



Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2022 – 06:16 PM JST

PDB ID : 7VMJ
Title : Crystal structure of tubulin with 17a
Authors : Jifa, Z.; Lun, T.
Deposited on : 2021-10-08
Resolution : 2.90 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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.31.3
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

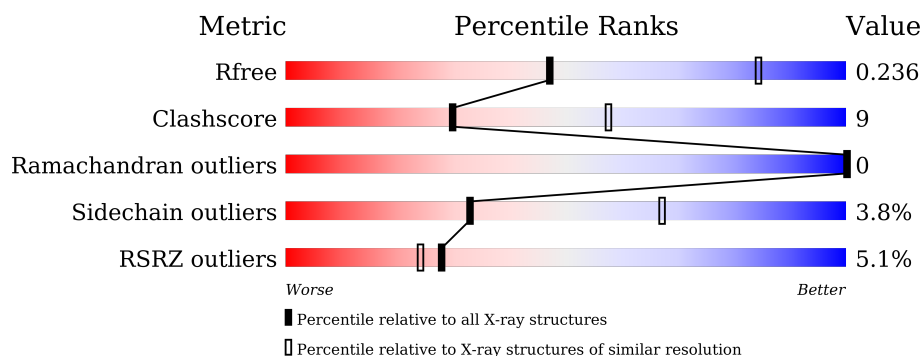
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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	450	<div> <div>76%</div> <div>21%</div> <div>.</div> </div>
1	C	450	<div> <div>80%</div> <div>17%</div> <div>.</div> </div>
2	B	445	<div> <div>75%</div> <div>18%</div> <div>5%</div> </div>
2	D	445	<div> <div>7%</div> <div>65%</div> <div>28%</div> <div>6%</div> </div>
3	E	143	<div> <div>4%</div> <div>66%</div> <div>18%</div> <div>14%</div> </div>
4	F	384	<div> <div>18%</div> <div>63%</div> <div>25%</div> <div>10%</div> </div>

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17608 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-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	4	0
			3427	2170	580	653	24			
1	C	440	Total	C	N	O	S	0	8	0
			3465	2193	585	662	25			

- Molecule 2 is a protein called Tubulin beta-2B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	4	0
			3364	2116	575	647	26			
2	D	420	Total	C	N	O	S	0	1	0
			3291	2069	557	639	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	2	0
			1026	633	186	202	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	346	Total	C	N	O	S	0	5	0
			2856	1835	487	519	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- 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		
5	C	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		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	1	0
			1	1		

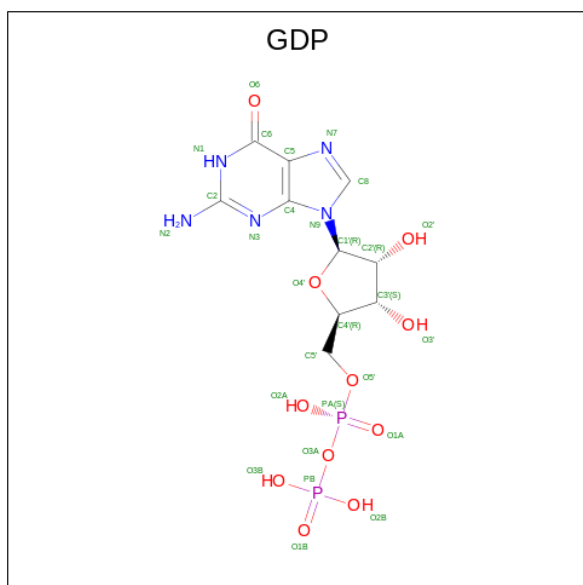
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	1	0
			1	1		
7	C	1	Total	Ca	1	0
			1	1		

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

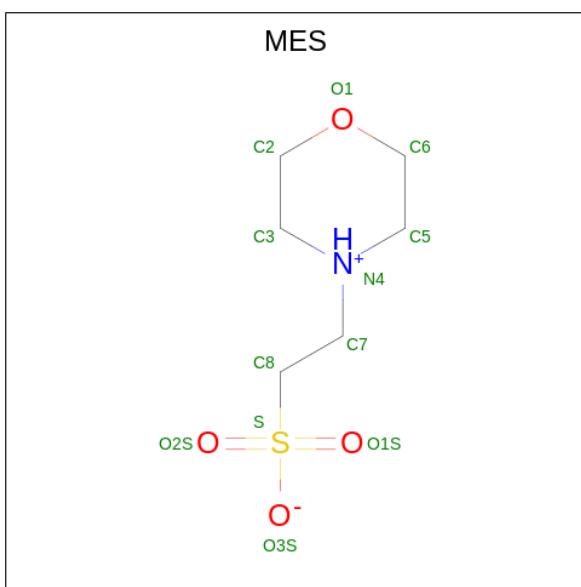
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	1	0
			1	1		

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



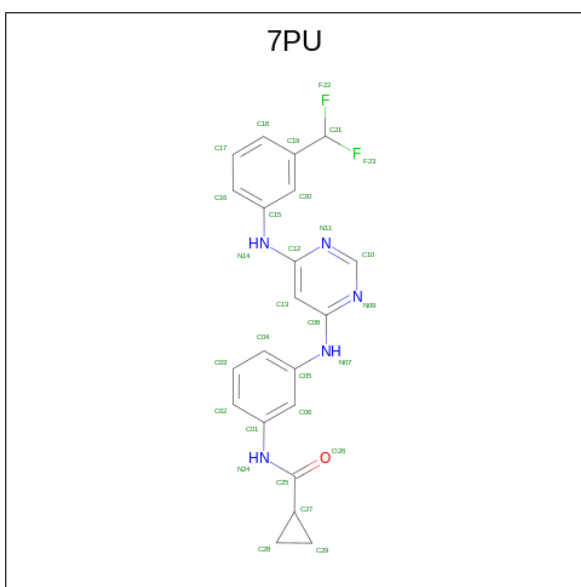
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
9	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 11 is N-[3-[[6-[[3-[bis(fluoranyl)methyl]phenyl]amino]pyrimidin-4-yl]amino]phenyl]cyclopropanecarboxamide (three-letter code: 7PU) (formula: C₂₁H₁₉F₂N₅O) (labeled as "Ligand of Interest" by depositor).

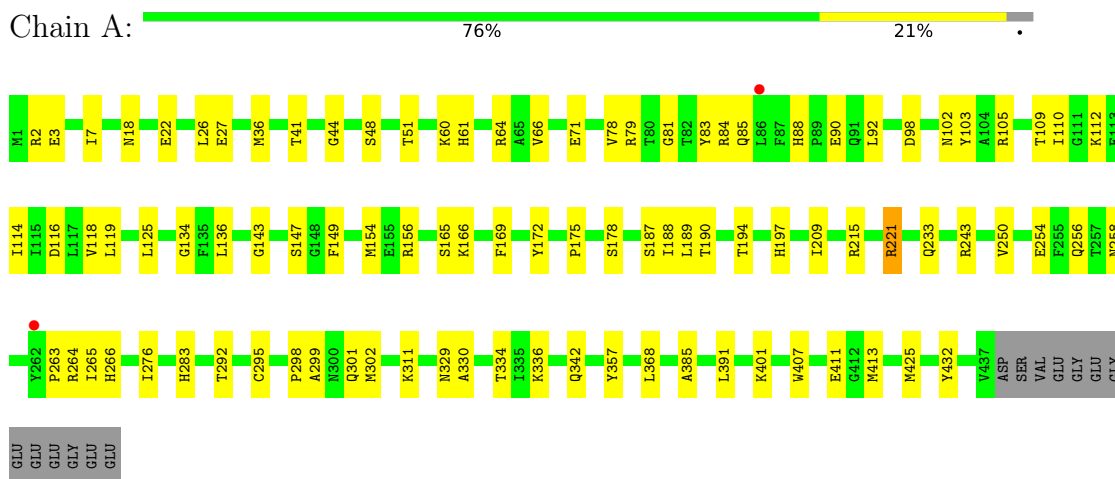


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	F	N	O	0	0
			29	21	2	5	1		

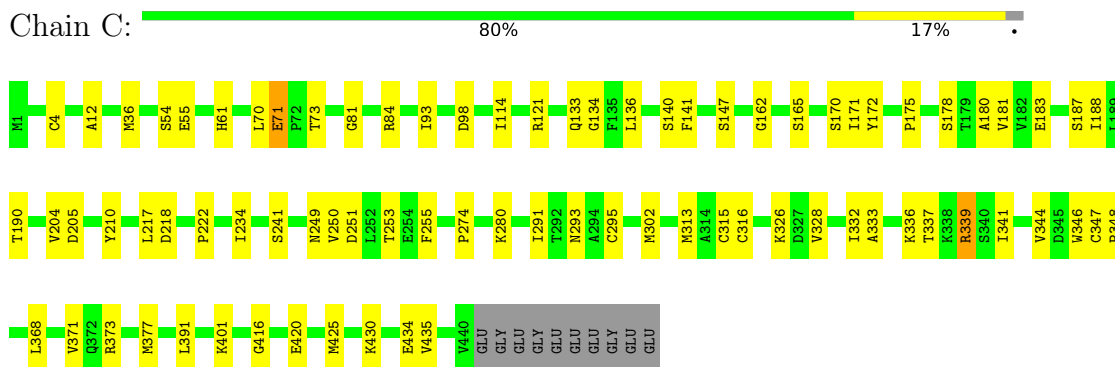
3 Residue-property plots

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.

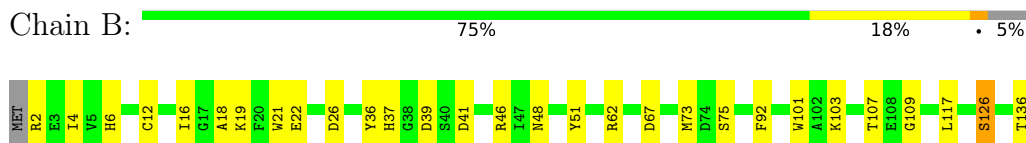
• Molecule 1: Tubulin alpha-1B chain

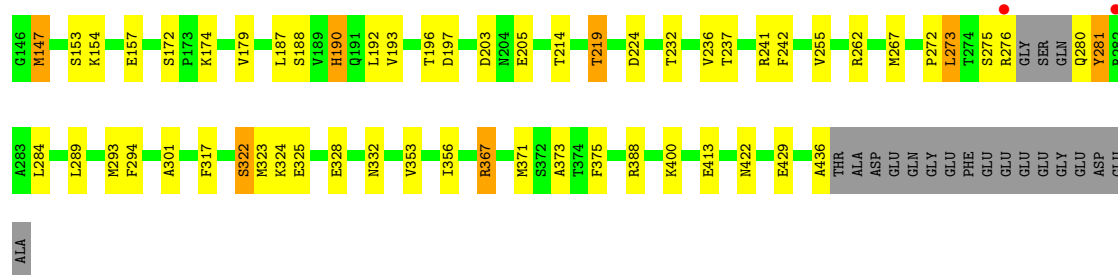


• Molecule 1: Tubulin alpha-1B chain

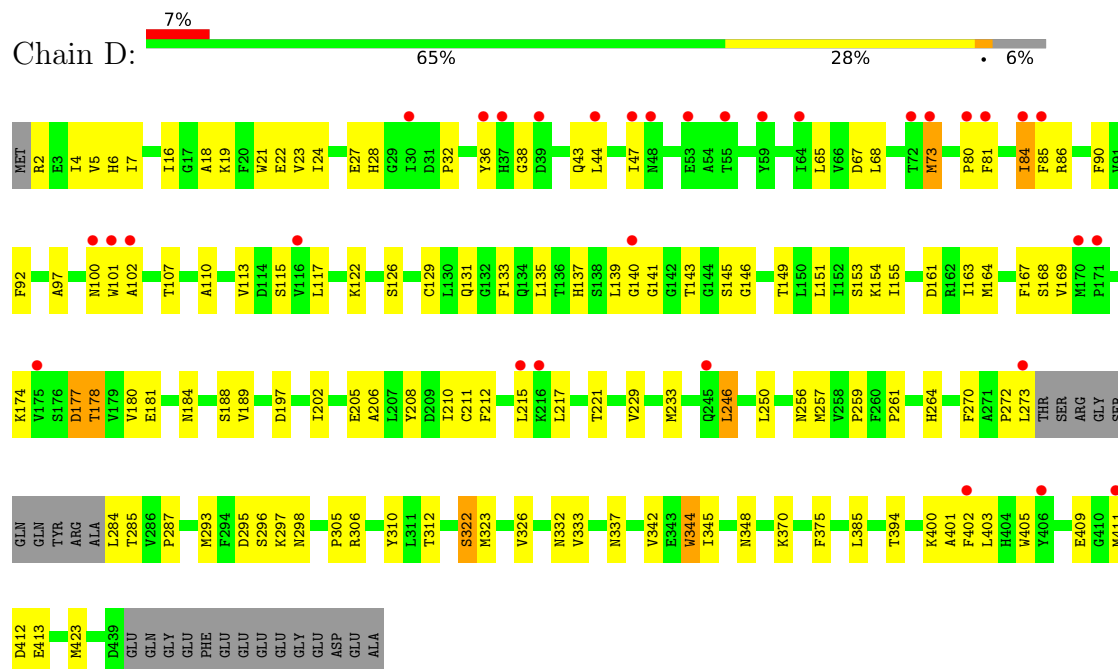


• Molecule 2: Tubulin beta-2B chain

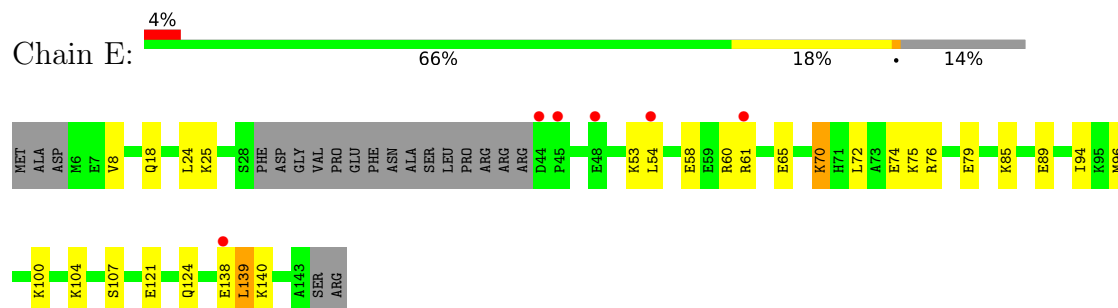




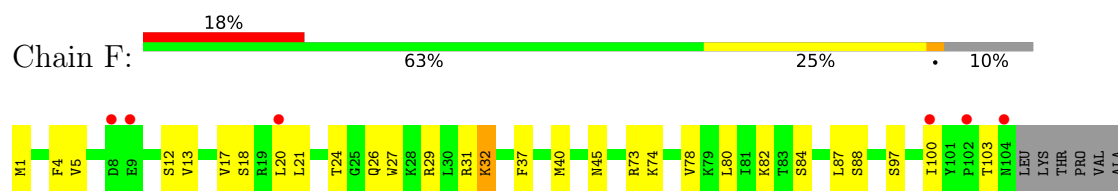
• Molecule 2: Tubulin beta-2B chain

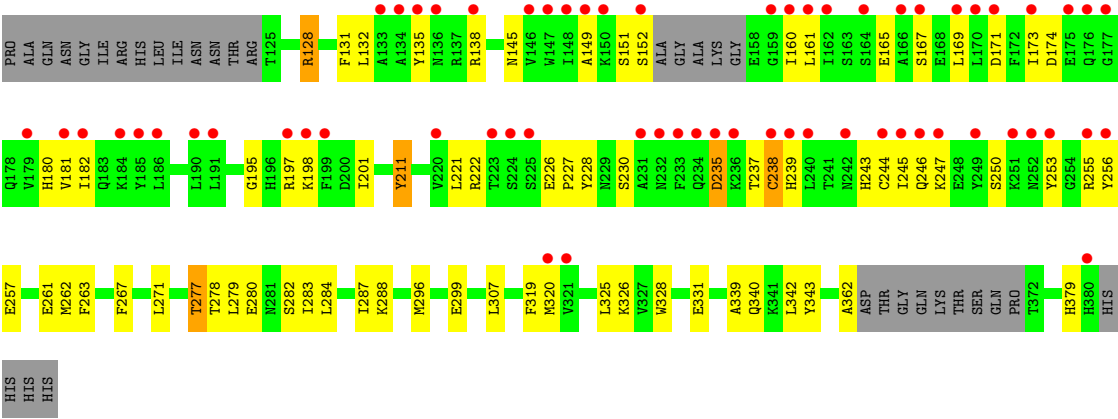


• Molecule 3: Stathmin-4



• Molecule 4: Tubulin tyrosine ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.98Å 157.93Å 182.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	87.43 – 2.90 87.43 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.7 (87.43-2.90) 99.7 (87.43-2.90)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 2.91Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.199 , 0.243 0.191 , 0.236	Depositor DCC
R_{free} test set	1995 reflections (2.95%)	wwPDB-VP
Wilson B-factor (Å ²)	64.0	Xtriage
Anisotropy	0.329	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 59.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17608	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.07% 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: GTP, MES, CL, 7PU, MG, CA, 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	0.48	0/3517	0.66	0/4776
1	C	0.58	1/3564 (0.0%)	0.71	0/4839
2	B	0.48	0/3447	0.69	1/4667 (0.0%)
2	D	0.45	0/3364	0.63	0/4560
3	E	0.51	0/1041	0.69	1/1382 (0.1%)
4	F	0.47	1/2935 (0.0%)	0.66	0/3966
All	All	0.50	2/17868 (0.0%)	0.67	2/24190 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	238	CYS	CB-SG	-9.16	1.66	1.82
1	C	295	CYS	CB-SG	-7.10	1.70	1.82

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	139	LEU	CA-CB-CG	6.04	129.18	115.30
2	B	273	LEU	CA-CB-CG	-5.12	103.53	115.30

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	3427	0	3340	64	0
1	C	3465	0	3383	47	0
2	B	3364	0	3250	59	0
2	D	3291	0	3155	84	0
3	E	1026	0	1042	23	0
4	F	2856	0	2837	66	0
5	A	32	0	12	1	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
9	B	28	0	12	1	0
9	D	28	0	12	2	0
10	B	24	0	24	2	0
11	B	29	0	0	0	0
All	All	17608	0	17079	326	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 (326) 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)
2:D:139:LEU:HD11	2:D:168:SER:HB3	1.38	1.04
1:C:234:ILE:HD13	1:C:302:MET:SD	2.18	0.84
1:A:154:MET:HG3	1:A:194:THR:HG23	1.63	0.80
2:D:65:LEU:HD11	2:D:85:PHE:HD2	1.47	0.78
4:F:135:TYR:OH	4:F:165:GLU:HA	1.84	0.78
2:D:206:ALA:O	2:D:210:ILE:HG13	1.84	0.78
4:F:31:ARG:HE	4:F:32:LYS:H	1.32	0.77
4:F:226:GLU:OE1	4:F:238:CYS:HB3	1.86	0.75
1:A:105:ARG:HG2	1:A:110:ILE:HD13	1.69	0.73
2:B:203:ASP:OD2	2:B:388:ARG:NH2	2.22	0.73
4:F:31:ARG:NE	4:F:32:LYS:H	1.88	0.72
4:F:103:THR:N	4:F:174:ASP:OD1	2.23	0.71
1:A:329:ASN:HD21	3:E:8:VAL:HG21	1.56	0.71
2:B:324:LYS:O	2:B:328:GLU:HG3	1.93	0.68
2:B:272:PRO:HB3	2:B:284:LEU:HD21	1.75	0.67
2:B:126:SER:O	2:B:126:SER:OG	2.14	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:322:SER:OG	2:B:325:GLU:HB2	1.95	0.66
1:A:2:ARG:O	1:A:51:THR:HG23	1.96	0.66
4:F:78:VAL:HG21	4:F:181:VAL:HG21	1.78	0.66
2:D:141:GLY:HA3	9:D:501:GDP:O3A	1.96	0.66
1:A:143:GLY:HA3	5:A:501:GTP:O3A	1.96	0.65
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.77	0.65
2:D:139:LEU:HA	2:D:145[A]:SER:HB3	1.78	0.64
2:D:81:PHE:O	2:D:84:ILE:HG22	1.99	0.63
4:F:326:LYS:HE2	4:F:328:TRP:CZ2	2.34	0.63
1:C:175:PRO:HA	1:C:178:SER:OG	1.99	0.63
2:D:177:ASP:N	2:D:177:ASP:OD1	2.32	0.62
1:A:88:HIS:CD2	1:A:90:GLU:HG3	2.34	0.62
1:A:88:HIS:HD2	1:A:90:GLU:H	1.47	0.62
1:C:188:ILE:HD12	1:C:425:MET:HG3	1.82	0.62
2:D:32:PRO:HB3	2:D:81:PHE:HA	1.82	0.61
1:A:109:THR:HG22	1:A:110:ILE:HD12	1.82	0.61
1:A:330:ALA:O	1:A:334:THR:HG23	2.00	0.61
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.41	0.60
2:B:289:LEU:HD22	2:B:371:MET:HE3	1.84	0.60
1:A:112:LYS:HD2	3:E:54:LEU:HB3	1.83	0.60
1:C:36:MET:HE3	1:C:61:HIS:CD2	2.37	0.60
1:C:430:LYS:O	1:C:434:GLU:HG3	2.00	0.60
2:D:44:LEU:HA	2:D:47:ILE:HB	1.84	0.60
2:D:140:GLY:O	2:D:184:ASN:ND2	2.31	0.60
2:D:16:ILE:HD11	2:D:169:VAL:HG21	1.83	0.60
3:E:96:MET:O	3:E:100:LYS:HG3	2.02	0.59
3:E:24:LEU:O	3:E:25:LYS:HG3	2.02	0.59
4:F:235:ASP:OD1	4:F:235:ASP:N	2.34	0.59
2:B:224:ASP:OD1	2:B:276:ARG:NH2	2.31	0.59
2:D:412:ASP:OD1	2:D:413:GLU:N	2.35	0.59
2:B:219:THR:HG21	1:C:326:LYS:HA	1.84	0.59
3:E:121:GLU:HA	3:E:124:GLN:HG2	1.84	0.59
2:B:145:SER:HB2	2:B:188:SER:OG	2.03	0.58
4:F:211:TYR:CE2	4:F:299:GLU:HG3	2.39	0.58
4:F:82:LYS:HE3	4:F:97:SER:O	2.03	0.58
2:D:272:PRO:HG3	2:D:284:LEU:CD2	2.34	0.58
2:B:293:MET:HE2	2:B:375:PHE:HB2	1.86	0.58
1:A:166:LYS:HE2	1:A:197:HIS:O	2.04	0.58
4:F:226:GLU:HG2	4:F:227:PRO:HD2	1.86	0.58
4:F:284:LEU:O	4:F:288:LYS:HG3	2.03	0.58
4:F:339:ALA:HB3	4:F:342:LEU:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:211:TYR:CD2	4:F:299:GLU:HG3	2.39	0.57
1:C:250:VAL:HG22	1:C:255:PHE:CE2	2.39	0.57
1:A:88:HIS:NE2	1:A:90:GLU:HG3	2.18	0.57
4:F:128:ARG:HA	4:F:131:PHE:HB3	1.86	0.57
2:B:275:SER:OG	2:B:276:ARG:N	2.37	0.57
1:C:71:GLU:OE1	1:C:73:THR:HG23	2.05	0.57
2:D:202:ILE:HD13	2:D:229:VAL:HG13	1.88	0.56
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.36	0.56
4:F:87:LEU:O	4:F:88:SER:CB	2.53	0.56
1:A:27:GLU:OE1	1:A:243:ARG:NH2	2.35	0.56
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.87	0.56
1:A:401:LYS:HE3	2:B:436:ALA:HB1	1.87	0.56
2:D:36:TYR:CD2	2:D:44:LEU:HD11	2.41	0.56
4:F:201:ILE:HD13	4:F:221:LEU:CD2	2.36	0.56
2:D:272:PRO:HG3	2:D:284:LEU:HD21	1.88	0.55
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.89	0.55
4:F:221:LEU:HD11	4:F:267:PHE:CG	2.41	0.55
1:C:332:ILE:O	1:C:336:LYS:HG2	2.07	0.55
4:F:13:VAL:O	4:F:17:VAL:HG23	2.07	0.55
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.72	0.54
2:B:46:ARG:HH11	2:B:46:ARG:HG2	1.73	0.54
1:A:79:ARG:HG2	1:A:92:LEU:HD12	1.89	0.54
2:D:4:ILE:HG12	2:D:250:LEU:HD11	1.89	0.54
2:B:18:ALA:O	2:B:22:GLU:HG3	2.08	0.54
2:D:65:LEU:HD21	2:D:85:PHE:CE2	2.43	0.54
2:D:189:VAL:HG11	2:D:423:MET:HG3	1.90	0.53
4:F:26:GLN:HE22	4:F:362:ALA:H	1.56	0.53
1:A:311:LYS:HZ2	1:A:342:GLN:HG2	1.73	0.53
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.26	0.53
1:C:313:MET:HE3	1:C:435:VAL:HB	1.89	0.53
2:D:19:LYS:O	2:D:23:VAL:HG23	2.08	0.53
3:E:139:LEU:HB2	3:E:140:LYS:NZ	2.23	0.53
4:F:221:LEU:HD12	4:F:262:MET:HE3	1.91	0.53
1:A:112:LYS:HG3	3:E:54:LEU:HD23	1.89	0.53
2:B:242:PHE:CD1	2:B:356:ILE:HD12	2.44	0.53
1:A:102:ASN:HB3	1:A:105:ARG:HB2	1.91	0.53
2:D:23:VAL:O	2:D:27:GLU:HG3	2.08	0.53
4:F:20:LEU:O	4:F:24:THR:HG23	2.09	0.53
2:D:18:ALA:O	2:D:22:GLU:HG3	2.09	0.53
2:D:22:GLU:OE2	2:D:80:PRO:HG2	2.09	0.53
2:D:117:LEU:HD11	2:D:154:LYS:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:267:MET:HG3	2:B:301:ALA:HB3	1.91	0.52
2:D:65:LEU:HD21	2:D:85:PHE:CD2	2.44	0.52
2:D:139:LEU:HD23	2:D:188:SER:HB3	1.91	0.52
4:F:340:GLN:HA	4:F:343:TYR:HD1	1.75	0.52
2:B:139:LEU:HA	2:B:145:SER:HB3	1.92	0.52
1:C:274:PRO:HG2	1:C:371:VAL:HG11	1.91	0.52
2:D:163:ILE:HA	2:D:197:ASP:OD2	2.10	0.52
2:D:5:VAL:HG13	2:D:133:PHE:CD2	2.44	0.52
1:C:140:SER:HA	1:C:171:ILE:HB	1.92	0.52
1:A:147:SER:HB2	1:A:190:THR:HB	1.92	0.52
4:F:31:ARG:HE	4:F:32:LYS:HG2	1.75	0.52
2:D:400:LYS:O	2:D:403:LEU:HB2	2.10	0.52
2:B:317:PHE:HB2	2:B:353:VAL:HG22	1.91	0.51
2:D:2:ARG:HG3	2:D:129:CYS:HB3	1.92	0.51
1:A:118:VAL:HG21	1:A:149:PHE:HZ	1.75	0.51
2:D:6:HIS:CD2	2:D:7:ILE:N	2.79	0.51
1:A:215:ARG:NH2	1:A:299:ALA:O	2.43	0.51
2:B:262:ARG:HH21	2:B:429[A]:GLU:CD	2.13	0.51
1:A:116:ASP:OD1	1:A:156:ARG:NH2	2.43	0.51
4:F:201:ILE:HB	4:F:319:PHE:HB2	1.92	0.51
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.91	0.51
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.93	0.51
4:F:151:SER:HB3	4:F:180:HIS:CE1	2.46	0.51
1:C:328:VAL:O	1:C:332:ILE:HG13	2.10	0.51
4:F:167:SER:O	4:F:171:ASP:HB2	2.10	0.50
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.92	0.50
3:E:85:LYS:O	3:E:89:GLU:HG2	2.10	0.50
1:C:134:GLY:HA3	1:C:165:SER:O	2.12	0.50
4:F:246:GLN:O	4:F:250:SER:HB3	2.10	0.50
2:D:65:LEU:HD11	2:D:85:PHE:CD2	2.38	0.50
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.47	0.50
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.47	0.50
4:F:128:ARG:O	4:F:132:LEU:HG	2.12	0.50
2:D:401:ALA:HB1	2:D:402:PHE:CD1	2.47	0.49
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.47	0.49
4:F:100:ILE:HD12	4:F:128:ARG:HB3	1.95	0.49
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.95	0.49
2:D:68:LEU:HD12	2:D:97:ALA:HB2	1.94	0.49
2:D:174:LYS:HD2	2:D:208:TYR:HD2	1.77	0.48
2:D:257:MET:HE2	2:D:257:MET:HA	1.95	0.48
4:F:228:TYR:HE1	4:F:239:HIS:HD1	1.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:190:HIS:NE2	2:B:422:ASN:OD1	2.47	0.48
2:D:139:LEU:HD23	2:D:188:SER:CB	2.44	0.48
1:A:357:TYR:OH	3:E:18:GLN:NE2	2.46	0.48
4:F:197:ARG:NH2	4:F:257:GLU:OE2	2.46	0.48
2:D:143:THR:HB	9:D:501:GDP:O2B	2.14	0.48
4:F:138:ARG:HB3	4:F:145:ASN:HD22	1.78	0.48
2:D:107:THR:HG21	2:D:409:GLU:HG3	1.96	0.48
2:D:322:SER:O	2:D:326:VAL:HG23	2.14	0.48
3:E:60:ARG:HG3	3:E:60:ARG:HH11	1.79	0.47
2:D:174:LYS:HD2	2:D:208:TYR:CD2	2.49	0.47
4:F:5:VAL:CG1	4:F:32:LYS:HA	2.44	0.47
2:D:167:PHE:CE2	2:D:233:MET:HG2	2.49	0.47
2:D:151:LEU:O	2:D:155:ILE:HG13	2.15	0.47
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.96	0.47
1:C:339:ARG:HB3	1:C:341:ILE:HD12	1.96	0.47
1:A:221:ARG:NH1	2:B:323:MET:HG3	2.29	0.47
1:C:291:ILE:HD13	1:C:373:ARG:HG3	1.96	0.47
4:F:279:LEU:HD12	4:F:283:ILE:HB	1.96	0.47
1:A:407:TRP:CE2	2:B:255:VAL:HA	2.50	0.47
1:C:55:GLU:HG2	1:C:61:HIS:CD2	2.50	0.47
4:F:261:GLU:HB3	4:F:263:PHE:HE2	1.79	0.47
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.44	0.47
1:C:180:ALA:HB3	1:C:183:GLU:HG3	1.97	0.47
4:F:255[B]:ARG:HD3	4:F:256:TYR:CE1	2.49	0.47
2:B:16[A]:ILE:HD11	2:B:136:THR:HB	1.97	0.47
2:D:19:LYS:NZ	2:D:22:GLU:OE1	2.48	0.47
2:D:270:PHE:O	2:D:298:ASN:HB3	2.15	0.47
2:B:272:PRO:HG3	2:B:284:LEU:HD11	1.97	0.47
2:D:401:ALA:HB1	2:D:402:PHE:HD1	1.79	0.46
3:E:70:LYS:O	3:E:74:GLU:HG3	2.15	0.46
1:A:336:LYS:HG3	3:E:24:LEU:CD1	2.45	0.46
1:A:136:LEU:HD23	1:A:169:PHE:HE2	1.80	0.46
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.96	0.46
2:B:48:ASN:HA	2:B:51:TYR:O	2.15	0.46
2:B:232:THR:O	2:B:236:VAL:HG13	2.15	0.46
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.69	0.46
2:B:197:ASP:OD1	10:B:503:MES:H72	2.14	0.46
1:C:133:GLN:NE2	1:C:253:THR:HG21	2.31	0.46
1:A:105:ARG:NH1	1:A:411:GLU:OE2	2.48	0.46
1:A:125:LEU:HD23	1:A:125:LEU:HA	1.76	0.46
2:B:26:ASP:OD2	2:B:367:ARG:HD2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:7:ILE:O	2:D:135:LEU:HD12	2.16	0.46
2:D:295:ASP:OD2	2:D:297:LYS:HG3	2.15	0.46
4:F:221:LEU:HD12	4:F:262:MET:CE	2.46	0.46
1:A:103:TYR:CD2	1:A:189:LEU:HD13	2.51	0.46
1:A:263:PRO:O	1:A:266:HIS:HD2	1.99	0.46
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.51	0.46
1:A:88:HIS:CD2	1:A:90:GLU:H	2.29	0.46
1:C:188:ILE:HG23	1:C:425:MET:HG2	1.98	0.46
2:B:101:TRP:CE3	2:B:187:LEU:HD13	2.50	0.46
2:D:100:ASN:ND2	2:D:405:TRP:HB3	2.31	0.46
4:F:138:ARG:CB	4:F:145:ASN:HD22	2.29	0.46
1:C:81:GLY:O	1:C:84:ARG:HG2	2.16	0.45
1:C:241:SER:HA	1:C:249:ASN:OD1	2.17	0.45
2:D:102:ALA:HB2	2:D:411:MET:CE	2.46	0.45
2:D:110:ALA:O	2:D:113:VAL:HG12	2.16	0.45
3:E:139:LEU:HB2	3:E:140:LYS:HZ2	1.79	0.45
4:F:173:ILE:HD11	4:F:182:ILE:HG23	1.98	0.45
4:F:263:PHE:HD2	4:F:263:PHE:N	2.14	0.45
2:D:261:PRO:O	2:D:264:HIS:ND1	2.42	0.45
4:F:37:PHE:CE1	4:F:40:MET:HB2	2.51	0.45
1:A:329:ASN:HD21	3:E:8:VAL:CG2	2.28	0.45
2:D:323:MET:HA	2:D:326:VAL:HG23	1.99	0.45
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.99	0.45
2:D:6:HIS:HD2	2:D:7:ILE:N	2.14	0.45
2:B:172:SER:HB2	2:B:205:GLU:HB2	1.98	0.45
4:F:149:ALA:HB2	4:F:182:ILE:HG22	1.99	0.45
2:B:273:LEU:HD23	2:B:273:LEU:HA	1.87	0.45
2:D:333:VAL:O	2:D:337:ASN:HB2	2.16	0.45
4:F:263:PHE:N	4:F:263:PHE:CD2	2.84	0.45
4:F:198:LYS:HE3	4:F:239:HIS:HA	1.99	0.45
2:D:169:VAL:HA	2:D:202:ILE:O	2.17	0.45
1:A:175:PRO:HA	1:A:178:SER:HB3	1.98	0.44
2:B:284:LEU:HD22	2:B:289:LEU:HD13	1.99	0.44
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.32	0.44
2:D:73:MET:HG2	2:D:90:PHE:HD2	1.83	0.44
1:A:292:THR:O	1:A:295:CYS:HB2	2.18	0.44
2:B:46:ARG:HG2	2:B:46:ARG:NH1	2.30	0.44
2:D:345:ILE:HG22	2:D:348:ASN:HB3	1.98	0.44
1:A:60:LYS:NZ	1:A:85:GLN:O	2.41	0.44
2:D:178:THR:O	2:D:181:GLU:HG3	2.17	0.44
3:E:58:GLU:HG3	3:E:61:ARG:NH2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:109:GLY:HA3	2:B:147:MET:HG3	2.00	0.44
2:B:262:ARG:NE	2:B:429[A]:GLU:OE1	2.40	0.44
1:C:416:GLY:O	1:C:420[B]:GLU:HB2	2.18	0.44
2:D:310:TYR:O	2:D:342:VAL:HG22	2.17	0.44
3:E:139:LEU:C	3:E:140:LYS:HD3	2.38	0.44
1:A:22:GLU:HG3	1:A:83:TYR:CE1	2.53	0.44
2:D:36:TYR:CE1	2:D:38:GLY:HA3	2.52	0.44
2:B:4:ILE:O	2:B:62:ARG:HD2	2.18	0.44
2:B:237:THR:O	2:B:241:ARG:HG3	2.18	0.43
2:B:400:LYS:HE3	2:B:413:GLU:OE2	2.18	0.43
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.99	0.43
2:D:257:MET:CE	2:D:312:THR:HB	2.47	0.43
1:A:41:THR:OG1	1:A:44:GLY:O	2.36	0.43
1:C:333:ALA:O	1:C:337:THR:HG23	2.18	0.43
2:D:257:MET:O	2:D:259:PRO:HD3	2.17	0.43
4:F:243:HIS:HE1	4:F:247:LYS:NZ	2.16	0.43
2:B:39:ASP:OD2	2:B:39:ASP:N	2.50	0.43
1:A:41:THR:OG1	1:A:41:THR:O	2.35	0.43
2:B:174:LYS:HE3	2:B:205:GLU:CG	2.48	0.43
2:B:332:ASN:HD22	2:B:332:ASN:N	2.16	0.43
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.52	0.43
2:D:28:HIS:O	2:D:43:GLN:HB3	2.18	0.43
1:C:181:VAL:N	2:D:256:ASN:OD1	2.50	0.43
2:D:285:THR:HB	2:D:287:PRO:HD2	2.00	0.43
2:D:296:SER:HB3	2:D:305:PRO:HD2	2.00	0.43
4:F:161:LEU:HD23	4:F:169:LEU:HA	2.00	0.43
1:A:385:ALA:HB2	1:A:432:TYR:CG	2.53	0.43
2:D:102:ALA:HB1	2:D:409:GLU:HB3	2.01	0.43
3:E:60:ARG:HG3	3:E:60:ARG:NH1	2.34	0.43
4:F:151:SER:HB3	4:F:180:HIS:CD2	2.54	0.43
4:F:284:LEU:HA	4:F:284:LEU:HD12	1.79	0.43
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.54	0.43
2:D:2:ARG:C	2:D:131:GLN:HE21	2.22	0.43
4:F:244:CYS:SG	4:F:245:ILE:N	2.92	0.43
2:B:103:LYS:HA	2:B:107:THR:OG1	2.19	0.42
1:C:293[A]:ASN:OD1	1:C:339:ARG:NH1	2.53	0.42
4:F:247:LYS:NZ	4:F:253:TYR:OH	2.53	0.42
2:B:190:HIS:CD2	2:B:422:ASN:OD1	2.72	0.42
2:D:86:ARG:HH22	2:D:122:LYS:NZ	2.17	0.42
3:E:75:LYS:O	3:E:79:GLU:HG3	2.20	0.42
4:F:87:LEU:O	4:F:88:SER:HB3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:LEU:HD23	1:C:70:LEU:HA	1.71	0.42
1:C:401:LYS:HG3	2:D:344:TRP:CE3	2.55	0.42
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.55	0.42
2:B:67:ASP:O	2:B:92:PHE:HA	2.20	0.42
1:A:209:ILE:HD11	1:A:302:MET:SD	2.60	0.42
2:B:153:SER:OG	3:E:76:ARG:NH2	2.50	0.42
4:F:195:GLY:HA3	4:F:197:ARG:HD3	2.01	0.42
1:A:134:GLY:HA3	1:A:165:SER:O	2.20	0.42
2:B:190:HIS:O	2:B:193:VAL:HG12	2.20	0.42
1:C:147:SER:HB2	1:C:190:THR:HB	2.02	0.42
2:B:12:CYS:HB2	9:B:501:GDP:C8	2.55	0.42
1:C:204:VAL:HG13	1:C:302:MET:HG3	2.02	0.42
2:D:246:LEU:HD23	2:D:246:LEU:HA	1.87	0.42
2:B:36:TYR:O	2:B:37:HIS:ND1	2.52	0.41
2:B:73:MET:CE	2:B:92:PHE:HB3	2.50	0.41
2:B:192:LEU:HD22	2:B:196:THR:HG21	2.01	0.41
2:D:47:ILE:HD12	2:D:47:ILE:HA	1.83	0.41
4:F:151:SER:HB3	4:F:180:HIS:NE2	2.35	0.41
1:A:188:ILE:HD12	1:A:425:MET:HG3	2.01	0.41
1:A:276:ILE:HD12	1:A:283:HIS:CE1	2.55	0.41
2:D:211:CYS:HA	2:D:215:LEU:HB2	2.01	0.41
4:F:74:LYS:NZ	4:F:331:GLU:OE1	2.52	0.41
4:F:80:LEU:O	4:F:84:SER:HB2	2.20	0.41
4:F:280:GLU:HA	4:F:284:LEU:HB2	2.01	0.41
1:A:81:GLY:O	1:A:84:ARG:NH1	2.52	0.41
1:A:81:GLY:O	1:A:84:ARG:HG2	2.21	0.41
1:A:298:PRO:HA	1:A:301:GLN:CD	2.41	0.41
1:C:217:LEU:HD21	1:C:368:LEU:HD23	2.02	0.41
3:E:53:LYS:HE2	3:E:53:LYS:HB3	1.89	0.41
2:D:273:LEU:HD23	2:D:273:LEU:HA	1.93	0.41
1:A:7:ILE:HG12	1:A:66:VAL:HG12	2.03	0.41
2:D:6:HIS:CE1	2:D:21:TRP:HE1	2.39	0.41
2:D:85:PHE:N	2:D:85:PHE:CD1	2.89	0.41
4:F:262:MET:HE3	4:F:262:MET:HB3	1.71	0.41
2:B:19:LYS:HB3	2:B:19:LYS:HE3	1.69	0.41
1:C:54:SER:O	1:C:61:HIS:HA	2.21	0.41
1:C:430:LYS:HE2	1:C:434:GLU:OE2	2.20	0.41
2:D:293:MET:HE2	2:D:375:PHE:HB2	2.03	0.41
1:C:12:ALA:HB3	1:C:140:SER:HB3	2.03	0.41
2:D:215:LEU:HB3	2:D:217:LEU:HD13	2.02	0.41
1:A:114:ILE:O	1:A:118:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:280:GLN:HG3	2:B:281:TYR:H	1.85	0.41
2:B:293:MET:HE3	2:B:373:ALA:HB1	2.03	0.41
2:B:294:PHE:HB3	10:B:504:MES:C3	2.51	0.41
1:C:93:ILE:HD11	1:C:121:ARG:HG3	2.02	0.41
1:C:313:MET:HE3	1:C:346:TRP:HZ2	1.85	0.41
2:D:101:TRP:NE1	2:D:146:GLY:HA2	2.36	0.41
2:D:385:LEU:HD23	2:D:385:LEU:C	2.41	0.41
4:F:4:PHE:CZ	4:F:29:ARG:HB2	2.56	0.41
2:B:117:LEU:HD11	2:B:154:LYS:HB3	2.02	0.41
2:D:67:ASP:HA	2:D:143:THR:HG21	2.02	0.41
4:F:277:THR:HG22	4:F:278:THR:H	1.86	0.41
4:F:307:LEU:HD12	4:F:307:LEU:HA	1.92	0.41
1:A:215:ARG:NH2	1:A:299:ALA:HB1	2.36	0.40
2:B:157:GLU:HB2	3:E:72:LEU:HD13	2.03	0.40
4:F:21:LEU:HD22	4:F:27:TRP:CD2	2.56	0.40
1:A:26:LEU:HD23	1:A:26:LEU:HA	1.83	0.40
1:A:154:MET:HG3	1:A:194:THR:CG2	2.41	0.40
2:B:262:ARG:NH2	2:B:429[A]:GLU:OE2	2.51	0.40
2:D:24:ILE:O	2:D:28:HIS:HD2	2.05	0.40
1:C:316:CYS:O	1:C:377:MET:HG3	2.21	0.40
4:F:326:LYS:HE2	4:F:328:TRP:CH2	2.56	0.40
4:F:282:SER:HB2	4:F:325:LEU:HD22	2.03	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	439/450 (98%)	421 (96%)	18 (4%)	0	100	100
1	C	445/450 (99%)	436 (98%)	9 (2%)	0	100	100
2	B	424/445 (95%)	406 (96%)	18 (4%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	416/445 (94%)	390 (94%)	26 (6%)	0	100	100
3	E	121/143 (85%)	118 (98%)	3 (2%)	0	100	100
4	F	343/384 (89%)	328 (96%)	15 (4%)	0	100	100
All	All	2188/2317 (94%)	2099 (96%)	89 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	371/378 (98%)	365 (98%)	6 (2%)	62	86
1	C	378/378 (100%)	369 (98%)	9 (2%)	49	79
2	B	370/383 (97%)	358 (97%)	12 (3%)	39	73
2	D	361/383 (94%)	339 (94%)	22 (6%)	18	48
3	E	112/127 (88%)	107 (96%)	5 (4%)	27	61
4	F	315/342 (92%)	294 (93%)	21 (7%)	16	43
All	All	1907/1991 (96%)	1832 (96%)	75 (4%)	33	66

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	SER
1	A	221	ARG
1	A	250	VAL
1	A	256	GLN
1	A	264	ARG
1	A	413	MET
2	B	2	ARG
2	B	41	ASP
2	B	75	SER
2	B	126	SER

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Mol	Chain	Res	Type
2	B	137	HIS
2	B	147	MET
2	B	190	HIS
2	B	214	THR
2	B	219	THR
2	B	281	TYR
2	B	322	SER
2	B	367	ARG
1	C	71	GLU
1	C	218	ASP
1	C	251	ASP
1	C	280	LYS
1	C	315[A]	CYS
1	C	315[B]	CYS
1	C	339	ARG
1	C	347[A]	CYS
1	C	347[B]	CYS
2	D	73	MET
2	D	84	ILE
2	D	92	PHE
2	D	115	SER
2	D	126	SER
2	D	137	HIS
2	D	153	SER
2	D	161	ASP
2	D	164	MET
2	D	177	ASP
2	D	178	THR
2	D	180	VAL
2	D	205	GLU
2	D	212	PHE
2	D	221	THR
2	D	246	LEU
2	D	306	ARG
2	D	322	SER
2	D	332	ASN
2	D	344	TRP
2	D	370	LYS
2	D	394	THR
3	E	65	GLU
3	E	70	LYS
3	E	104	LYS

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Mol	Chain	Res	Type
3	E	107	SER
3	E	138	GLU
4	F	1	MET
4	F	12	SER
4	F	18	SER
4	F	32	LYS
4	F	45	ASN
4	F	73	ARG
4	F	128	ARG
4	F	152	SER
4	F	160	ILE
4	F	211	TYR
4	F	222	ARG
4	F	230	SER
4	F	235	ASP
4	F	237	THR
4	F	271[A]	LEU
4	F	271[B]	LEU
4	F	277	THR
4	F	296[A]	MET
4	F	296[B]	MET
4	F	320	MET
4	F	379	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	61	HIS
1	A	88	HIS
1	A	329	ASN
2	B	332	ASN
1	C	301	GLN
2	D	8	GLN
3	E	18	GLN
4	F	26	GLN
4	F	145	ASN
4	F	243	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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 13 ligands modelled in this entry, 6 are monoatomic - leaving 7 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$
10	MES	B	503	-	12,12,12	1.83	2 (16%)	14,16,16	3.14	10 (71%)
9	GDP	D	501	-	24,30,30	1.04	2 (8%)	30,47,47	1.17	3 (10%)
11	7PU	B	505	-	31,32,32	1.79	8 (25%)	39,44,44	1.54	5 (12%)
5	GTP	A	501	6	26,34,34	1.14	2 (7%)	32,54,54	1.39	4 (12%)
5	GTP	C	501	6	26,34,34	1.36	3 (11%)	32,54,54	1.51	7 (21%)
10	MES	B	504	-	12,12,12	1.80	1 (8%)	14,16,16	2.79	8 (57%)
9	GDP	B	501	6	24,30,30	1.00	1 (4%)	30,47,47	1.26	5 (16%)

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
10	MES	B	503	-	-	4/6/14/14	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GDP	D	501	-	-	4/12/32/32	0/3/3/3
11	7PU	B	505	-	-	2/20/22/22	0/4/4/4
5	GTP	A	501	6	-	4/18/38/38	0/3/3/3
5	GTP	C	501	6	-	5/18/38/38	0/3/3/3
10	MES	B	504	-	-	2/6/14/14	0/1/1/1
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	504	MES	C8-S	-5.87	1.69	1.77
10	B	503	MES	C8-S	-5.73	1.69	1.77
11	B	505	7PU	C25-N24	5.20	1.47	1.35
5	C	501	GTP	C5-C6	-4.29	1.38	1.47
11	B	505	7PU	C12-N14	4.21	1.46	1.38
11	B	505	7PU	C08-N07	3.95	1.45	1.38
5	A	501	GTP	C5-C6	-3.70	1.39	1.47
11	B	505	7PU	C01-N24	2.75	1.47	1.41
9	D	501	GDP	C6-N1	-2.70	1.33	1.37
11	B	505	7PU	C15-N14	2.56	1.46	1.40
11	B	505	7PU	C27-C25	2.54	1.56	1.51
9	D	501	GDP	C2'-C1'	-2.36	1.50	1.53
11	B	505	7PU	C05-N07	2.31	1.45	1.40
5	A	501	GTP	C2-N3	2.26	1.38	1.33
5	C	501	GTP	C5-C4	-2.22	1.37	1.43
11	B	505	7PU	O26-C25	-2.14	1.19	1.23
5	C	501	GTP	PG-O1G	2.08	1.57	1.50
9	B	501	GDP	C2'-C1'	-2.04	1.50	1.53
10	B	503	MES	O2S-S	2.04	1.51	1.45

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	505	7PU	N11-C10-N09	-5.48	120.04	128.60
10	B	503	MES	C5-N4-C3	5.06	120.22	108.83
10	B	503	MES	C2-C3-N4	-4.96	102.58	110.10
10	B	504	MES	C2-C3-N4	-4.84	102.76	110.10
10	B	503	MES	O3S-S-C8	4.77	113.48	105.77
11	B	505	7PU	C29-C27-C25	4.40	121.33	117.21
10	B	504	MES	C5-N4-C3	4.38	118.70	108.83
10	B	503	MES	C7-N4-C5	4.12	121.76	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	503	MES	O2S-S-C8	4.11	111.86	106.92
10	B	504	MES	C7-N4-C3	4.00	121.47	111.23
5	C	501	GTP	C8-N7-C5	3.72	110.07	102.99
5	A	501	GTP	C8-N7-C5	3.55	109.76	102.99
10	B	504	MES	O2S-S-C8	3.55	111.19	106.92
5	C	501	GTP	PB-O3B-PG	-3.26	121.65	132.83
10	B	504	MES	C7-N4-C5	3.17	119.34	111.23
10	B	504	MES	C6-C5-N4	-3.17	105.30	110.10
5	A	501	GTP	C5-C6-N1	3.09	119.41	113.95
11	B	505	7PU	C15-N14-C12	-3.03	120.79	128.74
5	A	501	GTP	C2-N1-C6	-2.99	119.60	125.10
5	C	501	GTP	C5-C6-N1	2.94	119.15	113.95
10	B	504	MES	O3S-S-C8	2.91	110.47	105.77
10	B	503	MES	O1-C6-C5	2.80	117.96	111.80
9	D	501	GDP	PA-O3A-PB	-2.78	123.28	132.83
9	D	501	GDP	C8-N7-C5	2.55	107.84	102.99
9	B	501	GDP	C5-C6-N1	2.54	118.44	113.95
10	B	503	MES	C6-O1-C2	2.47	118.13	109.89
9	B	501	GDP	C8-N7-C5	2.46	107.67	102.99
10	B	503	MES	O3S-S-O1S	-2.42	105.35	111.27
9	B	501	GDP	O6-C6-C5	-2.41	119.66	124.37
5	C	501	GTP	N2-C2-N1	2.38	121.78	116.71
11	B	505	7PU	C13-C12-N11	-2.35	119.48	122.75
5	C	501	GTP	N1-C2-N3	-2.29	119.03	123.32
9	B	501	GDP	PA-O3A-PB	-2.28	125.01	132.83
9	D	501	GDP	C5-C6-N1	2.27	117.96	113.95
5	C	501	GTP	C2-N1-C6	-2.27	120.92	125.10
10	B	503	MES	O3S-S-O2S	-2.19	105.91	111.27
5	A	501	GTP	PA-O3A-PB	-2.17	125.39	132.83
10	B	504	MES	C6-O1-C2	2.15	117.06	109.89
5	C	501	GTP	C5'-C4'-C3'	-2.13	107.21	115.18
10	B	503	MES	C7-N4-C3	2.12	116.67	111.23
11	B	505	7PU	C10-N11-C12	2.12	122.26	115.25
9	B	501	GDP	O5'-C5'-C4'	-2.03	102.01	108.99

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O1A
10	B	503	MES	C8-C7-N4-C5
10	B	503	MES	C7-C8-S-O2S
10	B	503	MES	C7-C8-S-O3S
10	B	504	MES	C8-C7-N4-C3
10	B	504	MES	C8-C7-N4-C5
5	A	501	GTP	PB-O3B-PG-O2G
9	B	501	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O2A
10	B	503	MES	C7-C8-S-O1S
5	C	501	GTP	C4'-C5'-O5'-PA
11	B	505	7PU	C16-C15-N14-C12
9	D	501	GDP	PA-O3A-PB-O3B
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O3A
11	B	505	7PU	N09-C08-N07-C05

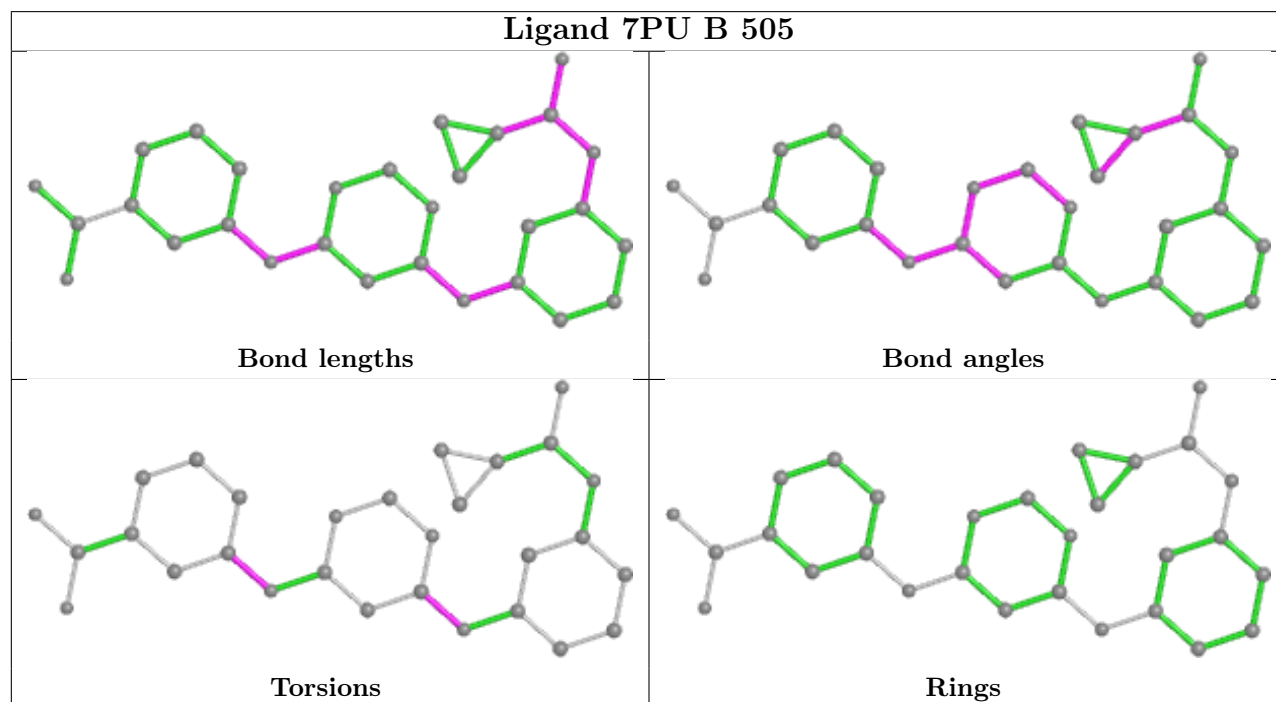
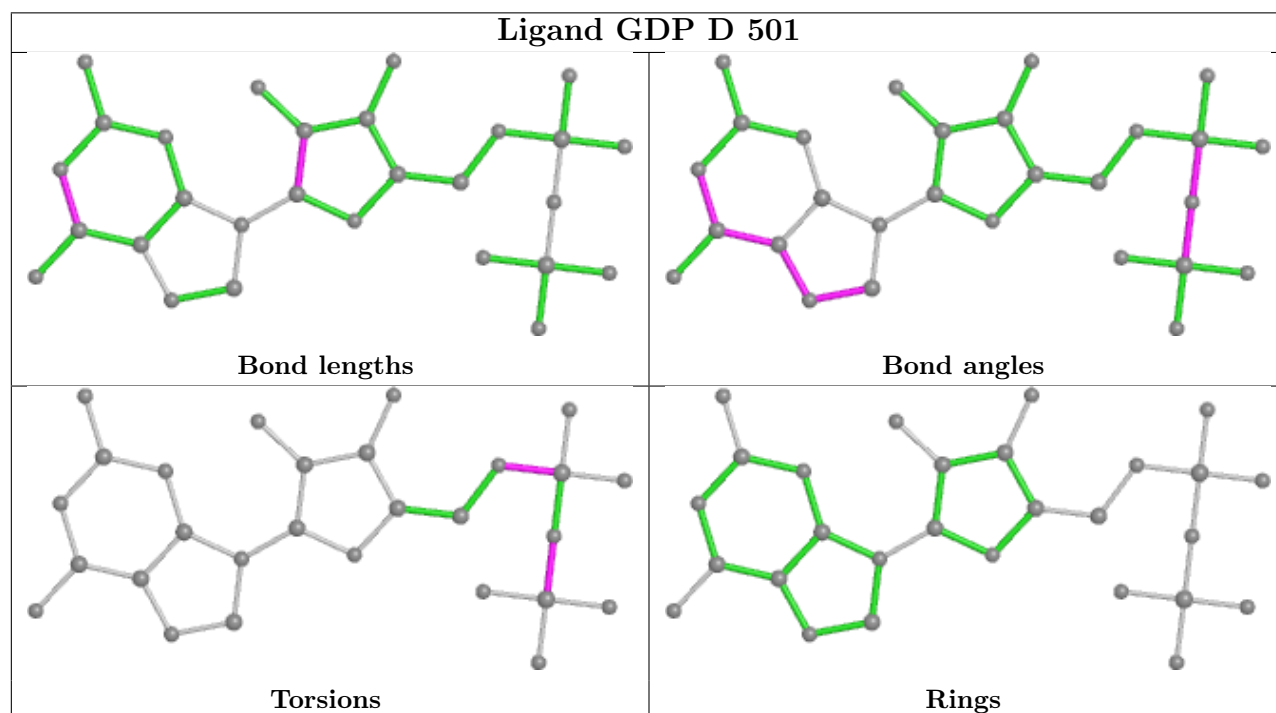
There are no ring outliers.

5 monomers are involved in 6 short contacts:

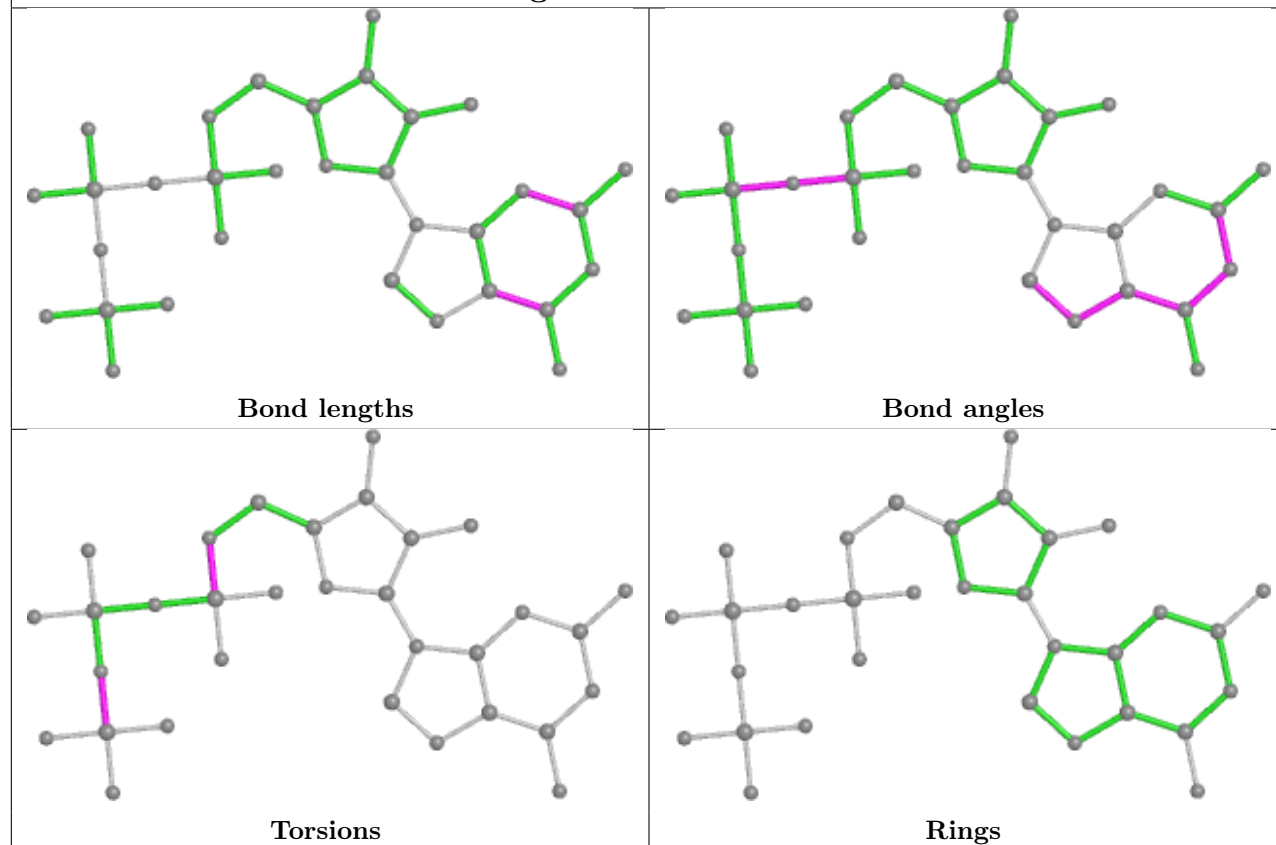
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	503	MES	1	0
9	D	501	GDP	2	0
5	A	501	GTP	1	0
10	B	504	MES	1	0
9	B	501	GDP	1	0

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.

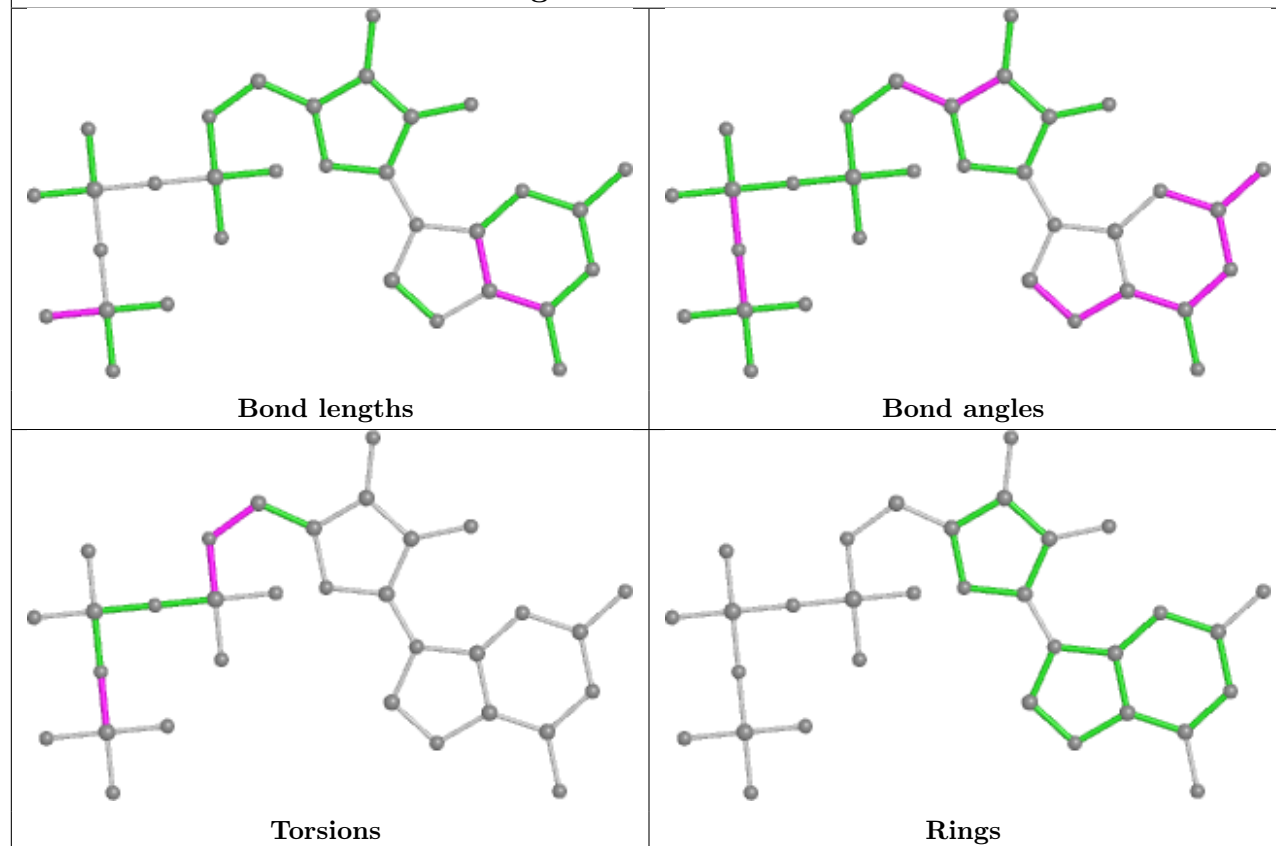
The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

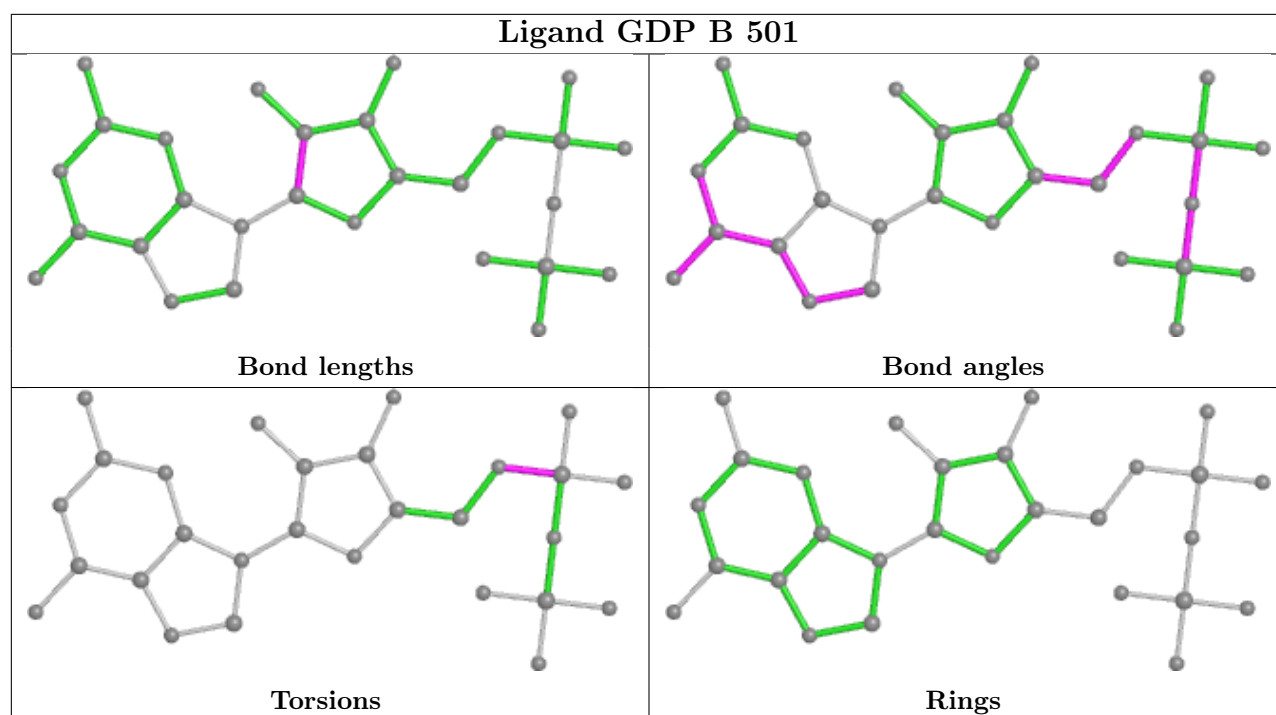


Ligand GTP A 501



Ligand GTP C 501





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	437/450 (97%)	0.16	2 (0%) 91 91	32, 49, 71, 90	0
1	C	440/450 (97%)	0.11	0 100 100	23, 41, 65, 85	0
2	B	424/445 (95%)	0.14	2 (0%) 91 91	28, 47, 75, 106	1 (0%)
2	D	420/445 (94%)	0.66	32 (7%) 13 10	36, 74, 103, 121	2 (0%)
3	E	123/143 (86%)	0.36	6 (4%) 29 26	40, 71, 107, 132	0
4	F	346/384 (90%)	1.16	69 (19%) 1 0	41, 75, 134, 152	0
All	All	2190/2317 (94%)	0.41	111 (5%) 28 24	23, 56, 104, 152	3 (0%)

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	169	LEU	7.0
4	F	233	PHE	6.5
4	F	159	GLY	5.8
4	F	152	SER	5.8
2	D	72	THR	5.5
4	F	182	ILE	5.4
4	F	149	ALA	5.2
4	F	239	HIS	5.2
4	F	225	SER	5.1
4	F	252	ASN	5.1
4	F	242	ASN	5.0
4	F	173	ILE	5.0
4	F	240	LEU	4.9
4	F	161	LEU	4.9
4	F	133	ALA	4.8
4	F	245	ILE	4.7
4	F	232	ASN	4.5
4	F	147	TRP	4.2
2	D	59	TYR	4.2

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Mol	Chain	Res	Type	RSRZ
4	F	100	ILE	4.2
2	D	44	LEU	4.1
4	F	231	ALA	4.0
2	D	37	HIS	4.0
2	D	175	VAL	3.9
4	F	255[A]	ARG	3.8
4	F	166	ALA	3.7
4	F	170	LEU	3.5
2	D	140	GLY	3.4
2	D	101	TRP	3.4
2	D	73	MET	3.4
2	D	30	ILE	3.4
2	D	273	LEU	3.4
4	F	224	SER	3.4
2	D	39	ASP	3.3
2	D	215	LEU	3.3
4	F	251	LYS	3.3
2	D	216	LYS	3.3
2	D	80	PRO	3.2
4	F	198	LYS	3.2
2	D	100	ASN	3.2
4	F	185	TYR	3.2
4	F	160	ILE	3.1
4	F	380	HIS	3.1
4	F	162	ILE	3.1
4	F	136	ASN	3.1
4	F	256	TYR	3.1
2	D	48	ASN	3.1
4	F	197	ARG	3.0
4	F	167	SER	2.9
4	F	176	GLN	2.9
4	F	253	TYR	2.9
3	E	54	LEU	2.9
4	F	164	SER	2.8
3	E	138	GLU	2.8
2	D	36	TYR	2.8
4	F	220[A]	VAL	2.7
4	F	223	THR	2.7
4	F	238	CYS	2.7
2	D	171	PRO	2.6
2	D	245	GLN	2.6
2	D	55	THR	2.6

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Mol	Chain	Res	Type	RSRZ
2	D	411	MET	2.6
4	F	249	TYR	2.6
4	F	179	VAL	2.6
2	D	402	PHE	2.6
2	D	84	ILE	2.6
4	F	186	LEU	2.6
4	F	177	GLY	2.5
4	F	148	ILE	2.5
3	E	48	GLU	2.5
2	B	282	ARG	2.5
4	F	181	VAL	2.5
4	F	236	LYS	2.5
2	D	53	GLU	2.5
4	F	9	GLU	2.5
4	F	134	ALA	2.5
4	F	8	ASP	2.5
4	F	246	GLN	2.4
4	F	104	ASN	2.4
4	F	135	TYR	2.4
4	F	320	MET	2.4
2	D	85	PHE	2.4
1	A	262	TYR	2.4
4	F	150	LYS	2.4
4	F	190	LEU	2.4
4	F	244	CYS	2.3
4	F	171	ASP	2.3
2	D	47	ILE	2.3
4	F	321	VAL	2.3
3	E	45	PRO	2.3
4	F	247	LYS	2.2
4	F	199	PHE	2.2
2	D	81	PHE	2.2
4	F	20	LEU	2.2
4	F	191	LEU	2.2
4	F	234	GLN	2.2
2	D	170	MET	2.2
2	B	276	ARG	2.2
2	D	116	VAL	2.1
2	D	102	ALA	2.1
2	D	406	TYR	2.1
1	A	86	LEU	2.1
4	F	146	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
3	E	61	ARG	2.1
4	F	102	PRO	2.1
3	E	44	ASP	2.1
4	F	184	LYS	2.1
2	D	64	ILE	2.0
4	F	175	GLU	2.0
4	F	138	ARG	2.0
4	F	235	ASP	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 monosaccharides in this entry.

6.4 Ligands [i](#)

LIGAND-RSR INFOmissingINFO

6.5 Other polymers [i](#)

There are no such residues in this entry.