



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:28 PM GMT

PDB ID : 4LNU
Title : Nucleotide-free kinesin motor domain in complex with tubulin and a DARPin
Authors : Cao, L.; Gigant, B.; Knossow, M.
Deposited on : 2013-07-12
Resolution : 2.19 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

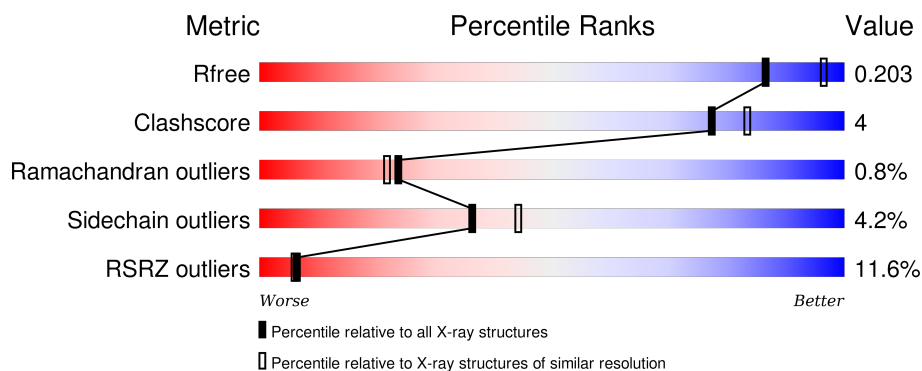
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (2.20-2.20)

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	451	<div> <div>7%</div> <div>86%</div> <div>9%</div> <div>• •</div> </div>
2	B	445	<div> <div>9%</div> <div>86%</div> <div>10%</div> <div>• •</div> </div>
3	D	169	<div> <div>5%</div> <div>85%</div> <div>8%</div> <div>7%</div> </div>
4	K	325	<div> <div>23%</div> <div>80%</div> <div>14%</div> <div>• 5%</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
10	GOL	B	503	-	-	-	X
10	GOL	B	504	-	-	-	X
10	GOL	D	201	-	-	-	X
10	GOL	K	401	-	-	-	X
7	SO4	A	505	-	-	-	X
7	SO4	B	510	-	-	-	X
7	SO4	K	403	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 11209 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 Tubulin alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	434	Total	C	N	O	S	0	3	0
			3410	2161	578	648	23			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	431	Total	C	N	O	S	0	5	0
			3424	2145	585	668	26			

- Molecule 3 is a protein called Designed ankyrin repeat protein (DARPIN) D1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	157	Total	C	N	O	S	0	0	0
			1170	737	201	229	3			

- Molecule 4 is a protein called Kinesin-1 heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	K	309	Total	C	N	O	S	0	0	0
			2420	1512	416	483	9			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
K	7	SER	CYS	ENGINEERED MUTATION	UNP P33176
K	65	ALA	CYS	ENGINEERED MUTATION	UNP P33176
K	168	ALA	CYS	ENGINEERED MUTATION	UNP P33176
K	174	SER	CYS	ENGINEERED MUTATION	UNP P33176
K	294	ALA	CYS	ENGINEERED MUTATION	UNP P33176

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

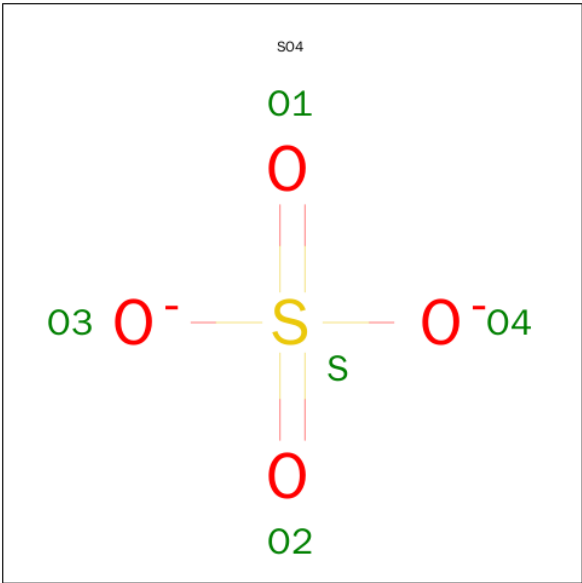


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

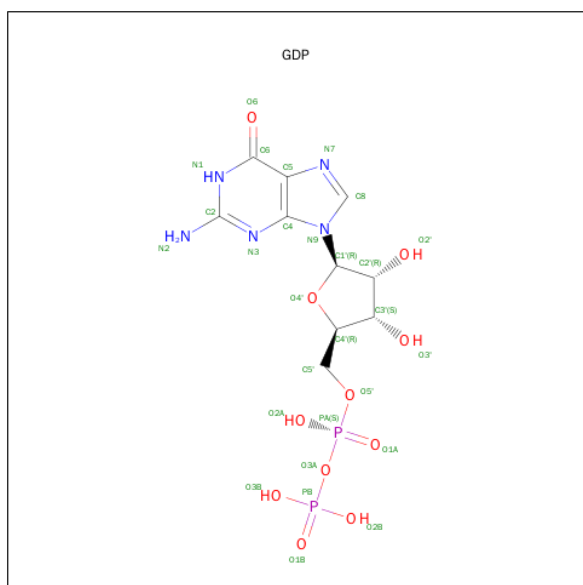
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		

- Molecule 7 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



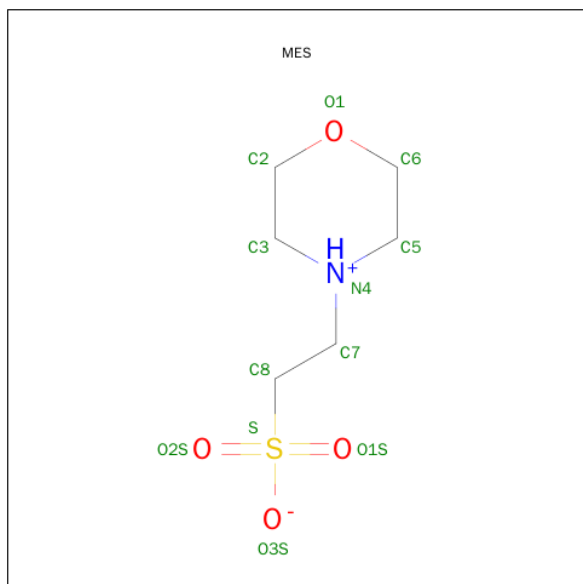
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0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

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



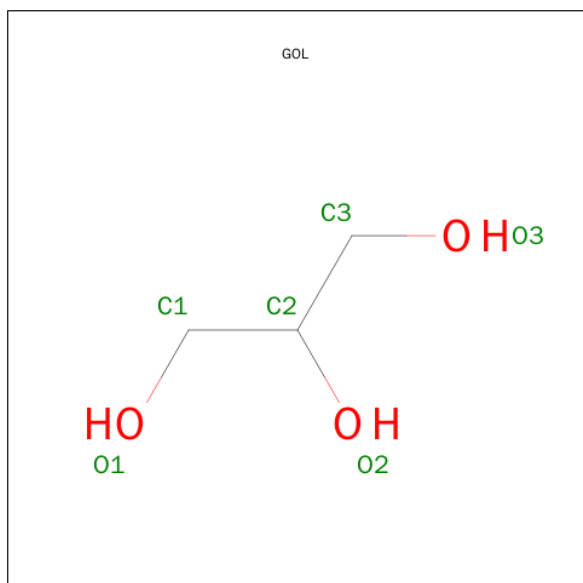
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			6	3	3		
10	B	1	Total	C	O	0	0
			6	3	3		
10	D	1	Total	C	O	0	0
			6	3	3		
10	K	1	Total	C	O	0	0
			6	3	3		

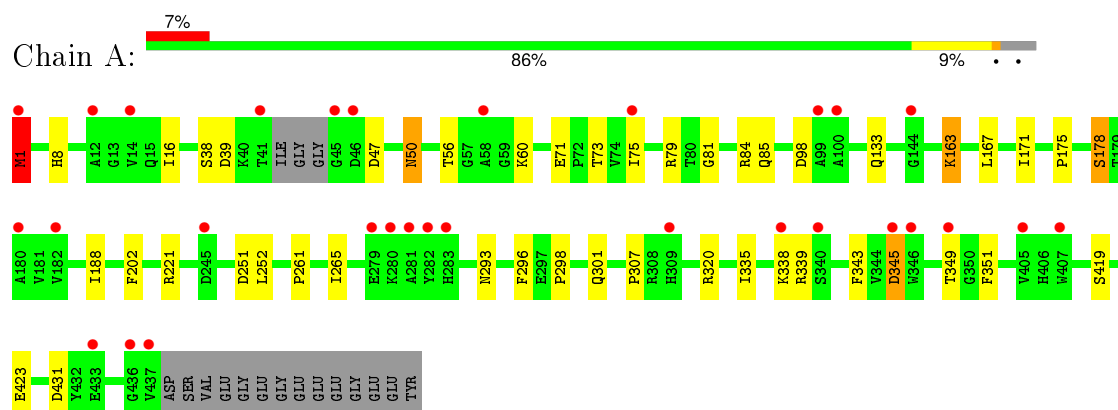
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	262	Total	O	0	0
			262	262		
11	B	219	Total	O	0	1
			219	219		
11	D	99	Total	O	0	0
			99	99		
11	K	53	Total	O	0	0
			53	53		

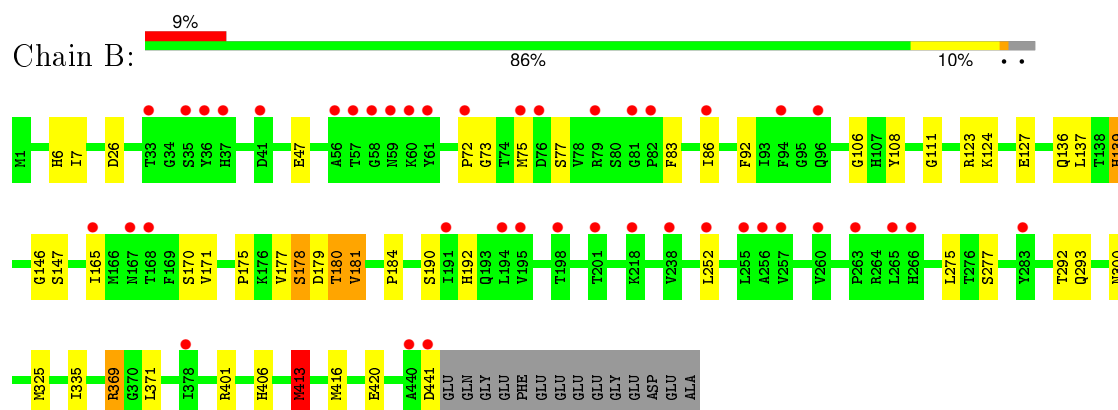
3 Residue-property plots

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.

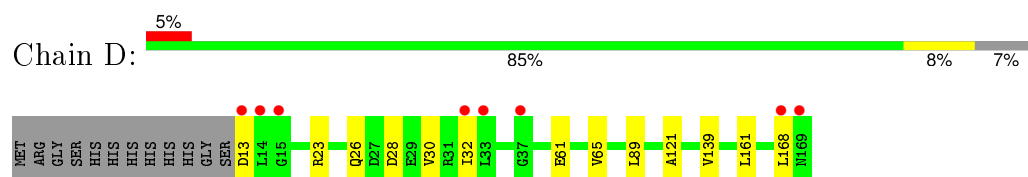
• Molecule 1: Tubulin alpha chain



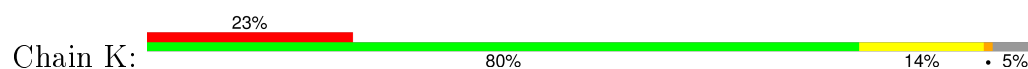
• Molecule 2: Tubulin beta chain

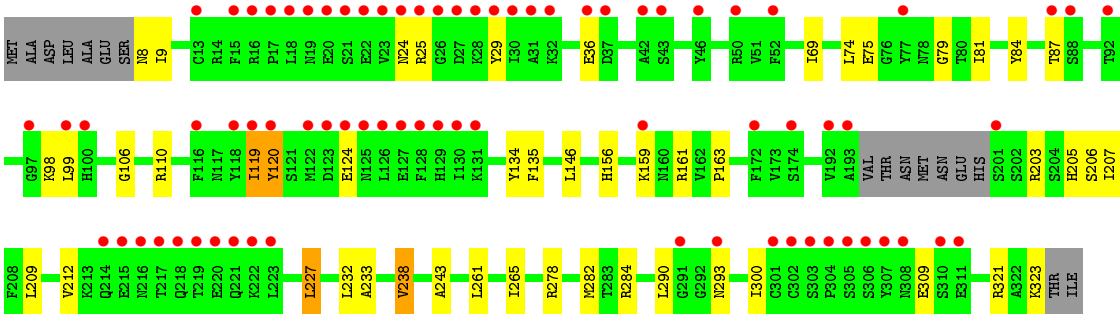


• Molecule 3: Designed ankyrin repeat protein (DARPIN) D1



• Molecule 4: Kinesin-1 heavy chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	73.40Å 83.01Å 83.31Å 116.16° 105.08° 97.57°	Depositor
Resolution (Å)	43.45 – 2.19 43.45 – 2.19	Depositor EDS
% Data completeness (in resolution range)	92.3 (43.45-2.19) 78.0 (43.45-2.19)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.18Å)	Xtriage
Refinement program	BUSTER 2.10.0	Depositor
R, R_{free}	0.155 , 0.195 0.162 , 0.203	Depositor DCC
R_{free} test set	3881 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 58.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 77634 reflections	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	11209	wwPDB-VP
Average B, all atoms (Å ²)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.12% 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: GDP, GOL, MG, GTP, SO4, MES

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	0.53	0/3495	0.71	2/4744 (0.0%)
2	B	0.53	0/3510	0.70	3/4754 (0.1%)
3	D	0.52	0/1186	0.74	0/1612
4	K	0.45	0/2457	0.69	0/3309
All	All	0.51	0/10648	0.71	5/14419 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	177	VAL	C-N-CA	5.38	135.15	121.70
2	B	178[A]	SER	N-CA-C	5.29	125.30	111.00
2	B	178[B]	SER	N-CA-C	5.29	125.30	111.00
1	A	1[A]	MET	C-N-CA	5.21	134.71	121.70
1	A	1[B]	MET	C-N-CA	5.21	134.71	121.70

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	3410	0	3323	30	0
2	B	3424	0	3292	27	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	D	1170	0	1173	8	0
4	K	2420	0	2397	16	1
5	A	32	0	12	0	0
6	A	1	0	0	0	0
7	A	15	0	0	0	0
7	B	30	0	0	0	0
7	K	10	0	0	0	0
8	B	28	0	12	0	0
9	B	12	0	13	1	0
10	B	12	0	16	1	0
10	D	6	0	8	1	0
10	K	6	0	8	0	0
11	A	262	0	0	3	1
11	B	219	0	0	1	0
11	D	99	0	0	0	0
11	K	53	0	0	1	0
All	All	11209	0	10254	77	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 4.

All (77) 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:71:GLU:OE2	1:A:73:THR:HB	1.63	0.98
2:B:6:HIS:HD2	2:B:136:GLN:HE21	1.20	0.87
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.58	0.84
1:A:133:GLN:HE22	1:A:252:LEU:H	1.34	0.74
2:B:192:HIS:HD2	11:B:767:HOH:O	1.75	0.70
1:A:133:GLN:NE2	1:A:252:LEU:H	1.92	0.67
2:B:292:THR:HG22	2:B:335:ILE:HG13	1.79	0.65
1:A:1[A]:MET:HG3	1:A:50:ASN:HB3	1.82	0.62
2:B:6:HIS:CD2	2:B:136:GLN:HE21	2.10	0.62
1:A:265:ILE:HD11	1:A:431:ASP:HB3	1.82	0.61
4:K:205:HIS:HD2	4:K:233:ALA:H	1.50	0.59
2:B:75:MET:HG3	2:B:92:PHE:CD2	2.38	0.59
2:B:275:LEU:HD11	2:B:300:ASN:HA	1.82	0.59
4:K:238:VAL:HG22	4:K:243:ALA:HB3	1.85	0.58
4:K:205:HIS:CD2	4:K:233:ALA:H	2.22	0.58
2:B:106:GLY:O	2:B:111:GLY:HA3	2.04	0.58
2:B:124:LYS:HB3	10:B:504:GOL:H12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:ARG:O	2:B:127:GLU:HG2	2.06	0.56
1:A:261:PRO:HD2	11:A:845:HOH:O	2.05	0.56
1:A:133:GLN:NE2	1:A:251:ASP:HB2	2.21	0.56
2:B:175:PRO:HA	2:B:178[A]:SER:HB3	1.87	0.56
3:D:61:GLU:O	3:D:65:VAL:HG23	2.07	0.54
3:D:61:GLU:H	3:D:61:GLU:CD	2.12	0.52
1:A:8:HIS:HE1	11:A:768:HOH:O	1.91	0.52
4:K:84:TYR:HB3	4:K:300:ILE:HG22	1.92	0.52
1:A:16:ILE:HD13	1:A:171:ILE:HD11	1.92	0.52
4:K:278:ARG:NH2	11:K:506:HOH:O	2.30	0.49
2:B:406[B]:HIS:CD2	3:D:23:ARG:HH22	2.30	0.49
2:B:420:GLU:OE1	4:K:156:HIS:HD2	1.96	0.49
3:D:121:ALA:HB1	3:D:161:LEU:HD21	1.96	0.48
4:K:261:LEU:HG	4:K:265:ILE:HD11	1.96	0.48
2:B:6:HIS:HD2	2:B:136:GLN:NE2	2.00	0.47
4:K:74:LEU:HD23	4:K:212:VAL:HG11	1.97	0.47
3:D:23:ARG:NH1	10:D:201:GOL:O2	2.48	0.47
1:A:298:PRO:HA	1:A:301:GLN:NE2	2.30	0.47
1:A:343:PHE:HB2	1:A:349:THR:HG22	1.96	0.47
3:D:28:ASP:O	3:D:32:ILE:HG12	2.16	0.46
2:B:165:ILE:HD13	9:B:502:MES:H82	1.98	0.46
2:B:401:ARG:HD3	3:D:89:LEU:HD22	1.96	0.46
1:A:16:ILE:HD13	1:A:171:ILE:CD1	2.46	0.45
2:B:75:MET:HG3	2:B:92:PHE:HD2	1.79	0.45
2:B:139:HIS:HD2	2:B:146:GLY:O	1.99	0.45
4:K:278:ARG:HG2	4:K:284:ARG:HD2	1.97	0.45
1:A:293:ASN:HA	1:A:335:ILE:HD11	1.99	0.45
1:A:175:PRO:HA	1:A:178:SER:HB2	1.99	0.45
1:A:47:ASP:O	1:A:50:ASN:HB2	2.17	0.45
2:B:83:PHE:O	2:B:86:ILE:HG22	2.17	0.44
1:A:338:LYS:HE2	1:A:339:ARG:HG2	2.00	0.44
1:A:221:ARG:HG2	2:B:325:MET:HB3	2.00	0.44
4:K:81:ILE:HD12	4:K:227:LEU:HD21	1.99	0.44
1:A:163:LYS:HE3	1:A:163:LYS:H	1.83	0.44
1:A:419:SER:O	1:A:423[A]:GLU:HG3	2.18	0.44
4:K:207:ILE:HD11	4:K:282:MET:HG3	2.00	0.43
1:A:60:LYS:NZ	1:A:85:GLN:O	2.49	0.43
1:A:296:PHE:HZ	1:A:351:PHE:HE2	1.64	0.43
2:B:165:ILE:HG21	2:B:252:LEU:HB3	2.01	0.43
1:A:133:GLN:HE22	1:A:252:LEU:N	2.09	0.43
1:A:75:ILE:O	1:A:79:ARG:HG3	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:SER:HB2	2:B:190:SER:OG	2.19	0.43
2:B:108:TYR:CE1	2:B:413:MET:HG3	2.54	0.42
2:B:139:HIS:HE1	2:B:170:SER:OG	2.02	0.42
2:B:7:ILE:O	2:B:137:LEU:HA	2.20	0.42
4:K:156:HIS:O	4:K:163:PRO:HA	2.20	0.42
1:A:301:GLN:HE22	1:A:307:PRO:CD	2.32	0.42
2:B:26:ASP:OD2	2:B:369:ARG:HD2	2.20	0.42
1:A:81:GLY:O	1:A:84:ARG:HD3	2.20	0.41
1:A:301:GLN:HE22	1:A:307:PRO:HD3	1.85	0.41
3:D:26:GLN:O	3:D:30:VAL:HG23	2.21	0.41
1:A:167[A]:LEU:HD13	1:A:252:LEU:HD22	2.03	0.41
4:K:106:GLY:O	4:K:110:ARG:HD2	2.21	0.41
4:K:205:HIS:HD2	4:K:232:LEU:HA	1.86	0.41
1:A:320:ARG:HB2	11:A:725:HOH:O	2.21	0.41
1:A:167[B]:LEU:HD13	1:A:202:PHE:HE1	1.86	0.41
2:B:181:VAL:O	2:B:184:PRO:HD2	2.21	0.40
4:K:69:ILE:HG23	4:K:79:GLY:HA3	2.03	0.40
4:K:119:ILE:O	4:K:120:TYR:HB3	2.21	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)
4:K:120:TYR:OH	11:A:861:HOH:O[1_454]	2.13	0.07

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	432/451 (96%)	412 (95%)	17 (4%)	3 (1%)	26	25
2	B	434/445 (98%)	420 (97%)	8 (2%)	6 (1%)	14	10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	D	155/169 (92%)	154 (99%)	0	1 (1%)	30	29
4	K	305/325 (94%)	289 (95%)	15 (5%)	1 (0%)	46	50
All	All	1326/1390 (95%)	1275 (96%)	40 (3%)	11 (1%)	24	22

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	345	ASP
2	B	181	VAL
3	D	168	LEU
4	K	99	LEU
2	B	73	GLY
2	B	180[A]	THR
2	B	180[B]	THR
2	B	413	MET
1	A	56	THR
2	B	72	PRO

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	368/379 (97%)	360 (98%)	8 (2%)	60	72
2	B	379/385 (98%)	366 (97%)	13 (3%)	44	54
3	D	122/132 (92%)	120 (98%)	2 (2%)	70	82
4	K	271/286 (95%)	244 (90%)	27 (10%)	9	8
All	All	1140/1182 (96%)	1090 (96%)	50 (4%)	36	42

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1[A]	MET

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Mol	Chain	Res	Type
1	A	1[B]	MET
1	A	39	ASP
1	A	50	ASN
1	A	163	LYS
1	A	178	SER
1	A	188	ILE
1	A	345	ASP
2	B	47	GLU
2	B	77	SER
2	B	139	HIS
2	B	171	VAL
2	B	180[A]	THR
2	B	180[B]	THR
2	B	277	SER
2	B	293	GLN
2	B	369	ARG
2	B	371	LEU
2	B	413	MET
2	B	416	MET
2	B	441	ASP
3	D	13	ASP
3	D	139	VAL
4	K	8	ASN
4	K	9	ILE
4	K	24	ASN
4	K	25	ARG
4	K	29	TYR
4	K	36	GLU
4	K	75	GLU
4	K	87	THR
4	K	98	LYS
4	K	119	ILE
4	K	120	TYR
4	K	124	GLU
4	K	134	TYR
4	K	135	PHE
4	K	146	LEU
4	K	159	LYS
4	K	161	ARG
4	K	203	ARG
4	K	206	SER
4	K	209	LEU

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Mol	Chain	Res	Type
4	K	227	LEU
4	K	238	VAL
4	K	290	LEU
4	K	293	ASN
4	K	309	GLU
4	K	321	ARG
4	K	323	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	50	ASN
1	A	107	HIS
1	A	133	GLN
1	A	139	HIS
1	A	216	ASN
1	A	285	GLN
1	A	301	GLN
1	A	309	HIS
2	B	6	HIS
2	B	139	HIS
2	B	247	GLN
2	B	282	GLN
2	B	394	GLN
4	K	156	HIS
4	K	205	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 19 ligands modelled in this entry, 1 is 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$
5	GTP	A	501	6	25,34,34	0.98	1 (4%)	34,54,54	1.99	4 (11%)
7	SO4	A	503	-	4,4,4	0.18	0	6,6,6	0.07	0
7	SO4	A	504	-	4,4,4	0.13	0	6,6,6	0.07	0
7	SO4	A	505	-	4,4,4	0.25	0	6,6,6	0.17	0
8	GDP	B	501	-	23,30,30	0.97	2 (8%)	30,47,47	2.24	5 (16%)
9	MES	B	502	-	11,12,12	0.85	0	14,16,16	0.58	0
10	GOL	B	503	-	5,5,5	0.13	0	5,5,5	0.34	0
10	GOL	B	504	-	5,5,5	0.12	0	5,5,5	0.19	0
7	SO4	B	505	-	4,4,4	0.15	0	6,6,6	0.14	0
7	SO4	B	506	-	4,4,4	0.12	0	6,6,6	0.15	0
7	SO4	B	507	-	4,4,4	0.16	0	6,6,6	0.13	0
7	SO4	B	508	-	4,4,4	0.12	0	6,6,6	0.09	0
7	SO4	B	509	-	4,4,4	0.11	0	6,6,6	0.09	0
7	SO4	B	510	-	4,4,4	0.19	0	6,6,6	0.18	0
10	GOL	D	201	-	5,5,5	0.16	0	5,5,5	0.41	0
10	GOL	K	401	-	5,5,5	0.11	0	5,5,5	0.25	0
7	SO4	K	402	-	4,4,4	0.22	0	6,6,6	0.11	0
7	SO4	K	403	-	4,4,4	0.22	0	6,6,6	0.19	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
5	GTP	A	501	6	-	0/18/38/38	0/3/3/3
7	SO4	A	503	-	-	0/0/0/0	0/0/0/0
7	SO4	A	504	-	-	0/0/0/0	0/0/0/0
7	SO4	A	505	-	-	0/0/0/0	0/0/0/0
8	GDP	B	501	-	-	0/12/32/32	0/3/3/3
9	MES	B	502	-	-	0/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GOL	B	503	-	-	0/4/4/4	0/0/0/0
10	GOL	B	504	-	-	0/4/4/4	0/0/0/0
7	SO4	B	505	-	-	0/0/0/0	0/0/0/0
7	SO4	B	506	-	-	0/0/0/0	0/0/0/0
7	SO4	B	507	-	-	0/0/0/0	0/0/0/0
7	SO4	B	508	-	-	0/0/0/0	0/0/0/0
7	SO4	B	509	-	-	0/0/0/0	0/0/0/0
7	SO4	B	510	-	-	0/0/0/0	0/0/0/0
10	GOL	D	201	-	-	0/4/4/4	0/0/0/0
10	GOL	K	401	-	-	0/4/4/4	0/0/0/0
7	SO4	K	402	-	-	0/0/0/0	0/0/0/0
7	SO4	K	403	-	-	0/0/0/0	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	501	GDP	C6-C5	2.47	1.46	1.41
8	B	501	GDP	C6-N1	2.82	1.38	1.33
5	A	501	GTP	C6-N1	3.23	1.39	1.33

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	GDP	C5-C6-N1	-8.28	112.27	123.59
5	A	501	GTP	C5-C6-N1	-8.06	112.57	123.59
5	A	501	GTP	N3-C2-N1	-2.75	123.26	127.44
8	B	501	GDP	C6-C5-C4	-2.72	117.64	120.90
8	B	501	GDP	N3-C2-N1	-2.60	123.49	127.44
5	A	501	GTP	C6-C5-C4	-2.28	118.17	120.90
8	B	501	GDP	O5'-PA-O1A	2.15	117.98	109.62
5	A	501	GTP	C6-N1-C2	6.59	125.08	115.94
8	B	501	GDP	C6-N1-C2	6.78	125.35	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	502	MES	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	504	GOL	1	0
10	D	201	GOL	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	434/451 (96%)	0.41	30 (6%) 20 19	27, 44, 90, 114	0
2	B	431/445 (96%)	0.50	42 (9%) 10 9	27, 45, 79, 120	5 (1%)
3	D	157/169 (92%)	0.00	8 (5%) 32 31	30, 46, 90, 124	0
4	K	309/325 (95%)	1.27	75 (24%) 1 1	34, 84, 153, 186	0
All	All	1331/1390 (95%)	0.59	155 (11%) 6 6	27, 50, 119, 186	5 (0%)

All (155) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	K	21	SER	11.5
4	K	99	LEU	10.1
4	K	218	GLN	9.8
4	K	31	ALA	8.5
4	K	307	TYR	8.5
1	A	346	TRP	8.3
4	K	29	TYR	7.9
4	K	20	GLU	7.8
1	A	437	VAL	7.8
4	K	30	ILE	7.3
4	K	22	GLU	7.2
2	B	57	THR	6.9
1	A	281	ALA	6.9
4	K	215	GLU	6.8
4	K	28	LYS	6.7
4	K	120	TYR	6.5
1	A	282	TYR	6.3
4	K	24	ASN	6.1
4	K	293	ASN	5.9
4	K	19	ASN	5.8
2	B	441	ASP	5.8

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Mol	Chain	Res	Type	RSRZ
1	A	45	GLY	5.7
4	K	223	LEU	5.7
2	B	59	ASN	5.7
4	K	125	ASN	5.7
1	A	345	ASP	5.7
1	A	349	THR	5.6
4	K	201	SER	5.5
4	K	27	ASP	5.5
4	K	219	THR	5.5
4	K	17	PRO	5.5
4	K	216	ASN	5.5
4	K	18	LEU	5.4
4	K	126	LEU	5.3
4	K	217	THR	5.2
4	K	88	SER	4.9
1	A	436	GLY	4.8
4	K	306	SER	4.7
4	K	15	PHE	4.7
4	K	130	ILE	4.6
2	B	37	HIS	4.6
2	B	33	THR	4.6
4	K	25	ARG	4.5
4	K	23	VAL	4.4
4	K	26	GLY	4.4
1	A	309	HIS	4.3
4	K	302	CYS	4.3
4	K	304	PRO	4.3
2	B	260	VAL	4.0
2	B	440	ALA	4.0
4	K	124	GLU	4.0
4	K	13	CYS	3.9
2	B	72	PRO	3.9
4	K	16	ARG	3.9
4	K	221	GLN	3.9
4	K	305	SER	3.8
4	K	43	SER	3.8
4	K	52	PHE	3.8
4	K	97	GLY	3.8
4	K	308	ASN	3.8
4	K	127	GLU	3.7
2	B	255	LEU	3.7
2	B	75	MET	3.7

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Mol	Chain	Res	Type	RSRZ
3	D	169	ASN	3.7
4	K	222	LYS	3.7
4	K	174	SER	3.7
2	B	60	LYS	3.7
4	K	159	LYS	3.7
4	K	220	GLU	3.6
2	B	56	ALA	3.6
4	K	87	THR	3.5
4	K	36	GLU	3.5
1	A	46	ASP	3.4
4	K	116	PHE	3.4
1	A	280	LYS	3.3
4	K	192	VAL	3.3
1	A	245	ASP	3.3
3	D	168	LEU	3.3
1	A	433	GLU	3.3
2	B	165	ILE	3.3
4	K	129	HIS	3.2
2	B	194	LEU	3.2
2	B	252	LEU	3.2
3	D	33	LEU	3.1
2	B	58	GLY	3.1
4	K	214	GLN	3.1
4	K	122	MET	3.1
3	D	13	ASP	3.1
1	A	407	TRP	3.1
2	B	36	TYR	3.0
4	K	311	GLU	3.0
2	B	257	VAL	3.0
2	B	283	TYR	3.0
4	K	77	TYR	3.0
4	K	46	TYR	2.9
4	K	37	ASP	2.9
2	B	82	PRO	2.9
2	B	198	THR	2.9
4	K	42	ALA	2.9
4	K	92	THR	2.9
1	A	338	LYS	2.9
4	K	123	ASP	2.8
4	K	32	LYS	2.8
4	K	131	LYS	2.8
2	B	35	SER	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	1[A]	MET	2.7
1	A	340	SER	2.7
4	K	172	PHE	2.7
2	B	61	TYR	2.7
4	K	291	GLY	2.7
1	A	279	GLU	2.7
4	K	128	PHE	2.7
2	B	265	LEU	2.6
4	K	193	ALA	2.6
4	K	301	CYS	2.6
4	K	119	ILE	2.6
1	A	12	ALA	2.6
1	A	41	THR	2.6
2	B	96	GLN	2.5
3	D	14	LEU	2.5
4	K	303	SER	2.5
2	B	168	THR	2.5
2	B	256	ALA	2.4
2	B	81	GLY	2.4
2	B	378	ILE	2.4
1	A	182	VAL	2.4
4	K	310	SER	2.4
2	B	195	VAL	2.4
2	B	167	ASN	2.4
2	B	41	ASP	2.4
4	K	50	ARG	2.4
2	B	263	PRO	2.3
2	B	79	ARG	2.3
2	B	191	ILE	2.3
1	A	283	HIS	2.2
1	A	100	ALA	2.2
3	D	15	GLY	2.2
1	A	58	ALA	2.2
1	A	405	VAL	2.2
2	B	238	VAL	2.2
1	A	99	ALA	2.2
2	B	266	HIS	2.1
3	D	37	GLY	2.1
1	A	14	VAL	2.1
2	B	76	ASP	2.1
4	K	118	TYR	2.1
2	B	86	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	201	THR	2.1
2	B	218	LYS	2.1
1	A	75	ILE	2.0
3	D	32	ILE	2.0
1	A	144	GLY	2.0
1	A	180	ALA	2.0
2	B	94	PHE	2.0
4	K	100	HIS	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, 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
7	SO4	B	510	5/5	0.87	0.28	12.23	126,126,126,127	0
7	SO4	K	403	5/5	0.73	0.38	4.66	143,143,144,145	0
10	GOL	B	504	6/6	0.83	0.28	3.60	92,94,95,95	0
10	GOL	K	401	6/6	0.84	0.34	3.30	71,76,77,78	0
10	GOL	D	201	6/6	0.85	0.22	3.18	59,65,66,66	0
7	SO4	A	505	5/5	0.93	0.27	2.84	106,109,109,111	0
10	GOL	B	503	6/6	0.91	0.25	2.62	85,86,87,87	0
7	SO4	A	503	5/5	0.85	0.20	1.96	134,134,135,136	0
9	MES	B	502	12/12	0.98	0.25	0.77	44,46,46,47	0
7	SO4	B	509	5/5	0.96	0.14	-0.15	99,99,100,101	0
8	GDP	B	501	28/28	0.98	0.10	-0.29	33,36,45,46	0
7	SO4	K	402	5/5	0.82	0.18	-0.46	134,134,135,135	0
5	GTP	A	501	32/32	0.99	0.16	-0.56	26,31,33,36	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	SO4	B	506	5/5	0.98	0.06	-	109,109,110,110	0
7	SO4	B	508	5/5	0.77	0.21	-	146,147,147,147	0
6	MG	A	502	1/1	0.85	0.21	-	36,36,36,36	0
7	SO4	A	504	5/5	0.96	0.09	-	106,107,108,108	0
7	SO4	B	507	5/5	0.92	0.15	-	121,121,121,122	0
7	SO4	B	505	5/5	0.95	0.24	-	122,122,123,124	0

6.5 Other polymers [i](#)

There are no such residues in this entry.