



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:48 AM UTC

PDB ID : 4LNU / pdb_00004lnu
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

<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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

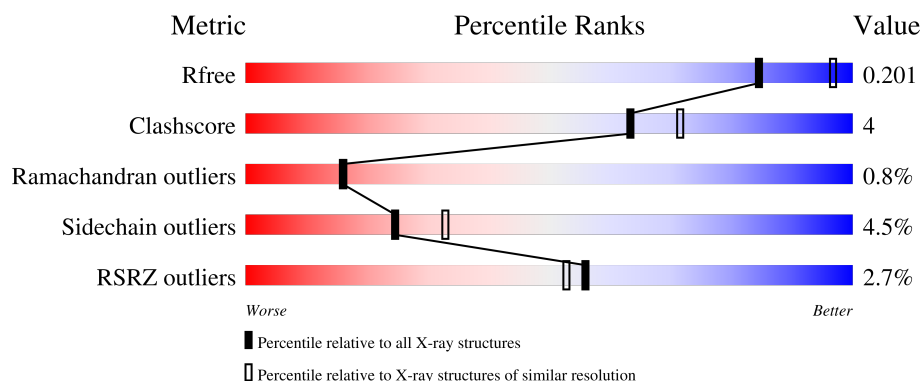
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.19 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}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (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 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	451	2% 84% 10% • •
2	B	445	83% 13% • •
3	D	169	4% 79% 13% • 7%
4	K	325	6% 78% 16% • 5%

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 (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

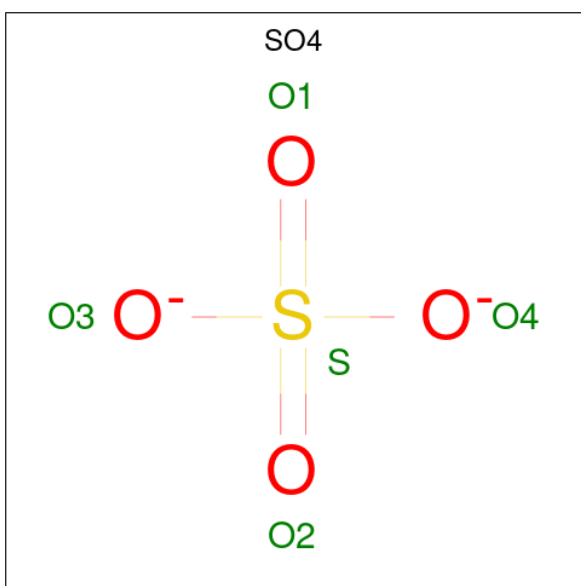


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

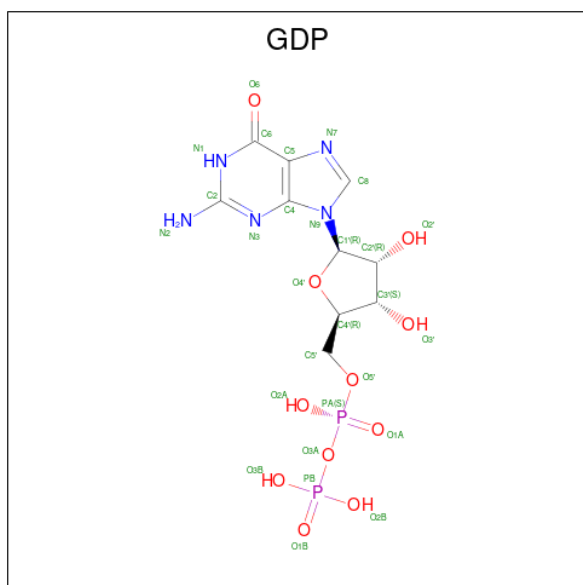
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0

- Molecule 7 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



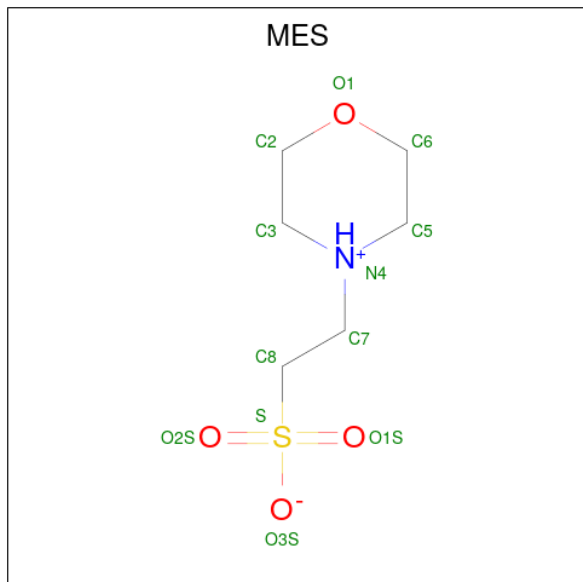
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	A	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
7	B	1	Total O S 5 4 1	0	0
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 (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



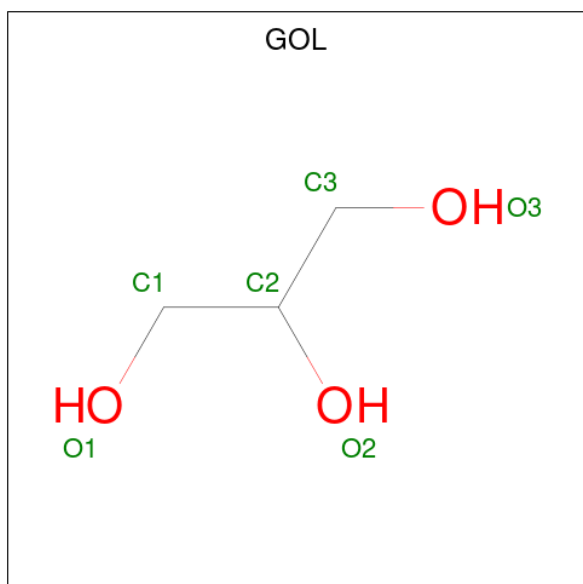
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: 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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
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		

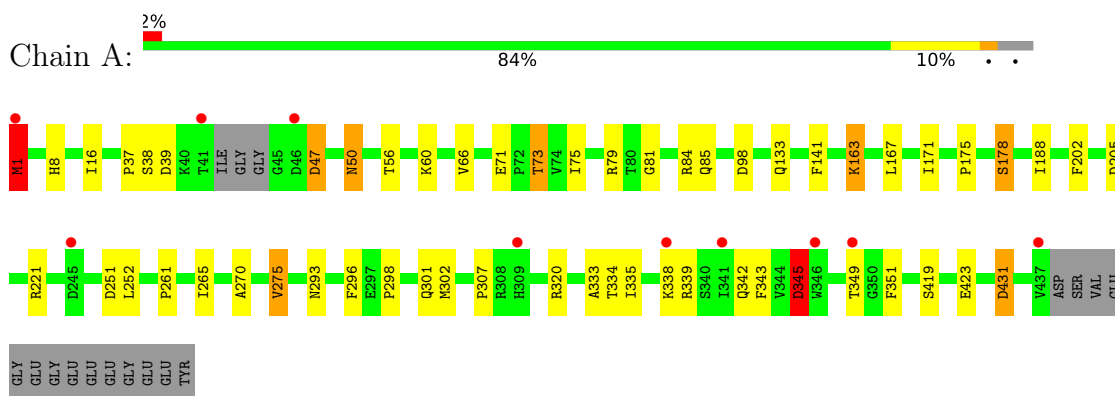
- Molecule 11 is water.

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		

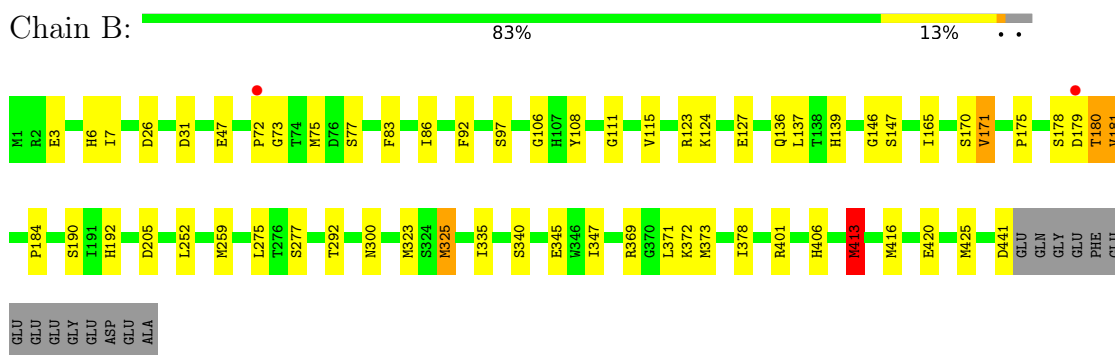
3 Residue-property plots [i](#)

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.

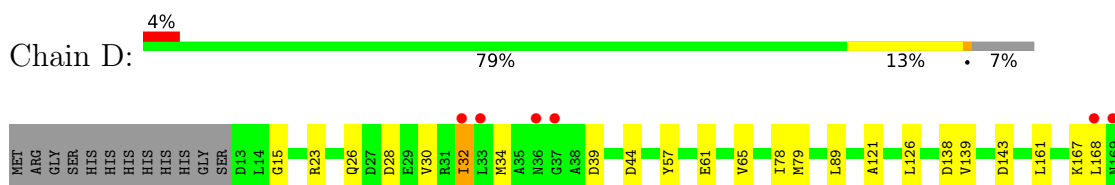
- Molecule 1: Tubulin alpha chain



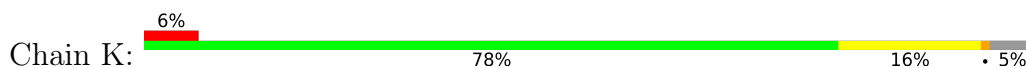
- Molecule 2: Tubulin beta chain

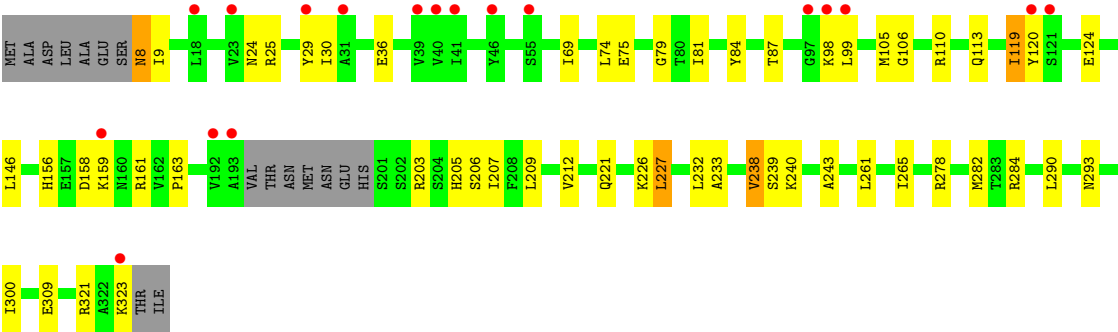


- Molecule 3: Designed ankyrin repeat protein (DARPIN) D1



- 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) 92.2 (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 0.165 , 0.201	Depositor DCC
R_{free} test set	3882 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	38.2	Xtriage
Anisotropy	0.440	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 70.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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, 0.333 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: SO4, GTP, MES, MG, GDP, GOL

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	0.89	0/3495	1.35	21/4744 (0.4%)
2	B	0.89	1/3510 (0.0%)	1.30	11/4754 (0.2%)
3	D	0.91	0/1186	1.49	8/1612 (0.5%)
4	K	0.80	0/2457	1.34	4/3309 (0.1%)
All	All	0.87	1/10648 (0.0%)	1.35	44/14419 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	425	MET	SD-CE	-6.92	1.62	1.79

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	VAL	N-CA-CB	8.25	121.72	111.41
2	B	171	VAL	N-CA-CB	7.53	119.58	111.00
1	A	1[A]	MET	CA-C-N	7.23	134.71	121.70
1	A	1[A]	MET	C-N-CA	7.23	134.71	121.70
1	A	1[B]	MET	CA-C-N	7.23	134.71	121.70
1	A	1[B]	MET	C-N-CA	7.23	134.71	121.70
1	A	205	ASP	CA-CB-CG	6.79	119.39	112.60
2	B	115	VAL	N-CA-C	6.59	117.28	110.36
2	B	372	LYS	N-CA-C	-6.51	104.38	112.90
2	B	205	ASP	CA-CB-CG	6.28	118.88	112.60
4	K	240	LYS	N-CA-C	-6.26	102.09	110.55
3	D	44	ASP	CA-CB-CG	6.04	118.64	112.60
3	D	39	ASP	CA-CB-CG	6.02	118.62	112.60
4	K	8	ASN	CA-CB-CG	6.00	118.60	112.60
1	A	333	ALA	CA-C-N	5.97	128.20	120.44
1	A	333	ALA	C-N-CA	5.97	128.20	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	GLU	N-CA-C	5.89	118.80	109.96
3	D	126	LEU	N-CA-C	5.80	117.61	111.28
2	B	31	ASP	CA-CB-CG	5.78	118.38	112.60
1	A	73	THR	N-CA-C	5.68	117.92	111.11
2	B	345	GLU	CB-CG-CD	5.66	122.22	112.60
1	A	345	ASP	CA-CB-CG	5.56	118.16	112.60
2	B	97	SER	N-CA-C	5.48	119.13	112.23
2	B	171	VAL	CB-CA-C	5.39	117.48	110.96
1	A	37	PRO	CA-C-N	5.37	131.80	121.54
1	A	37	PRO	C-N-CA	5.37	131.80	121.54
4	K	239	SER	N-CA-C	-5.29	105.41	111.07
2	B	347	ILE	N-CA-CB	5.27	118.59	111.21
3	D	138	ASP	CA-CB-CG	5.25	117.85	112.60
4	K	158	ASP	CA-CB-CG	5.16	117.76	112.60
1	A	47	ASP	CA-C-N	5.14	127.12	120.44
1	A	47	ASP	C-N-CA	5.14	127.12	120.44
3	D	57	TYR	N-CA-C	5.14	119.19	113.02
2	B	340	SER	N-CA-C	5.12	118.31	111.75
3	D	143	ASP	CA-CB-CG	5.07	117.67	112.60
1	A	334	THR	CA-C-N	5.06	126.94	120.56
1	A	334	THR	C-N-CA	5.06	126.94	120.56
1	A	141	PHE	CA-C-N	5.05	126.70	120.34
1	A	141	PHE	C-N-CA	5.05	126.70	120.34
1	A	275	VAL	CB-CA-C	5.04	118.36	111.31
1	A	37	PRO	N-CA-C	5.02	118.61	111.13
1	A	431	ASP	CA-CB-CG	5.02	117.62	112.60
3	D	15	GLY	CA-C-N	5.02	126.96	120.44
3	D	15	GLY	C-N-CA	5.02	126.96	120.44

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	32	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3424	0	3292	29	0
3	D	1170	0	1173	10	0
4	K	2420	0	2397	17	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	84	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 (84) 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:270:ALA:HB3	1:A:302:MET:HE2	1.66	0.77
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
3:D:78:ILE:HG23	3:D:79:MET:HE2	1.76	0.68
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:61:GLU:CD	3:D:61:GLU:H	2.12	0.57
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
1:A:270:ALA:CB	1:A:302:MET:HE2	2.37	0.54
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:105:MET:HE3	4:K:110:ARG:HG3	1.91	0.52
3:D:30:VAL:HG12	3:D:34:MET:HE2	1.91	0.51
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:259:MET:HE2	2:B:378:ILE:HG22	1.94	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:175:PRO:HA	1:A:178:SER:HB2	1.99	0.45
1:A:293:ASN:HA	1:A:335:ILE:HD11	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:163:LYS:HE3	1:A:163:LYS:H	1.83	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:SER:O	1:A:423[A]:GLU:HG3	2.18	0.44
1:A:60:LYS:NZ	1:A:85:GLN:O	2.49	0.43
4:K:207:ILE:HD11	4:K:282:MET:HG3	2.00	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
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:323:MET:HE2	2:B:373:MET:HG2	2.01	0.42
2:B:7:ILE:O	2:B:137:LEU:HA	2.20	0.42
2:B:139:HIS:HE1	2:B:170:SER:OG	2.02	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
1:A:320:ARG:HB2	11:A:725:HOH:O	2.21	0.41
4:K:205:HIS:HD2	4:K:232:LEU:HA	1.86	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%)	18	19
2	B	434/445 (98%)	420 (97%)	8 (2%)	6 (1%)	9	7
3	D	155/169 (92%)	154 (99%)	0	1 (1%)	21	23
4	K	305/325 (94%)	289 (95%)	15 (5%)	1 (0%)	36	42
All	All	1326/1390 (95%)	1275 (96%)	40 (3%)	11 (1%)	16	16

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%)	357 (97%)	11 (3%)	36	49
2	B	379/385 (98%)	368 (97%)	11 (3%)	37	51
3	D	122/132 (92%)	119 (98%)	3 (2%)	42	56
4	K	271/286 (95%)	243 (90%)	28 (10%)	7	7
All	All	1140/1182 (96%)	1087 (95%)	53 (5%)	24	32

All (53) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1[A]	MET
1	A	1[B]	MET
1	A	39	ASP
1	A	50	ASN
1	A	66	VAL
1	A	163	LYS
1	A	178	SER
1	A	188	ILE
1	A	275	VAL
1	A	342	GLN
1	A	345	ASP
2	B	47	GLU
2	B	77	SER
2	B	171	VAL
2	B	180[A]	THR
2	B	180[B]	THR
2	B	277	SER
2	B	325	MET
2	B	371	LEU
2	B	413	MET
2	B	416	MET
2	B	441	ASP
3	D	32	ILE
3	D	139	VAL
3	D	167	LYS
4	K	8	ASN
4	K	9	ILE
4	K	24	ASN
4	K	25	ARG
4	K	29	TYR
4	K	30	ILE
4	K	36	GLU
4	K	75	GLU
4	K	87	THR
4	K	98	LYS
4	K	113	GLN
4	K	119	ILE
4	K	124	GLU
4	K	146	LEU
4	K	159	LYS
4	K	161	ARG
4	K	203	ARG

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Mol	Chain	Res	Type
4	K	206	SER
4	K	209	LEU
4	K	221	GLN
4	K	226	LYS
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	15	GLN
1	A	50	ASN
1	A	107	HIS
1	A	133	GLN
1	A	139	HIS
1	A	216	ASN
1	A	233	GLN
1	A	285	GLN
1	A	301	GLN
1	A	309	HIS
2	B	6	HIS
2	B	139	HIS
2	B	192	HIS
2	B	193	GLN
2	B	293	GLN
2	B	336	GLN
2	B	434	GLN
3	D	36	ASN
3	D	166	GLN
4	K	24	ASN
4	K	63	ASN
4	K	125	ASN
4	K	156	HIS
4	K	205	HIS
4	K	216	ASN

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 oligosaccharides 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	$\# Z > 2$
7	SO4	B	506	-	4,4,4	0.23	0	6,6,6	0.15	0
7	SO4	B	509	-	4,4,4	0.26	0	6,6,6	0.08	0
7	SO4	A	505	-	4,4,4	0.33	0	6,6,6	0.23	0
7	SO4	K	402	-	4,4,4	0.29	0	6,6,6	0.14	0
7	SO4	B	510	-	4,4,4	0.21	0	6,6,6	0.14	0
7	SO4	A	504	-	4,4,4	0.26	0	6,6,6	0.07	0
9	MES	B	502	-	12,12,12	0.90	0	15,16,16	0.44	0
7	SO4	A	503	-	4,4,4	0.24	0	6,6,6	0.08	0
10	GOL	B	504	-	5,5,5	0.06	0	5,5,5	0.21	0
7	SO4	B	505	-	4,4,4	0.23	0	6,6,6	0.14	0
10	GOL	K	401	-	5,5,5	0.06	0	5,5,5	0.21	0
8	GDP	B	501	-	29,30,30	0.39	0	45,47,47	0.78	2 (4%)
7	SO4	B	508	-	4,4,4	0.25	0	6,6,6	0.10	0
7	SO4	K	403	-	4,4,4	0.27	0	6,6,6	0.19	0
5	GTP	A	501	6	33,34,34	2.16	2 (6%)	50,54,54	0.56	0
10	GOL	B	503	-	5,5,5	0.05	0	5,5,5	0.25	0
7	SO4	B	507	-	4,4,4	0.25	0	6,6,6	0.14	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
10	GOL	D	201	-	5,5,5	0.13	0	5,5,5	0.38	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
9	MES	B	502	-	-	0/6/14/14	0/1/1/1
10	GOL	B	504	-	-	2/4/4/4	-
10	GOL	K	401	-	-	0/4/4/4	-
8	GDP	B	501	-	-	3/16/32/32	0/3/3/3
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3
10	GOL	B	503	-	-	1/4/4/4	-
10	GOL	D	201	-	-	0/4/4/4	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	501	GTP	PB-O3B	-8.56	1.50	1.59
5	A	501	GTP	PA-O3A	-8.56	1.50	1.59

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	GDP	O5'-PA-O1A	2.28	117.98	108.94
8	B	501	GDP	PA-O5'-C5'	2.27	134.38	121.35

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
10	B	503	GOL	C1-C2-C3-O3
10	B	504	GOL	O1-C1-C2-C3
8	B	501	GDP	C3'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O1G

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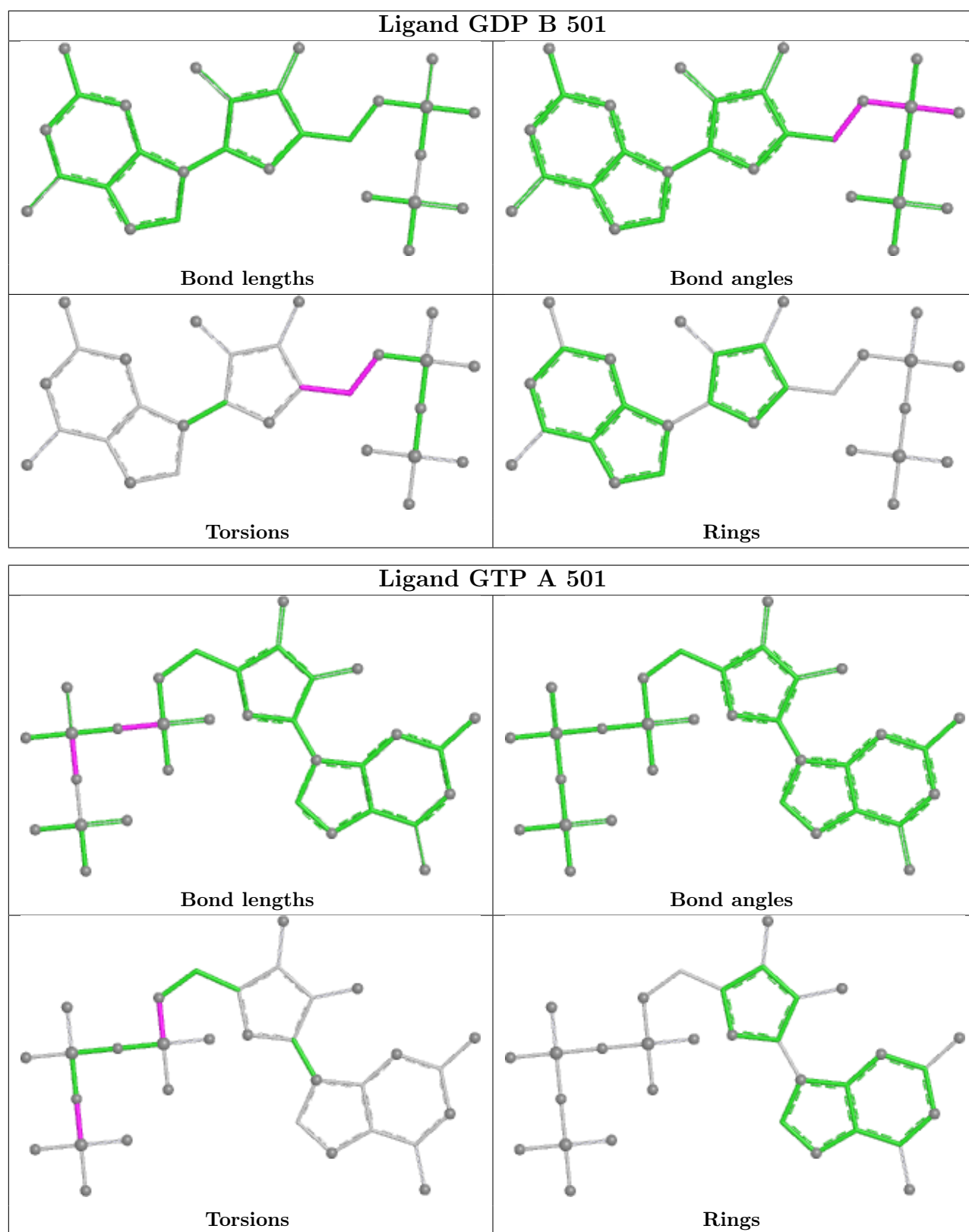
Mol	Chain	Res	Type	Atoms
8	B	501	GDP	C4'-C5'-O5'-PA
8	B	501	GDP	O4'-C4'-C5'-O5'
10	B	504	GOL	O1-C1-C2-O2
5	A	501	GTP	PB-O3B-PG-O2G

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
10	B	504	GOL	1	0
10	D	201	GOL	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.22	10 (2%) 61 58	20, 44, 90, 114	3 (0%)
2	B	431/445 (96%)	-0.22	2 (0%) 87 85	24, 44, 78, 120	10 (2%)
3	D	157/169 (92%)	-0.20	6 (3%) 44 41	30, 46, 90, 124	0
4	K	309/325 (95%)	0.48	18 (5%) 29 25	34, 84, 153, 186	0
All	All	1331/1390 (95%)	-0.05	36 (2%) 56 53	20, 50, 119, 186	13 (0%)

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	K	99	LEU	4.0
4	K	120	TYR	3.9
3	D	168	LEU	3.9
1	A	437	VAL	3.7
2	B	179[A]	ASP	3.6
4	K	323	LYS	3.1
4	K	193	ALA	3.0
4	K	23	VAL	2.8
3	D	36	ASN	2.8
1	A	46	ASP	2.8
1	A	245	ASP	2.7
1	A	346	TRP	2.6
4	K	121	SER	2.6
3	D	32	ILE	2.5
4	K	159	LYS	2.5
4	K	31	ALA	2.5
1	A	349	THR	2.5
4	K	41	ILE	2.5
4	K	40	VAL	2.4
2	B	72	PRO	2.3
1	A	1[A]	MET	2.3

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Mol	Chain	Res	Type	RSRZ
4	K	192	VAL	2.3
3	D	169	ASN	2.3
3	D	37	GLY	2.2
1	A	41	THR	2.2
4	K	39	VAL	2.2
1	A	309	HIS	2.2
4	K	55	SER	2.2
4	K	98	LYS	2.2
4	K	29	TYR	2.1
4	K	97	GLY	2.1
4	K	18	LEU	2.1
3	D	33	LEU	2.0
1	A	338	LYS	2.0
1	A	341	ILE	2.0
4	K	46	TYR	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 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
7	SO4	K	402	5/5	0.67	0.11	134,134,135,135	0
10	GOL	B	504	6/6	0.78	0.15	92,94,95,95	0
7	SO4	B	510	5/5	0.82	0.11	126,126,126,127	0
10	GOL	B	503	6/6	0.84	0.21	85,86,87,87	0
10	GOL	K	401	6/6	0.84	0.20	71,76,77,78	0
7	SO4	B	509	5/5	0.86	0.10	99,99,100,101	0
7	SO4	K	403	5/5	0.87	0.12	143,143,144,145	0
10	GOL	D	201	6/6	0.87	0.12	59,65,66,66	0

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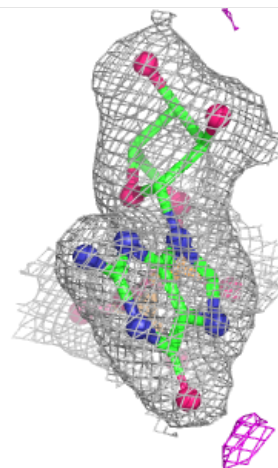
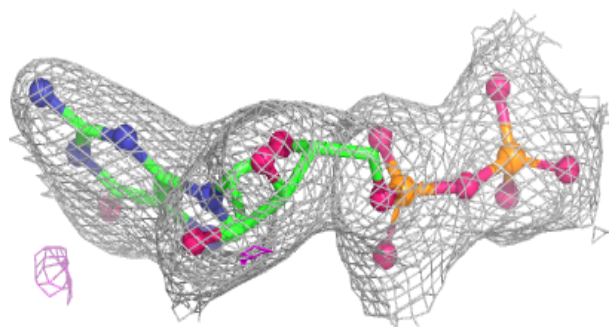
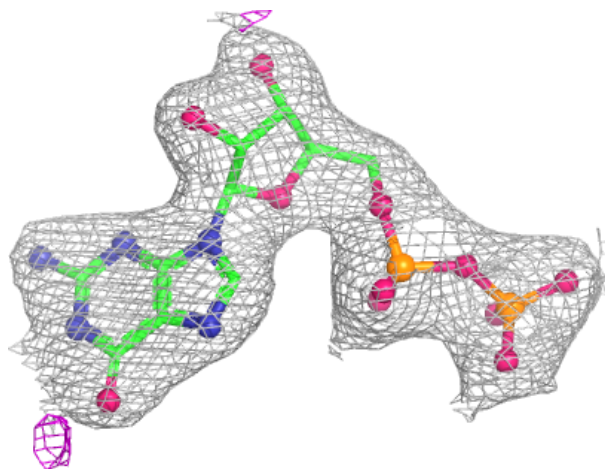
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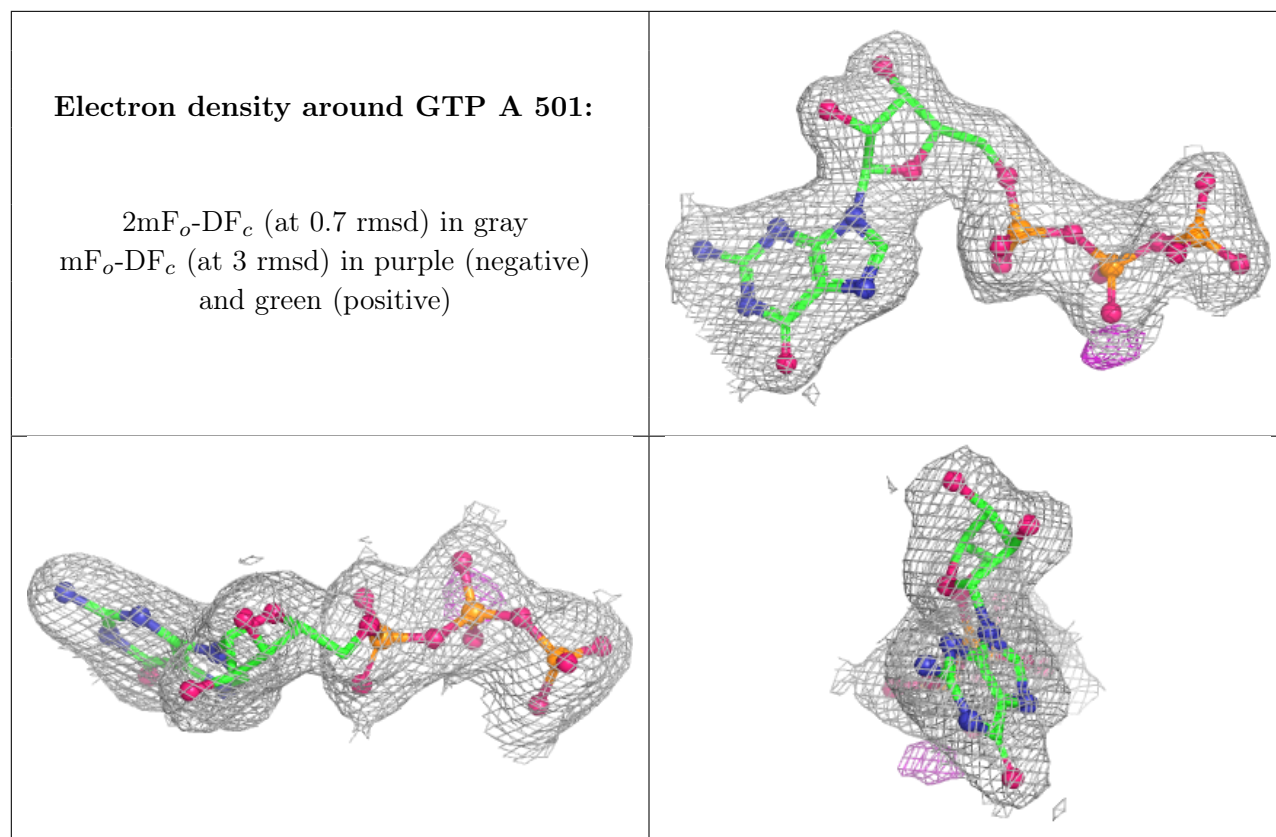
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	SO4	B	507	5/5	0.87	0.08	121,121,121,122	0
7	SO4	A	504	5/5	0.88	0.07	106,107,108,108	0
7	SO4	B	508	5/5	0.88	0.10	146,147,147,147	0
7	SO4	B	506	5/5	0.89	0.06	109,109,110,110	0
7	SO4	A	505	5/5	0.90	0.16	106,109,109,111	0
7	SO4	A	503	5/5	0.91	0.12	134,134,135,136	0
7	SO4	B	505	5/5	0.92	0.10	122,122,123,124	0
9	MES	B	502	12/12	0.97	0.06	44,46,46,47	0
8	GDP	B	501	28/28	0.98	0.05	33,36,45,46	0
6	MG	A	502	1/1	0.98	0.06	36,36,36,36	0
5	GTP	A	501	32/32	0.99	0.04	26,31,33,36	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around GDP B 501:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.