



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:47 AM UTC

PDB ID : 4EB6 / pdb_00004eb6
Title : Tubulin-Vinblastine: Stathmin-like complex
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Deposited on : 2012-03-23
Resolution : 3.47 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

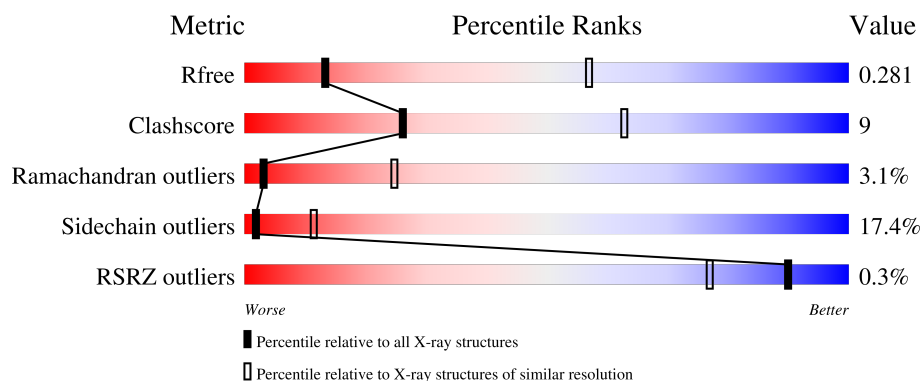
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

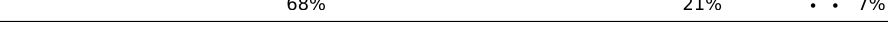
The reported resolution of this entry is 3.47 Å.

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	1083 (3.52-3.44)
Clashscore	190562	1139 (3.52-3.44)
Ramachandran outliers	187476	1111 (3.52-3.44)
Sidechain outliers	187428	1112 (3.52-3.44)
RSRZ outliers	180081	1082 (3.52-3.44)

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	
1	C	451	
2	B	445	
2	D	445	
3	E	142	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 14918 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	433	Total	C	N	O	S	0	1	0
			3399	2153	577	647	22			
1	C	432	Total	C	N	O	S	0	4	0
			3408	2161	576	648	23			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
A	340	SER	THR	SEE REMARK 999	UNP D0VWZ0
C	232	SER	GLY	SEE REMARK 999	UNP D0VWZ0
C	340	SER	THR	SEE REMARK 999	UNP D0VWZ0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	432	Total	C	N	O	S	0	2	0
			3400	2130	582	662	26			
2	D	432	Total	C	N	O	S	0	1	0
			3394	2127	580	661	26			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	317	THR	ALA	SEE REMARK 999	UNP D0VWY9
B	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9
B	335	ILE	VAL	SEE REMARK 999	UNP D0VWY9
B	375	SER	ALA	SEE REMARK 999	UNP D0VWY9
D	317	THR	ALA	SEE REMARK 999	UNP D0VWY9
D	318	ILE	VAL	SEE REMARK 999	UNP D0VWY9
D	335	ILE	VAL	SEE REMARK 999	UNP D0VWY9
D	375	SER	ALA	SEE REMARK 999	UNP D0VWY9

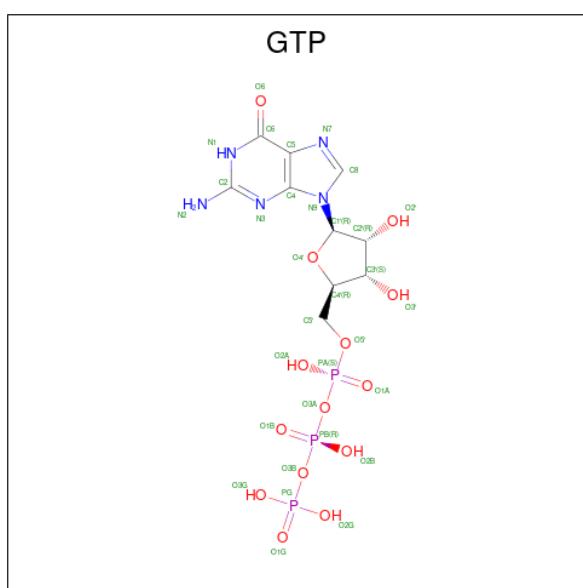
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	132	Total	C	N	O	S	0	1	0
			1080	669	195	212	4			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	4	ALA	-	expression tag	UNP P63043
E	14	ALA	CYS	engineered mutation	UNP P63043
E	20	TRP	PHE	engineered mutation	UNP P63043

- Molecule 4 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).

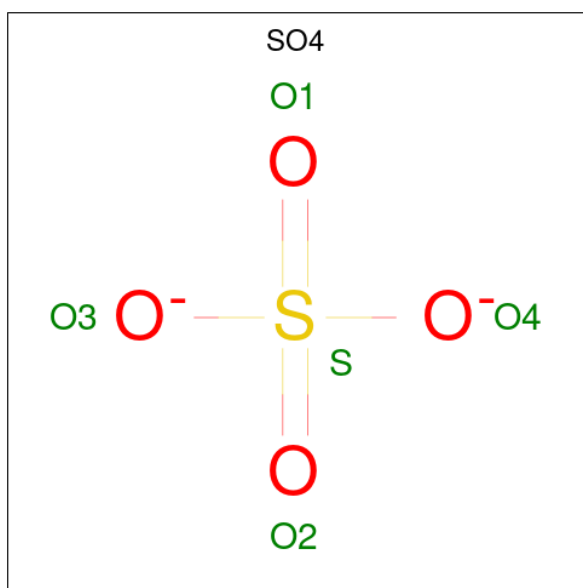


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
4	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

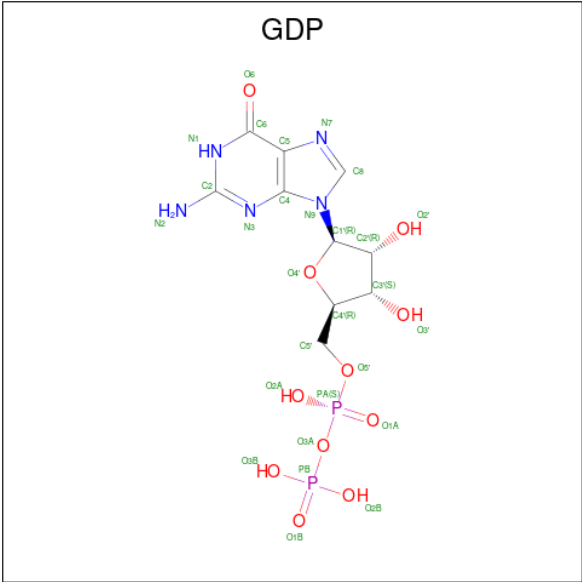
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	C	1	Total	Mg	0	0
			1	1		

- Molecule 6 is SULFATE ION (CCD ID: SO4) (formula: O_4S).



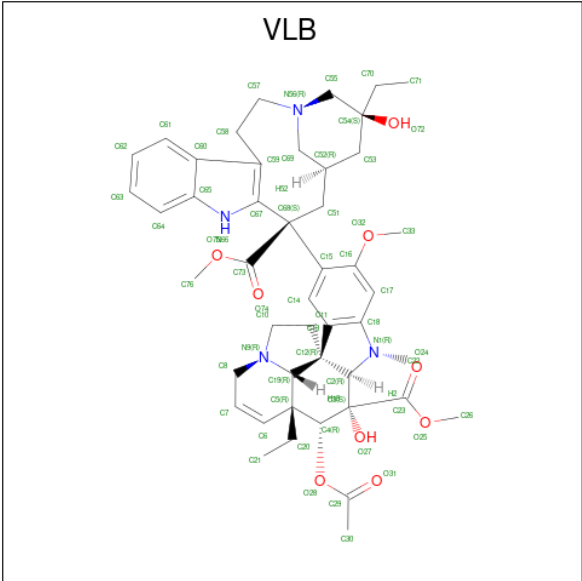
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	B	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

- Molecule 7 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

- Molecule 8 is (2ALPHA,2'BETA,3BETA,4ALPHA,5BETA)-VINCALEUKOBLASTINE (CCD ID: VLB) (formula: C₄₆H₅₈N₄O₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	C	1	Total	C	N	O	0	0
			59	46	4	9		

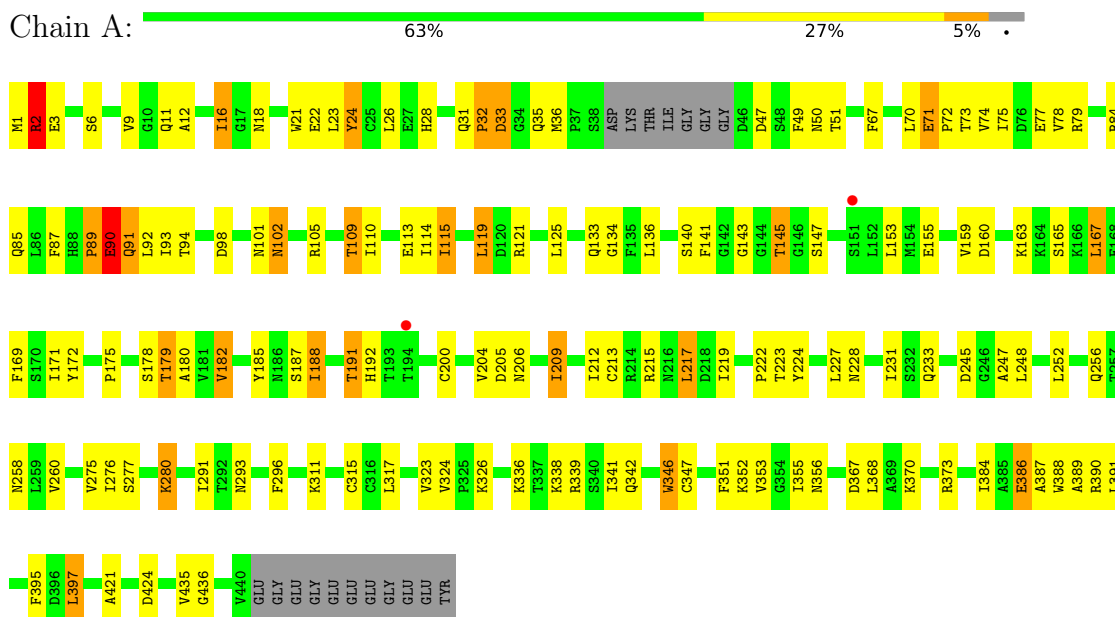
- Molecule 9 is water.

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

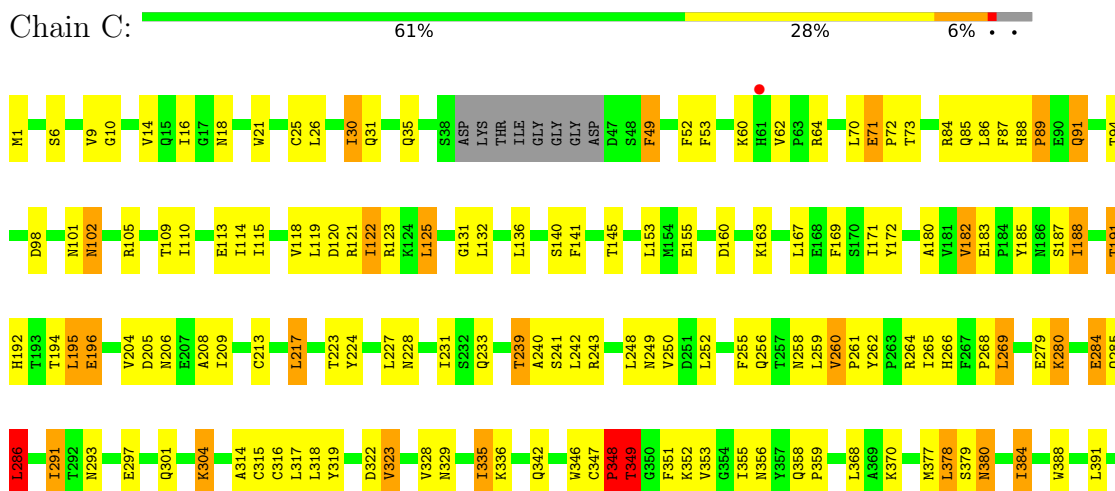
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Tubulin alpha chain



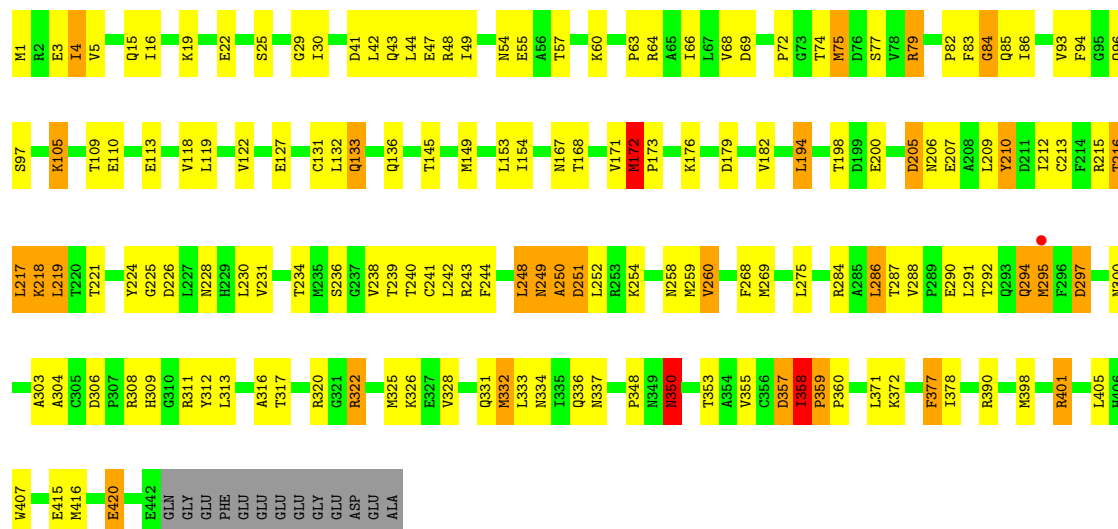
• Molecule 1: Tubulin alpha chain





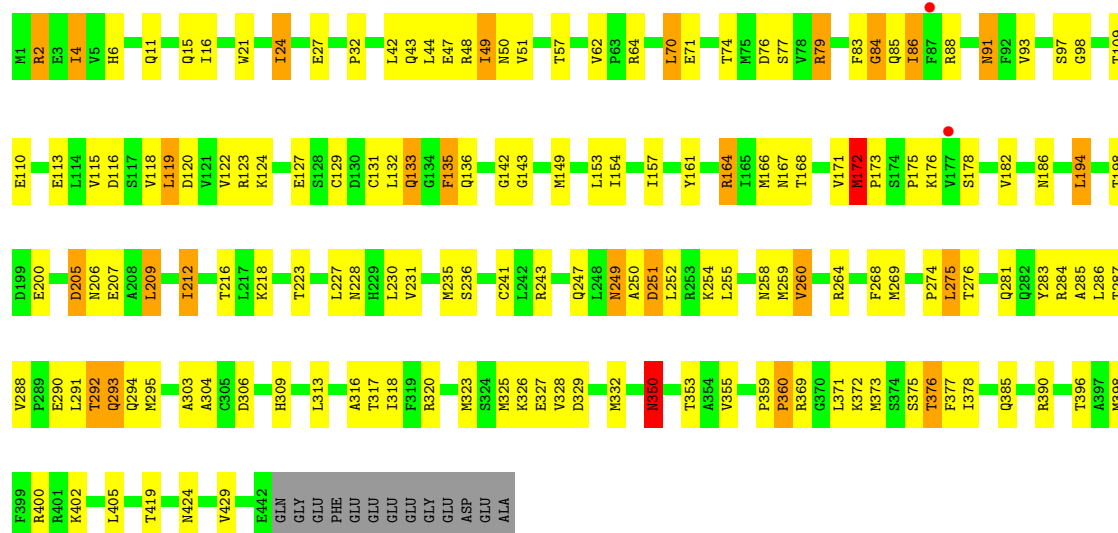
• Molecule 2: Tubulin beta chain

Chain B: 61% 29% 7% . .



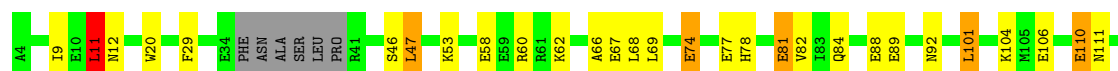
• Molecule 2: Tubulin beta chain

Chain D: 61% 30% 6% . .



• Molecule 3: Stathmin-4

Chain E: 68% 21% . . 7%





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	64.69Å 129.68Å 252.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	43.06 – 3.47 43.06 – 3.47	Depositor EDS
% Data completeness (in resolution range)	(Not available) (43.06-3.47) 99.1 (43.06-3.47)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 3.48Å)	Xtriage
Refinement program	BUSTER 2.8.0	Depositor
R, R_{free}	0.213 , 0.253 0.232 , 0.281	Depositor DCC
R_{free} test set	1424 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	119.2	Xtriage
Anisotropy	0.677	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 206.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	14918	wwPDB-VP
Average B, all atoms (Å ²)	174.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.88% 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: VLB, MG, SO4, GTP, GDP

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	0.74	0/3479	1.41	15/4723 (0.3%)
1	C	0.73	1/3495 (0.0%)	1.47	18/4745 (0.4%)
2	B	0.74	1/3485 (0.0%)	1.43	21/4720 (0.4%)
2	D	0.76	0/3471	1.42	20/4701 (0.4%)
3	E	0.76	0/1095	1.47	2/1459 (0.1%)
All	All	0.74	2/15025 (0.0%)	1.43	76/20348 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	209	ILE	CG1-CD1	-5.54	1.30	1.51
2	B	288	VAL	CA-CB	5.29	1.56	1.54

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	256	GLN	N-CA-C	-8.74	101.83	111.36
1	C	120[A]	ASP	N-CA-C	-8.33	105.12	114.62
1	C	120[B]	ASP	N-CA-C	-8.33	105.12	114.62
2	D	76	ASP	CA-CB-CG	7.46	120.06	112.60
3	E	124	GLN	N-CA-C	-7.45	106.13	114.62
2	B	219	LEU	N-CA-C	7.35	120.39	108.34
1	C	348	PRO	CA-C-N	7.22	134.70	121.70
1	C	348	PRO	C-N-CA	7.22	134.70	121.70
2	B	206	ASN	CA-CB-CG	7.11	119.71	112.60
2	B	260	VAL	N-CA-C	6.91	114.39	107.55
2	D	260	VAL	N-CA-C	6.87	114.35	107.55
2	B	249	ASN	N-CA-C	-6.82	102.08	110.61
2	D	4	ILE	N-CA-C	6.81	117.71	108.17
1	A	89	PRO	N-CA-C	6.65	126.17	112.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	131	GLU	N-CA-C	-6.57	107.13	114.62
2	B	334	ASN	CA-CB-CG	6.38	118.98	112.60
1	C	346	TRP	N-CA-C	6.29	120.21	112.54
2	B	216	THR	N-CA-C	-6.23	103.87	112.03
2	D	172	MET	CB-CA-C	6.16	119.19	109.27
2	B	287	THR	CA-C-N	6.12	126.30	120.43
2	B	287	THR	C-N-CA	6.12	126.30	120.43
2	D	86	ILE	N-CA-C	6.09	116.83	110.62
2	B	172	MET	CB-CA-C	6.09	119.07	109.27
2	B	251	ASP	CA-CB-CG	5.96	118.56	112.60
1	C	428	LEU	CD1-CG-CD2	5.93	123.86	110.80
2	D	350	ASN	CA-CB-CG	5.93	118.53	112.60
1	A	90	GLU	CA-C-N	5.89	128.98	120.38
1	A	90	GLU	C-N-CA	5.89	128.98	120.38
2	B	210	TYR	N-CA-C	-5.84	104.83	111.14
2	D	173	PRO	N-CA-C	5.82	120.42	111.57
1	A	115	ILE	N-CA-C	5.82	116.28	110.23
2	B	173	PRO	N-CA-C	5.79	120.38	111.57
1	A	390	ARG	CA-C-N	5.79	128.31	120.44
1	A	390	ARG	C-N-CA	5.79	128.31	120.44
2	D	251	ASP	CA-CB-CG	5.75	118.36	112.60
2	B	337	ASN	CA-CB-CG	5.71	118.31	112.60
2	B	350	ASN	CA-CB-CG	5.71	118.31	112.60
2	D	135	PHE	CA-CB-CG	5.66	119.46	113.80
2	B	218	LYS	N-CA-C	5.59	122.70	110.80
1	A	32	PRO	N-CA-C	5.57	123.95	112.47
1	A	145	THR	N-CA-C	-5.54	102.28	110.48
1	C	115	ILE	N-CA-C	5.51	116.15	110.36
1	C	49	PHE	CA-CB-CG	5.50	119.30	113.80
1	C	121	ARG	N-CA-C	-5.50	106.41	113.23
1	C	21	TRP	CA-C-N	5.49	127.64	120.28
1	C	21	TRP	C-N-CA	5.49	127.64	120.28
2	D	205	ASP	CA-CB-CG	5.44	118.04	112.60
1	C	86	LEU	N-CA-C	-5.43	106.61	113.18
2	D	120	ASP	CA-CB-CG	5.40	118.00	112.60
1	A	276	ILE	N-CA-C	5.39	116.34	108.53
2	D	325	MET	CA-C-N	5.36	127.46	120.28
2	D	325	MET	C-N-CA	5.36	127.46	120.28
2	B	294	GLN	N-CA-C	5.27	116.88	111.03
1	A	24	TYR	N-CA-C	-5.26	105.72	113.61
2	B	205	ASP	CA-CB-CG	5.21	117.81	112.60
2	D	376	THR	CB-CA-C	5.21	118.48	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	89	PRO	CA-C-N	5.20	128.62	120.82
1	C	89	PRO	C-N-CA	5.20	128.62	120.82
1	C	347	CYS	N-CA-C	5.20	121.31	109.81
2	B	85	GLN	CA-C-N	5.16	127.53	120.46
2	B	85	GLN	C-N-CA	5.16	127.53	120.46
2	D	235	MET	CA-C-N	5.16	127.46	120.65
2	D	235	MET	C-N-CA	5.16	127.46	120.65
1	C	91	GLN	N-CA-C	5.14	119.41	113.18
2	B	357	ASP	N-CA-C	5.13	118.68	112.93
2	D	329	ASP	CA-C-N	5.13	127.11	120.44
2	D	329	ASP	C-N-CA	5.13	127.11	120.44
1	C	85	GLN	N-CA-C	5.09	119.08	112.86
1	A	386	GLU	CA-C-N	5.08	131.25	121.54
1	A	386	GLU	C-N-CA	5.08	131.25	121.54
2	D	236	SER	CA-C-N	5.08	125.72	120.03
2	D	236	SER	C-N-CA	5.08	125.72	120.03
2	B	358	ILE	N-CA-CB	5.08	118.32	111.21
1	A	389	ALA	CA-C-N	5.06	127.02	120.44
1	A	389	ALA	C-N-CA	5.06	127.02	120.44
1	A	346	TRP	N-CA-C	5.03	116.84	111.36

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	3399	0	3312	56	0
1	C	3408	0	3322	64	0
2	B	3400	0	3266	75	0
2	D	3394	0	3268	71	0
3	E	1080	0	1077	10	0
4	A	32	0	12	4	0
4	C	32	0	12	3	0
5	A	1	0	0	0	0
5	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	10	0	0	0	0
6	B	5	0	0	0	0
6	D	10	0	0	0	0
7	B	28	0	12	0	0
7	D	28	0	12	2	0
8	C	59	0	58	13	0
9	A	5	0	0	0	0
9	B	3	0	0	0	0
9	C	13	0	0	0	0
9	D	9	0	0	0	0
9	E	1	0	0	0	0
All	All	14918	0	14351	275	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 9.

All (275) 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)
8:C:503:VLB:H213	8:C:503:VLB:H303	1.50	0.93
2:B:212:ILE:HA	2:B:217:LEU:HG	1.55	0.86
2:B:221:THR:HA	8:C:503:VLB:H761	1.61	0.83
8:C:503:VLB:H582	8:C:503:VLB:H511	1.64	0.78
2:B:5:VAL:HG12	2:B:64:ARG:HG2	1.67	0.77
2:D:62:VAL:HG21	2:D:88:ARG:HG3	1.68	0.76
2:D:2:ARG:HB2	2:D:131:CYS:HB3	1.67	0.76
2:D:317:THR:HG22	2:D:377:PHE:HD1	1.52	0.74
1:C:259:LEU:HD21	1:C:378:LEU:HB3	1.71	0.73
1:A:180:ALA:HA	2:B:258:ASN:HD21	1.53	0.73
2:B:359:PRO:HB2	2:B:360:PRO:CD	2.18	0.73
2:D:212:ILE:HD11	2:D:230:LEU:HD22	1.72	0.71
1:C:206:ASN:HD21	4:C:501:GTP:HN22	1.38	0.70
1:A:206:ASN:HD21	4:A:501:GTP:HN22	1.38	0.69
2:B:359:PRO:HB2	2:B:360:PRO:HD2	1.74	0.69
1:A:167:LEU:HD21	1:A:252:LEU:HB2	1.75	0.68
2:D:21:TRP:HA	2:D:24:ILE:HG22	1.75	0.68
1:C:213:CYS:HA	1:C:217:LEU:HB2	1.77	0.66
2:D:320:ARG:HB3	2:D:359:PRO:HA	1.76	0.66
2:B:407:TRP:HZ2	1:C:260:VAL:HG13	1.62	0.65
2:B:297:ASP:HA	2:B:308:ARG:HH12	1.62	0.64
2:B:248:LEU:HG	2:B:249:ASN:H	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:11:GLN:HE21	2:D:15:GLN:HE22	1.47	0.63
2:B:228:ASN:HA	2:B:231:VAL:HG12	1.81	0.63
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.79	0.63
2:B:1:MET:N	2:B:131:CYS:SG	2.72	0.63
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.81	0.62
8:C:503:VLB:H332	8:C:503:VLB:H512	1.80	0.62
1:C:101:ASN:HD22	1:C:180:ALA:HB2	1.64	0.62
1:A:70:LEU:HD23	1:A:110:ILE:HG23	1.81	0.61
1:C:25:CYS:HB2	1:C:30:ILE:HB	1.83	0.61
2:B:216:THR:H	2:B:217:LEU:HD22	1.66	0.60
2:D:320:ARG:HE	2:D:360:PRO:HG3	1.65	0.60
2:D:157:ILE:HG13	2:D:166:MET:HE1	1.84	0.60
1:C:191:THR:HG21	1:C:388:TRP:CH2	2.36	0.60
2:D:133:GLN:HG2	2:D:252:LEU:HB2	1.83	0.59
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.82	0.59
1:A:87:PHE:HB3	1:A:91:GLN:HG3	1.83	0.59
1:A:101:ASN:HD22	1:A:180:ALA:HB2	1.66	0.59
3:E:11:LEU:H	3:E:20:TRP:HA	1.68	0.59
2:B:210:TYR:HE2	8:C:503:VLB:H333	1.67	0.59
1:C:241:SER:HA	1:C:249:ASN:HD21	1.66	0.59
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.84	0.58
2:D:209:LEU:HB3	2:D:230:LEU:HD11	1.86	0.58
1:C:239:THR:O	1:C:241:SER:N	2.36	0.58
1:A:2:ARG:HB2	1:A:133[A]:GLN:HE21	1.67	0.57
1:C:262:TYR:HB2	1:C:265:ILE:HD12	1.86	0.57
1:A:247:ALA:HB1	3:E:12:ASN:HB2	1.85	0.57
2:B:172:MET:CE	2:B:390:ARG:HH22	2.18	0.57
2:B:401:ARG:HH11	2:B:401:ARG:HB3	1.69	0.57
2:D:172:MET:CE	2:D:390:ARG:HH22	2.18	0.57
1:C:208:ALA:HB2	1:C:304:LYS:HG2	1.88	0.56
8:C:503:VLB:H691	8:C:503:VLB:C59	2.35	0.56
1:A:191:THR:HG21	1:A:388:TRP:CH2	2.41	0.56
2:D:142:GLY:HA3	7:D:501:GDP:H4'	1.88	0.56
2:D:133:GLN:HE21	2:D:252:LEU:H	1.53	0.56
1:A:33:ASP:HA	1:A:85:GLN:HG3	1.88	0.55
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.88	0.55
2:B:306:ASP:HB3	2:B:309:HIS:HB2	1.88	0.55
2:D:21:TRP:HA	2:D:24:ILE:CG2	2.37	0.55
1:A:28:HIS:CD2	1:A:49:PHE:HB2	2.42	0.55
2:B:79:ARG:HA	2:B:84:GLY:HA3	1.89	0.55
2:B:172:MET:HE3	2:B:390:ARG:HH22	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ILE:HD11	1:A:231:ILE:HG13	1.89	0.54
1:A:11:GLN:HG3	1:A:74:VAL:HG11	1.90	0.54
2:B:96:GLN:HE22	1:C:1:MET:HE3	1.73	0.54
1:A:28:HIS:HB3	1:A:36:MET:HE3	1.87	0.54
1:A:213:CYS:SG	1:A:222:PRO:HG3	2.48	0.53
2:D:172:MET:HE3	2:D:390:ARG:HH22	1.72	0.53
1:A:217:LEU:HA	1:A:277:SER:HB3	1.89	0.53
1:C:87:PHE:HB2	1:C:91:GLN:NE2	2.23	0.53
2:D:318:ILE:HB	2:D:376:THR:HG23	1.91	0.53
2:D:249:ASN:HB2	2:D:255:LEU:HA	1.91	0.52
1:A:67:PHE:HB2	1:A:92:LEU:HD22	1.91	0.52
2:B:86:ILE:H	2:B:86:ILE:HD12	1.74	0.52
2:B:407:TRP:CZ2	1:C:260:VAL:HG13	2.43	0.52
2:B:241:CYS:SG	2:B:248:LEU:HD11	2.49	0.52
2:D:116:ASP:HA	2:D:119:LEU:HG	1.92	0.52
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.90	0.52
1:C:196:GLU:CD	1:C:196:GLU:H	2.18	0.52
2:D:24:ILE:HD11	2:D:243:ARG:HD3	1.91	0.51
2:D:182:VAL:HA	2:D:398:MET:HE1	1.92	0.51
1:A:93:ILE:HD11	1:A:121:ARG:HG2	1.92	0.51
1:C:206:ASN:ND2	4:C:501:GTP:HN22	2.07	0.51
1:A:206:ASN:ND2	4:A:501:GTP:HN22	2.08	0.51
2:B:5:VAL:HG22	2:B:132:LEU:HD11	1.93	0.51
2:D:205:ASP:HB3	2:D:303:ALA:HA	1.93	0.51
2:D:241:CYS:HB2	2:D:250:ALA:HA	1.93	0.51
1:C:204:VAL:HG11	1:C:231:ILE:HD12	1.92	0.51
1:A:397:LEU:HD23	2:B:348:PRO:HG3	1.93	0.50
1:C:318:LEU:HD13	1:C:378:LEU:HD23	1.94	0.50
1:A:159:VAL:HG11	3:E:47:LEU:HB2	1.94	0.50
1:A:204:VAL:HG11	1:A:231:ILE:HD12	1.93	0.50
2:D:161:TYR:HB3	2:D:164:ARG:HG3	1.92	0.50
2:D:251:ASP:HB3	2:D:254:LYS:HB2	1.93	0.50
2:B:269:MET:HG3	2:B:303:ALA:HB3	1.93	0.50
1:C:31:GLN:HB2	1:C:35:GLN:HB2	1.93	0.50
1:A:175:PRO:HA	1:A:179:THR:HG21	1.93	0.50
1:A:140:SER:HA	1:A:171:ILE:HB	1.94	0.50
2:B:234:THR:O	2:B:238:VAL:HG23	2.11	0.50
1:C:242:LEU:HD11	1:C:252:LEU:HB3	1.94	0.50
2:D:396:THR:O	2:D:400:ARG:HB2	2.11	0.50
1:A:90:GLU:C	1:A:121:ARG:HH12	2.20	0.50
2:B:205:ASP:HB3	2:B:303:ALA:HA	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:153:LEU:O	2:D:157:ILE:HG12	2.11	0.49
2:B:149:MET:HE2	2:B:153:LEU:HD21	1.93	0.49
2:B:251:ASP:HB3	2:B:254:LYS:HB2	1.94	0.49
2:D:149:MET:HE2	2:D:153:LEU:HD21	1.93	0.49
2:B:63:PRO:HD3	2:B:86:ILE:HG22	1.95	0.49
2:B:66:ILE:HD13	2:B:122:VAL:HG12	1.94	0.49
2:B:286:LEU:HD11	2:B:291:LEU:HD13	1.95	0.49
2:D:175:PRO:HA	2:D:178:SER:HB3	1.95	0.49
2:B:41:ASP:HA	2:B:44:LEU:HD12	1.95	0.49
2:B:182:VAL:HA	2:B:398:MET:HE1	1.94	0.49
1:C:259:LEU:HD11	1:C:316:CYS:HB2	1.95	0.49
1:A:105:ARG:HA	1:A:109:THR:HG23	1.95	0.48
2:B:236:SER:HA	2:B:239:THR:OG1	2.13	0.48
1:C:269:LEU:HD12	1:C:384:ILE:HD12	1.96	0.48
2:D:2:ARG:HB2	2:D:131:CYS:CB	2.41	0.48
2:D:79:ARG:HA	2:D:84:GLY:HA3	1.94	0.48
3:E:66:ALA:HA	3:E:69:LEU:HD12	1.94	0.48
1:C:70:LEU:HD22	1:C:145:THR:HG22	1.96	0.48
2:D:316:ALA:HB3	2:D:378:ILE:HB	1.94	0.48
8:C:503:VLB:H511	8:C:503:VLB:C58	2.40	0.48
1:C:136:LEU:HD22	1:C:169:PHE:HE1	1.79	0.47
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.96	0.47
1:A:143:GLY:O	1:A:147:SER:OG	2.32	0.47
2:D:291:LEU:HG	2:D:375:SER:HB2	1.95	0.47
2:B:172:MET:HE1	2:B:205:ASP:OD1	2.15	0.47
2:B:4:ILE:HD11	2:B:252:LEU:HD13	1.96	0.47
1:C:140:SER:HA	1:C:171:ILE:HB	1.97	0.47
1:C:328:VAL:HG21	1:C:355:ILE:HD11	1.96	0.47
1:C:356:ASN:HD21	1:C:358:GLN:HB2	1.80	0.47
2:B:133:GLN:HE21	2:B:252:LEU:H	1.63	0.47
2:B:225:GLY:HA2	2:B:228:ASN:HB2	1.97	0.46
2:B:77:SER:H	2:B:79:ARG:HH21	1.64	0.46
2:B:316:ALA:HB3	2:B:378:ILE:HB	1.96	0.46
1:C:206:ASN:HD21	4:C:501:GTP:N2	2.10	0.46
1:A:2:ARG:HG3	1:A:51:THR:HG22	1.97	0.46
2:B:22:GLU:HB3	2:B:83:PHE:HB2	1.98	0.46
1:A:219:ILE:HD12	1:A:222:PRO:HB3	1.96	0.46
1:A:317:LEU:HB2	1:A:353:VAL:HG13	1.98	0.46
2:D:172:MET:HE1	2:D:205:ASP:OD1	2.16	0.45
7:D:501:GDP:H5''	7:D:501:GDP:H8	1.80	0.45
2:B:259:MET:HE2	2:B:378:ILE:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:THR:HG21	2:B:332:MET:HE2	1.98	0.45
1:A:21:TRP:HA	1:A:24:TYR:HB2	1.97	0.45
2:D:264:ARG:NH2	2:D:424:ASN:O	2.43	0.45
1:A:145:THR:O	4:A:501:GTP:O2B	2.35	0.45
2:B:44:LEU:O	2:B:49:ILE:HG13	2.17	0.45
2:B:48:ARG:HH22	2:B:250:ALA:HB1	1.82	0.45
1:C:314:ALA:HB3	1:C:380:ASN:H	1.82	0.45
2:D:77:SER:H	2:D:79:ARG:HH21	1.65	0.45
1:C:329:ASN:HD21	8:C:503:VLB:H66	1.62	0.45
1:A:167:LEU:HD12	1:A:200:CYS:HB3	1.98	0.45
2:B:243:ARG:HD2	2:B:243:ARG:N	2.32	0.45
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.99	0.45
2:D:216:THR:HG21	2:D:275:LEU:HD13	1.99	0.45
1:C:88:HIS:HB2	1:C:89:PRO:HD2	1.98	0.45
1:C:123:ARG:C	1:C:125:LEU:H	2.24	0.45
2:D:323:MET:HE2	2:D:373:MET:HG2	1.98	0.45
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.99	0.44
1:A:209:ILE:HD11	1:A:227:LEU:HG	2.00	0.44
1:A:311:LYS:HD2	1:A:436:GLY:HA2	1.99	0.44
2:D:143:GLY:O	2:D:186:ASN:ND2	2.50	0.44
2:D:227:LEU:O	2:D:230:LEU:HG	2.17	0.44
2:B:350:ASN:H	2:B:350:ASN:HD22	1.65	0.44
2:D:205:ASP:CB	2:D:303:ALA:HA	2.48	0.44
1:C:286:LEU:HD21	1:C:291:ILE:HG23	1.99	0.44
1:C:319:TYR:HB2	1:C:355:ILE:HG12	1.99	0.44
2:D:176:LYS:HD2	2:D:207:GLU:HG3	1.98	0.44
2:D:274:PRO:HD2	2:D:371:LEU:HD23	1.99	0.44
2:B:176:LYS:HD2	2:B:207:GLU:HG3	1.98	0.44
2:D:350:ASN:HD22	2:D:350:ASN:H	1.66	0.44
2:B:238:VAL:HG22	2:B:378:ILE:HD11	1.99	0.44
3:E:106:GLU:O	3:E:110:GLU:HG3	2.18	0.44
2:B:68:VAL:HG22	2:B:93:VAL:HG13	2.00	0.44
2:D:292:THR:HG22	2:D:332:MET:HE2	1.99	0.44
2:B:350:ASN:HD22	2:B:350:ASN:N	2.16	0.44
1:A:31:GLN:O	1:A:33:ASP:N	2.51	0.43
2:B:312:TYR:CE2	2:B:377:PHE:HZ	2.36	0.43
1:C:239:THR:HB	1:C:243:ARG:HD3	2.01	0.43
2:D:228:ASN:HA	2:D:231:VAL:HB	2.00	0.43
2:B:205:ASP:CB	2:B:303:ALA:HA	2.48	0.43
1:C:10:GLY:O	1:C:14:VAL:HG22	2.18	0.43
2:B:322:ARG:HH12	2:B:325:MET:HE3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:32:PRO:HB3	2:D:83:PHE:HA	1.99	0.43
2:B:105:LYS:HG3	2:B:110:GLU:HG2	2.00	0.43
1:C:241:SER:HA	1:C:249:ASN:ND2	2.32	0.43
3:E:74:GLU:HA	3:E:77:GLU:HG2	2.00	0.43
1:A:136:LEU:HD22	1:A:169:PHE:HE1	1.84	0.43
2:B:248:LEU:CG	2:B:249:ASN:H	2.30	0.43
1:C:195:LEU:HD12	1:C:264:ARG:HG2	2.00	0.43
8:C:503:VLB:H713	8:C:503:VLB:H692	2.01	0.43
2:B:25:SER:HB3	2:B:30:ILE:HG13	2.00	0.43
2:B:48:ARG:NH2	2:B:250:ALA:HB1	2.34	0.43
2:D:49:ILE:C	2:D:51:VAL:H	2.27	0.43
2:D:115:VAL:HG22	2:D:119:LEU:HD23	2.01	0.43
1:C:180:ALA:O	1:C:183:GLU:HG3	2.19	0.43
1:C:180:ALA:HA	2:D:258:ASN:HD21	1.84	0.43
1:C:319:TYR:HB3	1:C:323:VAL:HG21	2.01	0.43
1:C:88:HIS:HB2	1:C:89:PRO:CD	2.49	0.43
1:C:118:VAL:O	1:C:122:ILE:HB	2.18	0.43
1:A:134:GLY:HA3	1:A:165:SER:O	2.19	0.43
1:C:228:ASN:HA	1:C:231:ILE:HG12	2.01	0.43
1:C:358:GLN:HA	1:C:359:PRO:HD3	1.95	0.43
1:C:378:LEU:HD13	1:C:378:LEU:HA	1.85	0.43
1:A:192:HIS:CG	1:A:421:ALA:HA	2.54	0.42
1:C:155:GLU:HB3	3:E:101:LEU:HD11	2.01	0.42
1:C:192:HIS:CG	1:C:421:ALA:HA	2.54	0.42
2:D:350:ASN:HD22	2:D:350:ASN:N	2.17	0.42
3:E:78:HIS:O	3:E:81:GLU:HG3	2.19	0.42
1:C:255:PHE:HA	1:C:258:ASN:HD22	1.83	0.42
2:D:259:MET:HE2	2:D:378:ILE:HG22	2.01	0.42
1:A:87:PHE:C	1:A:91:GLN:HE21	2.28	0.42
2:D:259:MET:HB3	2:D:268:PHE:CE2	2.53	0.42
2:D:286:LEU:HD22	2:D:290:GLU:HB3	2.00	0.42
1:A:12:ALA:O	1:A:16:ILE:HB	2.20	0.42
1:A:102:ASN:HD22	1:A:105:ARG:H	1.67	0.42
2:D:200:GLU:HB2	2:D:268:PHE:HE1	1.84	0.42
2:B:176:LYS:O	8:C:503:VLB:H222	2.20	0.42
1:C:102:ASN:HD22	1:C:105:ARG:H	1.67	0.42
2:D:62:VAL:HG23	2:D:86:ILE:O	2.19	0.42
1:A:91:GLN:HA	1:A:121:ARG:NH1	2.35	0.42
1:A:206:ASN:HD21	4:A:501:GTP:N2	2.10	0.42
1:A:28:HIS:HD2	1:A:49:PHE:HB2	1.84	0.42
2:B:240:THR:HG21	2:B:320:ARG:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:292:THR:HG21	2:B:331:GLN:HB3	2.01	0.42
2:D:172:MET:SD	2:D:205:ASP:HA	2.60	0.42
1:A:91:GLN:CD	1:A:92:LEU:HG	2.45	0.42
1:A:228:ASN:HA	1:A:231:ILE:HG12	2.01	0.42
8:C:503:VLB:H582	8:C:503:VLB:C51	2.44	0.42
2:D:2:ARG:NH2	2:D:132:LEU:H	2.18	0.42
1:A:182:VAL:O	1:A:185:TYR:HB2	2.20	0.42
2:D:132:LEU:HD23	2:D:164:ARG:HD3	2.01	0.42
2:D:293:GLN:C	2:D:295:MET:H	2.27	0.42
2:B:19:LYS:HA	2:B:22:GLU:HG2	2.00	0.41
2:B:200:GLU:HB2	2:B:268:PHE:HE2	1.84	0.41
1:C:182:VAL:O	1:C:185:TYR:HB2	2.20	0.41
2:B:240:THR:HA	2:B:244:PHE:HD1	1.85	0.41
2:B:401:ARG:HH21	1:C:435:VAL:HG12	1.84	0.41
1:C:70:LEU:HD23	1:C:110:ILE:HB	2.02	0.41
2:D:70:LEU:HB3	2:D:98:GLY:HA2	2.02	0.41
3:E:58:GLU:HG2	3:E:62:LYS:HD2	2.03	0.41
1:A:79:ARG:HG3	1:A:92:LEU:HD12	2.02	0.41
2:B:69:ASP:HB3	2:B:94:PHE:CD1	2.55	0.41
2:B:72:PRO:HA	2:B:75:MET:HG2	2.02	0.41
1:C:266:HIS:O	1:C:268:PRO:HD3	2.20	0.41
8:C:503:VLB:H212	8:C:503:VLB:N1	2.36	0.41
2:D:306:ASP:HB3	2:D:309:HIS:CG	2.55	0.41
2:D:136:GLN:HA	2:D:167:ASN:O	2.21	0.41
2:B:416:MET:O	2:B:420:GLU:HG3	2.21	0.41
2:D:129:CYS:HB3	2:D:131:CYS:O	2.21	0.41
2:B:136:GLN:HA	2:B:167:ASN:O	2.21	0.41
1:C:188:ILE:HD13	1:C:395:PHE:HB2	2.02	0.41
8:C:503:VLB:C14	8:C:503:VLB:H52	2.51	0.41
2:B:275:LEU:HD11	2:B:300:ASN:HA	2.03	0.41
1:C:335:ILE:HD11	1:C:351:PHE:CZ	2.56	0.41
1:A:346:TRP:HB3	3:E:29:PHE:HD2	1.85	0.41
2:B:194:LEU:HD23	2:B:198:THR:HG21	2.02	0.41
2:B:259:MET:HB3	2:B:268:PHE:CE1	2.56	0.41
1:C:224:TYR:HA	1:C:227:LEU:HB2	2.03	0.41
2:D:27:GLU:CD	2:D:320:ARG:HH22	2.28	0.41
2:D:88:ARG:HB2	2:D:91:ASN:OD1	2.21	0.41
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.39	0.41
1:A:188:ILE:HD13	1:A:395:PHE:HB2	2.02	0.40
1:C:259:LEU:O	1:C:261:PRO:HD3	2.21	0.40
1:C:348:PRO:HA	1:C:349:THR:C	2.47	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:194:LEU:HD23	2:D:198:THR:HG21	2.02	0.40
1:A:115:ILE:O	1:A:119:LEU:HD13	2.22	0.40
2:B:69:ASP:HA	2:B:145:THR:HG21	2.03	0.40
2:D:43:GLN:C	2:D:47:GLU:H	2.30	0.40
1:A:224:TYR:HA	1:A:227:LEU:HB2	2.03	0.40
2:B:172:MET:SD	2:B:205:ASP:HA	2.61	0.40
1:C:285:GLN:O	1:C:286:LEU:HB3	2.22	0.40

There are no symmetry-related clashes.

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	430/451 (95%)	374 (87%)	43 (10%)	13 (3%)	3	25
1	C	432/451 (96%)	382 (88%)	35 (8%)	15 (4%)	3	22
2	B	432/445 (97%)	380 (88%)	38 (9%)	14 (3%)	3	24
2	D	431/445 (97%)	385 (89%)	33 (8%)	13 (3%)	3	25
3	E	129/142 (91%)	114 (88%)	13 (10%)	2 (2%)	7	36
All	All	1854/1934 (96%)	1635 (88%)	162 (9%)	57 (3%)	3	25

All (57) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	32	PRO
1	A	89	PRO
1	A	179	THR
1	A	245	ASP
2	B	215	ARG
2	B	359	PRO
1	C	240	ALA

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Mol	Chain	Res	Type
1	C	379	SER
1	C	437	VAL
2	D	369	ARG
3	E	11	LEU
1	A	2	ARG
1	A	3	GLU
1	A	178	SER
2	B	82	PRO
2	B	109	THR
2	B	224	TYR
2	B	372	LYS
1	C	109	THR
1	C	239	THR
1	C	284	GLU
1	C	286	LEU
1	C	322	ASP
1	C	348	PRO
2	D	84	GLY
2	D	97	SER
2	D	109	THR
1	A	280	LYS
2	B	84	GLY
2	B	295	MET
2	D	281	GLN
2	D	285	ALA
2	B	57	THR
2	B	286	LEU
2	B	304	ALA
2	B	358	ILE
1	C	280	LYS
2	D	50	ASN
2	D	249	ASN
2	D	283	TYR
2	D	294	GLN
2	D	304	ALA
2	D	360	PRO
3	E	46	SER
1	A	338	LYS
1	A	387	ALA
2	B	250	ALA
1	C	342	GLN
1	C	349	THR

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Mol	Chain	Res	Type
2	D	57	THR
1	A	260	VAL
1	C	438	ASP
1	A	72	PRO
1	C	72	PRO
1	C	131	GLY
2	B	29	GLY
1	A	212	ILE

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%)	296 (80%)	72 (20%)	1	8
1	C	370/379 (98%)	305 (82%)	65 (18%)	2	11
2	B	375/385 (97%)	315 (84%)	60 (16%)	2	14
2	D	374/385 (97%)	317 (85%)	57 (15%)	3	16
3	E	114/125 (91%)	91 (80%)	23 (20%)	1	7
All	All	1601/1653 (97%)	1324 (83%)	277 (17%)	2	12

All (277) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	2	ARG
1	A	6	SER
1	A	9	VAL
1	A	16	ILE
1	A	18	ASN
1	A	22	GLU
1	A	23	LEU
1	A	26	LEU
1	A	33	ASP
1	A	35	GLN

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Mol	Chain	Res	Type
1	A	47	ASP
1	A	50	ASN
1	A	71	GLU
1	A	73	THR
1	A	75	ILE
1	A	77	GLU
1	A	78	VAL
1	A	84	ARG
1	A	90	GLU
1	A	91	GLN
1	A	94	THR
1	A	102	ASN
1	A	109	THR
1	A	113	GLU
1	A	114	ILE
1	A	119	LEU
1	A	125	LEU
1	A	141	PHE
1	A	153	LEU
1	A	155	GLU
1	A	160	ASP
1	A	163	LYS
1	A	167	LEU
1	A	182	VAL
1	A	188	ILE
1	A	191	THR
1	A	209	ILE
1	A	215	ARG
1	A	217	LEU
1	A	223	THR
1	A	233	GLN
1	A	248	LEU
1	A	256	GLN
1	A	258	ASN
1	A	275	VAL
1	A	280	LYS
1	A	291	ILE
1	A	293	ASN
1	A	296	PHE
1	A	315	CYS
1	A	323	VAL
1	A	324	VAL

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Mol	Chain	Res	Type
1	A	326	LYS
1	A	336	LYS
1	A	339	ARG
1	A	341	ILE
1	A	342	GLN
1	A	347	CYS
1	A	351	PHE
1	A	352	LYS
1	A	355	ILE
1	A	356	ASN
1	A	367	ASP
1	A	368	LEU
1	A	370	LYS
1	A	373	ARG
1	A	384	ILE
1	A	386	GLU
1	A	397	LEU
1	A	424	ASP
1	A	435	VAL
2	B	3	GLU
2	B	4	ILE
2	B	15	GLN
2	B	16	ILE
2	B	42	LEU
2	B	43	GLN
2	B	47	GLU
2	B	54	ASN
2	B	55	GLU
2	B	60	LYS
2	B	74	THR
2	B	75	MET
2	B	79	ARG
2	B	97	SER
2	B	105	LYS
2	B	113	GLU
2	B	118	VAL
2	B	119	LEU
2	B	127	GLU
2	B	133	GLN
2	B	154	ILE
2	B	168	THR
2	B	171	VAL

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Mol	Chain	Res	Type
2	B	172	MET
2	B	179	ASP
2	B	194	LEU
2	B	209	LEU
2	B	213	CYS
2	B	217	LEU
2	B	218	LYS
2	B	219	LEU
2	B	226	ASP
2	B	230	LEU
2	B	242	LEU
2	B	248	LEU
2	B	260	VAL
2	B	284	ARG
2	B	290	GLU
2	B	294	GLN
2	B	295	MET
2	B	297	ASP
2	B	311	ARG
2	B	313	LEU
2	B	322	ARG
2	B	326	LYS
2	B	328	VAL
2	B	332	MET
2	B	333	LEU
2	B	336	GLN
2	B	350	ASN
2	B	353	THR
2	B	355	VAL
2	B	357	ASP
2	B	358	ILE
2	B	371	LEU
2	B	377	PHE
2	B	401	ARG
2	B	405	LEU
2	B	415	GLU
2	B	420	GLU
1	C	6	SER
1	C	9	VAL
1	C	16	ILE
1	C	18	ASN
1	C	26	LEU

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Mol	Chain	Res	Type
1	C	30	ILE
1	C	49	PHE
1	C	52	PHE
1	C	53	PHE
1	C	60	LYS
1	C	62	VAL
1	C	64	ARG
1	C	71	GLU
1	C	73	THR
1	C	84	ARG
1	C	94	THR
1	C	102	ASN
1	C	113	GLU
1	C	114	ILE
1	C	119	LEU
1	C	122	ILE
1	C	125	LEU
1	C	132	LEU
1	C	141	PHE
1	C	153	LEU
1	C	160	ASP
1	C	163	LYS
1	C	167	LEU
1	C	182	VAL
1	C	188	ILE
1	C	191	THR
1	C	194	THR
1	C	195	LEU
1	C	196	GLU
1	C	217	LEU
1	C	223	THR
1	C	233	GLN
1	C	248	LEU
1	C	260	VAL
1	C	269	LEU
1	C	279	GLU
1	C	280	LYS
1	C	284	GLU
1	C	286	LEU
1	C	291	ILE
1	C	293	ASN
1	C	297	GLU

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Mol	Chain	Res	Type
1	C	301	GLN
1	C	304	LYS
1	C	315	CYS
1	C	317	LEU
1	C	323	VAL
1	C	335	ILE
1	C	336	LYS
1	C	349	THR
1	C	353	VAL
1	C	368	LEU
1	C	370	LYS
1	C	377	MET
1	C	378	LEU
1	C	380	ASN
1	C	384	ILE
1	C	397	LEU
1	C	424	ASP
1	C	428	LEU
2	D	2	ARG
2	D	4	ILE
2	D	16	ILE
2	D	24	ILE
2	D	42	LEU
2	D	44	LEU
2	D	48	ARG
2	D	49	ILE
2	D	64	ARG
2	D	70	LEU
2	D	71	GLU
2	D	74	THR
2	D	79	ARG
2	D	85	GLN
2	D	91	ASN
2	D	93	VAL
2	D	110	GLU
2	D	113	GLU
2	D	118	VAL
2	D	119	LEU
2	D	122	VAL
2	D	123	ARG
2	D	124	LYS
2	D	127	GLU

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Mol	Chain	Res	Type
2	D	133	GLN
2	D	135	PHE
2	D	154	ILE
2	D	164	ARG
2	D	168	THR
2	D	171	VAL
2	D	172	MET
2	D	194	LEU
2	D	206	ASN
2	D	209	LEU
2	D	212	ILE
2	D	218	LYS
2	D	223	THR
2	D	247	GLN
2	D	260	VAL
2	D	275	LEU
2	D	276	THR
2	D	284	ARG
2	D	287	THR
2	D	288	VAL
2	D	292	THR
2	D	293	GLN
2	D	313	LEU
2	D	326	LYS
2	D	327	GLU
2	D	328	VAL
2	D	350	ASN
2	D	353	THR
2	D	355	VAL
2	D	372	LYS
2	D	402	LYS
2	D	405	LEU
2	D	419	THR
3	E	9	ILE
3	E	11	LEU
3	E	47	LEU
3	E	53	LYS
3	E	60	ARG
3	E	67	GLU
3	E	68	LEU
3	E	74	GLU
3	E	81	GLU

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Mol	Chain	Res	Type
3	E	82	VAL
3	E	84	GLN
3	E	88	GLU
3	E	89	GLU
3	E	92	ASN
3	E	101	LEU
3	E	104	LYS
3	E	110	GLU
3	E	111	ASN
3	E	116	LEU
3	E	120	LEU
3	E	123	LEU
3	E	128	LYS
3	E	134	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	HIS
1	A	35	GLN
1	A	50	ASN
1	A	101	ASN
1	A	102	ASN
1	A	206	ASN
1	A	249	ASN
1	A	256	GLN
1	A	283	HIS
1	A	301	GLN
1	A	358	GLN
1	A	380	ASN
2	B	11	GLN
2	B	50	ASN
2	B	54	ASN
2	B	96	GLN
2	B	133	GLN
2	B	139	HIS
2	B	186	ASN
2	B	192	HIS
2	B	249	ASN
2	B	258	ASN
2	B	300	ASN
2	B	309	HIS

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Mol	Chain	Res	Type
2	B	331	GLN
2	B	339	ASN
2	B	350	ASN
2	B	380	ASN
2	B	424	ASN
2	B	433	GLN
1	C	8	HIS
1	C	50	ASN
1	C	85	GLN
1	C	101	ASN
1	C	102	ASN
1	C	128	GLN
1	C	206	ASN
1	C	226	ASN
1	C	249	ASN
1	C	293	ASN
1	C	356	ASN
2	D	15	GLN
2	D	59	ASN
2	D	85	GLN
2	D	133	GLN
2	D	139	HIS
2	D	186	ASN
2	D	192	HIS
2	D	247	GLN
2	D	258	ASN
2	D	300	ASN
2	D	331	GLN
2	D	334	ASN
2	D	336	GLN
2	D	350	ASN
2	D	380	ASN
2	D	424	ASN
2	D	433	GLN
3	E	12	ASN
3	E	90	ASN
3	E	91	ASN
3	E	115	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 2 are monoatomic - leaving 10 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	$\# Z > 2$
6	SO4	D	502	-	4,4,4	0.27	0	6,6,6	0.08	0
8	VLB	C	503	-	66,67,67	1.75	15 (22%)	82,108,108	2.43	26 (31%)
6	SO4	A	503	-	4,4,4	0.31	0	6,6,6	0.05	0
4	GTP	A	501	5	33,34,34	1.38	3 (9%)	50,54,54	1.67	8 (16%)
7	GDP	B	501	-	29,30,30	1.09	1 (3%)	45,47,47	1.67	8 (17%)
6	SO4	A	504	-	4,4,4	0.25	0	6,6,6	0.08	0
7	GDP	D	501	-	29,30,30	1.42	5 (17%)	45,47,47	1.73	7 (15%)
6	SO4	B	502	-	4,4,4	0.27	0	6,6,6	0.09	0
4	GTP	C	501	5	33,34,34	1.54	4 (12%)	50,54,54	1.73	10 (20%)
6	SO4	D	503	-	4,4,4	0.26	0	6,6,6	0.07	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
8	VLB	C	503	-	-	21/40/131/131	0/7/9/9
4	GTP	A	501	5	-	6/22/38/38	0/3/3/3
7	GDP	B	501	-	-	2/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	GDP	D	501	-	-	1/16/32/32	0/3/3/3
4	GTP	C	501	5	-	6/22/38/38	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	C	503	VLB	C5-C6	-5.18	1.42	1.51
8	C	503	VLB	C6-C7	4.80	1.41	1.32
4	C	501	GTP	PA-O3A	4.37	1.64	1.59
4	A	501	GTP	PA-O3A	3.73	1.63	1.59
8	C	503	VLB	C8-C7	-3.66	1.39	1.49
4	C	501	GTP	PB-O3B	3.65	1.63	1.59
8	C	503	VLB	C67-C59	3.47	1.42	1.37
7	D	501	GDP	PA-O3A	3.29	1.63	1.59
4	C	501	GTP	PB-O3A	3.22	1.63	1.59
8	C	503	VLB	C18-N1	-2.98	1.34	1.39
8	C	503	VLB	C60-C59	-2.85	1.38	1.44
4	A	501	GTP	PB-O3B	2.83	1.62	1.59
7	B	501	GDP	PA-O3A	2.82	1.62	1.59
4	A	501	GTP	PB-O3A	2.80	1.62	1.59
8	C	503	VLB	C68-C67	2.68	1.57	1.52
8	C	503	VLB	O75-C73	2.61	1.38	1.33
7	D	501	GDP	PB-O2B	2.60	1.64	1.54
8	C	503	VLB	C58-C59	2.60	1.55	1.51
8	C	503	VLB	C65-N66	-2.57	1.34	1.38
8	C	503	VLB	C30-C29	-2.54	1.41	1.49
8	C	503	VLB	C16-C15	2.51	1.44	1.39
7	D	501	GDP	O4'-C1'	2.51	1.47	1.42
8	C	503	VLB	C19-N9	2.19	1.50	1.47
7	D	501	GDP	C2-N2	2.16	1.39	1.34
8	C	503	VLB	O25-C23	2.14	1.37	1.33
7	D	501	GDP	PB-O3B	2.09	1.62	1.54
4	C	501	GTP	C5'-C4'	2.03	1.57	1.51
8	C	503	VLB	C5-C19	2.01	1.58	1.53

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	503	VLB	O32-C16-C15	8.26	124.78	116.59
8	C	503	VLB	O28-C29-C30	6.96	123.50	111.09
8	C	503	VLB	O75-C73-C68	6.73	122.08	111.21
8	C	503	VLB	C33-O32-C16	-6.33	108.23	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	503	VLB	O32-C16-C17	-5.73	114.21	124.08
7	D	501	GDP	C5-C4-N3	-5.41	119.78	128.39
7	B	501	GDP	C2-N3-C4	5.28	121.40	112.30
4	C	501	GTP	C2-N3-C4	5.22	121.30	112.30
7	B	501	GDP	C5-C4-N3	-5.22	120.08	128.39
7	D	501	GDP	C2-N3-C4	5.18	121.22	112.30
4	A	501	GTP	C2-N3-C4	5.02	120.95	112.30
4	C	501	GTP	C5-C4-N3	-4.94	120.53	128.39
4	A	501	GTP	C5-C4-N3	-4.73	120.85	128.39
7	D	501	GDP	N9-C4-N3	4.46	134.88	125.95
8	C	503	VLB	C22-N1-C2	-4.35	108.60	119.14
8	C	503	VLB	C22-N1-C18	-4.23	107.82	120.94
8	C	503	VLB	C69-N56-C55	3.83	116.05	110.87
8	C	503	VLB	C17-C18-C13	-3.77	117.67	121.99
7	B	501	GDP	N9-C4-N3	3.75	133.46	125.95
8	C	503	VLB	O25-C23-C3	3.66	118.24	112.21
4	C	501	GTP	N9-C4-N3	3.64	133.24	125.95
4	A	501	GTP	N9-C4-N3	3.53	133.01	125.95
8	C	503	VLB	C20-C5-C6	-3.52	103.80	107.99
4	C	501	GTP	C6-C5-N7	3.34	136.38	130.29
8	C	503	VLB	C64-C65-C60	-3.11	119.18	122.19
4	C	501	GTP	C8-N7-C5	3.05	109.69	104.26
4	A	501	GTP	C6-C5-N7	3.01	135.77	130.29
4	A	501	GTP	C8-N7-C5	3.01	109.62	104.26
8	C	503	VLB	O74-C73-C68	-2.96	117.77	124.81
8	C	503	VLB	C59-C67-N66	-2.95	106.82	109.95
8	C	503	VLB	C13-C12-C19	-2.90	105.62	115.26
4	A	501	GTP	O2G-PG-O3B	2.85	114.18	104.64
7	B	501	GDP	C8-N7-C5	2.82	109.28	104.26
8	C	503	VLB	C2-C12-C19	2.72	118.66	114.07
4	A	501	GTP	C4-C5-N7	-2.71	106.38	110.67
4	C	501	GTP	C4-C5-N7	-2.67	106.43	110.67
7	B	501	GDP	C6-C5-N7	2.59	135.00	130.29
7	B	501	GDP	C4-C5-N7	-2.55	106.64	110.67
8	C	503	VLB	O28-C29-O31	-2.50	118.16	122.99
4	C	501	GTP	O2G-PG-O3B	2.47	112.92	104.64
8	C	503	VLB	C61-C60-C65	2.46	121.39	118.84
7	D	501	GDP	O2B-PB-O3A	2.42	112.76	104.64
4	C	501	GTP	C2-N1-C6	-2.42	120.72	125.11
8	C	503	VLB	C76-O75-C73	-2.41	111.95	115.91
4	C	501	GTP	N9-C8-N7	-2.38	108.99	113.40
4	C	501	GTP	C5-C6-N1	2.38	119.31	113.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	501	GDP	C6-C5-N7	2.38	134.61	130.29
7	D	501	GDP	C8-N7-C5	2.36	108.46	104.26
8	C	503	VLB	C12-C19-C5	-2.31	116.49	118.20
8	C	503	VLB	C5-C19-N9	2.25	116.47	111.72
8	C	503	VLB	O75-C73-O74	-2.21	120.14	123.95
8	C	503	VLB	C8-C7-C6	-2.18	119.74	123.13
7	D	501	GDP	C4-C5-N7	-2.16	107.25	110.67
8	C	503	VLB	C14-C13-C18	2.13	122.06	120.29
4	A	501	GTP	N9-C8-N7	-2.13	109.46	113.40
7	B	501	GDP	C2-N1-C6	-2.12	121.27	125.11
7	B	501	GDP	O6-C6-C5	-2.12	120.95	126.53
8	C	503	VLB	C11-C12-C19	2.11	106.33	101.85
8	C	503	VLB	O28-C4-C3	2.01	109.43	106.29

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	501	GTP	PB-O3B-PG-O2G
4	A	501	GTP	C5'-O5'-PA-O3A
4	A	501	GTP	C5'-O5'-PA-O1A
4	A	501	GTP	C5'-O5'-PA-O2A
4	C	501	GTP	PB-O3B-PG-O2G
4	C	501	GTP	C5'-O5'-PA-O3A
4	C	501	GTP	C5'-O5'-PA-O1A
4	C	501	GTP	C5'-O5'-PA-O2A
8	C	503	VLB	O72-C54-C70-C71
8	C	503	VLB	C55-C54-C70-C71
8	C	503	VLB	C53-C54-C70-C71
8	C	503	VLB	C51-C68-C73-O74
8	C	503	VLB	C51-C68-C73-O75
8	C	503	VLB	C67-C68-C73-O74
8	C	503	VLB	C67-C68-C73-O75
8	C	503	VLB	C15-C68-C73-O75
8	C	503	VLB	C21-C20-C5-C19
8	C	503	VLB	C21-C20-C5-C6
8	C	503	VLB	C21-C20-C5-C4
8	C	503	VLB	C30-C29-O28-C4
8	C	503	VLB	O31-C29-O28-C4
8	C	503	VLB	C3-C23-O25-C26
8	C	503	VLB	C68-C73-O75-C76
8	C	503	VLB	O24-C23-O25-C26

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Mol	Chain	Res	Type	Atoms
8	C	503	VLB	O74-C73-O75-C76
8	C	503	VLB	C15-C16-O32-C33
8	C	503	VLB	C17-C16-O32-C33
7	B	501	GDP	PB-O3A-PA-O2A
7	D	501	GDP	PB-O3A-PA-O2A
8	C	503	VLB	C58-C57-N56-C69
7	B	501	GDP	C5'-O5'-PA-O2A
4	A	501	GTP	PB-O3A-PA-O1A
4	C	501	GTP	PB-O3A-PA-O1A
8	C	503	VLB	C15-C68-C73-O74
4	A	501	GTP	PB-O3B-PG-O3G
4	C	501	GTP	PB-O3B-PG-O3G

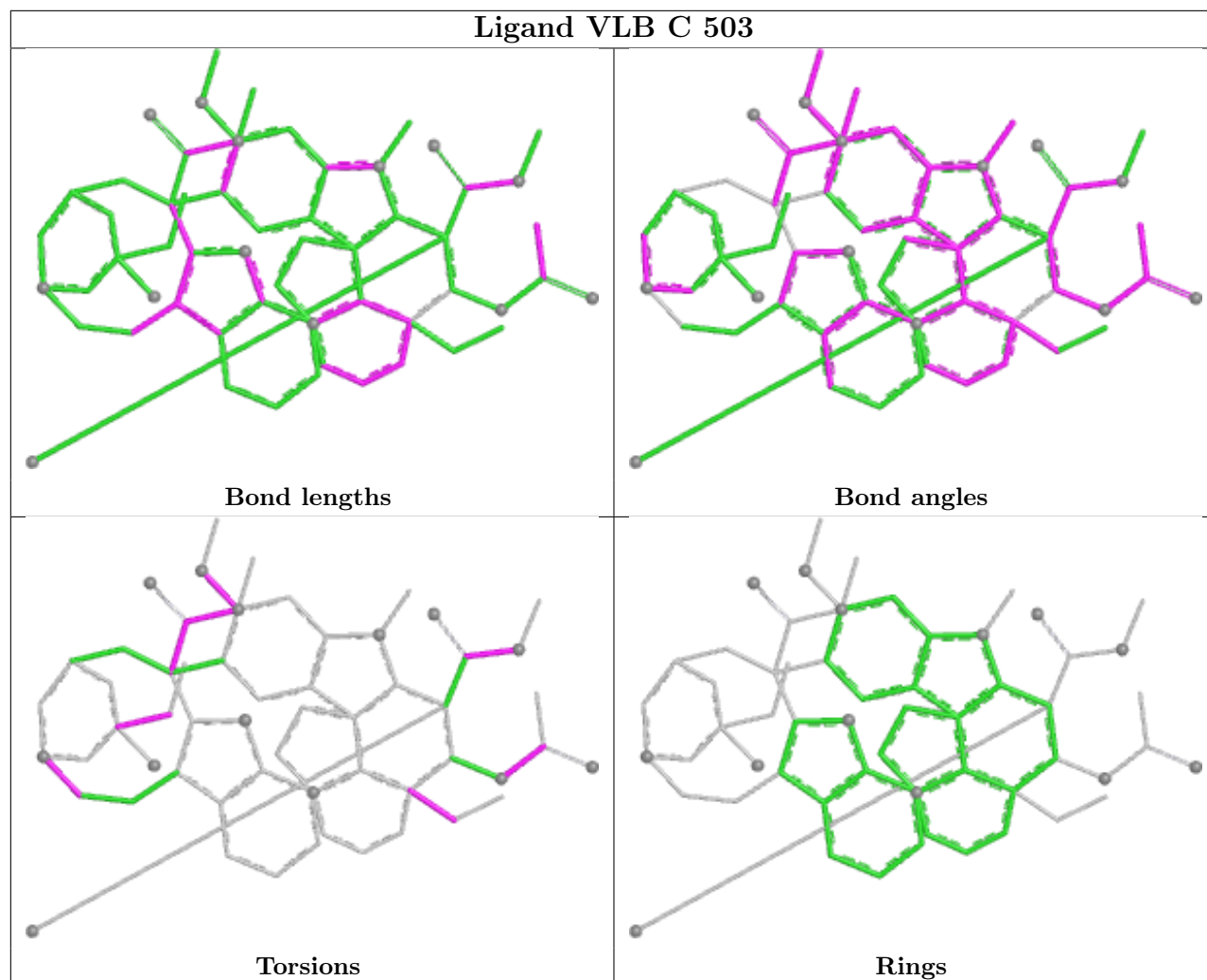
There are no ring outliers.

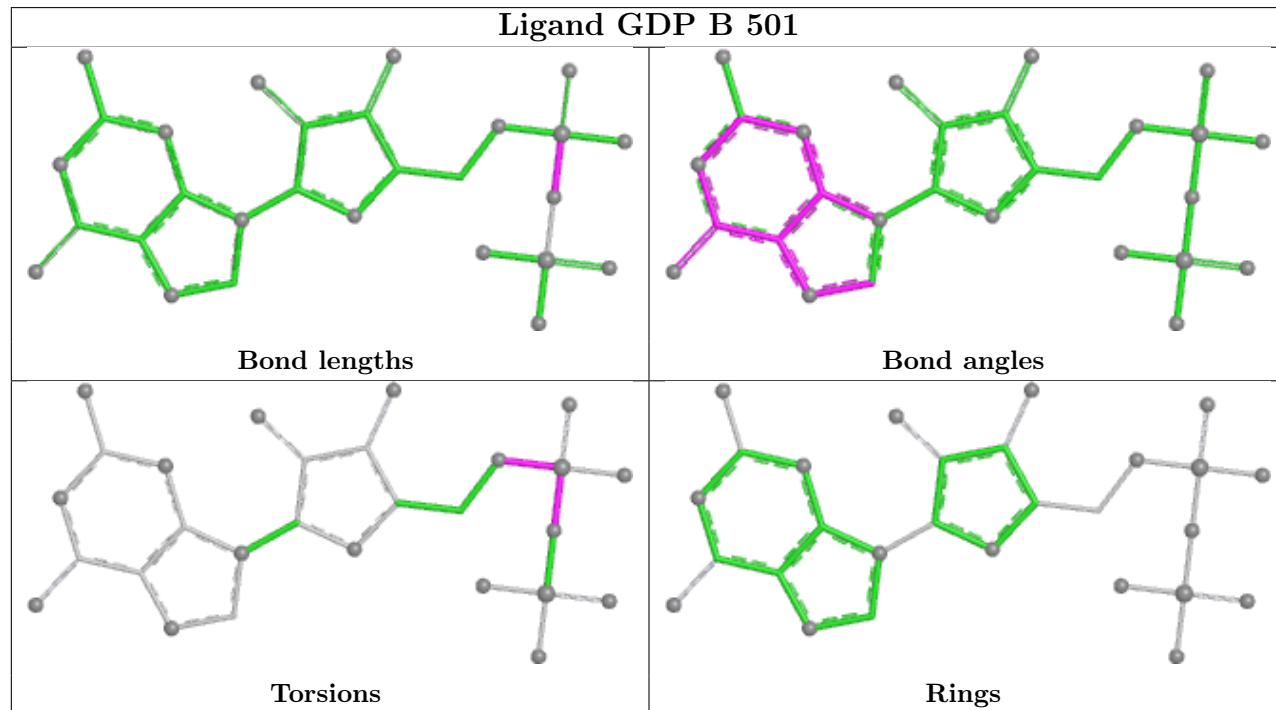
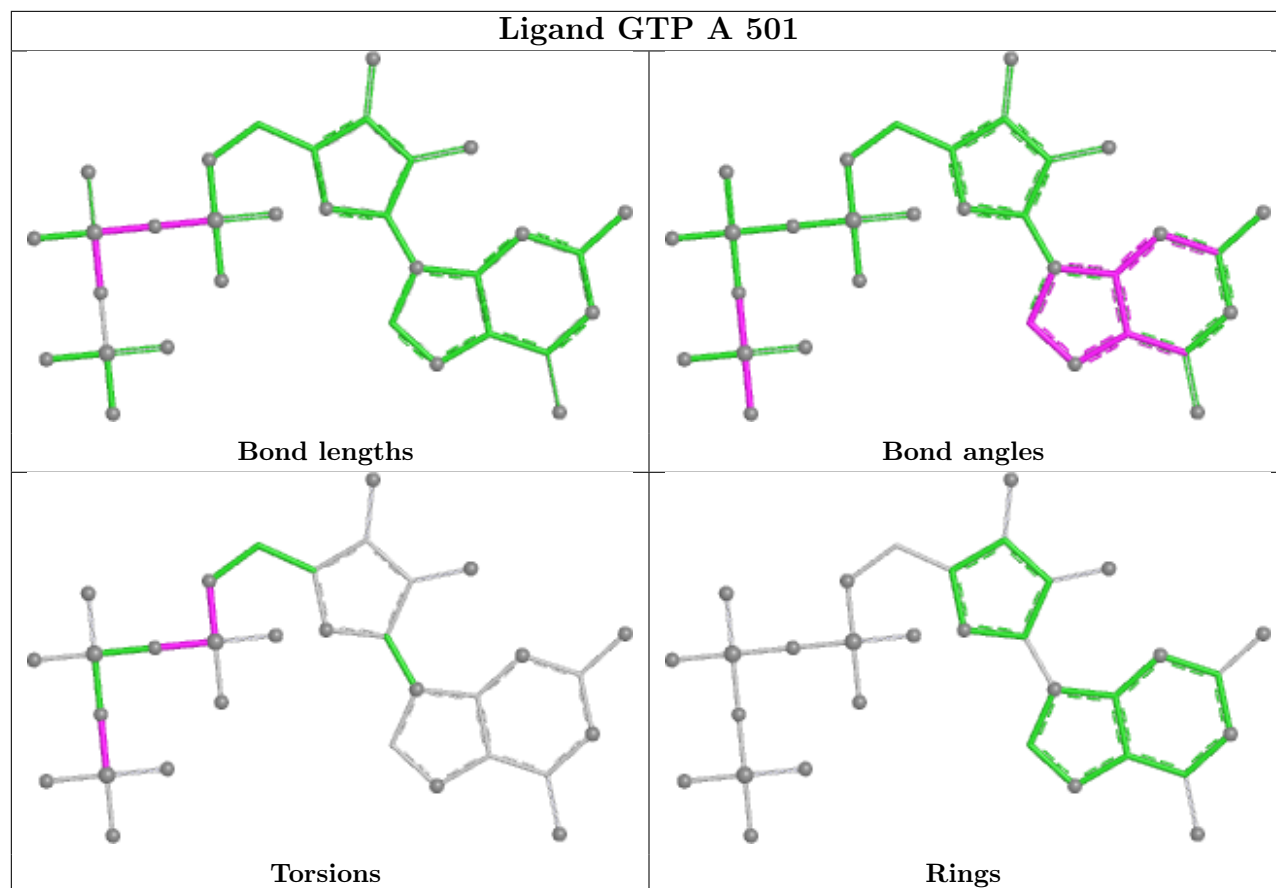
4 monomers are involved in 22 short contacts:

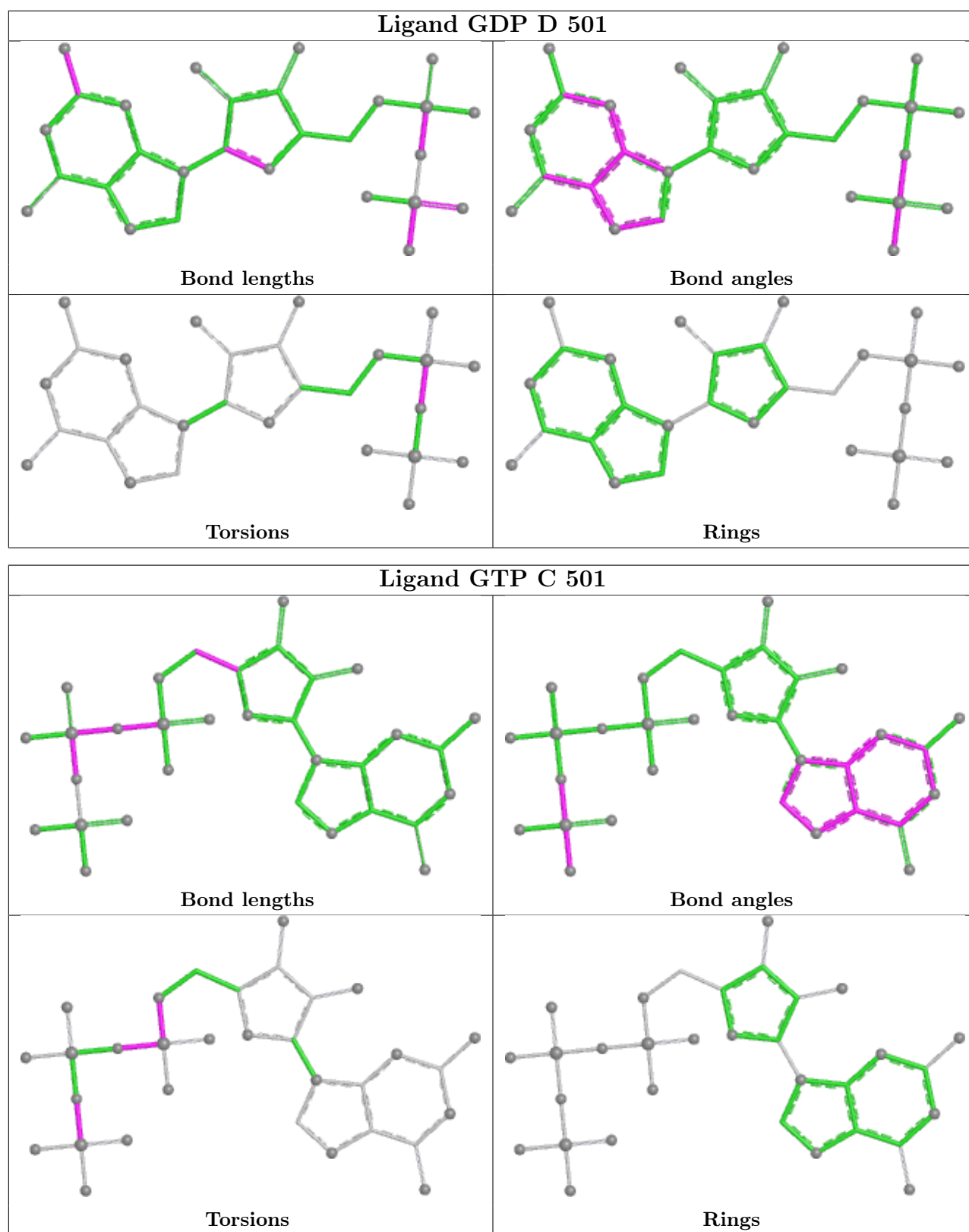
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	503	VLB	13	0
4	A	501	GTP	4	0
7	D	501	GDP	2	0
4	C	501	GTP	3	0

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.

Ligand VLB C 503







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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	433/451 (96%)	-0.49	2 (0%) 87 69	98, 187, 248, 265	1 (0%)
1	C	432/451 (95%)	-0.46	1 (0%) 91 82	79, 169, 233, 267	4 (0%)
2	B	432/445 (97%)	-0.49	1 (0%) 91 82	90, 165, 242, 269	4 (0%)
2	D	432/445 (97%)	-0.43	2 (0%) 87 69	73, 142, 233, 251	3 (0%)
3	E	132/142 (92%)	-0.67	0 100 100	86, 209, 254, 266	1 (0%)
All	All	1861/1934 (96%)	-0.48	6 (0%) 90 77	73, 170, 243, 269	13 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	177	VAL	2.4
1	A	151	SER	2.3
1	C	61	HIS	2.2
2	D	87	PHE	2.1
1	A	194	THR	2.1
2	B	295	MET	2.1

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

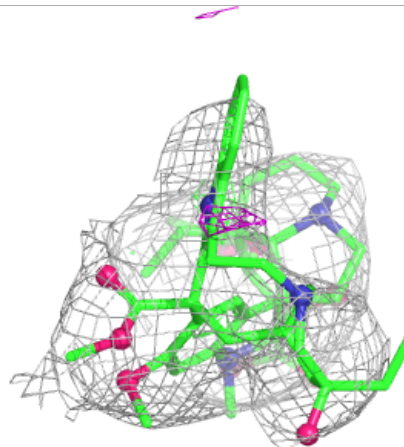
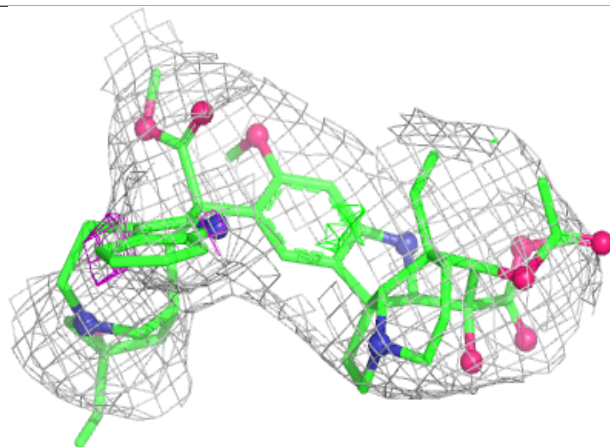
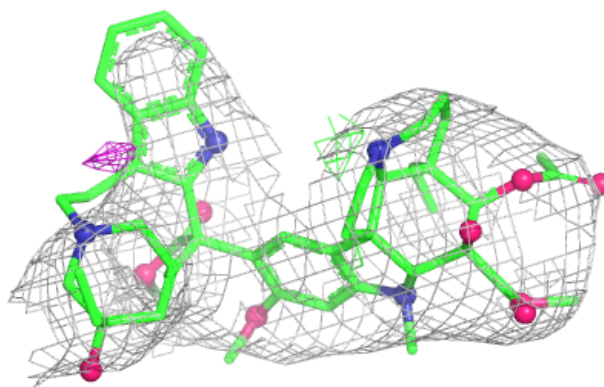
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	SO4	A	503	5/5	0.55	0.07	232,237,238,238	0
6	SO4	A	504	5/5	0.63	0.07	246,250,251,251	0
6	SO4	B	502	5/5	0.66	0.05	243,248,249,249	0
6	SO4	D	502	5/5	0.89	0.06	219,223,224,224	0
8	VLB	C	503	59/59	0.89	0.09	154,159,166,170	0
6	SO4	D	503	5/5	0.91	0.05	159,164,165,165	0
7	GDP	D	501	28/28	0.93	0.07	113,117,125,130	0
4	GTP	C	501	32/32	0.94	0.07	134,138,144,149	0
7	GDP	B	501	28/28	0.97	0.05	126,131,138,140	0
5	MG	C	502	1/1	0.97	0.04	121,121,121,121	0
4	GTP	A	501	32/32	0.97	0.06	140,148,158,159	0
5	MG	A	502	1/1	0.99	0.04	116,116,116,116	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.

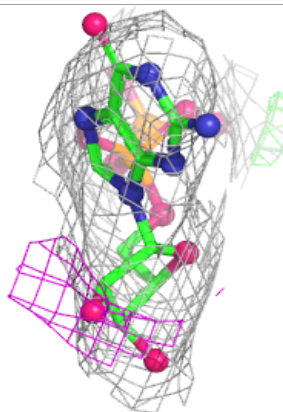
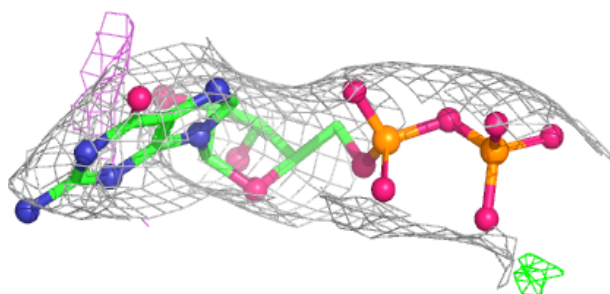
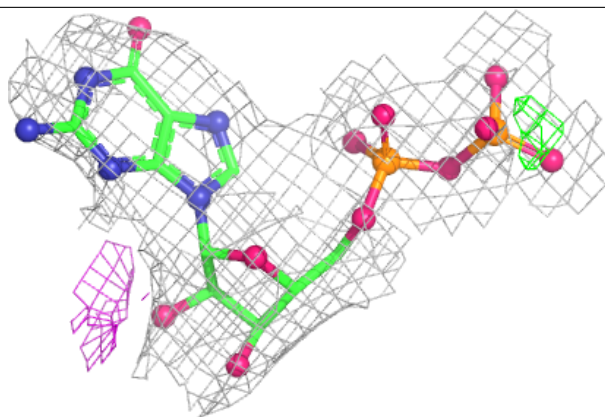
Electron density around VLB C 503:

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

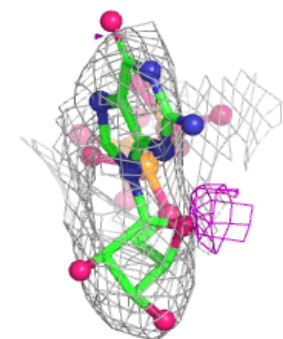
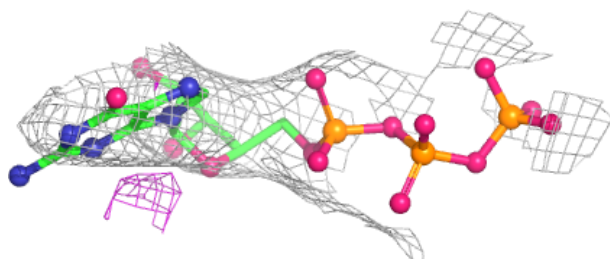
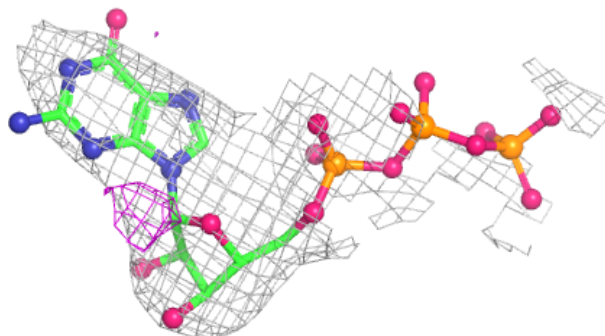


Electron density around GDP D 501:

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

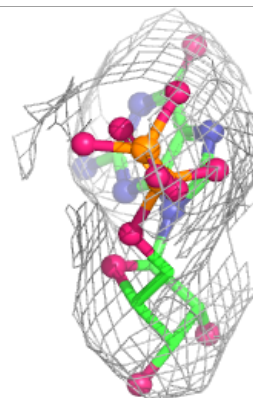
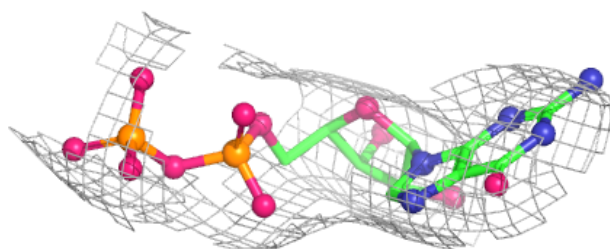
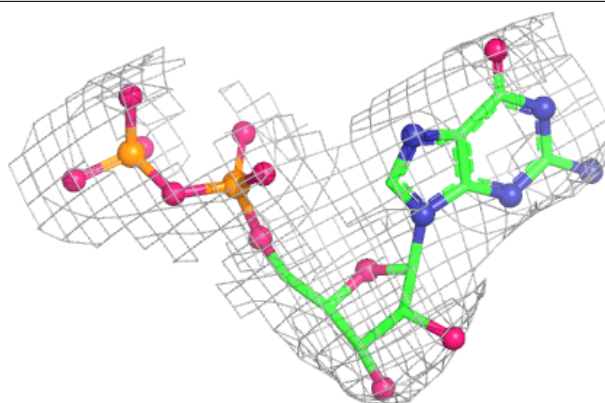
**Electron density around GTP C 501:**

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

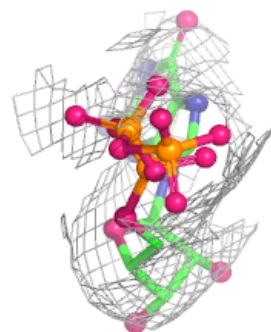
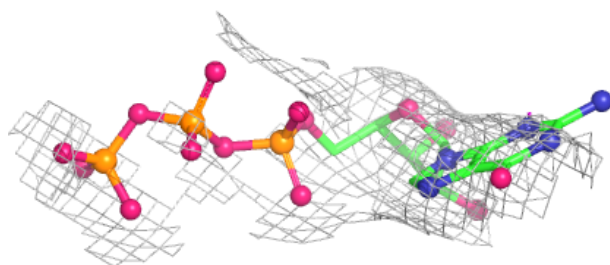
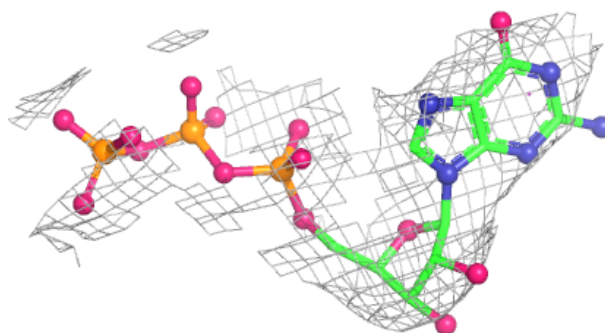


Electron density around GDP B 501:

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

**Electron density around GTP A 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.