



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 7, 2024 – 04:15 pm GMT

PDB ID : 5NJH
Title : Triazolopyrimidines stabilize microtubules by binding to the vinca inhibitor site of tubulin
Authors : Sharma, A.; Calvo, G.S.; Prota, A.E.; Diaz, J.F.; Steinmetz, M.O.
Deposited on : 2017-03-28
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4.02b-467
Mogul : 1.8.4, CSD as541be (2020)
Xtrriage (Phenix) : 1.13
EDS : 2.36
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) : 2.36

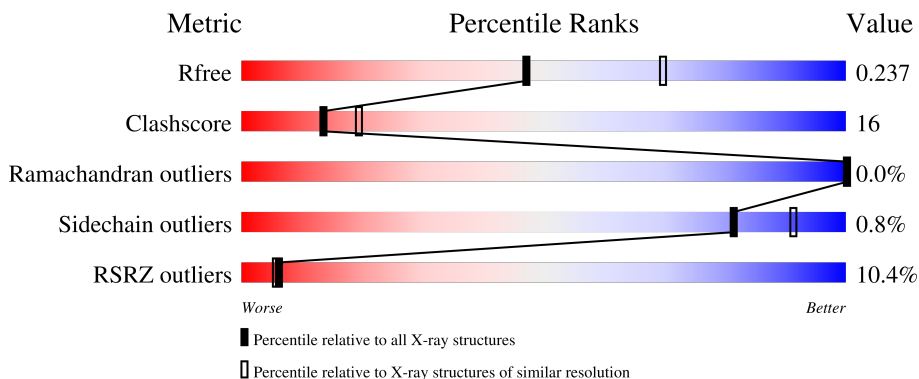
1 Overall quality at a glance i

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.



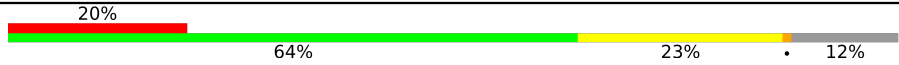
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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 ≥ 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	 6% 74% 21%
1	C	450	 5% 79% 18%
2	B	445	 8% 71% 21% 7%
2	D	445	 11% 75% 20% 5%
3	E	143	 10% 69% 15% 15%

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Mol	Chain	Length	Quality of chain
4	F	384	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into four segments: a red segment (20%), a green segment (64%), a yellow segment (23%), and a grey segment (12%). The percentages are labeled below the bar.</p>

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 17810 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
			Total	C	N	O	S			
1	A	435	Total	C	N	O	S	0	0	0
			3393	2147	577	647	22			
1	C	439	Total	C	N	O	S	0	11	0
			3480	2207	585	665	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	413	Total	C	N	O	S	3	4	0
			3258	2049	552	631	26			
2	D	424	Total	C	N	O	S	1	5	0
			3350	2107	568	647	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	E	121	Total	C	N	O	S	0	1	0
			1006	621	182	198	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	ILE	conflict	UNP P63043
E	4	ALA	SER	conflict	UNP P63043

- Molecule 4 is a protein called tubulin tyrosine ligase TTL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	F	339	Total	C	N	O	S	0	0	0
			2777	1781	475	507	14			

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
			Total	C	N	O	P		
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).

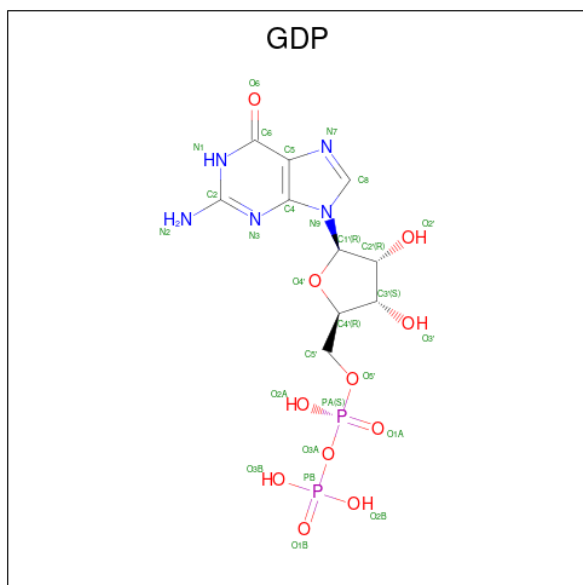
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

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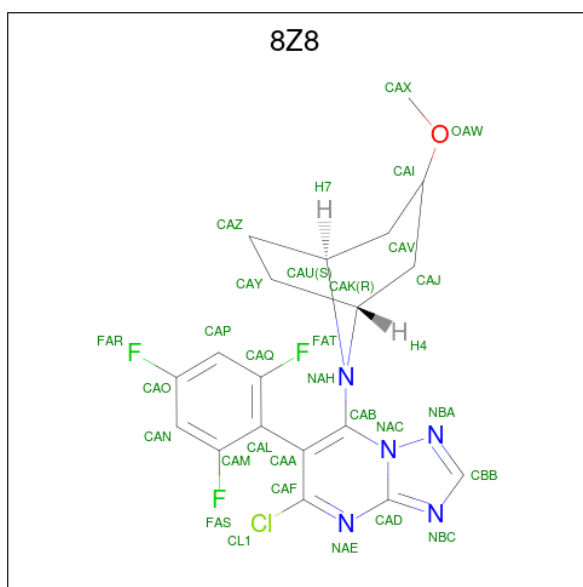
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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



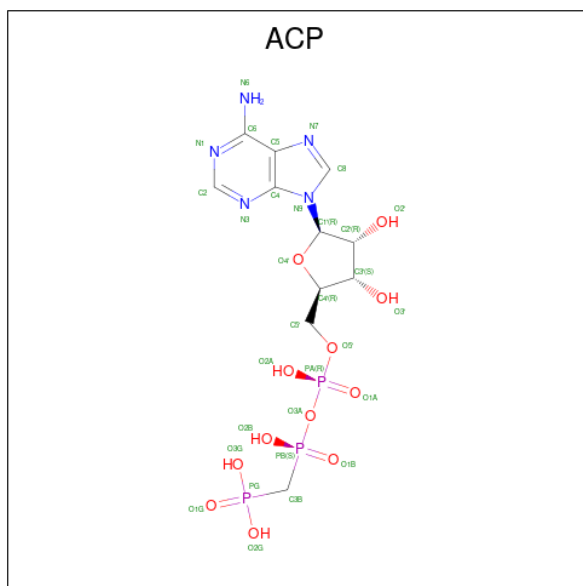
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
7	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
7	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 8 is 5-chloranyl-7-[(1 {R},5 {S})-3-methoxy-8-azabicyclo[3.2.1]octan-8-yl]-6-[2,4,6-tris(fluoranyl)phenyl]-[1,2,4]triazolo[1,5-a]pyrimidine (three-letter code: 8Z8) (formula: $C_{19}H_{17}ClF_3N_5O$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Cl	F	N		
8	B	1	29	19	1	3	5	0	0

- Molecule 9 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	
			Total	C	N	O			P
9	F	1	31	11	5	12	3	0	0

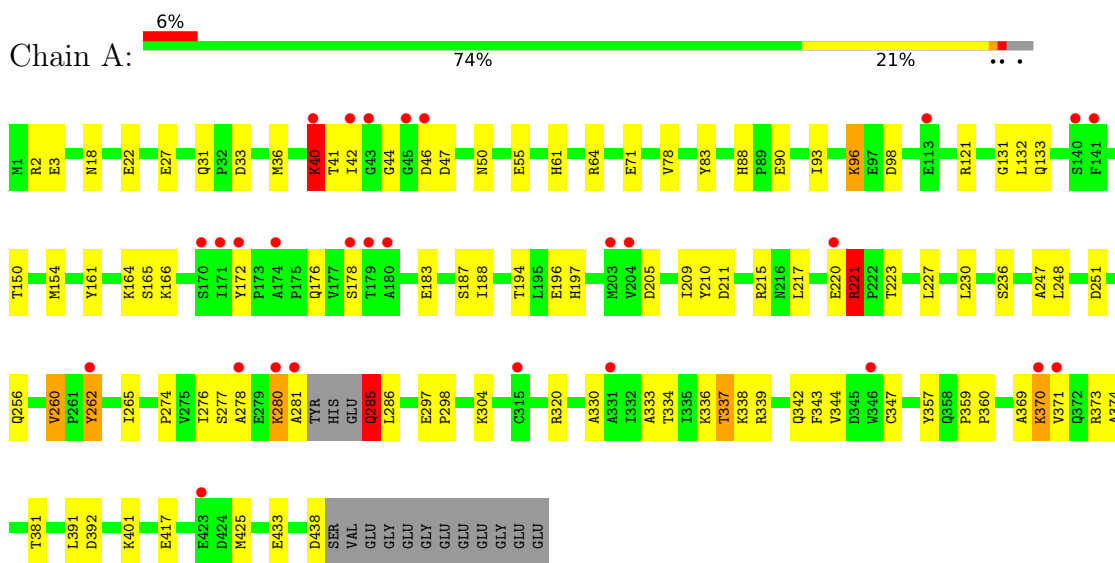
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	79	Total O 79 79	0	0
10	B	59	Total O 59 59	0	0
10	C	98	Total O 98 98	0	0
10	D	62	Total O 62 62	0	0
10	E	18	Total O 18 18	0	0
10	F	45	Total O 45 45	0	0

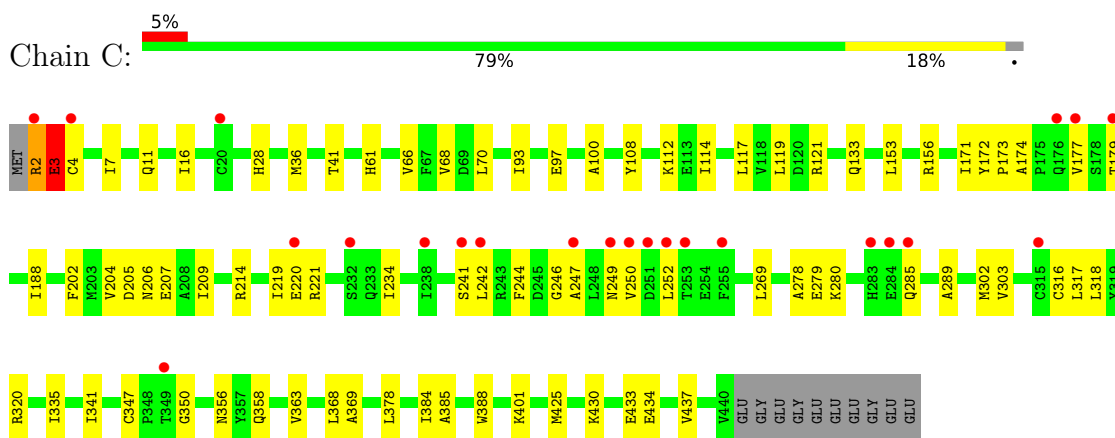
3 Residue-property plots [i](#)

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

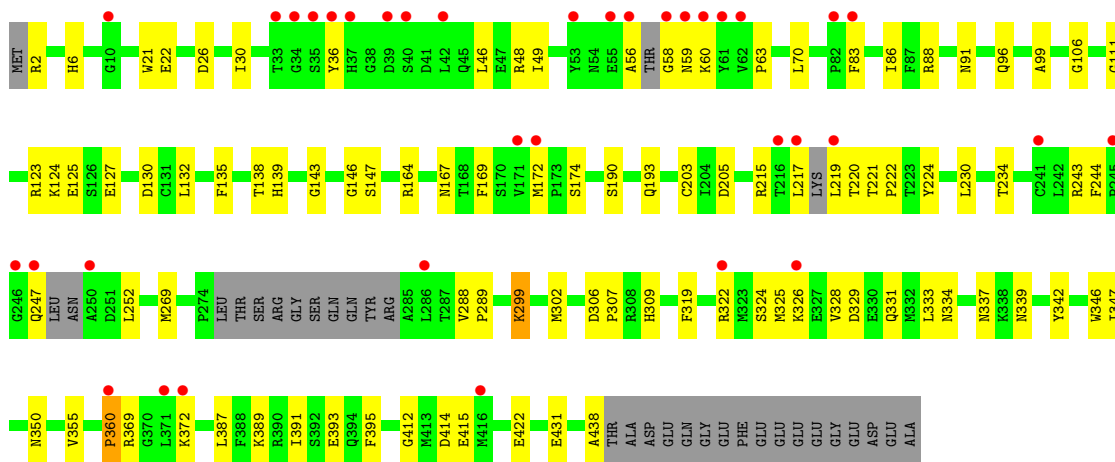


- Molecule 1: Tubulin alpha-1B chain

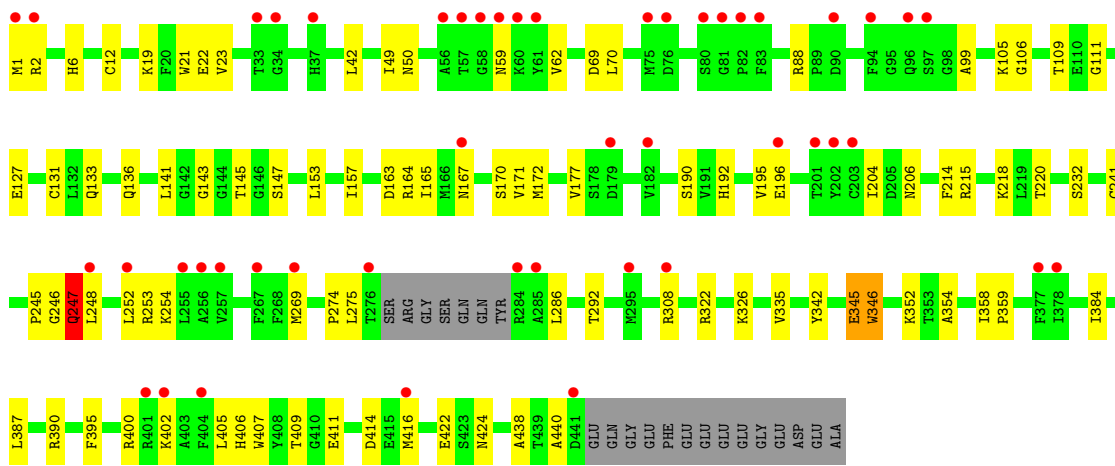
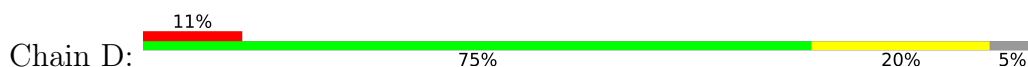


- Molecule 2: Tubulin beta-2B chain

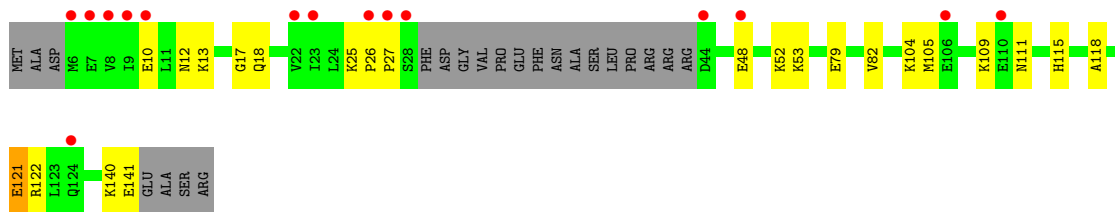




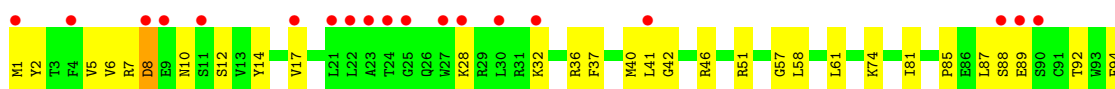
• Molecule 2: Tubulin beta-2B chain

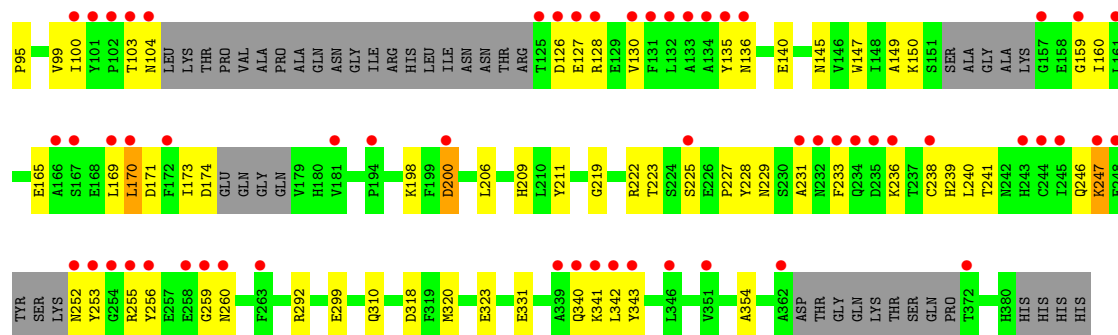


• Molecule 3: Stathmin-4



• Molecule 4: tubulin tyrosine ligase TTL





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.43Å 158.35Å 173.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.09 – 2.39 48.09 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.09-2.39) 99.7 (48.09-2.39)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.18 (at 2.39Å)	Xtrriage
Refinement program	PHENIX (dev_2420: ???)	Depositor
R, R_{free}	0.217 , 0.237 0.217 , 0.237	Depositor DCC
R_{free} test set	2000 reflections (1.78%)	wwPDB-VP
Wilson B-factor (Å ²)	50.9	Xtrriage
Anisotropy	0.106	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17810	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.63% 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: GDP, 8Z8, GTP, ACP, MG

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	0.45	0/3468	0.66	4/4706 (0.1%)
1	C	0.35	0/3591	0.61	5/4878 (0.1%)
2	B	0.46	1/3340 (0.0%)	0.57	2/4519 (0.0%)
2	D	0.50	2/3438 (0.1%)	0.57	3/4657 (0.1%)
3	E	0.33	0/1017	0.58	1/1349 (0.1%)
4	F	0.28	0/2838	0.56	3/3832 (0.1%)
All	All	0.42	3/17692 (0.0%)	0.60	18/23941 (0.1%)

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	6
1	C	0	2
2	D	0	3
3	E	0	1
4	F	0	1
All	All	0	13

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	360	PRO	C-N	-20.77	0.86	1.34
2	D	345	GLU	C-N	-17.66	0.93	1.34
2	D	346	TRP	C-N	-17.37	0.94	1.34

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	3	GLU	C-N-CA	12.26	152.36	121.70
2	D	346	TRP	O-C-N	-10.51	105.88	122.70
1	A	285	GLN	O-C-N	-7.88	110.10	122.70
1	C	4[A]	CYS	CA-C-O	7.24	135.30	120.10
1	C	4[B]	CYS	CA-C-O	7.24	135.30	120.10
2	D	346	TRP	CA-C-N	7.16	132.96	117.20
2	D	247	GLN	O-C-N	-6.51	112.28	122.70
1	A	221	ARG	O-C-N	6.25	132.97	121.10
4	F	8	ASP	O-C-N	6.12	132.50	122.70
1	C	4[A]	CYS	CA-C-N	-6.02	103.96	117.20
1	C	4[B]	CYS	CA-C-N	-6.02	103.96	117.20
3	E	121	GLU	O-C-N	-5.90	113.26	122.70
2	B	360	PRO	C-N-CA	5.50	135.44	121.70
1	A	40	LYS	O-C-N	-5.47	113.95	122.70
4	F	170	LEU	C-N-CA	-5.42	108.16	121.70
4	F	8	ASP	CA-C-N	-5.40	105.33	117.20
1	A	260	VAL	C-N-CD	5.08	139.08	128.40
2	B	244	PHE	C-N-CD	5.04	138.99	128.40

There are no chirality outliers.

All (13) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	196	GLU	Mainchain
1	A	285	GLN	Mainchain
1	A	337	THR	Mainchain
1	A	40	LYS	Mainchain
1	A	46	ASP	Mainchain
1	A	96	LYS	Mainchain
1	C	280	LYS	Mainchain
1	C	3	GLU	Peptide
2	D	127	GLU	Mainchain
2	D	247	GLN	Mainchain
2	D	59	ASN	Mainchain
3	E	121	GLU	Mainchain
4	F	171	ASP	Mainchain

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within

the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3393	0	3312	138	0
1	C	3480	0	3409	78	0
2	B	3258	0	3134	128	0
2	D	3350	0	3245	84	0
3	E	1006	0	1026	29	0
4	F	2777	0	2743	136	0
5	A	32	0	12	0	0
5	C	32	0	12	3	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	B	28	0	12	1	0
7	D	28	0	12	1	0
8	B	29	0	0	1	0
9	F	31	0	14	6	0
10	A	79	0	0	7	0
10	B	59	0	0	2	0
10	C	98	0	0	10	0
10	D	62	0	0	9	0
10	E	18	0	0	3	0
10	F	45	0	0	8	0
All	All	17810	0	16931	548	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 16.

All (548) 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)
4:F:252:ASN:HD22	4:F:255:ARG:NH2	1.09	1.44
2:B:59:ASN:HB2	2:B:60:LYS:NZ	1.36	1.34
4:F:1:MET:HB3	4:F:28:LYS:NZ	1.42	1.33
4:F:252:ASN:ND2	4:F:255:ARG:NH2	1.80	1.29
2:B:59:ASN:CB	2:B:60:LYS:HZ2	1.52	1.22
1:A:336:LYS:HD3	1:A:336:LYS:O	1.42	1.20
4:F:100:ILE:HG23	4:F:128:ARG:CG	1.70	1.19
2:B:56:ALA:C	2:B:58:GLY:HA3	1.63	1.18
2:B:360:PRO:O	2:B:369:ARG:N	1.78	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:370:LYS:HD2	1:A:371:VAL:N	1.60	1.15
4:F:150:LYS:HB3	4:F:160:ILE:CD1	1.76	1.15
1:A:220:GLU:OE2	2:B:326:LYS:HD3	1.46	1.14
1:A:188:ILE:HG23	1:A:425:MET:HG3	1.26	1.14
4:F:5:VAL:CG1	4:F:32:LYS:HA	1.77	1.13
2:B:360:PRO:C	2:B:369:ARG:CA	2.15	1.13
4:F:1:MET:CB	4:F:28:LYS:HZ2	1.63	1.12
2:B:360:PRO:CA	2:B:369:ARG:N	2.13	1.10
1:A:88:HIS:ND1	1:A:90:GLU:HG3	1.67	1.08
4:F:100:ILE:CG2	4:F:128:ARG:HG2	1.84	1.07
2:B:30:ILE:HD11	2:B:49:ILE:HD11	1.29	1.07
1:A:221:ARG:NE	2:B:325:MET:HE2	1.69	1.06
4:F:1:MET:CB	4:F:28:LYS:NZ	2.18	1.06
4:F:252:ASN:HB3	4:F:255:ARG:HD2	1.36	1.06
2:D:269:MET:HG3	2:D:384[A]:ILE:HD13	1.38	1.05
2:B:322:ARG:HE	2:B:372:LYS:CE	1.67	1.04
4:F:150:LYS:HB3	4:F:160:ILE:HD11	1.37	1.02
2:B:56:ALA:C	2:B:58:GLY:CA	2.30	1.00
1:A:188:ILE:HG23	1:A:425:MET:CG	1.92	1.00
2:B:59:ASN:C	2:B:60:LYS:HD3	1.81	0.99
4:F:5:VAL:HG13	4:F:32:LYS:HA	1.41	0.98
4:F:150:LYS:CB	4:F:160:ILE:HD11	1.94	0.97
1:A:370:LYS:NZ	1:A:371:VAL:O	1.98	0.96
4:F:200:ASP:OD2	4:F:222:ARG:HB2	1.66	0.96
2:D:215:ARG:O	2:D:218:LYS:HE3	1.66	0.95
1:A:88:HIS:CE1	1:A:90:GLU:HG3	2.02	0.95
1:A:188:ILE:CG2	1:A:425:MET:HG3	1.96	0.95
1:A:221:ARG:NE	2:B:325:MET:CE	2.30	0.95
1:A:248:LEU:O	10:A:601:HOH:O	1.84	0.95
2:D:246:GLY:CA	10:D:601:HOH:O	2.15	0.94
1:A:221:ARG:CZ	2:B:325:MET:HE3	1.97	0.94
4:F:252:ASN:CB	4:F:255:ARG:HD2	1.98	0.93
3:E:53:LYS:O	10:E:201:HOH:O	1.85	0.93
4:F:81:ILE:HA	4:F:87:LEU:HD12	1.49	0.93
4:F:100:ILE:HG23	4:F:128:ARG:HG2	0.95	0.93
2:B:59:ASN:HB2	2:B:60:LYS:HZ2	0.83	0.92
1:A:41:THR:OG1	10:A:602:HOH:O	1.85	0.92
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.48	0.92
2:B:360:PRO:C	2:B:369:ARG:N	0.86	0.91
2:D:246:GLY:N	10:D:601:HOH:O	2.02	0.91
1:A:215:ARG:HH11	1:A:215:ARG:HB3	1.32	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:62:VAL:HG11	2:D:88:ARG:CG	2.02	0.90
4:F:150:LYS:HB3	4:F:160:ILE:HD12	1.52	0.90
1:A:133:GLN:HE22	1:A:251:ASP:HA	1.37	0.90
2:D:345:GLU:HG3	2:D:440:ALA:HB2	1.52	0.89
1:A:221:ARG:CZ	2:B:325:MET:CE	2.50	0.89
1:A:371:VAL:CG1	1:A:373:ARG:O	2.20	0.89
4:F:252:ASN:ND2	4:F:255:ARG:HH21	1.51	0.89
4:F:5:VAL:HG11	4:F:32:LYS:HA	1.53	0.89
2:B:59:ASN:O	2:B:60:LYS:HD3	1.71	0.89
2:B:431:GLU:OE1	10:B:602:HOH:O	1.90	0.88
4:F:150:LYS:CB	4:F:160:ILE:CD1	2.50	0.88
4:F:225:SER:CB	4:F:252:ASN:O	2.22	0.88
4:F:225:SER:HB3	4:F:252:ASN:O	1.72	0.88
1:A:41:THR:OG1	1:A:44:GLY:O	1.91	0.87
4:F:241:THR:OG1	9:F:402:ACP:O3'	1.92	0.87
1:A:336:LYS:HD3	1:A:336:LYS:C	1.95	0.87
2:B:58:GLY:O	2:B:60:LYS:NZ	2.07	0.86
2:B:289:PRO:HG3	2:B:331:GLN:NE2	1.90	0.86
1:A:370:LYS:HD2	1:A:371:VAL:H	1.40	0.86
1:A:215:ARG:NH1	1:A:215:ARG:CB	2.39	0.86
4:F:233:PHE:CD1	4:F:239:HIS:CE1	2.64	0.86
5:C:501:GTP:O1A	10:C:602:HOH:O	1.93	0.85
2:D:195:VAL:HG13	2:D:196:GLU:HG3	1.58	0.85
1:C:289:ALA:HB2	10:C:679:HOH:O	1.76	0.85
2:B:322:ARG:HH11	2:B:372:LYS:NZ	1.72	0.85
2:B:322:ARG:NE	2:B:372:LYS:CE	2.39	0.84
4:F:159:GLY:O	4:F:160:ILE:HD13	1.78	0.84
1:A:40:LYS:O	1:A:42:ILE:HD12	1.77	0.84
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.58	0.83
4:F:341:LYS:O	10:F:501:HOH:O	1.95	0.83
1:A:40:LYS:O	1:A:42:ILE:CD1	2.26	0.83
2:B:143:GLY:O	2:B:147[B]:SER:OG	1.94	0.83
2:D:62:VAL:HG11	2:D:88:ARG:HG3	1.58	0.83
2:D:269:MET:CG	2:D:384[A]:ILE:HD13	2.07	0.83
4:F:233:PHE:HD1	4:F:239:HIS:CE1	1.97	0.83
3:E:79:GLU:O	10:E:202:HOH:O	1.97	0.82
4:F:247:LYS:O	4:F:247:LYS:HD3	1.78	0.82
2:B:288:VAL:HG12	2:B:331:GLN:HG3	1.62	0.82
2:B:172:MET:CE	2:B:203:CYS:SG	2.69	0.80
1:A:221:ARG:HE	2:B:325:MET:HE2	1.44	0.79
1:A:359:PRO:HB2	1:A:370:LYS:NZ	1.98	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:149:ALA:O	4:F:160:ILE:HD12	1.81	0.79
1:A:371:VAL:HG11	1:A:373:ARG:O	1.82	0.79
1:A:215:ARG:HB3	1:A:215:ARG:NH1	1.97	0.78
1:A:133:GLN:NE2	1:A:251:ASP:HA	1.99	0.78
4:F:7:ARG:HG3	4:F:42:GLY:HA2	1.65	0.78
2:D:62:VAL:CG1	2:D:88:ARG:HG3	2.12	0.78
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.19	0.78
4:F:219:GLY:O	10:F:502:HOH:O	2.01	0.78
4:F:223:THR:OG1	4:F:260:ASN:HB3	1.84	0.78
1:A:215:ARG:HH11	1:A:215:ARG:CB	1.96	0.77
4:F:150:LYS:HA	4:F:160:ILE:CD1	2.13	0.77
2:B:30:ILE:CD1	2:B:49:ILE:HD11	2.14	0.77
4:F:7:ARG:CG	4:F:42:GLY:HA2	2.15	0.77
2:D:245:PRO:C	10:D:601:HOH:O	2.23	0.77
1:A:221:ARG:CZ	2:B:329:ASP:OD2	2.33	0.77
1:A:417:GLU:OE2	10:A:603:HOH:O	2.02	0.77
1:C:285:GLN:CD	1:C:285:GLN:H	1.88	0.76
1:C:112:LYS:HD3	3:E:109:LYS:NZ	2.00	0.76
1:A:3:GLU:OE1	1:A:131:GLY:O	2.04	0.76
1:A:336:LYS:HE2	1:A:336:LYS:HA	1.67	0.76
2:B:322:ARG:HE	2:B:372:LYS:HE2	1.50	0.75
3:E:10:GLU:CG	3:E:10:GLU:O	2.34	0.75
4:F:104:ASN:OD1	4:F:104:ASN:O	2.03	0.75
2:D:143:GLY:O	2:D:147[A]:SER:OG	2.04	0.75
2:D:19:LYS:HE2	2:D:22:GLU:CD	2.07	0.74
1:A:220:GLU:CD	2:B:326:LYS:HD3	2.08	0.74
3:E:140:LYS:HG2	3:E:141:GLU:OE2	1.86	0.74
1:A:370:LYS:CD	1:A:371:VAL:N	2.46	0.74
2:B:59:ASN:CB	2:B:60:LYS:NZ	2.25	0.74
3:E:48:GLU:O	3:E:52:LYS:HG2	1.88	0.74
1:A:274:PRO:HB2	1:A:276:ILE:CD1	2.18	0.73
2:B:172:MET:HE2	2:B:203:CYS:SG	2.28	0.73
3:E:140:LYS:CG	3:E:141:GLU:OE2	2.35	0.73
1:C:430:LYS:NZ	1:C:434:GLU:OE2	2.21	0.73
1:A:188:ILE:CG2	1:A:425:MET:CG	2.63	0.73
4:F:331:GLU:OE2	9:F:402:ACP:O3G	2.07	0.72
2:B:56:ALA:O	2:B:58:GLY:HA3	1.89	0.72
1:A:215:ARG:NH1	1:A:215:ARG:HB2	2.03	0.72
3:E:10:GLU:O	3:E:10:GLU:HG2	1.88	0.72
4:F:1:MET:CB	4:F:28:LYS:HZ1	2.03	0.72
1:C:108:TYR:O	1:C:112:LYS:HG3	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:211:TYR:CD2	4:F:299:GLU:HG3	2.24	0.72
2:B:322:ARG:NE	2:B:372:LYS:HE3	2.05	0.72
1:C:316:CYS:SG	1:C:318:LEU:HD11	2.29	0.71
2:B:172:MET:HE3	2:B:203:CYS:SG	2.30	0.71
2:B:217:LEU:HD12	2:B:217:LEU:O	1.90	0.71
4:F:81:ILE:HA	4:F:87:LEU:CD1	2.21	0.71
1:C:2:ARG:HD3	1:C:2:ARG:N	2.06	0.71
2:B:59:ASN:HB2	2:B:60:LYS:HZ3	1.51	0.71
4:F:150:LYS:CA	4:F:160:ILE:CD1	2.68	0.71
1:A:330:ALA:HB3	10:A:614:HOH:O	1.89	0.71
1:C:356[B]:ASN:HD21	1:C:358[B]:GLN:HB2	1.56	0.71
4:F:51:ARG:O	10:F:504:HOH:O	2.10	0.70
4:F:85:PRO:O	4:F:88:SER:HB2	1.90	0.70
1:A:220:GLU:HG2	2:B:326:LYS:NZ	2.05	0.70
1:A:274:PRO:HG2	1:A:371:VAL:HG21	1.74	0.70
4:F:323:GLU:OE2	10:F:503:HOH:O	2.09	0.70
1:A:215:ARG:HB2	1:A:215:ARG:CZ	2.23	0.69
1:C:28:HIS:CE1	1:C:244:PHE:CZ	2.81	0.69
1:C:119:LEU:HD11	1:C:156:ARG:HB3	1.73	0.69
2:B:322:ARG:HH11	2:B:372:LYS:HZ2	1.41	0.69
4:F:126:ASP:OD1	4:F:128:ARG:HG3	1.93	0.69
4:F:198:LYS:HD3	4:F:239:HIS:O	1.93	0.69
1:A:286:LEU:O	1:A:373:ARG:HD2	1.93	0.69
9:F:402:ACP:O2B	10:F:505:HOH:O	2.10	0.68
2:D:153:LEU:O	2:D:157:ILE:HG13	1.93	0.68
2:D:406:HIS:NE2	2:D:407:TRP:CD1	2.61	0.68
2:D:414:ASP:OD2	2:D:416:MET:CB	2.42	0.68
1:C:179:THR:HG21	10:C:602:HOH:O	1.92	0.68
1:A:96:LYS:HE3	2:B:130:ASP:OD1	1.94	0.68
4:F:7:ARG:HB2	4:F:42:GLY:HA2	1.75	0.68
4:F:128:ARG:HH21	4:F:170:LEU:HD22	1.59	0.68
4:F:233:PHE:HA	4:F:239:HIS:NE2	2.09	0.67
2:D:42:LEU:HD22	2:D:245:PRO:HG2	1.76	0.67
2:D:248:LEU:HD21	2:D:352:LYS:HB3	1.75	0.67
1:A:336:LYS:O	1:A:336:LYS:CD	2.32	0.67
2:D:195:VAL:CG1	2:D:196:GLU:HG3	2.25	0.67
1:A:2:ARG:HB3	1:A:133:GLN:HG3	1.77	0.67
2:D:402:LYS:HD2	2:D:402:LYS:N	2.08	0.66
4:F:1:MET:HB3	4:F:28:LYS:HZ2	0.69	0.66
3:E:111:ASN:O	3:E:115:HIS:CD2	2.49	0.66
4:F:252:ASN:HD22	4:F:255:ARG:HH21	0.67	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:1:MET:C	4:F:28:LYS:NZ	2.49	0.65
4:F:7:ARG:CB	4:F:42:GLY:HA2	2.26	0.65
2:B:322:ARG:HE	2:B:372:LYS:NZ	1.93	0.65
1:A:27:GLU:CD	1:A:320:ARG:HH22	1.99	0.65
1:A:265:ILE:O	1:A:265:ILE:HG22	1.95	0.65
2:D:215:ARG:O	2:D:218:LYS:CE	2.43	0.65
1:A:220:GLU:HG2	2:B:326:LYS:CD	2.27	0.64
1:A:359:PRO:HB2	1:A:370:LYS:HZ1	1.61	0.64
4:F:149:ALA:O	4:F:160:ILE:CD1	2.44	0.64
5:C:501:GTP:PA	10:C:602:HOH:O	2.53	0.64
1:C:285:GLN:CD	1:C:285:GLN:N	2.50	0.64
1:C:214:ARG:HG2	1:C:219:ILE:O	1.98	0.64
1:A:2:ARG:HB3	1:A:133:GLN:CG	2.28	0.64
1:A:188:ILE:HD13	1:A:392:ASP:OD1	1.97	0.64
2:D:438:ALA:O	10:D:602:HOH:O	2.15	0.64
3:E:109:LYS:HD3	3:E:109:LYS:N	2.12	0.64
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.21	0.64
4:F:92:THR:OG1	10:F:506:HOH:O	2.15	0.64
2:B:289:PRO:HG3	2:B:331:GLN:HE21	1.63	0.63
2:D:12:CYS:SG	2:D:171:VAL:HG21	2.37	0.63
1:A:217:LEU:HA	1:A:277:SER:HB2	1.80	0.63
4:F:5:VAL:HG12	4:F:6:VAL:N	2.14	0.63
4:F:37:PHE:O	4:F:58:LEU:HD13	1.99	0.63
4:F:28:LYS:HD3	4:F:28:LYS:N	2.13	0.63
2:D:406:HIS:CD2	2:D:407:TRP:HD1	2.16	0.63
4:F:7:ARG:HG3	4:F:40:MET:CE	2.29	0.63
2:B:139:HIS:HD2	2:B:146:GLY:O	1.82	0.63
1:C:220:GLU:HB3	2:D:326:LYS:HE2	1.80	0.63
2:D:147[B]:SER:OG	2:D:190:SER:OG	2.15	0.62
1:A:220:GLU:CG	2:B:326:LYS:CD	2.77	0.62
1:C:285:GLN:H	1:C:285:GLN:NE2	1.97	0.62
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.79	0.62
2:D:62:VAL:HG11	2:D:88:ARG:HG2	1.82	0.62
1:A:359:PRO:CB	1:A:370:LYS:HZ1	2.12	0.62
1:A:370:LYS:CD	1:A:371:VAL:H	2.12	0.61
2:B:230:LEU:HG	2:B:302:MET:CE	2.30	0.61
1:A:336:LYS:HE2	1:A:336:LYS:CA	2.29	0.61
1:A:220:GLU:CB	2:B:326:LYS:HD2	2.30	0.61
4:F:81:ILE:HG12	4:F:87:LEU:HD13	1.82	0.61
2:B:83:PHE:HB3	2:B:86:ILE:HD13	1.81	0.61
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:368:LEU:CD2	10:C:667:HOH:O	2.48	0.61
1:C:368:LEU:HD22	10:C:667:HOH:O	1.99	0.61
2:D:163:ASP:O	2:D:253:ARG:NH2	2.34	0.61
4:F:74:LYS:HE3	4:F:331:GLU:HG3	1.82	0.61
1:A:359:PRO:HB2	1:A:370:LYS:CE	2.31	0.61
1:A:370:LYS:HD2	1:A:370:LYS:C	2.21	0.61
1:C:100:ALA:HA	2:D:254:LYS:HG3	1.81	0.61
4:F:100:ILE:CG2	4:F:128:ARG:CG	2.59	0.61
1:C:108:TYR:CD1	3:E:105:MET:HE2	2.36	0.61
2:B:30:ILE:HD11	2:B:49:ILE:CD1	2.19	0.61
4:F:2:TYR:N	4:F:28:LYS:NZ	2.48	0.60
2:B:60:LYS:HD3	2:B:60:LYS:N	2.05	0.60
4:F:150:LYS:HA	4:F:160:ILE:HD13	1.84	0.60
2:B:319:PHE:HB2	2:B:355:VAL:HG22	1.84	0.60
1:A:133:GLN:HE21	1:A:251:ASP:CG	2.04	0.60
1:C:335:ILE:HG23	1:C:341:ILE:HD13	1.84	0.60
3:E:140:LYS:HG3	3:E:141:GLU:OE2	2.01	0.59
1:A:248:LEU:N	10:A:601:HOH:O	2.33	0.59
4:F:227:PRO:O	4:F:238:CYS:SG	2.60	0.59
1:C:206:ASN:HB2	10:C:606:HOH:O	2.01	0.59
1:C:249:ASN:O	10:C:603:HOH:O	2.17	0.59
1:C:108:TYR:CD1	3:E:105:MET:CE	2.85	0.59
4:F:7:ARG:HB2	4:F:42:GLY:CA	2.33	0.59
1:A:357:TYR:CZ	3:E:17:GLY:HA2	2.37	0.58
2:D:136:GLN:HA	2:D:167:ASN:O	2.03	0.58
2:B:322:ARG:NH1	2:B:372:LYS:NZ	2.48	0.58
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.86	0.58
4:F:136:ASN:O	4:F:140:GLU:HG3	2.04	0.58
2:D:345:GLU:CG	2:D:440:ALA:HB2	2.29	0.58
1:A:223:THR:O	1:A:227:LEU:HG	2.04	0.57
1:C:269:LEU:HD21	1:C:384:ILE:HD13	1.85	0.57
4:F:2:TYR:N	4:F:28:LYS:HZ3	2.02	0.57
2:B:26:ASP:OD1	2:B:369:ARG:HG3	2.04	0.57
1:A:221:ARG:NH2	2:B:325:MET:SD	2.77	0.57
1:A:133:GLN:NE2	1:A:251:ASP:OD1	2.32	0.57
2:D:1:MET:HG3	2:D:50:ASN:HD21	1.69	0.57
2:B:322:ARG:HH11	2:B:372:LYS:HZ1	1.49	0.56
2:D:172:MET:HG2	2:D:204:ILE:O	2.05	0.56
2:B:221:THR:N	2:B:222:PRO:HD3	2.21	0.56
2:B:215:ARG:HD2	2:B:299:LYS:NZ	2.20	0.56
2:D:414:ASP:OD2	2:D:416:MET:HB3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:126:ASP:OD1	4:F:127:GLU:N	2.38	0.56
4:F:160:ILE:O	4:F:236:LYS:HE2	2.05	0.56
1:A:215:ARG:CB	1:A:215:ARG:CZ	2.83	0.56
1:A:360:PRO:HG2	1:A:374:ALA:HB3	1.88	0.56
4:F:7:ARG:HG3	4:F:40:MET:HE2	1.87	0.56
1:A:336:LYS:C	1:A:336:LYS:CD	2.63	0.56
2:D:196:GLU:HG2	10:D:648:HOH:O	2.06	0.55
4:F:127:GLU:HB2	4:F:130:VAL:CG1	2.35	0.55
4:F:211:TYR:CE2	4:F:299:GLU:HG3	2.41	0.55
2:B:56:ALA:C	2:B:58:GLY:N	2.59	0.55
2:B:224:TYR:OH	7:B:501:GDP:O2'	2.25	0.55
2:B:389:LYS:O	2:B:393:GLU:HG2	2.06	0.55
4:F:1:MET:C	4:F:28:LYS:HZ1	2.10	0.55
2:D:19:LYS:HE2	2:D:22:GLU:OE2	2.06	0.55
1:A:40:LYS:O	1:A:42:ILE:HD11	2.05	0.55
1:A:194:THR:O	1:A:194:THR:HG22	2.06	0.55
2:B:322:ARG:HE	2:B:372:LYS:HZ1	1.55	0.55
2:B:58:GLY:O	2:B:59:ASN:HB2	2.06	0.54
1:C:112:LYS:HD3	3:E:109:LYS:HZ1	1.71	0.54
3:E:25:LYS:HG3	3:E:26:PRO:HD2	1.89	0.54
1:A:276:ILE:HG23	1:A:280:LYS:HE3	1.88	0.54
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.89	0.54
1:A:360:PRO:HG2	1:A:374:ALA:CB	2.38	0.54
4:F:74:LYS:NZ	4:F:331:GLU:OE1	2.40	0.54
1:A:176:GLN:HG2	1:A:210:TYR:CE2	2.43	0.54
1:A:220:GLU:CG	2:B:326:LYS:HD2	2.36	0.54
1:C:278:ALA:HA	1:C:369:ALA:HB2	1.89	0.54
1:C:242:LEU:N	1:C:242:LEU:HD12	2.22	0.54
2:D:1:MET:O	2:D:131:CYS:HB3	2.06	0.54
2:B:88:ARG:HD2	2:B:91:ASN:OD1	2.08	0.54
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.89	0.54
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.91	0.53
1:A:188:ILE:CD1	1:A:392:ASP:OD1	2.56	0.53
2:D:248:LEU:HB3	2:D:354:ALA:HB2	1.91	0.53
1:A:166:LYS:HE2	1:A:197:HIS:O	2.09	0.53
1:A:221:ARG:HH21	2:B:325:MET:HG2	1.74	0.53
1:C:11:GLN:HE22	2:D:247:GLN:NE2	2.07	0.53
1:A:274:PRO:HB2	1:A:276:ILE:HD12	1.89	0.53
2:B:219:LEU:O	2:B:219:LEU:HG	2.09	0.53
2:D:1:MET:HG3	2:D:50:ASN:ND2	2.24	0.53
2:B:96:GLN:O	1:C:2:ARG:HD2	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:19:LYS:HE2	2:D:22:GLU:OE1	2.07	0.53
1:A:220:GLU:CG	2:B:326:LYS:HD3	2.39	0.52
1:A:342:GLN:HG3	1:A:343:PHE:N	2.24	0.52
1:C:385:ALA:HA	1:C:388:TRP:HD1	1.73	0.52
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.90	0.52
1:A:381:THR:OG1	10:A:604:HOH:O	2.19	0.52
1:C:108:TYR:CE1	3:E:105:MET:HE2	2.44	0.52
1:C:202:PHE:CE1	1:C:378:LEU:HD13	2.44	0.52
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.92	0.52
4:F:100:ILE:HG23	4:F:128:ARG:CD	2.35	0.52
1:A:71:GLU:OE1	2:B:247:GLN:NE2	2.43	0.52
2:B:387:LEU:O	2:B:391:ILE:HG12	2.10	0.52
4:F:160:ILE:O	4:F:236:LYS:CE	2.57	0.52
1:A:31:GLN:HB2	1:A:33:ASP:OD1	2.09	0.52
2:B:48:ARG:HB2	2:B:243:ARG:O	2.09	0.52
2:B:215:ARG:HD2	2:B:299:LYS:HZ1	1.74	0.52
2:B:288:VAL:HB	2:B:289:PRO:HD3	1.91	0.52
2:D:414:ASP:OD2	2:D:416:MET:HB2	2.10	0.52
1:C:363[B]:VAL:HG22	10:C:656:HOH:O	2.10	0.51
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.91	0.51
4:F:100:ILE:CG2	4:F:128:ARG:CD	2.87	0.51
1:C:108:TYR:CE1	3:E:105:MET:CE	2.92	0.51
1:C:112:LYS:HD3	3:E:109:LYS:HZ3	1.73	0.51
3:E:13:LYS:HG3	3:E:18:GLN:HB3	1.92	0.51
4:F:88:SER:O	4:F:88:SER:OG	2.28	0.51
4:F:223:THR:OG1	4:F:260:ASN:CB	2.56	0.51
2:B:269:MET:HE1	2:B:307:PRO:HG3	1.93	0.51
1:C:2:ARG:N	1:C:2:ARG:CD	2.73	0.51
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.93	0.51
4:F:252:ASN:HB3	4:F:255:ARG:CD	2.25	0.51
2:B:59:ASN:HB3	2:B:60:LYS:HZ2	1.63	0.51
4:F:74:LYS:HE3	4:F:331:GLU:CG	2.40	0.51
1:C:3:GLU:O	1:C:133:GLN:N	2.33	0.51
2:D:406:HIS:NE2	2:D:407:TRP:HD1	2.08	0.51
2:B:322:ARG:NH1	2:B:372:LYS:HZ1	2.07	0.51
2:D:141:LEU:HD12	2:D:172:MET:HE3	1.93	0.51
2:D:402:LYS:N	2:D:402:LYS:CD	2.73	0.51
3:E:118:ALA:O	3:E:122:ARG:HG3	2.11	0.51
1:A:433:GLU:OE2	4:F:46:ARG:NH2	2.43	0.50
3:E:105:MET:HE2	3:E:105:MET:HA	1.93	0.50
2:D:246:GLY:HA2	10:D:601:HOH:O	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:406:HIS:CD2	2:D:407:TRP:CD1	2.99	0.50
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.76	0.50
1:C:335:ILE:HG23	1:C:341:ILE:CD1	2.41	0.50
4:F:240:LEU:O	4:F:246:GLN:NE2	2.43	0.50
2:B:2:ARG:HD3	2:B:48:ARG:HH12	1.77	0.50
2:D:322:ARG:O	2:D:322:ARG:HG3	2.11	0.50
2:B:360:PRO:O	2:B:369:ARG:CA	2.43	0.50
1:C:174:ALA:HB3	1:C:177:VAL:HG12	1.93	0.50
4:F:103:THR:HG23	4:F:128:ARG:HH12	1.76	0.50
2:B:288:VAL:CG1	2:B:331:GLN:HG3	2.38	0.50
2:D:192:HIS:O	2:D:195:VAL:HG12	2.12	0.50
4:F:104:ASN:OD1	4:F:104:ASN:C	2.48	0.49
1:A:220:GLU:HB3	2:B:326:LYS:HD2	1.93	0.49
2:B:234:THR:OG1	2:B:302:MET:SD	2.61	0.49
2:D:141:LEU:HD21	2:D:170:SER:HB3	1.95	0.49
1:A:42:ILE:HD12	1:A:42:ILE:N	2.27	0.49
2:B:123:ARG:O	2:B:127:GLU:HG3	2.11	0.49
1:C:316:CYS:SG	1:C:318:LEU:CD1	2.98	0.49
4:F:99:VAL:HG23	4:F:127:GLU:OE2	2.12	0.49
4:F:252:ASN:CB	4:F:255:ARG:CD	2.83	0.49
2:B:174:SER:OG	2:B:205:ASP:OD2	2.17	0.49
1:C:242:LEU:HD21	1:C:252:LEU:HD13	1.95	0.49
2:D:195:VAL:HG11	2:D:424:ASN:HD21	1.76	0.49
1:A:247:ALA:HB1	3:E:12:ASN:HD22	1.76	0.49
1:A:220:GLU:HG2	2:B:326:LYS:HD2	1.95	0.49
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.28	0.49
4:F:7:ARG:HG3	4:F:40:MET:HE3	1.94	0.49
1:A:132:LEU:O	1:A:164:LYS:CD	2.61	0.48
2:B:220:THR:O	2:B:221:THR:OG1	2.25	0.48
4:F:5:VAL:CG1	4:F:6:VAL:N	2.76	0.48
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.48	0.48
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.94	0.48
2:B:217:LEU:O	2:B:217:LEU:CD1	2.61	0.48
1:C:279:GLU:OE1	1:C:279:GLU:N	2.36	0.48
1:A:359:PRO:HB2	1:A:370:LYS:HE2	1.95	0.48
1:C:66:VAL:HG12	1:C:68[A]:VAL:HG23	1.96	0.48
4:F:7:ARG:HB2	4:F:42:GLY:C	2.34	0.48
2:B:36:TYR:CE2	2:B:46:LEU:HD11	2.48	0.48
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.95	0.48
1:C:41:THR:O	1:C:41:THR:OG1	2.31	0.48
1:C:172:TYR:CD1	1:C:173:PRO:HD2	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.32	0.48
4:F:255:ARG:HG3	4:F:256:TYR:CD2	2.49	0.48
2:B:46:LEU:HA	2:B:49:ILE:HB	1.95	0.48
2:B:70:LEU:HD12	2:B:99:ALA:HB2	1.96	0.48
4:F:88:SER:O	4:F:89:GLU:HB2	2.12	0.48
1:A:438:ASP:OD1	1:A:438:ASP:N	2.46	0.48
1:C:108:TYR:CD1	3:E:105:MET:HE1	2.49	0.47
1:A:280:LYS:NZ	1:A:281:ALA:C	2.67	0.47
2:B:324:SER:O	2:B:328:VAL:HG23	2.14	0.47
2:B:139:HIS:CD2	2:B:146:GLY:O	2.66	0.47
1:C:205:ASP:CB	1:C:303:VAL:HA	2.45	0.47
2:D:177:VAL:HG21	2:D:206:ASN:HB3	1.96	0.47
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.33	0.47
4:F:135:TYR:OH	4:F:165:GLU:HA	2.15	0.47
2:B:88:ARG:HG3	2:B:88:ARG:HH11	1.78	0.47
1:C:205:ASP:O	1:C:209:ILE:HG12	2.14	0.47
2:D:195:VAL:CG1	2:D:196:GLU:N	2.78	0.47
4:F:150:LYS:CA	4:F:160:ILE:HD11	2.37	0.47
4:F:229:ASN:OD1	4:F:229:ASN:C	2.53	0.47
4:F:253:TYR:CZ	4:F:259:GLY:HA2	2.50	0.47
1:A:370:LYS:CD	1:A:370:LYS:C	2.80	0.47
1:C:97:GLU:CD	2:D:164:ARG:HH22	2.18	0.47
2:D:322:ARG:O	2:D:322:ARG:CG	2.63	0.47
1:A:178:SER:OG	1:A:183:GLU:OE1	2.30	0.47
1:A:210:TYR:OH	1:A:221:ARG:HD3	2.15	0.46
2:B:322:ARG:NE	2:B:372:LYS:HZ1	2.13	0.46
4:F:74:LYS:HE3	4:F:331:GLU:CD	2.35	0.46
4:F:150:LYS:CB	4:F:160:ILE:HD12	2.29	0.46
2:B:333:LEU:HD13	4:F:57:GLY:HA3	1.96	0.46
1:A:280:LYS:HZ2	1:A:281:ALA:C	2.18	0.46
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.98	0.46
1:C:241:SER:HB2	1:C:250:VAL:H	1.80	0.46
2:D:12:CYS:HB2	7:D:501:GDP:C8	2.50	0.46
2:D:241[B]:CYS:SG	10:D:625:HOH:O	2.61	0.46
3:E:104:LYS:NZ	10:E:204:HOH:O	2.30	0.46
1:A:22:GLU:HG3	1:A:83:TYR:CE1	2.51	0.46
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.45	0.46
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.50	0.46
1:A:220:GLU:HG2	2:B:326:LYS:HZ3	1.81	0.46
2:B:46:LEU:HD23	2:B:49:ILE:HD12	1.96	0.46
2:D:69:ASP:HA	2:D:145:THR:HG21	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ARG:NH2	2:B:325:MET:CE	2.77	0.46
1:C:347:CYS:SG	1:C:350:GLY:HA2	2.55	0.45
2:D:2:ARG:HB3	2:D:133:GLN:HB2	1.97	0.45
2:B:339:ASN:HB3	2:B:342:TYR:HD2	1.81	0.45
1:C:97:GLU:OE2	2:D:164:ARG:NH2	2.48	0.45
1:A:370:LYS:NZ	1:A:371:VAL:C	2.67	0.45
1:A:188:ILE:CG2	1:A:425:MET:HG2	2.46	0.45
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.52	0.45
2:D:274:PRO:HB3	2:D:286:LEU:HD11	1.99	0.45
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.82	0.45
1:A:47:ASP:O	1:A:50:ASN:HB2	2.17	0.45
1:A:274:PRO:HB2	1:A:276:ILE:HD11	1.97	0.45
2:B:132:LEU:O	2:B:164:ARG:NH1	2.41	0.45
3:E:25:LYS:CG	3:E:26:PRO:HD2	2.47	0.44
1:C:204:VAL:HG13	1:C:209:ILE:HD11	1.98	0.44
2:D:308:ARG:HD2	2:D:342:TYR:CZ	2.51	0.44
4:F:100:ILE:HD12	4:F:128:ARG:HG2	1.99	0.44
4:F:126:ASP:CG	4:F:128:ARG:HG3	2.37	0.44
2:B:414:ASP:OD1	2:B:415:GLU:N	2.51	0.44
2:D:358:ILE:HA	2:D:359:PRO:HD3	1.84	0.44
2:D:390:ARG:NH1	10:D:612:HOH:O	2.49	0.44
1:A:2:ARG:O	1:A:133:GLN:OE1	2.36	0.44
1:A:220:GLU:HG2	2:B:326:LYS:HZ2	1.78	0.44
2:B:26:ASP:OD1	2:B:369:ARG:NE	2.50	0.44
2:D:109:THR:HG21	2:D:411:GLU:OE1	2.17	0.44
1:A:344:VAL:HG23	1:A:347:CYS:HB2	2.00	0.44
4:F:225:SER:HB2	4:F:252:ASN:O	2.09	0.44
4:F:173:ILE:O	4:F:174:ASP:C	2.55	0.44
2:D:275:LEU:HD23	2:D:275:LEU:HA	1.85	0.43
4:F:252:ASN:ND2	4:F:255:ARG:CZ	2.70	0.43
2:D:292:THR:HG22	2:D:335:VAL:HG21	2.01	0.43
1:A:248:LEU:CA	10:A:601:HOH:O	2.66	0.43
1:C:317:LEU:C	1:C:318:LEU:HD12	2.39	0.43
1:A:338:LYS:HE2	1:A:339:ARG:HG3	2.01	0.43
2:B:63:PRO:HG2	2:B:86:ILE:HG13	2.01	0.43
2:B:322:ARG:O	2:B:322:ARG:HG3	2.18	0.43
2:B:334:ASN:O	2:B:334:ASN:ND2	2.52	0.43
4:F:229:ASN:OD1	4:F:231:ALA:N	2.47	0.43
1:A:161:TYR:HB3	1:A:164:LYS:HG3	2.00	0.43
1:A:360:PRO:CG	1:A:374:ALA:HB3	2.48	0.43
2:B:306:ASP:HB3	2:B:309:HIS:ND1	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ARG:HD3	2:B:48:ARG:NH1	2.34	0.43
4:F:253:TYR:OH	4:F:259:GLY:HA2	2.18	0.43
1:C:433:GLU:O	1:C:437:VAL:HG23	2.18	0.43
4:F:233:PHE:HA	4:F:239:HIS:CD2	2.53	0.43
4:F:255:ARG:HD3	4:F:256:TYR:CE2	2.54	0.42
2:B:124:LYS:HD3	2:B:124:LYS:C	2.39	0.42
2:D:106:GLY:O	2:D:111:GLY:HA3	2.19	0.42
2:D:395:PHE:CE1	2:D:422:GLU:HB2	2.54	0.42
1:A:27:GLU:OE1	1:A:236:SER:OG	2.32	0.42
1:A:55:GLU:HG2	1:A:61:HIS:CD2	2.55	0.42
1:A:210:TYR:OH	1:A:221:ARG:CD	2.68	0.42
4:F:94:PHE:HA	4:F:95:PRO:HD3	1.91	0.42
4:F:252:ASN:HD22	4:F:255:ARG:CZ	2.07	0.42
2:B:138:THR:HG22	2:B:169:PHE:HB2	2.01	0.42
1:C:119:LEU:HD11	1:C:156:ARG:CB	2.47	0.42
2:D:1:MET:SD	10:D:656:HOH:O	2.62	0.42
1:A:71:GLU:HG2	1:A:98:ASP:HB3	2.01	0.42
2:D:406:HIS:HA	2:D:409:THR:OG1	2.19	0.42
4:F:342:LEU:HA	10:F:501:HOH:O	2.19	0.42
1:A:280:LYS:HE3	1:A:280:LYS:HB3	1.85	0.42
4:F:128:ARG:HH12	4:F:173:ILE:CD1	2.32	0.42
2:B:337:ASN:OD1	4:F:36:ARG:NH2	2.45	0.42
1:C:156:ARG:NH1	10:C:612:HOH:O	2.52	0.42
2:B:124:LYS:HD3	2:B:125:GLU:N	2.34	0.42
1:C:234:ILE:HD11	1:C:302[B]:MET:SD	2.59	0.42
4:F:8:ASP:OD2	4:F:8:ASP:C	2.58	0.42
4:F:10:ASN:OD1	4:F:10:ASN:N	2.53	0.42
4:F:100:ILE:HD12	4:F:128:ARG:HA	2.01	0.42
2:B:347:ILE:HG22	2:B:350:ASN:HB3	2.01	0.42
4:F:14:TYR:HA	4:F:17:VAL:HB	2.02	0.42
4:F:150:LYS:HA	4:F:160:ILE:HD11	1.99	0.42
1:A:338:LYS:HG3	1:A:339:ARG:N	2.35	0.41
8:B:503:8Z8:CAK	8:B:503:8Z8:NBA	2.83	0.41
1:A:260:VAL:CG1	1:A:262:TYR:O	2.68	0.41
2:B:22:GLU:HG3	2:B:83:PHE:CD1	2.55	0.41
2:B:289:PRO:CG	2:B:331:GLN:NE2	2.73	0.41
4:F:318:ASP:OD2	9:F:402:ACP:O3G	2.37	0.41
1:A:221:ARG:HH21	2:B:325:MET:CG	2.32	0.41
2:D:49:ILE:O	2:D:49:ILE:HG13	2.20	0.41
2:D:214:PHE:CE1	2:D:220:THR:HG22	2.55	0.41
2:B:106:GLY:O	2:B:111:GLY:HA3	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:209:HIS:ND1	10:F:509:HOH:O	2.37	0.41
1:A:333:ALA:O	1:A:337:THR:HG23	2.19	0.41
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.55	0.41
1:C:70:LEU:HD23	1:C:70:LEU:HA	1.86	0.41
2:D:402:LYS:HA	2:D:405:LEU:HD12	2.01	0.41
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.50	0.41
4:F:320:MET:CE	9:F:402:ACP:O2'	2.68	0.41
2:B:412:GLY:C	3:E:82:VAL:HG13	2.40	0.41
2:D:105:LYS:HE2	2:D:411:GLU:OE2	2.21	0.41
4:F:61:LEU:HD12	4:F:310:GLN:O	2.21	0.41
4:F:331:GLU:OE2	9:F:402:ACP:PG	2.79	0.41
1:A:150:THR:O	1:A:154:MET:HG2	2.21	0.41
2:B:167:ASN:ND2	2:B:252:LEU:HD22	2.35	0.41
2:D:165:ILE:HG21	2:D:252:LEU:HB3	2.02	0.41
2:D:406:HIS:CE1	2:D:407:TRP:CD1	3.08	0.41
1:A:285:GLN:OE1	1:A:285:GLN:HA	2.19	0.41
1:A:297:GLU:HA	1:A:298:PRO:HD3	1.95	0.41
1:A:401:LYS:HE3	2:B:438:ALA:HB1	2.02	0.41
1:C:205:ASP:HB2	1:C:303:VAL:HA	2.02	0.41
1:C:356[B]:ASN:ND2	1:C:358[B]:GLN:HB2	2.31	0.41
4:F:5:VAL:HG11	4:F:32:LYS:CA	2.37	0.41
4:F:128:ARG:HH12	4:F:173:ILE:HD11	1.86	0.41
4:F:206:LEU:HD21	4:F:354:ALA:HB2	2.02	0.41
1:A:330:ALA:O	1:A:334:THR:HG23	2.21	0.41
2:B:132:LEU:HD21	2:B:135:PHE:CZ	2.55	0.41
1:C:117:LEU:O	1:C:121:ARG:HG2	2.21	0.41
1:C:246:GLY:O	1:C:247:ALA:C	2.59	0.41
1:A:221:ARG:HG3	2:B:326:LYS:HA	2.02	0.40
2:B:193:GLN:HB3	10:B:611:HOH:O	2.21	0.40
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.53	0.40
2:D:402:LYS:HA	2:D:405:LEU:CD1	2.51	0.40
4:F:247:LYS:HD3	4:F:247:LYS:C	2.36	0.40
1:C:16:ILE:HD11	1:C:171:ILE:HD11	2.03	0.40
1:C:179:THR:CG2	5:C:501:GTP:H5'	2.51	0.40
3:E:111:ASN:O	3:E:115:HIS:HD2	2.00	0.40
4:F:128:ARG:NH2	4:F:170:LEU:HD22	2.32	0.40
4:F:228:TYR:HA	4:F:238:CYS:SG	2.61	0.40
2:B:217:LEU:O	2:B:217:LEU:CG	2.70	0.40
1:C:93:ILE:CG2	1:C:114:ILE:HD11	2.42	0.40
1:C:205:ASP:HB3	1:C:303:VAL:HA	2.03	0.40
1:C:401:LYS:HG3	2:D:346:TRP:CE3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:172:MET:HE2	2:D:387:LEU:HD21	2.02	0.40
4:F:7:ARG:CD	4:F:40:MET:HE3	2.51	0.40
4:F:58:LEU:HD23	4:F:58:LEU:HA	1.86	0.40
2:B:147[B]:SER:HB2	2:B:190:SER:HG	1.85	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	431/450 (96%)	423 (98%)	8 (2%)	0	100	100
1	C	448/450 (100%)	436 (97%)	12 (3%)	0	100	100
2	B	407/445 (92%)	402 (99%)	5 (1%)	0	100	100
2	D	425/445 (96%)	416 (98%)	9 (2%)	0	100	100
3	E	118/143 (82%)	115 (98%)	2 (2%)	1 (1%)	19	29
4	F	327/384 (85%)	322 (98%)	5 (2%)	0	100	100
All	All	2156/2317 (93%)	2114 (98%)	41 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	E	27	PRO

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	366/378 (97%)	360 (98%)	6 (2%)	62	79
1	C	381/378 (101%)	379 (100%)	2 (0%)	88	95
2	B	360/383 (94%)	359 (100%)	1 (0%)	92	97
2	D	371/383 (97%)	370 (100%)	1 (0%)	92	97
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	305/342 (89%)	300 (98%)	5 (2%)	62	79
All	All	1893/1991 (95%)	1878 (99%)	15 (1%)	81	91

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	165	SER
1	A	221	ARG
1	A	256	GLN
1	A	262	TYR
1	A	280	LYS
1	A	370	LYS
2	B	299	LYS
1	C	2	ARG
1	C	221	ARG
2	D	400	ARG
4	F	12	SER
4	F	145	ASN
4	F	200	ASP
4	F	247	LYS
4	F	292	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	133	GLN
1	A	256	GLN
2	B	139	HIS
2	B	334	ASN
1	C	11	GLN
1	C	285	GLN
1	C	293	ASN

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Mol	Chain	Res	Type
2	D	167	ASN
2	D	247	GLN
2	D	394	GLN
3	E	12	ASN
3	E	108	ASN
3	E	115	HIS
3	E	124	GLN
4	F	234	GLN
4	F	252	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 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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$
9	ACP	F	402	6	27,33,33	1.27	2 (7%)	32,52,52	1.47	4 (12%)
7	GDP	B	501	-	24,30,30	0.94	1 (4%)	30,47,47	1.22	4 (13%)
5	GTP	A	501	6	26,34,34	1.34	3 (11%)	32,54,54	1.22	4 (12%)
7	GDP	D	501	6	24,30,30	0.95	1 (4%)	30,47,47	1.16	3 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	8Z8	B	503	-	27,33,33	3.66	7 (25%)	33,50,50	3.32	15 (45%)
5	GTP	C	501	6	26,34,34	1.13	2 (7%)	32,54,54	1.50	6 (18%)

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
9	ACP	F	402	6	-	5/15/38/38	0/3/3/3
7	GDP	B	501	-	-	7/12/32/32	0/3/3/3
5	GTP	A	501	6	-	3/18/38/38	0/3/3/3
7	GDP	D	501	6	-	5/12/32/32	0/3/3/3
8	8Z8	B	503	-	-	0/6/31/31	0/6/5/5
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	503	8Z8	CAK-NAH	-11.09	1.36	1.47
8	B	503	8Z8	CAU-NAH	-10.98	1.37	1.47
8	B	503	8Z8	CAZ-CAY	-6.28	1.36	1.54
8	B	503	8Z8	OAW-CAI	-6.02	1.29	1.43
5	C	501	GTP	C5-C6	-3.96	1.39	1.47
5	A	501	GTP	C6-N1	-3.87	1.32	1.37
8	B	503	8Z8	CAF-NAE	3.44	1.33	1.30
9	F	402	ACP	PG-O3G	2.73	1.61	1.54
9	F	402	ACP	PG-O2G	2.58	1.60	1.54
7	B	501	GDP	C6-N1	-2.32	1.34	1.37
7	D	501	GDP	C6-N1	-2.27	1.34	1.37
8	B	503	8Z8	CAF-CL1	-2.26	1.70	1.74
5	A	501	GTP	C2'-C1'	-2.11	1.50	1.53
5	C	501	GTP	C2-N3	2.10	1.38	1.33
5	A	501	GTP	PG-O2G	-2.05	1.46	1.54
8	B	503	8Z8	FAR-CAO	-2.01	1.31	1.36

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	503	8Z8	CAQ-CAL-CAM	8.24	122.65	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	503	8Z8	CAF-NAE-CAD	7.04	120.52	116.64
8	B	503	8Z8	CAY-CAK-NAH	-6.52	97.76	102.11
8	B	503	8Z8	CAZ-CAU-NAH	-5.77	98.27	102.11
8	B	503	8Z8	CAA-CAF-NAE	-5.50	119.45	125.91
8	B	503	8Z8	CL1-CAF-NAE	5.36	121.16	115.55
8	B	503	8Z8	CAB-CAA-CAF	4.77	117.97	113.40
9	F	402	ACP	PB-O3A-PA	-4.49	118.33	132.56
8	B	503	8Z8	CAN-CAM-CAL	-3.86	119.04	123.45
8	B	503	8Z8	CAP-CAQ-CAL	-3.69	119.24	123.45
7	B	501	GDP	PA-O3A-PB	-3.50	120.82	132.83
9	F	402	ACP	C3'-C2'-C1'	3.29	105.93	100.98
5	C	501	GTP	PA-O3A-PB	-3.29	121.55	132.83
5	C	501	GTP	PB-O3B-PG	-3.26	121.64	132.83
7	D	501	GDP	PA-O3A-PB	-3.21	121.80	132.83
5	C	501	GTP	C5-C6-N1	3.21	119.63	113.95
8	B	503	8Z8	CAA-CAL-CAM	-3.11	117.98	122.24
5	C	501	GTP	C8-N7-C5	3.08	108.86	102.99
8	B	503	8Z8	CAF-CAA-CAL	-3.04	118.00	123.88
5	C	501	GTP	C2-N1-C6	-2.86	119.83	125.10
9	F	402	ACP	N3-C2-N1	-2.85	124.23	128.68
5	A	501	GTP	C5-C6-N1	2.79	118.89	113.95
9	F	402	ACP	C4-C5-N7	-2.77	106.51	109.40
8	B	503	8Z8	CAV-CAI-CAJ	2.42	116.72	112.07
7	B	501	GDP	C8-N7-C5	2.40	107.56	102.99
7	D	501	GDP	C8-N7-C5	2.38	107.52	102.99
7	B	501	GDP	C5-C6-N1	2.35	118.10	113.95
7	D	501	GDP	C5-C6-N1	2.29	118.00	113.95
8	B	503	8Z8	CAI-CAV-CAU	-2.24	109.33	112.69
5	A	501	GTP	O6-C6-C5	-2.20	120.07	124.37
5	C	501	GTP	O6-C6-C5	-2.18	120.11	124.37
8	B	503	8Z8	CAI-CAJ-CAK	-2.18	109.42	112.69
5	A	501	GTP	C8-N7-C5	2.13	107.05	102.99
7	B	501	GDP	O4'-C1'-C2'	-2.10	103.86	106.93
8	B	503	8Z8	CAA-CAL-CAQ	-2.10	119.36	122.24
5	A	501	GTP	O2B-PB-O1B	2.00	122.14	112.24

There are no chirality outliers.

All (27) 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

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Mol	Chain	Res	Type	Atoms
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
7	D	501	GDP	C5'-O5'-PA-O1A
7	D	501	GDP	C5'-O5'-PA-O2A
9	F	402	ACP	PG-C3B-PB-O1B
9	F	402	ACP	PG-C3B-PB-O2B
9	F	402	ACP	PG-C3B-PB-O3A
9	F	402	ACP	O4'-C4'-C5'-O5'
9	F	402	ACP	C3'-C4'-C5'-O5'
7	B	501	GDP	C3'-C4'-C5'-O5'
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	C5'-O5'-PA-O3A
7	D	501	GDP	C5'-O5'-PA-O3A
7	B	501	GDP	C5'-O5'-PA-O2A
7	B	501	GDP	O4'-C4'-C5'-O5'
5	C	501	GTP	PB-O3A-PA-O2A
7	D	501	GDP	PB-O3A-PA-O2A
7	B	501	GDP	C4'-C5'-O5'-PA
5	A	501	GTP	C5'-O5'-PA-O3A
7	B	501	GDP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O1A
7	B	501	GDP	PB-O3A-PA-O1A
7	B	501	GDP	PB-O3A-PA-O2A
7	D	501	GDP	PB-O3A-PA-O1A
5	C	501	GTP	C4'-C5'-O5'-PA

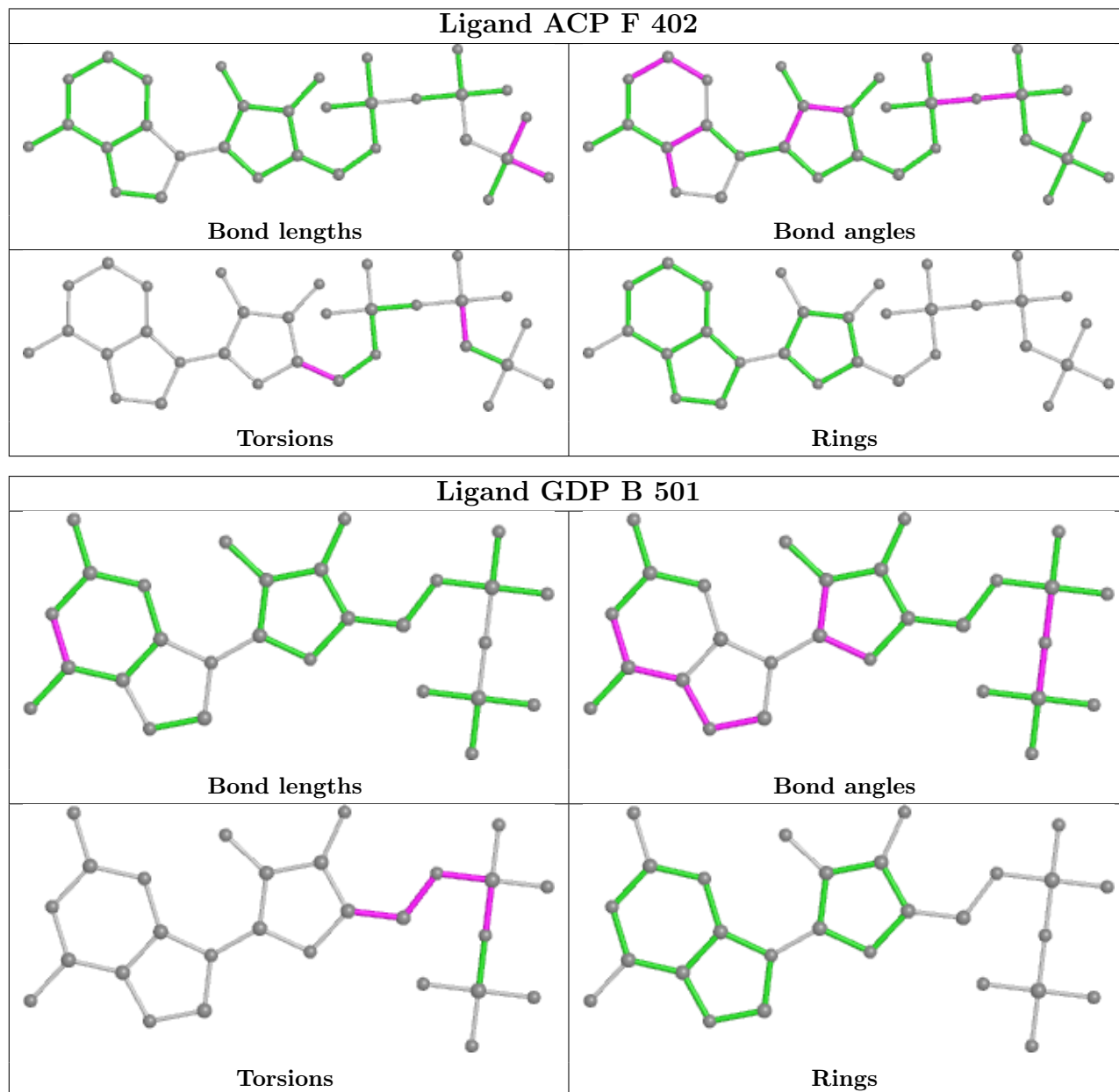
There are no ring outliers.

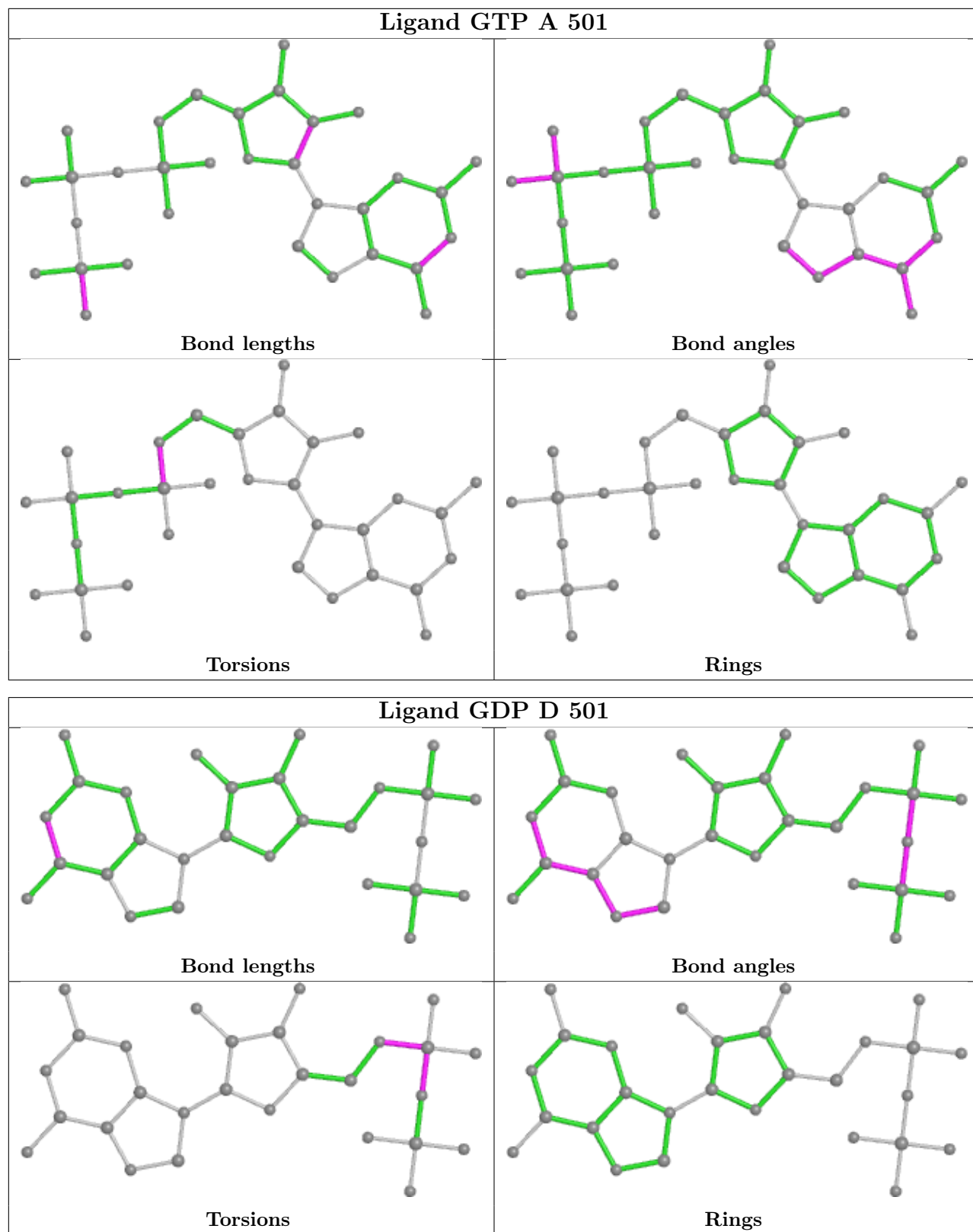
5 monomers are involved in 12 short contacts:

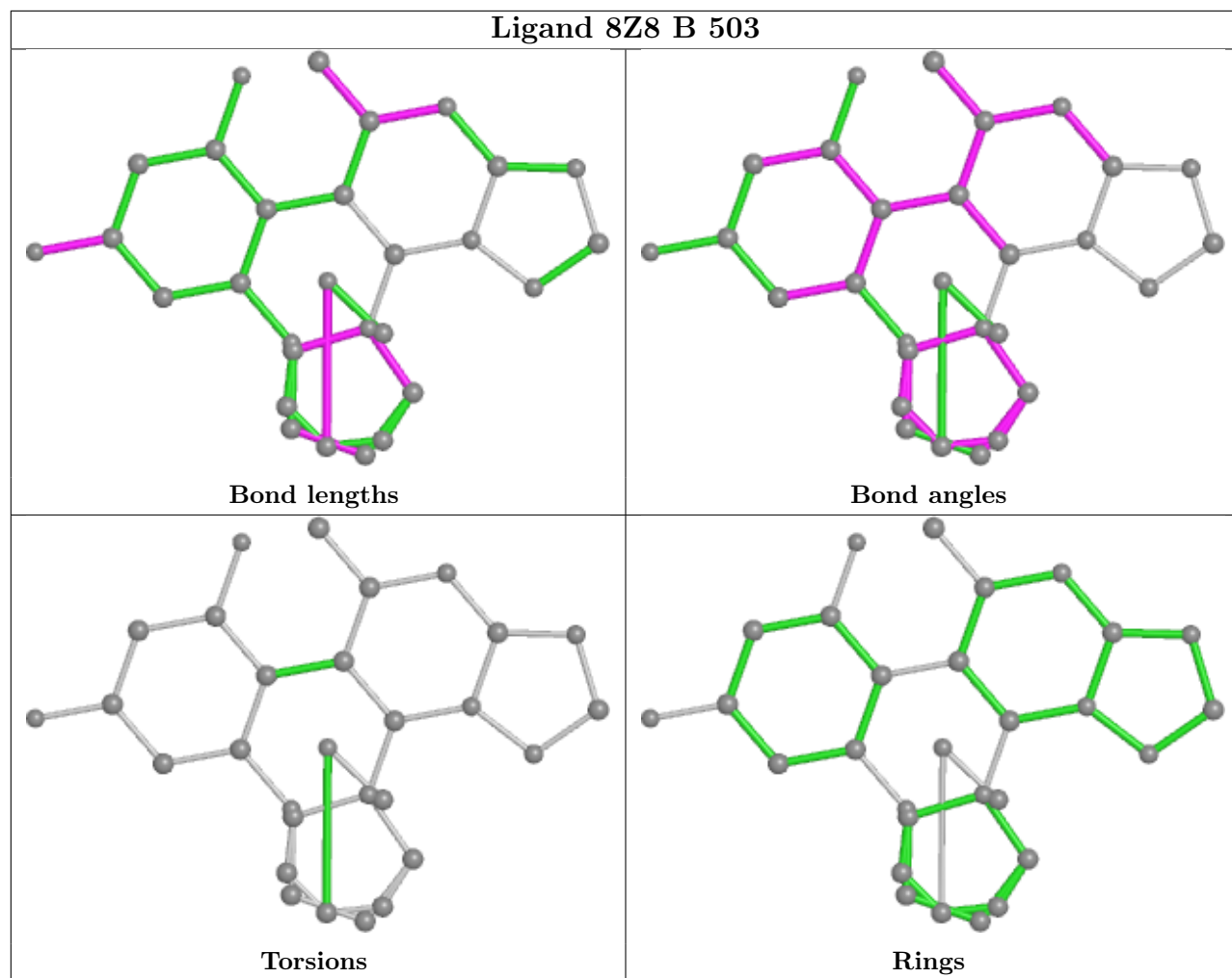
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	F	402	ACP	6	0
7	B	501	GDP	1	0
7	D	501	GDP	1	0
8	B	503	8Z8	1	0
5	C	501	GTP	3	0

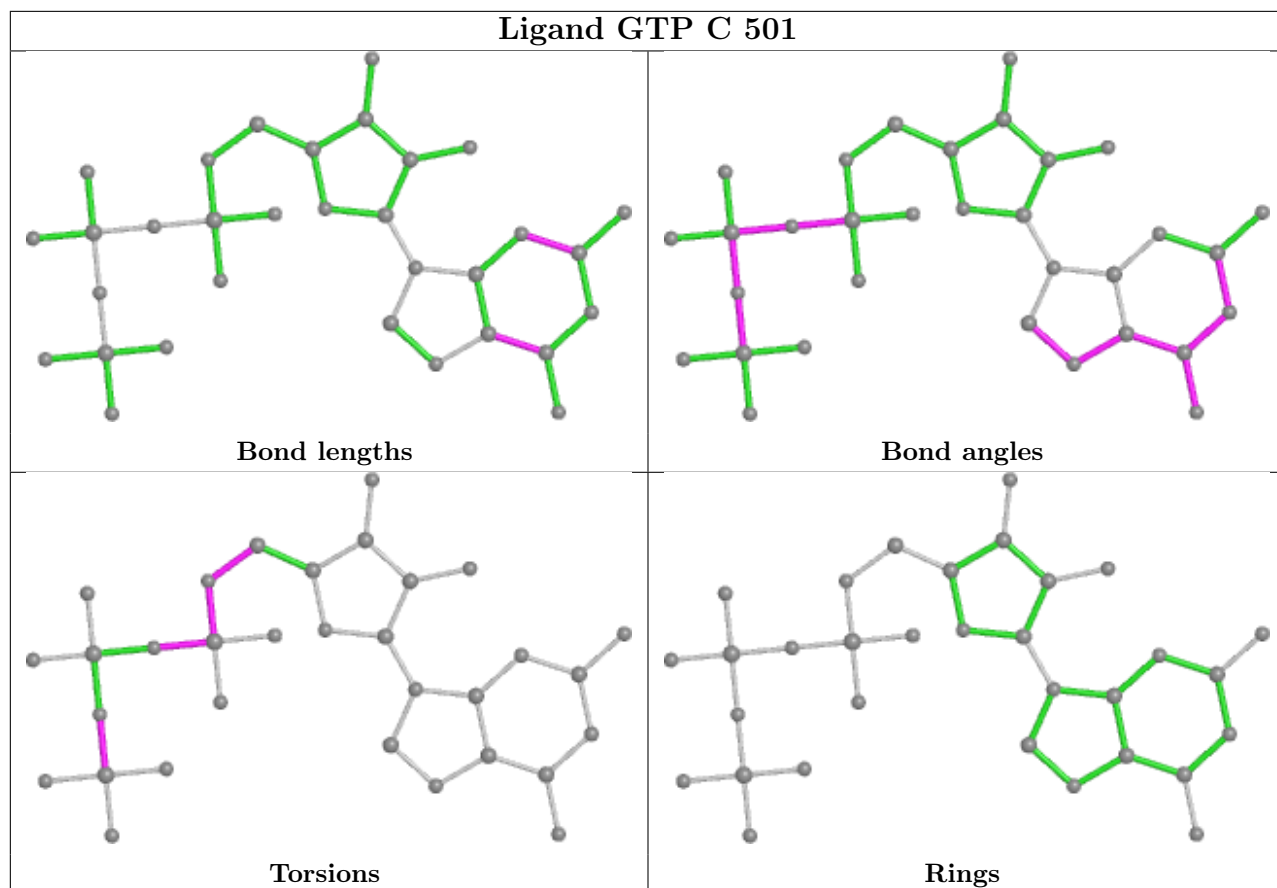
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [\(i\)](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	2
2	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	346:TRP	C	347:ILE	N	0.94
1	D	345:GLU	C	346:TRP	N	0.93
1	B	360:PRO	C	369:ARG	N	0.86

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	435/450 (96%)	0.60	28 (6%) 19 18	35, 56, 94, 123	0
1	C	439/450 (97%)	0.44	23 (5%) 27 26	30, 48, 81, 129	0
2	B	413/445 (92%)	0.71	36 (8%) 10 9	32, 54, 97, 146	1 (0%)
2	D	424/445 (95%)	0.73	47 (11%) 5 4	35, 59, 97, 140	3 (0%)
3	E	121/143 (84%)	0.91	15 (12%) 4 3	40, 68, 108, 146	0
4	F	339/384 (88%)	1.06	77 (22%) 0 0	42, 77, 129, 171	0
All	All	2171/2317 (93%)	0.70	226 (10%) 6 6	30, 57, 105, 171	4 (0%)

All (226) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1	MET	7.8
2	D	57	THR	7.1
1	A	262	TYR	6.9
2	B	59	ASN	6.6
3	E	7	GLU	6.6
2	B	56	ALA	6.0
4	F	161	LEU	5.9
4	F	252	ASN	5.7
3	E	6	MET	5.5
2	D	285	ALA	5.2
4	F	253	TYR	4.9
1	A	42	ILE	4.8
2	D	58	GLY	4.7
4	F	255	ARG	4.6
4	F	169	LEU	4.5
2	D	276	THR	4.5
1	C	2	ARG	4.5
2	D	56	ALA	4.4
2	B	61	TYR	4.4

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Mol	Chain	Res	Type	RSRZ
4	F	21	LEU	4.4
4	F	245	ILE	4.4
4	F	236	LYS	4.3
3	E	26	PRO	4.2
2	B	250	ALA	4.2
2	B	82	PRO	4.2
2	B	58	GLY	4.2
4	F	128	ARG	4.2
1	A	180	ALA	4.1
4	F	1	MET	4.0
2	D	59	ASN	4.0
1	C	250	VAL	3.9
2	D	179	ASP	3.9
4	F	22	LEU	3.9
3	E	8	VAL	3.8
1	A	45	GLY	3.8
4	F	167	SER	3.8
4	F	342	LEU	3.8
4	F	89	GLU	3.8
1	C	285	GLN	3.7
2	D	284	ARG	3.7
2	D	441	ASP	3.7
3	E	28	SER	3.7
4	F	244	CYS	3.6
1	A	280	LYS	3.6
2	B	322	ARG	3.6
4	F	256	TYR	3.6
3	E	9	ILE	3.6
4	F	9	GLU	3.5
2	D	37	HIS	3.5
2	B	60	LYS	3.5
4	F	259	GLY	3.4
4	F	125	THR	3.4
2	D	167	ASN	3.4
4	F	25	GLY	3.4
1	A	179	THR	3.4
2	B	36	TYR	3.3
4	F	234	GLN	3.3
4	F	166	ALA	3.3
4	F	130	VAL	3.3
4	F	104	ASN	3.3
3	E	124	GLN	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	346	TRP	3.2
1	C	4[A]	CYS	3.2
4	F	135	TYR	3.2
4	F	233	PHE	3.2
3	E	44	ASP	3.2
2	D	308	ARG	3.2
4	F	11	SER	3.2
1	A	43	GLY	3.2
2	B	35	SER	3.1
4	F	263	PHE	3.1
4	F	88	SER	3.1
4	F	102	PRO	3.1
2	B	83	PHE	3.1
4	F	258	GLU	3.1
4	F	159	GLY	3.1
1	C	177	VAL	3.1
4	F	103	THR	3.1
2	D	60	LYS	3.0
1	C	249	ASN	3.0
1	A	315	CYS	3.0
4	F	100	ILE	3.0
4	F	157	GLY	3.0
2	B	326	LYS	3.0
2	B	39	ASP	3.0
2	B	42	LEU	2.9
4	F	134	ALA	2.9
4	F	235	ASP	2.9
1	A	140	SER	2.9
4	F	232	ASN	2.9
2	B	219	LEU	2.9
2	B	286	LEU	2.9
2	B	416	MET	2.9
2	B	372	LYS	2.8
4	F	260	ASN	2.8
2	B	371	LEU	2.8
4	F	343	TYR	2.8
1	C	238	ILE	2.8
4	F	247	LYS	2.8
4	F	136	ASN	2.8
4	F	372	THR	2.8
4	F	27	TRP	2.8
2	D	269	MET	2.8

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Mol	Chain	Res	Type	RSRZ
4	F	170	LEU	2.8
4	F	248	GLU	2.8
2	D	416	MET	2.7
4	F	132	LEU	2.7
2	B	37	HIS	2.7
1	A	141	PHE	2.7
4	F	346	LEU	2.7
2	B	216	THR	2.7
1	A	171	ILE	2.7
4	F	194	PRO	2.7
4	F	351	VAL	2.7
2	B	55	GLU	2.7
1	A	203	MET	2.7
4	F	127	GLU	2.6
2	D	248	LEU	2.6
2	D	76	ASP	2.6
1	A	40	LYS	2.6
4	F	32	LYS	2.6
2	D	203	CYS	2.6
2	B	247	GLN	2.6
4	F	101	TYR	2.6
4	F	172	PHE	2.6
1	C	283	HIS	2.6
4	F	238	CYS	2.6
3	E	27	PRO	2.6
2	D	401	ARG	2.6
2	B	172	MET	2.6
4	F	181	VAL	2.6
3	E	106	GLU	2.5
4	F	28	LYS	2.5
1	C	242	LEU	2.5
2	B	246	GLY	2.5
1	A	46	ASP	2.5
4	F	231	ALA	2.5
4	F	340	GLN	2.5
2	D	402	LYS	2.5
2	D	75	MET	2.5
2	D	80	SER	2.5
2	D	94	PHE	2.5
2	D	82	PRO	2.5
4	F	254	GLY	2.5
2	B	245	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
4	F	225	SER	2.4
2	D	33	THR	2.4
2	D	267	PHE	2.4
1	A	370	LYS	2.4
1	A	170	SER	2.4
2	B	62	VAL	2.4
1	C	252	LEU	2.4
1	A	278	ALA	2.4
1	C	251	ASP	2.4
1	A	178	SER	2.4
2	D	90	ASP	2.4
4	F	131	PHE	2.4
1	C	241	SER	2.4
2	D	404	PHE	2.3
3	E	48	GLU	2.3
2	D	378	ILE	2.3
4	F	133	ALA	2.3
2	B	10	GLY	2.3
4	F	8	ASP	2.3
2	D	83	PHE	2.2
4	F	17	VAL	2.2
4	F	362	ALA	2.2
1	C	179	THR	2.2
2	D	201	THR	2.2
1	A	172	TYR	2.2
2	D	377	PHE	2.2
1	A	281	ALA	2.2
2	B	34	GLY	2.2
2	D	34	GLY	2.2
4	F	30	LEU	2.2
2	D	202	TYR	2.2
1	A	371	VAL	2.2
1	A	113	GLU	2.2
2	B	53	TYR	2.2
4	F	90	SER	2.2
2	B	33	THR	2.2
1	C	20	CYS	2.2
3	E	23	ILE	2.2
3	E	110	GLU	2.2
2	D	61	TYR	2.1
4	F	126	ASP	2.1
1	C	176	GLN	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	40	SER	2.1
3	E	10	GLU	2.1
1	A	331	ALA	2.1
4	F	341	LYS	2.1
2	B	241	CYS	2.1
4	F	23	ALA	2.1
2	B	360	PRO	2.1
2	D	196	GLU	2.1
4	F	243	HIS	2.1
1	C	315	CYS	2.1
1	A	204	VAL	2.1
2	D	182	VAL	2.1
4	F	200	ASP	2.1
1	A	423	GLU	2.1
1	C	220	GLU	2.1
1	A	174	ALA	2.1
1	C	247	ALA	2.1
1	C	349	THR	2.1
2	D	2	ARG	2.1
1	C	232	SER	2.1
2	D	81	GLY	2.1
4	F	41	LEU	2.1
1	C	284	GLU	2.1
4	F	24	THR	2.1
3	E	22	VAL	2.1
4	F	4	PHE	2.1
2	D	252	LEU	2.0
2	D	295	MET	2.0
1	C	253	THR	2.0
2	D	256	ALA	2.0
4	F	339	ALA	2.0
1	A	220	GLU	2.0
2	D	257	VAL	2.0
2	D	255	LEU	2.0
2	D	96	GLN	2.0
2	B	171	VAL	2.0
1	C	255	PHE	2.0
2	B	217	LEU	2.0
2	D	97	SER	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](#)

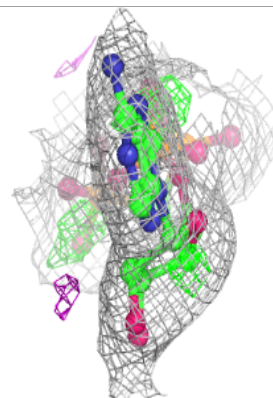
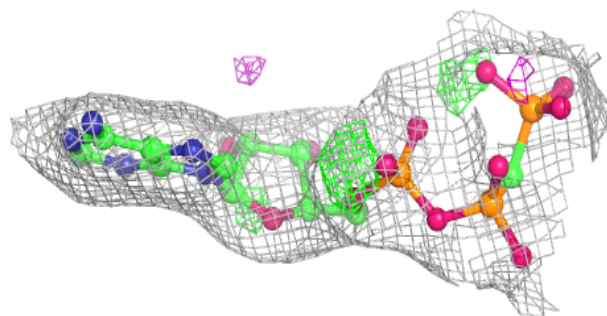
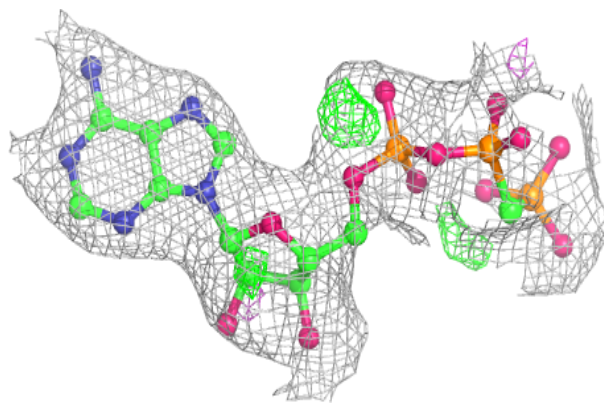
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	F	401	1/1	0.80	0.12	110,110,110,110	0
6	MG	A	502	1/1	0.81	0.12	45,45,45,45	0
9	ACP	F	402	31/31	0.89	0.13	58,86,141,142	0
6	MG	B	502	1/1	0.90	1.03	73,73,73,73	0
6	MG	D	502	1/1	0.91	0.08	54,54,54,54	0
6	MG	C	502	1/1	0.92	0.14	44,44,44,44	0
8	8Z8	B	503	29/29	0.96	0.15	45,52,58,62	0
7	GDP	D	501	28/28	0.96	0.13	49,55,61,63	0
7	GDP	B	501	28/28	0.97	0.23	40,57,66,73	0
5	GTP	C	501	32/32	0.97	0.16	38,47,61,71	0
5	GTP	A	501	32/32	0.98	0.22	36,45,51,55	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

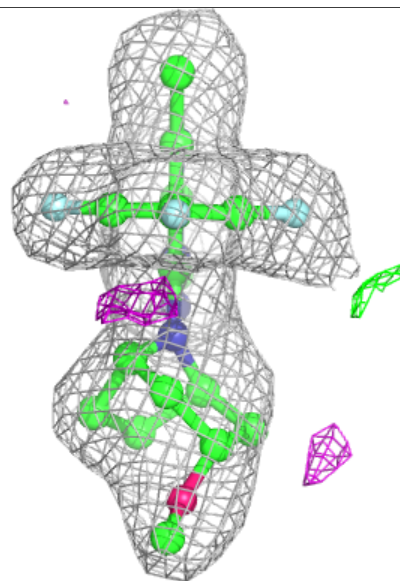
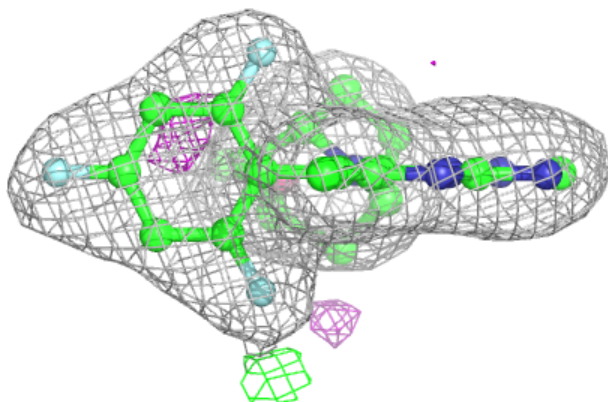
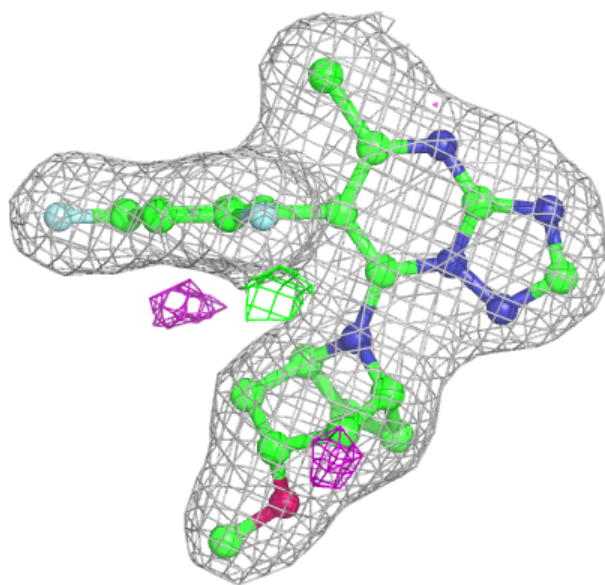
Electron density around ACP F 402:

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



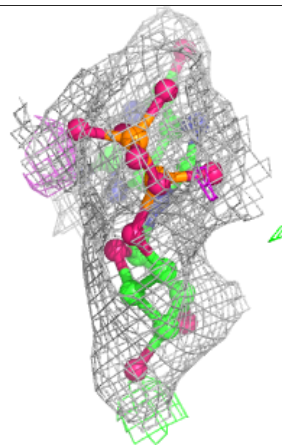
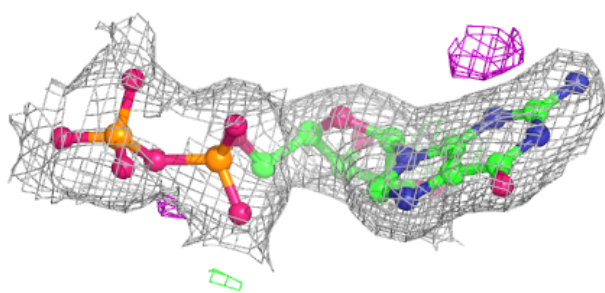
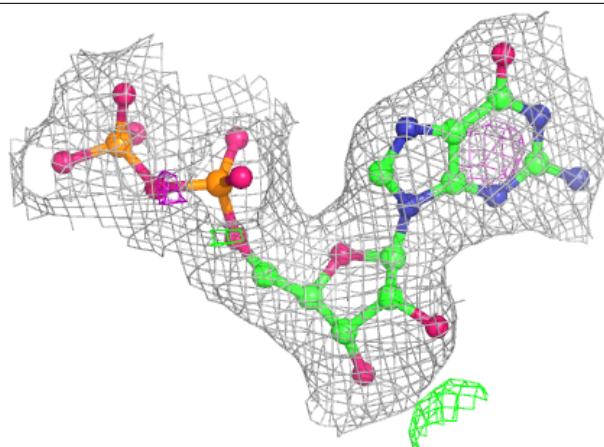
Electron density around 8Z8 B 503:

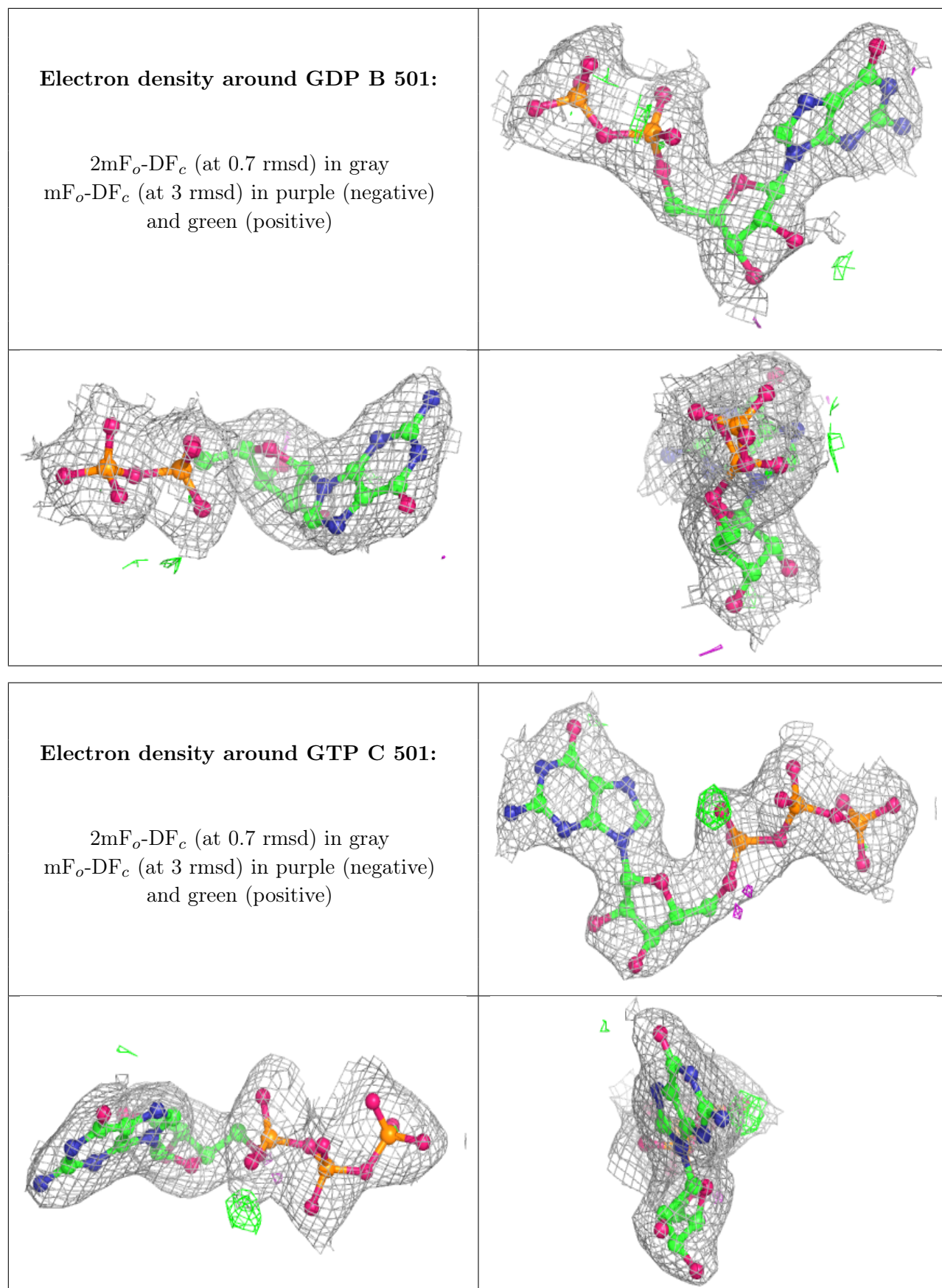
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

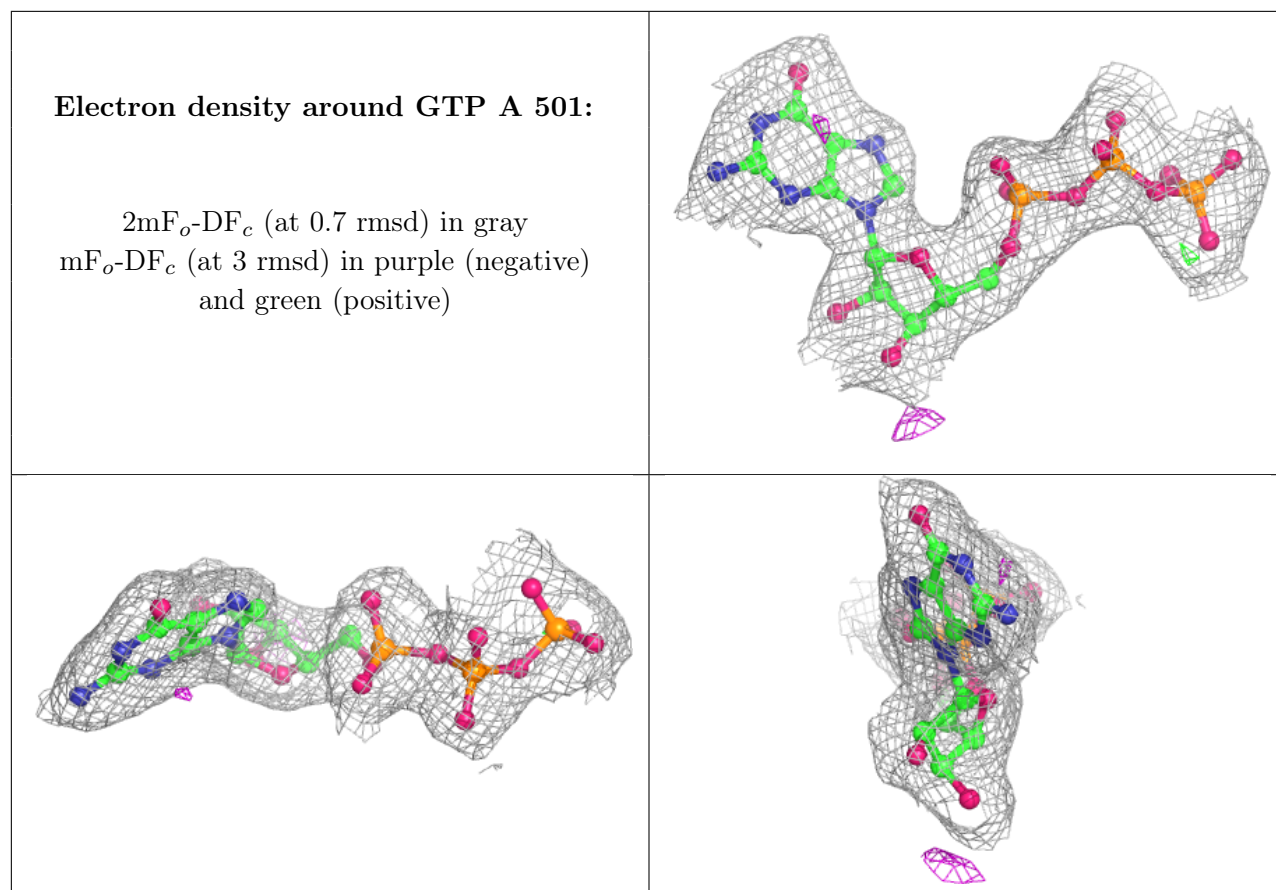


Electron density around GDP D 501:

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







6.5 Other polymers [i](#)

There are no such residues in this entry.