



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 12, 2022 – 06:17 PM JST

PDB ID : 7VMG  
Title : Crystal structure of tubulin with 17j  
Authors : Jifa, Z.; Lun, T.  
Deposited on : 2021-10-08  
Resolution : 2.39 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<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>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (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

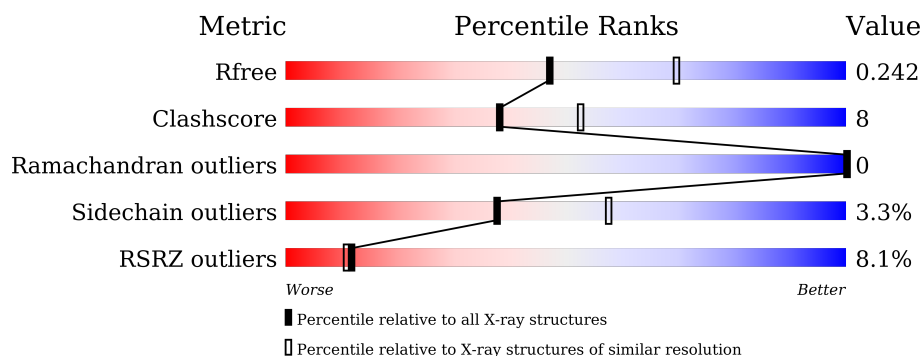
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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  $\geq 3$ , 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>2%</div> <div>85%</div> <div>12%</div> <div>•</div> </div>
1	C	450	<div> <div>2%</div> <div>83%</div> <div>14%</div> <div>••</div> </div>
2	B	445	<div> <div>2%</div> <div>82%</div> <div>13%</div> <div>• 5%</div> </div>
2	D	445	<div> <div>13%</div> <div>66%</div> <div>27%</div> <div>• 6%</div> </div>
3	E	143	<div> <div>13%</div> <div>65%</div> <div>17%</div> <div>• 14%</div> </div>
4	F	384	<div> <div>20%</div> <div>70%</div> <div>18%</div> <div>• 10%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	CL	D	503	-	-	-	X

## 2 Entry composition [i](#)

There are 12 unique types of molecules in this entry. The entry contains 17851 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	9	0
			3468	2195	585	663	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

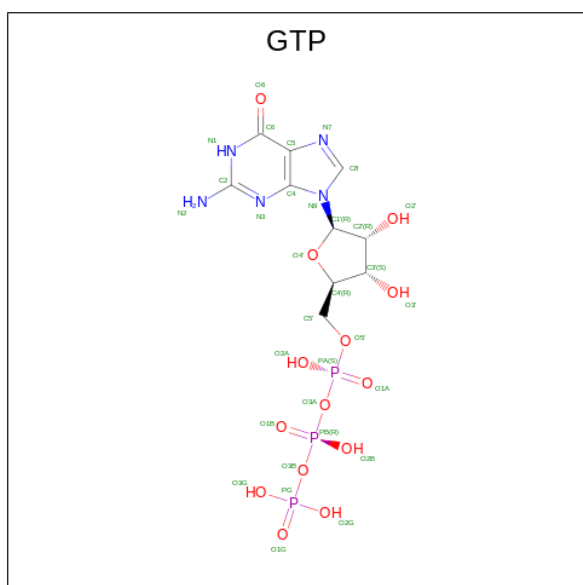
- Molecule 4 is a protein called TTL.

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	0	0
			1	1		

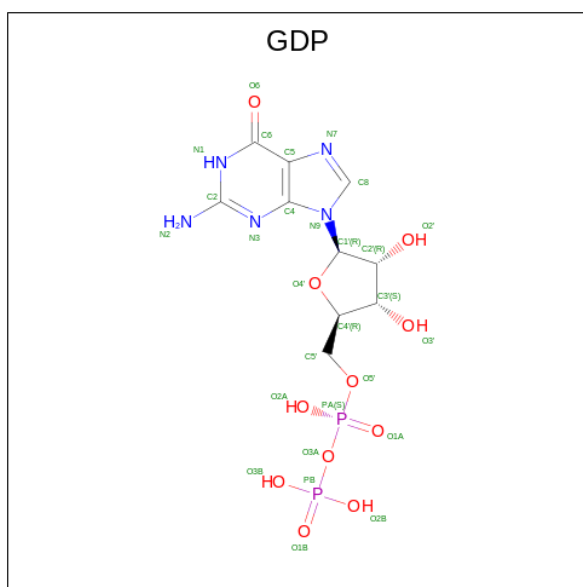
- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

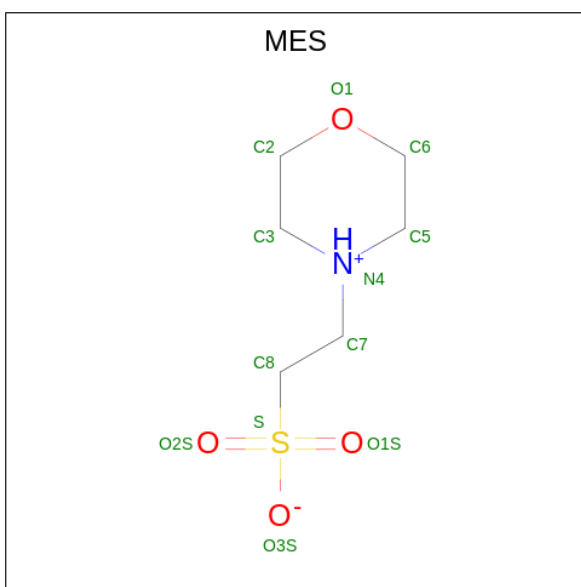
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	1	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

- 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		
8	D	1	Total	Cl	0	0
			1	1		

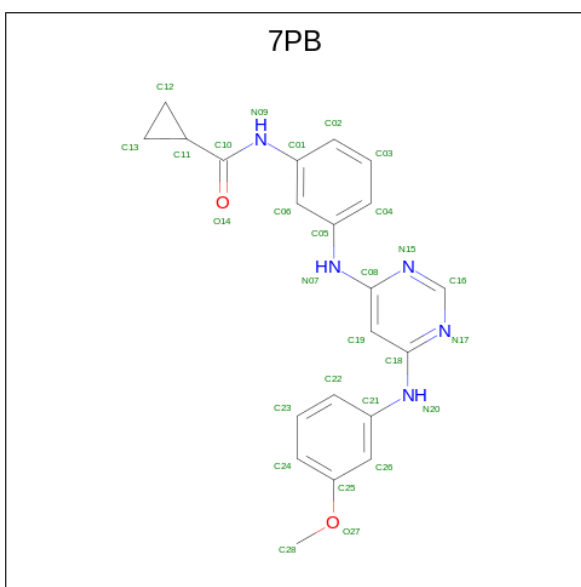
- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>11</sub>P<sub>2</sub>).





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-methoxyphenyl)amino]pyrimidin-4-yl]amino]phenyl]cyclopropanecarboxamide (three-letter code: 7PB) (formula: C<sub>21</sub>H<sub>21</sub>N<sub>5</sub>O<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			28	21	5	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	D	1	Total	C	N	O	0	0
			28	21	5	2		

- Molecule 12 is water.

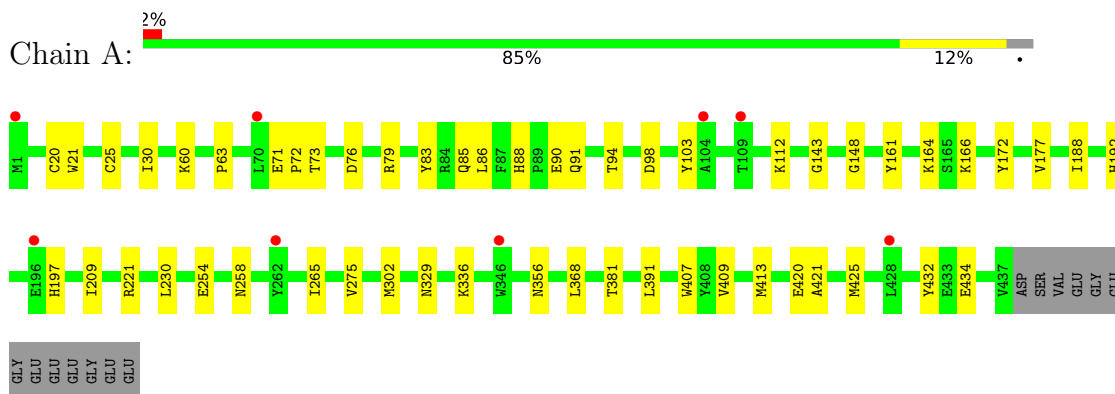
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	55	Total	O	0	0
			55	55		
12	B	51	Total	O	0	0
			51	51		
12	C	82	Total	O	0	0
			82	82		
12	D	4	Total	O	0	0
			4	4		
12	E	5	Total	O	0	0
			5	5		
12	F	15	Total	O	0	0
			15	15		



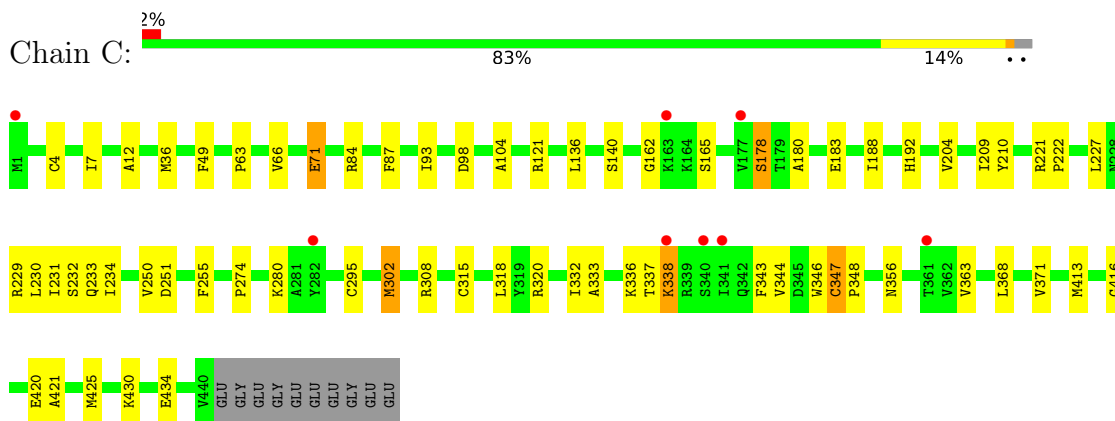
### 3 Residue-property plots [i](#)

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.

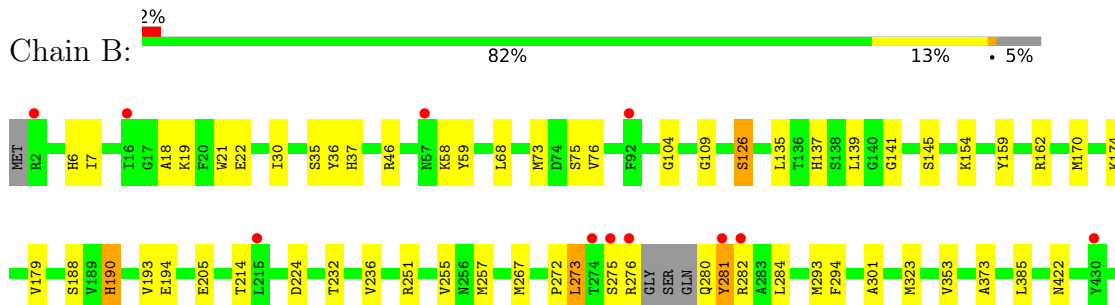
#### • Molecule 1: Tubulin alpha-1B chain

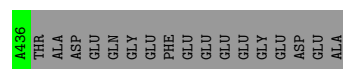


#### • Molecule 1: Tubulin alpha-1B chain

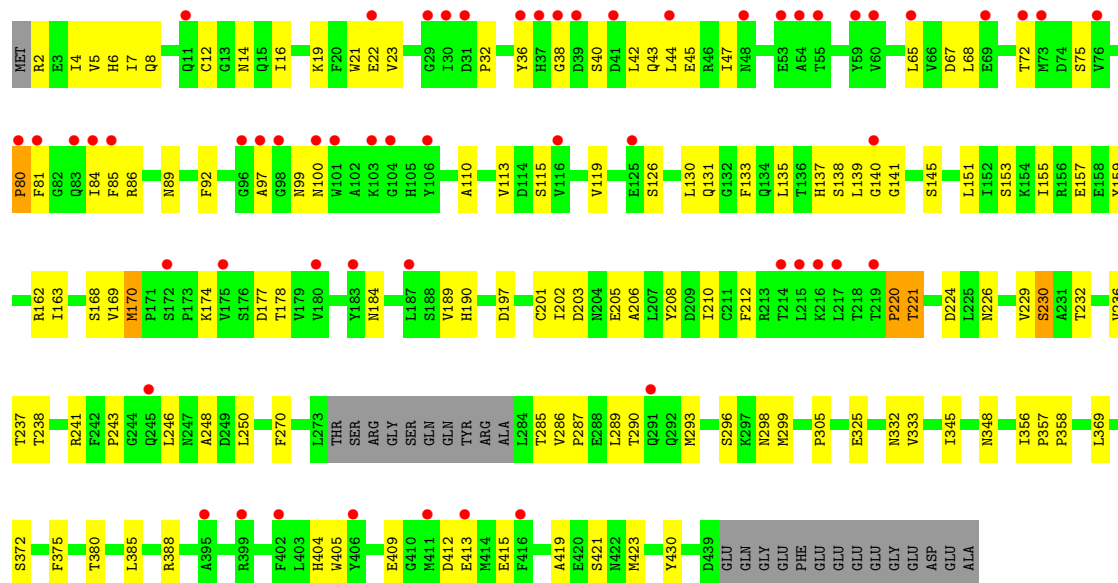


#### • Molecule 2: Tubulin beta-2B chain

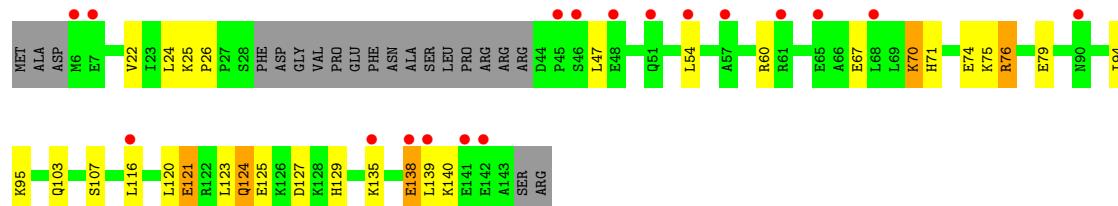




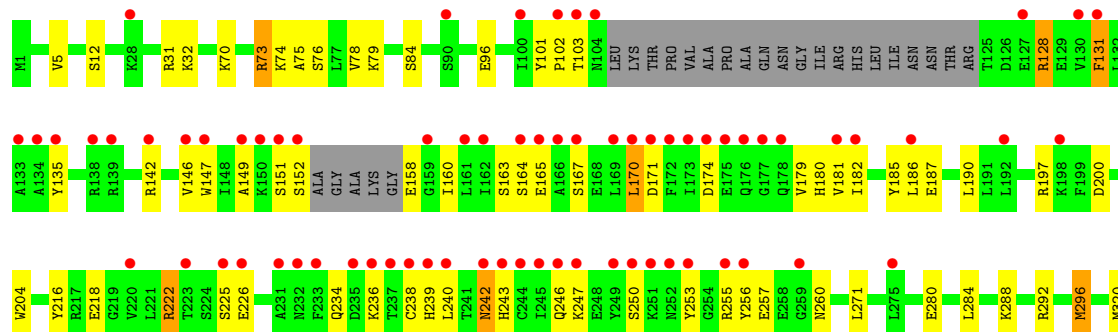
• Molecule 2: Tubulin beta-2B chain

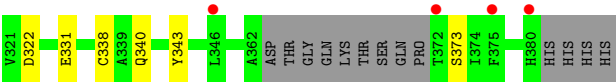


• Molecule 3: Stathmin-4



• Molecule 4: TTL





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.33Å 158.21Å 182.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.24 – 2.39 119.54 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.7 (91.24-2.39) 95.6 (119.54-2.39)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, $R_{free}$	0.210 , 0.250 0.204 , 0.242	Depositor DCC
$R_{free}$ test set	2000 reflections (1.65%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	52.2	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 50.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	17851	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CA, GDP, GTP, 7PB, MES, MG, CL

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	0.46	1/3517 (0.0%)	0.63	0/4776
1	C	0.53	2/3570 (0.1%)	0.68	1/4847 (0.0%)
2	B	0.52	1/3447 (0.0%)	0.68	1/4667 (0.0%)
2	D	0.47	0/3364	0.68	1/4560 (0.0%)
3	E	0.51	0/1041	0.67	0/1382
4	F	0.39	0/2935	0.61	0/3966
All	All	0.48	4/17874 (0.0%)	0.66	3/24198 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	F	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	281	TYR	CD2-CE2	-6.84	1.29	1.39
1	C	295	CYS	CB-SG	-5.71	1.72	1.81
1	A	20	CYS	CB-SG	-5.49	1.72	1.81
1	C	338	LYS	CD-CE	5.25	1.64	1.51

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	220	PRO	N-CA-C	6.12	128.03	112.10
1	C	338	LYS	CA-CB-CG	6.07	126.74	113.40
2	B	273	LEU	CA-CB-CG	-5.08	103.61	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	F	234	GLN	Peptide

## 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	3427	0	3340	34	0
1	C	3468	0	3388	38	0
2	B	3364	0	3249	41	0
2	D	3291	0	3155	86	0
3	E	1026	0	1042	26	0
4	F	2856	0	2837	50	0
5	A	32	0	12	2	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
8	D	1	0	0	0	0
9	B	28	0	12	1	0
9	D	28	0	12	1	0
10	B	24	0	26	4	0
11	B	28	0	0	1	0
11	D	28	0	0	2	0
12	A	55	0	0	1	0
12	B	51	0	0	0	0
12	C	82	0	0	2	0
12	D	4	0	0	1	0
12	E	5	0	0	0	0
12	F	15	0	0	0	0
All	All	17851	0	17085	265	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 8.

All (265) 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:B:251:ARG:NH2	10:B:503:MES:O1S	2.02	0.92
2:D:99:ASN:HD22	2:D:178:THR:HG21	1.39	0.87
1:A:112:LYS:HD2	3:E:54:LEU:HB3	1.56	0.87
2:D:131:GLN:HB2	2:D:250:LEU:HD12	1.57	0.86
1:A:88:HIS:NE2	1:A:90:GLU:HG3	1.98	0.79
2:B:36:TYR:O	2:B:37:HIS:ND1	2.15	0.79
1:C:229:ARG:HD2	1:C:363:VAL:HG11	1.64	0.78
4:F:128:ARG:HE	4:F:170:LEU:HD22	1.50	0.76
2:D:221:THR:HG23	2:D:224:ASP:H	1.51	0.76
4:F:128:ARG:HH21	4:F:170:LEU:HB3	1.52	0.73
2:D:206:ALA:O	2:D:210:ILE:HG13	1.87	0.73
1:A:60:LYS:NZ	1:A:85:GLN:O	2.23	0.71
1:A:88:HIS:CD2	1:A:90:GLU:HG3	2.27	0.69
2:D:221:THR:HG22	2:D:224:ASP:HB2	1.75	0.68
4:F:31:ARG:HE	4:F:32:LYS:H	1.40	0.68
2:B:251:ARG:CZ	10:B:503:MES:O1S	2.08	0.68
1:A:161:TYR:HB3	1:A:164:LYS:HD3	1.75	0.67
4:F:135:TYR:OH	4:F:165:GLU:HA	1.93	0.67
2:D:67:ASP:OD2	2:D:72:THR:HG21	1.95	0.67
2:B:280:GLN:HG3	2:B:281:TYR:H	1.59	0.67
2:D:220:PRO:O	2:D:221:THR:HG22	1.96	0.66
2:B:73:MET:HA	2:B:76:VAL:HG12	1.78	0.66
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.78	0.66
2:B:267:MET:HG3	2:B:301:ALA:HB3	1.80	0.64
2:D:99:ASN:ND2	2:D:178:THR:HG21	2.12	0.64
4:F:226:GLU:OE1	4:F:238:CYS:HB3	1.98	0.63
2:B:154:LYS:NZ	3:E:76:ARG:HD2	2.13	0.63
3:E:121:GLU:HA	3:E:124:GLN:HG2	1.81	0.62
2:D:65:LEU:HD11	2:D:85:PHE:HD2	1.64	0.61
4:F:246:GLN:O	4:F:250:SER:HB3	1.99	0.61
2:D:202:ILE:HD13	2:D:229:VAL:HG13	1.82	0.61
2:D:2:ARG:N	2:D:131:GLN:HG2	2.16	0.61
2:D:40:SER:H	2:D:43:GLN:HE22	1.49	0.61
2:D:236:VAL:O	11:D:502:7PB:N09	2.34	0.61
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.83	0.60
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.29	0.60
1:C:178:SER:HB2	1:C:183:GLU:OE2	2.00	0.60
2:D:141:GLY:HA3	9:D:501:GDP:O3A	2.01	0.60
2:D:139:LEU:HD21	2:D:168:SER:HB3	1.82	0.60
2:D:139:LEU:HA	2:D:145[A]:SER:HB3	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:MET:HG3	2:B:385:LEU:HD21	1.83	0.59
2:B:323:MET:SD	2:B:353:VAL:HG21	2.42	0.59
1:A:79:ARG:NH2	1:A:94:THR:OG1	2.35	0.58
4:F:128:ARG:HA	4:F:131:PHE:HB3	1.85	0.58
2:D:32:PRO:HB3	2:D:81:PHE:HA	1.86	0.58
2:D:221:THR:CG2	2:D:224:ASP:H	2.16	0.58
3:E:67:GLU:O	3:E:70:LYS:HE3	2.04	0.57
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.84	0.57
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.44	0.57
2:D:45:GLU:OE1	2:D:243:PRO:HG2	2.03	0.57
2:D:412:ASP:OD1	2:D:413:GLU:N	2.38	0.57
2:B:126:SER:OG	2:B:126:SER:O	2.23	0.57
4:F:103:THR:HG22	4:F:174:ASP:HB3	1.88	0.56
1:C:234:ILE:HD13	1:C:302:MET:SD	2.45	0.56
4:F:78:VAL:HG21	4:F:181:VAL:HG21	1.88	0.56
2:D:130:LEU:O	2:D:162:ARG:NH1	2.35	0.55
4:F:103:THR:N	4:F:174:ASP:OD1	2.39	0.55
2:D:44:LEU:HA	2:D:47:ILE:HB	1.87	0.55
4:F:236:LYS:HB2	4:F:240:LEU:HD22	1.87	0.55
2:D:285:THR:HB	2:D:287:PRO:HD2	1.87	0.55
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.72	0.55
2:B:145:SER:HB2	2:B:188:SER:OG	2.07	0.55
2:B:104:GLY:O	2:B:109:GLY:HA3	2.06	0.55
2:D:140:GLY:O	2:D:184:ASN:ND2	2.31	0.54
2:B:190:HIS:O	2:B:193:VAL:HG12	2.06	0.54
2:D:19:LYS:O	2:D:23:VAL:HG23	2.08	0.54
4:F:5:VAL:HG13	4:F:32:LYS:HA	1.89	0.54
2:B:174:LYS:HD2	2:B:205:GLU:OE1	2.08	0.54
2:D:16:ILE:HD11	2:D:169:VAL:HG21	1.89	0.53
2:B:236:VAL:O	11:B:505:7PB:N09	2.42	0.52
1:A:209:ILE:HD11	1:A:302:MET:SD	2.49	0.52
2:B:154:LYS:HZ3	3:E:76:ARG:HD2	1.74	0.52
2:B:224:ASP:OD1	2:B:276:ARG:NH2	2.41	0.52
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.92	0.52
2:B:18:ALA:O	2:B:22:GLU:HG3	2.10	0.52
2:D:189:VAL:HG11	2:D:423:MET:HG3	1.91	0.52
2:D:44:LEU:HD23	2:D:47:ILE:HD13	1.91	0.52
2:D:248:ALA:HB1	11:D:502:7PB:N07	2.24	0.52
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.45	0.51
2:D:36:TYR:CD2	2:D:44:LEU:HD11	2.46	0.51
4:F:190:LEU:HB2	4:F:322:ASP:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:155:ILE:O	2:D:159:TYR:N	2.40	0.51
2:D:270:PHE:O	2:D:298:ASN:HB3	2.11	0.51
2:B:275:SER:OG	2:B:276:ARG:N	2.44	0.51
3:E:60:ARG:HG3	3:E:60:ARG:HH11	1.76	0.51
2:D:65:LEU:HD11	2:D:85:PHE:CD2	2.46	0.51
3:E:47:LEU:HD12	3:E:47:LEU:O	2.11	0.51
2:D:293:MET:HE2	2:D:375:PHE:HB2	1.94	0.50
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.46	0.50
1:A:83:TYR:HD2	1:A:86:LEU:HD22	1.77	0.50
2:D:67:ASP:OD1	2:D:68:LEU:N	2.45	0.49
2:D:232:THR:O	2:D:236:VAL:HG13	2.12	0.49
4:F:186:LEU:HD12	4:F:320:MET:HE2	1.94	0.49
2:D:174:LYS:HD2	2:D:208:TYR:CD2	2.47	0.49
4:F:31:ARG:NE	4:F:32:LYS:H	2.09	0.49
1:C:84:ARG:HG2	1:C:84:ARG:HH11	1.77	0.49
4:F:151:SER:HB3	4:F:180:HIS:CE1	2.47	0.49
4:F:31:ARG:HE	4:F:31:ARG:HA	1.78	0.49
1:A:275:VAL:HG13	1:A:368:LEU:HD21	1.94	0.49
2:D:19:LYS:NZ	2:D:22:GLU:OE1	2.36	0.49
2:D:22:GLU:OE2	2:D:80:PRO:HG2	2.13	0.49
2:D:409:GLU:OE1	2:D:409:GLU:HA	2.12	0.49
1:A:177:VAL:O	1:A:177:VAL:HG22	2.12	0.48
1:C:227:LEU:O	1:C:231:ILE:HG13	2.13	0.48
3:E:116:LEU:O	3:E:120:LEU:HD12	2.13	0.48
2:B:281:TYR:O	2:B:281:TYR:CD1	2.66	0.48
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.49	0.48
3:E:70:LYS:HD2	3:E:71:HIS:N	2.28	0.48
3:E:124:GLN:HG3	3:E:125:GLU:N	2.28	0.48
4:F:74:LYS:NZ	4:F:331:GLU:OE1	2.46	0.48
3:E:60:ARG:HG3	3:E:60:ARG:NH1	2.29	0.48
4:F:247:LYS:NZ	4:F:253:TYR:OH	2.46	0.48
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.96	0.48
1:C:430:LYS:O	1:C:434:GLU:HG3	2.13	0.48
4:F:102:PRO:HA	4:F:174:ASP:OD1	2.14	0.48
1:A:83:TYR:CD2	1:A:86:LEU:HD22	2.49	0.48
4:F:31:ARG:HE	4:F:32:LYS:N	2.11	0.48
1:A:420:GLU:OE1	12:A:601:HOH:O	2.20	0.47
1:A:25:CYS:HB3	1:A:30:ILE:O	2.15	0.47
2:D:89:ASN:HA	2:D:119:VAL:HG11	1.95	0.47
3:E:70:LYS:O	3:E:74:GLU:HG3	2.13	0.47
3:E:75:LYS:O	3:E:79:GLU:HG3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ILE:HG23	1:A:425:MET:HG3	1.96	0.47
2:B:35:SER:OG	2:B:58:LYS:HE2	2.14	0.47
2:B:139:LEU:HA	2:B:145:SER:HB3	1.95	0.47
4:F:73:ARG:O	4:F:76:SER:HB2	2.14	0.47
1:C:250:VAL:HG22	1:C:255:PHE:CZ	2.48	0.47
1:C:255:PHE:CZ	1:C:318:LEU:HD22	2.50	0.47
2:D:6:HIS:HD1	2:D:21:TRP:HE1	1.62	0.47
1:A:166:LYS:HE2	1:A:197:HIS:O	2.14	0.47
3:E:139:LEU:C	3:E:140:LYS:HD3	2.34	0.47
4:F:292:ARG:NH1	4:F:296[B]:MET:SD	2.88	0.47
1:A:143:GLY:HA3	5:A:501:GTP:O3A	2.14	0.47
1:C:416:GLY:O	1:C:420[B]:GLU:HB2	2.15	0.47
2:D:4:ILE:HG12	2:D:250:LEU:HD11	1.97	0.47
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.50	0.46
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.97	0.46
2:D:246:LEU:HD23	2:D:246:LEU:HA	1.67	0.46
2:D:290:THR:HG22	2:D:333:VAL:HG21	1.96	0.46
4:F:103:THR:CG2	4:F:174:ASP:HB3	2.44	0.46
3:E:25:LYS:HD3	3:E:26:PRO:O	2.15	0.46
4:F:167:SER:O	4:F:171:ASP:HB2	2.15	0.46
1:C:204:VAL:HG13	1:C:302:MET:HG3	1.98	0.46
2:D:110:ALA:O	2:D:113:VAL:HG12	2.16	0.46
2:D:356:ILE:HD12	2:D:357:PRO:HD2	1.96	0.46
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.33	0.46
2:B:7:ILE:O	2:B:135:LEU:HA	2.15	0.46
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.98	0.46
2:D:12:CYS:CB	2:D:138:SER:HB3	2.46	0.45
2:D:36:TYR:CZ	2:D:38:GLY:HA3	2.51	0.45
2:D:100:ASN:ND2	2:D:405:TRP:HB3	2.32	0.45
4:F:75:ALA:O	4:F:79:LYS:HG3	2.16	0.45
4:F:260:ASN:N	4:F:260:ASN:HD22	2.15	0.45
1:C:332:ILE:O	1:C:336:LYS:HG2	2.16	0.45
4:F:151:SER:HB3	4:F:180:HIS:NE2	2.32	0.45
2:D:68:LEU:HD12	2:D:97:ALA:HB2	1.98	0.45
2:D:81:PHE:O	2:D:84:ILE:HG22	2.16	0.45
1:C:274:PRO:HG2	1:C:371:VAL:HG11	1.99	0.45
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.17	0.45
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.89	0.44
4:F:255[B]:ARG:HD3	4:F:256:TYR:CE1	2.52	0.44
1:C:104:ALA:HB2	1:C:413:MET:SD	2.57	0.44
1:C:320:ARG:HA	1:C:356:ASN:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:237:THR:O	2:D:241:ARG:HG3	2.17	0.44
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.17	0.44
1:A:192:HIS:CG	1:A:421:ALA:HA	2.53	0.44
2:D:203:ASP:OD2	2:D:388:ARG:NH1	2.44	0.44
4:F:31:ARG:NE	4:F:31:ARG:HA	2.32	0.44
4:F:243:HIS:ND1	4:F:243:HIS:O	2.50	0.44
1:A:72:PRO:HB2	1:A:76:ASP:OD2	2.17	0.44
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.52	0.44
2:B:154:LYS:HZ1	3:E:76:ARG:HD2	1.81	0.44
2:B:294:PHE:HB3	10:B:504:MES:H31	1.98	0.44
1:C:229:ARG:O	1:C:232:SER:OG	2.34	0.44
2:D:6:HIS:CE1	2:D:21:TRP:HE1	2.35	0.44
4:F:284:LEU:O	4:F:288:LYS:HG3	2.17	0.44
2:D:7:ILE:O	2:D:135:LEU:HD12	2.17	0.44
2:D:163:ILE:HA	2:D:197:ASP:OD2	2.17	0.44
3:E:25:LYS:HD3	3:E:25:LYS:C	2.38	0.44
1:C:229:ARG:HD2	1:C:363:VAL:CG1	2.40	0.44
4:F:158:GLU:N	4:F:160:ILE:HD11	2.33	0.44
1:A:71:GLU:OE1	1:A:73:THR:OG1	2.29	0.44
1:C:233:GLN:HG3	1:C:368:LEU:HD12	2.00	0.43
2:D:221:THR:HG22	2:D:224:ASP:CB	2.45	0.43
1:A:409:VAL:HA	1:A:413:MET:O	2.18	0.43
2:D:170:MET:HE1	2:D:201:CYS:CA	2.48	0.43
3:E:135:LYS:O	3:E:138:GLU:HG3	2.18	0.43
4:F:200:ASP:OD1	4:F:222:ARG:NE	2.49	0.43
1:C:12:ALA:HB3	1:C:140:SER:HB3	2.00	0.43
1:A:88:HIS:HB3	1:A:91:GLN:OE1	2.18	0.43
2:B:159:TYR:HB3	2:B:162[B]:ARG:HG2	2.00	0.43
2:B:68:LEU:HA	2:B:68:LEU:HD23	1.74	0.43
2:D:404:HIS:CD2	2:D:405:TRP:HD1	2.36	0.43
4:F:146:VAL:HG23	4:F:187:GLU:OE2	2.18	0.43
2:B:30:ILE:HD13	2:B:59:TYR:HB2	2.01	0.43
2:D:8:GLN:NE2	2:D:14:ASN:HA	2.33	0.43
4:F:101:TYR:CD2	4:F:179:VAL:HG22	2.54	0.43
2:B:139:LEU:HD12	2:B:170:MET:SD	2.59	0.43
2:B:257:MET:HE3	2:B:257:MET:HB3	1.76	0.43
2:D:22:GLU:HG3	2:D:81:PHE:CD1	2.53	0.43
4:F:163:SER:OG	4:F:164:SER:N	2.51	0.43
1:C:93:ILE:HD11	1:C:121:ARG:HG3	2.00	0.42
1:C:308:ARG:HD2	12:C:664:HOH:O	2.19	0.42
2:D:296:SER:HB3	2:D:305:PRO:HD2	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:190:HIS:ND1	2:D:419:ALA:HA	2.34	0.42
4:F:242:ASN:OD1	4:F:242:ASN:N	2.52	0.42
4:F:340:GLN:HA	4:F:343:TYR:CD2	2.53	0.42
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.34	0.42
1:A:329:ASN:OD1	3:E:22:VAL:HG21	2.19	0.42
2:D:293:MET:HE3	2:D:293:MET:HB2	1.82	0.42
4:F:96:GLU:HG2	4:F:147:TRP:HH2	1.83	0.42
1:C:333:ALA:O	1:C:337:THR:HG23	2.20	0.42
2:D:5:VAL:HG13	2:D:133:PHE:CD2	2.55	0.42
2:B:293:MET:HE3	2:B:373:ALA:HB1	2.00	0.42
2:D:5:VAL:HG12	2:D:130:LEU:HD11	2.02	0.42
2:D:286:VAL:HB	2:D:325:GLU:HG2	2.01	0.42
2:D:157:GLU:HA	3:E:123:LEU:HD13	2.01	0.42
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.55	0.42
2:D:68:LEU:HD23	2:D:68:LEU:HA	1.90	0.42
2:D:345:ILE:HG22	2:D:348:ASN:HB3	2.01	0.42
2:B:190:HIS:CD2	2:B:422:ASN:OD1	2.73	0.42
2:B:272:PRO:HB3	2:B:284:LEU:HD22	2.02	0.42
1:C:192:HIS:CG	1:C:421:ALA:HA	2.55	0.42
2:D:380:THR:HA	2:D:430:TYR:CD1	2.55	0.42
1:C:36:MET:HE1	1:C:49:PHE:CE1	2.55	0.42
2:D:65:LEU:HD21	2:D:85:PHE:CE2	2.55	0.42
2:D:415:GLU:OE1	3:E:129:HIS:NE2	2.48	0.41
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.55	0.41
2:D:2:ARG:C	2:D:131:GLN:HE21	2.24	0.41
2:D:358:PRO:HB2	12:D:602:HOH:O	2.20	0.41
2:B:141:GLY:HA3	9:B:501:GDP:O3A	2.21	0.41
4:F:246:GLN:NE2	4:F:260:ASN:OD1	2.41	0.41
1:C:180:ALA:HB3	1:C:183:GLU:HG3	2.02	0.41
4:F:149:ALA:HB2	4:F:182:ILE:HG22	2.03	0.41
2:D:40:SER:N	2:D:43:GLN:HE22	2.16	0.41
1:A:72:PRO:HA	1:A:94:THR:HG21	2.02	0.41
1:C:356:ASN:ND2	12:C:607:HOH:O	2.53	0.41
2:D:40:SER:HB3	2:D:42:LEU:H	1.85	0.41
1:A:88:HIS:CD2	1:A:90:GLU:H	2.38	0.41
2:B:280:GLN:HG3	2:B:281:TYR:N	2.30	0.41
2:D:65:LEU:HD21	2:D:85:PHE:CD2	2.56	0.41
3:E:139:LEU:HB3	3:E:140:LYS:HE3	2.01	0.41
4:F:70:LYS:HB2	4:F:70:LYS:HE3	1.78	0.41
4:F:185:TYR:OH	4:F:239:HIS:HB3	2.21	0.41
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:296:SER:HA	2:D:299:MET:HG2	2.03	0.41
3:E:67:GLU:O	3:E:70:LYS:HG3	2.20	0.41
1:C:7:ILE:HG23	1:C:66:VAL:HG13	2.02	0.40
2:D:12:CYS:SG	2:D:138:SER:HB3	2.61	0.40
2:D:170:MET:HE1	2:D:201:CYS:C	2.41	0.40
1:A:407:TRP:CE2	2:B:255:VAL:HA	2.56	0.40
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.56	0.40
1:C:343:PHE:HD2	1:C:347[A]:CYS:SG	2.43	0.40
2:D:36:TYR:CE1	2:D:38:GLY:HA3	2.56	0.40
2:D:151:LEU:O	2:D:155:ILE:HG13	2.21	0.40
2:D:177:ASP:OD1	2:D:177:ASP:N	2.48	0.40
2:D:226:ASN:O	2:D:230:SER:HB2	2.22	0.40
4:F:204:TRP:CZ2	4:F:338:CYS:HA	2.56	0.40
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.56	0.40
2:B:19:LYS:HE3	2:B:19:LYS:HB3	1.66	0.40
2:B:273:LEU:HD23	2:B:273:LEU:HA	1.57	0.40
2:B:232:THR:O	2:B:236:VAL:HG13	2.22	0.40
1:C:338:LYS:HG2	1:C:338:LYS:O	2.22	0.40
3:E:95:LYS:HA	3:E:95:LYS:HD2	1.92	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%)	427 (97%)	12 (3%)	0	100	100
1	C	446/450 (99%)	437 (98%)	9 (2%)	0	100	100
2	B	424/445 (95%)	412 (97%)	12 (3%)	0	100	100
2	D	416/445 (94%)	397 (95%)	19 (5%)	0	100	100
3	E	121/143 (85%)	119 (98%)	2 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	F	343/384 (89%)	322 (94%)	21 (6%)	0	100	100
All	All	2189/2317 (94%)	2114 (97%)	75 (3%)	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%)	367 (99%)	4 (1%)	73	87
1	C	379/378 (100%)	367 (97%)	12 (3%)	39	59
2	B	370/383 (97%)	362 (98%)	8 (2%)	52	71
2	D	361/383 (94%)	341 (94%)	20 (6%)	21	35
3	E	112/127 (88%)	104 (93%)	8 (7%)	14	23
4	F	315/342 (92%)	299 (95%)	16 (5%)	24	39
All	All	1908/1991 (96%)	1840 (96%)	68 (4%)	38	54

All (68) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	ARG
1	A	356	ASN
1	A	381	THR
1	A	434	GLU
2	B	46	ARG
2	B	75	SER
2	B	126	SER
2	B	137	HIS
2	B	190	HIS
2	B	194	GLU
2	B	214	THR
2	B	282	ARG
1	C	71	GLU

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Mol	Chain	Res	Type
1	C	165[A]	SER
1	C	165[B]	SER
1	C	178	SER
1	C	221	ARG
1	C	251	ASP
1	C	280	LYS
1	C	302	MET
1	C	315[A]	CYS
1	C	315[B]	CYS
1	C	347[A]	CYS
1	C	347[B]	CYS
2	D	75	SER
2	D	80	PRO
2	D	86	ARG
2	D	92	PHE
2	D	115	SER
2	D	126	SER
2	D	137	HIS
2	D	153	SER
2	D	170	MET
2	D	205	GLU
2	D	212	PHE
2	D	221	THR
2	D	230	SER
2	D	238	THR
2	D	289	LEU
2	D	332	ASN
2	D	369	LEU
2	D	372	SER
2	D	385	LEU
2	D	421	SER
3	E	70	LYS
3	E	76	ARG
3	E	103	GLN
3	E	107	SER
3	E	121	GLU
3	E	124	GLN
3	E	127	ASP
3	E	138	GLU
4	F	12	SER
4	F	73	ARG
4	F	84	SER

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Mol	Chain	Res	Type
4	F	128	ARG
4	F	131	PHE
4	F	142	ARG
4	F	152	SER
4	F	170	LEU
4	F	222	ARG
4	F	225	SER
4	F	242	ASN
4	F	271[A]	LEU
4	F	271[B]	LEU
4	F	296[A]	MET
4	F	296[B]	MET
4	F	373	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	356	ASN
2	B	48	ASN
2	B	332	ASN
2	D	99	ASN
3	E	103	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 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	2	12,12,12	1.05	1 (8%)	14,16,16	3.11	4 (28%)
11	7PB	D	502	-	31,31,31	3.22	17 (54%)	42,42,42	4.77	21 (50%)
9	GDP	B	501	6	24,30,30	0.94	1 (4%)	30,47,47	1.47	5 (16%)
10	MES	B	504	-	12,12,12	1.51	1 (8%)	14,16,16	2.80	8 (57%)
11	7PB	B	505	-	31,31,31	2.46	11 (35%)	42,42,42	3.38	13 (30%)
9	GDP	D	501	-	24,30,30	0.90	1 (4%)	30,47,47	1.35	4 (13%)
5	GTP	C	501	6	26,34,34	1.14	2 (7%)	32,54,54	1.41	4 (12%)
5	GTP	A	501	6	26,34,34	1.07	2 (7%)	32,54,54	1.32	5 (15%)

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	2	-	3/6/14/14	0/1/1/1
11	7PB	D	502	-	-	0/18/20/20	0/4/4/4
9	GDP	B	501	6	-	3/12/32/32	0/3/3/3
10	MES	B	504	-	-	0/6/14/14	0/1/1/1
11	7PB	B	505	-	-	1/18/20/20	0/4/4/4
9	GDP	D	501	-	-	4/12/32/32	0/3/3/3
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
5	GTP	A	501	6	-	6/18/38/38	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	502	7PB	C08-N07	8.01	1.52	1.38
11	D	502	7PB	O27-C25	6.91	1.52	1.37
11	B	505	7PB	C08-N07	6.50	1.50	1.38
11	B	505	7PB	O27-C25	5.83	1.49	1.37
11	D	502	7PB	C21-N20	5.54	1.53	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	502	7PB	C10-N09	5.49	1.48	1.35
11	D	502	7PB	C18-N20	5.49	1.48	1.38
11	B	505	7PB	C21-N20	5.38	1.52	1.40
11	D	502	7PB	C01-N09	4.68	1.51	1.41
10	B	504	MES	C8-S	4.30	1.83	1.77
11	B	505	7PB	C18-N20	3.87	1.45	1.38
11	B	505	7PB	C10-N09	3.77	1.44	1.35
11	D	502	7PB	C05-N07	3.61	1.48	1.40
5	C	501	GTP	C5-C6	-3.61	1.40	1.47
11	D	502	7PB	C23-C22	3.46	1.46	1.38
5	A	501	GTP	C5-C6	-3.43	1.40	1.47
11	D	502	7PB	O27-C28	3.27	1.52	1.42
11	D	502	7PB	C16-N15	2.92	1.39	1.33
11	B	505	7PB	C05-N07	2.87	1.47	1.40
11	B	505	7PB	C23-C24	2.83	1.44	1.38
11	D	502	7PB	C23-C24	2.66	1.44	1.38
11	D	502	7PB	C06-C05	2.66	1.43	1.39
11	D	502	7PB	C13-C12	2.64	1.58	1.48
11	D	502	7PB	C03-C04	2.56	1.44	1.38
11	D	502	7PB	C02-C01	2.42	1.43	1.39
11	D	502	7PB	C16-N17	2.40	1.38	1.33
10	B	503	MES	C8-S	2.35	1.80	1.77
11	B	505	7PB	O27-C28	2.25	1.49	1.42
5	A	501	GTP	C2-N3	2.19	1.38	1.33
5	C	501	GTP	C2-N3	2.18	1.38	1.33
11	B	505	7PB	C16-N15	2.18	1.38	1.33
11	B	505	7PB	C01-N09	2.18	1.46	1.41
11	D	502	7PB	O14-C10	2.17	1.27	1.23
9	D	501	GDP	C6-N1	-2.13	1.34	1.37
11	B	505	7PB	C23-C22	2.11	1.43	1.38
9	B	501	GDP	C2'-C1'	-2.00	1.50	1.53

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	502	7PB	C13-C11-C10	-24.01	94.73	117.21
11	B	505	7PB	C12-C11-C10	-13.19	104.86	117.21
11	B	505	7PB	C13-C11-C10	-10.99	106.92	117.21
11	D	502	7PB	C12-C11-C10	-9.61	108.21	117.21
11	B	505	7PB	N17-C16-N15	-7.94	116.18	128.60
10	B	503	MES	O3S-S-O1S	-7.76	92.31	111.27
11	D	502	7PB	N17-C16-N15	-7.17	117.38	128.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	502	7PB	C04-C05-C06	6.19	126.98	119.65
10	B	503	MES	O3S-S-C8	5.54	114.73	105.77
10	B	504	MES	C5-N4-C3	5.11	120.33	108.83
11	B	505	7PB	O14-C10-C11	-5.08	115.50	122.12
11	D	502	7PB	C23-C22-C21	-4.91	113.85	119.72
10	B	503	MES	O1S-S-C8	4.90	112.82	106.92
11	D	502	7PB	C05-C06-C01	-4.47	112.86	119.64
11	D	502	7PB	C28-O27-C25	-4.30	108.17	117.51
10	B	504	MES	O3S-S-O2S	-4.17	101.09	111.27
11	D	502	7PB	C01-N09-C10	-4.08	117.64	127.40
11	B	505	7PB	C11-C10-N09	3.92	120.78	115.02
10	B	504	MES	C6-C5-N4	3.90	116.02	110.10
10	B	504	MES	O2S-S-C8	3.73	111.41	106.92
9	D	501	GDP	PA-O3A-PB	-3.64	120.34	132.83
5	A	501	GTP	C8-N7-C5	3.63	109.91	102.99
11	D	502	7PB	C02-C01-N09	-3.52	108.56	120.40
11	B	505	7PB	C04-C05-C06	3.44	123.73	119.65
11	D	502	7PB	C02-C01-C06	3.40	123.68	119.65
5	C	501	GTP	C8-N7-C5	3.40	109.46	102.99
11	D	502	7PB	C11-C10-N09	3.22	119.75	115.02
11	D	502	7PB	C04-C05-N07	-3.08	110.34	120.64
5	C	501	GTP	C5-C6-N1	3.00	119.26	113.95
11	D	502	7PB	C03-C04-C05	-2.95	116.20	119.72
9	B	501	GDP	O6-C6-C5	-2.94	118.64	124.37
10	B	503	MES	C5-N4-C3	2.90	115.35	108.83
10	B	504	MES	C7-N4-C5	-2.87	103.91	111.23
9	B	501	GDP	C8-N7-C5	2.87	108.45	102.99
9	B	501	GDP	PA-O3A-PB	-2.86	123.01	132.83
10	B	504	MES	C2-C3-N4	2.85	114.42	110.10
10	B	504	MES	O3S-S-C8	2.82	110.33	105.77
10	B	504	MES	C7-N4-C3	-2.77	104.16	111.23
11	B	505	7PB	C02-C01-C06	2.76	122.92	119.65
11	B	505	7PB	C05-C06-C01	-2.76	115.45	119.64
11	B	505	7PB	C21-N20-C18	-2.75	121.52	128.74
11	D	502	7PB	C22-C23-C24	2.74	124.14	120.25
5	C	501	GTP	C2-N1-C6	-2.70	120.12	125.10
9	B	501	GDP	C5-C6-N1	2.53	118.42	113.95
9	D	501	GDP	C8-N7-C5	2.51	107.77	102.99
5	A	501	GTP	C5'-C4'-C3'	-2.49	105.87	115.18
11	D	502	7PB	O14-C10-C11	-2.45	118.92	122.12
11	D	502	7PB	C21-N20-C18	-2.45	122.30	128.74
11	B	505	7PB	C16-N15-C08	2.45	123.37	115.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C5-C6-N1	2.37	118.14	113.95
11	B	505	7PB	C19-C08-N15	-2.37	119.45	122.75
11	B	505	7PB	C05-N07-C08	-2.34	122.61	128.74
11	B	505	7PB	C01-N09-C10	-2.33	121.83	127.40
11	D	502	7PB	C06-C01-N09	2.32	127.76	120.18
11	D	502	7PB	C16-N15-C08	2.31	122.92	115.25
11	D	502	7PB	C21-C26-C25	2.27	122.74	119.17
5	C	501	GTP	PA-O3A-PB	-2.17	125.39	132.83
9	D	501	GDP	C5-C6-N1	2.15	117.75	113.95
9	B	501	GDP	O2B-PB-O3A	2.14	111.81	104.64
11	D	502	7PB	C19-C08-N15	-2.11	119.80	122.75
5	A	501	GTP	PB-O3B-PG	-2.10	125.62	132.83
5	A	501	GTP	C2-N1-C6	-2.07	121.29	125.10
9	D	501	GDP	C3'-C2'-C1'	2.03	104.03	100.98
11	D	502	7PB	C19-C08-N07	2.01	126.61	120.24

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	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A
10	B	503	MES	C7-C8-S-O3S
5	A	501	GTP	PB-O3B-PG-O1G
9	D	501	GDP	PA-O3A-PB-O3B
5	A	501	GTP	C5'-O5'-PA-O3A
10	B	503	MES	C7-C8-S-O1S
10	B	503	MES	C7-C8-S-O2S
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	C4'-C5'-O5'-PA
11	B	505	7PB	C19-C08-N07-C05
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O3A

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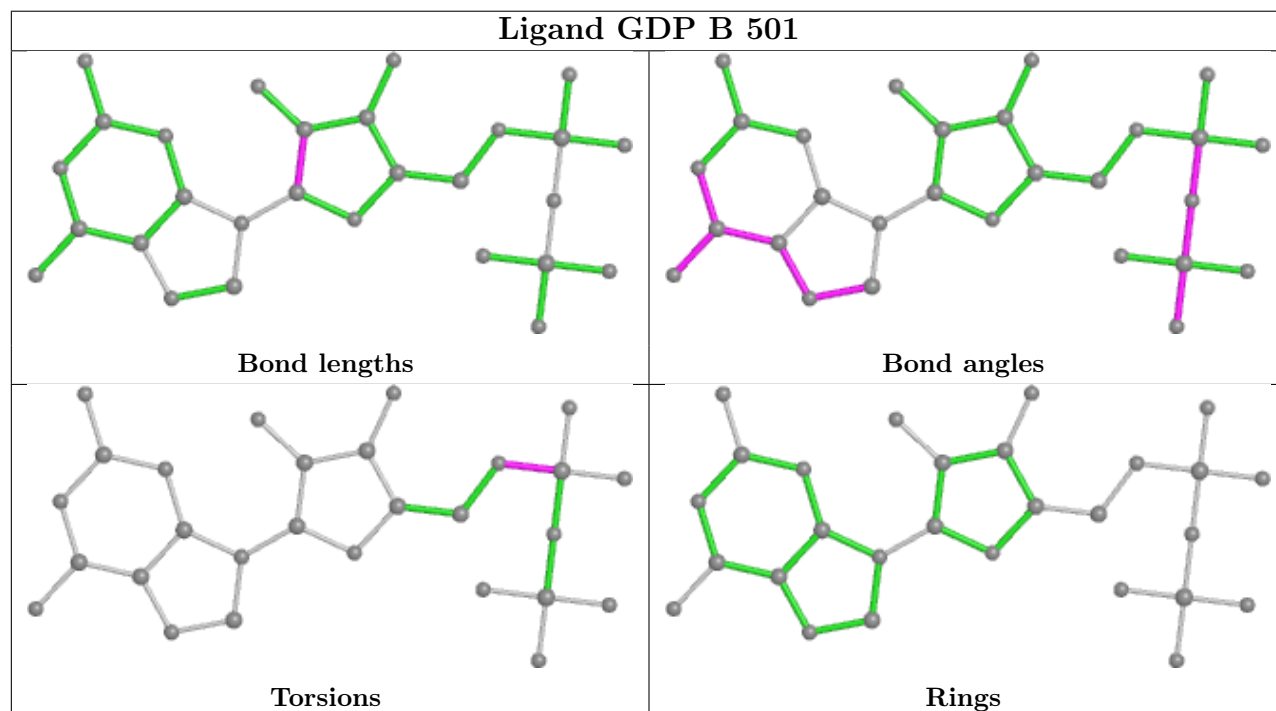
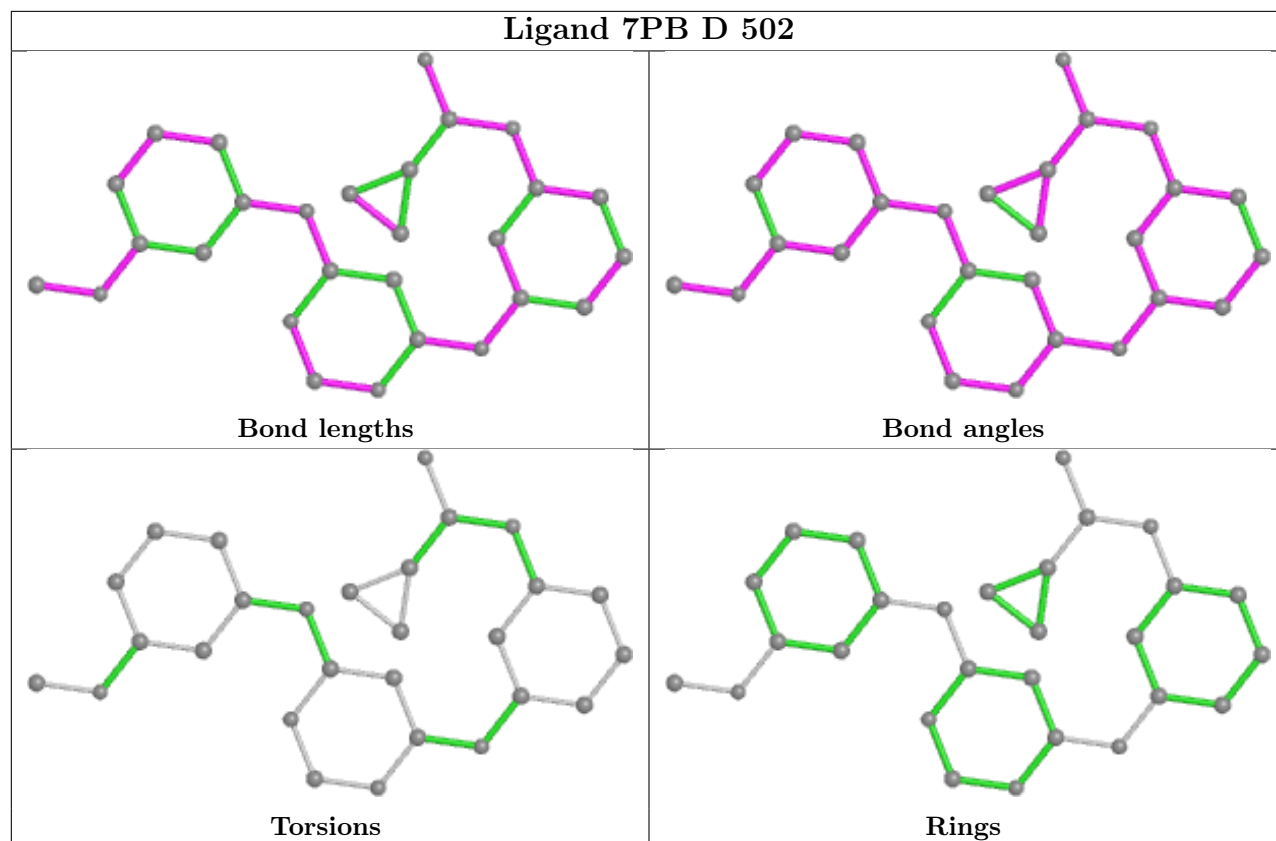
Mol	Chain	Res	Type	Atoms
9	D	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O2A

There are no ring outliers.

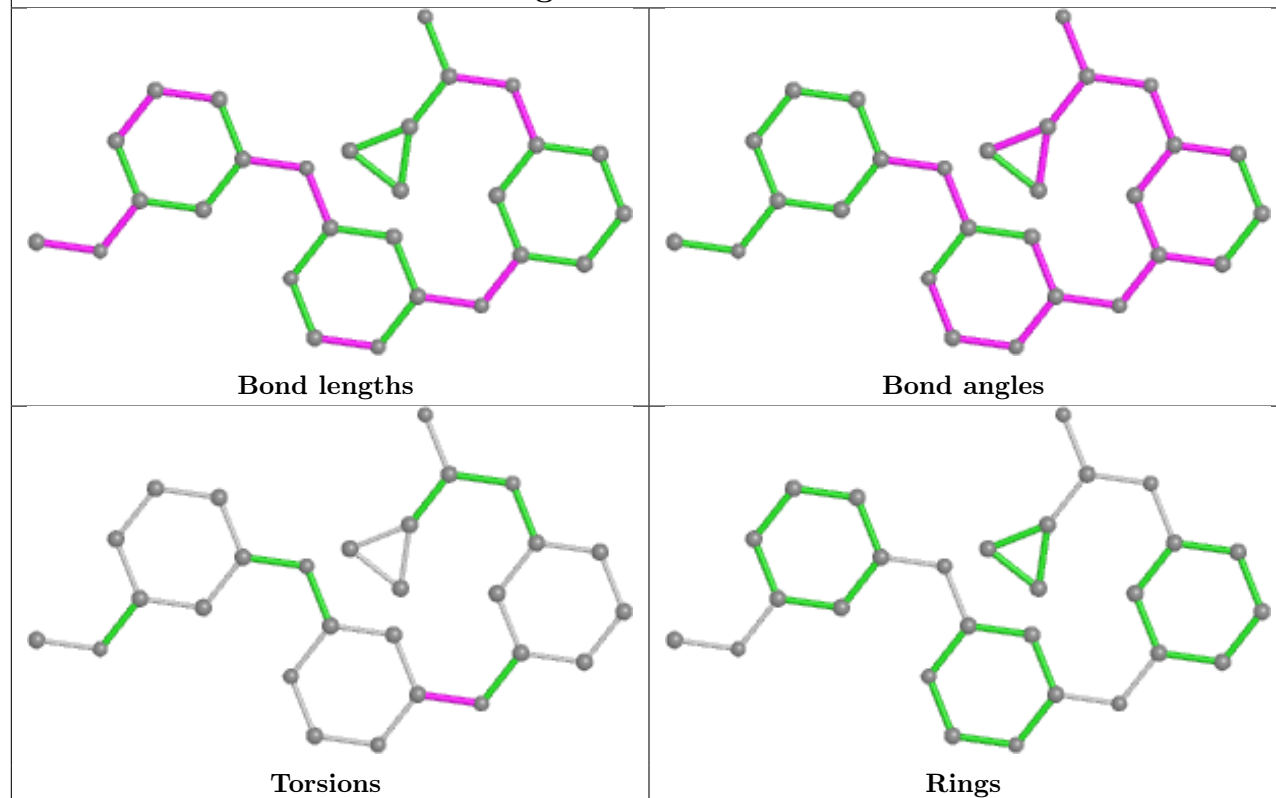
7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	503	MES	3	0
11	D	502	7PB	2	0
9	B	501	GDP	1	0
10	B	504	MES	1	0
11	B	505	7PB	1	0
9	D	501	GDP	1	0
5	A	501	GTP	2	0

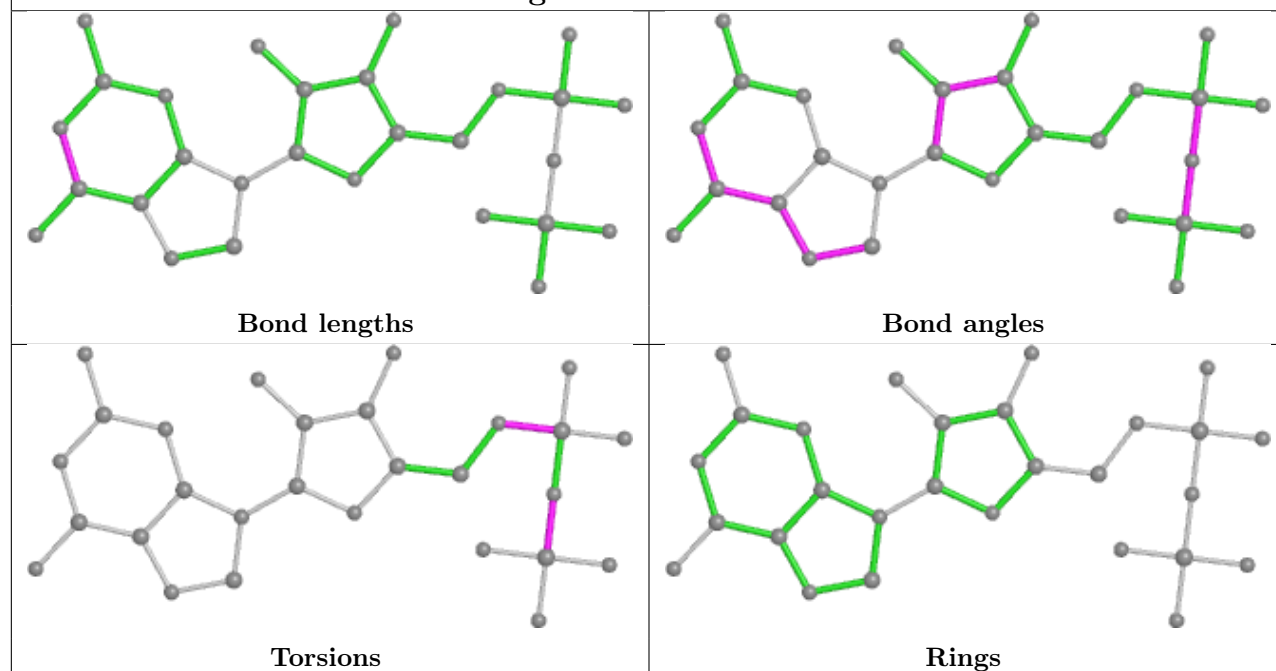
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



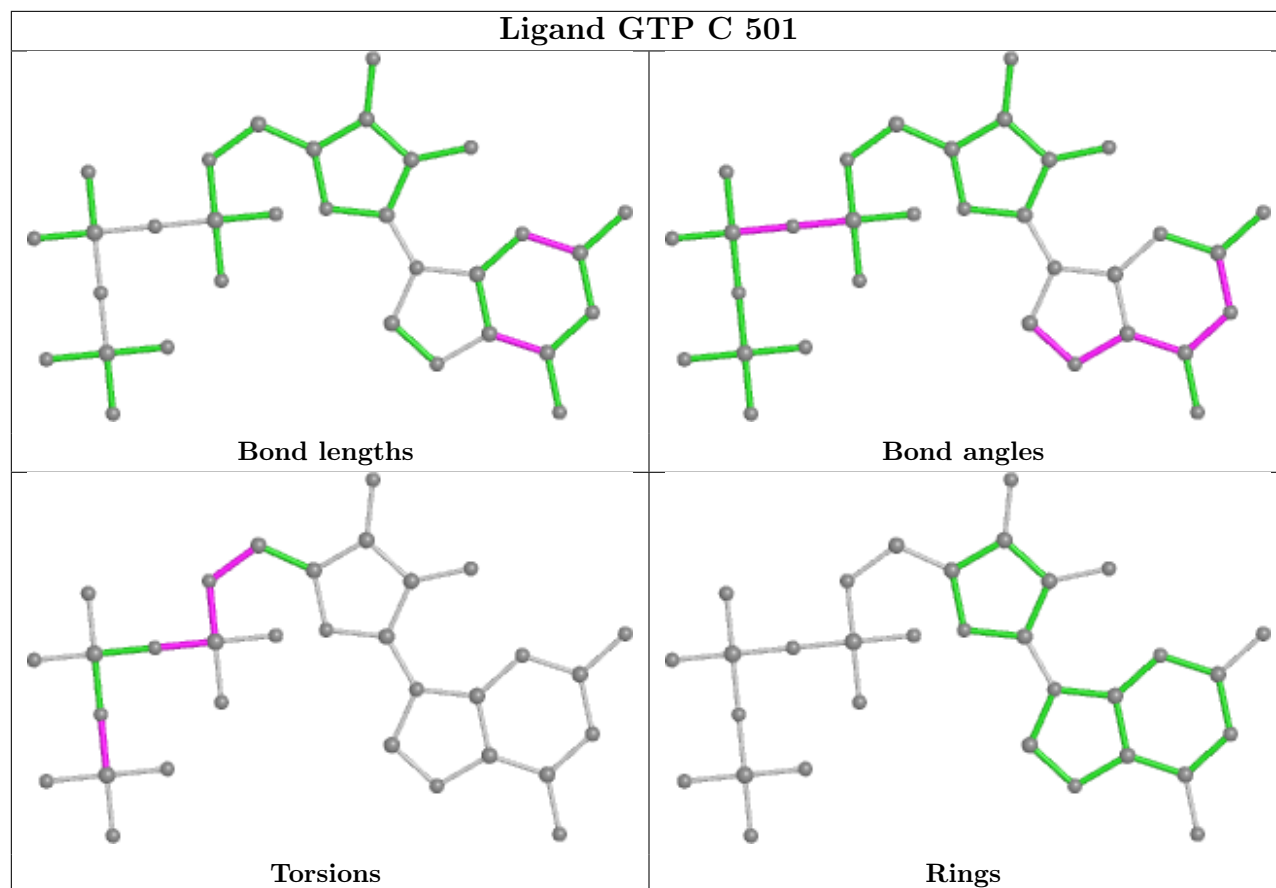
## Ligand 7PB B 505



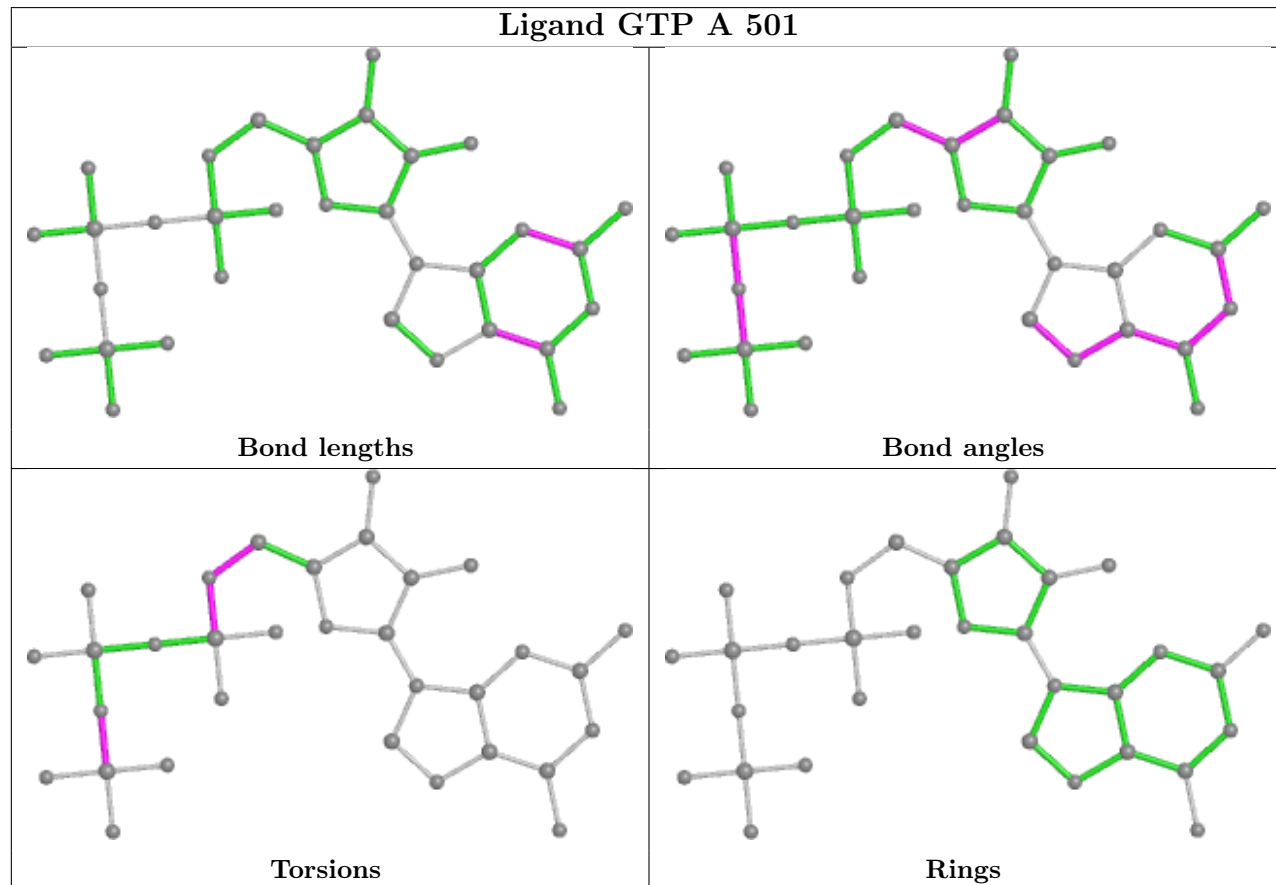
## Ligand GDP D 501



## Ligand GTP C 501



## Ligand GTP A 501





## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	437/450 (97%)	0.56	8 (1%) 68 66	39, 53, 74, 89	0
1	C	440/450 (97%)	0.62	8 (1%) 68 66	32, 46, 68, 88	0
2	B	424/445 (95%)	0.62	11 (2%) 56 54	34, 51, 78, 116	3 (0%)
2	D	420/445 (94%)	1.05	57 (13%) 3 2	44, 75, 100, 126	2 (0%)
3	E	123/143 (86%)	1.02	18 (14%) 2 2	46, 74, 104, 130	0
4	F	346/384 (90%)	1.18	75 (21%) 0 0	46, 78, 142, 163	0
All	All	2190/2317 (94%)	0.80	177 (8%) 12 11	32, 59, 104, 163	5 (0%)

All (177) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	169	LEU	12.7
4	F	173	ILE	10.9
4	F	161	LEU	10.0
2	D	72	THR	7.1
2	D	73	MET	6.7
4	F	166	ALA	6.6
2	D	81	PHE	6.3
1	C	340	SER	6.2
2	D	84	ILE	6.2
4	F	240	LEU	6.1
4	F	233	PHE	6.0
4	F	133	ALA	5.8
2	D	36	TYR	5.8
2	B	282	ARG	5.8
4	F	177	GLY	5.5
4	F	170	LEU	5.5
2	D	37	HIS	5.4
4	F	159	GLY	5.4
4	F	225	SER	5.3

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Mol	Chain	Res	Type	RSRZ
4	F	245	ILE	5.2
4	F	252	ASN	5.2
3	E	46	SER	5.0
2	D	44	LEU	5.0
4	F	100	ILE	4.9
1	A	262	TYR	4.9
2	D	216	LYS	4.9
3	E	138	GLU	4.8
4	F	239	HIS	4.7
2	D	217	LEU	4.6
2	D	402	PHE	4.6
4	F	226	GLU	4.5
4	F	103	THR	4.4
2	B	281	TYR	4.3
2	D	38	GLY	4.3
2	D	175	VAL	4.3
2	D	215	LEU	4.3
2	D	80	PRO	4.3
4	F	246	GLN	4.2
4	F	255[A]	ARG	4.1
4	F	134	ALA	4.1
2	D	97	ALA	4.0
2	D	85	PHE	4.0
2	D	55	THR	4.0
3	E	48	GLU	4.0
4	F	256	TYR	3.9
4	F	251	LYS	3.9
4	F	236	LYS	3.9
4	F	135	TYR	3.8
2	D	39	ASP	3.8
1	C	338	LYS	3.8
2	D	53	GLU	3.6
2	B	275	SER	3.5
2	D	406	TYR	3.5
4	F	175	GLU	3.4
4	F	244	CYS	3.4
4	F	102	PRO	3.4
2	B	57	ASN	3.3
4	F	249	TYR	3.3
4	F	182	ILE	3.3
4	F	149	ALA	3.3
2	D	59	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
2	D	103	LYS	3.3
2	D	291	GLN	3.2
4	F	242	ASN	3.2
4	F	164	SER	3.2
2	D	411	MET	3.2
4	F	162	ILE	3.1
4	F	147	TRP	3.1
2	D	413	GLU	3.1
3	E	142	GLU	3.1
1	C	282	TYR	3.1
2	D	76	VAL	3.0
4	F	238	CYS	3.0
4	F	346	LEU	3.0
4	F	380	HIS	3.0
4	F	152	SER	2.9
2	D	140	GLY	2.9
4	F	259	GLY	2.9
2	D	416	PHE	2.9
2	D	183	TYR	2.9
4	F	28	LYS	2.9
3	E	61	ARG	2.9
4	F	90	SER	2.9
2	D	187	LEU	2.9
2	D	245	GLN	2.9
2	D	41	ASP	2.9
3	E	54	LEU	2.9
3	E	68	LEU	2.9
4	F	127	GLU	2.9
4	F	151	SER	2.8
2	D	29	GLY	2.8
2	D	98	GLY	2.8
4	F	223	THR	2.8
2	D	30	ILE	2.8
1	A	104	ALA	2.8
1	A	70	LEU	2.8
4	F	198	LYS	2.7
4	F	174	ASP	2.7
1	C	177	VAL	2.7
4	F	375	PHE	2.7
4	F	171	ASP	2.7
3	E	57	ALA	2.7
4	F	181	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
3	E	45	PRO	2.7
2	D	101	TRP	2.6
2	D	219	THR	2.6
3	E	65	GLU	2.6
4	F	146	VAL	2.6
4	F	138	ARG	2.6
4	F	247	LYS	2.6
4	F	131	PHE	2.6
2	B	276	ARG	2.6
1	C	1	MET	2.6
2	D	83	GLN	2.6
4	F	172	PHE	2.5
4	F	176	GLN	2.5
2	D	172	SER	2.5
2	D	214	THR	2.5
4	F	150	LYS	2.5
4	F	250	SER	2.5
4	F	130	VAL	2.5
4	F	243	HIS	2.5
4	F	167	SER	2.4
2	D	125	GLU	2.4
4	F	372	THR	2.4
3	E	141	GLU	2.4
4	F	235	ASP	2.4
3	E	139	LEU	2.4
2	D	100	ASN	2.4
1	A	196	GLU	2.4
2	B	16[A]	ILE	2.4
2	D	96	GLY	2.4
4	F	104	ASN	2.4
1	A	346	TRP	2.3
4	F	186	LEU	2.3
2	B	274	THR	2.3
2	D	60	VAL	2.3
1	C	341	ILE	2.3
4	F	142	ARG	2.3
4	F	232	ASN	2.3
4	F	231	ALA	2.3
2	D	180	VAL	2.3
4	F	253	TYR	2.3
3	E	51	GLN	2.3
2	B	2	ARG	2.3

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
4	F	139	ARG	2.3
2	D	106	TYR	2.3
4	F	178	GLN	2.3
3	E	135	LYS	2.3
2	D	104	GLY	2.2
2	D	116	VAL	2.2
1	A	109	THR	2.2
2	D	395	ALA	2.2
4	F	165	GLU	2.2
2	D	65	LEU	2.2
2	D	31	ASP	2.2
2	D	69	GLU	2.2
3	E	7	GLU	2.2
3	E	90[A]	ASN	2.2
4	F	275[A]	LEU	2.2
3	E	6	MET	2.2
4	F	220[A]	VAL	2.1
4	F	237	THR	2.1
1	C	163	LYS	2.1
2	B	92	PHE	2.1
2	D	48	ASN	2.1
2	D	54	ALA	2.1
1	A	428	LEU	2.1
1	A	1	MET	2.1
2	D	22	GLU	2.1
2	D	399	ARG	2.1
2	B	430	TYR	2.1
4	F	192	LEU	2.1
2	D	11	GLN	2.0
2	B	215	LEU	2.0
3	E	116	LEU	2.0
1	C	361	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

## 6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

LIGAND-RSR INFOmissingINFO

## 6.5 Other polymers [i](#)

There are no such residues in this entry.