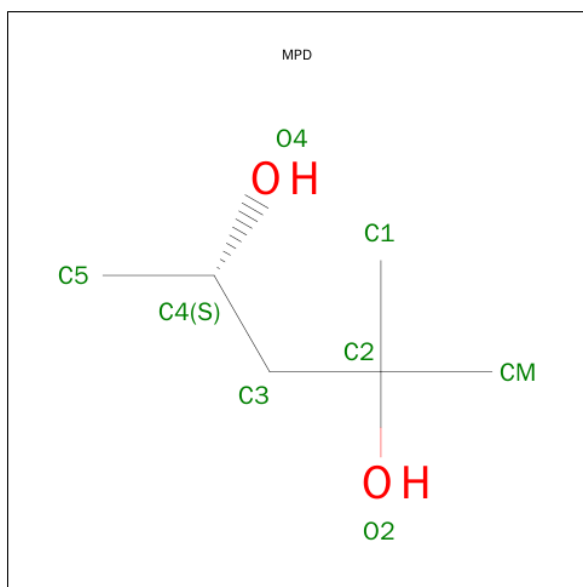
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Na	0	0
			1	1		
2	A	1	Total	Na	0	0
			1	1		

- Molecule 3 is THEOPHYLLINE (three-letter code: TEP) (formula: C<sub>7</sub>H<sub>8</sub>N<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			13	7	4	2		
3	B	1	Total	C	N	O	0	1
			13	7	4	2		

- Molecule 4 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



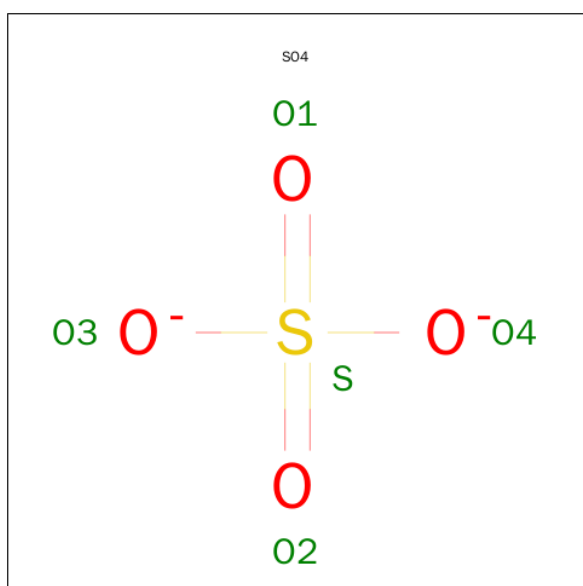
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	1
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	A	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	1
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		
4	B	1	Total	C	O	0	0
			8	6	2		

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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



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

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

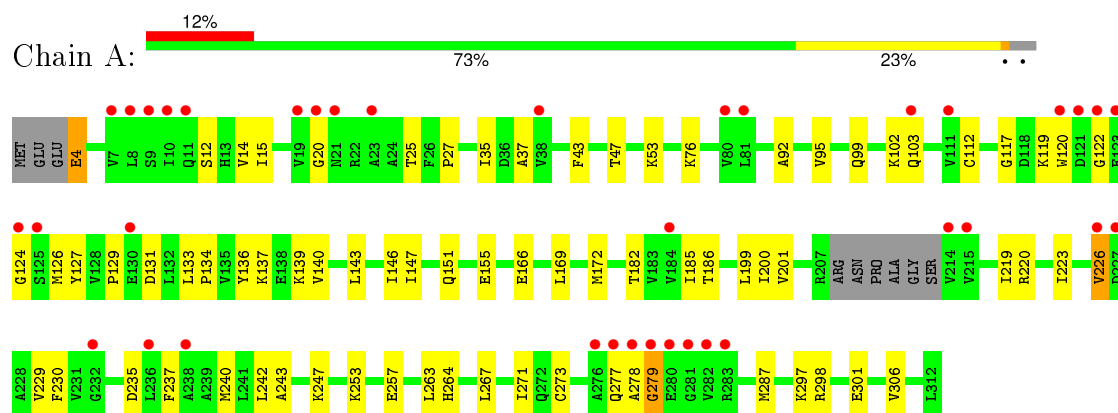
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	158	Total	O	0	0
			158	158		
6	B	197	Total	O	0	0
			197	197		

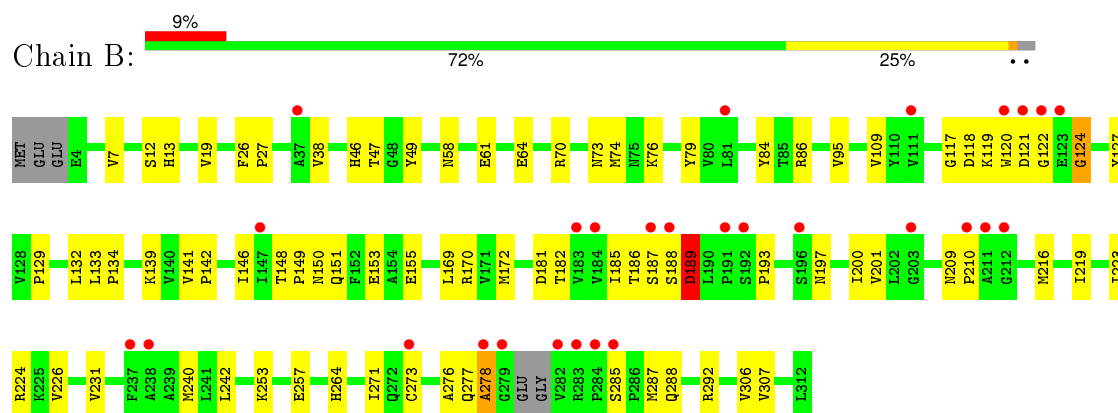
### 3 Residue-property plots [i](#)

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: 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, $\alpha$ , $\beta$ , $\gamma$	92.30Å 115.85Å 171.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.19 – 2.10 32.96 – 2.10	Depositor EDS
% Data completeness (in resolution range)	98.0 (29.19-2.10) 98.1 (32.96-2.10)	Depositor EDS
$R_{merge}$	0.03	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.38 (at 2.10Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.205 , 0.254 0.206 , 0.256	Depositor DCC
$R_{free}$ test set	2688 reflections (5.07%)	DCC
Wilson B-factor (Å <sup>2</sup> )	40.4	Xtriage
Anisotropy	0.436	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 72.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 52988 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	5348	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.79% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TEP, NA, MPD, SO4

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	0.32	0/2439	0.58	0/3305
1	B	0.32	0/2468	0.61	0/3345
All	All	0.32	0/4907	0.60	0/6650

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	2395	0	2407	55	0
1	B	2423	0	2437	81	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	13	0	8	5	0
3	B	13	0	8	8	0
4	A	40	0	70	16	0
4	B	72	0	126	49	0
5	A	15	0	0	0	0
5	B	20	0	0	0	0
6	A	158	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	197	0	0	10	1
All	All	5348	0	5056	179	1

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 (179) 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)
4:B:406:MPD:H53	4:B:406:MPD:HM1	1.37	1.06
4:A:406:MPD:H52	4:A:406:MPD:HM2	1.37	1.02
4:B:411:MPD:HM2	4:B:411:MPD:H52	1.45	0.98
1:A:226:VAL:HG13	4:A:406:MPD:H13	1.46	0.94
1:B:264:HIS:HD1	4:B:410:MPD:HO2	1.14	0.94
1:A:76:LYS:HB3	4:A:405:MPD:H11	1.54	0.89
1:A:12:SER:HB2	3:A:402[A]:TEP:H31	1.59	0.83
1:B:95:VAL:HG11	1:B:139:LYS:HE3	1.62	0.81
1:B:120:TRP:HH2	1:B:127:TYR:HE1	1.27	0.79
1:B:120:TRP:HH2	1:B:127:TYR:CE1	2.01	0.79
1:B:12:SER:CB	3:B:402[A]:TEP:H31	2.13	0.78
1:B:12:SER:OG	3:B:402[A]:TEP:H31	1.83	0.77
1:B:193:PRO:HG3	4:B:405:MPD:H11	1.65	0.77
1:B:188:SER:HB3	1:B:200:ILE:O	1.87	0.75
1:B:285:SER:H	1:B:288:GLN:NE2	1.84	0.75
4:B:408:MPD:H53	4:B:408:MPD:O2	1.87	0.74
1:B:197:ASN:HB3	1:B:224:ARG:NH2	2.04	0.73
1:A:169:LEU:HD23	1:A:172:MET:HE1	1.70	0.73
1:A:119:LYS:HG2	1:A:124:GLY:HA2	1.70	0.73
4:B:411:MPD:CM	4:B:411:MPD:H52	2.18	0.72
4:B:408:MPD:HM1	4:B:408:MPD:O4	1.90	0.72
1:B:12:SER:HB2	3:B:402[A]:TEP:H31	1.70	0.72
4:B:409:MPD:H11	6:B:684:HOH:O	1.89	0.72
1:B:84:TYR:HB3	3:B:402[A]:TEP:H32	1.72	0.71
1:B:150:ASN:OD1	1:B:153:GLU:HG3	1.89	0.71
1:A:223:ILE:HG23	4:A:406:MPD:H51	1.73	0.71
1:B:188:SER:HG	1:B:200:ILE:H	1.36	0.71
1:B:226:VAL:CG2	4:B:410:MPD:HM3	2.22	0.70
4:B:405:MPD:O2	4:B:405:MPD:H53	1.92	0.70
1:A:267:LEU:O	1:A:271:ILE:HG13	1.92	0.69
4:B:410:MPD:O4	4:B:410:MPD:HM1	1.93	0.68
4:B:410:MPD:H53	4:B:410:MPD:O2	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:405:MPD:H12	4:A:405:MPD:O4	1.94	0.68
1:B:188:SER:OG	1:B:200:ILE:N	2.19	0.68
4:A:406:MPD:H52	4:A:406:MPD:CM	2.20	0.67
1:B:253:LYS:O	1:B:257:GLU:HG3	1.94	0.67
4:B:405:MPD:HM1	4:B:405:MPD:O4	1.94	0.67
1:B:226:VAL:HG21	4:B:410:MPD:HM3	1.77	0.66
4:B:409:MPD:H12	4:B:409:MPD:O4	1.95	0.66
4:A:404:MPD:HM1	4:A:404:MPD:O4	1.96	0.65
4:B:406:MPD:H53	4:B:406:MPD:CM	2.21	0.64
1:A:229:VAL:HG12	6:A:576:HOH:O	1.96	0.64
4:A:405:MPD:H53	4:A:405:MPD:O2	1.96	0.64
4:B:404:MPD:O2	4:B:404:MPD:H52	1.98	0.64
1:B:285:SER:H	1:B:288:GLN:HE21	1.43	0.64
1:B:216:MET:HE1	6:B:602:HOH:O	1.98	0.64
1:B:181:ASP:OD2	4:B:404:MPD:HM3	1.98	0.63
4:B:409:MPD:O2	4:B:409:MPD:H53	2.00	0.62
3:B:402[A]:TEP:C3	6:B:660:HOH:O	2.47	0.62
4:B:409:MPD:H32	6:B:572:HOH:O	1.99	0.62
1:A:230:PHE:HZ	1:A:271:ILE:HG12	1.65	0.62
1:A:172:MET:HE2	1:A:185:ILE:HD12	1.83	0.61
4:A:406:MPD:C5	4:A:406:MPD:HM2	2.22	0.61
4:B:407:MPD:H11	4:B:407:MPD:O4	2.00	0.61
1:B:170:ARG:HD2	1:B:170:ARG:O	2.00	0.61
1:A:253:LYS:O	1:A:257:GLU:HG3	2.02	0.60
1:A:133:LEU:HB3	1:A:134:PRO:HD3	1.83	0.59
1:B:46:HIS:HA	4:B:403[B]:MPD:H13	1.84	0.59
1:A:200:ILE:HD13	1:A:220:ARG:HE	1.67	0.59
1:B:133:LEU:HB3	1:B:134:PRO:HD3	1.84	0.59
4:B:410:MPD:C5	4:B:410:MPD:O2	2.51	0.59
1:B:118:ASP:O	1:B:124:GLY:HA3	2.03	0.58
1:A:119:LYS:HG2	1:A:124:GLY:CA	2.32	0.58
4:A:407:MPD:HM1	4:A:407:MPD:O4	2.03	0.58
4:B:410:MPD:O4	4:B:410:MPD:CM	2.52	0.57
1:A:12:SER:CB	3:A:402[A]:TEP:H31	2.32	0.57
1:A:199:LEU:C	1:A:199:LEU:HD12	2.23	0.57
4:B:406:MPD:C5	4:B:406:MPD:HM1	2.22	0.57
1:A:169:LEU:HD23	1:A:172:MET:CE	2.34	0.56
1:B:193:PRO:CG	4:B:405:MPD:H11	2.33	0.56
1:B:7:VAL:HG22	1:B:79:TYR:HB2	1.88	0.56
1:B:120:TRP:CH2	1:B:127:TYR:HE1	2.17	0.55
1:A:297:LYS:O	1:A:301:GLU:HG3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:GLY:HA2	1:A:127:TYR:CD2	2.41	0.55
4:B:408:MPD:C5	4:B:408:MPD:O2	2.54	0.55
1:B:216:MET:HE3	6:B:645:HOH:O	2.07	0.54
1:B:47:THR:H	4:B:403[B]:MPD:H13	1.72	0.54
1:B:223:ILE:N	1:B:223:ILE:HD12	2.23	0.53
1:B:26:PHE:HB3	1:B:27:PRO:HD3	1.90	0.53
3:A:402[A]:TEP:H32	6:A:546:HOH:O	2.08	0.53
1:B:242:LEU:HD23	1:B:242:LEU:C	2.28	0.53
1:A:298:ARG:HH11	1:A:298:ARG:HG3	1.73	0.53
1:B:19:VAL:CG1	1:B:231:VAL:HG12	2.39	0.53
1:A:298:ARG:NH1	1:A:298:ARG:HG3	2.25	0.52
1:B:223:ILE:CG2	4:B:410:MPD:H4	2.40	0.52
1:A:20:GLY:CA	3:A:402[A]:TEP:H33	2.40	0.52
4:B:403[B]:MPD:O4	4:B:403[B]:MPD:H11	2.10	0.51
1:B:119:LYS:HA	1:B:124:GLY:HA3	1.93	0.51
1:A:112:CYS:O	1:A:147:ILE:HA	2.11	0.51
1:B:240:MET:HE2	1:B:240:MET:HA	1.92	0.51
1:A:226:VAL:HG13	4:A:406:MPD:C1	2.32	0.51
1:B:209:ASN:HB2	1:B:210:PRO:HD2	1.91	0.51
1:B:226:VAL:HG11	1:B:271:ILE:HD11	1.93	0.51
1:B:277:GLN:O	1:B:278:ALA:HB2	2.11	0.50
1:B:188:SER:HG	1:B:189:ASP:H	1.55	0.50
1:B:150:ASN:HB2	1:B:187:SER:OG	2.11	0.50
1:B:151:GLN:O	1:B:155:GLU:HG3	2.11	0.50
4:B:411:MPD:CM	4:B:411:MPD:C5	2.90	0.50
1:B:12:SER:HB2	3:B:402[A]:TEP:C3	2.39	0.50
1:A:229:VAL:HG13	1:A:229:VAL:O	2.11	0.50
1:A:201:VAL:HG21	1:A:223:ILE:HD12	1.94	0.50
1:B:224:ARG:O	4:B:410:MPD:H31	2.12	0.49
1:A:53:LYS:HB3	1:B:64:GLU:HG2	1.93	0.49
1:B:73:ASN:HD21	1:B:76:LYS:HZ1	1.59	0.49
1:B:264:HIS:CD2	1:B:306:VAL:HG21	2.47	0.49
4:B:408:MPD:O4	4:B:408:MPD:CM	2.59	0.49
1:A:15:ILE:HD13	1:B:38:VAL:HG22	1.95	0.48
4:B:405:MPD:C5	4:B:405:MPD:O2	2.58	0.48
1:A:136:TYR:HA	1:A:140:VAL:HB	1.94	0.48
1:A:146:ILE:HG12	1:A:182:THR:HB	1.94	0.48
3:B:402[A]:TEP:H32	6:B:660:HOH:O	2.09	0.48
1:A:242:LEU:C	1:A:242:LEU:HD23	2.33	0.48
1:B:193:PRO:HG3	4:B:405:MPD:C1	2.41	0.48
1:B:117:GLY:HA2	1:B:127:TYR:CD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:209:ASN:HB2	1:B:210:PRO:CD	2.44	0.48
1:B:188:SER:CB	1:B:200:ILE:HB	2.44	0.47
1:A:129:PRO:HB2	1:A:131:ASP:OD1	2.14	0.47
1:B:149:PRO:O	1:B:185:ILE:HA	2.14	0.47
1:B:307:VAL:HB	4:B:411:MPD:H13	1.97	0.47
4:B:409:MPD:H13	6:B:514:HOH:O	2.14	0.47
1:B:141:VAL:HB	1:B:142:PRO:HD3	1.97	0.47
1:B:146:ILE:HG12	1:B:182:THR:HB	1.95	0.47
1:B:219:ILE:C	1:B:219:ILE:HD12	2.34	0.47
1:A:264:HIS:CD2	1:A:306:VAL:HG21	2.49	0.47
1:A:287:MET:CE	1:B:74:MET:HG2	2.45	0.47
1:B:186:THR:O	1:B:201:VAL:HG22	2.15	0.47
1:B:49:TYR:OH	1:B:287:MET:HA	2.15	0.47
1:B:74:MET:HE3	1:B:74:MET:HB2	1.84	0.47
1:A:235:ASP:OD1	3:A:402[A]:TEP:O2	2.33	0.46
1:A:133:LEU:HD11	1:A:137:LYS:HE3	1.98	0.46
1:A:240:MET:HA	1:A:240:MET:HE2	1.96	0.46
4:B:403[B]:MPD:O4	4:B:403[B]:MPD:C1	2.63	0.46
1:B:276:ALA:C	1:B:278:ALA:H	2.19	0.46
1:A:139:LYS:NZ	6:A:592:HOH:O	2.48	0.46
4:B:406:MPD:CM	4:B:406:MPD:C5	2.90	0.45
1:B:19:VAL:HG12	1:B:231:VAL:HG12	1.98	0.45
1:B:73:ASN:ND2	1:B:76:LYS:NZ	2.65	0.45
4:B:404:MPD:O2	4:B:404:MPD:C5	2.64	0.45
1:B:129:PRO:HB2	1:B:132:LEU:HD13	1.97	0.45
1:A:243:ALA:O	1:A:247:LYS:HG2	2.16	0.45
4:A:405:MPD:C1	4:A:405:MPD:O4	2.63	0.45
4:B:409:MPD:O4	4:B:409:MPD:C1	2.64	0.45
3:B:402[A]:TEP:C1	6:B:693:HOH:O	2.65	0.45
1:B:46:HIS:HB2	4:B:403[B]:MPD:C1	2.46	0.45
1:A:37:ALA:O	1:B:13:HIS:HE1	2.00	0.44
1:B:119:LYS:HA	1:B:124:GLY:CA	2.48	0.44
1:A:14:VAL:HA	1:A:43:PHE:O	2.18	0.43
4:A:405:MPD:C5	4:A:405:MPD:O2	2.64	0.43
1:B:169:LEU:HD23	1:B:172:MET:HE1	2.01	0.43
1:A:92:ALA:O	1:A:95:VAL:HG22	2.19	0.43
1:A:169:LEU:HA	1:A:172:MET:HE3	2.00	0.42
1:A:27:PRO:HB2	1:A:240:MET:HE1	2.01	0.42
1:A:186:THR:HG22	1:A:237:PHE:CE2	2.54	0.42
4:A:406:MPD:C5	4:A:406:MPD:CM	2.89	0.42
1:B:58:ASN:OD1	1:B:61:GLU:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:109:VAL:HG21	4:B:409:MPD:H12	2.01	0.42
1:A:278:ALA:O	1:A:279:GLY:O	2.38	0.42
1:B:223:ILE:HG21	4:B:410:MPD:H4	2.01	0.42
1:A:4:GLU:HB3	6:B:674:HOH:O	2.18	0.42
1:B:86:ARG:HD2	4:B:407:MPD:O4	2.19	0.42
1:B:273:CYS:HB3	1:B:292:ARG:NH1	2.34	0.42
1:A:219:ILE:C	1:A:219:ILE:HD12	2.40	0.42
4:B:405:MPD:CM	4:B:405:MPD:O4	2.64	0.42
4:B:407:MPD:O4	4:B:407:MPD:C1	2.66	0.42
1:B:19:VAL:HG11	1:B:231:VAL:HG12	2.02	0.42
1:A:99:GLN:O	1:A:103:GLN:HG3	2.20	0.42
1:A:166:GLU:CD	1:A:166:GLU:H	2.23	0.42
4:B:409:MPD:C5	4:B:409:MPD:O2	2.68	0.41
1:A:25:THR:HA	1:A:35:ILE:HD13	2.02	0.41
4:A:406:MPD:H11	4:A:406:MPD:H4	1.88	0.41
1:A:47:THR:HG23	4:A:403[B]:MPD:HM3	2.02	0.41
1:A:102:LYS:HD2	1:A:143:LEU:HD22	2.02	0.41
1:A:151:GLN:O	1:A:155:GLU:HG3	2.20	0.41
1:B:148:THR:HB	1:B:186:THR:CG2	2.51	0.41
1:B:120:TRP:CH2	1:B:127:TYR:CE1	2.92	0.41
1:A:273:CYS:O	1:A:277:GLN:HG3	2.21	0.41
1:B:187:SER:HB3	6:B:692:HOH:O	2.21	0.40
1:B:46:HIS:CA	4:B:403[B]:MPD:H13	2.49	0.40
1:B:70:ARG:HG2	1:B:70:ARG:HH11	1.86	0.40

All (1) 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)
6:B:503:HOH:O	6:B:503:HOH:O[3_555]	1.84	0.36

## 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	299/312 (96%)	287 (96%)	9 (3%)	3 (1%)	19	13
1	B	303/312 (97%)	287 (95%)	11 (4%)	5 (2%)	11	5
All	All	602/624 (96%)	574 (95%)	20 (3%)	8 (1%)	15	9

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	279	GLY
1	B	278	ALA
1	A	120	TRP
1	B	122	GLY
1	B	189	ASP
1	B	124	GLY
1	A	122	GLY
1	B	121	ASP

### 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	268/275 (98%)	264 (98%)	4 (2%)	72	78
1	B	271/275 (98%)	270 (100%)	1 (0%)	93	96
All	All	539/550 (98%)	534 (99%)	5 (1%)	84	89

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	GLU
1	A	126	MET
1	A	226	VAL
1	A	263	LEU
1	B	189	ASP



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	73	ASN
1	A	103	GLN
1	A	104	GLN
1	A	165	GLN
1	A	248	HIS
1	B	13	HIS
1	B	73	ASN
1	B	272	GLN
1	B	288	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 25 ligands modelled in this entry, 2 are monoatomic - leaving 23 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	TEP	A	402[A]	-	7,14,14	0.88	0	8,21,21	1.37	1 (12%)
4	MPD	A	403[B]	-	6,7,7	0.34	0	7,10,10	0.57	0
4	MPD	A	404	-	6,7,7	0.36	0	7,10,10	0.58	0
4	MPD	A	405	-	6,7,7	0.36	0	7,10,10	0.50	0
4	MPD	A	406	-	6,7,7	0.35	0	7,10,10	0.47	0
4	MPD	A	407	-	6,7,7	0.34	0	7,10,10	0.55	0
5	SO4	A	408	-	4,4,4	0.25	0	6,6,6	0.08	0
5	SO4	A	409	-	4,4,4	0.23	0	6,6,6	0.10	0
5	SO4	A	410	-	4,4,4	0.23	0	6,6,6	0.08	0
3	TEP	B	402[A]	-	7,14,14	0.83	0	8,21,21	1.33	1 (12%)
4	MPD	B	403[B]	-	6,7,7	0.34	0	7,10,10	0.51	0
4	MPD	B	404	-	6,7,7	0.36	0	7,10,10	0.56	0
4	MPD	B	405	-	6,7,7	0.34	0	7,10,10	2.15	2 (28%)
4	MPD	B	406	-	6,7,7	0.35	0	7,10,10	0.52	0
4	MPD	B	407	-	6,7,7	0.34	0	7,10,10	0.52	0
4	MPD	B	408	-	6,7,7	0.33	0	7,10,10	2.12	2 (28%)
4	MPD	B	409	-	6,7,7	0.35	0	7,10,10	0.48	0
4	MPD	B	410	-	6,7,7	0.34	0	7,10,10	2.08	2 (28%)
4	MPD	B	411	-	6,7,7	0.36	0	7,10,10	0.47	0
5	SO4	B	412	-	4,4,4	0.21	0	6,6,6	0.08	0
5	SO4	B	413	-	4,4,4	0.23	0	6,6,6	0.08	0
5	SO4	B	414	-	4,4,4	0.23	0	6,6,6	0.09	0
5	SO4	B	415	-	4,4,4	0.21	0	6,6,6	0.08	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
3	TEP	A	402[A]	-	-	0/0/0/0	0/2/2/2
4	MPD	A	403[B]	-	-	0/5/5/5	0/0/0/0
4	MPD	A	404	-	-	0/5/5/5	0/0/0/0
4	MPD	A	405	-	-	0/5/5/5	0/0/0/0
4	MPD	A	406	-	-	0/5/5/5	0/0/0/0
4	MPD	A	407	-	-	0/5/5/5	0/0/0/0
5	SO4	A	408	-	-	0/0/0/0	0/0/0/0
5	SO4	A	409	-	-	0/0/0/0	0/0/0/0
5	SO4	A	410	-	-	0/0/0/0	0/0/0/0
3	TEP	B	402[A]	-	-	0/0/0/0	0/2/2/2
4	MPD	B	403[B]	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	MPD	B	404	-	-	0/5/5/5	0/0/0/0
4	MPD	B	405	-	-	0/5/5/5	0/0/0/0
4	MPD	B	406	-	-	0/5/5/5	0/0/0/0
4	MPD	B	407	-	-	0/5/5/5	0/0/0/0
4	MPD	B	408	-	-	0/5/5/5	0/0/0/0
4	MPD	B	409	-	-	0/5/5/5	0/0/0/0
4	MPD	B	410	-	-	0/5/5/5	0/0/0/0
4	MPD	B	411	-	-	0/5/5/5	0/0/0/0
5	SO4	B	412	-	-	0/0/0/0	0/0/0/0
5	SO4	B	413	-	-	0/0/0/0	0/0/0/0
5	SO4	B	414	-	-	0/0/0/0	0/0/0/0
5	SO4	B	415	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	402[A]	TEP	C4-C5-N7	-2.73	106.97	109.48
3	B	402[A]	TEP	C4-C5-N7	-2.43	107.24	109.48
4	B	410	MPD	O2-C2-CM	3.09	119.42	108.09
4	B	408	MPD	O2-C2-CM	3.19	119.79	108.09
4	B	405	MPD	O2-C2-CM	3.24	119.97	108.09
4	B	408	MPD	CM-C2-C1	3.76	118.42	110.24
4	B	410	MPD	CM-C2-C1	3.76	118.43	110.24
4	B	405	MPD	CM-C2-C1	3.82	118.56	110.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

16 monomers are involved in 78 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	402[A]	TEP	5	0
4	A	403[B]	MPD	1	0
4	A	404	MPD	1	0
4	A	405	MPD	5	0
4	A	406	MPD	8	0
4	A	407	MPD	1	0
3	B	402[A]	TEP	8	0
4	B	403[B]	MPD	6	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	404	MPD	3	0
4	B	405	MPD	7	0
4	B	406	MPD	4	0
4	B	407	MPD	3	0
4	B	408	MPD	4	0
4	B	409	MPD	8	0
4	B	410	MPD	10	0
4	B	411	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	303/312 (97%)	0.53	37 (12%) <b>5</b> <b>7</b>	31, 46, 80, 99	0
1	B	307/312 (98%)	0.41	28 (9%) <b>11</b> <b>16</b>	28, 40, 74, 100	0
All	All	610/624 (97%)	0.47	65 (10%) <b>8</b> <b>11</b>	28, 43, 75, 100	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	279	GLY	8.2
1	B	282	VAL	7.5
1	A	120	TRP	7.1
1	A	282	VAL	5.4
1	B	283	ARG	5.2
1	B	122	GLY	5.0
1	B	278	ALA	4.7
1	A	81	LEU	4.7
1	A	121	ASP	4.6
1	B	121	ASP	4.6
1	A	280	GLU	4.6
1	A	281	GLY	4.6
1	A	125	SER	4.5
1	B	210	PRO	4.3
1	A	278	ALA	4.1
1	A	124	GLY	4.1
1	A	279	GLY	4.0
1	B	120	TRP	4.0
1	B	188	SER	3.5
1	B	123	GLU	3.4
1	A	123	GLU	3.4
1	A	215	VAL	3.4
1	A	214	VAL	3.3
1	B	211	ALA	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	10	ILE	3.3
1	A	122	GLY	3.2
1	A	227	ASP	3.1
1	A	80	VAL	3.1
1	A	226	VAL	3.1
1	B	212	GLY	3.1
1	A	238	ALA	3.1
1	A	9	SER	3.0
1	A	276	ALA	3.0
1	A	283	ARG	3.0
1	A	236	LEU	3.0
1	B	284	PRO	2.9
1	B	147	ILE	2.9
1	A	111	VAL	2.9
1	B	191	PRO	2.8
1	A	23	ALA	2.7
1	A	103	GLN	2.7
1	B	81	LEU	2.6
1	A	20	GLY	2.6
1	B	238	ALA	2.5
1	A	130	GLU	2.5
1	B	273	CYS	2.5
1	A	232	GLY	2.4
1	A	19	VAL	2.4
1	B	37	ALA	2.4
1	B	285	SER	2.4
1	A	277	GLN	2.4
1	A	11	GLN	2.3
1	B	237	PHE	2.3
1	A	21	ASN	2.3
1	B	187	SER	2.2
1	B	192	SER	2.2
1	A	38	VAL	2.2
1	B	111	VAL	2.2
1	B	183	VAL	2.2
1	A	8	LEU	2.2
1	A	184	VAL	2.1
1	B	196	SER	2.1
1	B	203	GLY	2.0
1	A	7	VAL	2.0
1	B	184	VAL	2.0

## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	MPD	B	410	8/8	0.76	0.40	9.39	81,85,89,92	0
4	MPD	B	409	8/8	0.67	0.37	6.15	63,78,87,88	0
4	MPD	B	406	8/8	0.76	0.21	5.56	70,75,83,85	0
4	MPD	A	404	8/8	0.89	0.34	5.55	51,56,58,67	0
4	MPD	B	408	8/8	0.88	0.37	4.70	69,77,81,86	0
4	MPD	B	411	8/8	0.83	0.27	4.64	69,79,94,98	0
5	SO4	B	413	5/5	0.94	0.28	3.64	93,96,100,100	0
3	TEP	B	402[A]	13/13	0.83	0.28	3.46	52,62,65,71	13
4	MPD	A	407	8/8	0.83	0.20	2.89	68,75,84,86	0
4	MPD	B	407	8/8	0.85	0.20	2.56	64,68,70,74	0
5	SO4	B	414	5/5	0.86	0.21	1.91	92,93,100,100	0
4	MPD	A	405	8/8	0.86	0.23	1.77	60,72,75,76	0
4	MPD	A	403[B]	8/8	0.85	0.24	1.33	49,55,70,79	8
5	SO4	A	410	5/5	0.90	0.20	1.26	97,97,100,100	0
4	MPD	B	403[B]	8/8	0.90	0.18	1.00	23,41,49,59	8
3	TEP	A	402[A]	13/13	0.86	0.26	0.99	53,63,73,74	13
4	MPD	A	406	8/8	0.89	0.17	0.29	55,62,68,68	0
5	SO4	B	412	5/5	0.96	0.13	0.15	93,94,97,99	0
5	SO4	A	409	5/5	0.94	0.11	-0.40	86,88,94,96	0
5	SO4	B	415	5/5	0.91	0.18	-	93,94,98,100	0
2	NA	B	401	1/1	0.78	0.87	-	89,89,89,89	0
4	MPD	B	404	8/8	0.92	0.18	-	60,71,79,83	0
2	NA	A	401	1/1	0.78	0.55	-	79,79,79,79	0
5	SO4	A	408	5/5	0.82	0.37	-	100,100,100,100	0
4	MPD	B	405	8/8	0.82	0.29	-	72,79,86,96	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.