



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2021 – 02:00 PM EDT

PDB ID : 5S5B  
Title : Tubulin-Z906021418-complex  
Authors : Muehlethaler, T.; Gioia, D.; Protá, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.  
Deposited on : 2020-11-08  
Resolution : 2.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

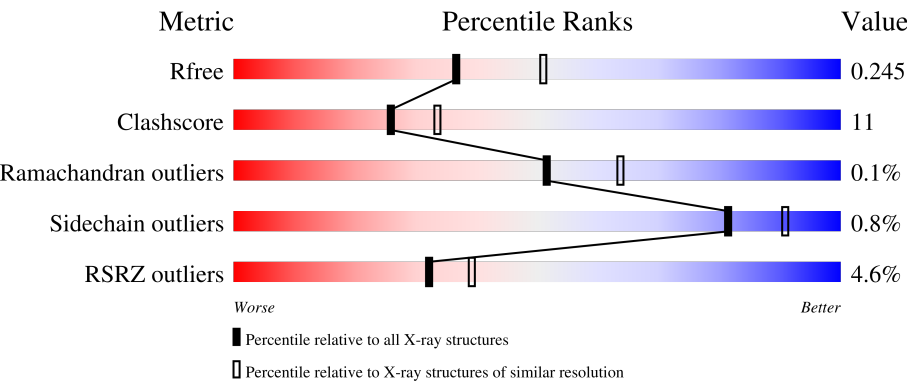
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.20
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.20

# 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 2.30 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 <sub>free</sub>	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	451	<div><div>3%</div><div></div><div>76%</div><div>21%</div><div></div><div></div></div>
1	C	451	<div><div>2%</div><div></div><div>79%</div><div>18%</div><div></div><div></div></div>
2	B	445	<div><div>2%</div><div></div><div>70%</div><div>24%</div><div>5%</div><div></div></div>
2	D	445	<div><div>5%</div><div></div><div>70%</div><div>27%</div><div></div><div></div></div>
3	E	143	<div><div>6%</div><div></div><div>67%</div><div>19%</div><div>14%</div><div></div></div>

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Mol	Chain	Length	Quality of chain
4	F	384	<div><div></div><div>10%</div><div>71%</div><div>21%</div><div>8%</div></div>

## 2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18043 atoms, of which 10 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	N	O	S	0	0	0
			3424	2167	582	653	22			
1	C	440	Total	C	N	O	S	0	1	0
			3443	2178	585	657	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	422	Total	C	N	O	S	2	0	0
			3329	2092	569	641	27			
2	D	429	Total	C	N	O	S	5	0	0
			3358	2107	573	651	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			1014	625	183	201	5			

There are 2 discrepancies between the modelled and reference sequences:

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

- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	352	Total	C	N	O	S	0	0	0
			2877	1843	495	525	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
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
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 CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula:  $C_{10}H_{15}N_5O_{11}P_2$ ).



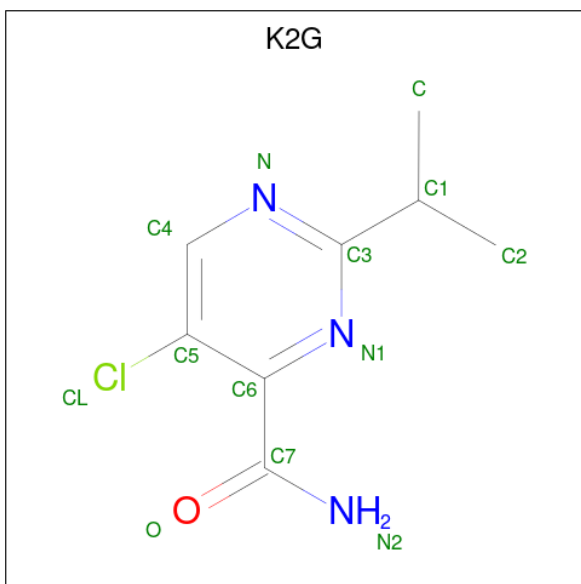
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

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



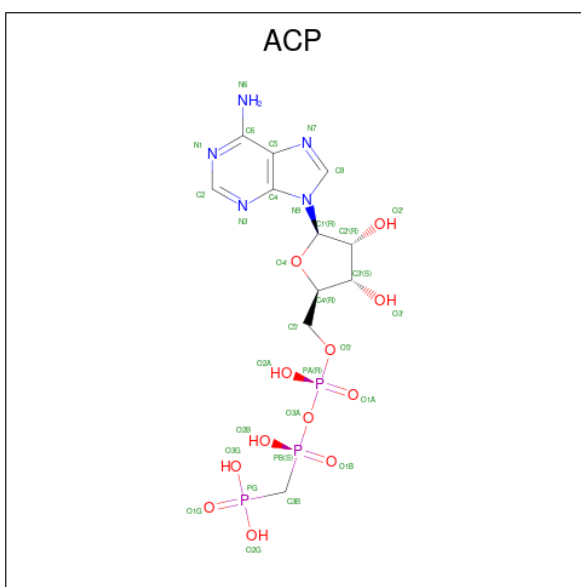
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is 5-chloro-2-(propan-2-yl)pyrimidine-4-carboxamide (three-letter code: K2G) (formula:  $C_8H_{10}ClN_3O$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
10	C	1	Total	C	Cl	H	N	O	0	0
			23	8	1	10	3	1		

- 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 31	C 11	N 5	O 12	P 3	0	0

- Molecule 12 is water.

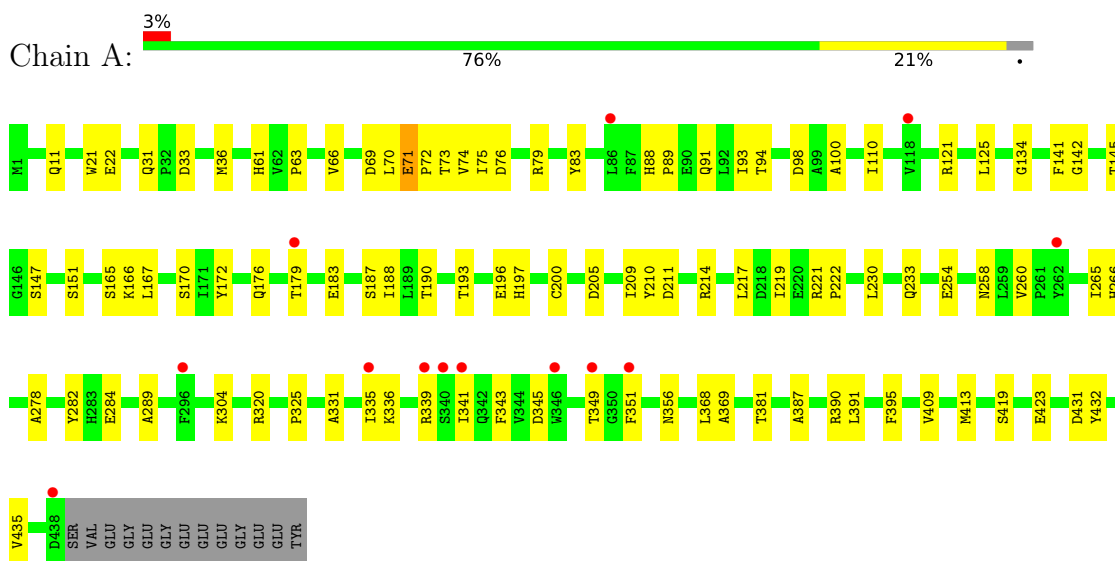
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	57	Total O 57 57	0	0
12	B	92	Total O 92 92	0	0
12	C	192	Total O 192 192	0	0
12	D	37	Total O 37 37	0	0
12	E	11	Total O 11 11	0	0
12	F	14	Total O 14 14	0	0



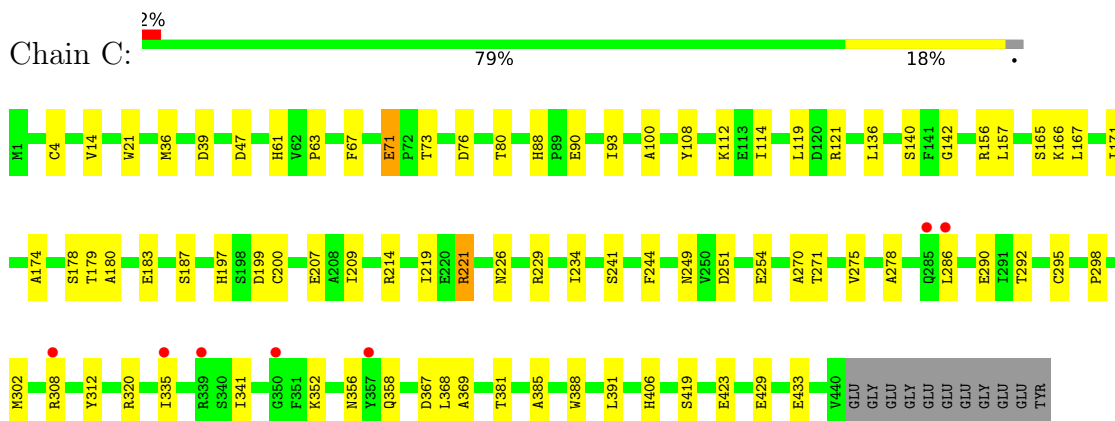
### 3 Residue-property plots [i](#)

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.

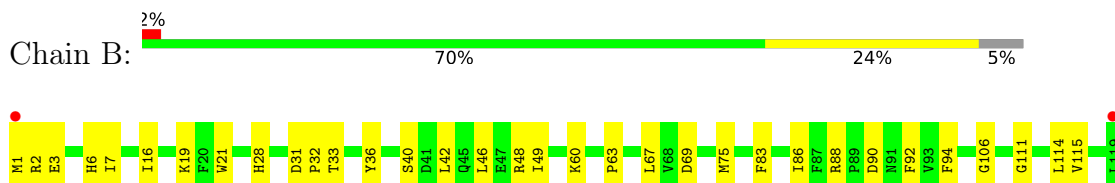
#### • Molecule 1: Tubulin alpha-1B chain

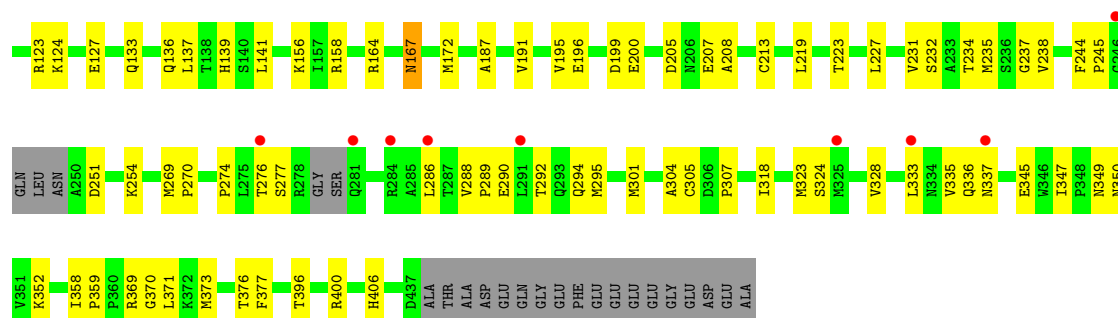


#### • Molecule 1: Tubulin alpha-1B chain

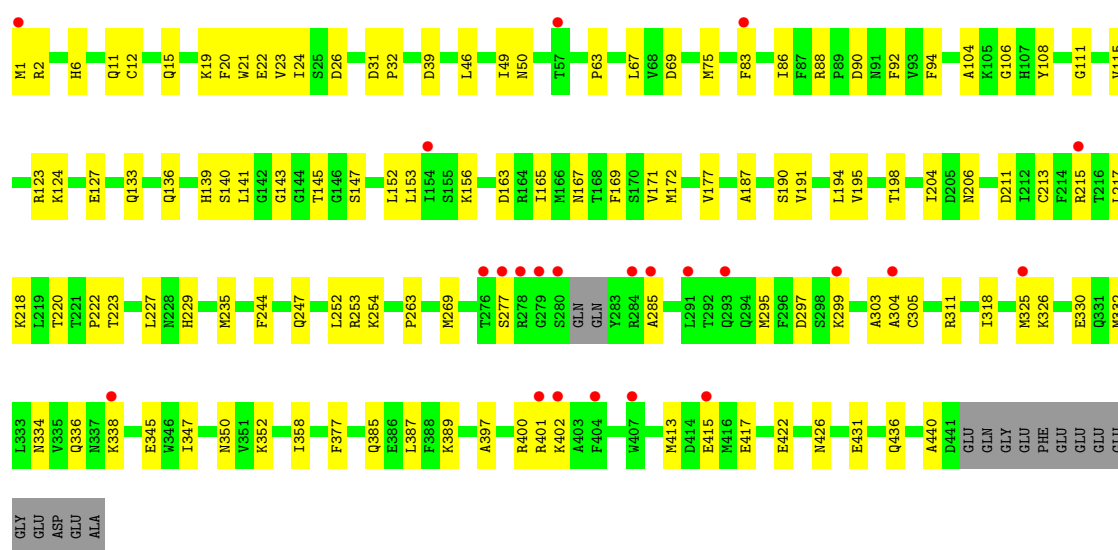


#### • Molecule 2: Tubulin beta-2B chain

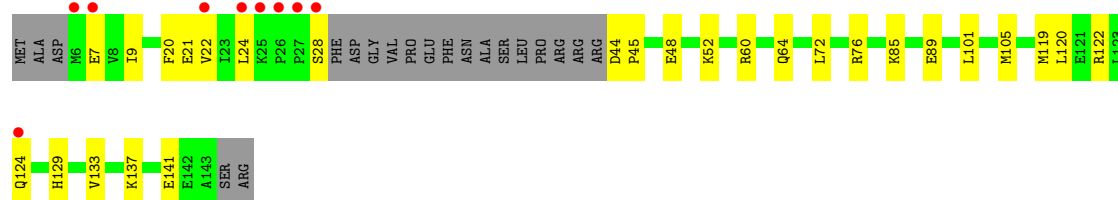




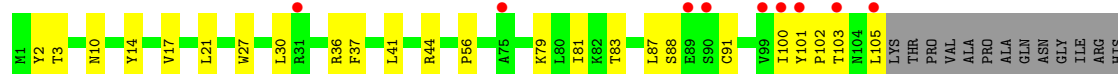
• Molecule 2: Tubulin beta-2B chain

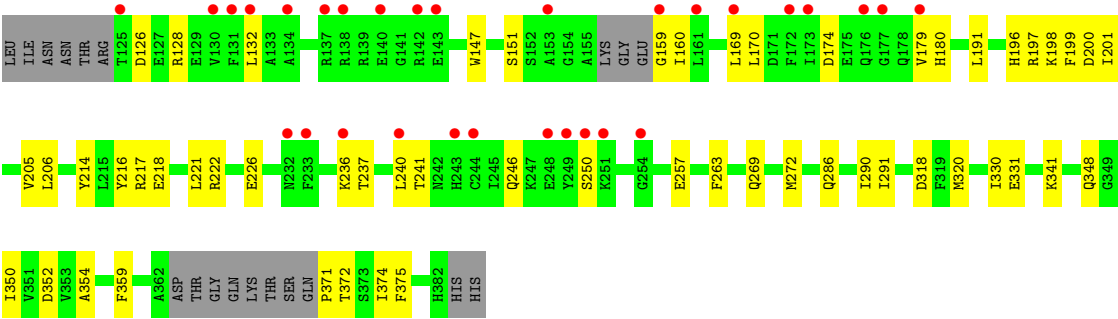


• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-Tyrosine Ligase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	105.02Å 158.92Å 179.41Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.37 – 2.30 118.96 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (63.37-2.30) 99.9 (118.96-2.30)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.11 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, $R_{free}$	0.209 , 0.244 0.210 , 0.245	Depositor DCC
$R_{free}$ test set	6614 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	57.4	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 46.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.52$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18043	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	74.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.38% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: ACP, MES, K2G, CA, GTP, GDP, 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	0.25	0/3502	0.42	0/4754
1	C	0.26	0/3521	0.43	0/4780
2	B	0.25	0/3402	0.41	0/4604
2	D	0.25	0/3431	0.41	0/4647
3	E	0.24	0/1022	0.35	0/1356
4	F	0.24	0/2944	0.40	0/3978
All	All	0.25	0/17822	0.41	0/24119

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3424	0	3334	73	0
1	C	3443	0	3352	61	0
2	B	3329	0	3210	80	0
2	D	3358	0	3231	81	0
3	E	1014	0	1029	21	0
4	F	2877	0	2839	64	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	3	0
9	B	12	0	12	1	0
10	C	13	10	0	0	0
11	F	31	0	14	5	0
12	A	57	0	0	3	0
12	B	92	0	0	3	0
12	C	192	0	0	4	0
12	D	37	0	0	3	0
12	E	11	0	0	1	0
12	F	14	0	0	1	0
All	All	18033	10	17069	365	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 11.

All (365) 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:102:PRO:HG2	4:F:105:LEU:HD13	1.44	0.99
2:D:217:LEU:HA	2:D:277:SER:HB3	1.48	0.95
1:C:209:ILE:HD11	1:C:302:MET:HE3	1.49	0.95
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.50	0.93
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.49	0.92
1:A:71:GLU:OE2	1:A:73:THR:OG1	1.94	0.84
2:B:2:ARG:HB2	2:B:133:GLN:HG3	1.58	0.84
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.65	0.77
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.18	0.76
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.67	0.76
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.67	0.76
4:F:318:ASP:OD2	11:F:401:ACP:O2G	2.05	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:406:HIS:ND1	12:B:601:HOH:O	2.21	0.74
1:C:47:ASP:OD2	12:C:601:HOH:O	2.06	0.74
4:F:371:PRO:HA	4:F:372:THR:HB	1.71	0.73
1:C:229:ARG:NH1	12:C:603:HOH:O	2.22	0.73
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.69	0.73
2:D:136:GLN:HA	2:D:167:ASN:O	1.89	0.72
1:C:270:ALA:O	1:C:302:MET:HG2	1.89	0.72
2:D:83:PHE:O	2:D:86:ILE:HG22	1.91	0.71
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.72	0.71
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.73	0.70
1:A:100:ALA:HA	2:B:254:LYS:HG3	1.73	0.70
1:C:76:ASP:O	1:C:80:THR:HG22	1.92	0.69
2:D:1:MET:HG3	2:D:50:ASN:HB2	1.73	0.69
2:B:337:ASN:OD1	4:F:36:ARG:HD3	1.92	0.69
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.58	0.69
4:F:331:GLU:OE2	11:F:401:ACP:O3G	2.11	0.68
1:C:367:ASP:OD1	12:C:602:HOH:O	2.11	0.67
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.75	0.67
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.08	0.67
1:C:209:ILE:CD1	1:C:302:MET:HE3	2.24	0.66
4:F:241:THR:HG1	11:F:401:ACP:HO3'	1.28	0.66
1:A:176:GLN:HG3	4:F:56:PRO:HB3	1.77	0.66
2:D:431:GLU:OE1	12:D:601:HOH:O	2.13	0.66
1:C:229:ARG:HG3	12:C:603:HOH:O	1.97	0.65
1:A:336:LYS:HD2	1:A:341:ILE:HD12	1.78	0.64
2:D:143:GLY:HA3	8:D:501:GDP:O3A	1.97	0.64
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.31	0.64
2:B:83:PHE:O	2:B:86:ILE:HG22	1.98	0.63
4:F:371:PRO:HA	4:F:372:THR:O	1.97	0.63
2:D:397:ALA:O	2:D:401:ARG:NH1	2.32	0.62
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.28	0.62
4:F:320:MET:CG	4:F:330:ILE:HD11	2.29	0.62
2:D:69:ASP:O	2:D:94:PHE:HA	1.99	0.62
1:A:70:LEU:HD22	1:A:110:ILE:CG2	2.30	0.61
2:B:69:ASP:O	2:B:94:PHE:HA	2.01	0.61
2:B:370:GLY:O	2:B:371:LEU:HD23	2.00	0.61
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.81	0.61
3:E:48:GLU:CG	3:E:52:LYS:HE3	2.31	0.60
4:F:320:MET:HG3	4:F:330:ILE:HD11	1.82	0.60
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.37	0.60
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ARG:HB2	2:B:133:GLN:CG	2.29	0.60
4:F:371:PRO:CA	4:F:372:THR:HB	2.32	0.60
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.83	0.59
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.37	0.59
4:F:132:LEU:HD21	4:F:170:LEU:HD11	1.83	0.59
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.67	0.59
1:A:70:LEU:HD12	1:A:145:THR:OG1	2.03	0.59
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.33	0.59
2:B:187:ALA:O	2:B:191:VAL:HG23	2.03	0.59
2:D:171:VAL:HA	2:D:204:ILE:O	2.03	0.59
4:F:159:GLY:C	4:F:160:ILE:HD12	2.23	0.59
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.02	0.59
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.37	0.59
2:D:211:ASP:O	2:D:215:ARG:HB2	2.03	0.58
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.84	0.58
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.85	0.58
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.86	0.58
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.34	0.58
1:C:320:ARG:HA	1:C:356:ASN:O	2.03	0.58
4:F:17:VAL:O	4:F:21:LEU:HG	2.03	0.58
4:F:101:TYR:N	4:F:126:ASP:OD1	2.23	0.58
2:D:215:ARG:O	2:D:218:LYS:HE3	2.04	0.58
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.37	0.58
1:A:70:LEU:HD22	1:A:110:ILE:HG21	1.85	0.58
2:D:1:MET:HG3	2:D:50:ASN:CB	2.34	0.57
2:D:345:GLU:HG3	2:D:440:ALA:HB2	1.87	0.57
4:F:91:CYS:HA	12:F:513:HOH:O	2.04	0.57
1:A:351:PHE:O	3:E:22:VAL:HG12	2.04	0.57
4:F:269:GLN:HA	4:F:272:MET:HE2	1.87	0.56
1:A:179:THR:HA	2:B:352:LYS:HD2	1.87	0.56
2:B:396:THR:O	2:B:400:ARG:HG2	2.05	0.56
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.88	0.56
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.41	0.56
3:E:85:LYS:O	3:E:89:GLU:HG3	2.05	0.56
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.36	0.56
1:C:108:TYR:O	1:C:112:LYS:HG2	2.06	0.55
1:A:88:HIS:CD2	1:A:91:GLN:HG3	2.40	0.55
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.41	0.55
4:F:102:PRO:HG2	4:F:105:LEU:CD1	2.29	0.55
4:F:241:THR:OG1	11:F:401:ACP:O3'	2.06	0.55
2:B:167:ASN:OD1	2:B:200:GLU:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.88	0.55
2:B:123:ARG:O	2:B:127:GLU:HG3	2.07	0.55
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.06	0.55
2:B:323:MET:HE2	2:B:373:MET:HB2	1.88	0.55
3:E:72:LEU:O	3:E:76:ARG:HG2	2.07	0.55
1:C:271:THR:HG21	1:C:295:CYS:O	2.06	0.55
1:A:11:GLN:HG3	1:A:74:VAL:HG21	1.89	0.55
2:B:124:LYS:HD3	2:B:124:LYS:C	2.27	0.54
2:B:223:THR:O	2:B:227:LEU:HD13	2.08	0.54
1:A:320:ARG:HD2	12:A:644:HOH:O	2.07	0.54
3:E:9:ILE:HG13	3:E:21:GLU:HB3	1.89	0.54
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.08	0.54
1:C:180:ALA:O	1:C:183:GLU:HG3	2.07	0.54
1:A:166:LYS:HE2	1:A:197:HIS:O	2.08	0.54
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.43	0.54
2:D:106:GLY:O	2:D:111:GLY:HA3	2.09	0.53
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.23	0.53
3:E:48:GLU:HG2	3:E:52:LYS:HE3	1.89	0.53
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.91	0.53
2:B:46:LEU:HA	2:B:49:ILE:HB	1.91	0.53
2:B:305:CYS:O	2:B:307:PRO:HD3	2.09	0.53
4:F:246:GLN:O	4:F:250:SER:HB3	2.09	0.53
1:A:419:SER:O	1:A:423:GLU:HG3	2.10	0.52
2:B:323:MET:HB3	2:B:373:MET:CE	2.39	0.52
2:D:115:VAL:HG23	2:D:153:LEU:HD23	1.91	0.52
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.45	0.52
1:C:241:SER:HA	1:C:249:ASN:OD1	2.10	0.52
4:F:269:GLN:HA	4:F:272:MET:CE	2.40	0.52
2:B:295:MET:CG	2:B:377:PHE:HB2	2.40	0.52
2:D:194:LEU:HD22	2:D:198:THR:HG21	1.91	0.52
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.44	0.52
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.27	0.52
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.92	0.52
1:A:69:ASP:O	1:A:94:THR:HA	2.10	0.52
2:B:106:GLY:O	2:B:111:GLY:HA3	2.09	0.52
2:D:108:TYR:OH	2:D:417:GLU:OE2	2.20	0.52
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.45	0.51
1:C:292:THR:HG22	1:C:335:ILE:HD12	1.91	0.51
2:B:141:LEU:HD12	2:B:172:MET:SD	2.50	0.51
2:D:1:MET:CG	2:D:50:ASN:HB2	2.41	0.51
2:B:345:GLU:OE1	2:B:345:GLU:N	2.36	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:10:ASN:CB	4:F:44:ARG:HH22	2.23	0.51
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.92	0.51
4:F:226:GLU:HG3	4:F:237:THR:HG22	1.93	0.51
4:F:151:SER:HB3	4:F:180:HIS:CD2	2.46	0.51
4:F:263:PHE:CZ	4:F:341:LYS:HE2	2.46	0.50
1:A:336:LYS:NZ	1:A:341:ILE:HB	2.26	0.50
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.92	0.50
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.75	0.50
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.25	0.50
1:A:141:PHE:HB3	1:A:187:SER:OG	2.12	0.50
1:A:151:SER:HB2	1:A:193:THR:OG1	2.11	0.50
1:C:174:ALA:HB2	1:C:207:GLU:HB2	1.93	0.50
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.47	0.50
4:F:217:ARG:NH2	4:F:374:ILE:HA	2.27	0.50
2:D:318:ILE:N	2:D:318:ILE:HD12	2.27	0.50
2:D:402:LYS:HE2	2:D:415:GLU:OE1	2.11	0.50
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.42	0.50
1:A:176:GLN:CG	4:F:56:PRO:HB3	2.40	0.50
2:D:191:VAL:O	2:D:195:VAL:HG23	2.12	0.50
4:F:371:PRO:HA	4:F:372:THR:C	2.32	0.50
4:F:81:ILE:HA	4:F:87:LEU:HD12	1.94	0.49
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.94	0.49
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.46	0.49
2:B:1:MET:HB3	2:B:3:GLU:OE2	2.12	0.49
2:B:205:ASP:OD1	2:B:207:GLU:N	2.44	0.49
2:D:147:SER:HB2	2:D:190:SER:OG	2.11	0.49
1:A:176:GLN:HB2	12:A:625:HOH:O	2.12	0.49
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.48	0.49
1:C:419:SER:O	1:C:423:GLU:HG3	2.12	0.49
2:D:303:ALA:O	2:D:305:CYS:N	2.40	0.49
4:F:201:ILE:HG12	4:F:221:LEU:HG	1.92	0.49
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.43	0.49
2:B:136:GLN:HA	2:B:167:ASN:O	2.11	0.49
2:D:163:ASP:O	2:D:253:ARG:NH2	2.45	0.49
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.93	0.49
2:D:311:ARG:NH1	2:D:436:GLN:O	2.46	0.49
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.95	0.49
2:D:145:THR:HB	8:D:501:GDP:O2B	2.13	0.49
4:F:3:THR:HB	4:F:30:LEU:HD11	1.94	0.49
2:B:42:LEU:H	2:B:42:LEU:HD12	1.79	0.48
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:7:GLU:O	3:E:22:VAL:HA	2.13	0.48
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.48	0.48
2:B:191:VAL:O	2:B:195:VAL:HG23	2.12	0.48
2:B:244:PHE:HB3	2:B:245:PRO:HD2	1.95	0.48
2:D:115:VAL:HG23	2:D:153:LEU:CD2	2.44	0.48
2:D:187:ALA:O	2:D:191:VAL:HG23	2.14	0.48
3:E:60:ARG:O	3:E:64:GLN:HG3	2.13	0.48
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.48	0.48
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.95	0.48
3:E:120:LEU:O	3:E:124:GLN:HG3	2.13	0.48
2:D:217:LEU:CA	2:D:277:SER:HB3	2.34	0.48
1:A:335:ILE:CG2	1:A:339:ARG:HG3	2.42	0.48
1:A:351:PHE:HB2	3:E:22:VAL:CG1	2.44	0.48
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.48	0.48
2:D:124:LYS:C	2:D:124:LYS:HD3	2.34	0.48
1:C:179:THR:HG21	12:D:614:HOH:O	2.14	0.48
2:D:152:LEU:O	2:D:156:LYS:HG2	2.13	0.48
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.96	0.48
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.36	0.48
2:B:244:PHE:CE1	2:B:358:ILE:HD12	2.48	0.47
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.95	0.47
4:F:371:PRO:HA	4:F:372:THR:CB	2.36	0.47
1:C:71:GLU:OE1	1:C:73:THR:HG23	2.14	0.47
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.49	0.47
1:C:136:LEU:HD23	1:C:167:LEU:HB2	1.96	0.47
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.96	0.47
2:D:31:ASP:HB2	2:D:32:PRO:HD2	1.95	0.47
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.96	0.47
2:B:349:ASN:O	2:B:352:LYS:HE2	2.15	0.47
2:D:67:LEU:N	2:D:67:LEU:HD12	2.29	0.47
3:E:129:HIS:O	3:E:133:VAL:HG23	2.14	0.47
1:A:325:PRO:HB3	3:E:20:PHE:CE1	2.49	0.47
2:D:177:VAL:HG21	2:D:206:ASN:HB3	1.97	0.47
3:E:137:LYS:HE2	3:E:141:GLU:OE2	2.15	0.47
2:B:231:VAL:O	2:B:235:MET:HG3	2.15	0.47
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.49	0.47
1:C:39:ASP:OD2	1:C:61:HIS:NE2	2.38	0.47
2:B:199:ASP:OD1	9:B:504:MES:H62	2.15	0.46
1:A:214:ARG:HG2	1:A:219:ILE:O	2.16	0.46
2:B:269:MET:HE1	2:B:307:PRO:HG3	1.97	0.46
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:198:LYS:HG2	4:F:199:PHE:H	1.80	0.46
1:C:234:ILE:HG12	1:C:302:MET:HE2	1.98	0.46
3:E:9:ILE:CG1	3:E:21:GLU:HB3	2.45	0.46
1:A:188:ILE:HD12	1:A:395:PHE:HB2	1.96	0.46
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.98	0.46
1:A:431:ASP:O	1:A:435:VAL:HG23	2.15	0.46
1:C:341:ILE:HD12	1:C:341:ILE:N	2.31	0.46
1:C:142:GLY:HA3	1:C:183:GLU:OE1	2.16	0.46
3:E:101:LEU:O	3:E:105:MET:HG2	2.15	0.46
4:F:350:ILE:O	4:F:354:ALA:HB3	2.15	0.46
1:A:187:SER:CB	1:A:391:LEU:HD21	2.46	0.46
2:B:234:THR:O	2:B:238:VAL:HG13	2.16	0.46
2:D:11:GLN:O	2:D:15:GLN:HG2	2.16	0.46
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.43	0.45
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.46	0.45
2:D:46:LEU:HA	2:D:49:ILE:HB	1.98	0.45
2:B:164:ARG:HD2	12:B:673:HOH:O	2.16	0.45
1:C:226:ASN:ND2	1:C:367:ASP:OD2	2.49	0.45
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.97	0.45
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.56	0.45
2:D:169:PHE:CE2	2:D:235:MET:HG2	2.52	0.45
4:F:79:LYS:O	4:F:83:THR:OG1	2.29	0.45
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.99	0.45
2:D:15:GLN:O	2:D:19:LYS:HG2	2.17	0.45
3:E:44:ASP:HB3	3:E:45:PRO:HD2	1.99	0.45
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.51	0.45
2:B:88:ARG:HH11	2:B:90:ASP:HB2	1.82	0.45
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.47	0.45
1:C:429:GLU:O	1:C:433:GLU:HG3	2.17	0.44
2:B:324:SER:O	2:B:328:VAL:HG23	2.17	0.44
1:A:142:GLY:HA3	1:A:183:GLU:OE2	2.17	0.44
2:B:318:ILE:N	2:B:318:ILE:HD12	2.32	0.44
2:D:326:LYS:O	2:D:330:GLU:HG3	2.17	0.44
2:D:332:MET:O	2:D:336:GLN:HG3	2.18	0.44
1:A:196:GLU:OE1	1:A:196:GLU:HA	2.17	0.44
1:C:286:LEU:HA	1:C:290:GLU:OE1	2.18	0.44
2:D:385:GLN:O	2:D:389:LYS:HG3	2.18	0.44
2:B:288:VAL:HB	2:B:289:PRO:HD3	2.00	0.44
2:B:323:MET:HB3	2:B:373:MET:HE2	2.00	0.44
2:D:75:MET:HE3	2:D:92:PHE:CD2	2.52	0.44
2:D:67:LEU:HD22	2:D:92:PHE:CE2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.00	0.44
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.48	0.44
1:A:343:PHE:CD1	1:A:349:THR:HG23	2.53	0.44
2:B:333:LEU:HD23	2:B:336:GLN:NE2	2.33	0.44
1:C:21:TRP:CE3	1:C:63:PRO:HB3	2.53	0.44
4:F:263:PHE:CE1	4:F:341:LYS:HE2	2.53	0.44
1:A:289:ALA:HA	1:A:331:ALA:CB	2.47	0.43
1:C:119:LEU:HD11	1:C:156:ARG:HB3	2.00	0.43
2:D:1:MET:CE	2:D:50:ASN:HB2	2.48	0.43
2:D:140:SER:HB2	12:D:605:HOH:O	2.16	0.43
1:A:284:GLU:CD	1:A:284:GLU:H	2.21	0.43
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.52	0.43
1:C:178:SER:OG	2:D:352:LYS:NZ	2.50	0.43
1:A:70:LEU:HD22	1:A:110:ILE:HG22	2.00	0.43
2:D:115:VAL:CG2	2:D:153:LEU:HD23	2.49	0.43
2:D:297:ASP:OD2	2:D:299:LYS:HB2	2.18	0.43
1:A:141:PHE:O	1:A:147:SER:HB3	2.17	0.43
1:A:320:ARG:HA	1:A:356:ASN:O	2.19	0.43
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.48	0.43
2:B:133:GLN:OE1	2:B:251:ASP:HB2	2.18	0.43
2:B:158:ARG:NH1	2:B:196:GLU:O	2.52	0.43
2:B:7:ILE:O	2:B:137:LEU:HA	2.19	0.43
2:B:67:LEU:N	2:B:67:LEU:HD12	2.33	0.43
1:C:278:ALA:HA	1:C:369:ALA:HB2	2.01	0.43
1:A:22:GLU:HG3	1:A:83:TYR:HE1	1.84	0.43
4:F:191:LEU:HD12	4:F:196:HIS:CE1	2.54	0.43
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.33	0.42
2:D:88:ARG:NH1	2:D:90:ASP:HB2	2.34	0.42
4:F:101:TYR:CD2	4:F:179:VAL:HG22	2.55	0.42
2:B:42:LEU:HD12	2:B:42:LEU:N	2.35	0.42
2:B:290:GLU:O	2:B:294:GLN:HG3	2.20	0.42
4:F:87:LEU:O	4:F:88:SER:OG	2.31	0.42
2:B:31:ASP:HB2	2:B:32:PRO:HD2	2.01	0.42
1:C:214:ARG:HG2	1:C:219:ILE:O	2.20	0.42
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.55	0.42
2:B:237:GLY:HA3	2:B:376:THR:OG1	2.19	0.42
1:C:174:ALA:HB1	1:C:207:GLU:HB2	2.00	0.42
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.00	0.42
1:C:140:SER:HA	1:C:171:ILE:HB	2.02	0.42
2:D:2:ARG:HB3	2:D:133:GLN:HG2	2.02	0.42
4:F:126:ASP:OD2	4:F:128:ARG:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LEU:HD21	1:A:368:LEU:HD23	2.02	0.42
1:A:387:ALA:HA	1:A:390:ARG:HD3	2.02	0.42
2:B:19:LYS:HB3	2:B:232:SER:OG	2.18	0.42
1:C:187:SER:CB	1:C:391:LEU:HD21	2.50	0.42
4:F:286:GLN:O	4:F:290:ILE:HG13	2.19	0.42
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.55	0.42
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.55	0.42
2:D:123:ARG:O	2:D:127:GLU:HG3	2.19	0.42
3:E:119:MET:HA	3:E:122:ARG:NH2	2.35	0.42
4:F:100:ILE:CD1	4:F:128:ARG:HA	2.49	0.42
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.55	0.42
1:A:345:ASP:HB3	3:E:28:SER:HB2	2.01	0.42
2:B:40:SER:OG	2:B:42:LEU:HD13	2.20	0.42
1:C:406:HIS:CG	2:D:263:PRO:HD3	2.54	0.42
4:F:341:LYS:HG2	4:F:341:LYS:O	2.20	0.42
2:B:270:PRO:HA	2:B:377:PHE:O	2.20	0.41
2:B:301:MET:HE3	2:B:307:PRO:HG2	2.01	0.41
1:C:406:HIS:CD2	2:D:263:PRO:HD3	2.54	0.41
2:D:19:LYS:O	2:D:23:VAL:HG23	2.20	0.41
2:D:169:PHE:CD2	2:D:235:MET:HG2	2.55	0.41
4:F:103:THR:HG23	4:F:128:ARG:NH2	2.34	0.41
2:B:396:THR:HG23	12:B:676:HOH:O	2.20	0.41
2:D:104:ALA:HB2	2:D:413:MET:SD	2.59	0.41
2:D:422:GLU:HG2	2:D:426:ASN:ND2	2.35	0.41
4:F:206:LEU:HD21	4:F:354:ALA:HB2	2.00	0.41
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.39	0.41
4:F:100:ILE:HD12	4:F:128:ARG:HA	2.01	0.41
2:B:276:THR:HG22	2:B:277:SER:O	2.20	0.41
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.86	0.41
2:D:220:THR:C	2:D:222:PRO:HD3	2.40	0.41
11:F:401:ACP:O3G	11:F:401:ACP:O1B	2.38	0.41
1:A:22:GLU:HG3	1:A:83:TYR:CE1	2.56	0.41
1:A:147:SER:HB2	1:A:190:THR:HB	2.02	0.41
1:C:100:ALA:HA	2:D:254:LYS:HG3	2.02	0.41
2:D:223:THR:O	2:D:227:LEU:HG	2.20	0.41
1:A:167:LEU:HG	1:A:200:CYS:HB3	2.03	0.41
1:C:93:ILE:HD11	1:C:121:ARG:CG	2.46	0.41
1:A:71:GLU:O	12:A:601:HOH:O	2.21	0.41
2:D:22:GLU:HG2	2:D:83:PHE:CD1	2.55	0.41
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.54	0.41
4:F:240:LEU:HD12	4:F:240:LEU:N	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:GLN:HB2	1:A:33:ASP:OD1	2.21	0.41
1:A:260:VAL:HG11	1:A:266:HIS:HB3	2.03	0.41
1:A:336:LYS:HG3	3:E:24:LEU:CD1	2.48	0.41
2:B:295:MET:HG2	2:B:377:PHE:HB2	2.02	0.41
1:C:165:SER:HA	1:C:199:ASP:OD2	2.20	0.41
3:E:85:LYS:NZ	12:E:301:HOH:O	2.53	0.41
4:F:3:THR:OG1	4:F:37:PHE:HA	2.20	0.41
2:B:28:HIS:HB3	2:B:49:ILE:HD13	2.02	0.41
2:B:205:ASP:OD1	2:B:207:GLU:HB3	2.21	0.41
1:C:166:LYS:HE2	1:C:197:HIS:O	2.21	0.41
2:D:20:PHE:CE1	2:D:24:ILE:HG21	2.56	0.41
2:B:114:LEU:HG	2:B:114:LEU:O	2.21	0.40
1:C:157:LEU:HD23	1:C:157:LEU:HA	1.89	0.40
4:F:103:THR:HG23	4:F:174:ASP:OD1	2.22	0.40
1:A:66:VAL:HG23	1:A:125:LEU:HD12	2.04	0.40
1:A:409:VAL:HA	1:A:413:MET:O	2.22	0.40
2:B:115:VAL:HG11	2:B:156:LYS:HE3	2.02	0.40
2:B:369:ARG:HA	2:B:369:ARG:HD3	1.98	0.40
4:F:2:TYR:HB2	4:F:27:TRP:CD2	2.56	0.40
1:A:134:GLY:HA3	1:A:165:SER:O	2.20	0.40
2:B:33:THR:O	2:B:60:LYS:NZ	2.49	0.40
2:B:213:CYS:HB3	2:B:219:LEU:HD12	2.02	0.40
2:B:359:PRO:HB2	2:B:371:LEU:O	2.21	0.40
2:D:141:LEU:HD12	2:D:172:MET:SD	2.62	0.40
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	436/451 (97%)	424 (97%)	12 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	439/451 (97%)	429 (98%)	10 (2%)	0	100	100
2	B	416/445 (94%)	405 (97%)	11 (3%)	0	100	100
2	D	425/445 (96%)	416 (98%)	7 (2%)	2 (0%)	29	35
3	E	119/143 (83%)	119 (100%)	0	0	100	100
4	F	344/384 (90%)	327 (95%)	17 (5%)	0	100	100
All	All	2179/2319 (94%)	2120 (97%)	57 (3%)	2 (0%)	51	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	304	ALA
2	D	285	ALA

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/379 (97%)	365 (99%)	4 (1%)	73	86
1	C	372/379 (98%)	368 (99%)	4 (1%)	73	86
2	B	366/383 (96%)	363 (99%)	3 (1%)	81	91
2	D	368/383 (96%)	363 (99%)	5 (1%)	67	81
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	315/342 (92%)	315 (100%)	0	100	100
All	All	1900/1993 (95%)	1884 (99%)	16 (1%)	81	91

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	221	ARG
1	A	282	TYR
1	A	381	THR

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Mol	Chain	Res	Type
2	B	48	ARG
2	B	139	HIS
2	B	167	ASN
1	C	71	GLU
1	C	221	ARG
1	C	251	ASP
1	C	381	THR
2	D	26	ASP
2	D	39	ASP
2	D	139	HIS
2	D	229	HIS
2	D	247	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	101	ASN
1	A	301	GLN
2	B	15	GLN
2	B	282	GLN
2	B	294	GLN
1	C	11	GLN
1	C	85	GLN
1	C	300	ASN
1	C	342	GLN
2	D	294	GLN
2	D	300	ASN
4	F	196	HIS
4	F	229	ASN
4	F	269	GLN
4	F	333	ASN

### 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 [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 9 are monoatomic - leaving 7 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
10	K2G	C	504	-	11,13,13	0.37	0	13,18,18	1.40	2 (15%)
11	ACP	F	401	6	27,33,33	1.38	5 (18%)	32,52,52	1.50	4 (12%)
5	GTP	A	501	6	26,34,34	0.98	1 (3%)	33,54,54	1.75	7 (21%)
8	GDP	B	501	6	24,30,30	1.16	2 (8%)	31,47,47	1.93	7 (22%)
9	MES	B	504	-	12,12,12	2.25	1 (8%)	14,16,16	1.90	4 (28%)
8	GDP	D	501	6	24,30,30	1.17	2 (8%)	31,47,47	1.92	7 (22%)
5	GTP	C	501	6	26,34,34	0.98	1 (3%)	33,54,54	1.61	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
10	K2G	C	504	-	-	2/8/8/8	0/1/1/1
11	ACP	F	401	6	-	12/15/38/38	0/3/3/3
5	GTP	A	501	6	-	9/18/38/38	0/3/3/3
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
9	MES	B	504	-	-	1/6/14/14	0/1/1/1
8	GDP	D	501	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	6/18/38/38	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.51	1.66	1.77
8	D	501	GDP	C6-C5	4.06	1.48	1.41
8	B	501	GDP	C6-C5	3.90	1.48	1.41
5	A	501	GTP	C6-N1	3.21	1.38	1.33
5	C	501	GTP	C6-N1	3.13	1.38	1.33
11	F	401	ACP	PG-O2G	2.96	1.61	1.54
11	F	401	ACP	PG-O3G	2.91	1.61	1.54
11	F	401	ACP	PB-O3A	2.62	1.61	1.58
11	F	401	ACP	C5-C4	2.50	1.47	1.40
8	D	501	GDP	C5-C4	2.43	1.47	1.40
8	B	501	GDP	C5-C4	2.27	1.46	1.40
11	F	401	ACP	PB-O2B	2.23	1.61	1.56

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	N3-C2-N1	-5.35	120.08	127.22
8	B	501	GDP	C2-N3-C4	5.21	121.30	115.36
5	C	501	GTP	N3-C2-N1	-5.10	120.42	127.22
8	D	501	GDP	C2-N3-C4	4.86	120.91	115.36
5	A	501	GTP	C2-N3-C4	4.49	120.49	115.36
9	B	504	MES	C5-N4-C3	4.40	118.74	108.83
11	F	401	ACP	PA-O3A-PB	-4.32	118.87	132.56
8	B	501	GDP	C6-C5-C4	-4.18	116.80	120.80
8	D	501	GDP	C6-N1-C2	4.11	122.47	115.93
8	D	501	GDP	C5-C6-N1	-4.08	117.85	123.43
8	B	501	GDP	C6-N1-C2	4.03	122.34	115.93
10	C	504	K2G	C4-C5-C6	-3.91	118.47	120.39
8	D	501	GDP	C6-C5-C4	-3.80	117.17	120.80
8	B	501	GDP	C5-C6-N1	-3.77	118.28	123.43
5	C	501	GTP	C2-N3-C4	3.73	119.62	115.36
8	B	501	GDP	N3-C2-N1	-3.69	122.30	127.22
8	D	501	GDP	N3-C2-N1	-3.37	122.73	127.22
11	F	401	ACP	C3'-C2'-C1'	3.37	106.05	100.98
5	C	501	GTP	C5-C6-N1	-3.28	118.95	123.43
11	F	401	ACP	N3-C2-N1	-3.17	123.72	128.68
5	A	501	GTP	C5-C6-N1	-2.90	119.46	123.43
5	A	501	GTP	PA-O3A-PB	-2.90	122.88	132.83
9	B	504	MES	O1S-S-C8	2.89	110.40	106.92
8	D	501	GDP	PA-O3A-PB	-2.89	122.91	132.83
8	D	501	GDP	C4-C5-N7	-2.76	106.52	109.40
5	A	501	GTP	PB-O3B-PG	-2.76	123.36	132.83
8	B	501	GDP	C4-C5-N7	-2.67	106.61	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	C6-N1-C2	2.65	120.14	115.93
9	B	504	MES	O3S-S-C8	2.58	109.94	105.77
11	F	401	ACP	C4-C5-N7	-2.58	106.71	109.40
5	A	501	GTP	C6-N1-C2	2.53	119.95	115.93
8	B	501	GDP	PA-O3A-PB	-2.52	124.19	132.83
5	C	501	GTP	PA-O3A-PB	-2.35	124.78	132.83
10	C	504	K2G	C5-C4-N	-2.34	120.83	122.84
5	A	501	GTP	N2-C2-N1	2.18	120.65	117.25
5	C	501	GTP	PB-O3B-PG	-2.16	125.43	132.83
9	B	504	MES	C7-N4-C5	2.10	116.60	111.23

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	PA-O3A-PB-O2B
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O2A
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O2B
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
10	C	504	K2G	C-C1-C3-N1
10	C	504	K2G	C2-C1-C3-N
11	F	401	ACP	C3'-C4'-C5'-O5'
9	B	504	MES	C8-C7-N4-C3
5	C	501	GTP	PB-O3B-PG-O1G
11	F	401	ACP	O4'-C4'-C5'-O5'
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
5	C	501	GTP	PB-O3B-PG-O3G
11	F	401	ACP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
11	F	401	ACP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA

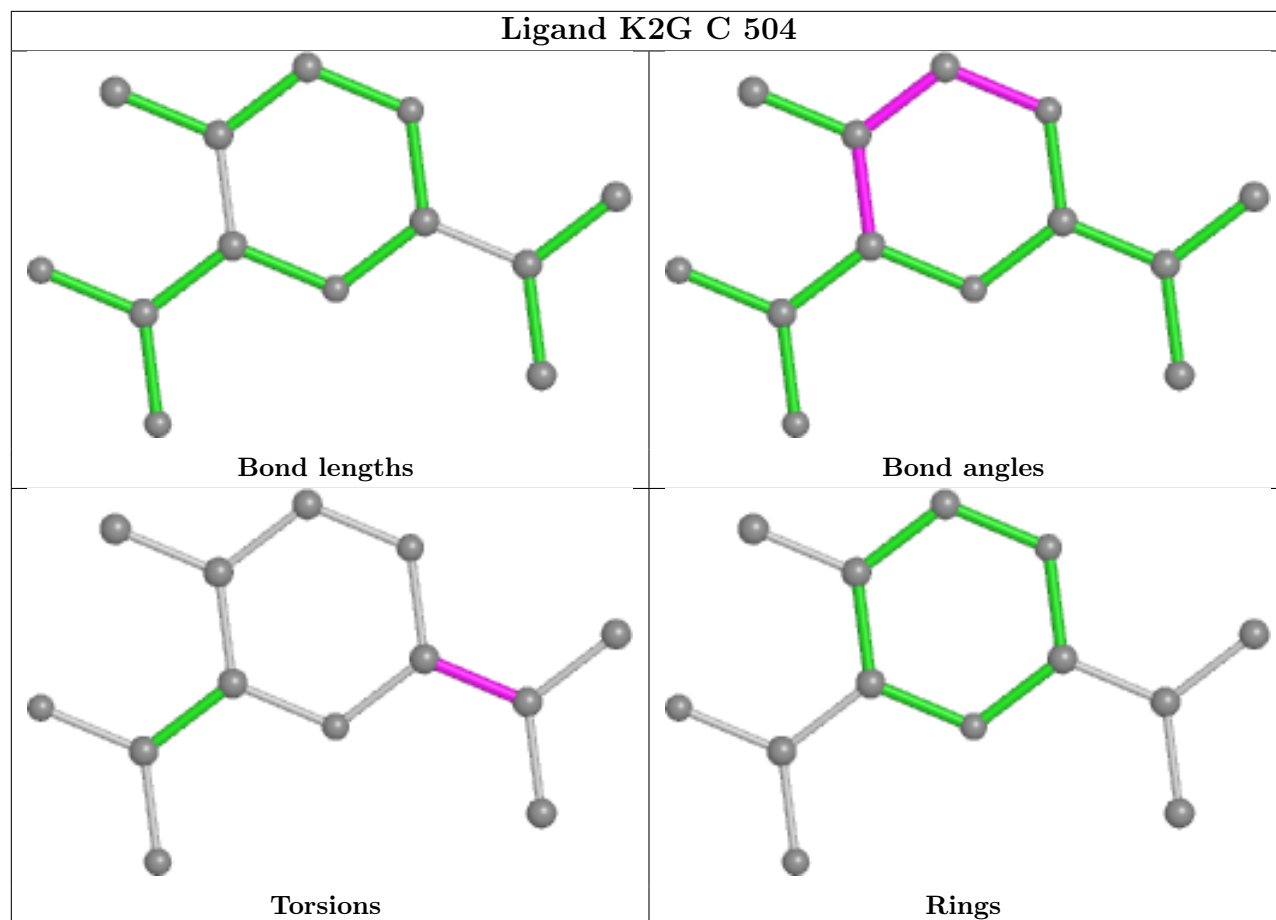
There are no ring outliers.

4 monomers are involved in 10 short contacts:

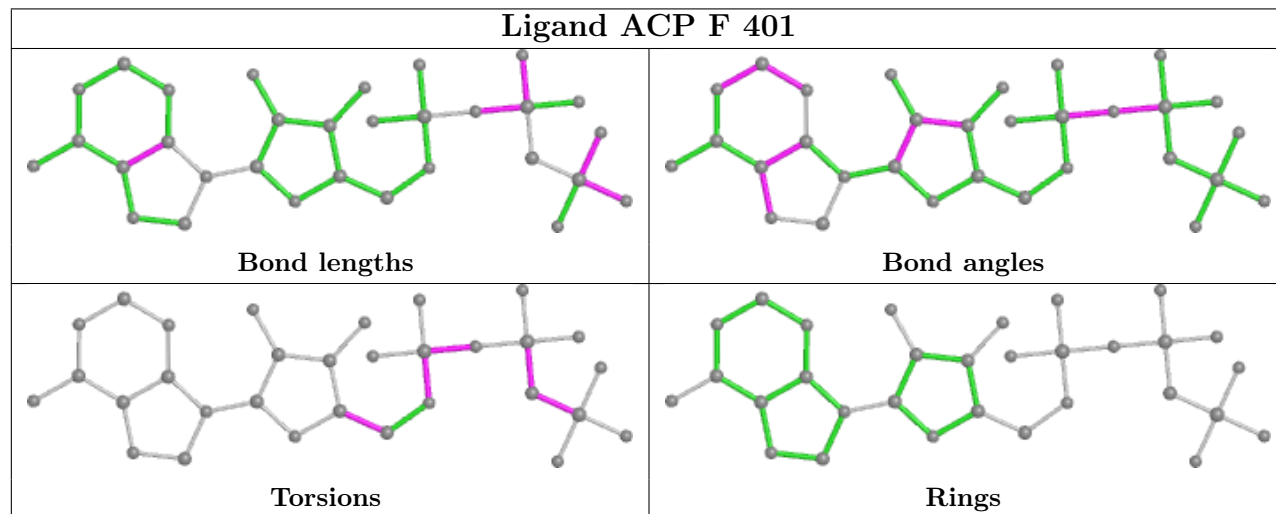
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	401	ACP	5	0
5	A	501	GTP	1	0
9	B	504	MES	1	0
8	D	501	GDP	3	0

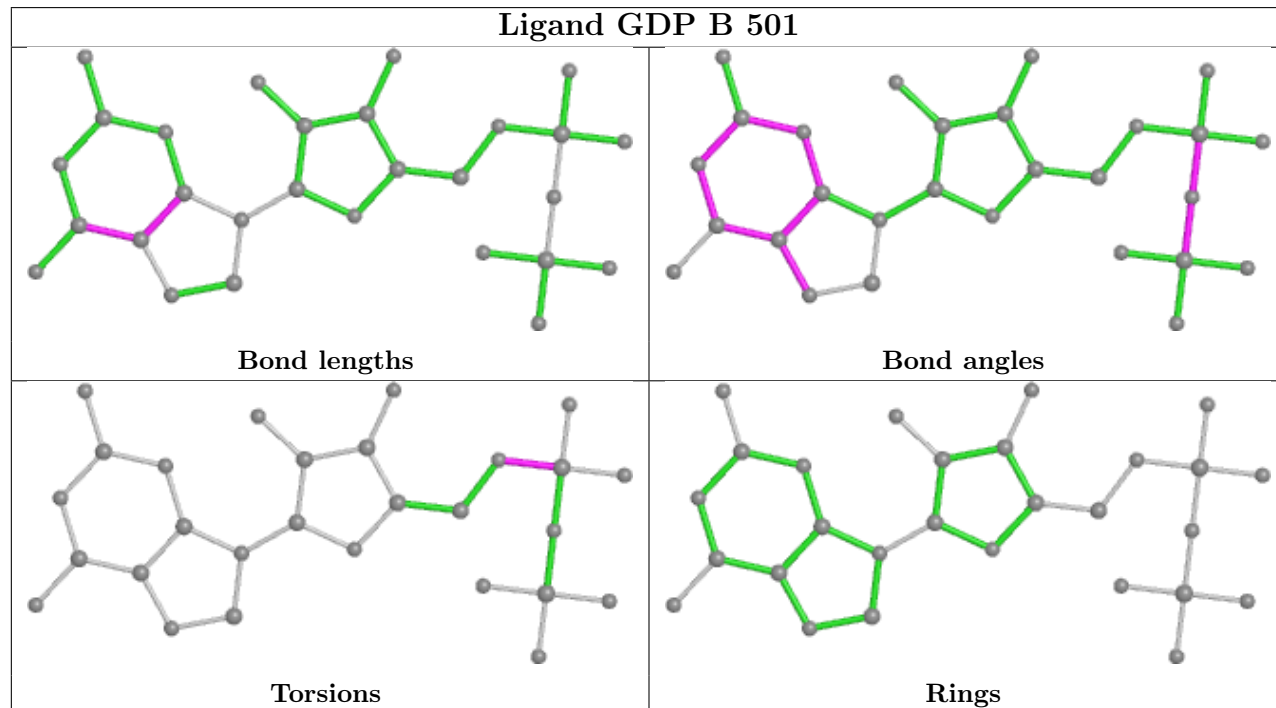
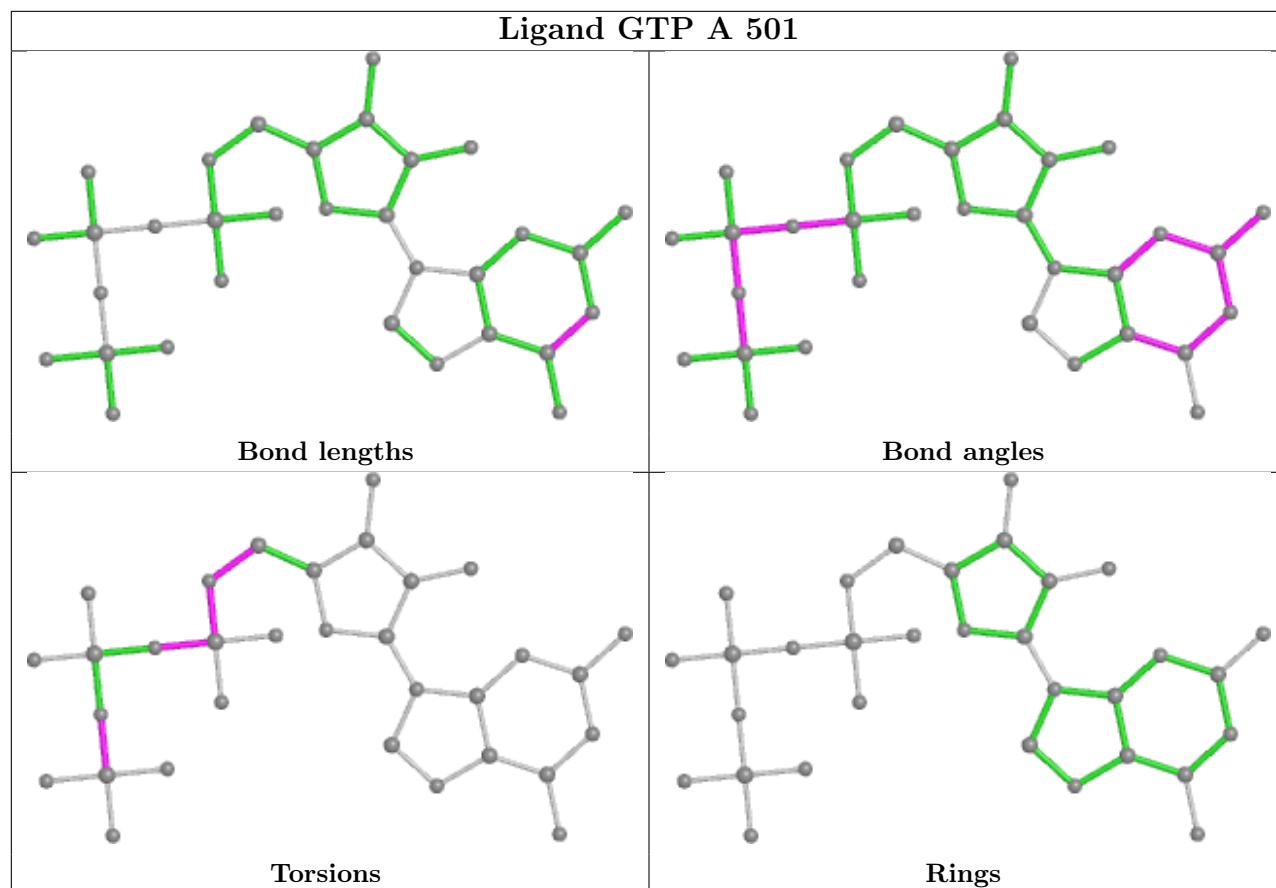
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

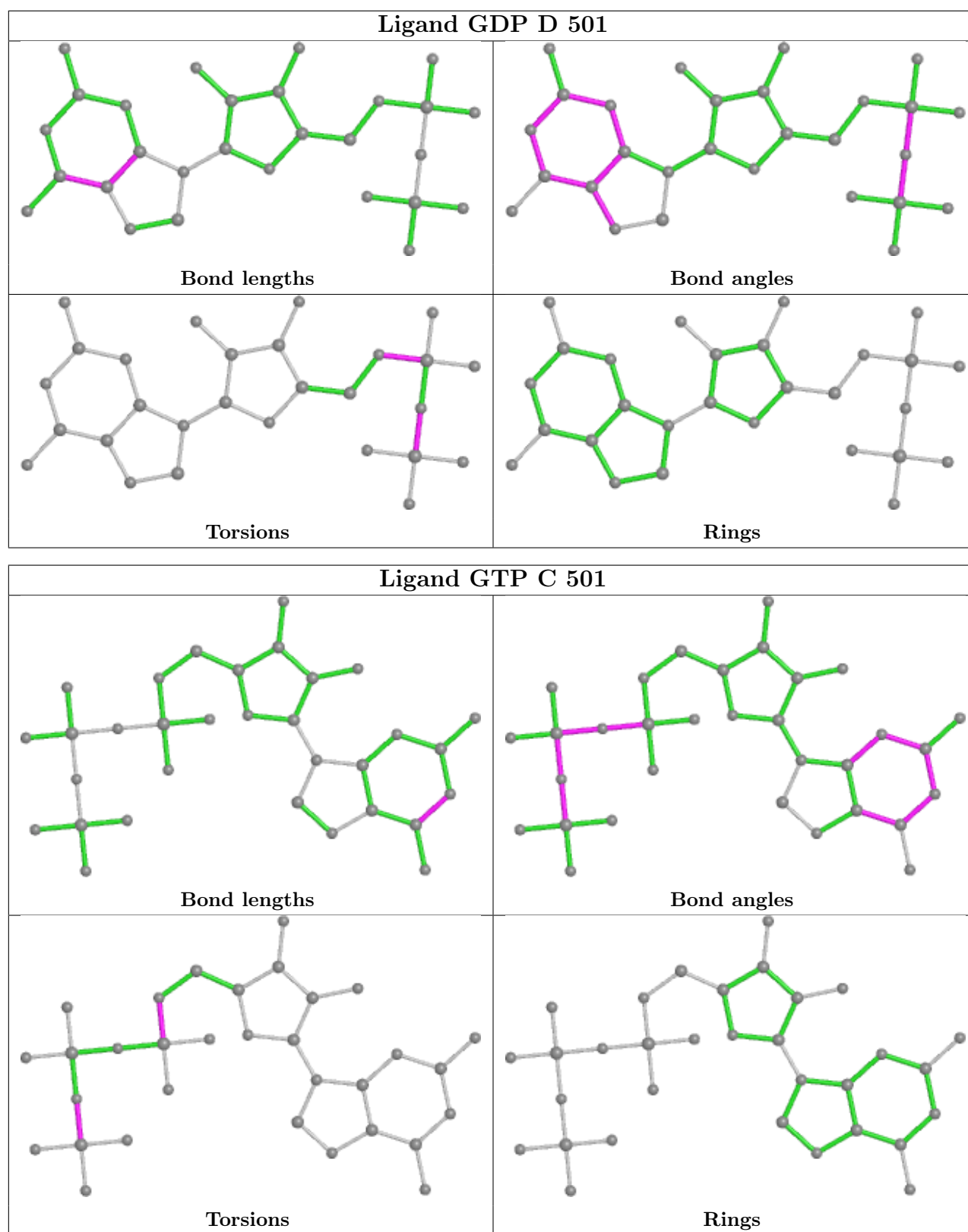
## Ligand K2G C 504



## Ligand ACP F 401







## 5.7 Other polymers [i](#)

There are no such residues in this entry.



## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	438/451 (97%)	0.35	13 (2%) 50 57	48, 68, 105, 170	0
1	C	440/451 (97%)	0.30	7 (1%) 72 77	40, 54, 79, 113	0
2	B	422/445 (94%)	0.44	11 (2%) 56 63	38, 64, 107, 146	3 (0%)
2	D	429/445 (96%)	0.40	23 (5%) 25 32	50, 73, 106, 148	4 (0%)
3	E	123/143 (86%)	0.69	9 (7%) 15 20	53, 78, 127, 150	0
4	F	352/384 (91%)	0.63	39 (11%) 5 7	61, 95, 162, 187	0
All	All	2204/2319 (95%)	0.43	102 (4%) 32 39	38, 69, 125, 187	7 (0%)

All (102) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	177	GLY	8.6
4	F	173	ILE	7.4
4	F	240	LEU	6.4
3	E	26	PRO	6.3
3	E	27	PRO	6.2
4	F	249	TYR	6.2
2	D	278	ARG	6.1
4	F	90	SER	6.1
4	F	142	ARG	6.1
3	E	6	MET	6.0
2	B	281	GLN	5.9
3	E	24	LEU	5.8
2	D	276	THR	5.6
3	E	22	VAL	4.6
4	F	232	ASN	4.3
1	A	349	THR	4.2
4	F	89	GLU	4.2
4	F	105	LEU	4.1
4	F	134	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
3	E	25	LYS	4.0
1	A	351	PHE	3.9
4	F	169	LEU	3.8
2	D	280	SER	3.7
2	B	1	MET	3.7
2	D	279	GLY	3.6
1	A	346	TRP	3.5
2	D	293	GLN	3.5
1	A	262	TYR	3.4
4	F	243	HIS	3.4
1	A	339	ARG	3.4
4	F	137	ARG	3.3
3	E	28	SER	3.3
2	B	337	ASN	3.3
2	D	1	MET	3.3
4	F	159	GLY	3.2
2	B	286	LEU	3.2
1	A	341	ILE	3.1
2	D	83	PHE	3.1
2	D	404	PHE	3.1
4	F	31	ARG	3.1
4	F	140	GLU	3.1
2	B	284	ARG	3.0
4	F	254	GLY	3.0
4	F	103	THR	3.0
2	D	277	SER	2.9
4	F	153	ALA	2.9
4	F	251	LYS	2.8
4	F	138	ARG	2.8
4	F	143	GLU	2.8
4	F	236	LYS	2.8
4	F	179	VAL	2.8
1	C	357	TYR	2.8
1	C	350	GLY	2.8
1	A	340	SER	2.7
2	B	276	THR	2.7
4	F	101	TYR	2.7
2	D	57	THR	2.7
2	B	246	GLY	2.6
4	F	130	VAL	2.6
1	A	335	ILE	2.6
4	F	100	ILE	2.6

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Mol	Chain	Res	Type	RSRZ
4	F	75	ALA	2.6
1	A	438	ASP	2.6
2	B	333	LEU	2.6
4	F	250	SER	2.5
4	F	99	VAL	2.5
1	C	335	ILE	2.5
2	D	401	ARG	2.5
2	D	285	ALA	2.5
4	F	248	GLU	2.5
4	F	132	LEU	2.5
4	F	233	PHE	2.4
1	C	286	LEU	2.4
1	C	308	ARG	2.4
2	D	325	MET	2.4
4	F	131	PHE	2.4
2	D	291	LEU	2.3
2	D	407	TRP	2.3
2	D	215	ARG	2.2
4	F	176	GLN	2.2
2	D	415	GLU	2.2
1	A	179	THR	2.2
2	D	304	ALA	2.2
2	B	325	MET	2.2
3	E	7	GLU	2.2
2	B	291	LEU	2.2
2	D	299	LYS	2.1
2	B	119	LEU	2.1
4	F	172	PHE	2.1
2	D	154	ILE	2.1
2	D	338	LYS	2.1
4	F	244	CYS	2.1
1	C	339	ARG	2.1
2	D	284	ARG	2.1
1	A	296	PHE	2.1
2	D	402	LYS	2.1
4	F	161	LEU	2.1
1	A	86	LEU	2.0
4	F	125	THR	2.0
1	A	118	VAL	2.0
1	C	285	GLN	2.0
3	E	124	GLN	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](#)

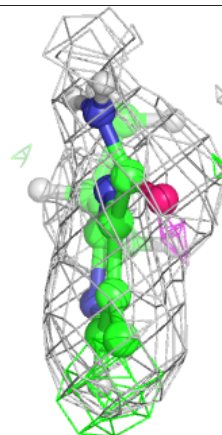
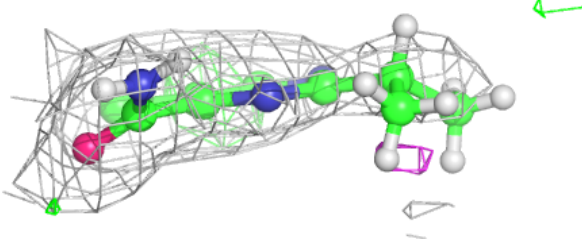
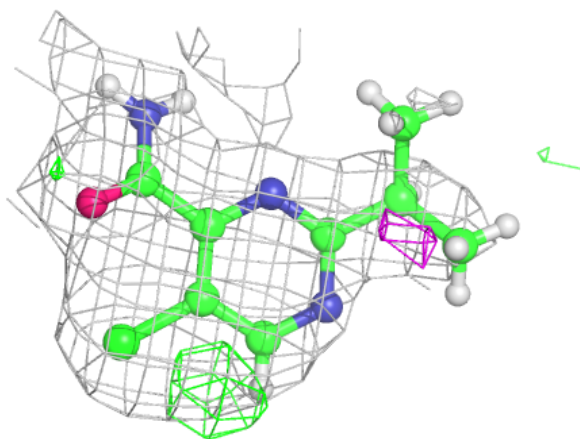
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
10	K2G	C	504	13/13	0.81	0.25	45,59,76,76	23
7	CA	B	503	1/1	0.85	0.15	101,101,101,101	0
11	ACP	F	401	31/31	0.85	0.14	93,107,117,118	0
7	CA	E	201	1/1	0.86	0.13	99,99,99,99	0
9	MES	B	504	12/12	0.88	0.16	78,84,94,104	0
8	GDP	D	501	28/28	0.94	0.17	66,70,79,88	0
6	MG	D	502	1/1	0.95	0.14	71,71,71,71	0
6	MG	F	402	1/1	0.95	0.11	98,98,98,98	0
7	CA	C	503	1/1	0.96	0.14	66,66,66,66	0
7	CA	A	503	1/1	0.97	0.14	89,89,89,89	0
6	MG	B	502	1/1	0.97	0.11	36,36,36,36	0
6	MG	A	502	1/1	0.98	0.12	47,47,47,47	0
5	GTP	A	501	32/32	0.98	0.15	42,50,54,55	0
5	GTP	C	501	32/32	0.98	0.17	41,44,51,51	0
6	MG	C	502	1/1	0.99	0.12	44,44,44,44	0
8	GDP	B	501	28/28	0.99	0.15	38,46,52,55	0

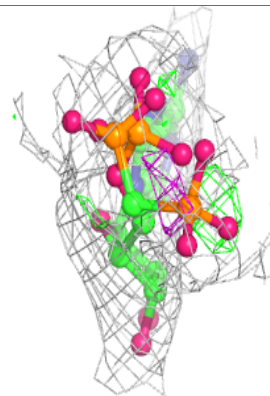
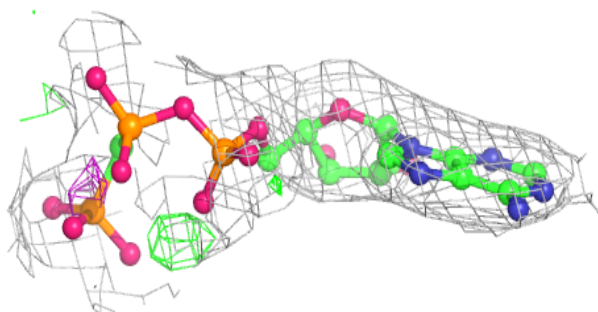
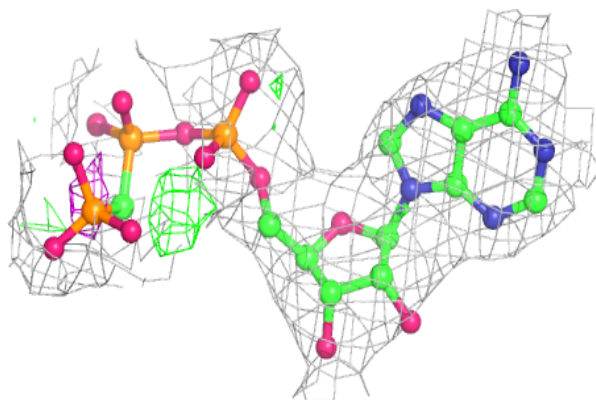
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around K2G C 504:**

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

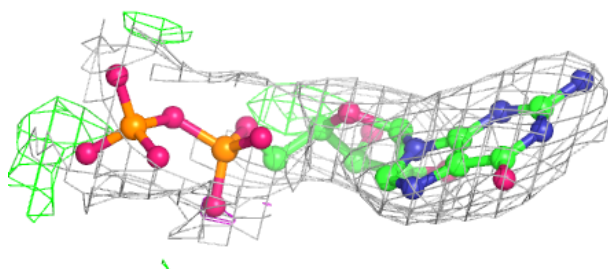
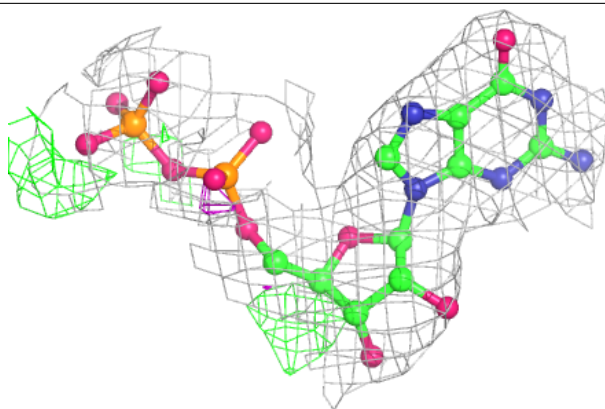
**Electron density around ACP F 401:**

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

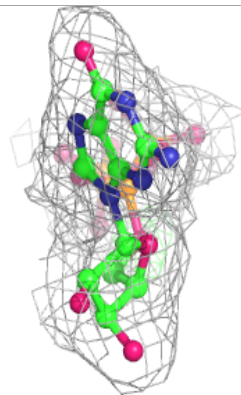
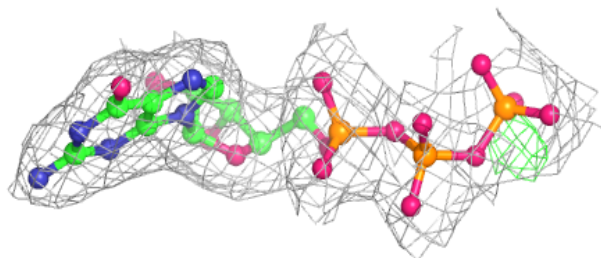
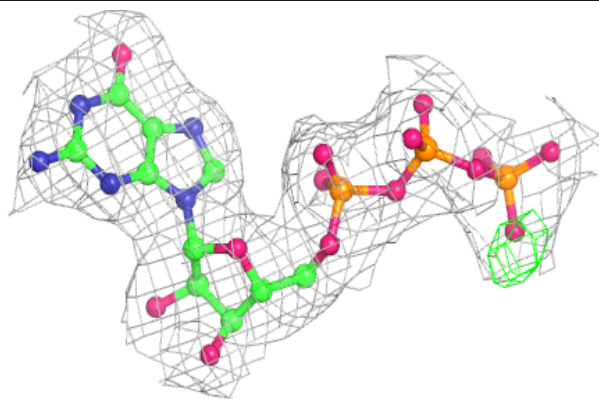


**Electron density around GDP D 501:**

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

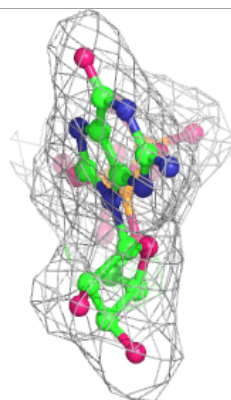
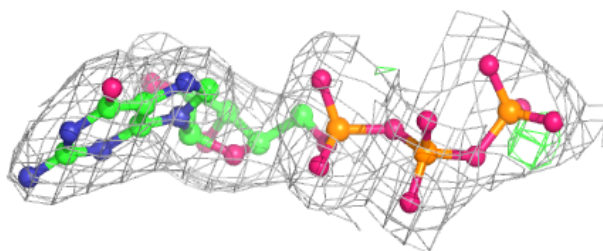
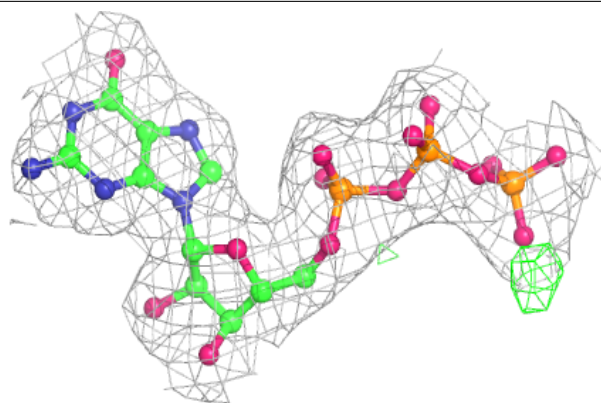
**Electron density around GTP A 501:**

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

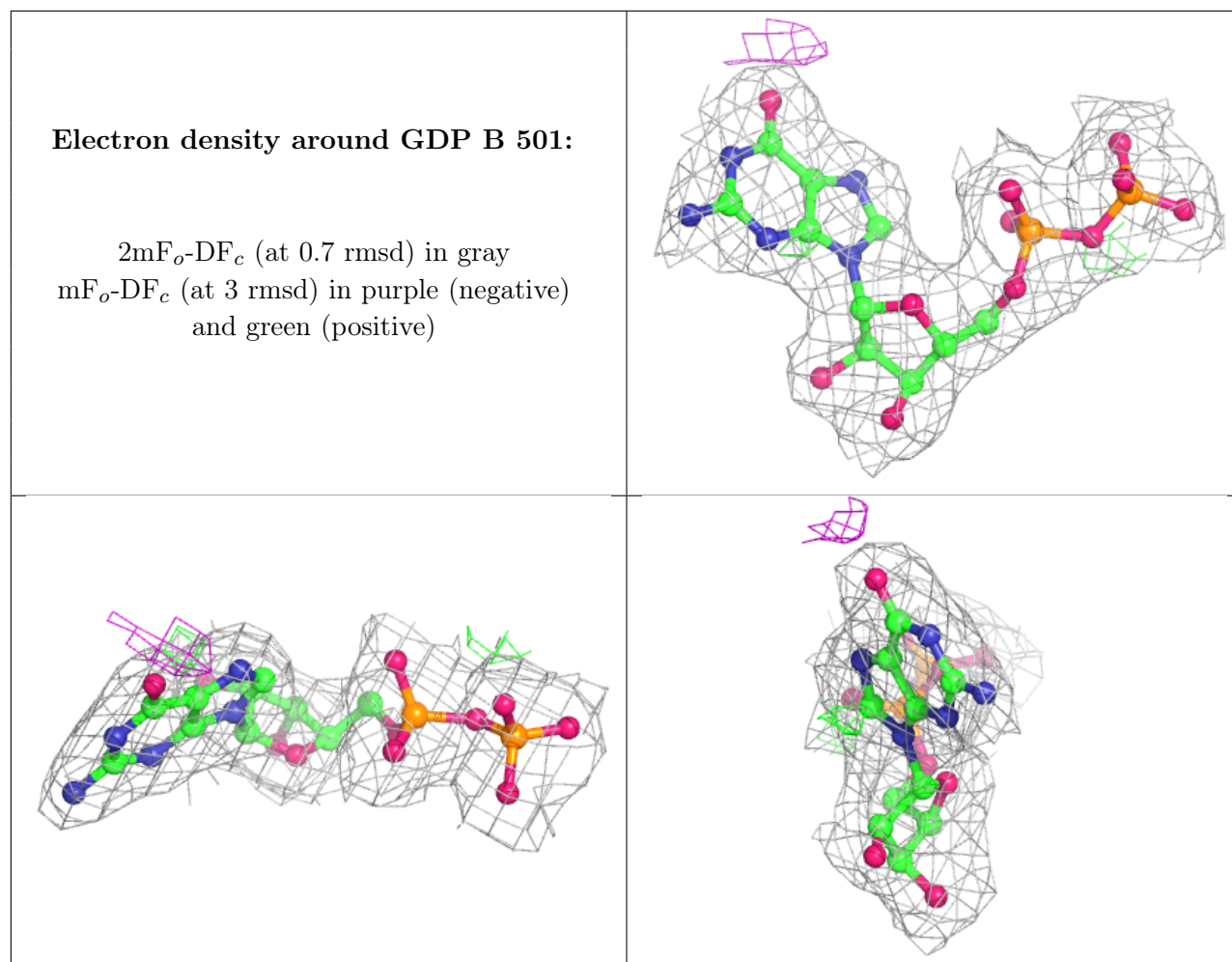


**Electron density around GTP C 501:**

$2mF_o-DF_c$  (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.