



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 29, 2021 – 12:39 AM JST

PDB ID : 7CBZ  
Title : Crystal structure of T2R-TTL-A31 complex  
Authors : Yang, J.H.; Yan, W.  
Deposited on : 2020-06-15  
Resolution : 2.61 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.

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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 : 2.25  
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) : 2.25

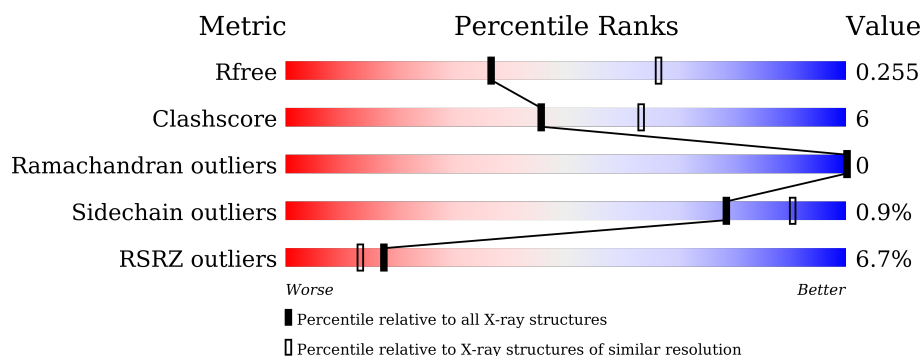
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.61 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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	451	<div> <div>2%</div> <div>83% 14% .</div> </div>
1	C	451	<div> <div>%</div> <div>87% 10% .</div> </div>
2	B	445	<div> <div>4%</div> <div>82% 13% 5%</div> </div>
2	D	445	<div> <div>7%</div> <div>79% 16% .</div> </div>
3	E	189	<div> <div>9%</div> <div>54% 11% 35%</div> </div>
4	F	383	<div> <div>16%</div> <div>70% 11% . 18%</div> </div>

## 2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 34298 atoms, of which 16837 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	438	Total	C	H	N	O	S	0	1	0
			6769	2170	3341	582	654	22			
1	C	440	Total	C	H	N	O	S	0	5	0
			6836	2190	3380	584	659	23			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	424	Total	C	H	N	O	S	0	1	0
			6565	2101	3222	570	646	26			
2	D	425	Total	C	H	N	O	S	0	1	0
			6553	2095	3215	569	648	26			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	57	THR	ALA	conflict	UNP P02554
B	172	MET	VAL	conflict	UNP P02554
B	298	SER	ALA	conflict	UNP P02554
B	318	ILE	VAL	conflict	UNP P02554
D	57	THR	ALA	conflict	UNP P02554
D	172	MET	VAL	conflict	UNP P02554
D	298	SER	ALA	conflict	UNP P02554
D	318	ILE	VAL	conflict	UNP P02554

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	E	123	Total	C	H	N	O	S	0	3	0
			2085	638	1049	188	205	5			

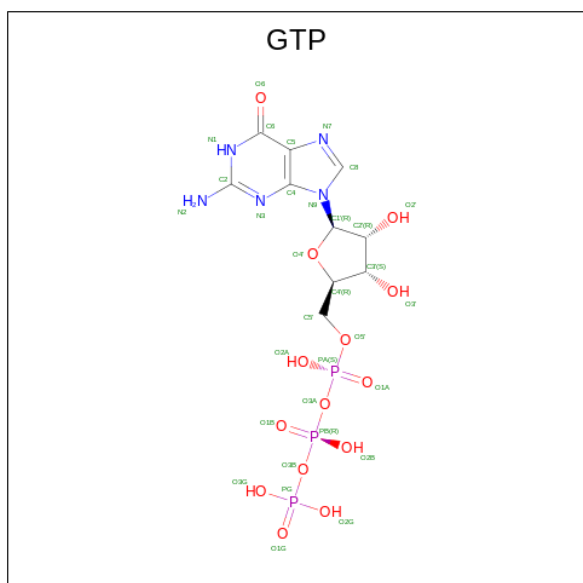
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	313	Total	C	H	N	O	S	0	0	0
			5032	1626	2507	425	462	12			

There are 5 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

- 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	H	N	O	P	41	0
			41	10	9	5	14	3		
5	C	1	Total	C	H	N	O	P	41	0
			41	10	9	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	1	0
			1	1		

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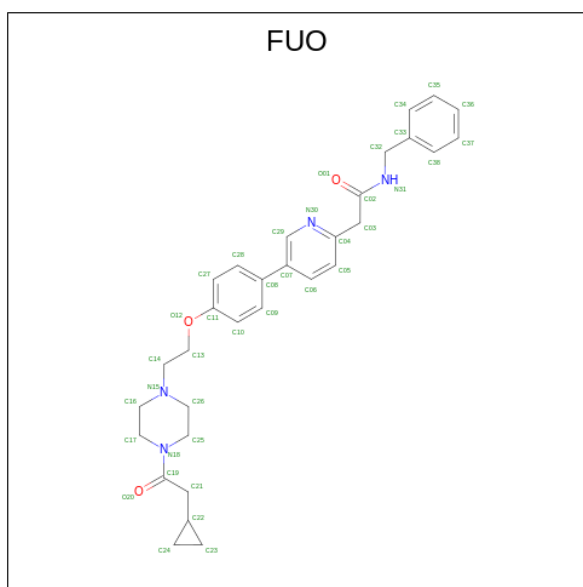
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total Mg 1 1	1	0
6	C	1	Total Mg 1 1	1	0
6	D	1	Total Mg 1 1	1	0
6	F	1	Total Mg 1 1	1	0

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

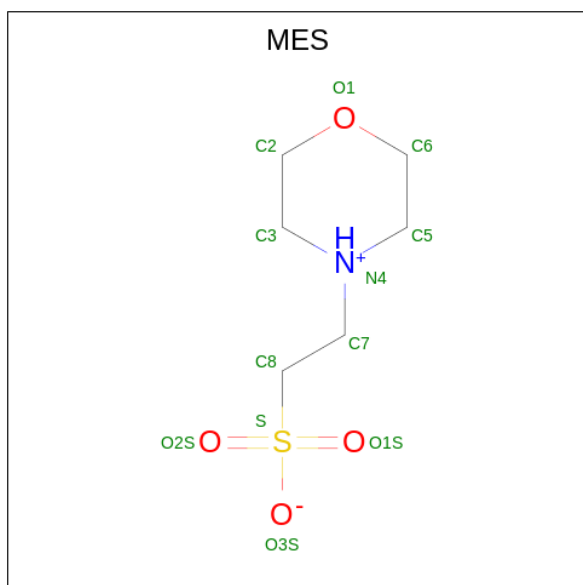
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Ca 2 2	2	0
7	B	2	Total Ca 2 2	2	0
7	C	1	Total Ca 1 1	1	0
7	D	1	Total Ca 1 1	1	0

- Molecule 8 is 2-[5-[4-[2-[4-(2-cyclopropylethanoyl)piperazin-1-yl]ethoxy]phenyl]pyridin-2-yl]-N-(phenylmethyl)ethanamide (three-letter code: FUU) (formula:  $C_{31}H_{36}N_4O_3$ ) (labeled as "Ligand of Interest" by depositor).



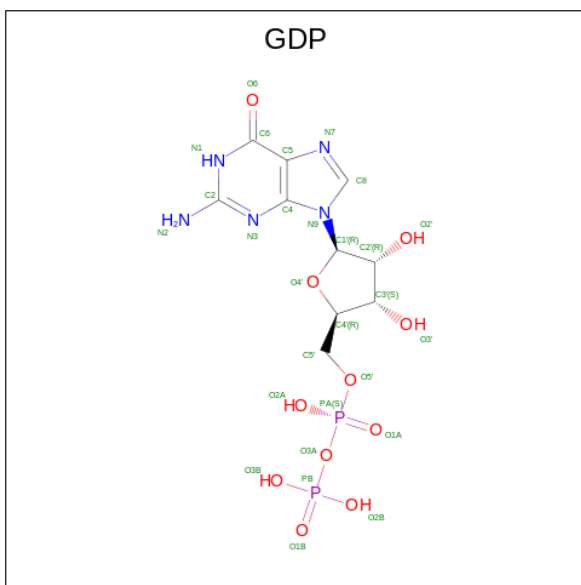
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	H	N	O	0	0
			74	31	36	4	3		
8	D	1	Total	C	H	N	O	0	0
			74	31	36	4	3		

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	S	25	0
			25	6	13	1	4	1		

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



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
10	B	1	Total 38	C 10	H 10	N 5	O 11	P 2	38	0
10	D	1	Total 38	C 10	H 10	N 5	O 11	P 2	38	0

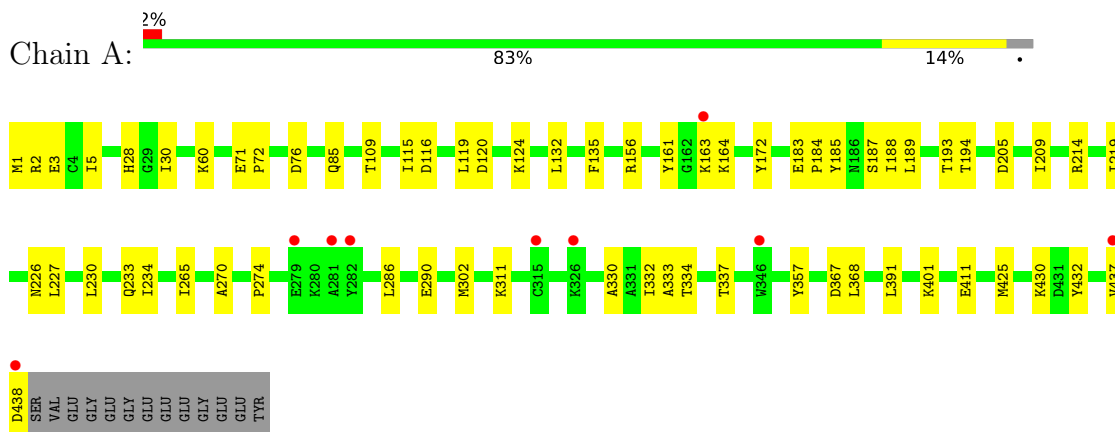
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	21	Total O 21 21	0	0
11	B	35	Total O 35 35	0	0
11	C	27	Total O 27 27	0	0
11	D	14	Total O 14 14	0	0
11	E	9	Total O 9 9	0	0
11	F	10	Total O 10 10	0	0

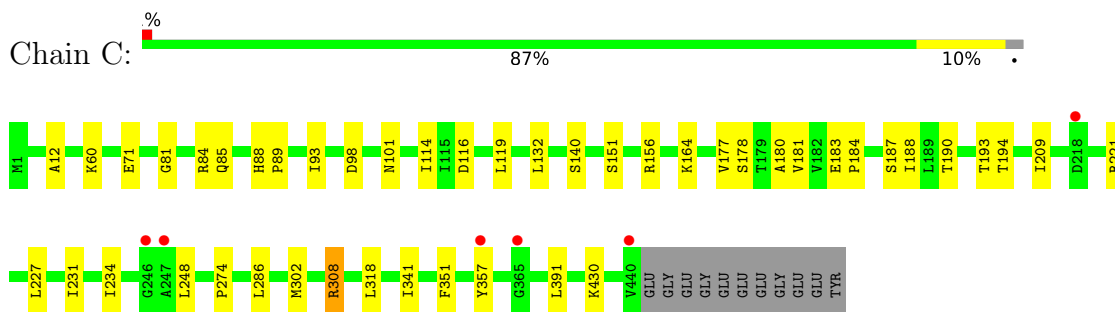
### 3 Residue-property plots [i](#)

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.

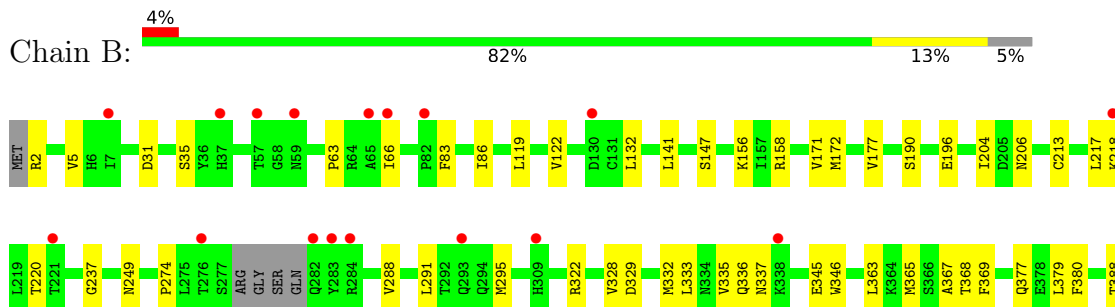
- Molecule 1: Tubulin alpha-1B chain



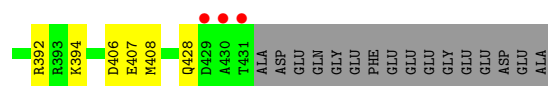
- Molecule 1: Tubulin alpha-1B chain



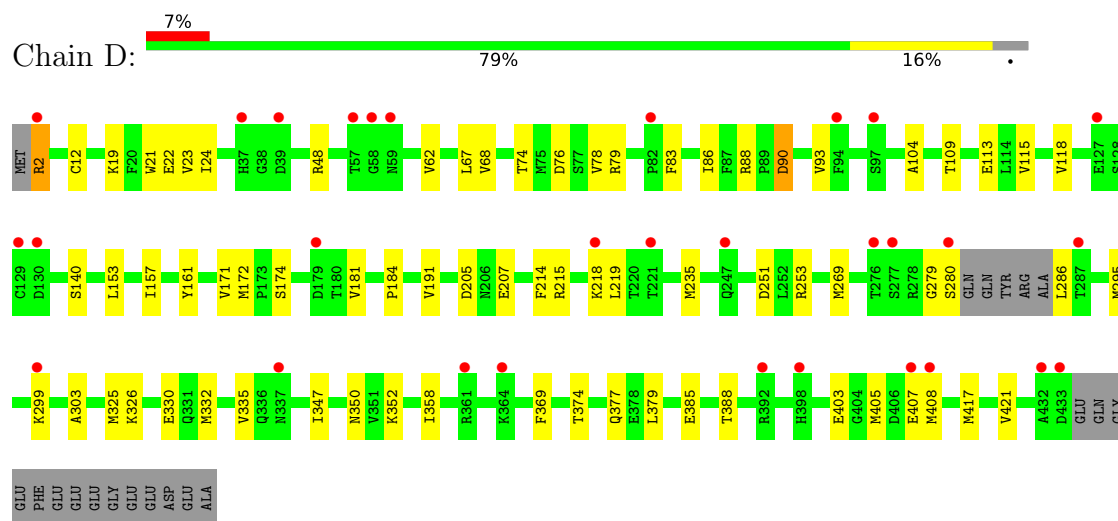
- Molecule 2: Tubulin beta chain



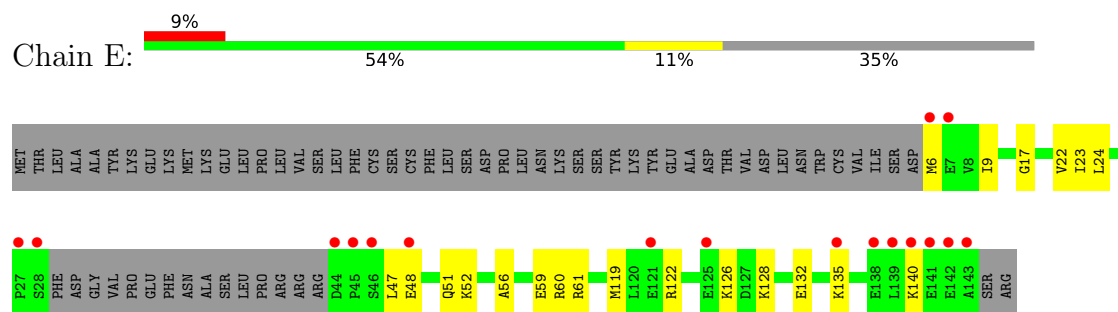




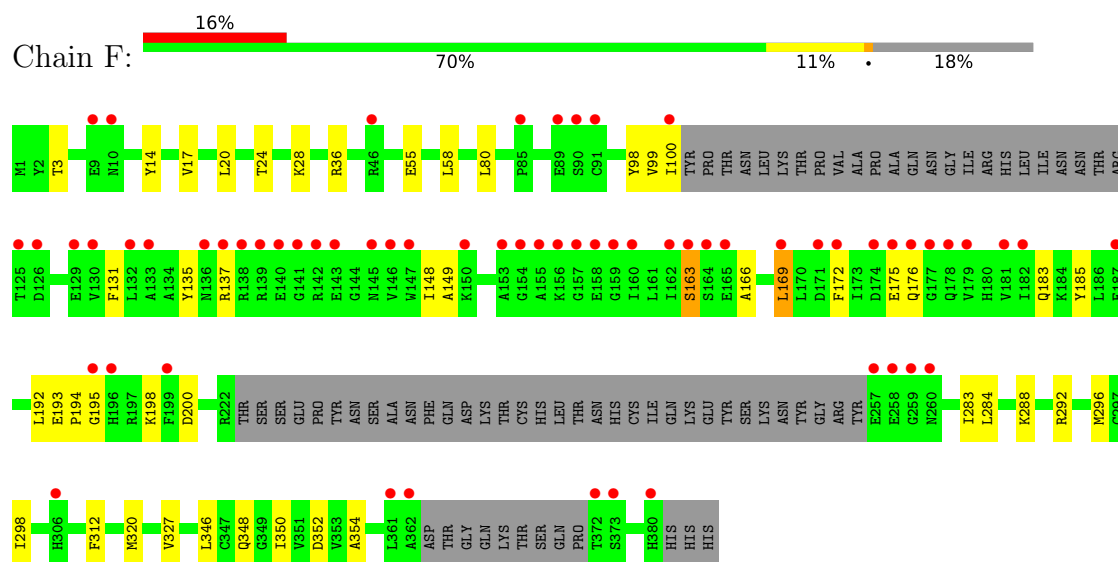
- Molecule 2: Tubulin beta chain



- 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, $\alpha$ , $\beta$ , $\gamma$	104.81Å 156.63Å 181.47Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.76 – 2.61 19.76 – 2.61	Depositor EDS
% Data completeness (in resolution range)	92.9 (19.76-2.61) 92.9 (19.76-2.61)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.95 (at 2.59Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.206 , 0.255 0.206 , 0.255	Depositor DCC
$R_{free}$ test set	4262 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	58.4	Xtriage
Anisotropy	0.211	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 51.6	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	0.94	EDS
Total number of atoms	34298	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.34% 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: MG, CA, MES, GDP, FUO, GTP

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	0.30	0/3509	0.48	0/4764
1	C	0.34	0/3549	0.49	0/4819
2	B	0.48	0/3420	0.55	0/4633
2	D	0.39	0/3414	0.52	1/4624 (0.0%)
3	E	0.46	0/1048	0.59	0/1391
4	F	0.31	0/2578	0.52	0/3482
All	All	0.38	0/17518	0.52	1/23713 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	251	ASP	O-C-N	-5.25	114.31	122.70

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	3428	3341	3341	43	3
1	C	3456	3380	3380	38	3
2	B	3343	3222	3221	41	0
2	D	3338	3215	3215	51	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	1036	1049	1047	13	0
4	F	2525	2507	2506	40	0
5	A	32	9	12	0	0
5	C	32	9	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	B	38	36	0	0	0
8	D	38	36	0	2	0
9	B	12	13	13	0	0
10	B	28	10	12	0	0
10	D	28	10	12	0	0
11	A	21	0	0	2	0
11	B	35	0	0	4	0
11	C	27	0	0	0	0
11	D	14	0	0	1	0
11	E	9	0	0	1	0
11	F	10	0	0	0	0
All	All	17461	16837	16771	218	3

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 6.

All (218) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:248:LEU:CD1	1:C:357:TYR:OH	1.99	1.11
1:C:248:LEU:HD12	1:C:357:TYR:OH	1.51	1.09
1:A:290:GLU:OE2	11:A:601:HOH:O	1.89	0.89
4:F:163:SER:HB2	4:F:169:LEU:CD2	2.03	0.88
3:E:9:ILE:HD12	3:E:23:ILE:HD12	1.60	0.84
1:C:248:LEU:HD12	1:C:357:TYR:CZ	2.15	0.82
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.17	0.80
4:F:149:ALA:HB3	4:F:169:LEU:HD11	1.70	0.73
1:A:333:ALA:O	1:A:337:THR:HG23	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:172:MET:HG3	2:B:379:LEU:HD11	1.72	0.71
1:C:248:LEU:HD11	1:C:357:TYR:OH	1.91	0.69
4:F:99:VAL:O	4:F:100:ILE:HD13	1.93	0.69
4:F:163:SER:HB2	4:F:169:LEU:HD23	1.75	0.69
1:C:177:VAL:HG12	1:C:177:VAL:O	1.91	0.69
2:D:172:MET:HG3	2:D:379:LEU:HD11	1.75	0.67
2:D:2:ARG:HH11	2:D:48:ARG:CZ	2.08	0.66
2:B:329:ASP:O	2:B:333:LEU:HD13	1.97	0.65
2:D:93:VAL:HG11	2:D:118:VAL:HG22	1.77	0.65
4:F:135:TYR:CE2	4:F:166:ALA:HB3	2.32	0.64
1:A:230:LEU:O	1:A:234:ILE:HD12	1.98	0.62
2:D:172:MET:HB2	2:D:205:ASP:HA	1.82	0.62
1:A:437:VAL:HG22	1:A:438:ASP:H	1.64	0.61
2:D:295:MET:CG	2:D:369:PHE:HB2	2.30	0.61
1:C:101:ASN:ND2	1:C:180:ALA:HB2	2.16	0.61
2:D:109:THR:HG21	2:D:403:GLU:OE1	2.02	0.60
2:D:115:VAL:HG23	2:D:153:LEU:HD13	1.84	0.60
2:D:172:MET:CE	2:D:379:LEU:HD21	2.32	0.59
4:F:137:ARG:HA	4:F:137:ARG:NE	2.18	0.59
2:D:286:LEU:N	11:D:601:HOH:O	2.34	0.59
1:C:81:GLY:O	1:C:84:ARG:NH1	2.36	0.58
1:C:187:SER:CB	1:C:391:LEU:HD21	2.34	0.58
2:D:326:LYS:O	2:D:330:GLU:HG3	2.03	0.58
2:D:377:GLN:HG3	2:D:421:VAL:HG13	1.86	0.58
4:F:149:ALA:CB	4:F:169:LEU:CD1	2.82	0.57
3:E:122:ARG:O	3:E:126:LYS:HG2	2.04	0.57
2:D:104:ALA:HB2	2:D:405:MET:SD	2.45	0.56
2:D:181:VAL:O	2:D:184:PRO:HD2	2.05	0.56
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.38	0.56
2:D:279:GLY:O	2:D:280:SER:OG	2.15	0.55
2:B:83:PHE:O	2:B:86:ILE:HG22	2.06	0.55
1:A:188:ILE:HG23	1:A:425:MET:HG3	1.86	0.55
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.89	0.55
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.88	0.54
2:B:177:VAL:HG11	2:B:206:ASN:HB3	1.90	0.54
3:E:61:ARG:HG3	3:E:61:ARG:HH11	1.71	0.54
1:A:311:LYS:NZ	1:A:438:ASP:OD1	2.37	0.54
2:B:291:LEU:HD11	2:B:365:MET:HB3	1.89	0.54
4:F:80:LEU:HD21	4:F:298:ILE:CG2	2.38	0.53
2:D:377:GLN:CG	2:D:421:VAL:HG13	2.39	0.53
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:358:ILE:O	2:D:358:ILE:HG13	2.07	0.53
1:C:190:THR:O	1:C:194:THR:HG23	2.08	0.53
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.90	0.53
4:F:200:ASP:CB	4:F:320:MET:HG2	2.39	0.53
4:F:149:ALA:CB	4:F:169:LEU:HD11	2.37	0.53
1:A:270:ALA:HB3	1:A:302:MET:HG3	1.90	0.52
4:F:172:PHE:HA	4:F:175:GLU:HB2	1.91	0.52
2:B:158:ARG:NH1	2:B:196:GLU:O	2.42	0.52
1:C:221:ARG:CD	2:D:325:MET:HG2	2.39	0.52
3:E:60:ARG:NH1	11:E:201:HOH:O	2.40	0.52
1:C:132:LEU:O	1:C:164:LYS:NZ	2.43	0.52
2:B:177:VAL:HG13	2:B:177:VAL:O	2.09	0.51
2:D:83:PHE:O	2:D:86:ILE:HG22	2.10	0.51
4:F:20:LEU:O	4:F:24:THR:HG23	2.10	0.51
1:A:430:LYS:HE2	1:A:430:LYS:HA	1.92	0.51
2:B:274:PRO:HD2	2:B:363:LEU:HD13	1.92	0.51
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.44	0.51
2:B:63:PRO:CD	2:B:86:ILE:HG12	2.40	0.51
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.93	0.51
2:D:67:LEU:N	2:D:67:LEU:HD12	2.26	0.51
1:A:163:LYS:HE2	1:A:163:LYS:HA	1.93	0.50
1:C:234:ILE:HD13	1:C:302:MET:SD	2.51	0.50
3:E:56:ALA:O	3:E:59:GLU:HG2	2.11	0.50
4:F:346:LEU:O	4:F:350:ILE:HG13	2.10	0.50
1:A:2:ARG:N	1:A:2:ARG:HD2	2.26	0.50
2:B:218:LYS:NZ	11:B:606:HOH:O	2.43	0.50
2:D:172:MET:HE1	2:D:379:LEU:HD21	1.94	0.50
1:A:187:SER:CB	1:A:391:LEU:HD21	2.42	0.50
2:D:90:ASP:OD1	2:D:90:ASP:N	2.44	0.50
4:F:36:ARG:NH1	4:F:55:GLU:HG3	2.27	0.50
4:F:172:PHE:HE2	4:F:176:GLN:HE21	1.59	0.50
1:A:116:ASP:OD1	1:A:156:ARG:NH2	2.45	0.49
4:F:148:ILE:HG23	4:F:183:GLN:HB2	1.94	0.49
4:F:193:GLU:O	4:F:195:GLY:N	2.42	0.49
1:C:231:ILE:HA	1:C:234:ILE:HD12	1.94	0.49
1:A:437:VAL:HG22	1:A:438:ASP:N	2.28	0.49
4:F:163:SER:CB	4:F:169:LEU:CD2	2.86	0.49
2:D:385:GLU:O	2:D:388:THR:HG22	2.13	0.49
2:D:218:LYS:O	2:D:219:LEU:HD12	2.13	0.48
2:B:428:GLN:NE2	11:B:605:HOH:O	2.42	0.48
2:B:394:LYS:HE3	2:B:407:GLU:CD	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:178:SER:HB2	1:C:183:GLU:OE2	2.13	0.48
1:A:72:PRO:O	1:A:76:ASP:N	2.41	0.48
4:F:193:GLU:N	4:F:194:PRO:HD2	2.29	0.48
2:D:157:ILE:O	2:D:161:TYR:N	2.43	0.47
1:A:132:LEU:HD23	1:A:164:LYS:HD3	1.96	0.47
1:A:1:MET:C	1:A:2:ARG:HD2	2.34	0.47
1:C:88:HIS:ND1	1:C:89:PRO:HD2	2.30	0.47
2:B:406:ASP:OD2	2:B:407:GLU:N	2.48	0.47
2:D:2:ARG:NH1	2:D:48:ARG:NH2	2.63	0.47
1:C:177:VAL:O	1:C:177:VAL:CG1	2.61	0.47
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.97	0.47
2:D:19:LYS:O	2:D:23:VAL:HG23	2.14	0.47
2:D:109:THR:O	2:D:113:GLU:HG3	2.14	0.47
2:D:214:PHE:C	2:D:214:PHE:CD1	2.86	0.47
3:E:132:GLU:OE1	3:E:132:GLU:HA	2.15	0.47
2:B:220:THR:N	11:B:610:HOH:O	2.49	0.46
2:B:332:MET:O	2:B:336:GLN:HG3	2.14	0.46
4:F:283:ILE:HG23	4:F:327:VAL:CG2	2.45	0.46
2:B:377:GLN:O	2:B:380:PHE:N	2.48	0.46
2:D:22:GLU:HG2	2:D:83:PHE:CD1	2.50	0.46
2:D:332:MET:O	2:D:335:VAL:HG12	2.16	0.46
1:A:109:THR:OG1	1:A:411:GLU:OE1	2.27	0.46
1:A:161:TYR:HB3	1:A:164:LYS:HD2	1.97	0.46
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.97	0.46
3:E:47:LEU:HD12	3:E:47:LEU:O	2.15	0.46
2:B:66:ILE:HD13	2:B:122:VAL:HG22	1.97	0.46
2:B:147:SER:HG	2:B:190:SER:HG	1.63	0.46
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.49	0.46
4:F:193:GLU:N	4:F:194:PRO:CD	2.79	0.46
2:B:295:MET:HG3	2:B:369:PHE:HB2	1.98	0.46
4:F:3:THR:HG22	4:F:28:LYS:HB3	1.98	0.46
1:A:28:HIS:HB2	1:A:30:ILE:HD12	1.97	0.45
2:B:394:LYS:HE3	2:B:407:GLU:OE1	2.16	0.45
4:F:99:VAL:C	4:F:100:ILE:HD13	2.37	0.45
2:D:67:LEU:CD2	2:D:78:VAL:HG11	2.46	0.45
4:F:14:TYR:HA	4:F:17:VAL:HB	1.99	0.45
2:B:333:LEU:O	2:B:337:ASN:ND2	2.49	0.45
2:B:333:LEU:N	2:B:333:LEU:HD12	2.32	0.45
2:B:31:ASP:OD1	2:B:35:SER:N	2.46	0.45
2:B:213:CYS:HA	2:B:217:LEU:HD12	1.99	0.45
1:C:341:ILE:HD13	1:C:351:PHE:HZ	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:SD	1:A:3:GLU:HG3	2.57	0.45
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.00	0.44
2:B:337:ASN:OD1	4:F:36:ARG:NE	2.51	0.44
2:D:21:TRP:CE3	2:D:24:ILE:HD11	2.53	0.44
3:E:48:GLU:O	3:E:52:LYS:HG2	2.16	0.44
2:D:374:THR:O	2:D:377:GLN:HB2	2.18	0.44
4:F:149:ALA:HB2	4:F:169:LEU:CD1	2.47	0.44
1:A:5:ILE:O	1:A:135:PHE:HA	2.18	0.44
2:B:333:LEU:N	2:B:333:LEU:CD1	2.81	0.44
2:D:115:VAL:HG23	2:D:153:LEU:CD1	2.47	0.44
4:F:98:TYR:CG	4:F:131:PHE:HB2	2.53	0.44
4:F:283:ILE:HG23	4:F:327:VAL:HG21	2.00	0.44
4:F:292:ARG:O	4:F:296:MET:HG2	2.18	0.44
1:A:214:ARG:HG2	1:A:219:ILE:O	2.17	0.43
1:A:438:ASP:N	11:A:604:HOH:O	2.51	0.43
2:D:352:LYS:HB3	8:D:501:FUO:C11	2.47	0.43
1:A:71:GLU:OE2	2:B:249:ASN:ND2	2.51	0.43
1:A:194:THR:O	1:A:194:THR:HG22	2.18	0.43
1:A:274:PRO:HB3	1:A:286:LEU:HD12	2.00	0.43
2:D:172:MET:HE2	2:D:379:LEU:HD21	1.99	0.43
4:F:149:ALA:HB2	4:F:169:LEU:HG	1.99	0.43
2:D:76:ASP:HA	2:D:79:ARG:HG2	2.01	0.43
2:D:295:MET:HG3	2:D:369:PHE:HB2	2.00	0.43
2:B:295:MET:CG	2:B:369:PHE:HB2	2.48	0.43
2:D:191:VAL:HG11	2:D:417:MET:HE2	2.00	0.43
2:B:295:MET:SD	2:B:367:ALA:HB1	2.58	0.43
1:C:227:LEU:O	1:C:231:ILE:HG13	2.19	0.43
2:B:171:VAL:HA	2:B:204:ILE:O	2.18	0.43
1:C:274:PRO:HB3	1:C:286:LEU:HD22	1.99	0.43
2:D:93:VAL:HG11	2:D:118:VAL:CG2	2.47	0.43
2:B:337:ASN:ND2	4:F:58:LEU:HD21	2.33	0.43
4:F:192:LEU:C	4:F:194:PRO:HD2	2.39	0.43
1:C:12:ALA:HB3	1:C:140:SER:HB3	2.01	0.42
2:D:235:MET:HE2	2:D:235:MET:HB3	1.90	0.42
2:B:141:LEU:HD12	2:B:172:MET:SD	2.58	0.42
2:B:337:ASN:OD1	4:F:36:ARG:NH2	2.52	0.42
2:D:2:ARG:NH1	2:D:48:ARG:CZ	2.81	0.42
2:D:74:THR:O	2:D:78:VAL:HG23	2.19	0.42
1:A:120:ASP:O	1:A:124:LYS:HG2	2.19	0.42
1:C:234:ILE:CD1	1:C:302:MET:SD	3.07	0.42
2:B:388:THR:O	2:B:392:ARG:HG2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:135:LYS:HD2	3:E:135:LYS:C	2.39	0.42
4:F:148:ILE:CG2	4:F:183:GLN:HB2	2.50	0.42
1:A:233:GLN:HG3	1:A:368:LEU:HD13	2.02	0.42
1:C:151[B]:SER:HA	1:C:194:THR:HG22	2.00	0.42
1:C:151[A]:SER:HB2	1:C:193:THR:HG21	2.02	0.42
1:C:209:ILE:HG22	1:C:227:LEU:CD2	2.49	0.42
4:F:149:ALA:HB3	4:F:169:LEU:CD1	2.40	0.42
1:A:115:ILE:HG13	1:A:119:LEU:HD12	2.02	0.42
1:A:401:LYS:HG3	2:B:346:TRP:CD2	2.54	0.42
2:B:288:VAL:HG11	2:B:328:VAL:HA	2.01	0.42
1:C:119:LEU:HD11	1:C:156:ARG:HB3	2.00	0.42
3:E:6:MET:HA	3:E:23:ILE:O	2.20	0.42
1:A:209:ILE:HG22	1:A:227:LEU:HD22	2.01	0.42
2:D:12:CYS:SG	2:D:171:VAL:HG21	2.60	0.42
2:D:68:VAL:HG21	2:D:118:VAL:HG11	2.01	0.42
1:C:151[A]:SER:HA	1:C:194:THR:HG22	2.01	0.41
2:D:174:SER:OG	2:D:207:GLU:HB2	2.20	0.41
1:A:183:GLU:N	1:A:184:PRO:CD	2.83	0.41
1:C:60:LYS:NZ	1:C:85:GLN:O	2.44	0.41
4:F:284:LEU:O	4:F:288:LYS:HG3	2.20	0.41
2:B:2:ARG:N	11:B:613:HOH:O	2.52	0.41
2:B:332:MET:O	2:B:335:VAL:HG12	2.20	0.41
1:C:151[B]:SER:HB3	1:C:193:THR:HG21	2.01	0.41
3:E:24:LEU:N	3:E:24:LEU:HD12	2.35	0.41
1:C:71:GLU:HG2	1:C:98:ASP:HB3	2.02	0.41
2:B:237:GLY:HA3	2:B:368:THR:OG1	2.19	0.41
1:A:60:LYS:NZ	1:A:85:GLN:O	2.37	0.41
1:A:189:LEU:O	1:A:193:THR:HG23	2.21	0.41
1:C:116:ASP:OD1	1:C:156:ARG:NH2	2.42	0.41
1:A:209:ILE:HG22	1:A:227:LEU:CD2	2.50	0.41
1:A:332:ILE:HD13	3:E:22:VAL:HG11	2.01	0.41
1:C:221:ARG:NH2	8:D:501:FUO:O20	2.52	0.41
2:D:62:VAL:HG11	2:D:88:ARG:NH1	2.36	0.41
4:F:312:PHE:CG	4:F:354:ALA:HB1	2.56	0.41
1:A:185:TYR:O	1:A:189:LEU:HG	2.21	0.41
1:A:330:ALA:O	1:A:334:THR:HG23	2.21	0.40
2:D:12:CYS:HB3	2:D:140:SER:HB3	2.03	0.40
2:D:299:LYS:HA	2:D:299:LYS:HD3	1.80	0.40
2:B:5:VAL:HG23	2:B:132:LEU:CD1	2.51	0.40
1:C:184:PRO:O	1:C:188:ILE:HG12	2.22	0.40
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:318:LEU:N	1:C:318:LEU:HD12	2.36	0.40
4:F:99:VAL:O	4:F:99:VAL:HG13	2.22	0.40

All (3) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:GLU:OE1	1:C:308:ARG:NH2[3_555]	1.59	0.61
1:A:290:GLU:OE1	1:C:308:ARG:HH21[3_555]	1.09	0.51
1:A:290:GLU:CD	1:C:308:ARG:NH2[3_555]	2.05	0.15

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	437/451 (97%)	425 (97%)	12 (3%)	0	100	100
1	C	443/451 (98%)	434 (98%)	9 (2%)	0	100	100
2	B	421/445 (95%)	405 (96%)	16 (4%)	0	100	100
2	D	422/445 (95%)	408 (97%)	14 (3%)	0	100	100
3	E	122/189 (65%)	120 (98%)	2 (2%)	0	100	100
4	F	305/383 (80%)	291 (95%)	14 (5%)	0	100	100
All	All	2150/2364 (91%)	2083 (97%)	67 (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	370/379 (98%)	370 (100%)	0	100	100
1	C	376/379 (99%)	374 (100%)	2 (0%)	88	95
2	B	368/383 (96%)	365 (99%)	3 (1%)	81	92
2	D	368/383 (96%)	362 (98%)	6 (2%)	62	81
3	E	113/171 (66%)	109 (96%)	4 (4%)	36	60
4	F	273/341 (80%)	271 (99%)	2 (1%)	84	93
All	All	1868/2036 (92%)	1851 (99%)	17 (1%)	78	90

All (17) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	322	ARG
2	B	345	GLU
2	B	408	MET
1	C	308	ARG
1	C	430	LYS
2	D	2	ARG
2	D	90	ASP
2	D	215	ARG
2	D	253	ARG
2	D	407	GLU
2	D	408	MET
3	E	51	GLN
3	E	119	MET
3	E	128	LYS
3	E	140	LYS
4	F	163	SER
4	F	169	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	101	ASN
2	D	294	GLN
3	E	92	ASN

### 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 18 ligands modelled in this entry, 11 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	$\# Z  > 2$
5	GTP	A	501	6	26,34,34	0.98	1 (3%)	33,54,54	1.97	8 (24%)
10	GDP	B	506	6	24,30,30	1.18	2 (8%)	31,47,47	1.97	8 (25%)
8	FUO	D	501	-	42,42,42	3.16	15 (35%)	55,56,56	1.88	11 (20%)
5	GTP	C	501	6	26,34,34	0.99	1 (3%)	33,54,54	1.90	8 (24%)
10	GDP	D	504	6	24,30,30	1.20	3 (12%)	31,47,47	2.10	9 (29%)
8	FUO	B	501	-	42,42,42	3.20	17 (40%)	55,56,56	2.97	19 (34%)
9	MES	B	503	-	12,12,12	2.27	1 (8%)	14,16,16	1.64	4 (28%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	GDP	B	506	6	-	2/12/32/32	0/3/3/3
8	FUO	D	501	-	-	6/27/39/39	0/5/5/5
5	GTP	C	501	6	-	4/18/38/38	0/3/3/3
10	GDP	D	504	6	-	3/12/32/32	0/3/3/3
8	FUO	B	501	-	-	5/27/39/39	1/5/5/5
9	MES	B	503	-	-	1/6/14/14	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	503	MES	C8-S	-7.60	1.66	1.77
8	B	501	FUO	C14-N15	-7.46	1.30	1.47
8	D	501	FUO	C37-C38	7.35	1.54	1.38
8	D	501	FUO	C34-C33	7.24	1.54	1.38
8	B	501	FUO	O01-C02	-6.85	1.09	1.23
8	D	501	FUO	C19-N18	6.58	1.48	1.35
8	D	501	FUO	C02-N31	6.36	1.47	1.33
8	B	501	FUO	C26-N15	-6.24	1.29	1.46
8	B	501	FUO	C16-N15	-6.04	1.30	1.46
8	D	501	FUO	C36-C35	5.99	1.53	1.38
8	B	501	FUO	C19-N18	5.82	1.47	1.35
8	D	501	FUO	C26-N15	-5.57	1.31	1.46
8	D	501	FUO	C14-N15	-5.56	1.34	1.47
8	D	501	FUO	C03-C04	5.56	1.56	1.51
8	D	501	FUO	C16-N15	-5.31	1.32	1.46
8	B	501	FUO	C38-C33	-5.16	1.27	1.38
8	B	501	FUO	C34-C33	5.12	1.49	1.38
8	B	501	FUO	C35-C34	-4.76	1.28	1.38
8	B	501	FUO	C29-C07	-4.37	1.31	1.39
8	B	501	FUO	C37-C38	4.33	1.48	1.38
10	B	506	GDP	C5-C6	4.22	1.48	1.41
8	B	501	FUO	C37-C36	-4.19	1.26	1.38
10	D	504	GDP	C5-C6	4.16	1.48	1.41
8	B	501	FUO	C36-C35	3.66	1.47	1.38
8	B	501	FUO	C02-N31	3.50	1.41	1.33
8	B	501	FUO	C32-N31	-3.24	1.39	1.46
8	B	501	FUO	O20-C19	-3.22	1.15	1.23
5	C	501	GTP	C6-N1	3.12	1.38	1.33
5	A	501	GTP	C6-N1	3.10	1.38	1.33
8	B	501	FUO	C06-C07	-2.86	1.33	1.39
8	D	501	FUO	C35-C34	-2.65	1.33	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	501	FUO	C08-C07	2.63	1.55	1.49
8	D	501	FUO	C38-C33	-2.59	1.33	1.38
8	D	501	FUO	C21-C19	2.59	1.56	1.51
8	D	501	FUO	O12-C11	2.57	1.43	1.37
10	D	504	GDP	O4'-C1'	2.50	1.44	1.41
10	B	506	GDP	C5-C4	2.43	1.47	1.40
8	D	501	FUO	C32-C33	2.34	1.56	1.51
10	D	504	GDP	C5-C4	2.23	1.46	1.40
8	B	501	FUO	C29-N30	-2.10	1.30	1.34

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	501	FUO	C03-C02-N31	14.08	135.21	116.19
8	B	501	FUO	O01-C02-N31	-7.86	108.19	123.01
8	D	501	FUO	C03-C02-N31	6.07	124.39	116.19
8	D	501	FUO	C17-C16-N15	5.67	122.28	110.64
8	B	501	FUO	C22-C21-C19	-5.57	105.37	113.02
10	D	504	GDP	C2-N3-C4	5.55	121.70	115.36
5	A	501	GTP	N3-C2-N1	-5.53	119.84	127.22
5	C	501	GTP	N3-C2-N1	-5.39	120.03	127.22
8	B	501	FUO	C29-C07-C08	-5.08	112.83	121.69
10	B	506	GDP	C2-N3-C4	4.89	120.94	115.36
5	A	501	GTP	C2-N3-C4	4.79	120.83	115.36
5	C	501	GTP	C2-N3-C4	4.51	120.51	115.36
5	A	501	GTP	PB-O3B-PG	-4.45	117.55	132.83
8	D	501	FUO	C03-C04-N30	4.39	122.44	116.41
8	B	501	FUO	C17-C16-N15	4.23	119.33	110.64
8	B	501	FUO	C23-C22-C21	-3.93	110.02	120.01
5	C	501	GTP	PB-O3B-PG	-3.82	119.73	132.83
10	B	506	GDP	C5-C6-N1	-3.80	118.24	123.43
10	D	504	GDP	PA-O3A-PB	-3.78	119.87	132.83
10	B	506	GDP	C2-N1-C6	3.73	121.86	115.93
10	D	504	GDP	C2-N1-C6	3.70	121.81	115.93
8	D	501	FUO	C14-N15-C16	-3.67	101.84	111.23
10	D	504	GDP	C5-C6-N1	-3.66	118.42	123.43
8	B	501	FUO	C06-C07-C08	3.66	127.69	121.36
8	B	501	FUO	C33-C32-N31	-3.64	105.24	113.05
8	B	501	FUO	C16-C17-N18	-3.58	102.76	110.44
10	B	506	GDP	C4-C5-C6	-3.57	117.39	120.80
10	B	506	GDP	PA-O3A-PB	-3.49	120.85	132.83
10	D	504	GDP	C4-C5-C6	-3.46	117.49	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	D	504	GDP	N3-C2-N1	-3.42	122.66	127.22
8	B	501	FUO	O20-C19-C21	-3.39	116.09	122.20
10	B	506	GDP	C3'-C2'-C1'	3.28	105.91	100.98
5	C	501	GTP	PA-O3A-PB	-3.18	121.90	132.83
8	B	501	FUO	C14-N15-C16	-3.14	103.19	111.23
10	D	504	GDP	C4-C5-N7	-3.14	106.13	109.40
8	B	501	FUO	C16-N15-C26	3.04	115.67	108.83
10	B	506	GDP	N3-C2-N1	-3.03	123.19	127.22
8	D	501	FUO	C22-C21-C19	-3.01	108.89	113.02
9	B	503	MES	C6-C5-N4	-2.88	105.73	110.10
8	D	501	FUO	O01-C02-N31	-2.85	117.63	123.01
10	D	504	GDP	C2'-C3'-C4'	2.85	108.18	102.64
5	A	501	GTP	PA-O3A-PB	-2.76	123.34	132.83
8	D	501	FUO	C05-C04-N30	-2.76	118.20	122.17
5	C	501	GTP	C5-C6-N1	-2.74	119.69	123.43
5	A	501	GTP	C2'-C3'-C4'	2.71	107.91	102.64
8	D	501	FUO	C33-C32-N31	-2.70	107.27	113.05
8	D	501	FUO	C25-N18-C17	2.67	117.77	112.62
9	B	503	MES	O3S-S-C8	2.67	110.09	105.77
5	C	501	GTP	C2'-C3'-C4'	2.65	107.78	102.64
8	B	501	FUO	C28-C08-C07	-2.64	116.78	121.36
10	D	504	GDP	C3'-C2'-C1'	2.63	104.94	100.98
10	B	506	GDP	C4-C5-N7	-2.61	106.68	109.40
5	C	501	GTP	C3'-C2'-C1'	2.59	104.88	100.98
8	D	501	FUO	C29-N30-C04	2.55	121.09	117.82
5	A	501	GTP	C5-C6-N1	-2.52	119.98	123.43
5	C	501	GTP	C2-N1-C6	2.49	119.88	115.93
5	A	501	GTP	C2-N1-C6	2.43	119.78	115.93
8	B	501	FUO	O01-C02-C03	-2.40	116.58	122.03
9	B	503	MES	C5-N4-C3	2.36	114.14	108.83
5	A	501	GTP	C3'-C2'-C1'	2.29	104.43	100.98
8	B	501	FUO	C38-C33-C34	-2.21	114.69	118.17
8	B	501	FUO	C21-C19-N18	2.20	122.77	118.52
9	B	503	MES	O2S-S-C8	2.18	109.54	106.92
8	B	501	FUO	C28-C27-C11	2.16	122.38	119.73
8	D	501	FUO	C07-C29-N30	-2.09	120.87	124.32
8	B	501	FUO	C09-C08-C07	2.04	124.89	121.36
8	B	501	FUO	C32-N31-C02	2.03	125.49	122.34

There are no chirality outliers.

All (28) 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-O3A
8	D	501	FUO	C19-C21-C22-C24
8	D	501	FUO	C19-C21-C22-C23
10	B	506	GDP	C5'-O5'-PA-O3A
10	D	504	GDP	C5'-O5'-PA-O3A
8	B	501	FUO	C03-C02-N31-C32
8	D	501	FUO	C03-C02-N31-C32
8	B	501	FUO	O01-C02-N31-C32
8	D	501	FUO	O01-C02-N31-C32
8	B	501	FUO	O12-C13-C14-N15
8	D	501	FUO	O12-C13-C14-N15
5	A	501	GTP	O4'-C4'-C5'-O5'
5	A	501	GTP	C3'-C4'-C5'-O5'
8	D	501	FUO	C14-C13-O12-C11
8	B	501	FUO	C10-C11-O12-C13
8	B	501	FUO	C27-C11-O12-C13
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C5'-O5'-PA-O2A
10	B	506	GDP	C5'-O5'-PA-O2A
10	D	504	GDP	C5'-O5'-PA-O2A
9	B	503	MES	C8-C7-N4-C3
5	A	501	GTP	C5'-O5'-PA-O3A
10	D	504	GDP	C3'-C4'-C5'-O5'
5	A	501	GTP	PA-O3A-PB-O2B

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	B	501	FUO	C16-C17-C25-C26-N15-N18

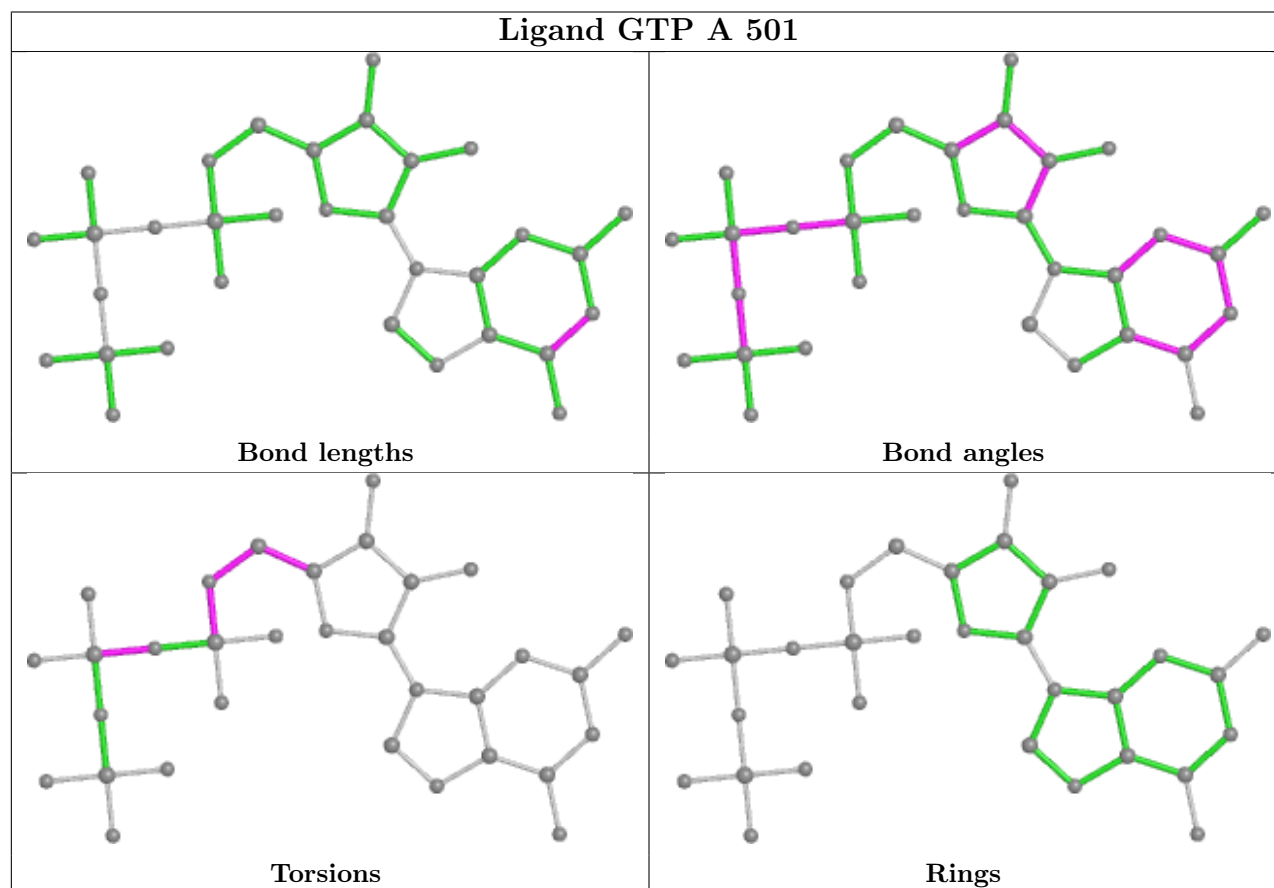
1 monomer is involved in 2 short contacts:

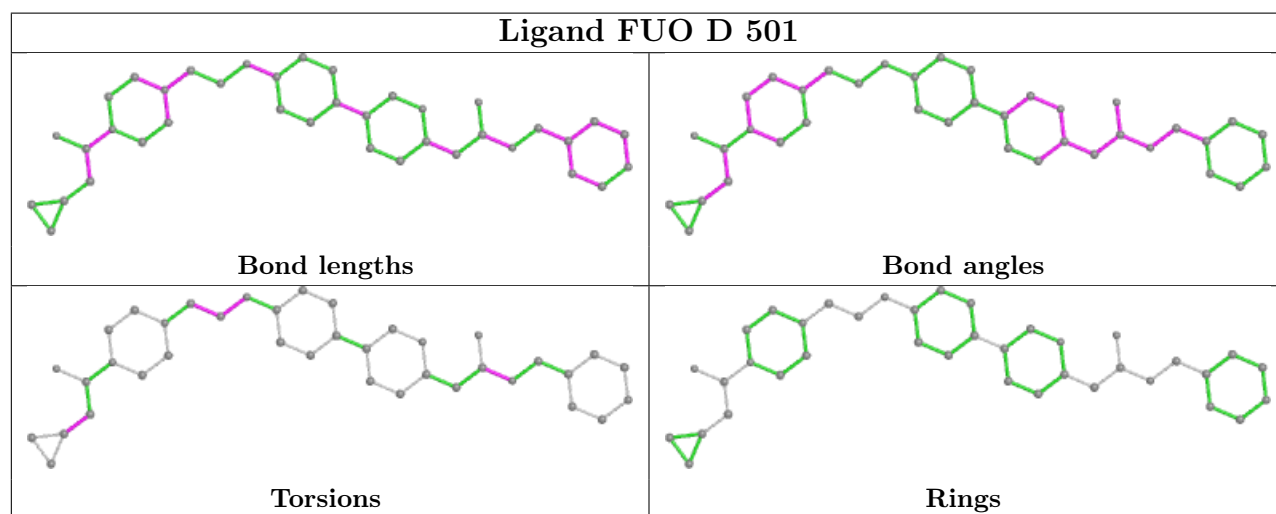
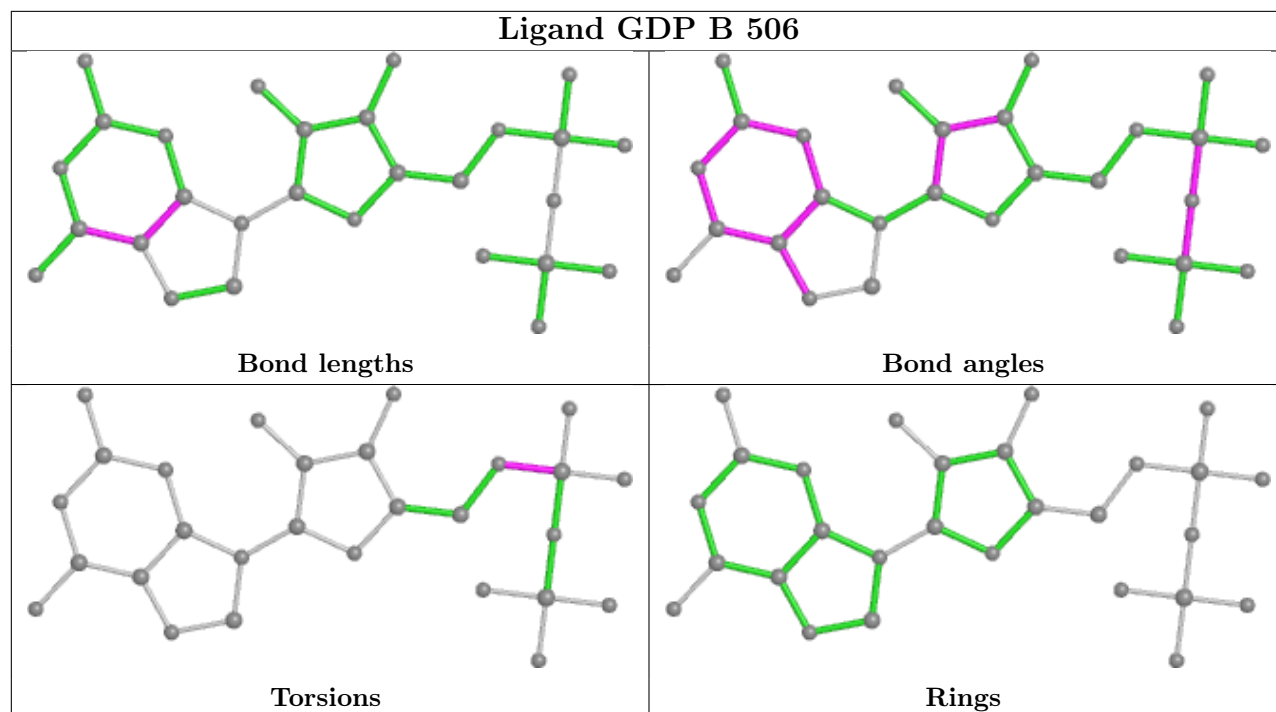
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	FUO	2	0

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

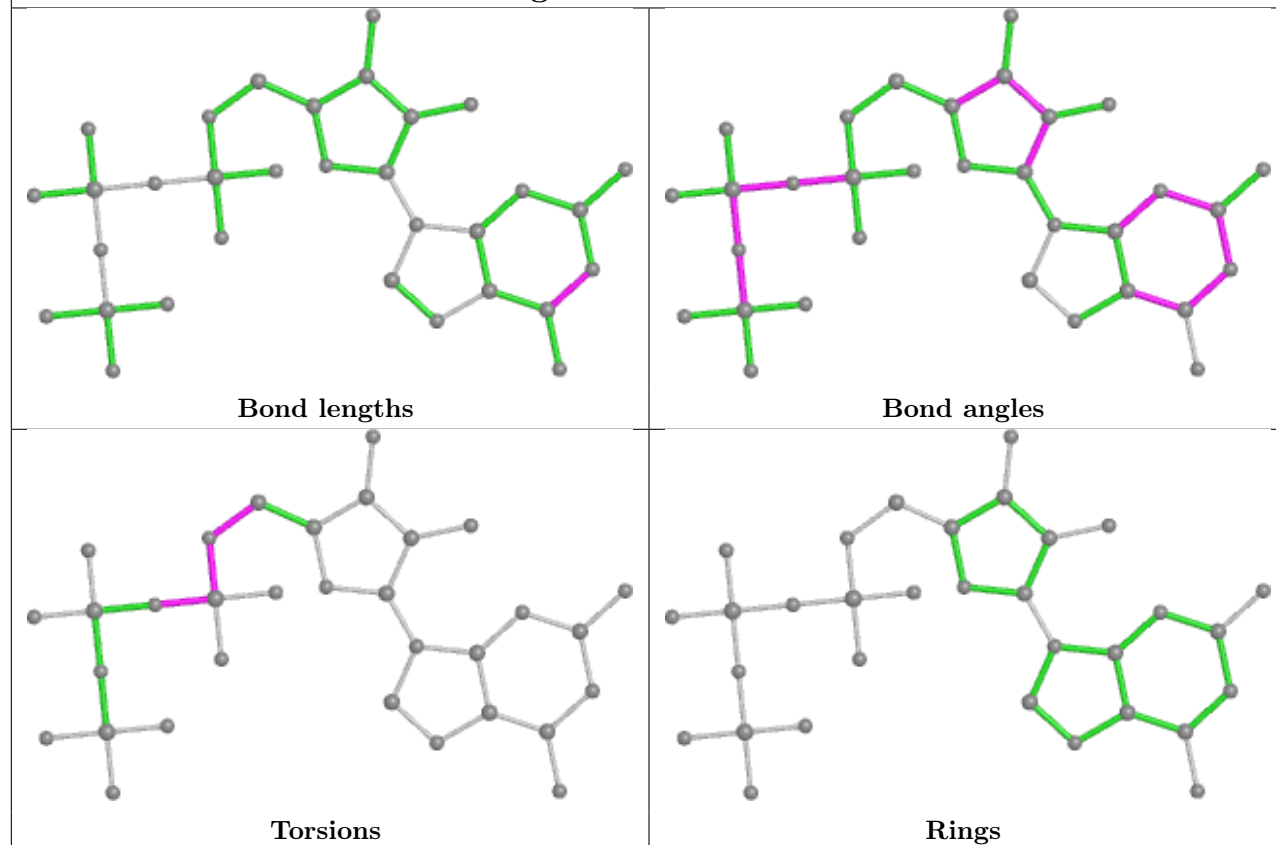


within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question 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.

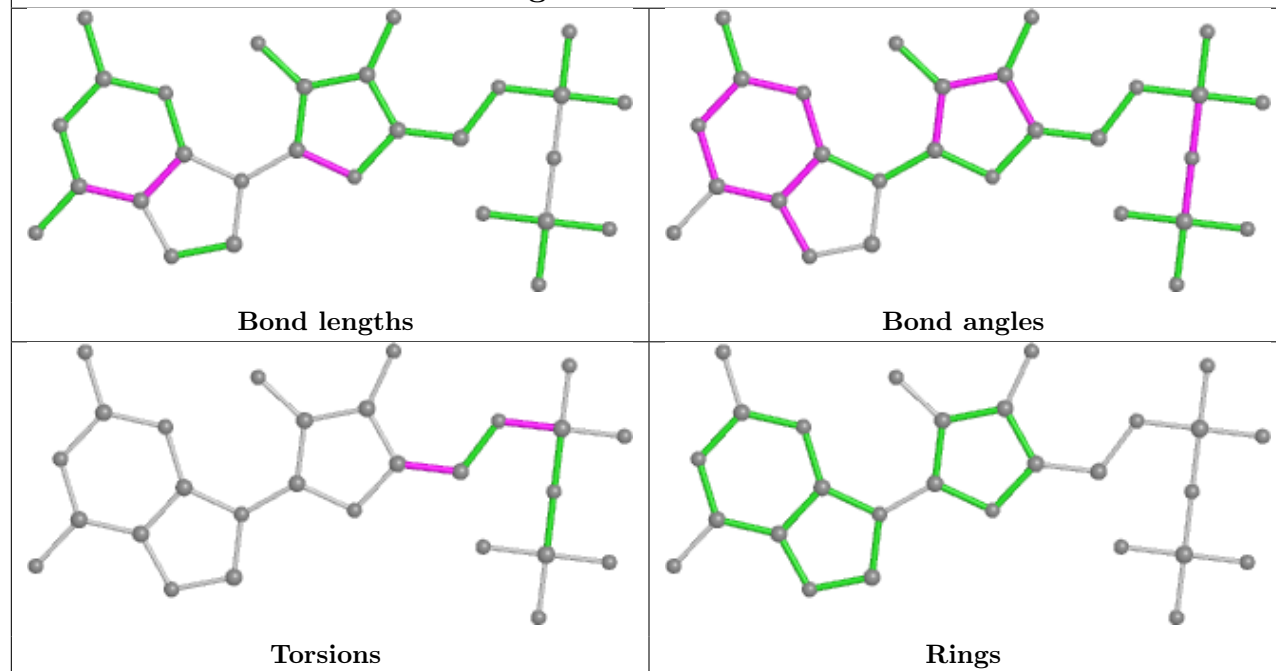


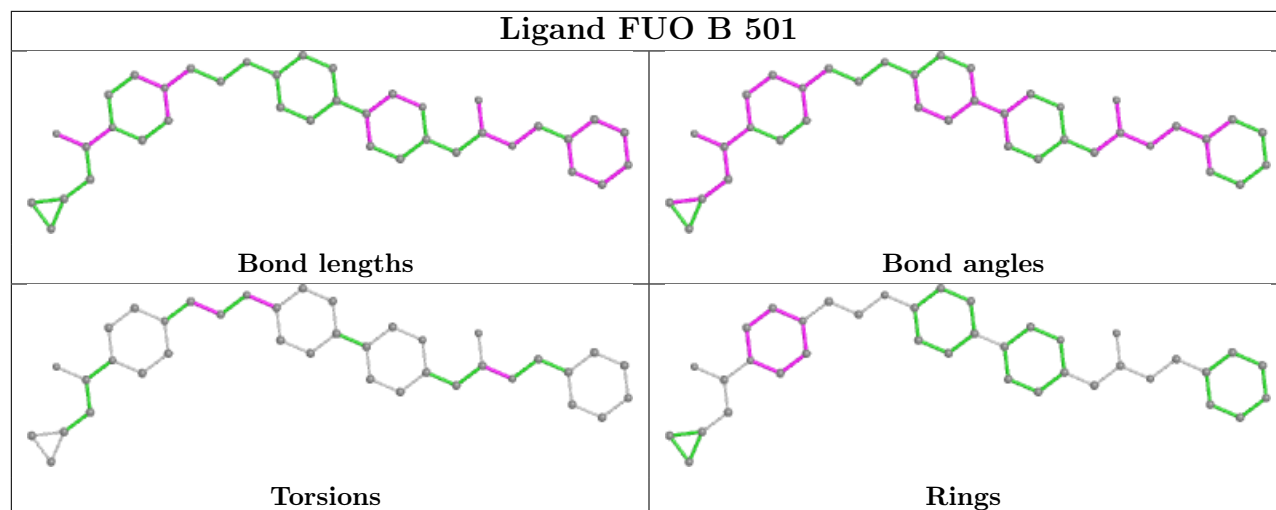


## Ligand GTP C 501



## Ligand GDP D 504





## 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, 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	438/451 (97%)	0.08	9 (2%) 63 58	41, 59, 86, 111	0
1	C	440/451 (97%)	-0.09	6 (1%) 75 71	37, 51, 79, 106	0
2	B	424/445 (95%)	0.18	20 (4%) 31 25	38, 58, 90, 118	0
2	D	425/445 (95%)	0.39	30 (7%) 16 11	44, 73, 102, 120	0
3	E	123/189 (65%)	0.71	17 (13%) 2 1	47, 75, 109, 127	0
4	F	313/383 (81%)	0.92	63 (20%) 1 0	49, 80, 146, 164	0
All	All	2163/2364 (91%)	0.28	145 (6%) 17 13	37, 63, 106, 164	0

All (145) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	125	THR	7.9
4	F	178	GLN	7.1
2	D	57	THR	6.7
4	F	157	GLY	6.7
4	F	259	GLY	6.5
4	F	153	ALA	6.3
4	F	156	LYS	6.0
4	F	160	ILE	5.7
4	F	154	GLY	5.4
4	F	143	GLU	5.2
4	F	158	GLU	5.2
1	A	281	ALA	5.0
4	F	362	ALA	4.9
4	F	136	ASN	4.9
4	F	155	ALA	4.8
3	E	140	LYS	4.7
4	F	258	GLU	4.7
4	F	162	ILE	4.7
3	E	45	PRO	4.7

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Mol	Chain	Res	Type	RSRZ
2	B	431	THR	4.6
4	F	140	GLU	4.4
1	A	438	ASP	4.4
4	F	177	GLY	4.4
4	F	132	LEU	4.3
2	D	82	PRO	4.3
4	F	133	ALA	4.3
2	B	57	THR	4.2
3	E	7	GLU	4.2
4	F	89	GLU	4.2
2	B	430	ALA	4.2
4	F	257	GLU	4.1
2	D	130	ASP	4.1
4	F	172	PHE	4.1
4	F	90	SER	4.0
2	B	293	GLN	4.0
4	F	145	ASN	3.9
4	F	142	ARG	3.8
4	F	179	VAL	3.8
2	B	59	ASN	3.8
3	E	143	ALA	3.8
4	F	260	ASN	3.7
2	B	338	LYS	3.7
4	F	175	GLU	3.7
2	D	179	ASP	3.7
4	F	141	GLY	3.7
2	D	276	THR	3.7
2	B	284	ARG	3.6
4	F	146	VAL	3.5
2	D	280	SER	3.5
2	D	408	MET	3.5
4	F	182	ILE	3.3
1	A	346	TRP	3.3
2	B	276	THR	3.3
2	D	337	ASN	3.2
4	F	163	SER	3.2
4	F	181	VAL	3.2
4	F	137	ARG	3.2
1	A	282	TYR	3.2
3	E	139	LEU	3.2
4	F	139	ARG	3.2
2	D	97	SER	3.2

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Mol	Chain	Res	Type	RSRZ
4	F	372	THR	3.2
2	B	130	ASP	3.2
4	F	164	SER	3.1
4	F	9	GLU	3.1
1	C	246	GLY	3.1
2	D	277	SER	3.0
4	F	100	ILE	3.0
3	E	27	PRO	3.0
1	C	440	VAL	3.0
4	F	159	GLY	3.0
2	B	282	GLN	3.0
2	B	429	ASP	3.0
2	D	364	LYS	3.0
3	E	142	GLU	2.9
1	A	437	VAL	2.9
2	D	361	ARG	2.9
2	D	94	PHE	2.9
2	D	433	ASP	2.8
2	D	247	GLN	2.8
2	D	58	GLY	2.8
3	E	46	SER	2.8
4	F	196	HIS	2.8
1	A	279	GLU	2.8
1	C	357	TYR	2.8
2	B	66	ILE	2.8
2	D	432	ALA	2.8
2	B	7	ILE	2.8
4	F	130	VAL	2.7
3	E	44	ASP	2.7
4	F	174	ASP	2.7
2	B	218	LYS	2.7
4	F	129	GLU	2.7
1	A	326	LYS	2.7
2	D	218	LYS	2.7
2	D	39	ASP	2.7
4	F	361	LEU	2.7
2	D	398	HIS	2.6
2	D	221	THR	2.6
4	F	46	ARG	2.6
1	C	247	ALA	2.6
1	A	163	LYS	2.6
2	B	37	HIS	2.5

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Mol	Chain	Res	Type	RSRZ
2	D	287	THR	2.5
4	F	150	LYS	2.5
2	D	37	HIS	2.5
2	D	299	LYS	2.5
3	E	141	GLU	2.5
1	C	365	GLY	2.4
2	B	82	PRO	2.4
2	B	221	THR	2.4
4	F	169	LEU	2.4
4	F	147	TRP	2.4
2	D	127	GLU	2.4
4	F	91	CYS	2.4
2	D	407	GLU	2.4
3	E	135	LYS	2.4
3	E	28	SER	2.3
4	F	10	ASN	2.3
4	F	126	ASP	2.3
1	A	315	CYS	2.3
2	D	392	ARG	2.3
3	E	6	MET	2.3
3	E	138	GLU	2.3
2	D	59	ASN	2.2
4	F	165	GLU	2.2
1	C	218	ASP	2.2
3	E	121	GLU	2.2
4	F	187	GLU	2.2
4	F	199	PHE	2.2
3	E	48	GLU	2.2
4	F	195	GLY	2.2
2	D	2	ARG	2.2
2	B	309	HIS	2.2
4	F	171	ASP	2.2
4	F	306	HIS	2.1
2	B	283	TYR	2.1
3	E	125	GLU	2.1
4	F	138	ARG	2.1
4	F	373	SER	2.1
4	F	176	GLN	2.0
4	F	380	HIS	2.0
2	B	65	ALA	2.0
2	D	129	CYS	2.0
4	F	85	PRO	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.