



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2021 – 03:39 PM EDT

PDB ID : 5S4T
Title : Tubulin-Z328695024-complex
Authors : Muehlethaler, T.; Gioia, D.; Protá, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.
Deposited on : 2020-11-08
Resolution : 2.27 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.20
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

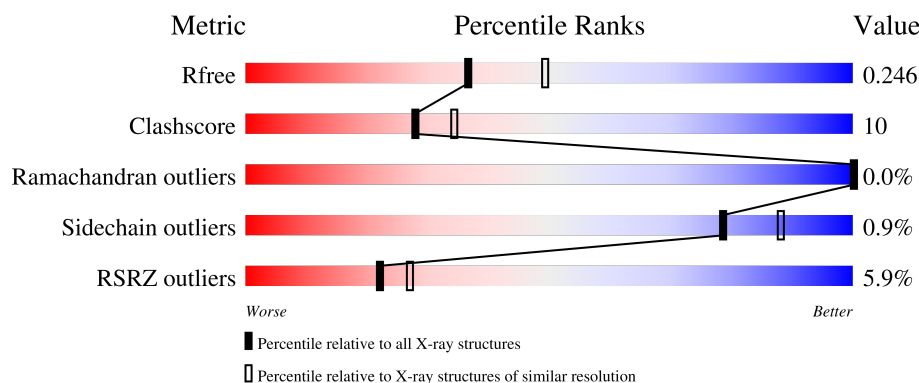
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.27 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	6980 (2.30-2.26)
Clashscore	141614	7711 (2.30-2.26)
Ramachandran outliers	138981	7597 (2.30-2.26)
Sidechain outliers	138945	7598 (2.30-2.26)
RSRZ outliers	127900	6849 (2.30-2.26)

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

Mol	Chain	Length	Quality of chain
1	A	451	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>19%</div> <div>..</div> </div> </div>
1	C	451	<div> <div>%</div> <div> <div></div> <div>79%</div> <div>18%</div> <div>.</div> </div> </div>
2	B	445	<div> <div>4%</div> <div> <div></div> <div>70%</div> <div>25%</div> <div>.</div> </div> </div>
2	D	445	<div> <div>4%</div> <div> <div></div> <div>71%</div> <div>24%</div> <div>.</div> </div> </div>
3	E	143	<div> <div>9%</div> <div> <div></div> <div>69%</div> <div>17%</div> <div>14%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
4	F	384	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
9	MES	B	504	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18029 atoms, of which 15 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	425	Total	C	N	O	S	1	2	0
			3365	2112	578	647	28			
2	D	426	Total	C	N	O	S	5	0	0
			3343	2098	570	648	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	348	Total	C	N	O	S	0	0	0
			2859	1833	491	521	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: $C_{10}H_{15}N_5O_{11}P_2$).



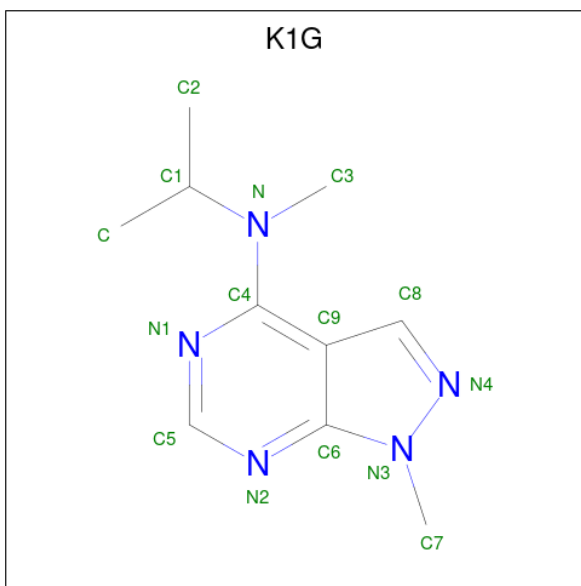
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

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



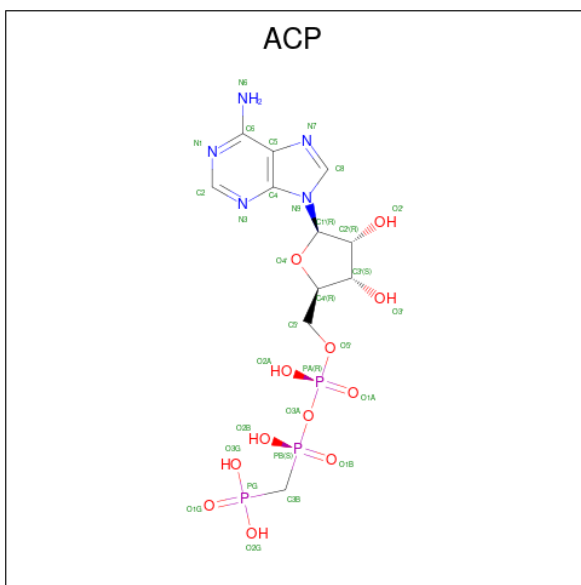
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is N,1-dimethyl-N-(propan-2-yl)-1H-pyrazolo[3,4-d]pyrimidin-4-amine (three-letter code: K1G) (formula: C₁₀H₁₅N₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	H	N	0	0
			30	10	15	5		

- Molecule 11 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	F	1	Total 31	C 11	N 5	O 12	P 3	0	0

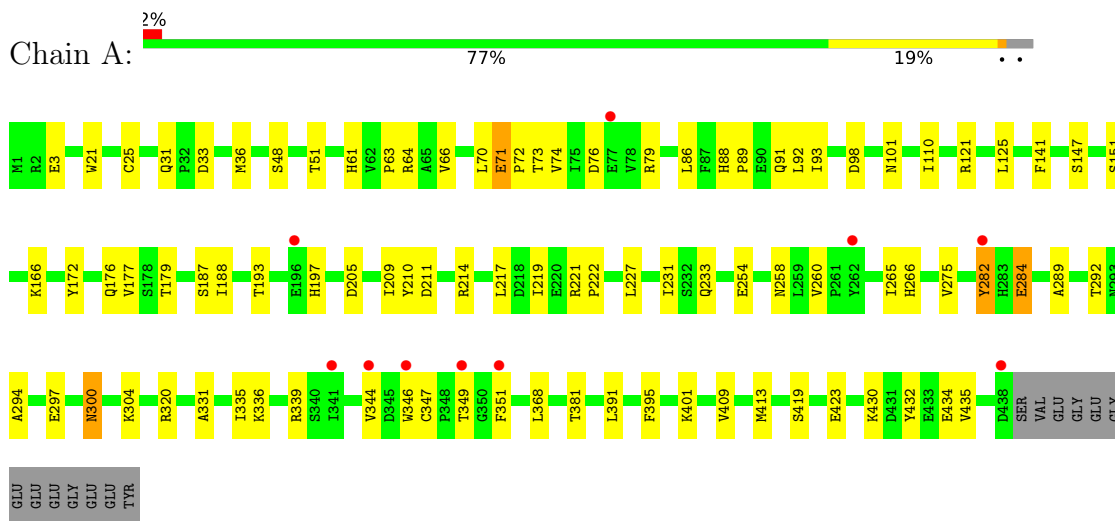
- Molecule 12 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
12	A	59	Total O 59 59	0	0
12	B	82	Total O 82 82	0	0
12	C	181	Total O 181 181	0	0
12	D	33	Total O 33 33	0	0
12	E	8	Total O 8 8	0	0
12	F	16	Total O 16 16	0	0

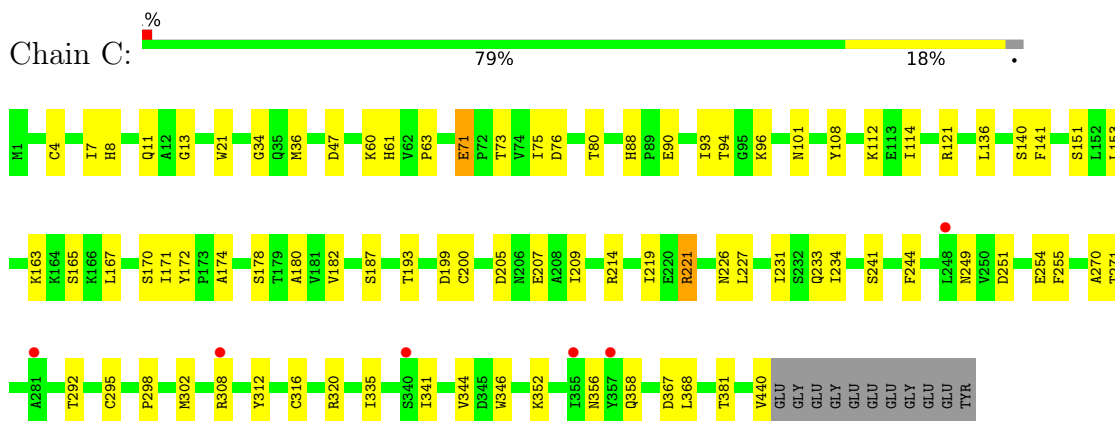
3 Residue-property plots [i](#)

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.

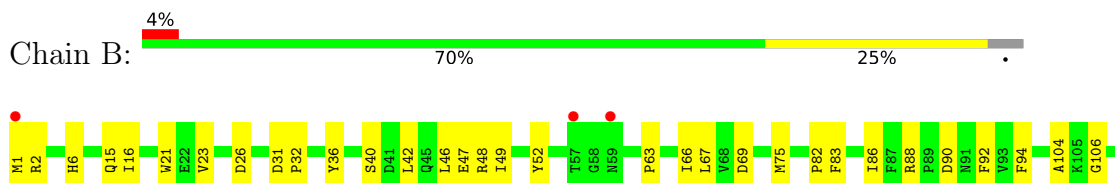
- Molecule 1: Tubulin alpha-1B chain

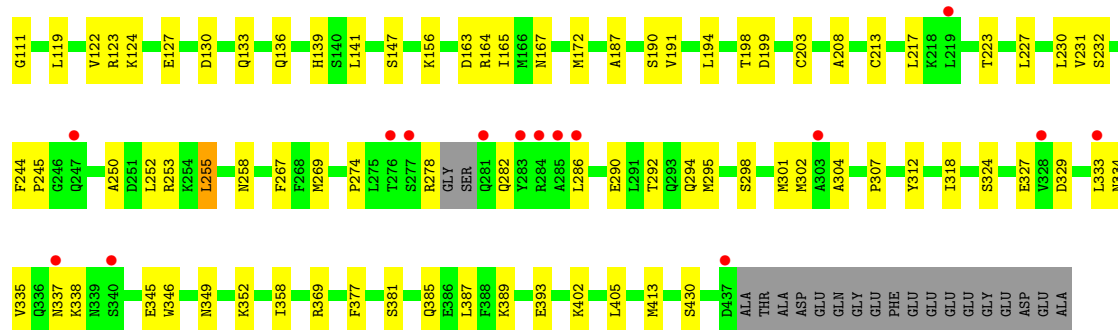


- Molecule 1: Tubulin alpha-1B chain

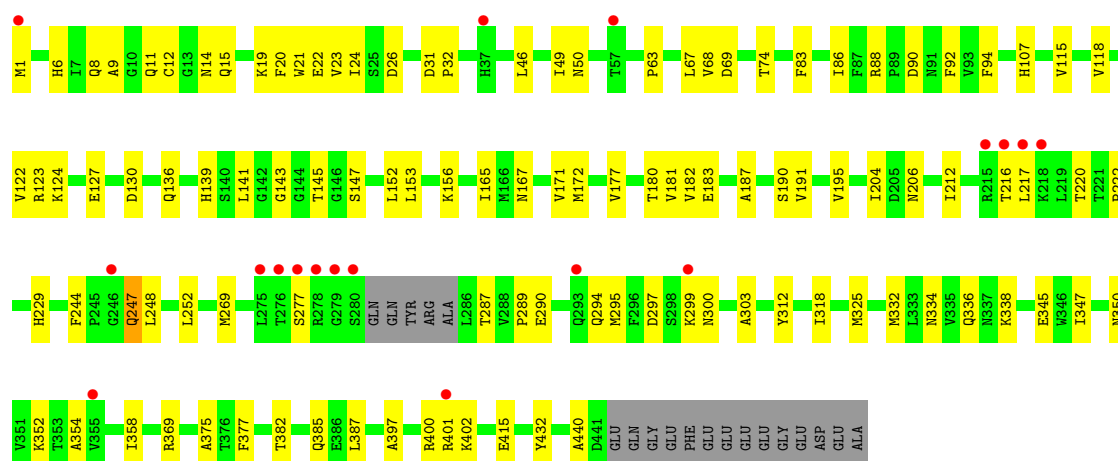


- Molecule 2: Tubulin beta-2B chain

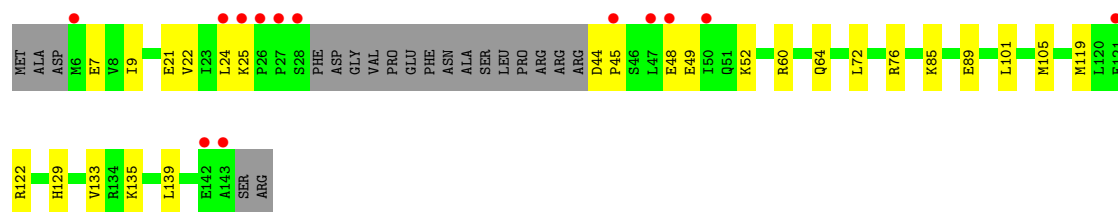




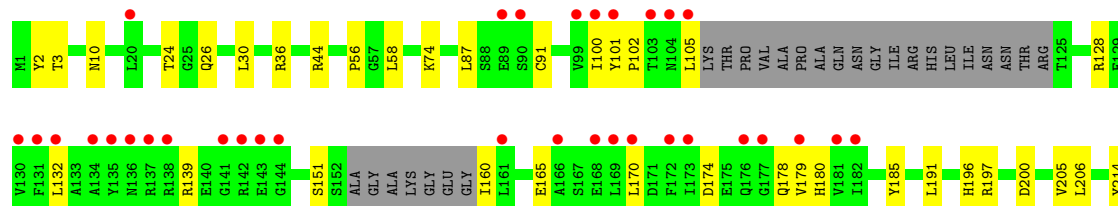
• Molecule 2: Tubulin beta-2B chain

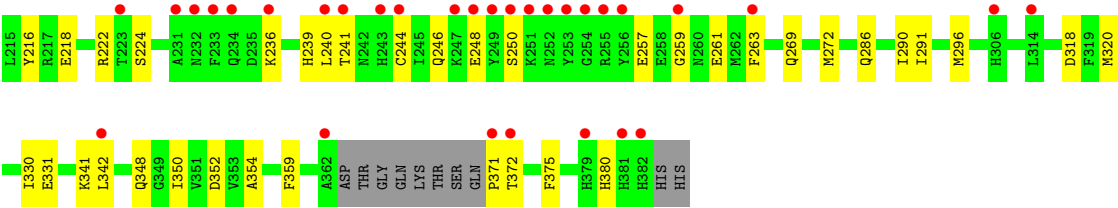


• Molecule 3: Stathmin-4



• 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, α , β , γ	104.77Å 158.42Å 179.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.53 – 2.27 87.39 – 2.27	Depositor EDS
% Data completeness (in resolution range)	99.8 (62.53-2.27) 99.8 (87.39-2.27)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.10 (at 2.27Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.206 , 0.246 0.206 , 0.246	Depositor DCC
R_{free} test set	6770 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å ²)	59.7	Xtriage
Anisotropy	0.252	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 49.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18029	wwPDB-VP
Average B, all atoms (Å ²)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.57% 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: CA, K1G, GTP, MG, MES, GDP, ACP

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	0/3439	0.42	0/4655
2	D	0.25	0/3416	0.41	0/4626
3	E	0.24	0/1022	0.34	0/1356
4	F	0.24	0/2926	0.39	0/3954
All	All	0.25	0/17826	0.41	0/24125

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	64	0
1	C	3443	0	3352	55	0
2	B	3365	0	3239	87	0
2	D	3343	0	3222	75	0
3	E	1014	0	1029	16	0
4	F	2859	0	2823	56	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	1	0
8	D	28	0	12	4	0
9	B	12	0	12	6	0
10	B	15	15	0	1	0
11	F	31	0	14	4	0
12	A	59	0	0	4	0
12	B	82	0	0	4	0
12	C	181	0	0	2	0
12	D	33	0	0	3	0
12	E	8	0	0	1	0
12	F	16	0	0	0	0
All	All	18014	15	17073	342	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 10.

All (342) 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	1.43	0.97
1:A:300:ASN:OD1	12:A:601:HOH:O	1.90	0.88
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.60	0.83
1:C:209:ILE:HD11	1:C:302:MET:HE3	1.59	0.82
1:A:71:GLU:OE2	1:A:73:THR:OG1	1.97	0.82
1:A:176:GLN:HG3	4:F:56:PRO:HB3	1.62	0.81
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.60	0.81
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.66	0.78
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.64	0.78
2:D:217:LEU:HA	2:D:277:SER:HB3	1.67	0.77
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.67	0.76
2:B:2:ARG:HB2	2:B:133:GLN:HG3	1.65	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.52	0.74
2:B:253[A]:ARG:NH1	9:B:504:MES:O3S	2.22	0.73
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.71	0.72
1:C:76:ASP:O	1:C:80:THR:HG22	1.90	0.72
2:D:397:ALA:O	2:D:401:ARG:NH1	2.23	0.71
2:D:136:GLN:HA	2:D:167:ASN:O	1.91	0.70
1:C:234:ILE:HG12	1:C:302:MET:HE2	1.73	0.70
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.72	0.70
3:E:85:LYS:NZ	12:E:301:HOH:O	2.25	0.70
2:B:2:ARG:HB2	2:B:133:GLN:CG	2.22	0.69
4:F:371:PRO:HA	4:F:372:THR:HB	1.74	0.69
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.73	0.69
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.32	0.69
2:B:69:ASP:O	2:B:94:PHE:HA	1.93	0.69
2:B:88:ARG:HH11	2:B:90:ASP:HB2	1.59	0.68
2:B:163:ASP:OD1	12:B:601:HOH:O	2.11	0.68
2:B:337:ASN:OD1	4:F:36:ARG:HD3	1.92	0.68
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.78	0.66
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.30	0.66
2:B:250:ALA:HB1	2:B:255:LEU:HD13	1.78	0.66
2:B:83:PHE:O	2:B:86:ILE:HG22	1.96	0.66
2:D:432:TYR:OH	12:D:601:HOH:O	2.13	0.66
2:D:83:PHE:O	2:D:86:ILE:HG22	1.97	0.65
4:F:241:THR:OG1	11:F:401:ACP:O3'	1.98	0.65
2:B:47:GLU:HG2	2:B:245:PRO:HB3	1.77	0.65
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.32	0.65
1:C:320:ARG:HA	1:C:356:ASN:O	1.97	0.64
1:C:270:ALA:O	1:C:302:MET:HG2	1.98	0.63
2:D:152:LEU:O	2:D:156:LYS:HG2	2.00	0.62
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.81	0.61
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.29	0.61
4:F:371:PRO:HA	4:F:372:THR:O	2.00	0.61
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.83	0.60
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.01	0.60
2:B:333:LEU:O	2:B:337:ASN:ND2	2.34	0.60
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.36	0.60
1:A:214:ARG:HG2	1:A:219:ILE:O	2.01	0.60
1:C:165:SER:HA	1:C:199:ASP:OD2	2.02	0.59
4:F:139:ARG:NH2	4:F:165:GLU:OE1	2.35	0.59
1:A:297:GLU:HB2	1:A:300:ASN:ND2	2.17	0.59
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:HIS:CD2	1:A:91:GLN:HG3	2.38	0.59
2:B:255:LEU:HG	10:B:505:K1G:C8	2.32	0.59
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.17	0.59
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.85	0.59
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.83	0.58
2:D:22:GLU:HG2	2:D:83:PHE:CD1	2.38	0.58
1:A:297:GLU:HB2	1:A:300:ASN:HD21	1.69	0.58
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.03	0.58
1:A:166:LYS:HE2	1:A:197:HIS:O	2.03	0.58
4:F:320:MET:HG3	4:F:330:ILE:HD11	1.86	0.58
2:B:345:GLU:OE1	2:B:345:GLU:N	2.30	0.57
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.37	0.57
4:F:371:PRO:CA	4:F:372:THR:HB	2.35	0.57
3:E:60:ARG:O	3:E:64:GLN:HG3	2.04	0.57
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.40	0.57
2:D:171:VAL:HA	2:D:204:ILE:O	2.05	0.57
2:D:69:ASP:O	2:D:94:PHE:HA	2.05	0.56
2:B:298:SER:HA	2:B:301:MET:HG3	1.86	0.56
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.35	0.56
2:D:118:VAL:O	2:D:122:VAL:HG23	2.04	0.56
4:F:197:ARG:HB2	4:F:224:SER:O	2.06	0.56
2:D:26:ASP:OD2	2:D:369:ARG:HD2	2.06	0.56
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.04	0.56
3:E:48:GLU:HG2	3:E:52:LYS:HE3	1.87	0.56
3:E:129:HIS:O	3:E:133:VAL:HG23	2.06	0.55
3:E:135:LYS:O	3:E:139:LEU:HG	2.05	0.55
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.42	0.55
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.88	0.55
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.87	0.55
2:D:141:LEU:HD12	2:D:172:MET:SD	2.46	0.55
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.42	0.55
3:E:85:LYS:O	3:E:89:GLU:HG3	2.06	0.55
2:D:332:MET:O	2:D:336:GLN:HG3	2.06	0.55
2:D:382:THR:O	2:D:385:GLN:HG2	2.06	0.55
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.42	0.54
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.89	0.54
1:A:289:ALA:HA	1:A:331:ALA:CB	2.38	0.54
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.90	0.54
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.89	0.54
4:F:246:GLN:O	4:F:250:SER:HB3	2.07	0.54
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.90	0.53
2:D:1:MET:HG3	2:D:50:ASN:HB2	1.90	0.53
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.44	0.53
4:F:320:MET:CG	4:F:330:ILE:HD11	2.38	0.53
4:F:371:PRO:HA	4:F:372:THR:C	2.29	0.53
1:C:271:THR:HG21	1:C:295:CYS:O	2.09	0.53
2:B:318:ILE:N	2:B:318:ILE:HD12	2.23	0.53
4:F:3:THR:HB	4:F:30:LEU:HD11	1.90	0.53
1:A:289:ALA:HA	1:A:331:ALA:HB1	1.90	0.53
2:D:46:LEU:HA	2:D:49:ILE:HB	1.90	0.53
2:D:187:ALA:O	2:D:191:VAL:HG23	2.09	0.53
4:F:151:SER:HB3	4:F:180:HIS:CD2	2.44	0.53
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.24	0.53
1:C:214:ARG:HG2	1:C:219:ILE:O	2.09	0.53
4:F:151:SER:HB3	4:F:180:HIS:CG	2.44	0.53
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.28	0.53
1:C:108:TYR:O	1:C:112:LYS:HG2	2.09	0.53
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.24	0.52
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.44	0.52
3:E:72:LEU:O	3:E:76:ARG:HG2	2.08	0.52
1:C:178:SER:OG	2:D:352:LYS:NZ	2.36	0.52
3:E:44:ASP:HB3	3:E:45:PRO:HD2	1.92	0.52
2:D:88:ARG:NH1	2:D:90:ASP:HB2	2.24	0.52
2:D:147:SER:HB2	2:D:190:SER:OG	2.10	0.52
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.92	0.52
2:D:1:MET:CE	2:D:50:ASN:HB2	2.40	0.52
2:D:9:ALA:HA	2:D:68:VAL:O	2.09	0.52
4:F:100:ILE:HD12	4:F:128:ARG:HA	1.92	0.52
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.32	0.51
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.92	0.51
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.93	0.51
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.37	0.51
2:B:124:LYS:HD3	2:B:124:LYS:C	2.31	0.51
2:B:295:MET:CG	2:B:377:PHE:HB2	2.41	0.51
2:B:295:MET:HG3	2:B:377:PHE:HB2	1.92	0.51
2:D:67:LEU:N	2:D:67:LEU:HD12	2.25	0.51
1:A:419:SER:O	1:A:423:GLU:HG3	2.11	0.51
2:B:250:ALA:HB1	2:B:255:LEU:CD1	2.40	0.51
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.41	0.51
1:A:31:GLN:HB2	1:A:33:ASP:OD1	2.10	0.51
2:B:244:PHE:CD1	2:B:358:ILE:HD12	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:367:ASP:OD1	12:C:601:HOH:O	2.19	0.51
1:A:409:VAL:HA	1:A:413:MET:O	2.11	0.51
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.76	0.51
2:B:136:GLN:HA	2:B:167:ASN:O	2.10	0.51
2:D:1:MET:HE2	2:D:50:ASN:HB2	1.93	0.51
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.45	0.51
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.93	0.51
1:C:71:GLU:OE1	1:C:73:THR:HG23	2.10	0.50
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.75	0.50
1:C:96:LYS:NZ	2:D:130:ASP:OD1	2.43	0.50
2:D:177:VAL:HG21	2:D:206:ASN:HB3	1.94	0.50
2:D:318:ILE:N	2:D:318:ILE:HD12	2.27	0.50
3:E:101:LEU:O	3:E:105:MET:HG2	2.11	0.50
2:B:253[A]:ARG:NH1	9:B:504:MES:O1S	2.41	0.50
2:D:145:THR:HB	8:D:501:GDP:O2B	2.11	0.50
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.47	0.50
2:B:278:ARG:HG2	2:B:282:GLN:NE2	2.27	0.49
4:F:160:ILE:HD12	4:F:160:ILE:N	2.27	0.49
4:F:318:ASP:OD2	11:F:401:ACP:O2G	2.30	0.49
1:C:209:ILE:HD11	1:C:302:MET:CE	2.35	0.49
2:B:253[A]:ARG:NH1	9:B:504:MES:S	2.78	0.49
2:D:115:VAL:HG23	2:D:153:LEU:HD23	1.94	0.49
1:C:8:HIS:HB3	1:C:13:GLY:O	2.13	0.49
2:B:290:GLU:O	2:B:294:GLN:HG3	2.13	0.49
2:D:11:GLN:HA	2:D:74:THR:HG21	1.94	0.49
2:D:402:LYS:HE2	2:D:415:GLU:OE1	2.13	0.49
4:F:178:GLN:N	4:F:178:GLN:OE1	2.46	0.49
3:E:7:GLU:O	3:E:22:VAL:HA	2.12	0.49
1:A:71:GLU:HG2	1:A:72:PRO:N	2.28	0.48
2:B:42:LEU:H	2:B:42:LEU:HD12	1.78	0.48
4:F:191:LEU:HD12	4:F:196:HIS:CE1	2.48	0.48
2:B:82:PRO:O	12:B:602:HOH:O	2.20	0.48
2:B:164:ARG:HD2	12:B:647:HOH:O	2.12	0.48
1:A:101:ASN:HD22	2:B:258:ASN:HD21	1.60	0.48
2:B:334:ASN:OD1	2:B:338:LYS:HD3	2.14	0.48
2:B:1:MET:HB2	2:B:130:ASP:OD2	2.14	0.48
12:B:655:HOH:O	1:C:163:LYS:HD2	2.14	0.48
2:D:67:LEU:HD22	2:D:92:PHE:CE2	2.48	0.48
2:B:141:LEU:HD12	2:B:172:MET:SD	2.54	0.48
1:C:234:ILE:HG12	1:C:302:MET:CE	2.42	0.48
4:F:371:PRO:HA	4:F:372:THR:CB	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.44	0.48
4:F:350:ILE:O	4:F:354:ALA:HB3	2.14	0.47
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.49	0.47
3:E:9:ILE:HG13	3:E:21:GLU:HB3	1.95	0.47
2:B:26:ASP:OD1	2:B:369:ARG:NH2	2.48	0.47
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.44	0.47
2:B:389:LYS:O	2:B:393:GLU:HG3	2.13	0.47
1:A:74:VAL:HB	12:A:610:HOH:O	2.15	0.47
1:A:275:VAL:HG13	1:A:368:LEU:CD2	2.45	0.47
1:A:294:ALA:O	1:A:300:ASN:ND2	2.47	0.47
2:B:40:SER:OG	2:B:42:LEU:HD13	2.14	0.47
2:B:147:SER:HG	2:B:190:SER:HG	1.61	0.47
4:F:100:ILE:CD1	4:F:128:ARG:HA	2.45	0.47
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.50	0.47
2:B:269:MET:HE1	2:B:307:PRO:HG3	1.96	0.47
2:D:212:ILE:O	2:D:216:THR:HB	2.14	0.47
4:F:286:GLN:O	4:F:290:ILE:HG13	2.14	0.47
2:B:46:LEU:HA	2:B:49:ILE:HB	1.97	0.47
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.96	0.47
2:B:47:GLU:HG2	2:B:245:PRO:CB	2.45	0.46
2:B:106:GLY:O	2:B:111:GLY:HA3	2.14	0.46
2:B:194:LEU:HD22	2:B:198:THR:HG21	1.98	0.46
4:F:132:LEU:HD21	4:F:170:LEU:HD11	1.96	0.46
4:F:244:CYS:O	4:F:248:GLU:HB2	2.15	0.46
4:F:296:MET:SD	4:F:380:HIS:HB2	2.54	0.46
1:A:176:GLN:CG	4:F:56:PRO:HB3	2.39	0.46
1:A:284:GLU:CD	1:A:284:GLU:H	2.17	0.46
2:B:15:GLN:NE2	8:B:501:GDP:O6	2.48	0.46
1:C:226:ASN:ND2	1:C:367:ASP:OD2	2.48	0.46
1:C:292:THR:HG22	1:C:335:ILE:HD12	1.97	0.46
8:D:501:GDP:O1A	12:D:602:HOH:O	2.20	0.46
3:E:45:PRO:HA	3:E:49:GLU:OE1	2.15	0.46
1:A:188:ILE:HD12	1:A:395:PHE:HB2	1.97	0.46
2:D:11:GLN:O	2:D:15:GLN:HG2	2.15	0.46
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.80	0.46
1:C:241:SER:HA	1:C:249:ASN:OD1	2.16	0.46
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.96	0.46
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.51	0.46
4:F:206:LEU:HD21	4:F:354:ALA:HB2	1.97	0.46
1:A:217:LEU:HD21	1:A:368:LEU:CD2	2.45	0.46
4:F:269:GLN:HA	4:F:272:MET:HE2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:123:ARG:O	2:B:127:GLU:HG3	2.16	0.46
1:C:341:ILE:HD12	1:C:341:ILE:N	2.30	0.46
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.34	0.46
2:D:181:VAL:HG13	2:D:182:VAL:HG13	1.98	0.45
1:A:346:TRP:HZ2	1:A:435:VAL:HG13	1.81	0.45
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.99	0.45
2:D:124:LYS:C	2:D:124:LYS:HD3	2.36	0.45
1:C:34:GLY:HA3	1:C:60:LYS:HG3	1.98	0.45
4:F:102:PRO:HG2	4:F:105:LEU:CD1	2.30	0.45
11:F:401:ACP:O3G	11:F:401:ACP:O1B	2.33	0.45
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.56	0.45
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.98	0.45
2:B:213:CYS:HA	2:B:217:LEU:HB2	1.98	0.45
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.51	0.45
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.99	0.45
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.51	0.45
1:A:430:LYS:O	1:A:434:GLU:HG3	2.17	0.45
1:A:227:LEU:O	1:A:231:ILE:HG13	2.17	0.45
1:C:47:ASP:OD2	12:C:602:HOH:O	2.21	0.45
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.52	0.45
2:D:295:MET:SD	2:D:375:ALA:HB1	2.57	0.45
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.52	0.44
2:D:294:GLN:HG2	2:D:300:ASN:HD21	1.81	0.44
4:F:10:ASN:CB	4:F:44:ARG:HH22	2.30	0.44
1:A:292:THR:HG22	1:A:335:ILE:CD1	2.48	0.44
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.47	0.44
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.52	0.44
1:A:66:VAL:HG23	1:A:125:LEU:HD12	1.99	0.44
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.39	0.44
1:C:101:ASN:ND2	1:C:180:ALA:HB2	2.32	0.44
2:B:67:LEU:N	2:B:67:LEU:HD12	2.33	0.44
2:D:172:MET:HG3	2:D:387:LEU:HD11	2.00	0.44
4:F:218:GLU:HB3	4:F:342:LEU:HD13	1.99	0.44
4:F:87:LEU:O	4:F:91:CYS:HB2	2.18	0.44
2:B:104:ALA:HB2	2:B:413:MET:SD	2.58	0.44
2:B:349:ASN:O	2:B:352:LYS:HE2	2.17	0.44
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.52	0.44
1:C:227:LEU:O	1:C:231:ILE:HG13	2.18	0.44
1:A:335:ILE:CG2	1:A:339:ARG:HG3	2.41	0.43
1:A:179:THR:HA	2:B:352:LYS:HD2	2.01	0.43
1:A:25:CYS:SG	1:A:86:LEU:HD11	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:177:VAL:HG23	1:A:177:VAL:O	2.18	0.43
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.18	0.43
4:F:241:THR:HG1	11:F:401:ACP:HO3'	1.26	0.43
1:A:48:SER:O	1:A:51:THR:HG23	2.18	0.43
1:A:79:ARG:HG2	1:A:92:LEU:HD12	2.00	0.43
1:A:344:VAL:HG23	1:A:347:CYS:HB2	2.01	0.43
1:C:75:ILE:HD12	1:C:94:THR:HG22	1.99	0.43
1:C:255:PHE:CD1	1:C:316:CYS:HB3	2.54	0.43
2:D:141:LEU:HA	2:D:147:SER:HB3	2.00	0.43
1:A:70:LEU:HD22	1:A:110:ILE:CG2	2.49	0.43
1:C:440:VAL:HG12	1:C:440:VAL:O	2.18	0.43
3:E:119:MET:HA	3:E:122:ARG:NH2	2.33	0.43
1:A:233:GLN:HG3	1:A:368:LEU:HD12	2.01	0.43
1:A:351:PHE:HE1	3:E:24:LEU:HD11	1.84	0.43
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.37	0.43
2:D:180:THR:HB	2:D:183:GLU:HG3	2.00	0.43
2:D:294:GLN:HG2	2:D:300:ASN:ND2	2.34	0.43
2:B:312:TYR:CD1	2:B:381:SER:HB2	2.54	0.43
2:B:329:ASP:O	2:B:333:LEU:HG	2.18	0.43
1:C:182:VAL:HG13	12:D:615:HOH:O	2.18	0.43
4:F:263:PHE:CZ	4:F:341:LYS:HE2	2.54	0.43
1:A:141:PHE:O	1:A:147:SER:HB3	2.20	0.42
2:B:324:SER:HB3	2:B:327:GLU:HB3	2.02	0.42
1:C:244:PHE:CE1	1:C:358:GLN:HG2	2.54	0.42
2:B:21:TRP:CH2	2:B:52:TYR:HB3	2.54	0.42
2:D:220:THR:C	2:D:222:PRO:HD3	2.39	0.42
9:B:504:MES:H51	9:B:504:MES:H81	1.60	0.42
2:B:42:LEU:HD12	2:B:42:LEU:N	2.34	0.42
2:B:164:ARG:O	9:B:504:MES:H31	2.19	0.42
2:D:19:LYS:O	2:D:23:VAL:HG23	2.20	0.42
4:F:24:THR:O	4:F:26:GLN:HG3	2.20	0.42
1:A:260:VAL:HG11	1:A:266:HIS:HB3	2.01	0.42
2:B:385:GLN:OE1	2:B:389:LYS:HE3	2.20	0.42
4:F:240:LEU:HD12	4:F:240:LEU:N	2.35	0.42
2:B:31:ASP:HB2	2:B:32:PRO:HD2	2.01	0.42
2:D:345:GLU:HG3	2:D:440:ALA:HB2	2.01	0.42
4:F:101:TYR:CD2	4:F:179:VAL:HG22	2.54	0.42
1:A:151:SER:HB2	1:A:193:THR:OG1	2.19	0.41
2:B:292:THR:HG22	2:B:335:VAL:HG21	2.01	0.41
2:D:8:GLN:NE2	2:D:14:ASN:HA	2.35	0.41
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.35	0.41
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.55	0.41
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.02	0.41
2:B:402:LYS:HB3	2:B:405:LEU:HD12	2.02	0.41
2:D:287:THR:OG1	2:D:289:PRO:HD2	2.20	0.41
2:D:387:LEU:HD23	2:D:387:LEU:C	2.40	0.41
1:A:93:ILE:HD11	1:A:121:ARG:HG3	2.02	0.41
2:B:88:ARG:NH1	2:B:90:ASP:OD2	2.54	0.41
2:D:191:VAL:O	2:D:195:VAL:HG23	2.21	0.41
2:B:217:LEU:HD11	2:B:230:LEU:HD21	2.03	0.41
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.56	0.41
2:B:199:ASP:OD1	9:B:504:MES:H62	2.21	0.41
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.02	0.41
2:D:107:HIS:O	2:D:152:LEU:HD22	2.20	0.41
2:D:312:TYR:CE1	2:D:377:PHE:HZ	2.39	0.41
4:F:185:TYR:OH	4:F:239:HIS:HB3	2.21	0.41
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.54	0.41
1:C:140:SER:HA	1:C:171:ILE:HB	2.03	0.41
2:D:216:THR:HG22	2:D:217:LEU:HD23	2.03	0.41
4:F:74:LYS:NZ	4:F:331:GLU:OE1	2.46	0.41
1:A:209:ILE:HG22	1:A:227:LEU:HD22	2.02	0.41
1:C:151:SER:HB2	1:C:193:THR:CG2	2.51	0.41
2:D:1:MET:HG3	2:D:50:ASN:CB	2.51	0.41
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.56	0.41
4:F:259:GLY:O	4:F:261:GLU:HG3	2.20	0.41
1:A:176:GLN:HB2	12:A:641:HOH:O	2.20	0.41
2:B:337:ASN:ND2	4:F:58:LEU:HD21	2.36	0.41
2:B:352:LYS:HD3	2:B:352:LYS:HA	1.90	0.41
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.56	0.41
1:C:11:GLN:HE22	2:D:247:GLN:NE2	2.19	0.40
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.51	0.40
2:D:297:ASP:OD2	2:D:299:LYS:HB2	2.21	0.40
2:B:165:ILE:HG21	2:B:252:LEU:HB3	2.02	0.40
2:B:187:ALA:O	2:B:191:VAL:HG23	2.21	0.40
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.57	0.40
2:D:123:ARG:O	2:D:127:GLU:HG3	2.21	0.40
2:B:223:THR:O	2:B:227:LEU:HD13	2.22	0.40
1:C:141:PHE:HB3	1:C:187:SER:OG	2.21	0.40
1:C:312:TYR:CE1	1:C:341:ILE:HG23	2.57	0.40
2:D:290:GLU:O	2:D:294:GLN:HB2	2.22	0.40
1:A:320:ARG:HD2	12:A:634:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:349:THR:HB	3:E:25:LYS:HB3	2.02	0.40
2:B:269:MET:HE3	2:B:301:MET:SD	2.62	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	436/451 (97%)	424 (97%)	11 (2%)	1 (0%)	47	57
1	C	439/451 (97%)	429 (98%)	10 (2%)	0	100	100
2	B	423/445 (95%)	407 (96%)	16 (4%)	0	100	100
2	D	422/445 (95%)	412 (98%)	10 (2%)	0	100	100
3	E	119/143 (83%)	117 (98%)	2 (2%)	0	100	100
4	F	340/384 (88%)	324 (95%)	16 (5%)	0	100	100
All	All	2179/2319 (94%)	2113 (97%)	65 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	TYR

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	369/379 (97%)	363 (98%)	6 (2%)	62	76
1	C	372/379 (98%)	368 (99%)	4 (1%)	73	84
2	B	369/383 (96%)	364 (99%)	5 (1%)	67	79
2	D	368/383 (96%)	365 (99%)	3 (1%)	81	90
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	315/342 (92%)	315 (100%)	0	100	100
All	All	1903/1993 (96%)	1885 (99%)	18 (1%)	78	88

All (18) 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	284	GLU
1	A	300	ASN
1	A	381	THR
2	B	48	ARG
2	B	139	HIS
2	B	255	LEU
2	B	302	MET
2	B	430	SER
1	C	71	GLU
1	C	221	ARG
1	C	251	ASP
1	C	381	THR
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 (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	88	HIS
1	A	101	ASN
1	A	300	ASN
2	B	15	GLN
2	B	282	GLN
2	B	294	GLN

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Mol	Chain	Res	Type
1	C	11	GLN
1	C	85	GLN
1	C	300	ASN
2	D	167	ASN
2	D	294	GLN
4	F	229	ASN
4	F	269	GLN
4	F	333	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 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	$\# Z > 2$
11	ACP	F	401	6	27,33,33	1.40	5 (18%)	32,52,52	1.47	4 (12%)
5	GTP	A	501	6	26,34,34	1.00	1 (3%)	33,54,54	1.72	7 (21%)
8	GDP	B	501	6	24,30,30	1.14	2 (8%)	31,47,47	1.86	7 (22%)
10	K1G	B	505	-	13,16,16	0.67	0	12,23,23	1.21	1 (8%)
9	MES	B	504	-	12,12,12	2.25	1 (8%)	14,16,16	2.05	5 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GDP	D	501	6	24,30,30	1.17	2 (8%)	31,47,47	1.90	7 (22%)
5	GTP	C	501	6	26,34,34	0.98	1 (3%)	33,54,54	1.65	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
11	ACP	F	401	6	-	9/15/38/38	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
10	K1G	B	505	-	-	0/8/8/8	0/2/2/2
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
8	GDP	D	501	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	9/18/38/38	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	-7.52	1.66	1.77
8	D	501	GDP	C6-C5	4.05	1.48	1.41
8	B	501	GDP	C6-C5	3.84	1.48	1.41
5	A	501	GTP	C6-N1	3.22	1.38	1.33
5	C	501	GTP	C6-N1	3.04	1.38	1.33
11	F	401	ACP	PG-O2G	2.97	1.61	1.54
11	F	401	ACP	PG-O3G	2.96	1.61	1.54
11	F	401	ACP	PB-O3A	2.68	1.61	1.58
11	F	401	ACP	C5-C4	2.55	1.47	1.40
8	D	501	GDP	C5-C4	2.43	1.47	1.40
8	B	501	GDP	C5-C4	2.38	1.47	1.40
11	F	401	ACP	PB-O2B	2.24	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	-5.41	120.00	127.22
5	C	501	GTP	N3-C2-N1	-5.16	120.34	127.22
8	B	501	GDP	C2-N3-C4	4.87	120.92	115.36
8	D	501	GDP	C2-N3-C4	4.80	120.84	115.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C2-N3-C4	4.30	120.27	115.36
8	B	501	GDP	C6-C5-C4	-4.19	116.80	120.80
8	D	501	GDP	C6-N1-C2	4.09	122.44	115.93
11	F	401	ACP	PA-O3A-PB	-4.09	119.60	132.56
8	D	501	GDP	C5-C6-N1	-4.01	117.94	123.43
8	B	501	GDP	C6-N1-C2	3.98	122.25	115.93
9	B	504	MES	C5-N4-C3	3.90	117.61	108.83
5	C	501	GTP	C2-N3-C4	3.83	119.73	115.36
8	D	501	GDP	C6-C5-C4	-3.81	117.16	120.80
8	B	501	GDP	C5-C6-N1	-3.78	118.27	123.43
11	F	401	ACP	C3'-C2'-C1'	3.51	106.26	100.98
8	B	501	GDP	N3-C2-N1	-3.41	122.67	127.22
8	D	501	GDP	N3-C2-N1	-3.35	122.75	127.22
9	B	504	MES	O1S-S-C8	3.26	110.84	106.92
9	B	504	MES	C6-C5-N4	-3.12	105.37	110.10
11	F	401	ACP	N3-C2-N1	-3.06	123.89	128.68
5	C	501	GTP	C5-C6-N1	-3.05	119.26	123.43
5	A	501	GTP	C5-C6-N1	-2.95	119.40	123.43
8	D	501	GDP	C4-C5-N7	-2.82	106.46	109.40
5	A	501	GTP	PA-O3A-PB	-2.65	123.72	132.83
8	D	501	GDP	PA-O3A-PB	-2.65	123.75	132.83
5	C	501	GTP	C6-N1-C2	2.62	120.09	115.93
11	F	401	ACP	C4-C5-N7	-2.61	106.68	109.40
5	A	501	GTP	PB-O3B-PG	-2.58	123.96	132.83
5	C	501	GTP	PA-O3A-PB	-2.58	123.97	132.83
5	A	501	GTP	C6-N1-C2	2.57	120.02	115.93
5	C	501	GTP	PB-O3B-PG	-2.52	124.17	132.83
8	B	501	GDP	PA-O3A-PB	-2.51	124.22	132.83
9	B	504	MES	O3S-S-C8	2.47	109.76	105.77
8	B	501	GDP	C4-C5-N7	-2.38	106.92	109.40
5	A	501	GTP	N2-C2-N1	2.34	120.89	117.25
9	B	504	MES	C7-N4-C5	2.22	116.92	111.23
10	B	505	K1G	C7-N3-C6	2.02	128.53	124.18

There are no chirality outliers.

All (37) 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

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Mol	Chain	Res	Type	Atoms
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O2A
9	B	504	MES	C8-C7-N4-C5
9	B	504	MES	C7-C8-S-O2S
9	B	504	MES	C7-C8-S-O3S
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-O3A
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O1G
8	D	501	GDP	C5'-O5'-PA-O1A
9	B	504	MES	C7-C8-S-O1S
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
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	C	501	GTP	PB-O3A-PA-O1A

There are no ring outliers.

6 monomers are involved in 17 short contacts:

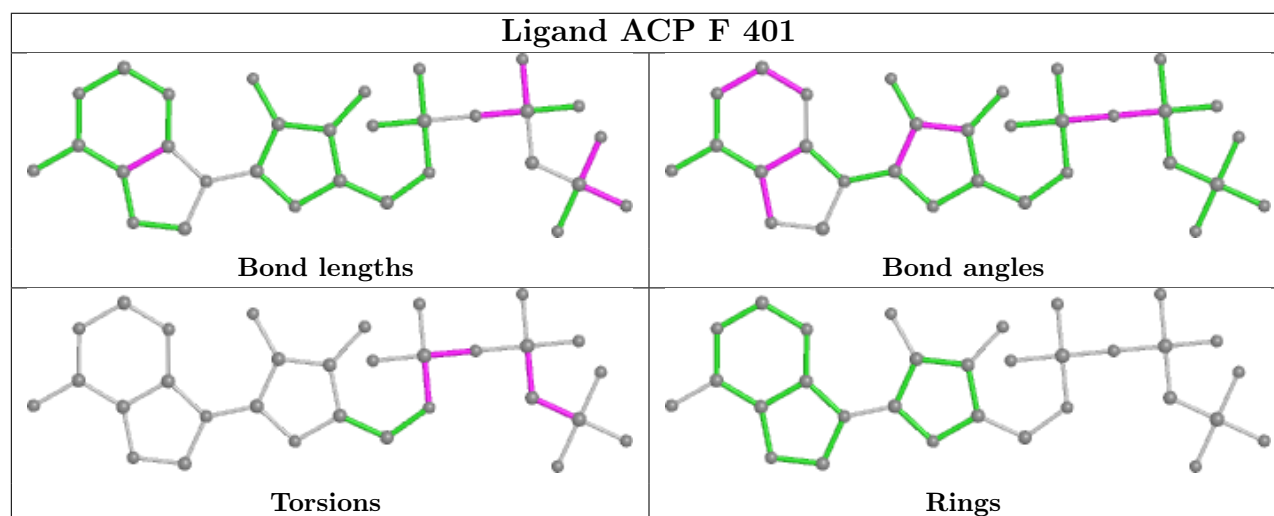
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	F	401	ACP	4	0
5	A	501	GTP	1	0
8	B	501	GDP	1	0
10	B	505	K1G	1	0

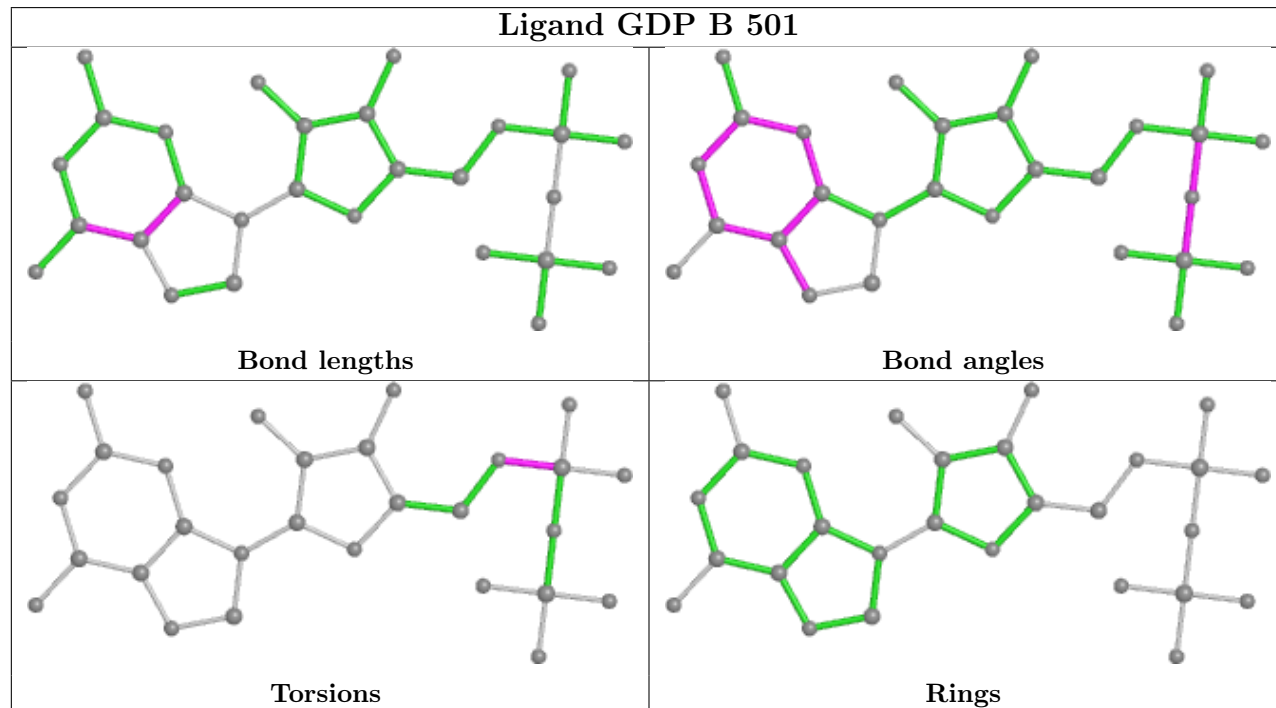
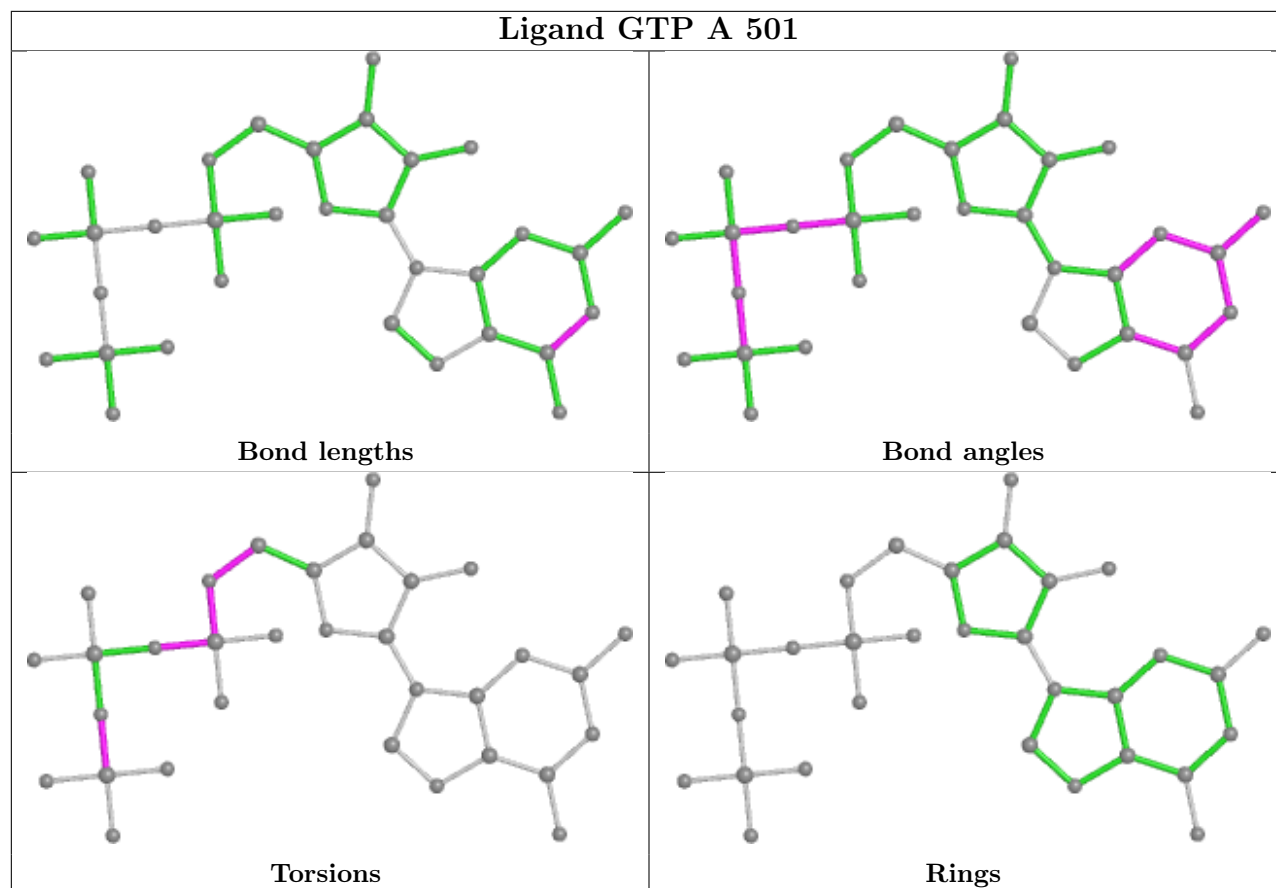
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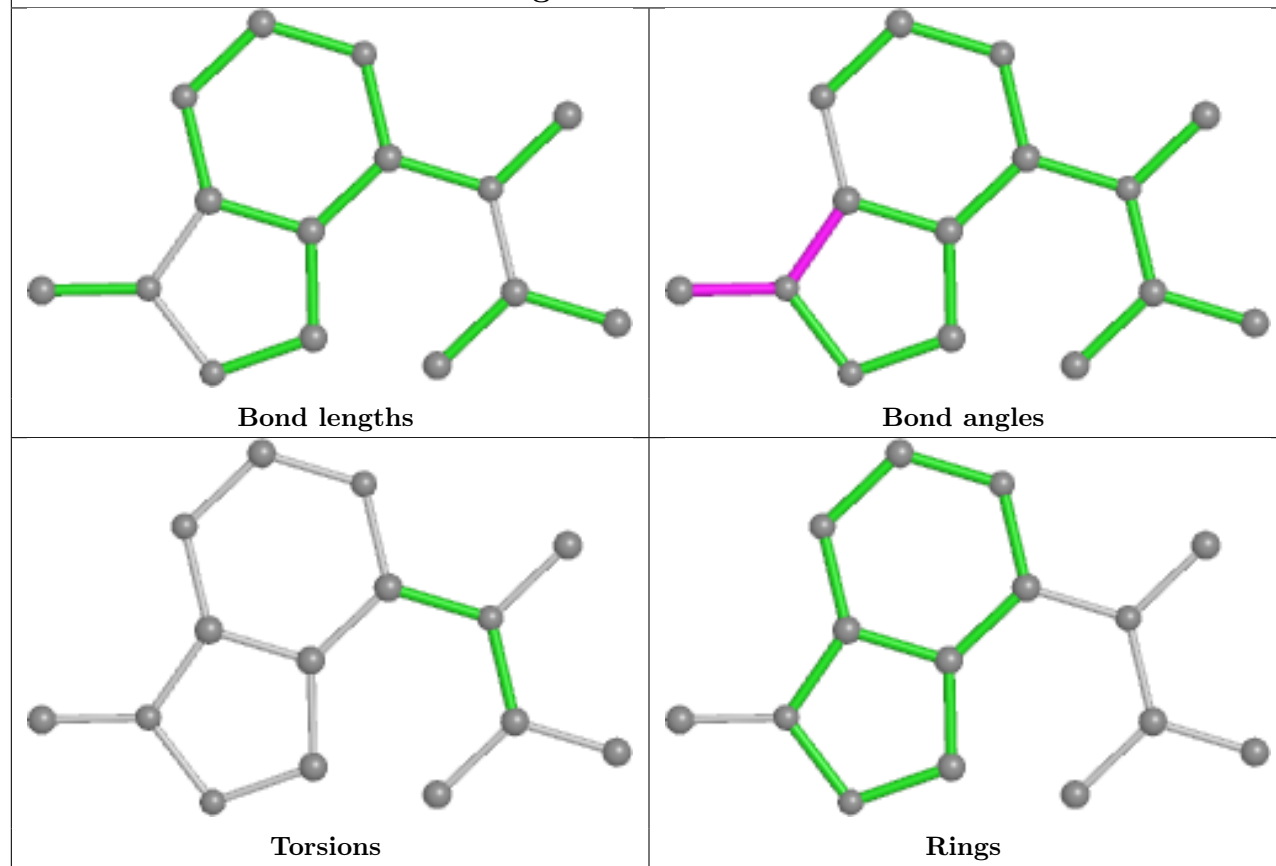
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	504	MES	6	0
8	D	501	GDP	4	0

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.

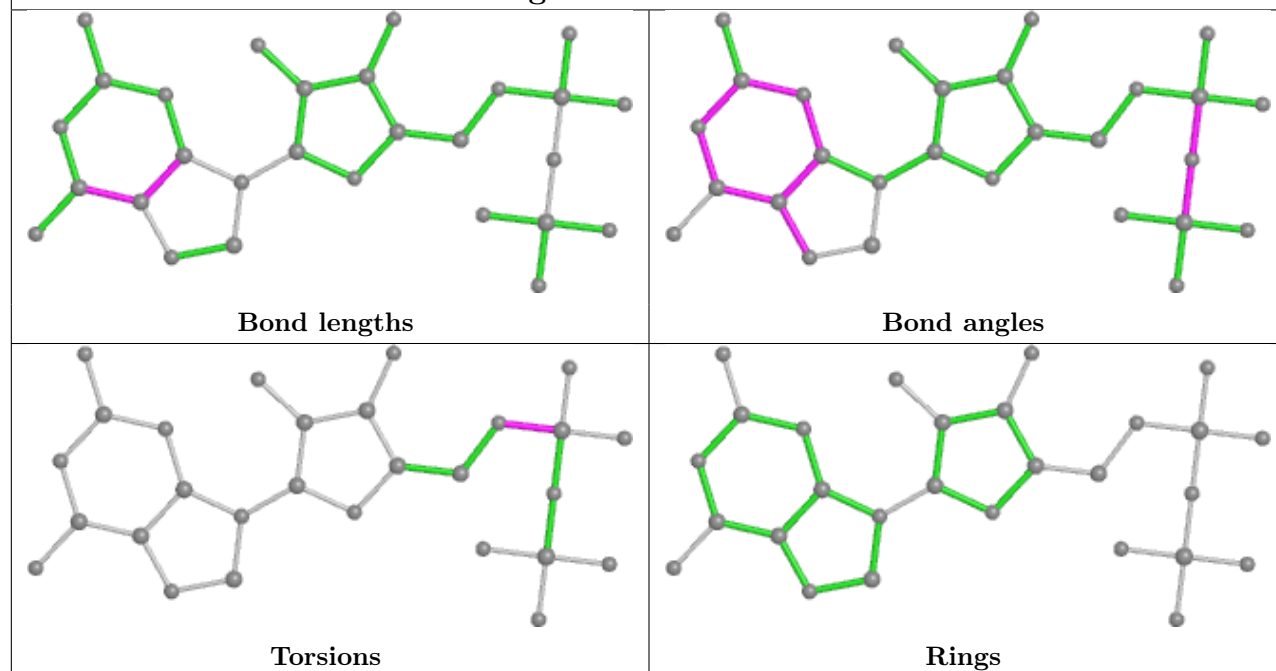


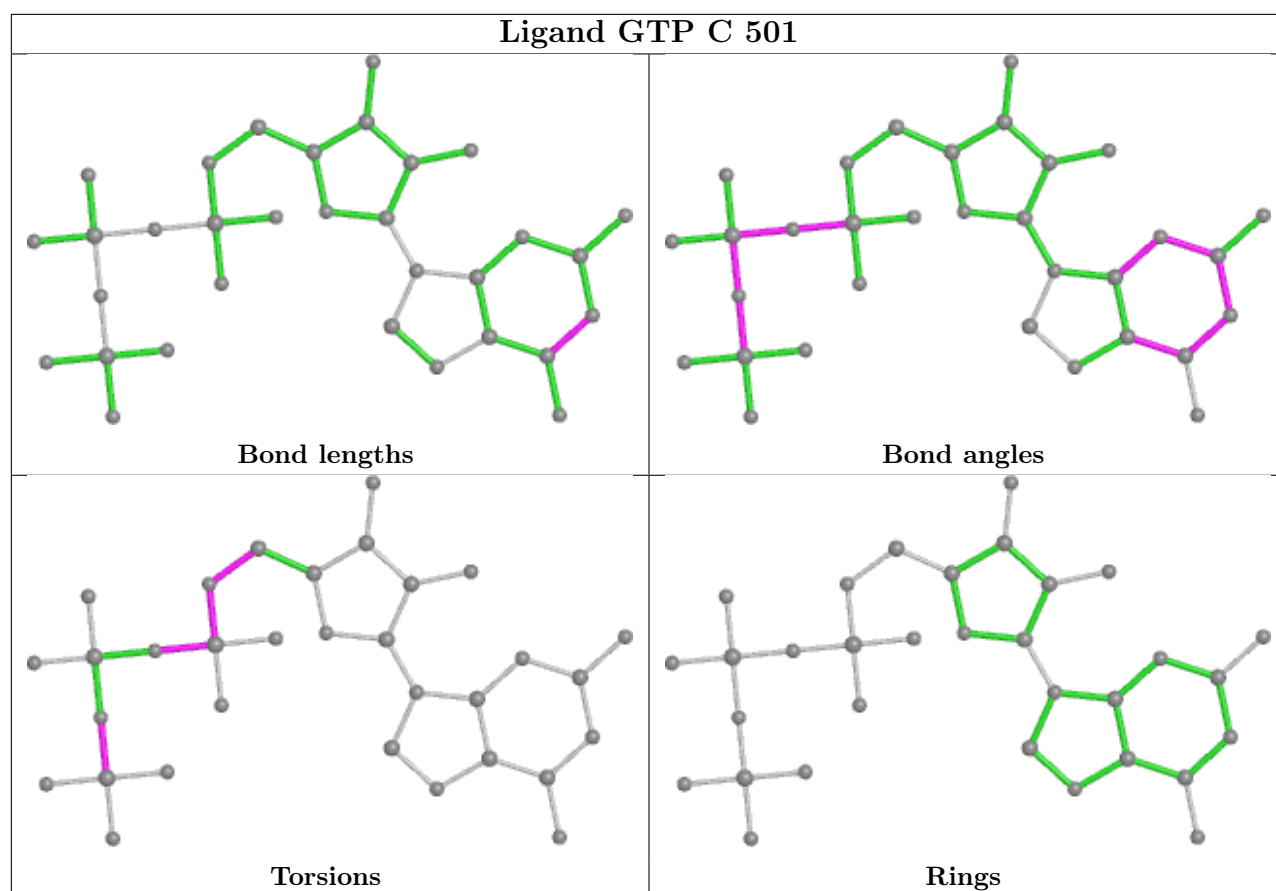


Ligand K1G B 505



Ligand GDP D 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	438/451 (97%)	0.25	10 (2%) 60 66	51, 70, 105, 173	0
1	C	440/451 (97%)	0.50	6 (1%) 75 79	44, 57, 82, 137	0
2	B	425/445 (95%)	0.45	18 (4%) 36 41	44, 67, 116, 149	2 (0%)
2	D	426/445 (95%)	0.26	18 (4%) 36 41	54, 78, 111, 137	4 (0%)
3	E	123/143 (86%)	0.84	13 (10%) 6 8	57, 86, 137, 183	0
4	F	348/384 (90%)	1.03	64 (18%) 1 1	65, 96, 165, 205	0
All	All	2200/2319 (94%)	0.50	129 (5%) 22 27	44, 72, 129, 205	6 (0%)

All (129) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	26	PRO	12.0
2	D	276	THR	8.9
3	E	27	PRO	7.6
4	F	90	SER	7.4
4	F	173	ILE	7.4
4	F	103	THR	6.1
4	F	254	GLY	6.0
4	F	89	GLU	6.0
2	D	279	GLY	5.9
2	B	284	ARG	5.9
3	E	24	LEU	5.8
4	F	240	LEU	5.8
3	E	25	LYS	5.7
4	F	251	LYS	5.6
4	F	105	LEU	5.6
4	F	104	ASN	5.5
4	F	253	TYR	5.1
4	F	249	TYR	4.9
4	F	182	ILE	4.7

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Mol	Chain	Res	Type	RSRZ
4	F	233	PHE	4.6
2	B	333	LEU	4.6
2	D	277	SER	4.6
3	E	6	MET	4.5
4	F	234	GLN	4.4
2	D	278	ARG	4.4
4	F	176	GLN	4.2
1	A	346	TRP	4.2
4	F	372	THR	4.2
4	F	169	LEU	4.1
4	F	99	VAL	4.1
4	F	243	HIS	4.1
4	F	131	PHE	4.0
4	F	250	SER	4.0
2	B	1	MET	3.9
1	A	351	PHE	3.7
2	B	276	THR	3.7
2	B	437	ASP	3.6
4	F	231	ALA	3.6
4	F	177	GLY	3.5
2	B	57	THR	3.5
4	F	132	LEU	3.5
2	B	281	GLN	3.5
2	B	247	GLN	3.5
4	F	100	ILE	3.4
1	A	438	ASP	3.4
2	B	285	ALA	3.4
4	F	137	ARG	3.4
1	A	341	ILE	3.4
4	F	244	CYS	3.3
4	F	170	LEU	3.3
3	E	28	SER	3.3
3	E	142	GLU	3.3
4	F	142	ARG	3.2
1	A	262	TYR	3.2
2	B	277	SER	3.1
2	B	340	SER	3.1
4	F	136	ASN	3.0
4	F	130	VAL	3.0
2	D	215	ARG	3.0
3	E	143	ALA	2.9
4	F	381	HIS	2.9

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Mol	Chain	Res	Type	RSRZ
4	F	135	TYR	2.9
4	F	259	GLY	2.9
4	F	143	GLU	2.9
4	F	241	THR	2.9
4	F	263	PHE	2.9
4	F	179	VAL	2.9
4	F	20	LEU	2.8
4	F	144	GLY	2.8
1	C	357	TYR	2.8
4	F	166	ALA	2.8
4	F	342	LEU	2.8
2	D	275	LEU	2.7
4	F	232	ASN	2.7
3	E	48	GLU	2.7
4	F	223	THR	2.7
2	B	286	LEU	2.7
2	B	59	ASN	2.6
4	F	371	PRO	2.6
3	E	50	ILE	2.6
1	A	282	TYR	2.6
4	F	161	LEU	2.5
4	F	247	LYS	2.5
2	D	401	ARG	2.5
2	D	217	LEU	2.5
4	F	101	TYR	2.5
4	F	255	ARG	2.4
4	F	134	ALA	2.4
2	D	280	SER	2.4
4	F	306	HIS	2.4
2	D	57	THR	2.4
2	D	299	LYS	2.3
4	F	138	ARG	2.3
4	F	256	TYR	2.3
2	D	355	VAL	2.3
1	C	308	ARG	2.3
4	F	181	VAL	2.3
4	F	252	ASN	2.3
1	A	77	GLU	2.3
1	A	344	VAL	2.3
4	F	168	GLU	2.3
2	B	219	LEU	2.3
2	B	283	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	1	MET	2.3
4	F	141	GLY	2.3
4	F	248	GLU	2.3
1	C	340	SER	2.2
4	F	362	ALA	2.2
2	D	246	GLY	2.2
2	B	328	VAL	2.1
4	F	172	PHE	2.1
1	C	248	LEU	2.1
1	A	349	THR	2.1
2	B	337	ASN	2.1
3	E	45	PRO	2.1
1	C	281	ALA	2.1
1	C	355	ILE	2.1
1	A	196	GLU	2.1
4	F	236	LYS	2.1
3	E	121	GLU	2.0
2	D	37	HIS	2.0
4	F	379	HIS	2.0
4	F	382	HIS	2.0
4	F	314	LEU	2.0
2	B	303	ALA	2.0
3	E	47	LEU	2.0
2	D	293	GLN	2.0
2	D	216	THR	2.0
2	D	218	LYS	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](#)

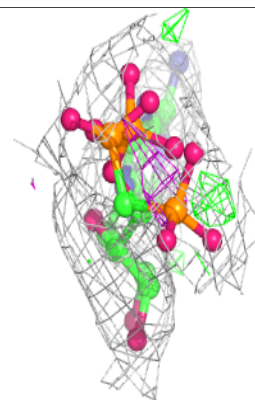
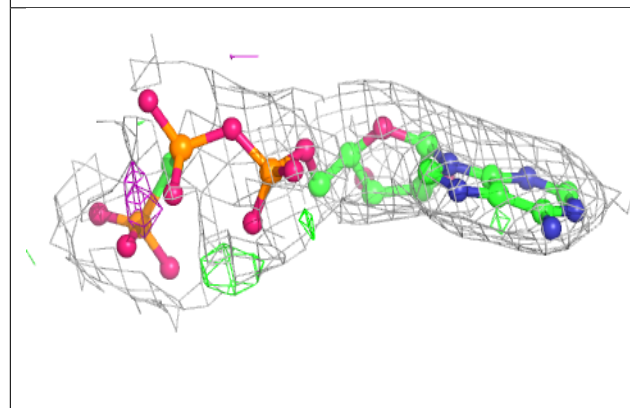
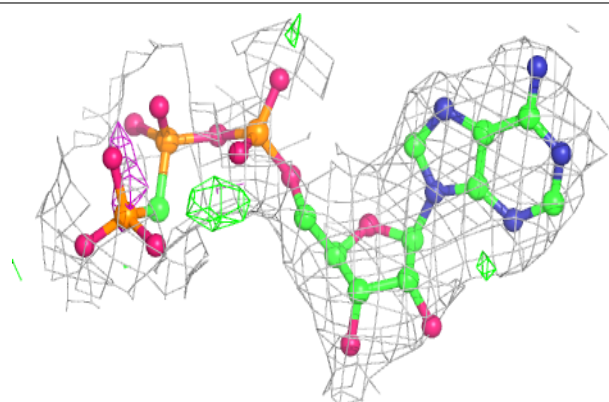
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
7	CA	B	503	1/1	0.82	0.22	106,106,106,106	0
7	CA	E	201	1/1	0.84	0.14	101,101,101,101	0
11	ACP	F	401	31/31	0.86	0.14	99,110,118,125	0
10	K1G	B	505	15/15	0.89	0.26	81,94,106,113	0
6	MG	A	502	1/1	0.90	0.11	53,53,53,53	0
9	MES	B	504	12/12	0.92	0.14	74,79,88,94	0
6	MG	B	502	1/1	0.92	0.15	41,41,41,41	0
6	MG	F	402	1/1	0.92	0.08	96,96,96,96	0
6	MG	C	502	1/1	0.94	0.17	51,51,51,51	0
7	CA	A	503	1/1	0.94	0.08	91,91,91,91	0
8	GDP	D	501	28/28	0.94	0.15	67,74,81,90	0
6	MG	D	502	1/1	0.96	0.11	77,77,77,77	0
5	GTP	A	501	32/32	0.97	0.15	46,53,58,59	0
7	CA	C	503	1/1	0.98	0.11	72,72,72,72	0
5	GTP	C	501	32/32	0.98	0.17	40,47,52,55	0
8	GDP	B	501	28/28	0.99	0.17	45,49,55,57	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.

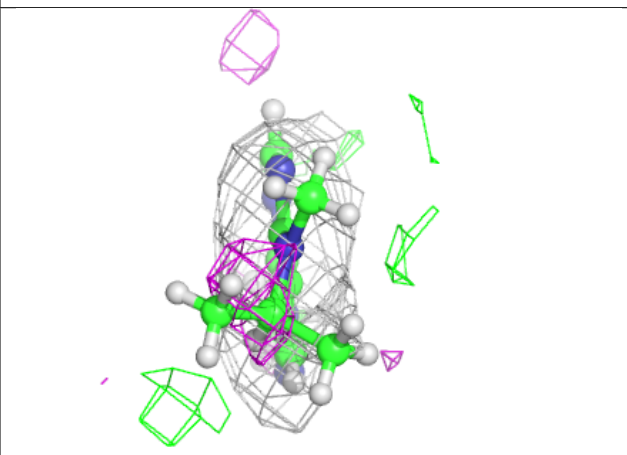
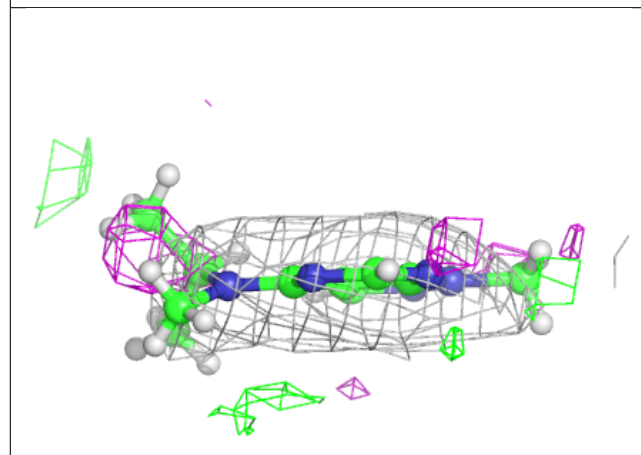
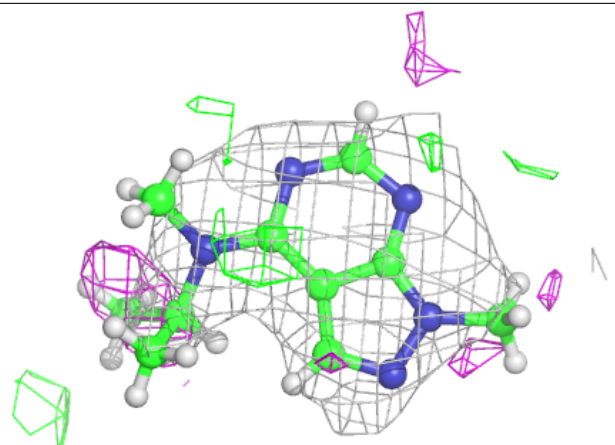
Electron density around ACP F 401:

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



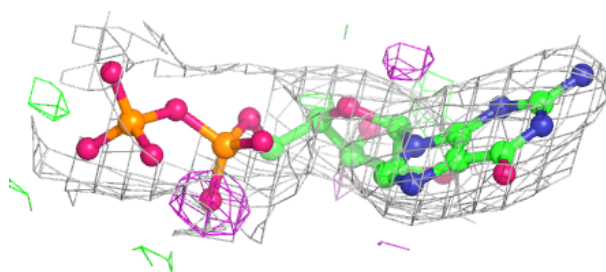
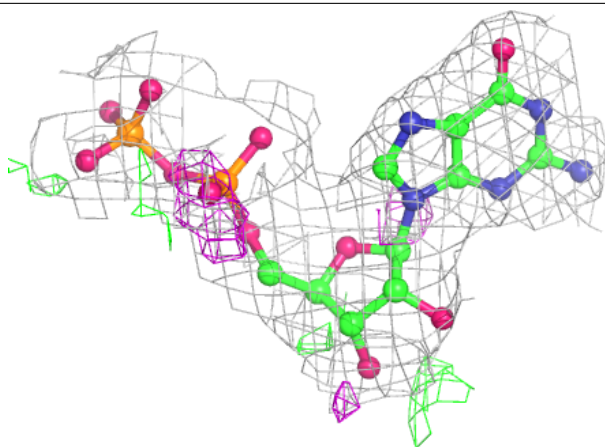
Electron density around K1G B 505:

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

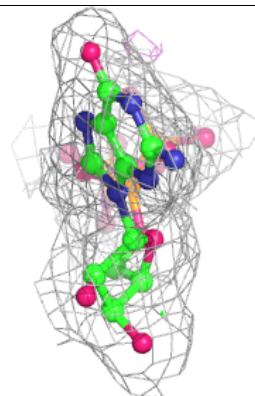
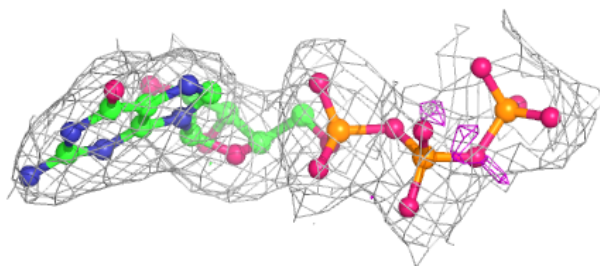
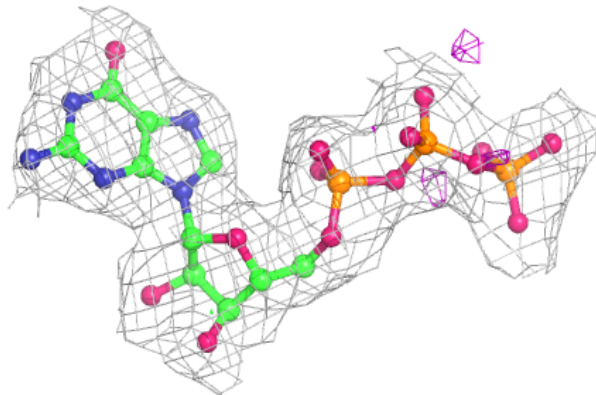


Electron density around GDP D 501:

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

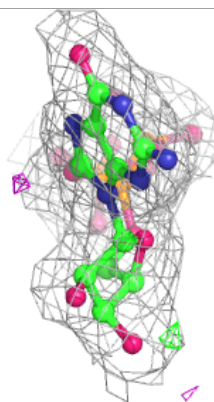
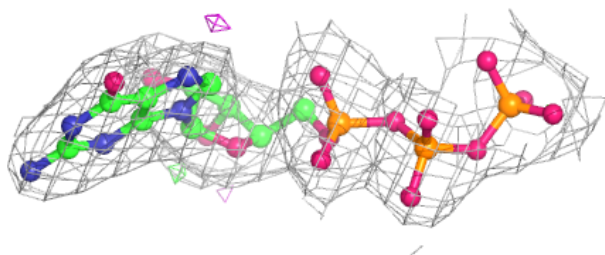
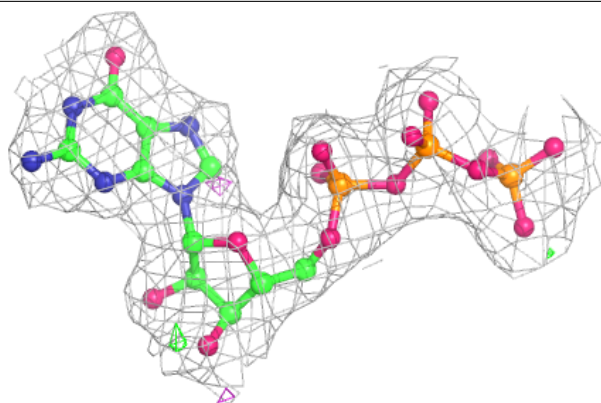
**Electron density around GTP A 501:**

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

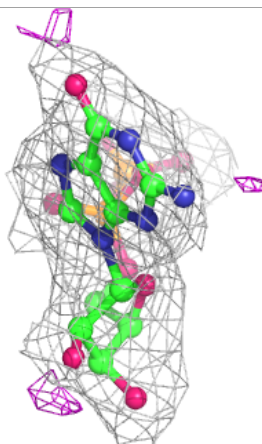
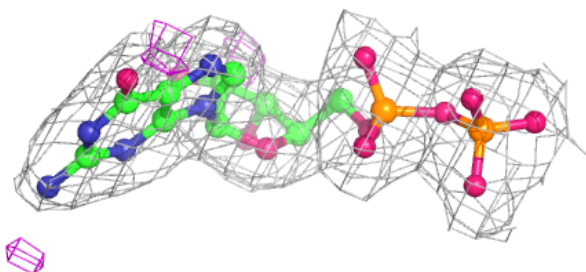
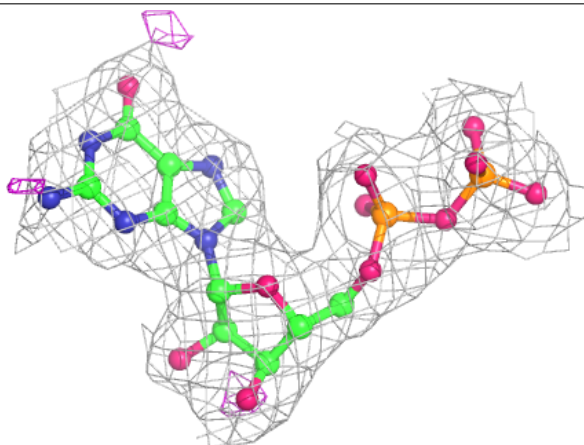


Electron density around GTP C 501:

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

**Electron density around GDP B 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.