



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 11, 2022 – 12:13 PM JST

PDB ID : 7EMJ
Title : Crystal structure of T2R-TTL-Barbigerone complex
Authors : Yang, J.H.; Yan, W.
Deposited on : 2021-04-14
Resolution : 2.33 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 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 : 2.27
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) : 2.27

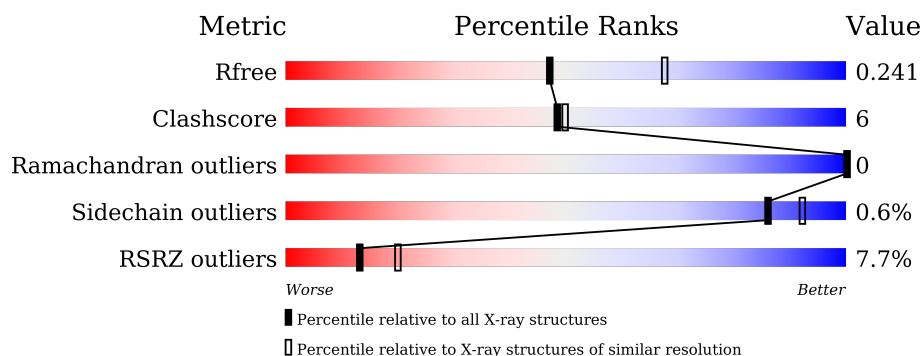
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.33 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	2096 (2.36-2.32)
Clashscore	141614	2193 (2.36-2.32)
Ramachandran outliers	138981	2159 (2.36-2.32)
Sidechain outliers	138945	2160 (2.36-2.32)
RSRZ outliers	127900	2067 (2.36-2.32)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	451	<div> <div></div> <div>86% 11% ..</div> </div>
1	C	451	<div> <div></div> <div>87% 10% .</div> </div>
2	B	445	<div> <div>4%</div> <div>84% 10% ..</div> </div>
2	D	445	<div> <div>6%</div> <div>80% 14% . 5%</div> </div>
3	E	189	<div> <div>4%</div> <div>54% 10% . 35%</div> </div>
4	F	384	<div> <div>29%</div> <div>71% 19% . 9%</div> </div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 35500 atoms, of which 17027 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	8	0
			6817	2187	3361	586	658	25			
1	C	440	Total	C	H	N	O	S	0	9	0
			6826	2189	3365	586	662	24			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	426	Total	C	H	N	O	S	0	1	0
			6528	2101	3184	573	644	26			
2	D	422	Total	C	H	N	O	S	0	1	0
			6481	2084	3167	563	641	26			

- 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	5	0
			2079	637	1044	188	205	5			

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	F	350	Total	C	H	N	O	S	0	1	0
			5682	1834	2818	490	525	15			

There are 6 discrepancies between the modelled and reference sequences:

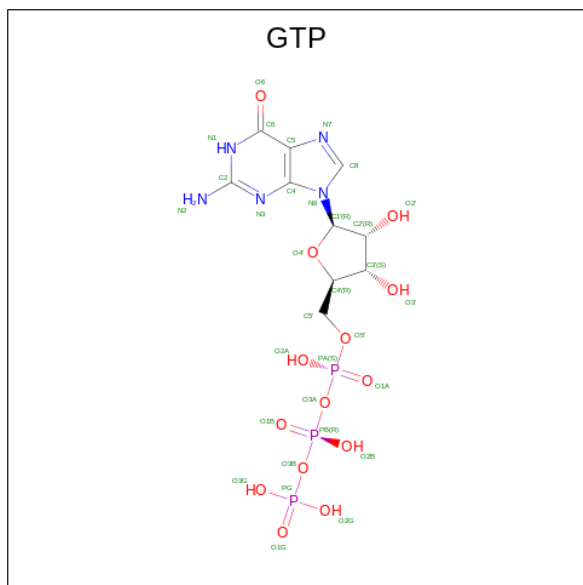
Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43

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Chain	Residue	Modelled	Actual	Comment	Reference
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

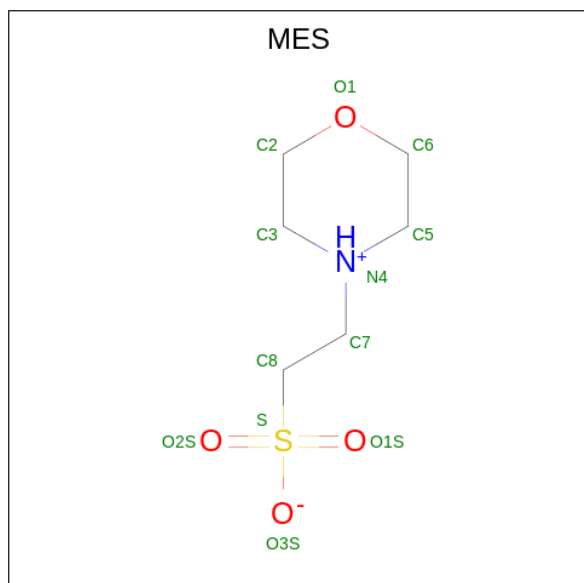
- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (three-letter code: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



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

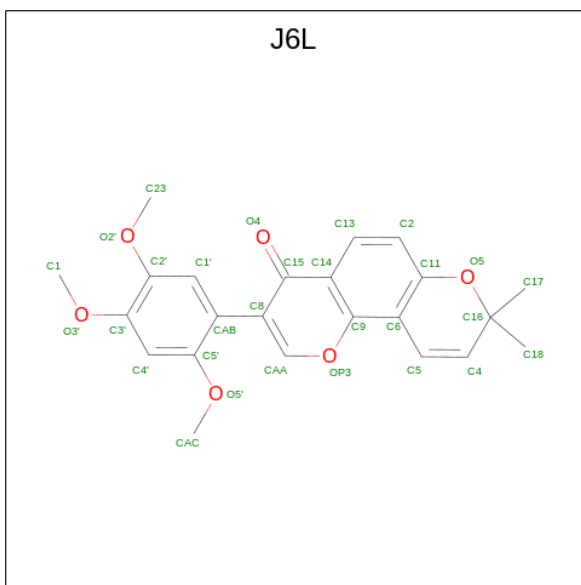
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	2	Total	Ca	2	0
			2	2		
7	B	2	Total	Ca	2	0
			2	2		
7	C	1	Total	Ca	1	0
			1	1		
7	D	1	Total	Ca	1	0
			1	1		

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (three-letter code: MES) (formula: C₆H₁₃NO₄S).



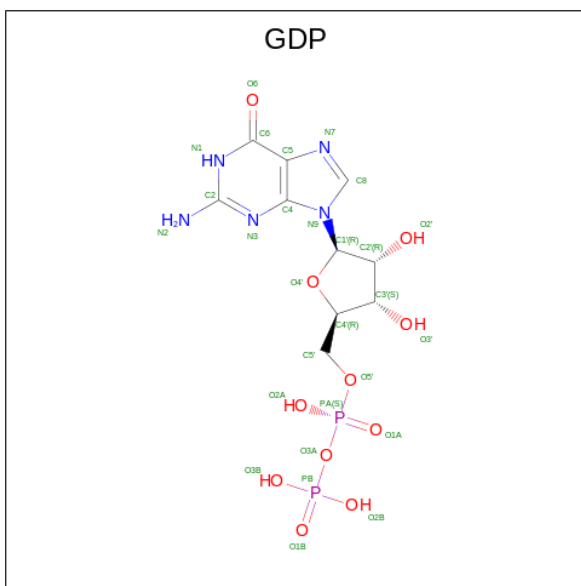
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	H	N	O	S	
			24	6	12	1	4	1	0

- Molecule 9 is 8,8-dimethyl-3-(2,4,5-trimethoxyphenyl)pyrano[2,3-f]chromen-4-one (three-letter code: J6L) (formula: C₂₃H₂₂O₆) (labeled as "Ligand of Interest" by depositor).



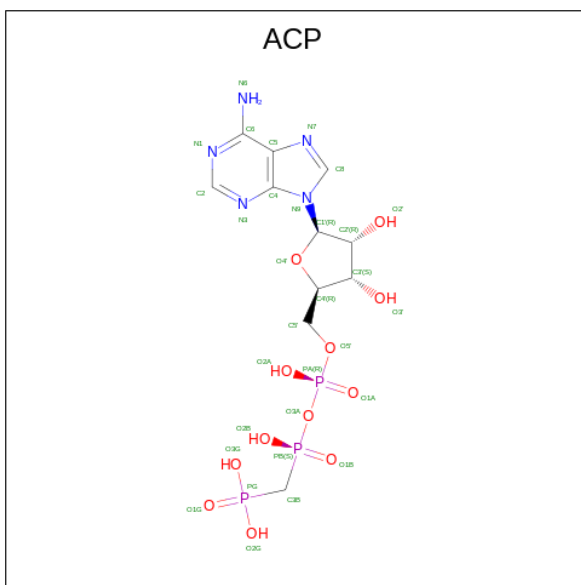
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	H	O	0	0
			51	23	22	6		

- Molecule 10 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).



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

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	
11	F	1	Total	C	H	N	O	P	45	0
			45	11	14	5	12	3		

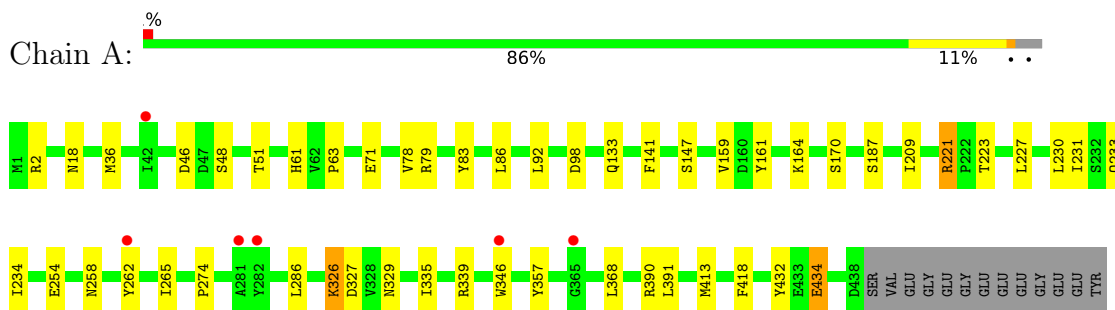
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	170	Total O 170 170	0	0
12	B	139	Total O 139 139	0	0
12	C	277	Total O 277 277	0	0
12	D	101	Total O 101 101	0	0
12	E	41	Total O 41 41	0	0
12	F	64	Total O 64 64	0	0

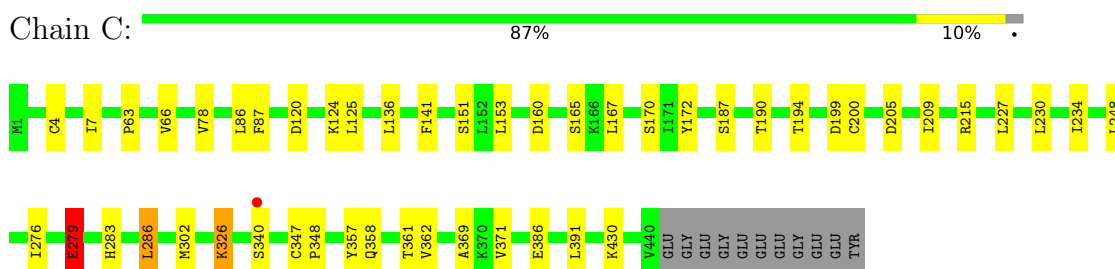
3 Residue-property plots

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.

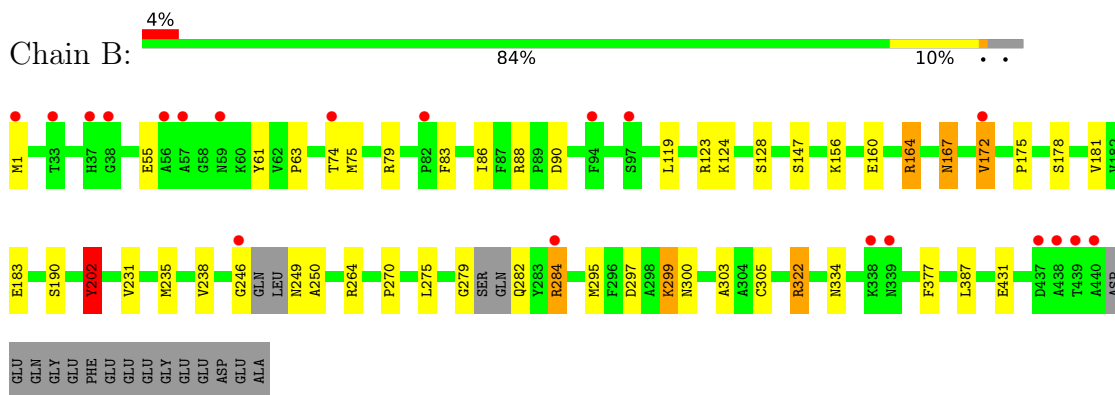
- Molecule 1: Tubulin alpha-1B chain

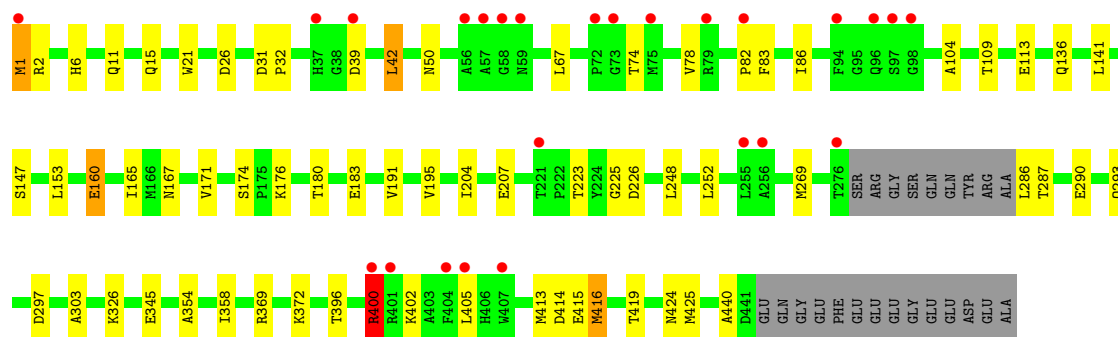


- Molecule 1: Tubulin alpha-1B chain

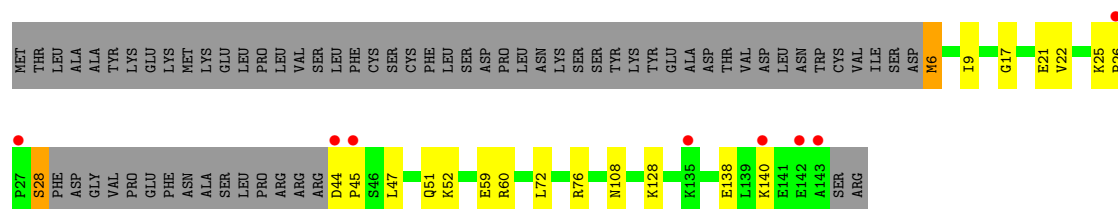


- Molecule 2: Tubulin beta chain

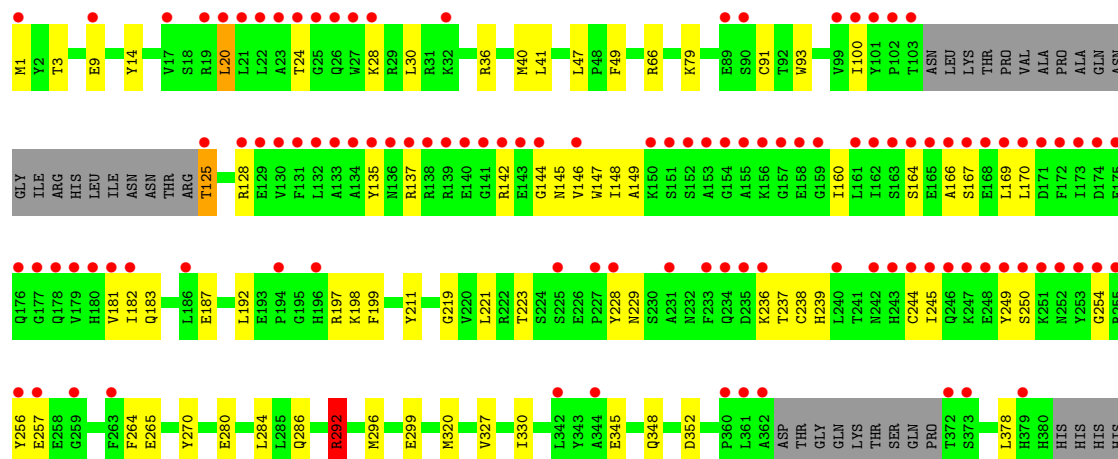




● Molecule 3: Stathmin-4



● 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	105.03Å 157.25Å 180.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.90 – 2.33 46.90 – 2.33	Depositor EDS
% Data completeness (in resolution range)	99.2 (46.90-2.33) 99.2 (46.90-2.33)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.47 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.198 , 0.241 0.198 , 0.241	Depositor DCC
R_{free} test set	6360 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	27.8	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 47.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	35500	wwPDB-VP
Average B, all atoms (Å ²)	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.67% 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: J6L, MG, GTP, GDP, MES, ACP, CA

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	0.42	3/3565 (0.1%)	0.69	4/4840 (0.1%)
1	C	0.48	1/3578 (0.0%)	0.65	8/4859 (0.2%)
2	B	0.63	5/3421 (0.1%)	0.72	12/4632 (0.3%)
2	D	0.46	5/3390 (0.1%)	0.96	15/4594 (0.3%)
3	E	0.55	0/1064	0.67	3/1412 (0.2%)
4	F	0.40	0/2929	0.73	8/3956 (0.2%)
All	All	0.49	14/17947 (0.1%)	0.75	50/24293 (0.2%)

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
1	A	0	1
1	C	0	2
2	B	0	1
2	D	0	1
4	F	0	2
All	All	0	7

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	293	GLN	C-O	-8.11	1.07	1.23
1	C	347	CYS	CB-SG	-7.46	1.69	1.82
2	B	183	GLU	CD-OE2	-6.31	1.18	1.25
2	B	183	GLU	CB-CG	-6.23	1.40	1.52
2	D	400	ARG	CD-NE	-6.15	1.35	1.46
2	B	172	VAL	C-O	-5.98	1.11	1.23
1	A	83	TYR	CG-CD1	-5.51	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	434	GLU	CD-OE2	-5.42	1.19	1.25
2	D	400	ARG	CZ-NH1	-5.36	1.26	1.33
2	B	202	TYR	CG-CD1	-5.35	1.32	1.39
2	B	167	ASN	C-O	-5.28	1.13	1.23
2	D	160	GLU	CG-CD	-5.16	1.44	1.51
2	D	400	ARG	NE-CZ	-5.05	1.26	1.33
1	A	434	GLU	CD-OE1	-5.04	1.20	1.25

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	400	ARG	NE-CZ-NH2	34.15	137.38	120.30
2	D	400	ARG	NE-CZ-NH1	-28.30	106.15	120.30
1	A	434	GLU	CG-CD-OE1	16.76	151.82	118.30
1	A	434	GLU	OE1-CD-OE2	-15.31	104.92	123.30
4	F	292	ARG	NE-CZ-NH1	-14.42	113.09	120.30
1	A	434	GLU	CG-CD-OE2	-12.83	92.64	118.30
4	F	292	ARG	NE-CZ-NH2	12.28	126.44	120.30
2	D	400	ARG	CB-CG-CD	10.23	138.20	111.60
2	D	400	ARG	CA-CB-CG	-9.53	92.42	113.40
2	D	400	ARG	CG-CD-NE	9.48	131.70	111.80
1	C	279	GLU	OE1-CD-OE2	-9.24	112.20	123.30
2	B	322	ARG	CG-CD-NE	8.66	129.98	111.80
2	B	297	ASP	CB-CG-OD2	8.60	126.04	118.30
1	C	430	LYS	CD-CE-NZ	-8.33	92.54	111.70
1	C	286	LEU	CB-CG-CD1	-8.21	97.05	111.00
4	F	36	ARG	NE-CZ-NH1	-8.07	116.27	120.30
2	B	164	ARG	NE-CZ-NH2	8.02	124.31	120.30
3	E	138	GLU	CA-CB-CG	7.75	130.45	113.40
1	C	286	LEU	CB-CG-CD2	7.66	124.02	111.00
2	D	326	LYS	CD-CE-NZ	7.52	128.99	111.70
4	F	20	LEU	CB-CG-CD2	-7.34	98.52	111.00
2	B	322	ARG	NE-CZ-NH2	-6.99	116.81	120.30
2	B	164	ARG	NE-CZ-NH1	-6.97	116.81	120.30
4	F	36	ARG	NE-CZ-NH2	6.92	123.76	120.30
2	B	322	ARG	CD-NE-CZ	6.84	133.18	123.60
2	D	372	LYS	CD-CE-NZ	6.70	127.10	111.70
1	C	326	LYS	CD-CE-NZ	6.58	126.83	111.70
2	B	1	MET	CG-SD-CE	-6.52	89.77	100.20
2	D	297	ASP	CB-CG-OD2	-6.47	112.48	118.30
2	D	416	MET	CB-CG-SD	-6.40	93.19	112.40
2	D	297	ASP	CB-CG-OD1	6.40	124.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	416	MET	CA-CB-CG	6.20	123.84	113.30
2	D	153	LEU	CB-CG-CD2	-6.08	100.66	111.00
1	C	86	LEU	CB-CG-CD1	-6.01	100.79	111.00
4	F	211	TYR	CB-CG-CD1	-5.93	117.44	121.00
2	D	42	LEU	CB-CG-CD1	-5.73	101.26	111.00
2	B	79	ARG	NE-CZ-NH2	-5.69	117.45	120.30
2	B	124	LYS	CA-CB-CG	5.62	125.76	113.40
4	F	137	ARG	CA-CB-CG	5.56	125.63	113.40
4	F	211	TYR	CB-CG-CD2	5.55	124.33	121.00
2	B	79	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	A	326	LYS	CB-CG-CD	-5.52	97.26	111.60
3	E	128	LYS	CD-CE-NZ	-5.44	99.19	111.70
2	B	183	GLU	CG-CD-OE1	5.38	129.05	118.30
2	D	1	MET	CA-CB-CG	5.32	122.34	113.30
2	B	284	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	C	279	GLU	CA-CB-CG	5.24	124.94	113.40
3	E	60	ARG	NE-CZ-NH1	5.24	122.92	120.30
2	D	400	ARG	CD-NE-CZ	-5.10	116.46	123.60
1	C	279	GLU	CG-CD-OE1	5.04	128.38	118.30

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	434	GLU	Sidechain
2	B	322	ARG	Sidechain
1	C	279	GLU	Sidechain
1	C	283	HIS	Mainchain
2	D	400	ARG	Sidechain
4	F	292	ARG	Sidechain
4	F	9	GLU	Sidechain

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	3456	3361	3342	36	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	3461	3365	3336	31	0
2	B	3344	3184	3221	37	2
2	D	3314	3167	3197	40	3
3	E	1035	1044	1023	14	1
4	F	2864	2818	2831	55	0
5	A	32	10	12	0	0
5	C	32	10	12	0	0
5	D	32	10	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	12	12	12	0	0
9	B	29	22	0	3	0
10	B	28	10	12	0	0
11	F	31	14	14	0	0
12	A	170	0	0	3	0
12	B	139	0	0	6	0
12	C	277	0	0	7	0
12	D	101	0	0	2	0
12	E	41	0	0	3	0
12	F	64	0	0	8	0
All	All	18473	17027	17024	208	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 (208) 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:167:ASN:HB3	9:B:505:J6L:C1	1.93	0.98
2:B:167:ASN:CB	9:B:505:J6L:C1	2.59	0.81
4:F:125:THR:OG1	12:F:501:HOH:O	2.04	0.75
2:B:202:TYR:CZ	2:B:270:PRO:HB3	2.21	0.75
4:F:345:GLU:O	12:F:502:HOH:O	2.09	0.69
1:C:215:ARG:NH1	12:C:607:HOH:O	2.25	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:279:GLY:O	12:B:601:HOH:O	2.09	0.69
2:D:402:LYS:HB3	2:D:405:LEU:HD12	1.73	0.69
3:E:28:SER:O	12:E:201:HOH:O	2.11	0.69
2:B:128:SER:O	12:B:602:HOH:O	2.10	0.68
1:A:46:ASP:OD2	12:A:601:HOH:O	2.10	0.68
2:B:250:ALA:O	12:B:604:HOH:O	2.12	0.68
2:D:225:GLY:O	12:D:601:HOH:O	2.12	0.67
4:F:270:TYR:OH	12:F:503:HOH:O	2.12	0.67
3:E:44:ASP:N	12:E:203:HOH:O	2.28	0.67
1:C:120[B]:ASP:OD2	1:C:124:LYS:NZ	2.27	0.67
2:B:282:GLN:N	12:B:609:HOH:O	2.28	0.67
4:F:79:LYS:HE2	4:F:79:LYS:HA	1.77	0.66
4:F:197:ARG:NH2	4:F:257:GLU:OE2	2.28	0.66
4:F:135:TYR:CE1	4:F:166:ALA:HB2	2.31	0.66
4:F:265:GLU:O	12:F:505:HOH:O	2.14	0.65
4:F:254:GLY:O	12:F:504:HOH:O	2.14	0.65
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.30	0.64
4:F:257:GLU:O	12:F:506:HOH:O	2.15	0.64
3:E:108:ASN:OD1	12:E:202:HOH:O	2.15	0.64
1:A:327:ASP:OD2	12:A:602:HOH:O	2.15	0.64
4:F:144:GLY:HA3	4:F:187:GLU:OE1	1.98	0.64
2:D:286:LEU:HD23	2:D:287:THR:N	2.13	0.63
2:B:264:ARG:NH1	2:B:431:GLU:OE1	2.28	0.63
1:A:329:ASN:O	3:E:6:MET:HE1	1.99	0.63
4:F:145:ASN:OD1	4:F:147:TRP:NE1	2.32	0.63
4:F:148:ILE:HD11	4:F:160:ILE:HG21	1.80	0.62
2:D:83:PHE:O	2:D:86:ILE:HG22	2.00	0.62
4:F:286:GLN:HG3	4:F:327:VAL:HB	1.82	0.62
1:C:286:LEU:HD12	1:C:286:LEU:N	2.14	0.61
2:D:223:THR:HG22	2:D:226:ASP:OD2	2.02	0.59
1:A:2:ARG:HB3	1:A:133:GLN:HG3	1.85	0.59
2:B:63:PRO:CD	2:B:86:ILE:HG12	2.33	0.59
1:A:329:ASN:O	3:E:6:MET:CE	2.50	0.59
1:C:326:LYS:NZ	12:C:616:HOH:O	2.35	0.58
4:F:166:ALA:O	4:F:169:LEU:HG	2.02	0.58
2:B:75:MET:N	12:B:615:HOH:O	2.36	0.58
2:B:295:MET:HG3	2:B:377:PHE:HB2	1.86	0.58
3:E:51:GLN:HA	3:E:51:GLN:OE1	2.04	0.58
2:D:345:GLU:HG2	2:D:440:ALA:HB2	1.86	0.57
2:B:295:MET:CG	2:B:377:PHE:HB2	2.34	0.57
4:F:3:THR:CG2	4:F:30:LEU:HD21	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:SER:OG	2:B:190:SER:OG	2.17	0.57
4:F:169:LEU:CD1	4:F:182:ILE:HD13	2.34	0.56
1:A:161:TYR:HB3	1:A:164:LYS:CG	2.35	0.56
2:B:246:GLY:O	2:B:249:ASN:N	2.38	0.56
3:E:44:ASP:N	3:E:45:PRO:CD	2.68	0.56
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.04	0.56
4:F:229:ASN:N	4:F:238:CYS:SG	2.78	0.56
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.88	0.55
1:A:209[A]:ILE:CD1	1:A:231:ILE:HD11	2.36	0.55
2:D:414:ASP:OD1	2:D:415:GLU:N	2.39	0.55
1:C:160:ASP:OD2	12:C:601:HOH:O	2.18	0.54
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.90	0.54
4:F:3:THR:HG21	4:F:30:LEU:HD21	1.88	0.54
2:D:345:GLU:CG	2:D:440:ALA:HB2	2.37	0.54
4:F:219:GLY:O	12:F:507:HOH:O	2.19	0.54
4:F:292:ARG:CD	4:F:378:LEU:HB3	2.38	0.53
4:F:125:THR:OG1	4:F:125:THR:O	2.22	0.53
4:F:320:MET:HG2	4:F:330:ILE:HD13	1.89	0.53
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.90	0.53
2:B:299:LYS:HD3	2:B:299:LYS:H	1.71	0.53
4:F:244:CYS:SG	4:F:245:ILE:N	2.82	0.53
2:B:83:PHE:O	2:B:86:ILE:HG22	2.08	0.53
2:B:172:VAL:HG11	2:B:387:LEU:HD21	1.90	0.53
2:B:202:TYR:CZ	2:B:238:VAL:HG11	2.44	0.53
4:F:256:TYR:HB2	4:F:257:GLU:OE1	2.08	0.53
2:D:416:MET:O	2:D:419:THR:N	2.42	0.52
2:D:136:GLN:HA	2:D:167:ASN:O	2.09	0.52
2:B:63:PRO:HD3	2:B:86:ILE:HG12	1.91	0.52
2:D:67:LEU:CD2	2:D:78:VAL:HG11	2.40	0.52
1:C:230:LEU:O	1:C:234:ILE:HD12	2.09	0.52
4:F:148:ILE:HD11	4:F:160:ILE:CG2	2.39	0.52
2:D:42:LEU:HD23	2:D:358:ILE:CD1	2.40	0.52
2:D:174:SER:OG	2:D:207:GLU:OE1	2.27	0.52
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.93	0.51
4:F:296[B]:MET:HE1	4:F:299:GLU:OE1	2.10	0.51
2:B:167:ASN:HB2	9:B:505:J6L:C1	2.40	0.51
2:B:202:TYR:CE1	2:B:238:VAL:HG11	2.45	0.51
1:C:371:VAL:HG12	12:C:861:HOH:O	2.11	0.51
4:F:169:LEU:HD13	4:F:182:ILE:HD13	1.92	0.51
2:B:181:VAL:HG12	1:C:348:PRO:HG2	1.93	0.51
2:D:223:THR:HG23	2:D:226:ASP:H	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.91	0.51
4:F:199:PHE:CD1	4:F:221:LEU:HD23	2.46	0.51
1:C:78:VAL:O	12:C:602:HOH:O	2.20	0.50
2:D:42:LEU:HD23	2:D:358:ILE:HD11	1.93	0.50
2:D:176:LYS:HE3	2:D:207:GLU:OE2	2.12	0.50
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.92	0.50
1:C:358:GLN:H	1:C:358:GLN:CD	2.15	0.50
4:F:91:CYS:SG	4:F:93:TRP:CE2	3.05	0.50
3:E:72:LEU:O	3:E:76:ARG:HG2	2.11	0.50
2:B:88:ARG:HH11	2:B:88:ARG:HG2	1.77	0.50
2:D:396:THR:O	2:D:400:ARG:HB2	2.12	0.50
4:F:292:ARG:HD2	4:F:378:LEU:HB3	1.94	0.49
4:F:237:THR:HG22	4:F:245:ILE:CG2	2.42	0.49
1:A:262:TYR:CZ	1:A:346:TRP:CZ2	3.01	0.49
2:B:119:LEU:HD11	2:B:156:LYS:CB	2.42	0.49
4:F:40:MET:HE1	4:F:47:LEU:HG	1.95	0.49
4:F:198:LYS:NZ	12:F:514:HOH:O	2.45	0.49
1:C:165:SER:HA	1:C:199:ASP:OD2	2.13	0.49
2:D:104:ALA:HB2	2:D:413:MET:SD	2.53	0.49
1:A:262:TYR:OH	1:A:346:TRP:CZ2	2.66	0.49
4:F:149:ALA:HA	4:F:181:VAL:O	2.13	0.49
3:E:44:ASP:N	3:E:45:PRO:HD3	2.28	0.48
1:A:161:TYR:HB3	1:A:164:LYS:HG2	1.94	0.48
2:B:250:ALA:HB3	12:B:604:HOH:O	2.13	0.48
1:C:136:LEU:HD23	1:C:167:LEU:HB2	1.95	0.48
2:D:171:VAL:HA	2:D:204:ILE:O	2.14	0.48
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.96	0.48
2:B:123:ARG:NE	2:B:160:GLU:OE2	2.39	0.48
4:F:237:THR:HB	4:F:250:SER:OG	2.13	0.48
1:C:386:GLU:OE1	12:C:603:HOH:O	2.20	0.47
2:B:231:VAL:O	2:B:235:MET:HG3	2.14	0.47
4:F:192:LEU:H	4:F:192:LEU:HD12	1.79	0.47
4:F:236:LYS:O	4:F:239:HIS:N	2.39	0.47
2:D:286:LEU:HD23	2:D:287:THR:H	1.79	0.47
1:C:209:ILE:HD11	1:C:302:MET:SD	2.54	0.47
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.95	0.47
4:F:237:THR:HG21	4:F:249:TYR:HB3	1.96	0.47
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.30	0.47
1:A:63:PRO:HD3	1:A:86:LEU:HG	1.96	0.46
1:C:190:THR:O	1:C:194[A]:THR:HG23	2.15	0.46
2:D:67:LEU:N	2:D:67:LEU:HD12	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.97	0.46
2:D:402:LYS:CB	2:D:405:LEU:HD12	2.42	0.46
1:A:79:ARG:HG2	1:A:92:LEU:HD12	1.98	0.46
4:F:228:TYR:HA	4:F:238:CYS:SG	2.55	0.46
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.98	0.46
2:D:2:ARG:NH1	12:D:609:HOH:O	2.37	0.45
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.16	0.45
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.31	0.45
4:F:146:VAL:HA	4:F:164:SER:HA	1.99	0.45
2:B:202:TYR:CE2	2:B:270:PRO:HB3	2.51	0.45
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.99	0.45
2:D:74:THR:O	2:D:78:VAL:HG23	2.17	0.45
1:A:230:LEU:O	1:A:234:ILE:HD12	2.17	0.45
1:C:4[B]:CYS:SG	1:C:136:LEU:HG	2.57	0.44
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.99	0.44
4:F:223:THR:HG21	4:F:257:GLU:OE2	2.16	0.44
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.52	0.44
4:F:20:LEU:HD22	4:F:348:GLN:OE1	2.18	0.44
3:E:25:LYS:HG3	3:E:26:PRO:HD2	1.99	0.44
1:C:361:THR:HG22	1:C:362:VAL:N	2.33	0.44
2:D:82:PRO:O	2:D:83:PHE:HB2	2.17	0.44
1:A:413:MET:CE	1:A:418:PHE:CE2	3.01	0.44
1:A:390:ARG:NH2	12:A:618:HOH:O	2.50	0.44
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.53	0.44
2:D:191:VAL:HB	2:D:425:MET:HE3	2.00	0.43
2:B:55:GLU:HG3	2:B:61:TYR:CE1	2.53	0.43
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.48	0.43
4:F:192:LEU:HD11	4:F:199:PHE:CD2	2.53	0.43
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.53	0.43
3:E:22:VAL:O	3:E:22:VAL:HG13	2.18	0.43
2:B:299:LYS:HD3	2:B:299:LYS:N	2.33	0.43
1:A:209[B]:ILE:HG22	1:A:227:LEU:HD22	2.00	0.43
4:F:100:ILE:HD12	4:F:128:ARG:HA	2.00	0.43
1:A:71:GLU:HG2	1:A:98:ASP:HB3	2.01	0.43
4:F:49:PHE:CD2	4:F:66:ARG:HG3	2.54	0.43
2:D:1:MET:HB2	2:D:50:ASN:OD1	2.19	0.43
2:B:303:ALA:O	2:B:305:CYS:N	2.49	0.43
2:B:334:ASN:OD1	2:B:334:ASN:C	2.57	0.42
1:C:187:SER:CB	1:C:391:LEU:HD21	2.50	0.42
2:B:275:LEU:HD11	2:B:300:ASN:HA	2.01	0.42
2:D:26:ASP:OD2	2:D:369:ARG:HD3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:400:ARG:HH11	2:D:400:ARG:HD3	1.54	0.42
3:E:9:ILE:HG12	3:E:21:GLU:HB3	2.00	0.42
1:A:335:ILE:HG23	1:A:339:ARG:HG3	2.02	0.42
2:D:180:THR:O	2:D:183:GLU:HG3	2.19	0.42
4:F:1:MET:SD	4:F:28:LYS:HB2	2.60	0.42
2:D:165:ILE:HG21	2:D:252:LEU:HB3	2.00	0.42
1:A:187:SER:CB	1:A:391:LEU:HD21	2.50	0.42
1:C:151[A]:SER:HA	1:C:194[A]:THR:HG22	2.02	0.42
2:D:195:VAL:HG11	2:D:424:ASN:ND2	2.34	0.42
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.38	0.41
2:D:11:GLN:O	2:D:15:GLN:HB2	2.20	0.41
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.55	0.41
4:F:20:LEU:O	4:F:24:THR:HG23	2.21	0.41
1:C:340:SER:OG	12:C:604:HOH:O	2.21	0.41
2:D:109:THR:O	2:D:113:GLU:HG3	2.20	0.41
4:F:3:THR:HG22	4:F:30:LEU:HD21	2.03	0.41
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.55	0.41
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.55	0.41
4:F:167:SER:HA	4:F:170:LEU:HB2	2.02	0.41
1:A:141:PHE:O	1:A:147:SER:HB3	2.21	0.41
1:A:223:THR:O	1:A:227:LEU:HG	2.20	0.41
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.56	0.41
1:A:48:SER:O	1:A:51[A]:THR:HG23	2.20	0.41
1:A:221:ARG:HD3	1:A:221:ARG:HA	1.81	0.41
1:A:233:GLN:HG3	1:A:368:LEU:HD22	2.03	0.41
2:B:175:PRO:HA	2:B:178:SER:HB2	2.03	0.41
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.51	0.41
1:C:279:GLU:OE1	1:C:279:GLU:N	2.42	0.41
4:F:3:THR:HA	4:F:28:LYS:O	2.21	0.41
1:C:276:ILE:HG23	1:C:369:ALA:HB3	2.01	0.40
2:D:286:LEU:CD2	2:D:290:GLU:HB2	2.51	0.40
4:F:197:ARG:HH12	4:F:256:TYR:HB2	1.86	0.40
1:A:326:LYS:HB3	1:A:326:LYS:HE2	1.75	0.40
2:D:141:LEU:HA	2:D:147:SER:HB3	2.03	0.40
1:A:63:PRO:CD	1:A:86:LEU:HG	2.51	0.40
1:A:159:VAL:HG11	3:E:47:LEU:HB2	2.02	0.40
2:B:74:THR:HG22	2:B:74:THR:O	2.22	0.40
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.57	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)
2:B:284:ARG:NH2	2:D:160:GLU:OE2[4_455]	1.68	0.52
2:B:284:ARG:HH22	2:D:160:GLU:OE2[4_455]	1.25	0.35
2:D:39:ASP:OD2	3:E:59:GLU:OE2[4_455]	2.11	0.09

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	444/451 (98%)	435 (98%)	9 (2%)	0	100	100
1	C	447/451 (99%)	435 (97%)	12 (3%)	0	100	100
2	B	421/445 (95%)	411 (98%)	10 (2%)	0	100	100
2	D	419/445 (94%)	410 (98%)	9 (2%)	0	100	100
3	E	124/189 (66%)	124 (100%)	0	0	100	100
4	F	345/384 (90%)	333 (96%)	12 (4%)	0	100	100
All	All	2200/2365 (93%)	2148 (98%)	52 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	377/379 (100%)	376 (100%)	1 (0%)	92	96
1	C	380/379 (100%)	380 (100%)	0	100	100
2	B	365/381 (96%)	362 (99%)	3 (1%)	81	89

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	364/381 (96%)	364 (100%)	0	100	100
3	E	115/171 (67%)	111 (96%)	4 (4%)	36	45
4	F	313/342 (92%)	310 (99%)	3 (1%)	76	85
All	All	1914/2033 (94%)	1903 (99%)	11 (1%)	86	92

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	221	ARG
2	B	164	ARG
2	B	202	TYR
2	B	299	LYS
3	E	6	MET
3	E	28	SER
3	E	52	LYS
3	E	140	LYS
4	F	125	THR
4	F	142	ARG
4	F	183	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
3	E	124	GLN

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 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
8	MES	B	502	-	12,12,12	2.24	1 (8%)	14,16,16	2.00	5 (35%)
9	J6L	B	505	-	27,32,32	3.43	9 (33%)	39,48,48	2.80	17 (43%)
11	ACP	F	401	6	27,33,33	1.35	6 (22%)	32,52,52	1.42	4 (12%)
10	GDP	B	506	6	24,30,30	1.26	2 (8%)	31,47,47	2.12	8 (25%)
5	GTP	A	501	6	26,34,34	0.96	1 (3%)	33,54,54	1.84	7 (21%)
5	GTP	D	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.86	6 (18%)
5	GTP	C	501	6	26,34,34	0.98	1 (3%)	33,54,54	1.84	7 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	MES	B	502	-	-	5/6/14/14	0/1/1/1
9	J6L	B	505	-	-	4/10/21/21	0/4/4/4
11	ACP	F	401	6	-	3/15/38/38	0/3/3/3
10	GDP	B	506	6	-	4/12/32/32	0/3/3/3
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3
5	GTP	D	501	6	-	7/18/38/38	0/3/3/3
5	GTP	C	501	6	-	6/18/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	505	J6L	O4-C15	-12.44	1.02	1.23
9	B	505	J6L	OP3-C9	-8.01	1.22	1.36
8	B	502	MES	C8-S	-7.50	1.66	1.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	505	J6L	O5-C16	-4.88	1.38	1.47
10	B	506	GDP	C5-C6	4.19	1.48	1.41
9	B	505	J6L	C13-C14	-3.71	1.33	1.41
9	B	505	J6L	O5'-C5'	-3.25	1.32	1.37
5	D	501	GTP	C6-N1	3.14	1.38	1.33
5	C	501	GTP	C6-N1	3.13	1.38	1.33
5	A	501	GTP	C6-N1	3.13	1.38	1.33
10	B	506	GDP	C5-C4	3.04	1.49	1.40
9	B	505	J6L	O5-C11	-2.95	1.33	1.37
9	B	505	J6L	C14-C9	-2.93	1.37	1.41
9	B	505	J6L	C4'-C5'	-2.90	1.33	1.38
11	F	401	ACP	PG-O2G	2.87	1.61	1.54
11	F	401	ACP	PG-O3G	2.85	1.61	1.54
11	F	401	ACP	PB-O3A	2.60	1.61	1.58
9	B	505	J6L	C2-C11	-2.31	1.34	1.39
11	F	401	ACP	C5-C4	2.17	1.46	1.40
11	F	401	ACP	PB-O2B	2.14	1.61	1.56
11	F	401	ACP	O4'-C1'	2.07	1.44	1.41

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	505	J6L	O3'-C3'-C2'	7.10	125.30	115.41
9	B	505	J6L	OP3-C9-C14	-5.96	114.86	121.30
9	B	505	J6L	O3'-C3'-C4'	-5.63	114.43	124.12
10	B	506	GDP	C2-N3-C4	5.44	121.56	115.36
8	B	502	MES	C5-N4-C3	5.42	121.03	108.83
5	D	501	GTP	N3-C2-N1	-5.36	120.08	127.22
5	A	501	GTP	N3-C2-N1	-5.33	120.11	127.22
9	B	505	J6L	O2'-C2'-C3'	5.33	122.83	115.41
5	C	501	GTP	N3-C2-N1	-5.31	120.13	127.22
9	B	505	J6L	C23-O2'-C2'	5.24	125.43	117.53
10	B	506	GDP	C5-C6-N1	-4.78	116.90	123.43
9	B	505	J6L	CAB-C8-C15	4.62	129.68	122.81
5	C	501	GTP	C2-N3-C4	4.41	120.39	115.36
5	A	501	GTP	C2-N3-C4	4.40	120.38	115.36
10	B	506	GDP	C4-C5-N7	-4.29	104.93	109.40
5	D	501	GTP	C2-N3-C4	4.18	120.13	115.36
9	B	505	J6L	CAC-O5'-C5'	4.15	123.79	117.53
9	B	505	J6L	C1-O3'-C3'	4.11	123.73	117.53
5	D	501	GTP	PB-O3B-PG	-3.99	119.12	132.83
10	B	506	GDP	C2-N1-C6	3.98	122.25	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	401	ACP	N3-C2-N1	-3.76	122.79	128.68
5	A	501	GTP	PB-O3B-PG	-3.72	120.06	132.83
11	F	401	ACP	PB-O3A-PA	-3.64	121.03	132.56
9	B	505	J6L	O5-C11-C6	3.59	125.26	121.85
5	C	501	GTP	PB-O3B-PG	-3.59	120.52	132.83
10	B	506	GDP	PA-O3A-PB	-3.57	120.59	132.83
5	C	501	GTP	PA-O3A-PB	-3.45	121.00	132.83
11	F	401	ACP	C3'-C2'-C1'	3.38	106.07	100.98
5	A	501	GTP	PA-O3A-PB	-3.33	121.41	132.83
5	D	501	GTP	PA-O3A-PB	-3.28	121.58	132.83
9	B	505	J6L	O2'-C2'-C1'	-3.07	118.83	124.12
10	B	506	GDP	C3'-C2'-C1'	3.06	105.58	100.98
10	B	506	GDP	N3-C2-N1	-3.05	123.16	127.22
5	C	501	GTP	C5-C6-N1	-2.87	119.51	123.43
5	D	501	GTP	C5-C6-N1	-2.85	119.54	123.43
5	A	501	GTP	C5-C6-N1	-2.79	119.61	123.43
9	B	505	J6L	O5'-C5'-C4'	-2.57	119.69	124.12
5	D	501	GTP	C2-N1-C6	2.57	120.01	115.93
9	B	505	J6L	C16-O5-C11	2.47	122.93	118.31
5	C	501	GTP	C2-N1-C6	2.47	119.86	115.93
5	A	501	GTP	C2-N1-C6	2.47	119.84	115.93
9	B	505	J6L	C6-C5-C4	-2.45	116.52	120.33
8	B	502	MES	O2S-S-C8	2.36	109.76	106.92
8	B	502	MES	O1S-S-C8	2.29	109.67	106.92
9	B	505	J6L	C13-C14-C9	2.25	119.10	116.50
8	B	502	MES	O3S-S-C8	2.24	109.39	105.77
5	A	501	GTP	C3'-C2'-C1'	2.21	104.30	100.98
11	F	401	ACP	C4-C5-N7	-2.19	107.12	109.40
8	B	502	MES	C7-N4-C5	2.16	116.76	111.23
5	C	501	GTP	C3'-C2'-C1'	2.11	104.15	100.98
9	B	505	J6L	C11-C6-C5	-2.07	113.68	117.12
9	B	505	J6L	O5'-C5'-CAB	2.07	119.34	116.26
9	B	505	J6L	C18-C16-C4	-2.02	107.71	111.45
10	B	506	GDP	C4-C5-C6	-2.02	118.87	120.80

There are no chirality outliers.

All (36) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
5	D	501	GTP	C5'-O5'-PA-O2A
8	B	502	MES	C7-C8-S-O2S
8	B	502	MES	C7-C8-S-O3S
10	B	506	GDP	O4'-C4'-C5'-O5'
10	B	506	GDP	C3'-C4'-C5'-O5'
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O3A
9	B	505	J6L	C4'-C3'-O3'-C1
9	B	505	J6L	C2'-C3'-O3'-C1
9	B	505	J6L	C1'-C2'-O2'-C23
9	B	505	J6L	C3'-C2'-O2'-C23
8	B	502	MES	C8-C7-N4-C5
5	D	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O1A
8	B	502	MES	C7-C8-S-O1S
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C4'-C5'-O5'-PA
8	B	502	MES	C8-C7-N4-C3
5	D	501	GTP	C4'-C5'-O5'-PA
10	B	506	GDP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
10	B	506	GDP	C5'-O5'-PA-O3A
5	D	501	GTP	C3'-C4'-C5'-O5'
5	D	501	GTP	PB-O3A-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O2A
5	D	501	GTP	O4'-C4'-C5'-O5'

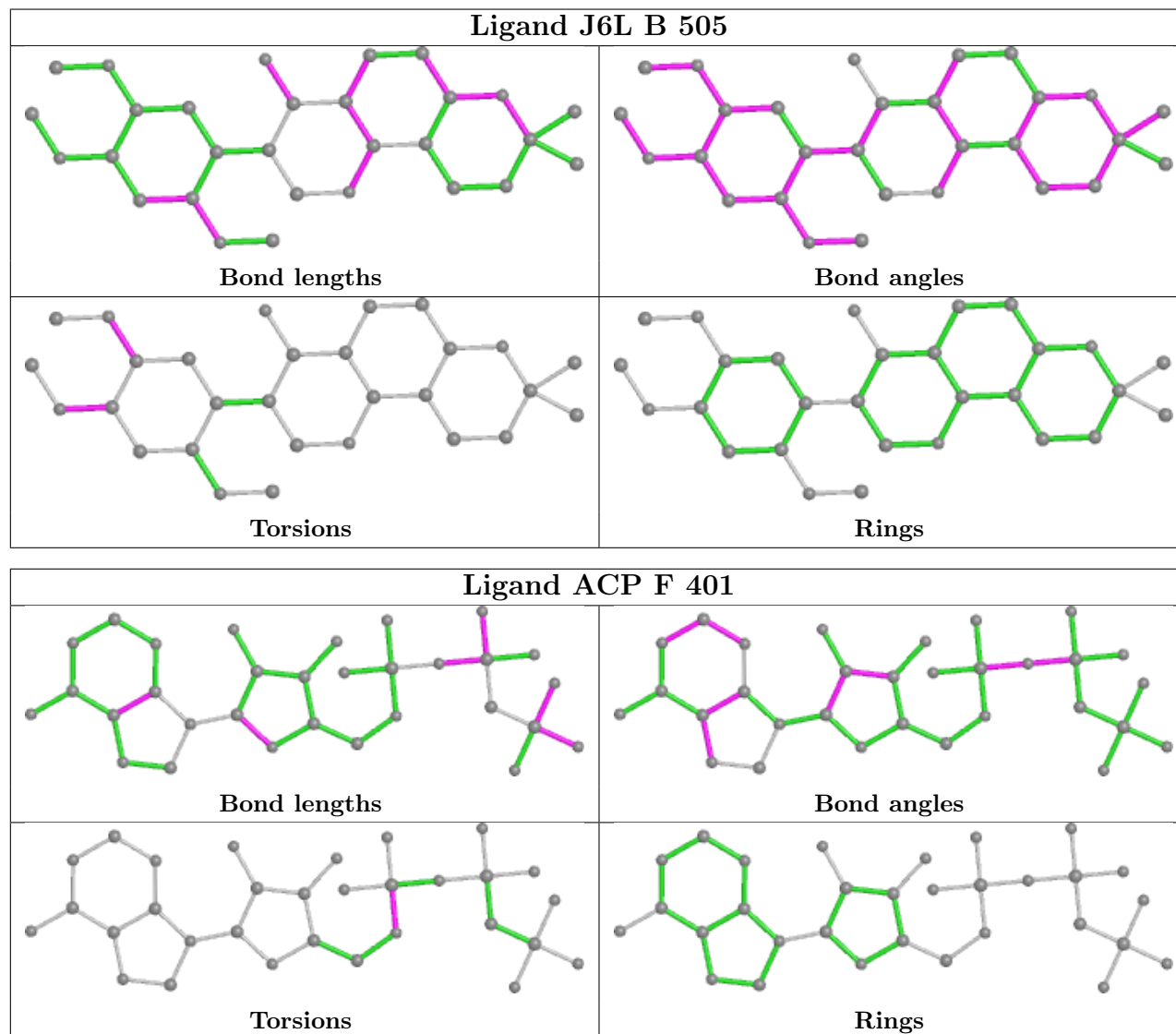
There are no ring outliers.

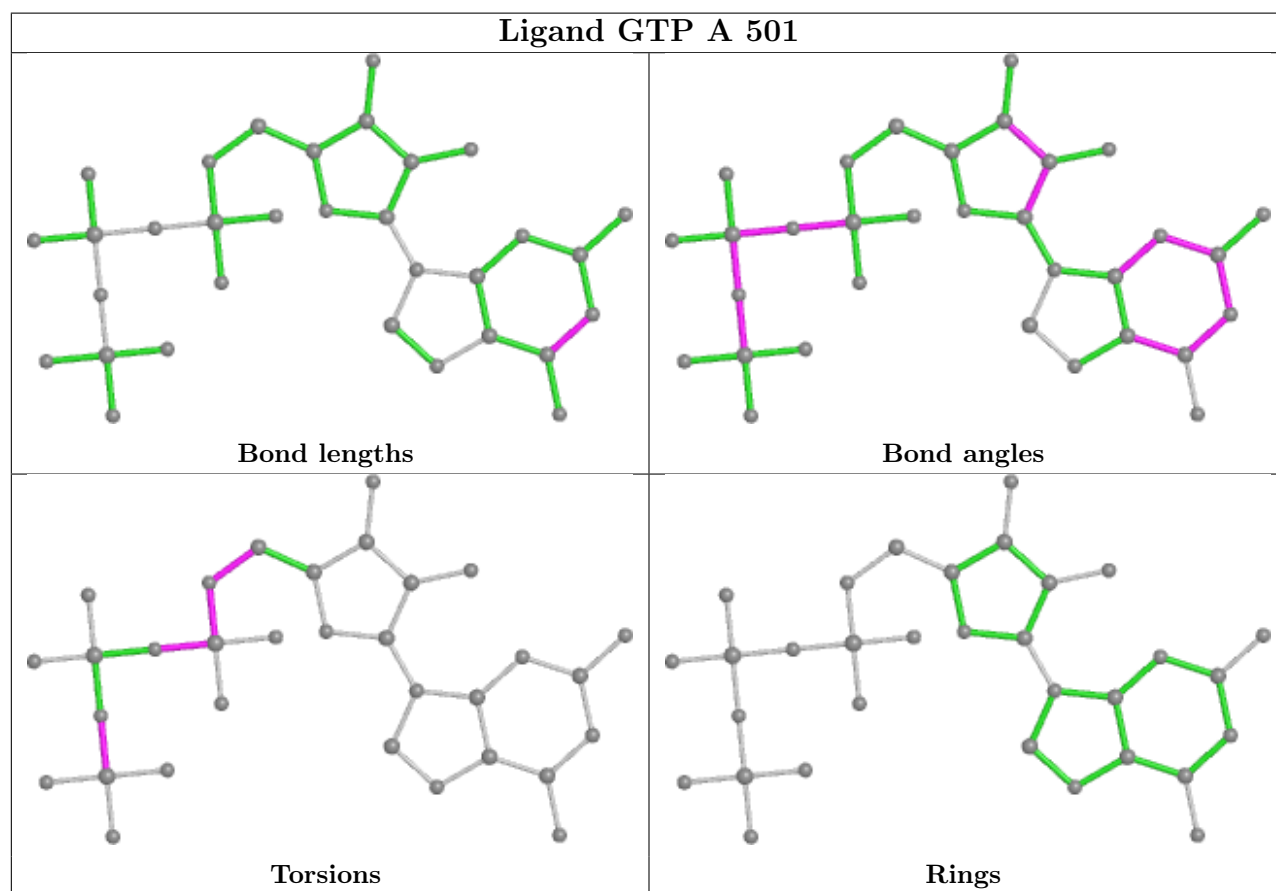
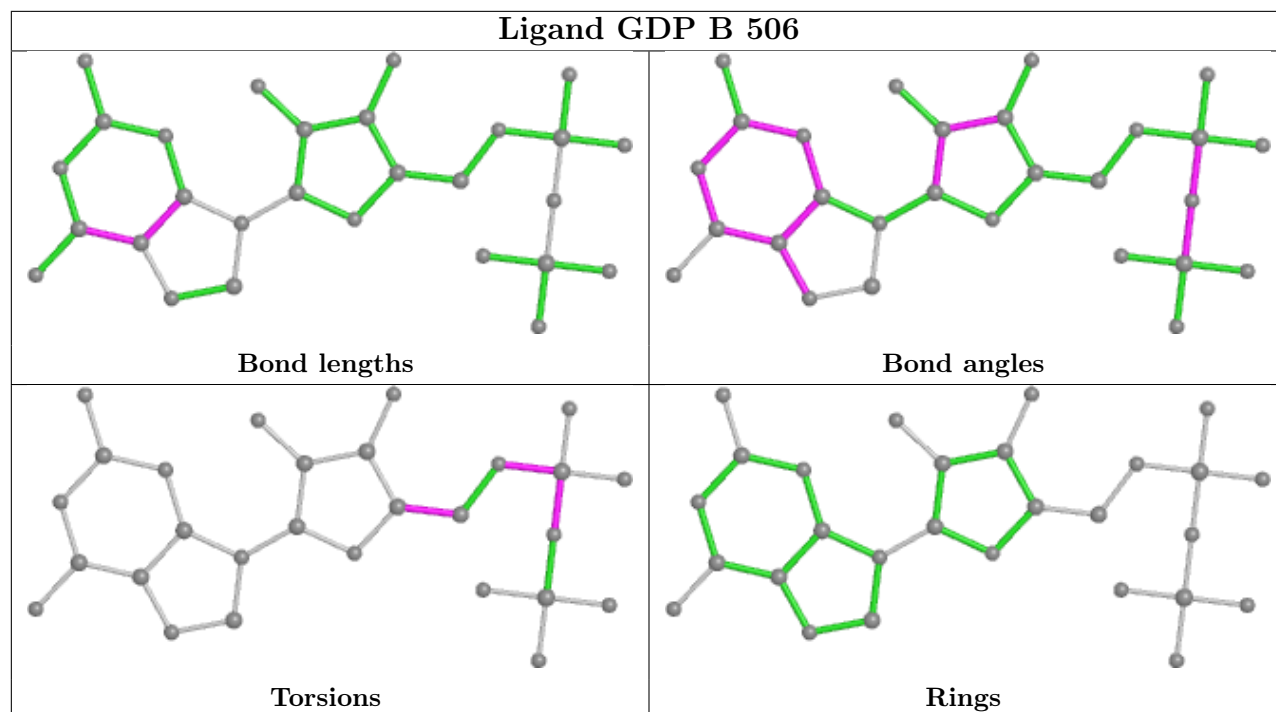
1 monomer is involved in 3 short contacts:

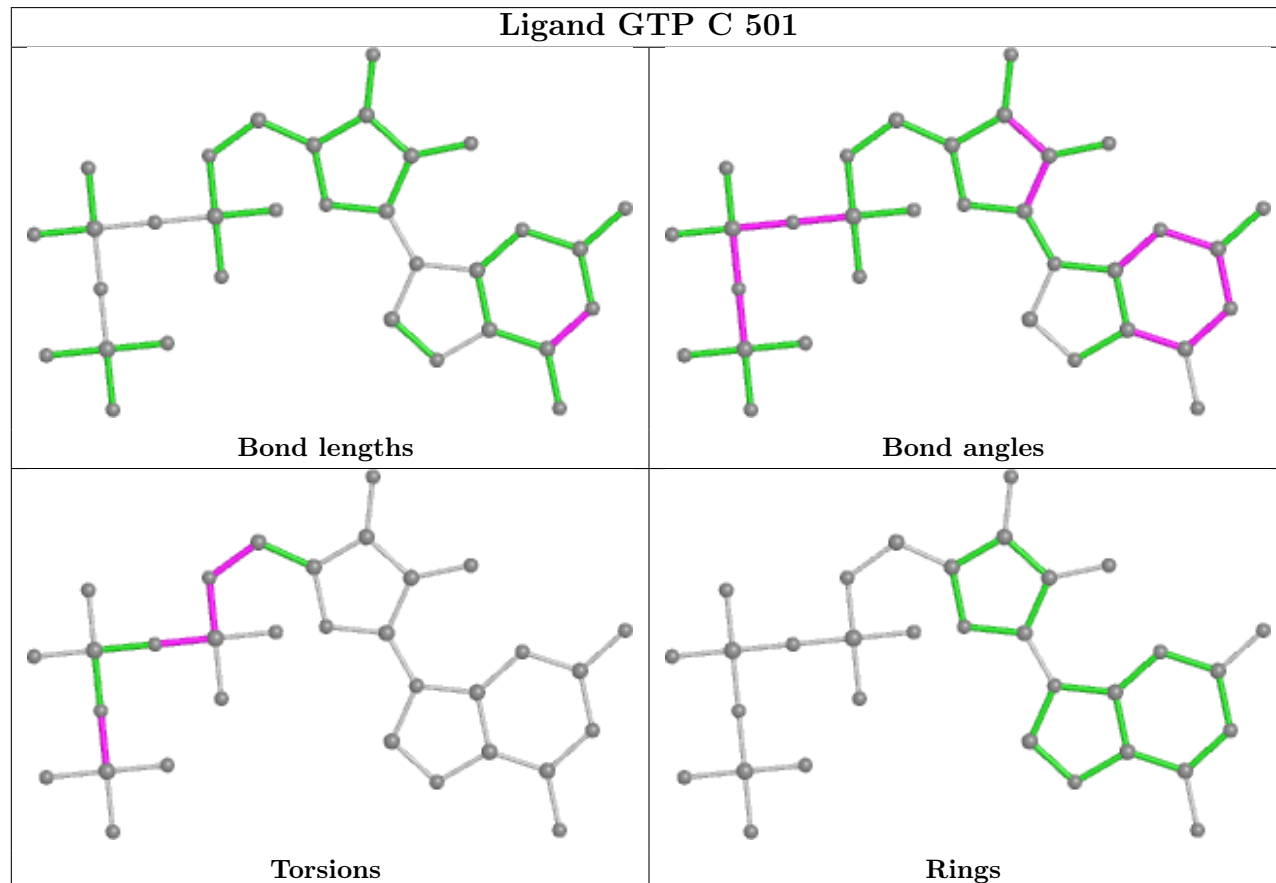
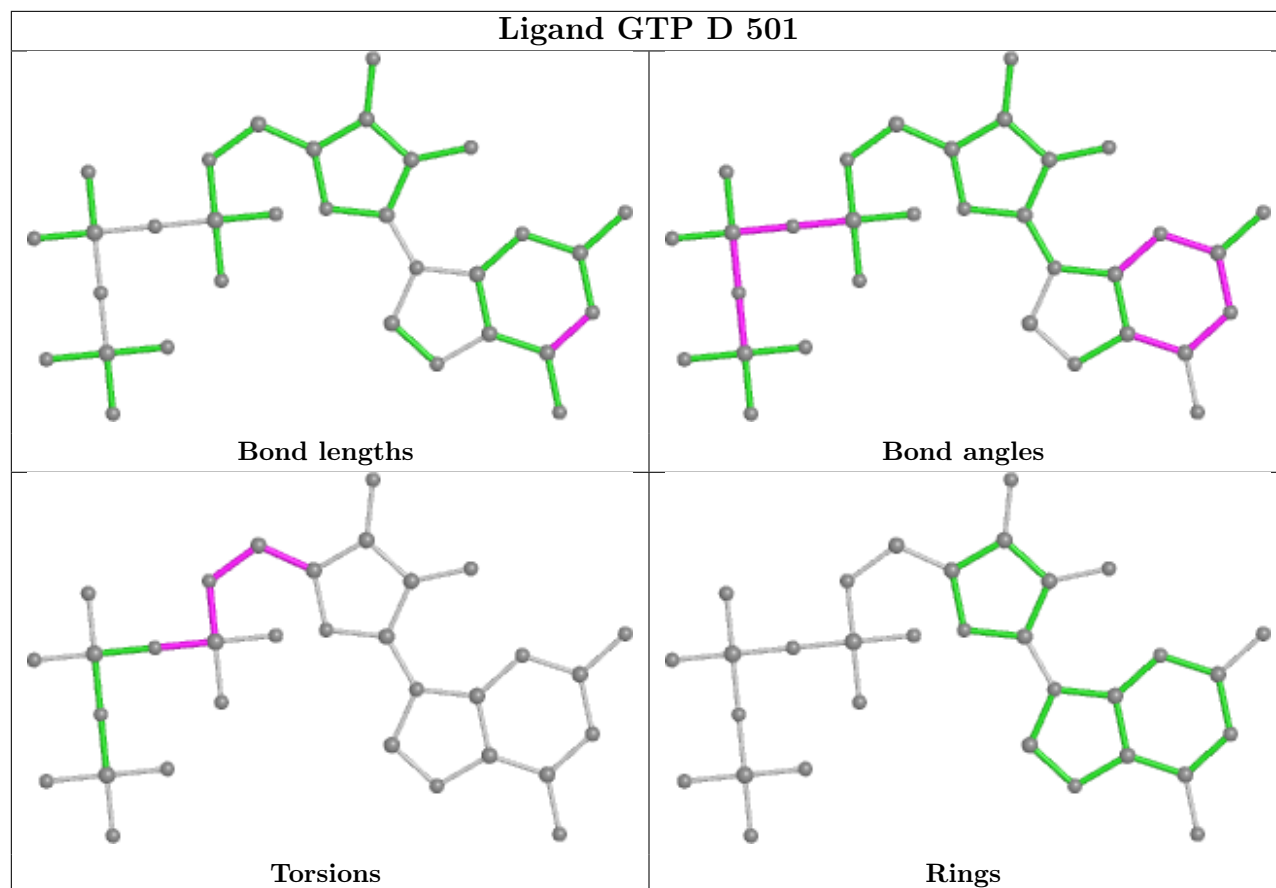
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	505	J6L	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In

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







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	438/451 (97%)	0.05	6 (1%) 75 82	18, 32, 64, 89	0
1	C	440/451 (97%)	-0.03	1 (0%) 95 97	14, 24, 50, 73	0
2	B	426/445 (95%)	0.21	20 (4%) 31 42	14, 33, 67, 97	0
2	D	422/445 (94%)	0.35	25 (5%) 22 31	21, 41, 73, 97	0
3	E	123/189 (65%)	0.39	8 (6%) 18 26	23, 49, 82, 99	0
4	F	350/384 (91%)	1.43	110 (31%) 0 0	25, 62, 109, 119	0
All	All	2199/2365 (92%)	0.36	170 (7%) 13 20	14, 36, 85, 119	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	169	LEU	10.4
4	F	173	ILE	9.9
4	F	172	PHE	8.6
4	F	130	VAL	8.0
4	F	103	THR	6.5
4	F	178	GLN	6.4
4	F	24	THR	6.2
2	B	59	ASN	6.0
4	F	155	ALA	5.9
2	B	439	THR	5.8
2	B	1	MET	5.8
4	F	134	ALA	5.7
4	F	142	ARG	5.7
4	F	177	GLY	5.6
4	F	256	TYR	5.5
4	F	251	LYS	5.5
4	F	138	ARG	5.5
4	F	154	GLY	5.5
4	F	158	GLU	5.5

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Mol	Chain	Res	Type	RSRZ
4	F	131	PHE	5.4
4	F	182	ILE	5.3
4	F	164	SER	5.3
4	F	248	GLU	5.2
4	F	135	TYR	5.2
4	F	161	LEU	5.2
4	F	101	TYR	5.2
4	F	372	THR	5.2
4	F	176	GLN	5.2
2	B	57	ALA	5.0
4	F	143	GLU	5.0
4	F	249	TYR	5.0
4	F	362	ALA	5.0
2	D	400	ARG	4.9
2	B	440	ALA	4.9
4	F	156	LYS	4.9
2	B	246	GLY	4.9
4	F	234	GLN	4.8
1	A	282	TYR	4.8
4	F	132	LEU	4.8
4	F	235	ASP	4.7
4	F	255	ARG	4.7
2	B	438	ALA	4.7
4	F	361	LEU	4.6
4	F	233	PHE	4.6
4	F	125	THR	4.6
4	F	20	LEU	4.6
2	D	97	SER	4.5
4	F	194	PRO	4.5
4	F	170	LEU	4.4
4	F	100	ILE	4.3
4	F	179	VAL	4.3
4	F	157	GLY	4.3
4	F	252	ASN	4.3
3	E	143	ALA	4.3
4	F	162	ILE	4.2
4	F	137	ARG	4.2
4	F	139	ARG	4.2
4	F	89	GLU	4.2
4	F	150	LYS	4.1
4	F	253	TYR	4.1
4	F	133	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
4	F	153	ALA	4.0
2	B	74	THR	4.0
4	F	22	LEU	3.9
4	F	102	PRO	3.9
4	F	165	GLU	3.9
4	F	99	VAL	3.9
4	F	136	ASN	3.8
4	F	129	GLU	3.7
2	D	57	ALA	3.7
4	F	379	HIS	3.6
4	F	159	GLY	3.6
3	E	26	PRO	3.6
3	E	142	GLU	3.6
4	F	180	HIS	3.6
4	F	231	ALA	3.6
2	D	94	PHE	3.6
4	F	250	SER	3.5
2	D	404	PHE	3.5
4	F	90	SER	3.4
1	A	262	TYR	3.4
2	D	98	GLY	3.4
4	F	175	GLU	3.4
2	D	96	GLN	3.4
1	A	281	ALA	3.4
1	A	42	ILE	3.4
2	D	58	GLY	3.3
2	D	75	MET	3.2
2	D	407	TRP	3.2
4	F	168	GLU	3.2
2	D	39	ASP	3.2
4	F	25	GLY	3.2
2	D	221	THR	3.1
3	E	45	PRO	3.1
4	F	1	MET	3.1
2	D	276	THR	3.1
4	F	17	VAL	3.0
4	F	181	VAL	3.0
4	F	146	VAL	3.0
4	F	152	SER	3.0
2	D	405	LEU	3.0
2	D	37	HIS	3.0
4	F	236	LYS	3.0

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Mol	Chain	Res	Type	RSRZ
3	E	135	LYS	3.0
4	F	163	SER	2.9
1	A	346	TRP	2.9
4	F	128	ARG	2.9
4	F	243	HIS	2.9
2	D	59	ASN	2.9
2	D	1	MET	2.9
2	B	437	ASP	2.8
2	B	82	PRO	2.8
4	F	167	SER	2.8
4	F	21	LEU	2.8
4	F	240	LEU	2.8
4	F	140	GLU	2.8
4	F	225	SER	2.7
2	B	38	GLY	2.7
4	F	360	PRO	2.7
2	B	284	ARG	2.7
3	E	140	LYS	2.7
4	F	27	TRP	2.7
4	F	141	GLY	2.7
4	F	247	LYS	2.7
3	E	44	ASP	2.6
2	D	82	PRO	2.6
2	D	79	ARG	2.6
4	F	28	LYS	2.6
2	B	33	THR	2.6
4	F	242	ASN	2.6
2	B	94	PHE	2.6
4	F	174	ASP	2.6
4	F	228	TYR	2.5
4	F	9	GLU	2.5
4	F	344	ALA	2.5
2	B	338	LYS	2.5
2	D	256	ALA	2.4
2	B	37	HIS	2.4
2	D	401	ARG	2.4
4	F	19	ARG	2.4
4	F	227	PRO	2.4
2	D	255	LEU	2.4
2	B	172	VAL	2.4
4	F	144	GLY	2.4
2	B	339	ASN	2.3

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Mol	Chain	Res	Type	RSRZ
4	F	151	SER	2.3
4	F	23	ALA	2.3
4	F	373	SER	2.3
4	F	26	GLN	2.3
4	F	244	CYS	2.3
4	F	32	LYS	2.3
4	F	254	GLY	2.2
1	A	365	GLY	2.2
2	B	56	ALA	2.2
4	F	186	LEU	2.2
1	C	340	SER	2.2
2	D	56	ALA	2.1
4	F	257	GLU	2.1
4	F	246	GLN	2.1
3	E	27	PRO	2.1
4	F	342	LEU	2.1
4	F	166	ALA	2.1
2	B	97	SER	2.1
2	D	72	PRO	2.1
4	F	245	ILE	2.1
4	F	259	GLY	2.1
4	F	196	HIS	2.0
4	F	171	ASP	2.0
2	D	73	GLY	2.0
4	F	263	PHE	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.