



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2021 – 02:34 PM EDT

PDB ID : 5S52
Title : Tubulin-Z50145861-complex
Authors : Muehlethaler, T.; Gioia, D.; Protá, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.
Deposited on : 2020-11-08
Resolution : 2.83 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

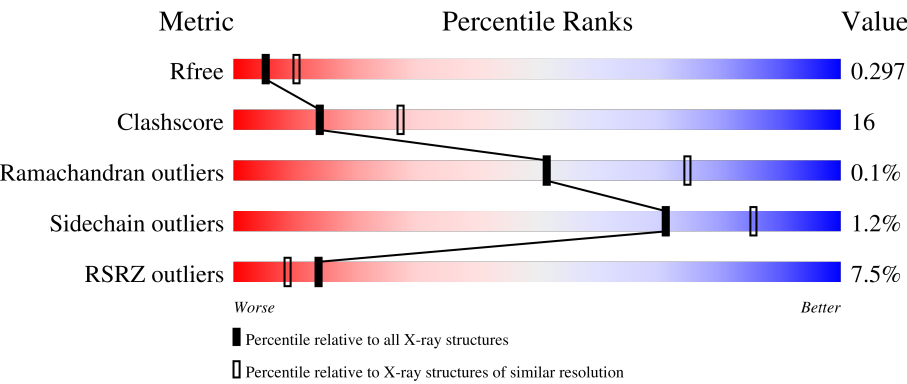
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.83 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	1031 (2.86-2.82)
Clashscore	141614	1078 (2.86-2.82)
Ramachandran outliers	138981	1050 (2.86-2.82)
Sidechain outliers	138945	1051 (2.86-2.82)
RSRZ outliers	127900	1019 (2.86-2.82)

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>9%</div><div>68%</div><div>29%</div><div>.</div></div>
1	C	451	<div><div>5%</div><div>65%</div><div>32%</div><div>..</div></div>
2	B	445	<div><div>7%</div><div>62%</div><div>33%</div><div>..</div></div>
2	D	445	<div><div>7%</div><div>60%</div><div>36%</div><div>.</div></div>
3	E	143	<div><div>8%</div><div>69%</div><div>17%</div><div>14%</div></div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	384	<div> <div>7%</div> <div>62%</div> <div>29%</div> <div>8%</div> </div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17803 atoms, of which 20 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	3	0	0
			3348	2103	573	645	27			
2	D	429	Total	C	N	O	S	6	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

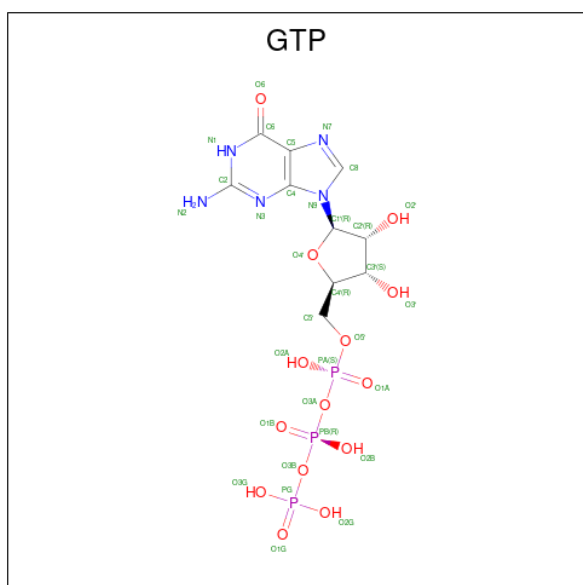
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

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		

Continued on next page...

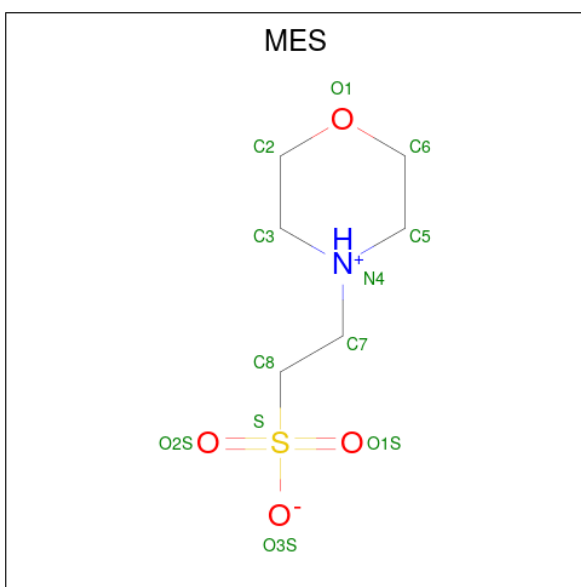
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total Mg 1 1	0	0

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

-
- The image displays the chemical structure of GDP (Guanosine Diphosphate). It consists of a guanine base (a purine derivative) linked to a ribose sugar, which is in turn linked to two phosphate groups. The guanine base is shown with its characteristic fused ring system, including atoms N1, N2, N3, N7, C2, C4, C5, C6, and C8. The ribose sugar is a five-membered ring with carbons C1', C2', C3', C4', and C5'. The two phosphate groups are represented by phosphorus atoms (P) and their associated oxygen atoms (O). The structure is color-coded: blue for nitrogen atoms, red for oxygen atoms, and purple for phosphorus atoms. Stereochemistry is indicated with wedges and dashes at the C1' and C4' positions of the ribose ring.

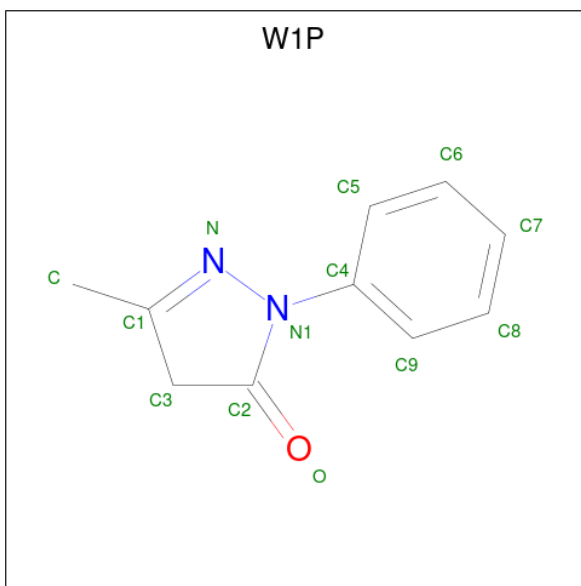
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- 



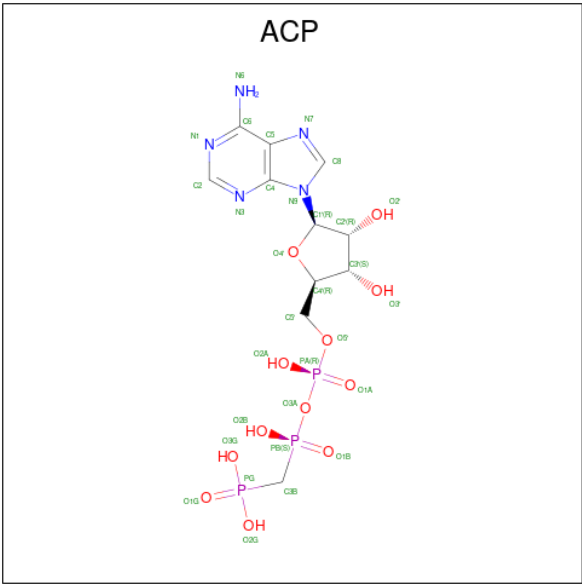
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is 5-methyl-2-phenyl-2,4-dihydro-3H-pyrazol-3-one (three-letter code: W1P) (formula: $C_{10}H_{10}N_2O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	0	0
			23	10	10	2	1		
10	B	1	Total	C	H	N	O	0	0
			23	10	10	2	1		

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



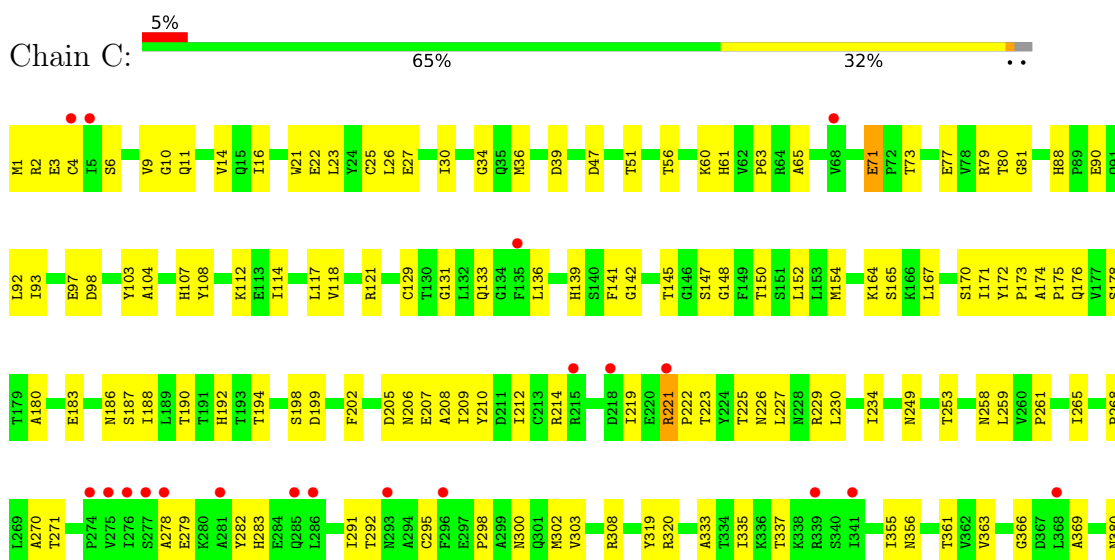
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Tubulin alpha-1B chain

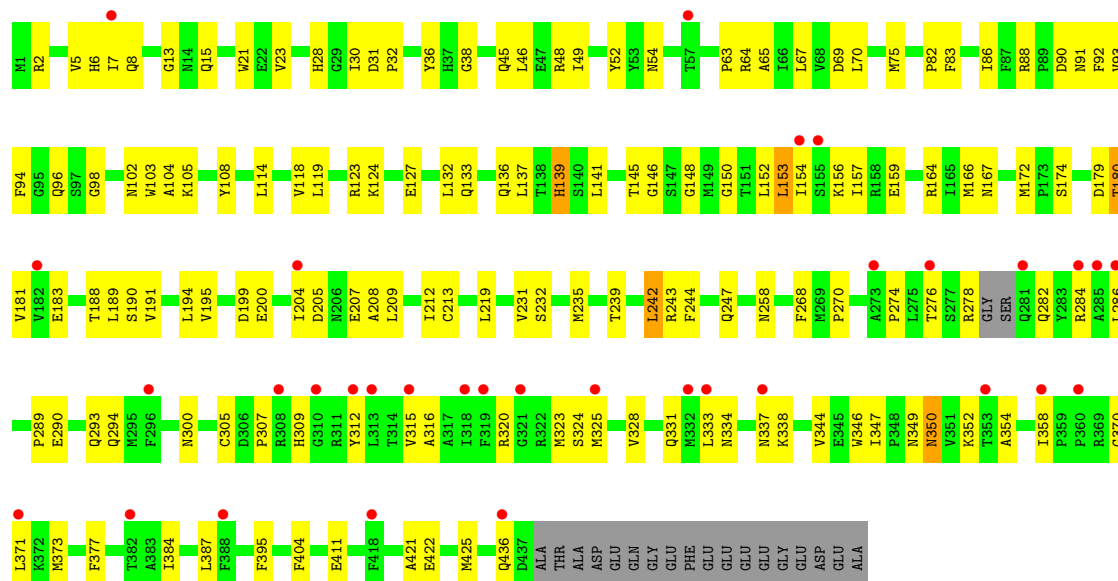


• Molecule 1: Tubulin alpha-1B chain

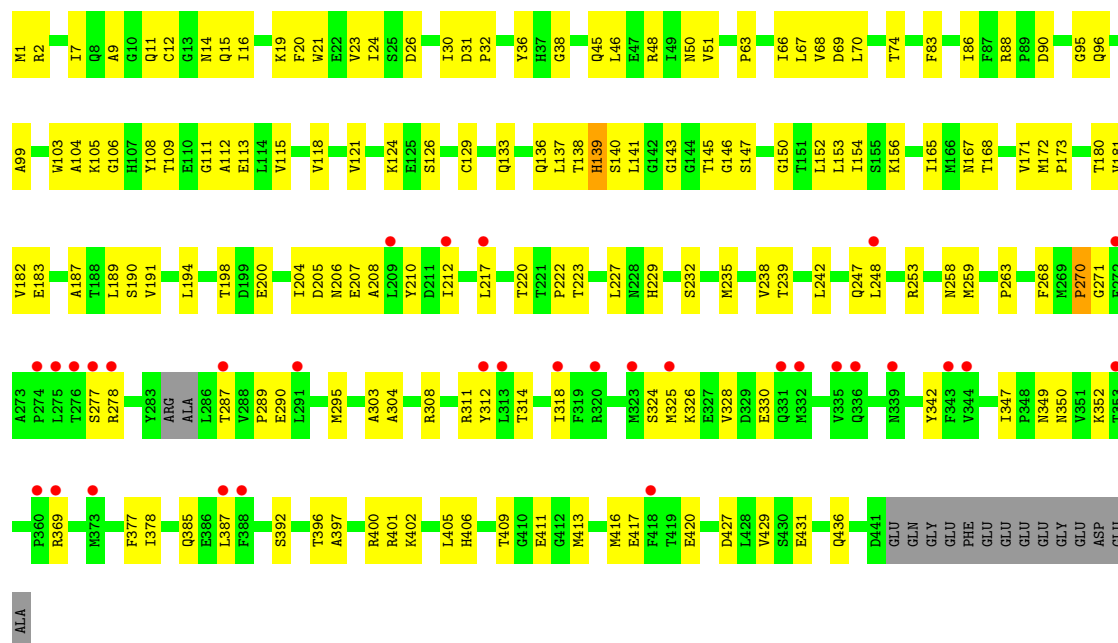




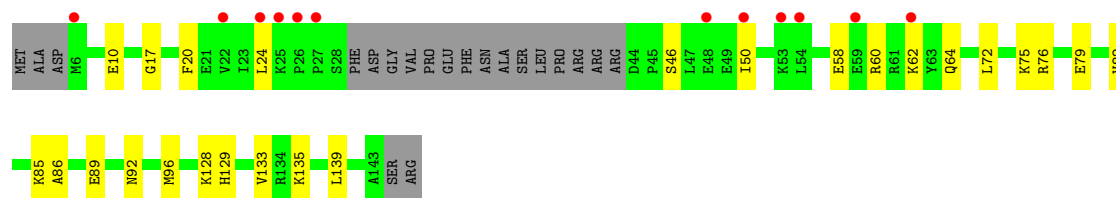
• Molecule 2: Tubulin beta-2B chain



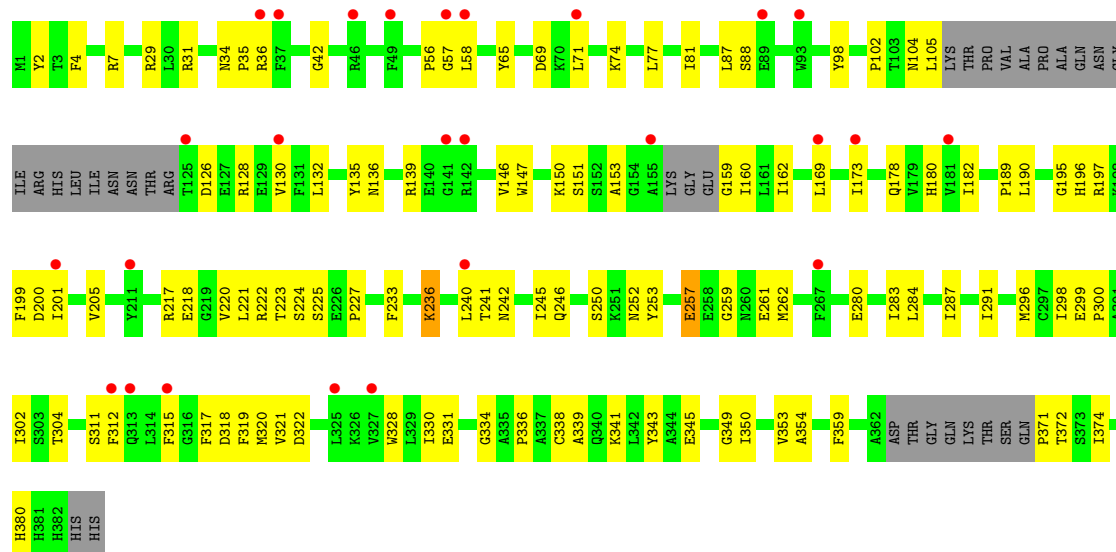
• Molecule 2: Tubulin beta-2B chain



• 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	105.09Å 161.57Å 174.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	118.67 – 2.83 118.67 – 2.83	Depositor EDS
% Data completeness (in resolution range)	97.3 (118.67-2.83) 97.3 (118.67-2.83)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.26 (at 2.82Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.238 , 0.297 0.238 , 0.297	Depositor DCC
R_{free} test set	3562 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	78.4	Xtriage
Anisotropy	0.224	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17803	wwPDB-VP
Average B, all atoms (Å ²)	94.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.76% 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: W1P, CA, GDP, MG, MES, ACP, GTP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.24	0/3502	0.40	0/4754
1	C	0.24	0/3521	0.40	0/4780
2	B	0.24	0/3422	0.40	0/4633
2	D	0.24	0/3431	0.39	0/4647
3	E	0.23	0/1022	0.33	0/1356
4	F	0.23	0/2944	0.39	0/3978
All	All	0.24	0/17842	0.39	0/24148

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	106	0
1	C	3443	0	3352	110	0
2	B	3348	0	3223	120	0
2	D	3358	0	3228	117	0
3	E	1014	0	1029	20	0
4	F	2877	0	2839	92	0
5	A	32	0	12	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	2	0
8	D	28	0	12	5	0
9	B	12	0	12	3	0
10	B	26	20	0	3	0
11	F	31	0	14	4	0
12	A	16	0	0	0	1
12	B	36	0	0	4	0
12	C	56	0	0	1	1
12	D	4	0	0	0	0
12	E	5	0	0	0	0
12	F	4	0	0	0	0
All	All	17783	20	17079	542	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 16.

All (542) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:381:THR:HG22	1:A:383:ALA:H	1.24	1.00
1:C:147:SER:HB2	1:C:190:THR:HB	1.61	0.83
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.63	0.80
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.63	0.79
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.63	0.78
2:D:136:GLN:HA	2:D:167:ASN:O	1.85	0.76
1:C:178:SER:OG	2:D:352:LYS:NZ	2.18	0.75
1:A:99:ALA:HA	1:A:105:ARG:HD3	1.67	0.74
4:F:280:GLU:OE1	4:F:284:LEU:HD23	1.88	0.74
1:C:165:SER:HA	1:C:199:ASP:OD2	1.88	0.74
2:D:217:LEU:HA	2:D:277:SER:HB3	1.70	0.73
1:C:79:ARG:HG2	1:C:92:LEU:HD12	1.71	0.72
1:A:286:LEU:O	1:A:373:ARG:NH1	2.23	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:271:THR:HG21	1:A:295:CYS:HA	1.73	0.71
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.72	0.71
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.72	0.71
4:F:371:PRO:HA	4:F:372:THR:O	1.91	0.70
2:B:2:ARG:HB2	2:B:133:GLN:HG3	1.73	0.70
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.74	0.69
1:C:93:ILE:CG2	1:C:114:ILE:HD11	2.22	0.69
1:C:136:LEU:HD23	1:C:167:LEU:HB2	1.74	0.69
2:B:284:ARG:NH2	2:B:290:GLU:OE2	2.26	0.68
2:D:311:ARG:NH1	2:D:436:GLN:O	2.25	0.68
2:D:402:LYS:HB3	2:D:405:LEU:HD12	1.75	0.68
4:F:320:MET:HG3	4:F:330:ILE:HD11	1.73	0.68
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.26	0.68
2:B:323:MET:HE1	2:B:373:MET:HB2	1.76	0.68
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.76	0.68
2:D:324:SER:O	2:D:328:VAL:HG23	1.93	0.68
2:B:152:LEU:HD11	2:B:156:LYS:HE2	1.75	0.68
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.75	0.68
2:B:167:ASN:ND2	2:B:200:GLU:HB2	2.09	0.68
2:B:352:LYS:HB2	10:B:505:W1P:C9	2.24	0.67
2:D:1:MET:HG3	2:D:50:ASN:HB2	1.77	0.67
4:F:153:ALA:HB3	4:F:178:GLN:HG3	1.77	0.67
2:B:204:ILE:HG22	2:B:209:LEU:HD11	1.75	0.67
1:C:270:ALA:O	1:C:302:MET:HG2	1.94	0.67
2:D:105:LYS:HE2	2:D:411:GLU:OE2	1.96	0.66
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.77	0.66
1:A:187:SER:CB	1:A:391:LEU:HD21	2.26	0.66
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.11	0.66
1:A:9:VAL:HG12	1:A:145:THR:HG22	1.77	0.66
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.77	0.65
2:B:337:ASN:OD1	4:F:36:ARG:HD3	1.96	0.65
1:C:136:LEU:CD2	1:C:167:LEU:HB2	2.26	0.65
2:B:118:VAL:HG11	2:B:153:LEU:HD11	1.76	0.65
2:D:154:ILE:HD11	2:D:168:THR:HG21	1.78	0.65
1:A:88:HIS:CD2	1:A:90:GLU:HB2	2.32	0.65
1:C:186:ASN:O	1:C:190:THR:HG22	1.96	0.65
2:B:141:LEU:HD12	2:B:172:MET:SD	2.37	0.64
1:C:221:ARG:HG3	2:D:325:MET:HG2	1.79	0.64
1:C:180:ALA:O	1:C:183:GLU:HG3	1.97	0.64
4:F:81:ILE:HA	4:F:87:LEU:HD12	1.80	0.64
2:B:276:THR:HG21	2:B:282:GLN:HA	1.79	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.33	0.63
2:B:324:SER:O	2:B:328:VAL:HG23	1.98	0.63
4:F:220:VAL:HG11	4:F:339:ALA:HB2	1.80	0.63
1:C:71:GLU:HB3	1:C:98:ASP:HB3	1.79	0.63
1:C:209:ILE:HD11	1:C:302:MET:HE3	1.80	0.63
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.33	0.63
1:A:274:PRO:HG2	1:A:371:VAL:HG11	1.81	0.63
9:B:504:MES:H81	12:B:614:HOH:O	1.98	0.63
4:F:371:PRO:HA	4:F:372:THR:HB	1.80	0.63
1:A:343:PHE:CD1	1:A:349:THR:HG23	2.33	0.63
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.79	0.63
2:B:180:THR:HG22	1:C:258:ASN:OD1	1.99	0.62
2:B:145:THR:HB	8:B:501:GDP:O2B	1.99	0.62
1:C:320:ARG:HA	1:C:356:ASN:O	1.99	0.62
1:C:214:ARG:HG2	1:C:219:ILE:O	1.99	0.62
2:D:19:LYS:O	2:D:23:VAL:HG23	1.99	0.62
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.82	0.62
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.82	0.62
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.28	0.62
2:D:200:GLU:HB2	2:D:268:PHE:CE2	2.34	0.62
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.35	0.61
4:F:241:THR:OG1	11:F:401:ACP:O3'	2.12	0.61
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.81	0.61
4:F:371:PRO:CA	4:F:372:THR:HB	2.30	0.61
2:B:204:ILE:CG2	2:B:209:LEU:HD11	2.30	0.61
2:B:333:LEU:O	2:B:337:ASN:ND2	2.33	0.61
2:D:287:THR:OG1	2:D:290:GLU:HG3	1.99	0.61
2:B:191:VAL:O	2:B:195:VAL:HG23	2.00	0.61
4:F:331:GLU:OE2	11:F:401:ACP:O3G	2.18	0.61
2:D:220:THR:O	2:D:222:PRO:HD3	2.00	0.61
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.01	0.60
1:C:10:GLY:O	1:C:14:VAL:HG23	2.00	0.60
1:A:68:VAL:HG11	1:A:149:PHE:CE2	2.35	0.60
2:D:2:ARG:HB3	2:D:133:GLN:HG2	1.82	0.60
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.15	0.60
2:D:12:CYS:HB3	2:D:140:SER:HB3	1.82	0.60
2:B:28:HIS:NE2	2:B:243:ARG:HD2	2.16	0.60
1:A:270:ALA:O	1:A:302:MET:HG2	2.01	0.60
1:A:291:ILE:HD13	1:A:373:ARG:HG3	1.84	0.60
2:B:199:ASP:OD1	9:B:504:MES:H62	2.01	0.60
4:F:349:GLY:O	4:F:353:VAL:HG22	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:199:PHE:CB	4:F:223:THR:HG22	2.31	0.60
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.19	0.59
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.36	0.59
2:B:65:ALA:O	2:B:91:ASN:ND2	2.33	0.59
1:C:175:PRO:HB3	2:D:349:ASN:ND2	2.17	0.59
2:D:95:GLY:O	2:D:96:GLN:NE2	2.35	0.59
1:A:292:THR:HG22	1:A:335:ILE:HD11	1.84	0.59
2:B:83:PHE:O	2:B:86:ILE:HG22	2.01	0.59
1:C:1:MET:O	1:C:51:THR:HG22	2.01	0.59
2:D:235:MET:O	2:D:239:THR:OG1	2.12	0.59
1:A:351:PHE:HE2	3:E:24:LEU:HD11	1.67	0.59
1:C:271:THR:HG23	1:C:300:ASN:O	2.02	0.59
1:C:1:MET:HE3	1:C:131:GLY:HA3	1.85	0.59
4:F:162:ILE:HD11	4:F:240:LEU:HD11	1.85	0.59
2:B:103:TRP:CD1	2:B:148:GLY:HA2	2.38	0.58
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.34	0.58
4:F:159:GLY:C	4:F:160:ILE:HD12	2.24	0.58
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.33	0.58
4:F:296:MET:SD	4:F:380:HIS:HB2	2.43	0.58
2:B:48:ARG:HH21	2:B:242:LEU:HA	1.68	0.58
4:F:199:PHE:HB2	4:F:223:THR:HG22	1.84	0.58
1:A:292:THR:HG22	1:A:335:ILE:CD1	2.33	0.58
2:B:69:ASP:O	2:B:94:PHE:HA	2.04	0.58
1:C:419:SER:O	1:C:423:GLU:HG3	2.03	0.58
2:D:154:ILE:CD1	2:D:168:THR:HG21	2.34	0.58
1:C:25:CYS:HB3	1:C:30:ILE:O	2.04	0.58
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.37	0.58
1:A:188:ILE:HD12	1:A:395:PHE:HB2	1.86	0.58
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.85	0.58
3:E:135:LYS:O	3:E:139:LEU:HG	2.02	0.58
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.85	0.58
1:A:22:GLU:HG3	1:A:83:TYR:CE2	2.39	0.57
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.84	0.57
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.86	0.57
2:D:146:GLY:N	8:D:501:GDP:O2B	2.31	0.57
4:F:320:MET:CG	4:F:330:ILE:HD11	2.34	0.57
1:C:97:GLU:HG3	2:D:2:ARG:CZ	2.35	0.57
2:D:210:TYR:CE1	2:D:222:PRO:HG2	2.39	0.57
1:A:270:ALA:HB3	1:A:302:MET:HG3	1.86	0.57
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.40	0.57
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:271:THR:HG21	1:C:295:CYS:HA	1.86	0.57
2:D:12:CYS:CB	2:D:140:SER:HB3	2.34	0.57
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.40	0.57
1:C:176:GLN:OE1	1:C:176:GLN:N	2.38	0.57
1:A:88:HIS:HD2	1:A:90:GLU:HB2	1.70	0.57
2:D:115:VAL:HG23	2:D:153:LEU:HD23	1.87	0.56
1:A:271:THR:CG2	1:A:295:CYS:HA	2.34	0.56
1:A:320:ARG:HA	1:A:356:ASN:O	2.04	0.56
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.70	0.56
1:C:209:ILE:HD11	1:C:302:MET:CE	2.34	0.56
2:D:2:ARG:O	2:D:133:GLN:NE2	2.29	0.56
1:A:224:TYR:H	2:B:247:GLN:HE21	1.54	0.56
4:F:318:ASP:OD2	11:F:401:ACP:O2G	2.23	0.56
1:C:333:ALA:O	1:C:337:THR:HG23	2.06	0.56
4:F:173:ILE:HD12	4:F:182:ILE:HD11	1.88	0.56
4:F:197:ARG:HB2	4:F:224:SER:O	2.05	0.56
1:A:331:ALA:O	1:A:335:ILE:HG13	2.05	0.56
2:D:124:LYS:C	2:D:124:LYS:HD3	2.26	0.56
1:A:317:LEU:HD23	1:A:377:MET:HG3	1.88	0.56
4:F:371:PRO:HA	4:F:372:THR:C	2.26	0.56
1:C:194:THR:HG22	1:C:198:SER:HB2	1.87	0.56
2:D:12:CYS:O	2:D:16:ILE:HG12	2.06	0.56
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.41	0.56
2:D:103:TRP:CE3	2:D:189:LEU:HD13	2.41	0.56
2:D:147:SER:HB2	2:D:190:SER:OG	2.06	0.56
2:D:83:PHE:O	2:D:86:ILE:HG22	2.06	0.55
1:C:71:GLU:OE1	1:C:73:THR:HG23	2.07	0.55
1:C:133:GLN:NE2	1:C:253:THR:HG21	2.21	0.55
4:F:87:LEU:O	4:F:88:SER:OG	2.22	0.55
1:C:107:HIS:CD2	1:C:152:LEU:HB2	2.41	0.55
4:F:153:ALA:CB	4:F:178:GLN:HG3	2.37	0.55
4:F:349:GLY:HA3	4:F:374:ILE:HD11	1.88	0.55
1:A:15:GLN:NE2	5:A:501:GTP:O6	2.38	0.55
2:B:349:ASN:O	2:B:352:LYS:HE2	2.07	0.55
4:F:317:PHE:HB3	4:F:319:PHE:CE1	2.42	0.55
2:B:105:LYS:HE2	2:B:411:GLU:OE2	2.07	0.55
2:B:124:LYS:HD3	2:B:124:LYS:C	2.27	0.55
2:B:294:GLN:O	2:B:300:ASN:HB2	2.07	0.55
2:B:103:TRP:CE3	2:B:189:LEU:HD13	2.42	0.55
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.89	0.55
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.37	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:GLY:O	1:A:14:VAL:HG23	2.07	0.54
1:A:188:ILE:HD12	1:A:395:PHE:CB	2.37	0.54
2:B:278:ARG:HG2	2:B:282:GLN:NE2	2.22	0.54
1:A:214:ARG:HG2	1:A:219:ILE:O	2.06	0.54
2:D:409:THR:HA	2:D:413:MET:O	2.08	0.54
4:F:280:GLU:HA	4:F:284:LEU:CB	2.38	0.54
2:B:108:TYR:CD2	3:E:82:VAL:HG11	2.43	0.54
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.90	0.54
3:E:60:ARG:O	3:E:64:GLN:HG3	2.06	0.54
3:E:72:LEU:O	3:E:76:ARG:HG2	2.06	0.54
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.43	0.54
2:B:93:VAL:HG11	2:B:118:VAL:HG22	1.90	0.54
1:C:114:ILE:O	1:C:118:VAL:HG23	2.07	0.54
2:D:180:THR:HB	2:D:183:GLU:HG3	1.89	0.54
1:A:25:CYS:HB3	1:A:30:ILE:O	2.07	0.53
2:B:69:ASP:HA	2:B:145:THR:HG21	1.90	0.53
4:F:132:LEU:O	4:F:136:ASN:ND2	2.41	0.53
1:A:250:VAL:HG12	1:A:254:GLU:OE1	2.07	0.53
2:B:181:VAL:HG13	1:C:258:ASN:ND2	2.23	0.53
2:B:188:THR:HG23	2:B:425:MET:HE2	1.90	0.53
1:A:221:ARG:HG3	2:B:325:MET:SD	2.48	0.53
2:D:112:ALA:O	2:D:115:VAL:HG12	2.08	0.53
4:F:135:TYR:OH	4:F:139:ARG:NH2	2.41	0.53
1:A:103:TYR:CE2	1:A:148:GLY:HA2	2.44	0.53
1:C:11:GLN:HE22	2:D:247:GLN:NE2	2.07	0.53
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.44	0.53
2:B:323:MET:HE1	2:B:373:MET:CB	2.39	0.53
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.44	0.53
2:D:88:ARG:NH1	2:D:90:ASP:HB2	2.24	0.53
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.24	0.52
4:F:102:PRO:HB2	4:F:104:ASN:OD1	2.09	0.52
2:D:11:GLN:O	2:D:15:GLN:HG2	2.09	0.52
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.91	0.52
4:F:189:PRO:HA	4:F:322:ASP:HA	1.91	0.52
2:B:309:HIS:O	2:B:436:GLN:NE2	2.42	0.52
2:B:333:LEU:HD13	4:F:57:GLY:HA3	1.91	0.52
2:D:208:ALA:O	2:D:212:ILE:HG13	2.09	0.52
1:A:132:LEU:O	1:A:164:LYS:NZ	2.42	0.52
1:C:1:MET:HG3	1:C:2:ARG:H	1.74	0.52
2:D:141:LEU:HD12	2:D:172:MET:SD	2.50	0.52
2:D:387:LEU:HD23	2:D:387:LEU:O	2.10	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:173:ILE:CD1	4:F:182:ILE:HD11	2.40	0.52
1:C:16:ILE:CD1	1:C:171:ILE:HD11	2.40	0.52
2:B:38:GLY:HA3	2:B:45:GLN:OE1	2.09	0.52
2:B:305:CYS:O	2:B:307:PRO:HD3	2.09	0.52
2:B:136:GLN:HA	2:B:167:ASN:O	2.10	0.52
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.45	0.52
2:B:30:ILE:HD13	2:B:36:TYR:HA	1.92	0.51
1:C:292:THR:HG22	1:C:335:ILE:HD11	1.91	0.51
4:F:246:GLN:O	4:F:250:SER:HB3	2.10	0.51
11:F:401:ACP:O3G	11:F:401:ACP:O1B	2.28	0.51
2:B:164:ARG:HD2	12:B:606:HOH:O	2.10	0.51
4:F:205:VAL:HG21	4:F:291:ILE:HG21	1.92	0.51
2:D:104:ALA:HB2	2:D:413:MET:SD	2.50	0.51
2:B:205:ASP:OD1	2:B:207:GLU:N	2.43	0.51
4:F:217:ARG:NH1	4:F:345:GLU:OE2	2.43	0.51
4:F:242:ASN:HD22	4:F:245:ILE:CD1	2.24	0.51
2:D:223:THR:O	2:D:227:LEU:HG	2.10	0.51
4:F:195:GLY:HA3	4:F:197:ARG:HE	1.75	0.51
2:B:2:ARG:HB2	2:B:133:GLN:CG	2.40	0.51
2:B:370:GLY:O	2:B:371:LEU:HD23	2.11	0.51
4:F:280:GLU:HA	4:F:284:LEU:HB3	1.93	0.51
2:B:108:TYR:CG	3:E:82:VAL:HG11	2.46	0.51
1:C:150:THR:O	1:C:154:MET:HG2	2.11	0.51
2:D:1:MET:HG3	2:D:50:ASN:CB	2.40	0.51
2:D:11:GLN:HG3	2:D:74:THR:OG1	2.10	0.51
1:C:117:LEU:HD11	1:C:121:ARG:NH2	2.26	0.51
4:F:304:THR:HG21	4:F:311:SER:OG	2.11	0.51
1:A:12:ALA:HB3	1:A:140:SER:HB3	1.93	0.50
1:A:270:ALA:HB3	1:A:302:MET:CG	2.41	0.50
2:D:427:ASP:O	2:D:431:GLU:HG3	2.11	0.50
1:C:97:GLU:HG3	2:D:2:ARG:NH1	2.26	0.50
2:B:244:PHE:CD1	2:B:358:ILE:HD12	2.47	0.50
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.93	0.50
1:A:99:ALA:CA	1:A:105:ARG:HD3	2.39	0.50
1:C:282:TYR:O	1:C:283:HIS:HB2	2.11	0.50
2:D:238:VAL:HA	2:D:378:ILE:HD11	1.93	0.50
3:E:85:LYS:O	3:E:89:GLU:HG3	2.11	0.50
4:F:221:LEU:HD13	4:F:262:MET:O	2.12	0.50
1:A:231:ILE:O	1:A:235:VAL:HG23	2.11	0.50
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.26	0.50
2:D:109:THR:O	2:D:113:GLU:HG2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:LEU:HB3	1:A:319:TYR:CE1	2.46	0.50
1:C:142:GLY:HA3	1:C:183:GLU:OE1	2.12	0.50
2:D:145:THR:HB	8:D:501:GDP:O2B	2.11	0.50
1:A:284:GLU:CD	1:A:284:GLU:H	2.14	0.50
2:B:96:GLN:HB3	1:C:1:MET:CE	2.41	0.50
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.94	0.50
2:B:179:ASP:N	2:B:183:GLU:OE2	2.42	0.50
2:D:30:ILE:CG2	2:D:86:ILE:HD11	2.42	0.50
2:D:137:LEU:HD12	2:D:138:THR:N	2.27	0.50
2:B:15:GLN:NE2	8:B:501:GDP:O6	2.44	0.49
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.47	0.49
4:F:71:LEU:HD12	4:F:77:LEU:HD13	1.94	0.49
1:A:103:TYR:CD2	1:A:148:GLY:HA2	2.48	0.49
1:A:101:ASN:HD22	2:B:258:ASN:HD21	1.59	0.49
1:A:357:TYR:CZ	3:E:17:GLY:HA2	2.48	0.49
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.51	0.49
4:F:287:ILE:HG23	4:F:319:PHE:CE1	2.48	0.49
4:F:338:CYS:HB3	4:F:343:TYR:CE1	2.47	0.49
2:D:207:GLU:HG2	2:D:304:ALA:CB	2.43	0.49
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.48	0.49
2:B:69:ASP:OD1	2:B:70:LEU:N	2.46	0.49
1:C:103:TYR:CD1	1:C:148:GLY:HA2	2.47	0.49
1:C:229:ARG:CZ	1:C:363:VAL:HG11	2.43	0.49
2:B:153:LEU:O	2:B:157:ILE:HG13	2.13	0.49
1:C:202:PHE:CE1	1:C:268:PRO:HG2	2.48	0.49
1:A:75:ILE:HD12	1:A:94:THR:CG2	2.42	0.49
2:B:7:ILE:O	2:B:137:LEU:HD12	2.13	0.49
2:D:48:ARG:O	2:D:51:VAL:HG23	2.13	0.49
4:F:126:ASP:OD2	4:F:128:ARG:HB2	2.13	0.49
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.13	0.49
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.41	0.48
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.48	0.48
1:A:216:ASN:HD22	1:A:275:VAL:HB	1.78	0.48
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.49	0.48
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.48	0.48
4:F:205:VAL:HG21	4:F:291:ILE:CG2	2.43	0.48
2:B:123:ARG:O	2:B:127:GLU:HG3	2.13	0.48
2:B:188:THR:HG22	2:B:421:ALA:HB1	1.95	0.48
2:D:205:ASP:HB3	2:D:303:ALA:HA	1.95	0.48
2:B:289:PRO:O	2:B:293:GLN:HG3	2.14	0.48
1:C:3:GLU:OE1	1:C:129:CYS:HB3	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:9:ALA:HA	2:D:68:VAL:O	2.13	0.48
2:D:171:VAL:HA	2:D:204:ILE:O	2.14	0.48
4:F:201:ILE:HG12	4:F:221:LEU:HG	1.95	0.48
1:A:93:ILE:CD1	1:A:121:ARG:HG3	2.39	0.48
2:B:204:ILE:HG21	2:B:231:VAL:HG22	1.95	0.48
2:B:270:PRO:HA	2:B:377:PHE:O	2.14	0.48
2:B:334:ASN:O	2:B:338:LYS:HG3	2.13	0.48
1:C:39:ASP:OD2	1:C:61:HIS:NE2	2.35	0.48
2:D:397:ALA:O	2:D:401:ARG:NH1	2.47	0.48
2:D:152:LEU:O	2:D:156:LYS:HG2	2.14	0.48
1:C:71:GLU:OE2	1:C:73:THR:OG1	2.31	0.48
2:D:68:VAL:HG21	2:D:118:VAL:HG11	1.95	0.48
1:C:34:GLY:HA3	1:C:60:LYS:HG3	1.95	0.47
3:E:46:SER:O	3:E:50:ILE:HG13	2.14	0.47
2:B:235:MET:O	2:B:239:THR:HG23	2.13	0.47
2:D:165:ILE:HD11	2:D:253:ARG:HG3	1.95	0.47
1:A:176:GLN:HG3	4:F:56:PRO:HB3	1.96	0.47
2:B:174:SER:OG	2:B:207:GLU:HB2	2.15	0.47
1:C:6:SER:O	1:C:65:ALA:HA	2.14	0.47
1:C:208:ALA:O	1:C:212:ILE:HG13	2.14	0.47
4:F:350:ILE:O	4:F:354:ALA:HB3	2.14	0.47
2:D:66:ILE:CD1	2:D:121:VAL:HG12	2.44	0.47
2:D:106:GLY:O	2:D:111:GLY:HA3	2.14	0.47
2:B:384:ILE:HD11	2:B:387:LEU:HD13	1.97	0.47
1:A:351:PHE:CE2	3:E:24:LEU:HD11	2.49	0.47
2:D:173:PRO:HB2	2:D:183:GLU:OE1	2.15	0.47
2:D:326:LYS:O	2:D:330:GLU:HG3	2.14	0.47
4:F:190:LEU:HB2	4:F:322:ASP:O	2.15	0.47
1:C:234:ILE:HG12	1:C:302:MET:CE	2.45	0.47
4:F:371:PRO:HA	4:F:372:THR:CB	2.43	0.47
1:A:419:SER:O	1:A:423:GLU:HG3	2.15	0.47
2:D:26:ASP:OD2	2:D:369:ARG:HD2	2.15	0.47
1:A:99:ALA:HA	1:A:105:ARG:CD	2.41	0.46
1:C:271:THR:CG2	1:C:295:CYS:HA	2.45	0.46
1:C:147:SER:HB2	1:C:190:THR:CB	2.40	0.46
1:C:77:GLU:O	1:C:81:GLY:N	2.48	0.46
1:C:234:ILE:HG12	1:C:302:MET:HE2	1.97	0.46
1:C:319:TYR:HB2	1:C:355:ILE:HG12	1.96	0.46
2:D:115:VAL:HG23	2:D:153:LEU:CD2	2.45	0.46
4:F:7:ARG:HB2	4:F:42:GLY:HA2	1.98	0.46
1:A:134:GLY:HA3	1:A:165:SER:O	2.14	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:188:ILE:HD12	1:A:395:PHE:CG	2.50	0.46
2:B:5:VAL:HG23	2:B:132:LEU:HD11	1.97	0.46
2:B:8:GLN:HB2	2:B:13:GLY:O	2.15	0.46
2:B:159:GLU:HB2	3:E:72:LEU:HD13	1.98	0.46
2:B:350:ASN:OD1	2:B:350:ASN:N	2.41	0.46
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.97	0.46
2:B:7:ILE:O	2:B:137:LEU:HA	2.15	0.46
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.51	0.46
2:D:248:LEU:CD2	2:D:352:LYS:HB3	2.45	0.46
2:D:312:TYR:CE1	2:D:377:PHE:HZ	2.34	0.46
1:A:215:ARG:NH1	1:A:299:ALA:HB1	2.30	0.46
2:B:2:ARG:HD3	2:B:133:GLN:NE2	2.31	0.46
2:B:213:CYS:HB3	2:B:219:LEU:HD12	1.97	0.46
2:B:320:ARG:O	2:B:373:MET:HA	2.16	0.46
2:D:220:THR:C	2:D:222:PRO:HD3	2.36	0.46
4:F:81:ILE:HG12	4:F:87:LEU:HD13	1.97	0.46
1:C:229:ARG:NH1	1:C:366:GLY:HA2	2.31	0.46
2:D:126:SER:O	2:D:129:CYS:HB2	2.16	0.46
2:D:295:MET:CE	2:D:377:PHE:HB2	2.45	0.46
1:A:2:ARG:HB3	1:A:133:GLN:HG3	1.98	0.46
2:B:337:ASN:ND2	4:F:58:LEU:HD21	2.30	0.46
2:D:238:VAL:CB	2:D:378:ILE:HD11	2.46	0.46
4:F:162:ILE:HD11	4:F:240:LEU:CD1	2.46	0.46
2:B:307:PRO:HB3	2:B:312:TYR:OH	2.16	0.46
2:B:334:ASN:ND2	2:B:338:LYS:HD2	2.30	0.46
1:C:23:LEU:O	1:C:27:GLU:HG3	2.15	0.46
1:C:265:ILE:HG23	1:C:432:TYR:CZ	2.51	0.46
2:D:318:ILE:N	2:D:318:ILE:HD12	2.31	0.46
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.97	0.45
2:D:308:ARG:HG2	2:D:342:TYR:CZ	2.51	0.45
1:C:223:THR:H	1:C:226:ASN:HB2	1.81	0.45
1:C:381:THR:O	1:C:384:ILE:HG22	2.16	0.45
2:D:259:MET:HA	2:D:314:THR:OG1	2.16	0.45
1:C:194:THR:HG22	1:C:194:THR:O	2.16	0.45
2:B:244:PHE:CE1	2:B:358:ILE:HD12	2.52	0.45
2:D:206:ASN:ND2	8:D:501:GDP:O2'	2.49	0.45
2:D:416:MET:O	2:D:420:GLU:HG3	2.16	0.45
4:F:240:LEU:HD12	4:F:240:LEU:N	2.31	0.45
4:F:283:ILE:HD11	4:F:321:VAL:HG11	1.99	0.45
1:A:21:TRP:CH2	1:A:63:PRO:HB3	2.51	0.45
2:B:67:LEU:N	2:B:67:LEU:HD12	2.32	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:VAL:HG12	1:C:145:THR:HG22	1.98	0.45
1:A:234:ILE:HD12	1:A:234:ILE:N	2.32	0.45
2:B:137:LEU:HD23	2:B:154:ILE:HD11	1.99	0.45
1:A:307:PRO:HA	1:A:383:ALA:HB2	1.97	0.45
1:A:317:LEU:HB3	1:A:319:TYR:HE1	1.81	0.45
2:D:108:TYR:OH	2:D:417:GLU:OE2	2.30	0.45
4:F:151:SER:HB3	4:F:180:HIS:CG	2.52	0.45
1:C:225:THR:O	1:C:229:ARG:HG2	2.16	0.45
1:A:201:ALA:O	1:A:268:PRO:HD2	2.16	0.45
1:C:104:ALA:HB2	1:C:413:MET:SD	2.58	0.45
4:F:4:PHE:CZ	4:F:29:ARG:HB2	2.52	0.45
2:B:146:GLY:O	2:B:150:GLY:HA3	2.16	0.44
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.98	0.44
1:A:307:PRO:HA	1:A:383:ALA:CB	2.47	0.44
2:B:404:PHE:CD1	1:C:261:PRO:HA	2.52	0.44
3:E:58:GLU:O	3:E:62:LYS:HG3	2.17	0.44
1:A:271:THR:HG21	1:A:295:CYS:CA	2.46	0.44
2:B:114:LEU:O	2:B:114:LEU:HG	2.17	0.44
4:F:334:GLY:C	4:F:336:PRO:HD3	2.38	0.44
2:B:54:ASN:OD1	2:B:64:ARG:NH2	2.47	0.44
1:C:103:TYR:CE1	1:C:148:GLY:HA2	2.53	0.44
2:D:67:LEU:N	2:D:67:LEU:HD12	2.32	0.44
2:D:99:ALA:HB2	2:D:145:THR:OG1	2.17	0.44
3:E:129:HIS:O	3:E:133:VAL:HG23	2.18	0.44
4:F:74:LYS:NZ	4:F:331:GLU:OE1	2.41	0.44
1:A:326:LYS:HE2	1:A:326:LYS:HB3	1.76	0.44
1:A:328:VAL:O	1:A:332:ILE:HG13	2.16	0.44
2:B:98:GLY:HA3	12:B:615:HOH:O	2.17	0.44
1:C:278:ALA:HA	1:C:369:ALA:HB2	1.99	0.44
1:C:56:THR:OG1	1:C:60:LYS:HB3	2.17	0.44
1:C:108:TYR:O	1:C:112:LYS:HG2	2.18	0.44
4:F:146:VAL:HG11	4:F:233:PHE:CE1	2.52	0.44
4:F:320:MET:HB2	4:F:328:TRP:HB2	1.99	0.44
1:C:271:THR:HG21	1:C:295:CYS:O	2.18	0.44
2:D:30:ILE:HG21	2:D:86:ILE:HD11	1.99	0.44
1:A:8:HIS:HB3	1:A:13:GLY:O	2.17	0.44
1:A:12:ALA:CB	1:A:140:SER:HB3	2.48	0.44
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.48	0.44
1:C:107:HIS:O	1:C:152:LEU:HD22	2.18	0.44
1:C:192:HIS:CG	1:C:421:ALA:HA	2.53	0.44
2:D:146:GLY:O	2:D:150:GLY:HA3	2.18	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:299:GLU:HB3	4:F:300:PRO:HD3	2.00	0.44
1:A:69:ASP:O	1:A:94:THR:HA	2.18	0.43
2:B:190:SER:O	2:B:194:LEU:HG	2.18	0.43
2:B:331:GLN:O	2:B:334:ASN:HB3	2.18	0.43
1:C:308:ARG:NE	12:C:605:HOH:O	2.51	0.43
1:A:343:PHE:CE1	1:A:349:THR:HG23	2.53	0.43
2:B:102:ASN:OD1	2:B:104:ALA:N	2.49	0.43
1:A:238:ILE:O	1:A:238:ILE:HG22	2.18	0.43
1:A:437:VAL:HG12	1:A:438:ASP:N	2.33	0.43
2:D:181:VAL:HG13	2:D:182:VAL:HG13	2.01	0.43
3:E:10:GLU:O	3:E:20:PHE:HA	2.18	0.43
4:F:69:ASP:N	4:F:69:ASP:OD1	2.52	0.43
4:F:150:LYS:HB3	4:F:160:ILE:HG13	2.00	0.43
1:A:227:LEU:O	1:A:231:ILE:HG13	2.18	0.43
1:A:277:SER:O	1:A:280:LYS:HB2	2.18	0.43
2:B:93:VAL:CG1	2:B:118:VAL:HG22	2.48	0.43
2:D:271:GLY:N	2:D:377:PHE:O	2.50	0.43
4:F:287:ILE:HG23	4:F:319:PHE:CZ	2.53	0.43
1:A:194:THR:O	1:A:194:THR:HG22	2.18	0.43
2:B:312:TYR:O	2:B:344:VAL:HG22	2.18	0.43
2:B:346:TRP:CE3	2:B:347:ILE:HG13	2.54	0.43
1:C:173:PRO:HG2	1:C:391:LEU:HD11	2.01	0.43
4:F:146:VAL:HG21	4:F:233:PHE:CZ	2.54	0.43
2:B:13:GLY:CA	2:B:139:HIS:HA	2.49	0.43
2:D:270:PRO:HA	2:D:377:PHE:O	2.19	0.43
4:F:280:GLU:HA	4:F:284:LEU:HB2	2.00	0.43
2:B:411:GLU:O	3:E:86:ALA:HB2	2.19	0.43
1:C:259:LEU:O	1:C:380:ASN:ND2	2.51	0.43
2:D:36:TYR:CD1	2:D:46:LEU:HD21	2.54	0.43
2:D:38:GLY:HA3	2:D:45:GLN:OE1	2.18	0.43
1:A:5:ILE:O	1:A:135:PHE:HA	2.19	0.43
2:B:323:MET:HB3	2:B:373:MET:HE2	2.01	0.43
1:A:188:ILE:HD12	1:A:395:PHE:CD2	2.54	0.42
2:B:21:TRP:CH2	2:B:52:TYR:HB3	2.54	0.42
1:C:141:PHE:HB2	1:C:173:PRO:HD3	2.00	0.42
2:B:354:ALA:HB2	10:B:505:W1P:C	2.49	0.42
1:C:117:LEU:O	1:C:121:ARG:HG2	2.19	0.42
1:A:25:CYS:SG	1:A:86:LEU:HD11	2.59	0.42
4:F:98:TYR:HE1	4:F:130:VAL:HG12	1.84	0.42
1:A:166:LYS:HE2	1:A:197:HIS:O	2.20	0.42
1:A:205:ASP:OD1	1:A:207:GLU:HB3	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:VAL:O	1:A:239:THR:HG23	2.18	0.42
2:B:67:LEU:HD12	2:B:67:LEU:H	1.83	0.42
2:D:14:ASN:HB2	2:D:74:THR:HG21	2.02	0.42
2:D:392:SER:O	2:D:396:THR:HG22	2.20	0.42
4:F:259:GLY:O	4:F:261:GLU:HG3	2.19	0.42
1:A:90:GLU:OE1	1:A:90:GLU:N	2.53	0.42
1:A:195:LEU:HD12	1:A:266:HIS:CE1	2.55	0.42
1:A:381:THR:HG22	1:A:383:ALA:N	2.10	0.42
3:E:128:LYS:O	3:E:128:LYS:HD3	2.19	0.42
1:A:16:ILE:CD1	1:A:171:ILE:HD11	2.50	0.42
2:B:164:ARG:NH1	12:B:606:HOH:O	2.53	0.42
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.85	0.42
1:C:292:THR:HG22	1:C:335:ILE:HD12	2.00	0.42
2:D:7:ILE:O	2:D:137:LEU:HA	2.18	0.42
3:E:92:ASN:O	3:E:96:MET:HG2	2.20	0.42
4:F:199:PHE:HB3	4:F:223:THR:HG22	2.01	0.42
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.50	0.42
2:D:248:LEU:HD21	2:D:352:LYS:HB3	2.02	0.42
4:F:34:ASN:OD1	4:F:35:PRO:HD2	2.20	0.42
2:D:137:LEU:HD11	2:D:139:HIS:HB3	2.02	0.41
2:D:295:MET:HE2	2:D:377:PHE:HB2	2.02	0.41
1:C:209:ILE:HG22	1:C:227:LEU:CD2	2.50	0.41
1:A:141:PHE:HB3	1:A:187:SER:OG	2.20	0.41
9:B:504:MES:H81	9:B:504:MES:H51	1.76	0.41
2:D:400:ARG:HG3	2:D:401:ARG:N	2.35	0.41
3:E:75:LYS:O	3:E:79:GLU:HG3	2.20	0.41
4:F:98:TYR:CE1	4:F:130:VAL:HG12	2.55	0.41
4:F:315:PHE:C	4:F:336:PRO:HG3	2.41	0.41
1:A:114:ILE:HG12	1:A:114:ILE:O	2.20	0.41
1:A:289:ALA:O	1:A:293:ASN:HB2	2.19	0.41
2:B:75:MET:CE	2:B:92:PHE:HD2	2.34	0.41
1:C:209:ILE:HG23	1:C:230:LEU:HD23	2.03	0.41
1:C:406:HIS:ND1	2:D:263:PRO:HD3	2.36	0.41
2:D:187:ALA:O	2:D:191:VAL:HG23	2.20	0.41
2:D:194:LEU:CD2	2:D:198:THR:HG21	2.51	0.41
2:B:157:ILE:HG21	2:B:166:MET:HE1	2.02	0.41
2:B:268:PHE:N	2:B:268:PHE:CD1	2.88	0.41
2:D:287:THR:HB	2:D:289:PRO:HD2	2.02	0.41
1:A:54:SER:O	1:A:61:HIS:HA	2.21	0.41
2:B:316:ALA:HB2	10:B:505:W1P:C9	2.50	0.41
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.02	0.41
2:D:51:VAL:HG21	2:D:242:LEU:O	2.20	0.41
4:F:253:TYR:CZ	4:F:259:GLY:HA2	2.56	0.41
1:C:206:ASN:OD1	5:C:501:GTP:N2	2.47	0.41
2:D:69:ASP:OD1	2:D:70:LEU:N	2.54	0.41
1:A:2:ARG:CB	1:A:133:GLN:HG3	2.51	0.41
1:A:196:GLU:HA	1:A:196:GLU:OE1	2.21	0.41
1:A:209:ILE:HG22	1:A:227:LEU:CD2	2.47	0.41
2:B:46:LEU:HA	2:B:49:ILE:HB	2.02	0.41
1:C:22:GLU:O	1:C:26:LEU:HG	2.21	0.41
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.52	0.41
1:C:291:ILE:HG13	1:C:292:THR:N	2.36	0.41
2:D:205:ASP:OD1	2:D:207:GLU:HB3	2.19	0.41
4:F:151:SER:HB3	4:F:180:HIS:CD2	2.56	0.41
4:F:196:HIS:O	4:F:227:PRO:HA	2.21	0.41
4:F:217:ARG:HG3	4:F:218:GLU:N	2.35	0.41
4:F:225:SER:HB2	4:F:252:ASN:O	2.21	0.41
4:F:298:ILE:O	4:F:302:ILE:HG12	2.21	0.41
4:F:341:LYS:O	4:F:341:LYS:HG2	2.21	0.41
2:B:88:ARG:HH11	2:B:90:ASP:HB2	1.82	0.41
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.56	0.41
1:C:205:ASP:HB2	1:C:303:VAL:HA	2.03	0.41
2:D:295:MET:HE2	2:D:295:MET:HB2	1.90	0.41
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.56	0.41
1:C:234:ILE:H	1:C:234:ILE:HD12	1.86	0.40
2:D:258:ASN:O	2:D:314:THR:HG21	2.22	0.40
2:B:119:LEU:HD11	2:B:156:LYS:CB	2.52	0.40
1:C:164:LYS:HE3	1:C:164:LYS:HB2	1.88	0.40
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.51	0.40
3:E:58:GLU:HG2	3:E:62:LYS:HE3	2.04	0.40
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.50	0.40
2:B:208:ALA:O	2:B:212:ILE:HG13	2.21	0.40
2:D:406:HIS:HA	2:D:409:THR:OG1	2.22	0.40
4:F:65:TYR:HE1	4:F:312:PHE:HA	1.86	0.40
4:F:217:ARG:HG3	4:F:218:GLU:HG2	2.04	0.40
1:A:5:ILE:HA	1:A:64:ARG:O	2.21	0.40
1:A:185:TYR:OH	1:A:398:MET:HB3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:610:HOH:O	12:C:605:HOH:O[3_555]	1.92	0.28

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%)	415 (95%)	21 (5%)	0	100	100
1	C	439/451 (97%)	425 (97%)	14 (3%)	0	100	100
2	B	421/445 (95%)	395 (94%)	25 (6%)	1 (0%)	47	69
2	D	425/445 (96%)	403 (95%)	21 (5%)	1 (0%)	47	69
3	E	119/143 (83%)	117 (98%)	2 (2%)	0	100	100
4	F	344/384 (90%)	321 (93%)	22 (6%)	1 (0%)	41	61
All	All	2184/2319 (94%)	2076 (95%)	105 (5%)	3 (0%)	51	75

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	82	PRO
4	F	236	LYS
2	D	278	ARG

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%)	365 (99%)	4 (1%)	73	86
1	C	372/379 (98%)	365 (98%)	7 (2%)	57	77
2	B	367/383 (96%)	361 (98%)	6 (2%)	62	81
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%)	313 (99%)	2 (1%)	86	93
All	All	1901/1993 (95%)	1879 (99%)	22 (1%)	71	85

All (22) 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
2	B	139	HIS
2	B	153	LEU
2	B	180	THR
2	B	242	LEU
2	B	315	VAL
2	B	350	ASN
1	C	47	ASP
1	C	71	GLU
1	C	80	THR
1	C	221	ARG
1	C	279	GLU
1	C	361	THR
1	C	406	HIS
2	D	139	HIS
2	D	229	HIS
2	D	270	PRO
4	F	31	ARG
4	F	257	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	88	HIS
1	A	101	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	107	HIS
2	B	15	GLN
2	B	167	ASN
2	B	206	ASN
2	B	247	GLN
2	B	282	GLN
2	B	294	GLN
2	B	300	ASN
1	C	11	GLN
1	C	15	GLN
1	C	133	GLN
2	D	96	GLN
2	D	107	HIS
2	D	294	GLN
4	F	136	ASN
4	F	180	HIS
4	F	229	ASN
4	F	242	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 17 ligands modelled in this entry, 9 are monoatomic - leaving 8 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
5	GTP	C	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.75	7 (21%)
9	MES	B	504	-	12,12,12	2.24	1 (8%)	14,16,16	1.99	6 (42%)
8	GDP	D	501	6	24,30,30	1.18	2 (8%)	31,47,47	1.94	8 (25%)
11	ACP	F	401	6	27,33,33	1.37	5 (18%)	32,52,52	1.51	4 (12%)
10	W1P	B	505	-	12,14,14	0.56	0	15,19,19	0.80	1 (6%)
10	W1P	B	506	-	12,14,14	0.58	0	15,19,19	0.74	0
5	GTP	A	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.75	6 (18%)
8	GDP	B	501	6	24,30,30	1.19	2 (8%)	31,47,47	2.04	8 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GTP	C	501	6	-	10/18/38/38	0/3/3/3
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
8	GDP	D	501	6	-	2/12/32/32	0/3/3/3
11	ACP	F	401	6	-	8/15/38/38	0/3/3/3
10	W1P	B	505	-	-	0/4/16/16	0/2/2/2
10	W1P	B	506	-	-	0/4/16/16	0/2/2/2
5	GTP	A	501	6	-	4/18/38/38	0/3/3/3
8	GDP	B	501	6	-	2/12/32/32	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	-7.47	1.66	1.77
8	D	501	GDP	C6-C5	4.20	1.48	1.41
8	B	501	GDP	C6-C5	4.16	1.48	1.41
5	C	501	GTP	C6-N1	3.03	1.38	1.33
5	A	501	GTP	C6-N1	3.01	1.38	1.33
11	F	401	ACP	PG-O2G	2.87	1.61	1.54
11	F	401	ACP	PG-O3G	2.87	1.61	1.54
11	F	401	ACP	PB-O3A	2.71	1.61	1.58
11	F	401	ACP	C5-C4	2.51	1.47	1.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	501	GDP	C5-C4	2.47	1.47	1.40
8	B	501	GDP	C5-C4	2.44	1.47	1.40
11	F	401	ACP	PB-O2B	2.17	1.61	1.56

All (40) 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
5	C	501	GTP	N3-C2-N1	-5.28	120.18	127.22
8	B	501	GDP	C2-N3-C4	5.00	121.07	115.36
8	D	501	GDP	C2-N3-C4	4.81	120.85	115.36
11	F	401	ACP	PA-O3A-PB	-4.43	118.51	132.56
5	C	501	GTP	C2-N3-C4	4.37	120.35	115.36
5	A	501	GTP	C2-N3-C4	4.24	120.20	115.36
8	B	501	GDP	C6-C5-C4	-4.21	116.78	120.80
8	B	501	GDP	C6-N1-C2	4.09	122.43	115.93
8	D	501	GDP	C6-N1-C2	4.03	122.33	115.93
8	D	501	GDP	C5-C6-N1	-3.95	118.03	123.43
8	D	501	GDP	C6-C5-C4	-3.84	117.13	120.80
8	B	501	GDP	C5-C6-N1	-3.81	118.23	123.43
11	F	401	ACP	C3'-C2'-C1'	3.57	106.35	100.98
8	B	501	GDP	PA-O3A-PB	-3.51	120.80	132.83
9	B	504	MES	C5-N4-C3	3.49	116.69	108.83
8	B	501	GDP	N3-C2-N1	-3.46	122.61	127.22
5	C	501	GTP	PA-O3A-PB	-3.32	121.42	132.83
5	A	501	GTP	PB-O3B-PG	-3.26	121.65	132.83
8	D	501	GDP	N3-C2-N1	-3.23	122.91	127.22
11	F	401	ACP	N3-C2-N1	-3.20	123.68	128.68
8	D	501	GDP	PA-O3A-PB	-3.09	122.22	132.83
9	B	504	MES	C6-C5-N4	-3.07	105.44	110.10
5	A	501	GTP	PA-O3A-PB	-3.04	122.38	132.83
8	B	501	GDP	C3'-C2'-C1'	2.97	105.45	100.98
8	D	501	GDP	C3'-C2'-C1'	2.80	105.20	100.98
9	B	504	MES	O1S-S-C8	2.77	110.25	106.92
5	C	501	GTP	PB-O3B-PG	-2.73	123.47	132.83
5	A	501	GTP	C5-C6-N1	-2.71	119.72	123.43
8	B	501	GDP	C4-C5-N7	-2.67	106.62	109.40
11	F	401	ACP	C4-C5-N7	-2.65	106.64	109.40
8	D	501	GDP	C4-C5-N7	-2.61	106.68	109.40
5	C	501	GTP	C5-C6-N1	-2.57	119.92	123.43
5	A	501	GTP	C6-N1-C2	2.50	119.91	115.93
9	B	504	MES	O3S-S-C8	2.43	109.70	105.77

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	C3'-C2'-C1'	2.38	104.57	100.98
5	C	501	GTP	C6-N1-C2	2.34	119.64	115.93
9	B	504	MES	C7-N4-C5	2.29	117.10	111.23
9	B	504	MES	O2S-S-C8	2.03	109.36	106.92
10	B	505	W1P	C-C1-N	2.03	123.44	121.70

There are no chirality outliers.

All (30) torsion outliers are listed below:

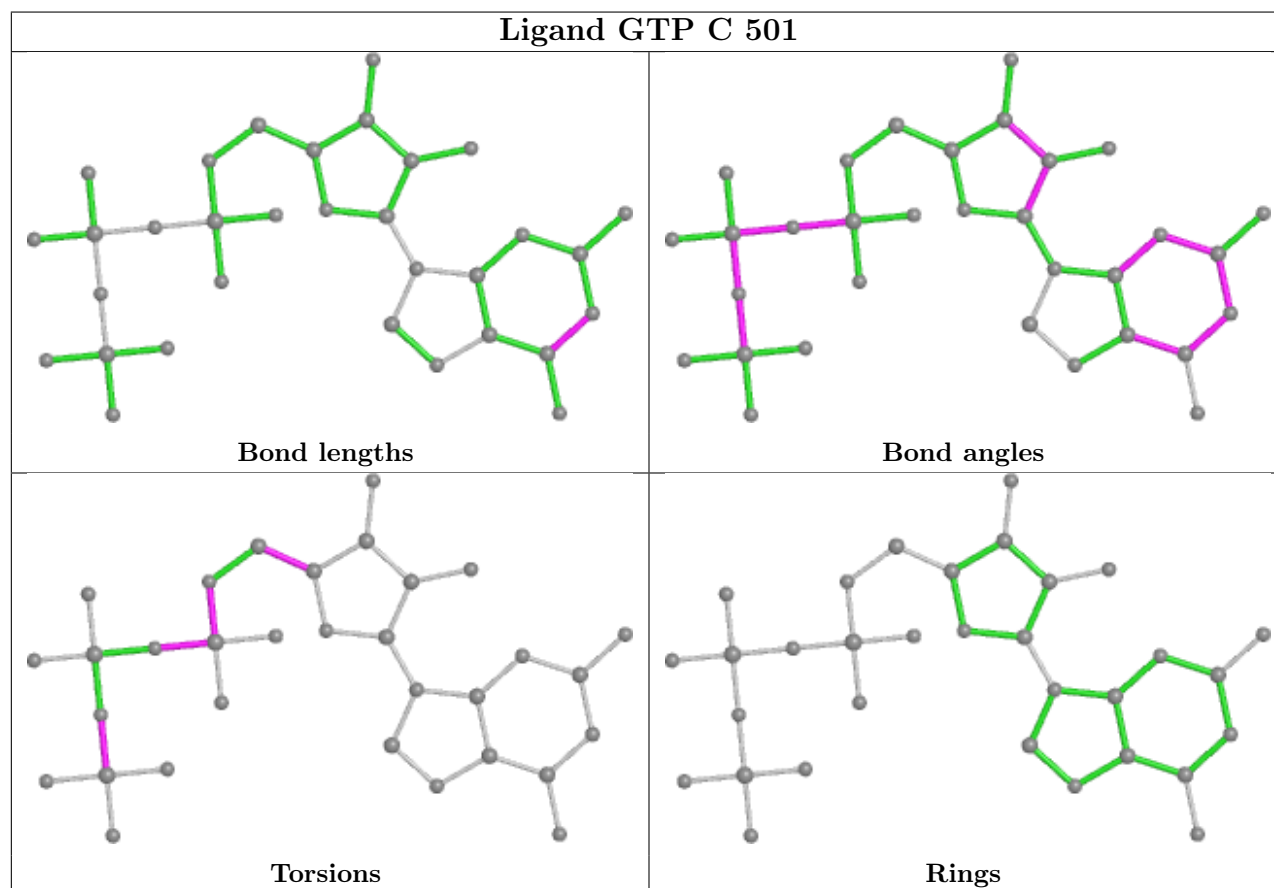
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O3A
9	B	504	MES	C8-C7-N4-C5
9	B	504	MES	C7-C8-S-O1S
9	B	504	MES	C7-C8-S-O2S
9	B	504	MES	C7-C8-S-O3S
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C5'-O5'-PA-O2A
11	F	401	ACP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C3'-C4'-C5'-O5'
5	C	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	O4'-C4'-C5'-O5'
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
11	F	401	ACP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O1A

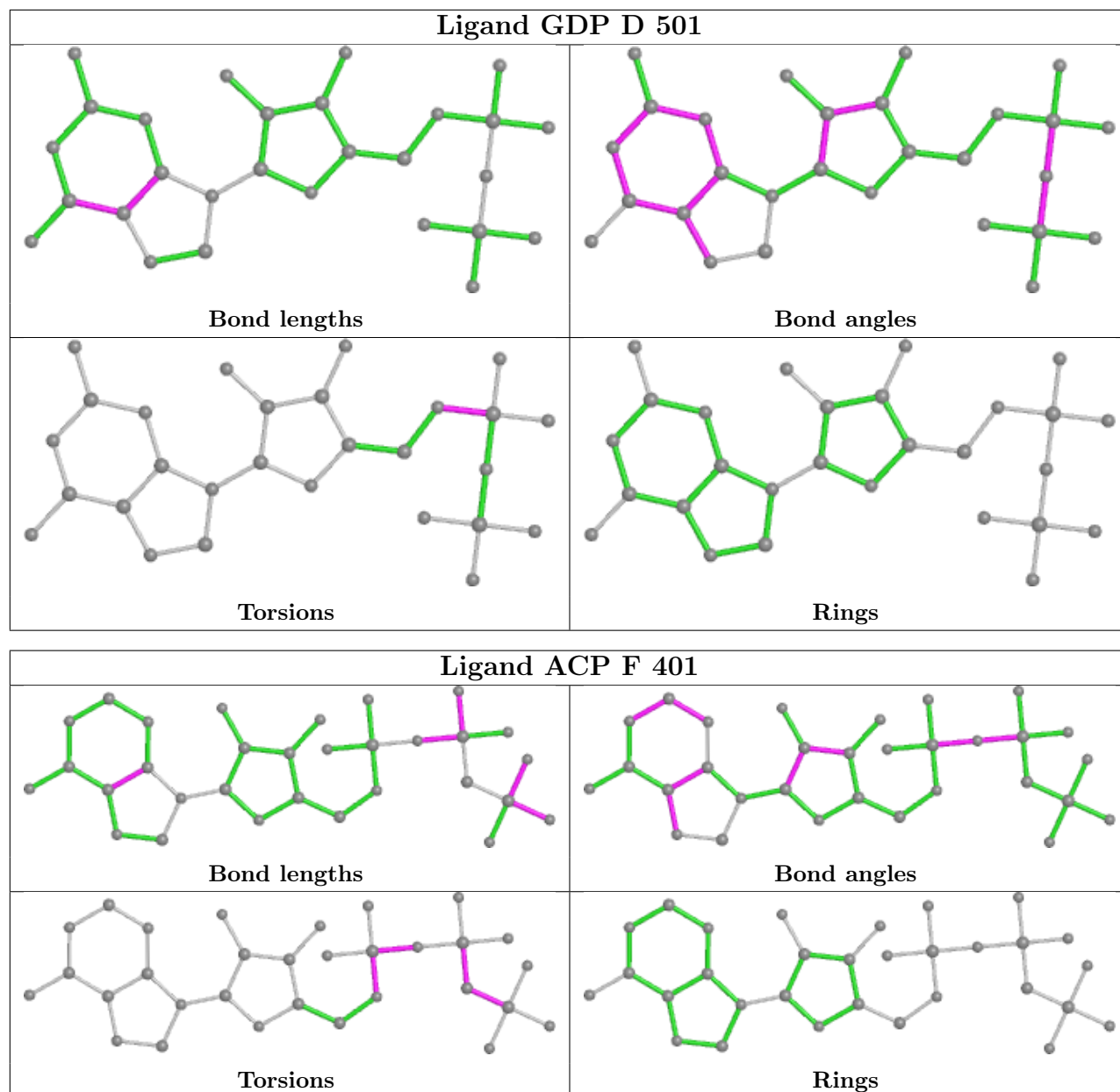
There are no ring outliers.

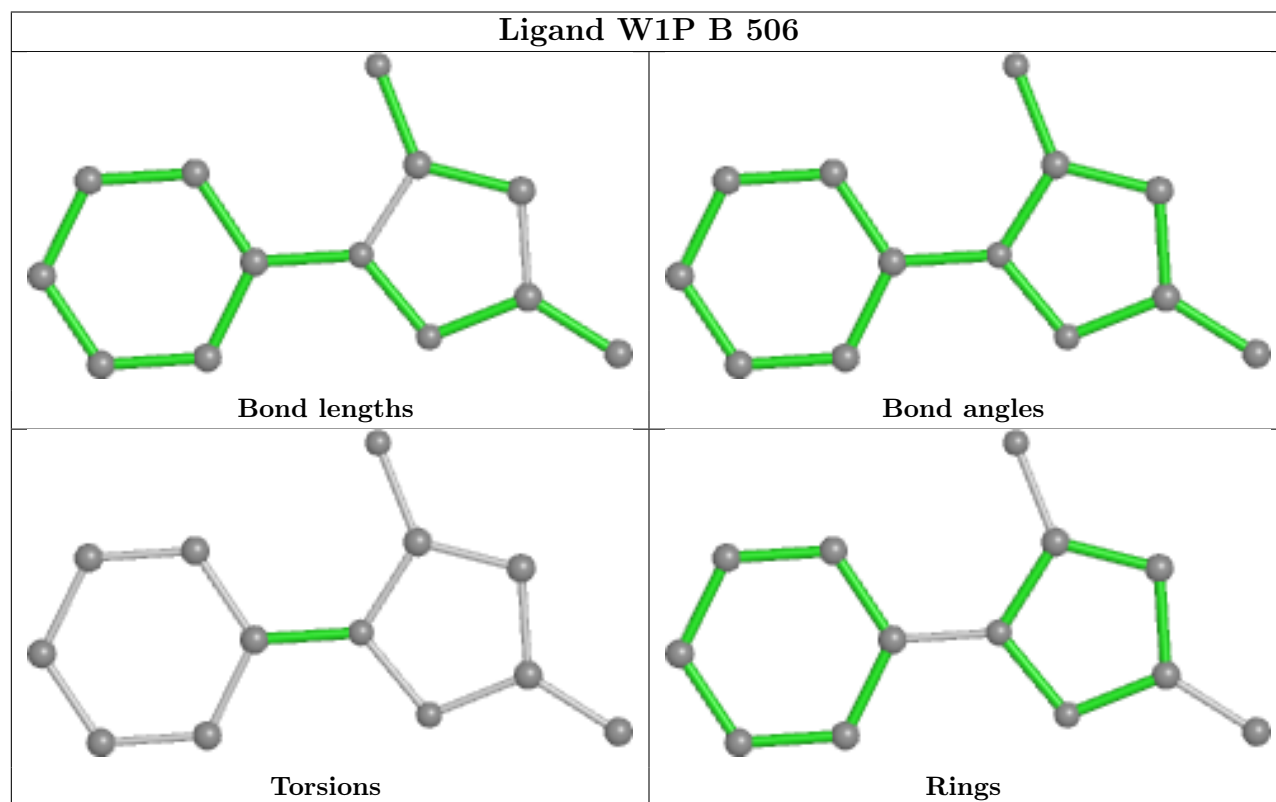
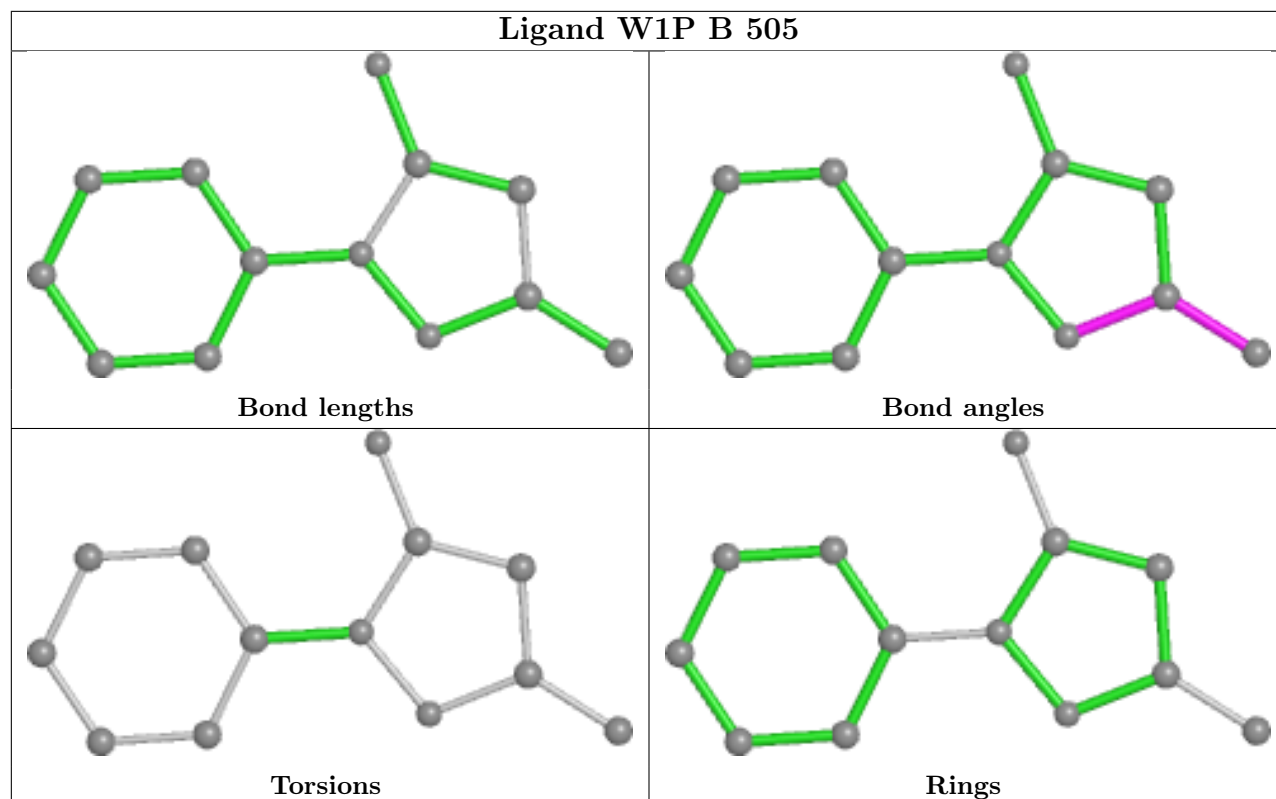
7 monomers are involved in 20 short contacts:

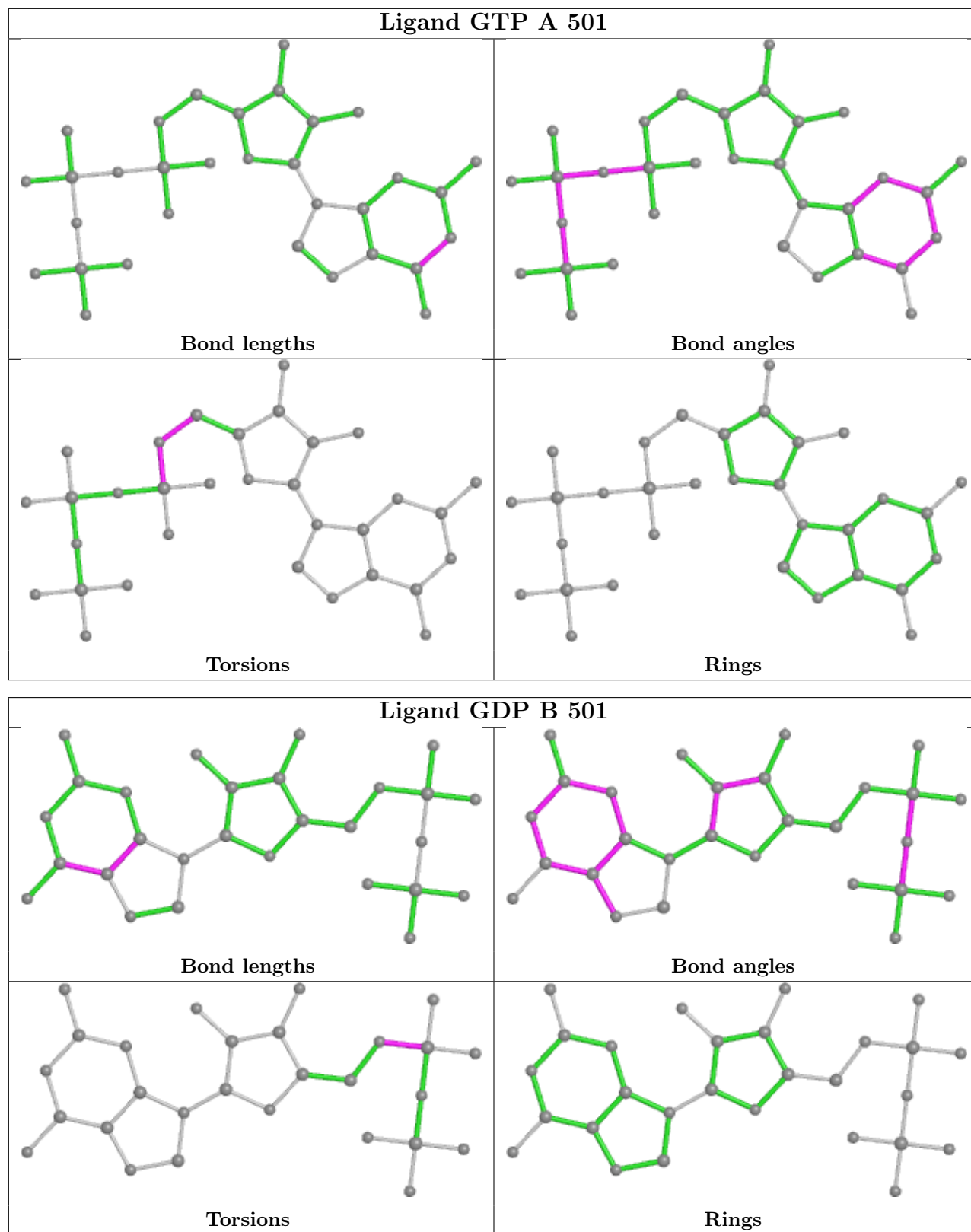
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	501	GTP	1	0
9	B	504	MES	3	0
8	D	501	GDP	5	0
11	F	401	ACP	4	0
10	B	505	W1P	3	0
5	A	501	GTP	2	0
8	B	501	GDP	2	0

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









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, 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%)	0.64	41 (9%) 8 4	58, 82, 130, 238	0
1	C	440/451 (97%)	0.39	21 (4%) 30 23	47, 69, 104, 154	0
2	B	425/445 (95%)	0.63	33 (7%) 13 8	52, 78, 151, 235	3 (0%)
2	D	429/445 (96%)	0.51	32 (7%) 14 9	68, 100, 138, 201	4 (0%)
3	E	123/143 (86%)	0.69	12 (9%) 7 4	72, 102, 156, 211	0
4	F	352/384 (91%)	0.46	26 (7%) 14 9	80, 116, 168, 211	0
All	All	2207/2319 (95%)	0.54	165 (7%) 14 9	47, 89, 153, 238	7 (0%)

All (165) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	285	ALA	11.0
2	D	278	ARG	7.4
2	B	337	ASN	6.6
2	B	333	LEU	6.5
3	E	24	LEU	6.2
2	B	360	PRO	6.0
1	C	286	LEU	5.6
2	B	284	ARG	5.2
1	A	299	ALA	5.1
2	D	274	PRO	4.6
2	B	276	THR	4.5
1	A	88	HIS	4.5
4	F	36	ARG	4.4
4	F	71	LEU	4.4
1	A	282	TYR	4.4
3	E	50	ILE	4.4
2	B	281	GLN	4.4
2	B	332	MET	4.3
1	A	323	VAL	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	342	GLN	4.2
2	D	373	MET	4.2
4	F	89	GLU	4.2
1	C	285	GLN	4.0
2	D	312	TYR	3.8
2	B	325	MET	3.7
4	F	325	LEU	3.7
1	C	368	LEU	3.7
1	A	221	ARG	3.7
1	A	438	ASP	3.5
1	A	351	PHE	3.5
1	A	316	CYS	3.5
4	F	142	ARG	3.4
1	A	341	ILE	3.4
1	A	338	LYS	3.3
4	F	155	ALA	3.3
2	D	275	LEU	3.3
2	D	369	ARG	3.3
4	F	315	PHE	3.2
3	E	26	PRO	3.2
2	D	339	ASN	3.1
2	D	332	MET	3.1
2	D	217	LEU	3.1
4	F	173	ILE	3.1
1	A	230	LEU	3.1
1	A	295	CYS	3.1
4	F	57	GLY	3.1
2	D	343	PHE	3.0
3	E	53	LYS	3.0
2	B	308	ARG	3.0
1	A	317	LEU	3.0
1	C	276	ILE	3.0
4	F	169	LEU	3.0
1	C	293	ASN	3.0
2	B	313	LEU	2.9
2	D	248	LEU	2.9
1	A	87	PHE	2.9
1	C	275	VAL	2.9
4	F	327	VAL	2.9
4	F	313	GLN	2.9
1	A	176	GLN	2.9
2	B	286	LEU	2.8

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	346	TRP	2.8
1	A	262	TYR	2.8
2	B	319	PHE	2.8
2	B	371	LEU	2.8
4	F	181	VAL	2.8
1	C	4[A]	CYS	2.7
1	C	339	ARG	2.7
3	E	25	LYS	2.7
2	D	272	PHE	2.7
1	A	276	ILE	2.7
1	C	277	SER	2.7
3	E	62	LYS	2.7
2	D	418	PHE	2.7
2	D	276	THR	2.6
1	A	149	PHE	2.6
2	D	320	ARG	2.6
4	F	312	PHE	2.6
2	B	358	ILE	2.6
1	A	215	ARG	2.6
1	A	265	ILE	2.6
3	E	22	VAL	2.6
1	C	274	PRO	2.6
2	D	318	ILE	2.6
3	E	6	MET	2.5
4	F	240	LEU	2.5
4	F	37	PHE	2.5
1	A	118	VAL	2.5
2	B	321	GLY	2.5
4	F	201	ILE	2.5
1	C	5	ILE	2.5
2	B	7	ILE	2.5
2	B	155	SER	2.5
2	D	388	PHE	2.5
1	A	391	LEU	2.5
2	D	313	LEU	2.4
4	F	211	TYR	2.4
2	D	353	THR	2.4
2	D	331	GLN	2.4
2	B	418	PHE	2.4
1	A	418	PHE	2.4
4	F	267	PHE	2.4
2	B	296	PHE	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	68	VAL	2.3
3	E	59	GLU	2.3
2	D	335	VAL	2.3
2	D	344	VAL	2.3
2	D	387	LEU	2.3
1	C	440	VAL	2.3
4	F	130	VAL	2.3
2	D	291	LEU	2.3
2	D	277	SER	2.3
1	C	218	ASP	2.3
1	C	135	PHE	2.3
3	E	48	GLU	2.3
1	C	215	ARG	2.3
1	A	371	VAL	2.3
2	B	204	ILE	2.3
2	B	436	GLN	2.3
1	A	26	LEU	2.3
2	B	273	ALA	2.3
4	F	141	GLY	2.3
1	A	68	VAL	2.2
3	E	27	PRO	2.2
2	B	318	ILE	2.2
2	D	209	LEU	2.2
1	A	377	MET	2.2
4	F	125	THR	2.2
1	C	221	ARG	2.2
2	B	310	GLY	2.2
2	B	382	THR	2.2
1	A	348	PRO	2.2
1	C	281	ALA	2.2
2	D	323	MET	2.2
2	D	325	MET	2.2
1	A	378	LEU	2.2
2	B	353	THR	2.2
1	A	315	CYS	2.2
2	D	212	ILE	2.2
4	F	49	PHE	2.2
1	A	283	HIS	2.2
1	A	349	THR	2.2
1	A	211	ASP	2.1
1	C	278	ALA	2.1
4	F	93	TRP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	332	ILE	2.1
1	A	296	PHE	2.1
1	A	303	VAL	2.1
2	B	182	VAL	2.1
1	C	296	PHE	2.1
3	E	54	LEU	2.1
2	D	360	PRO	2.1
1	A	21	TRP	2.1
1	A	339	ARG	2.1
2	B	154	ILE	2.1
4	F	46	ARG	2.1
2	B	57	THR	2.1
2	D	287	THR	2.1
1	C	341	ILE	2.1
2	B	315	VAL	2.1
2	D	336	GLN	2.0
4	F	58	LEU	2.0
2	B	312	TYR	2.0
1	A	313	MET	2.0
2	B	388	PHE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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	A	504	1/1	0.84	0.14	99,99,99,99	0
11	ACP	F	401	31/31	0.89	0.16	100,121,133,138	0
8	GDP	D	501	28/28	0.91	0.18	79,87,99,105	0

Continued on next page...

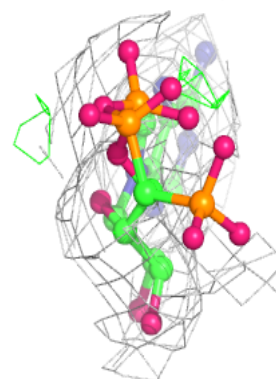
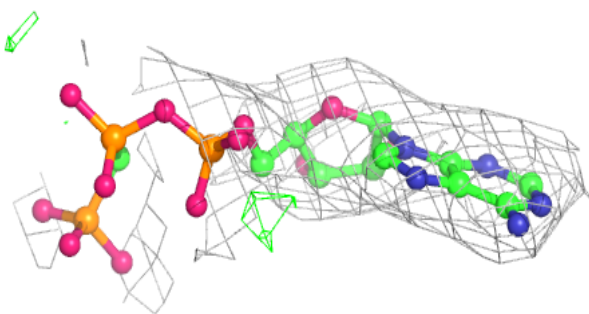
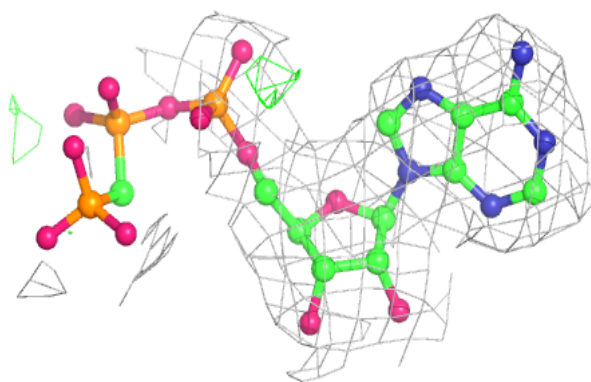
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	MG	D	502	1/1	0.91	0.21	83,83,83,83	0
10	W1P	B	506	13/13	0.92	0.45	61,68,84,84	23
9	MES	B	504	12/12	0.93	0.21	77,80,91,93	0
7	CA	A	503	1/1	0.95	0.18	102,102,102,102	0
10	W1P	B	505	13/13	0.95	0.45	64,71,86,86	23
5	GTP	A	501	32/32	0.96	0.17	58,63,72,77	0
5	GTP	C	501	32/32	0.96	0.17	50,59,67,69	0
8	GDP	B	501	28/28	0.97	0.17	49,56,63,64	0
6	MG	B	502	1/1	0.97	0.18	53,53,53,53	0
7	CA	B	503	1/1	0.97	0.17	112,112,112,112	0
6	MG	F	402	1/1	0.98	0.10	123,123,123,123	0
7	CA	C	503	1/1	0.98	0.20	73,73,73,73	0
6	MG	A	502	1/1	0.99	0.20	72,72,72,72	0
6	MG	C	502	1/1	0.99	0.17	58,58,58,58	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.

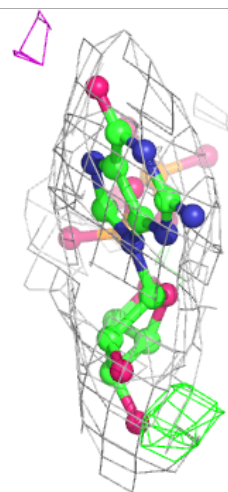
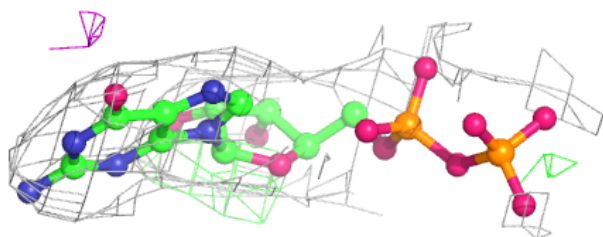
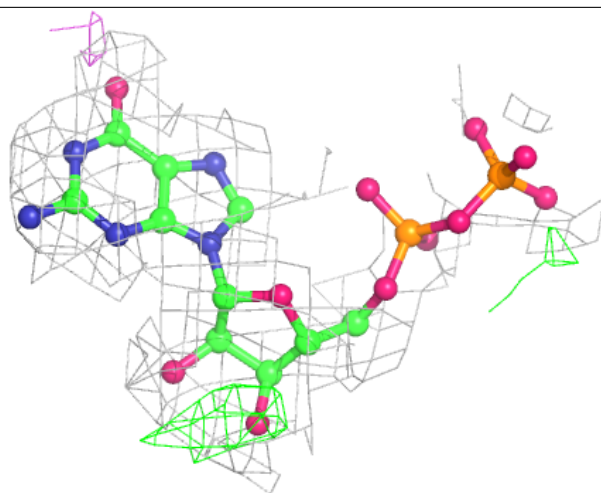
Electron density around ACP F 401:

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



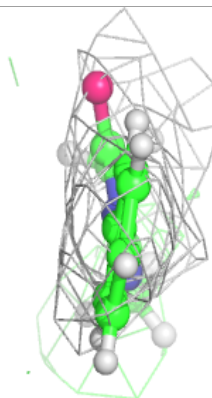
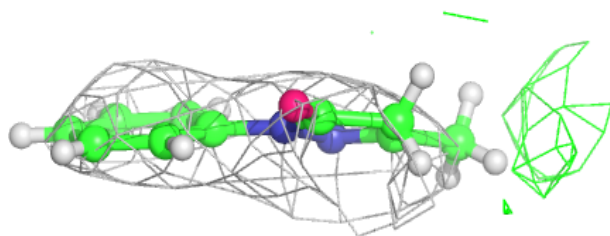
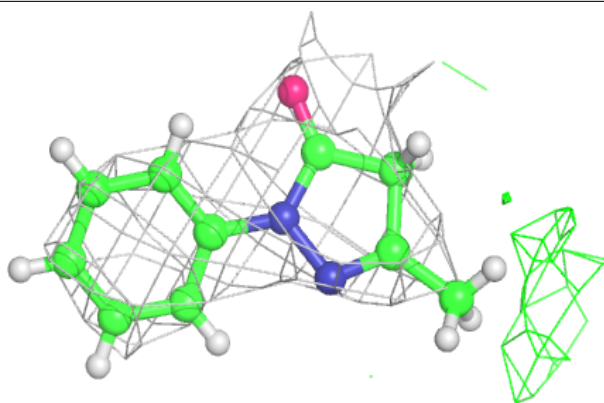
Electron density around GDP D 501:

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

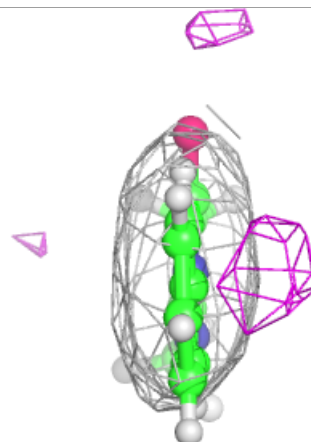
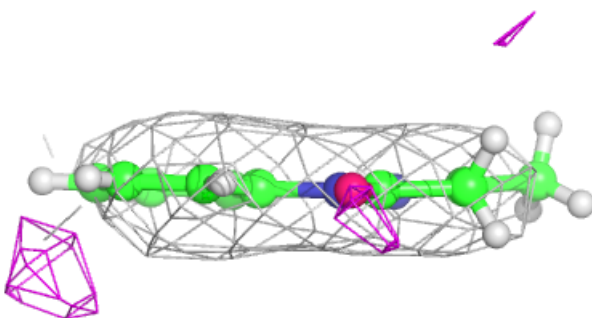
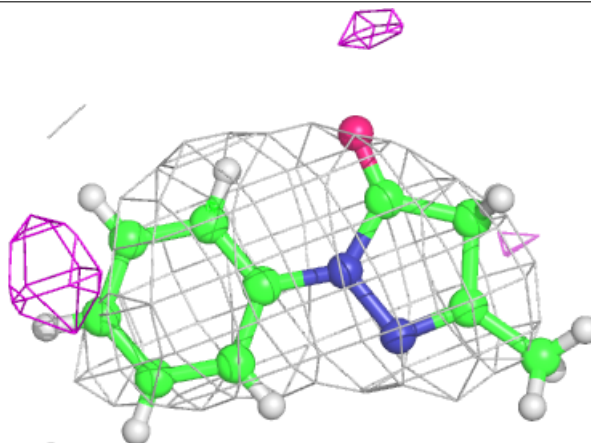


Electron density around W1P B 506:

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

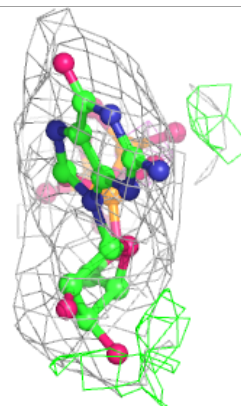
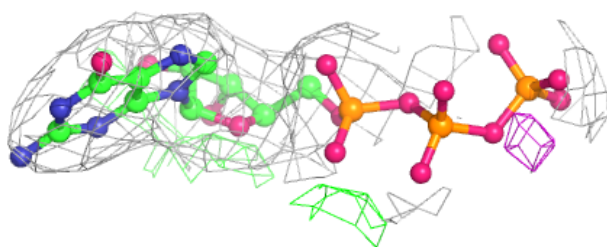
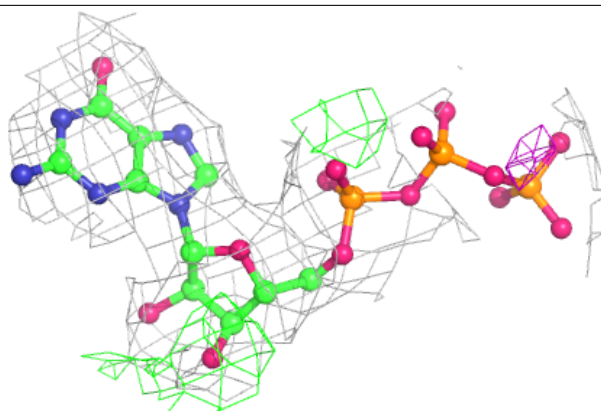
**Electron density around W1P B 505:**

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

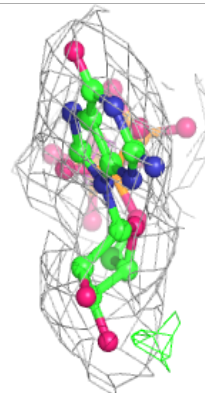
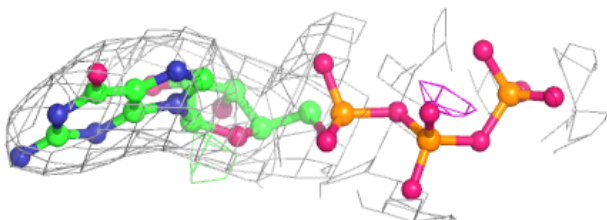
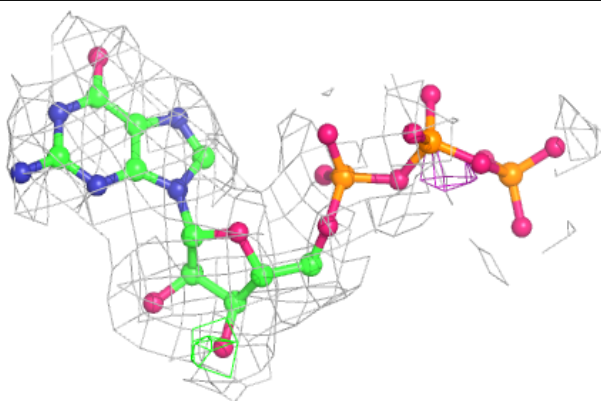


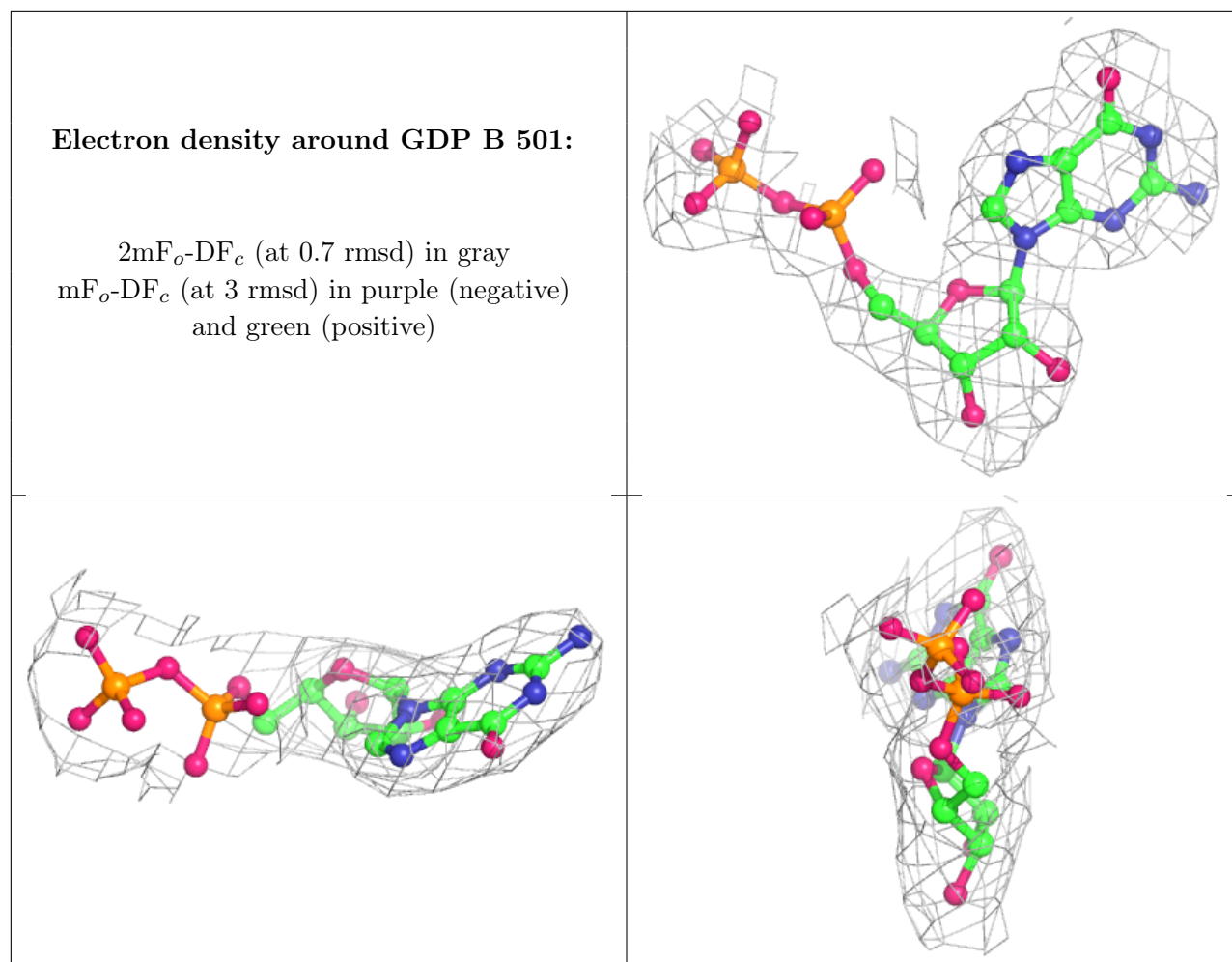
Electron density around GTP A 501:

$2mF_o-DF_c$ (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.