



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 01:36 AM UTC

PDB ID : 8WD0 / pdb_00008wd0
Title : Crystal structure of T2R-TTL-Erianin complex
Authors : Yang, J.
Deposited on : 2023-09-14
Resolution : 2.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	380	

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
10	W4F	B	503	-	X	-	-
10	W4F	D	503	-	X	-	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17492 atoms, of which 44 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	437	Total	C	N	O	S	0	0	0
			3402	2156	577	647	22			
1	C	440	Total	C	N	O	S	0	0	0
			3427	2169	580	656	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	428	Total	C	N	O	S	0	0	0
			3334	2095	566	647	26			
2	D	421	Total	C	N	O	S	0	0	0
			3280	2066	554	634	26			

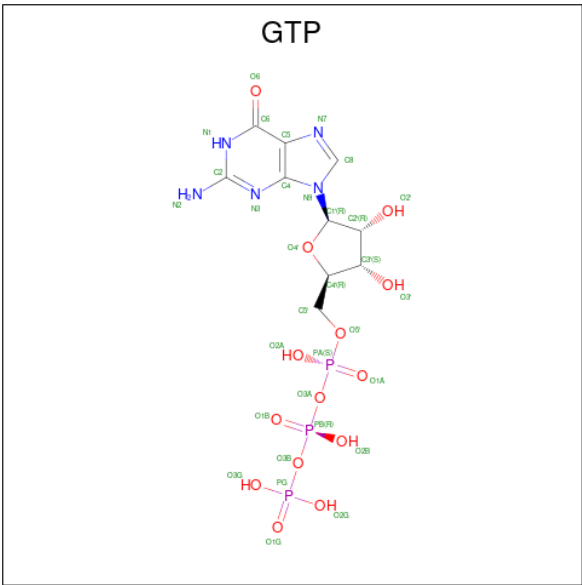
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	0	0
			996	614	180	197	5			

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	334	Total	C	N	O	S	0	0	0
			2717	1747	460	496	14			

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	32	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	32	0
			32	10	5	14	3		
5	D	1	Total	C	N	O	P	32	0
			32	10	5	14	3		

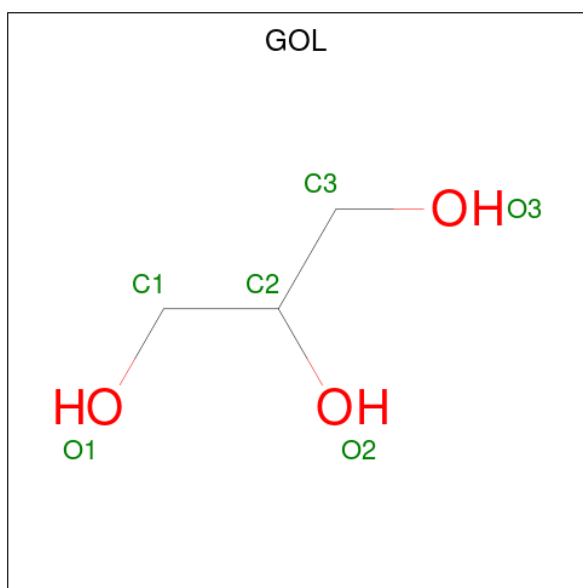
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

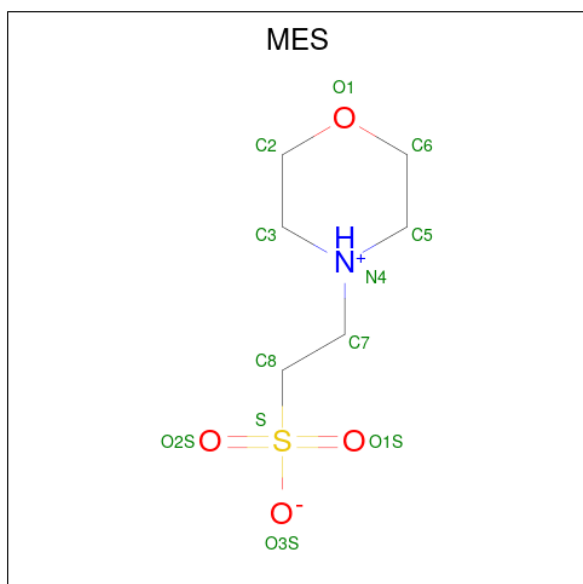
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	1	0
			1	1		
7	C	1	Total	Ca	1	0
			1	1		

- Molecule 8 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



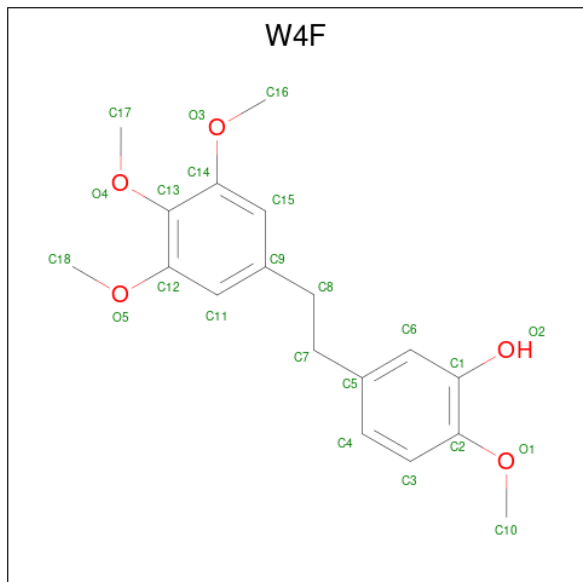
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	6	0
			6	3	3		

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



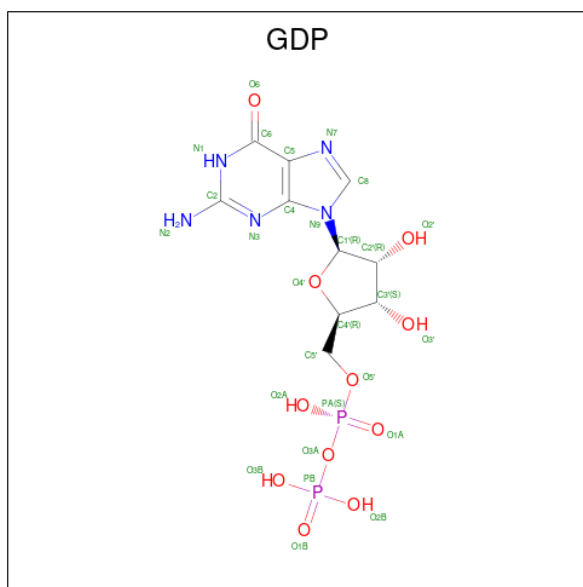
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	12	0
			12	6	1	4	1		

- Molecule 10 is 2-methoxy-5-[2-(3,4,5-trimethoxyphenyl)ethyl]phenol (CCD ID: W4F) (formula: $C_{18}H_{22}O_5$) (labeled as "Ligand of Interest" by depositor).



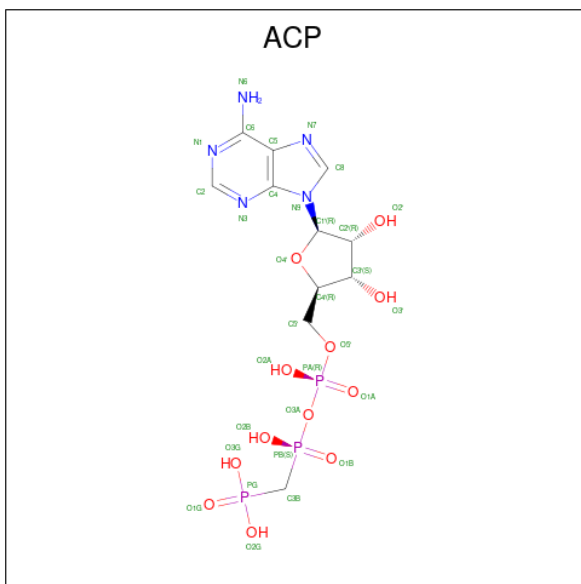
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	H	O	0	0
			45	18	22	5		
10	D	1	Total	C	H	O	0	0
			45	18	22	5		

- Molecule 11 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



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

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



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

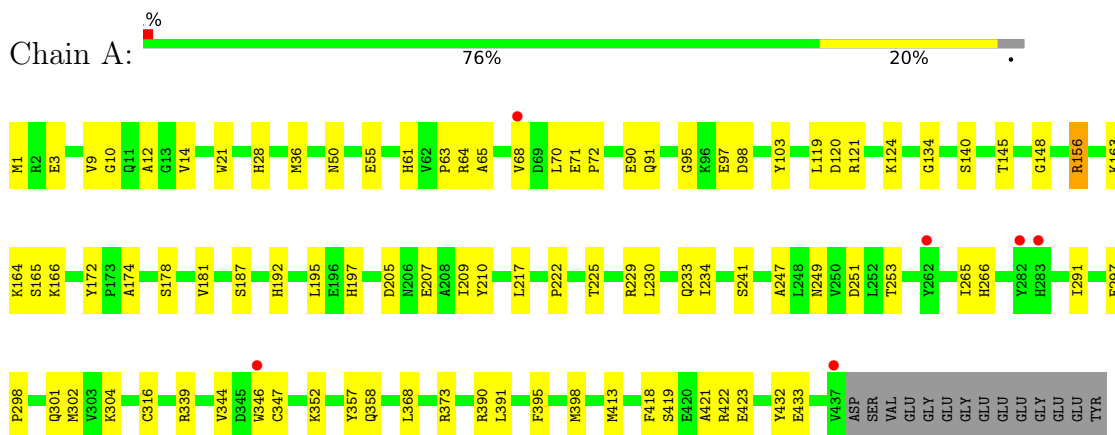
- Molecule 13 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
13	A	11	Total O 11 11	0	0
13	B	15	Total O 15 15	0	0
13	C	28	Total O 28 28	0	0
13	D	4	Total O 4 4	0	0
13	E	4	Total O 4 4	0	0
13	F	5	Total O 5 5	0	0

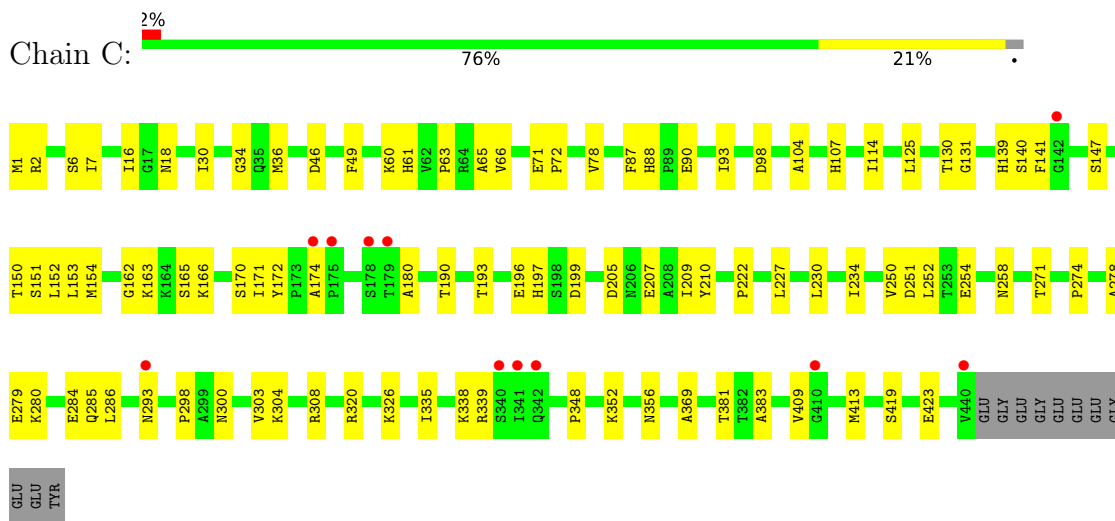
3 Residue-property plots [i](#)

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.

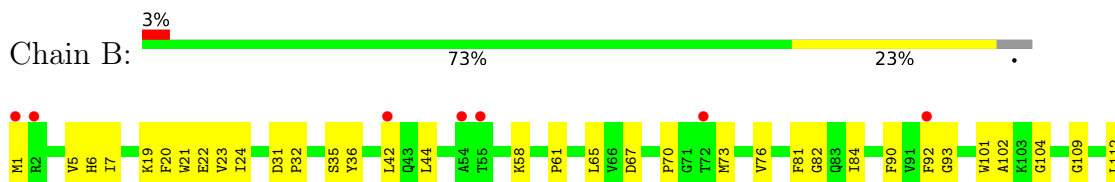
- Molecule 1: Tubulin alpha-1B chain

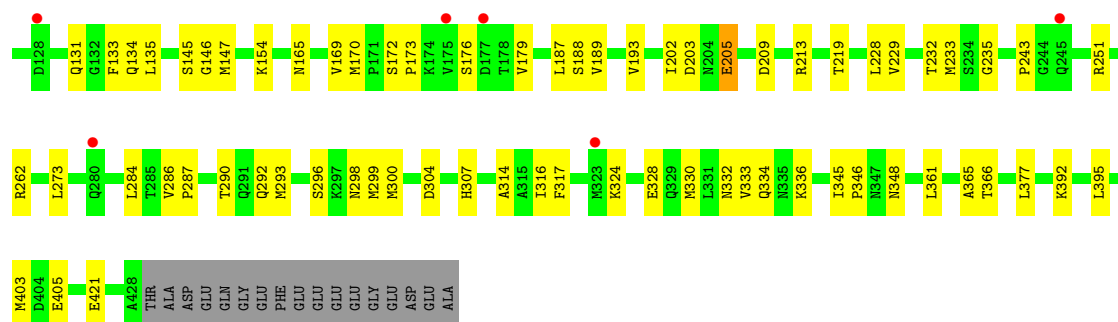


- Molecule 1: Tubulin alpha-1B chain

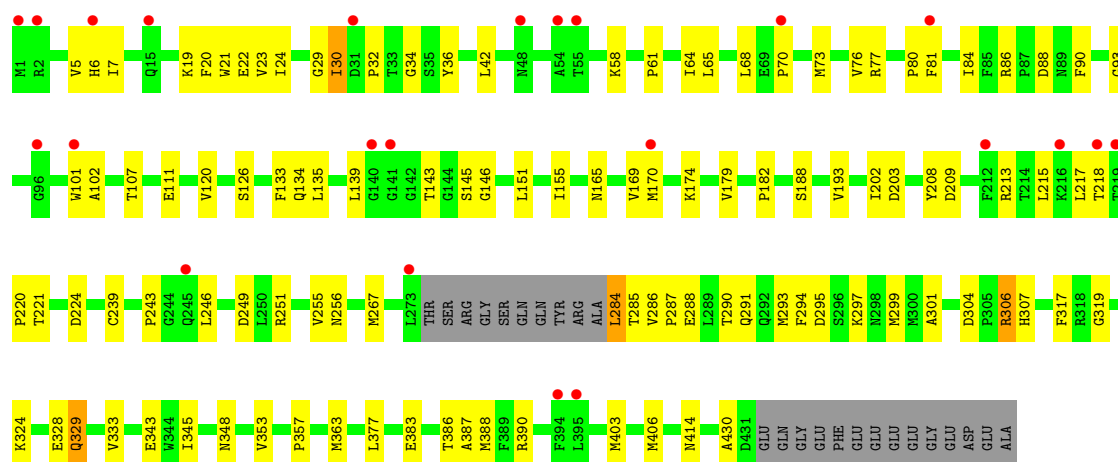


- Molecule 2: Tubulin beta chain

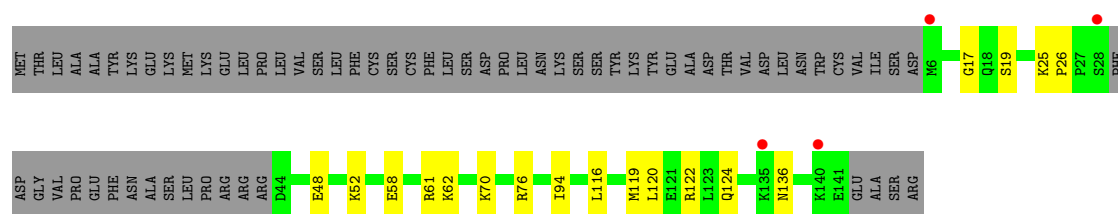




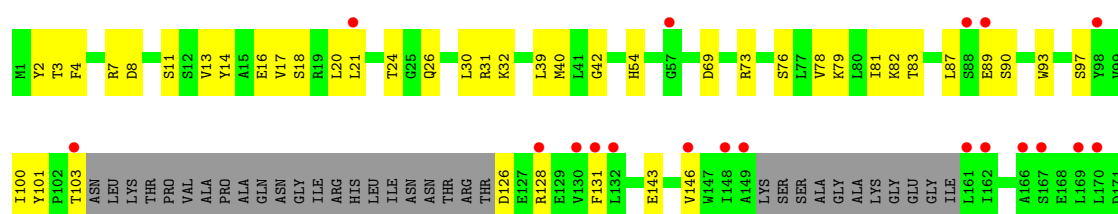
• Molecule 2: Tubulin beta chain

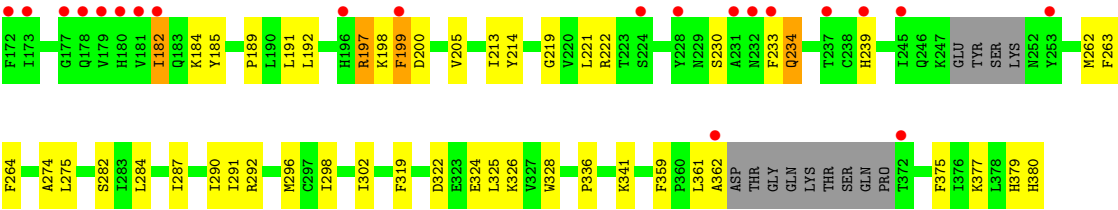


• Molecule 3: Stathmin-4



• Molecule 4: Tubulin tyrosine ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	156.56Å 181.54Å 104.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	38.26 – 2.60 38.26 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.8 (38.26-2.60) 98.8 (38.26-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.01 (at 2.61Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.227 , 0.258 0.228 , 0.259	Depositor DCC
R_{free} test set	2000 reflections (2.17%)	wwPDB-VP
Wilson B-factor (Å ²)	61.8	Xtriage
Anisotropy	0.192	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 38.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17492	wwPDB-VP
Average B, all atoms (Å ²)	68.0	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ACP, GTP, MES, GDP, W4F, GOL, CA

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.31	0/3480	0.47	0/4726
1	C	0.39	0/3505	0.50	0/4761
2	B	0.38	0/3409	0.57	0/4624
2	D	0.38	0/3353	0.56	0/4546
3	E	0.25	0/1004	0.36	0/1333
4	F	0.31	0/2778	0.53	1/3756 (0.0%)
All	All	0.35	0/17529	0.52	1/23746 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	89	GLU	N-CA-C	-5.50	105.70	112.90

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3402	0	3309	71	0
1	C	3427	0	3326	72	0
2	B	3334	0	3181	79	0
2	D	3280	0	3144	78	2

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	E	996	0	1007	20	0
4	F	2717	0	2662	82	2
5	A	32	0	12	0	0
5	C	32	0	12	0	0
5	D	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
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	6	0	8	0	0
9	B	12	0	12	0	0
10	B	23	22	0	2	0
10	D	23	22	0	1	0
11	B	28	0	12	0	0
12	F	31	0	14	0	0
13	A	11	0	0	1	0
13	B	15	0	0	0	0
13	C	28	0	0	1	0
13	D	4	0	0	0	0
13	E	4	0	0	0	0
13	F	5	0	0	0	0
All	All	17448	44	16711	389	2

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 12.

All (389) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1:MET:HB3	2:B:131:GLN:HB3	1.36	1.06
3:E:48:GLU:HG2	3:E:52:LYS:HE2	1.44	0.98
2:D:73:MET:HB3	2:D:77:ARG:HH21	1.31	0.94
4:F:200:ASP:OD1	4:F:222:ARG:HD3	1.68	0.94
1:A:119:LEU:HD11	1:A:156:ARG:HG2	1.52	0.91
4:F:192:LEU:HD22	4:F:262:MET:HE1	1.52	0.91
4:F:199:PHE:CE1	4:F:221:LEU:HG	2.06	0.90
4:F:263:PHE:CE2	4:F:341:LYS:HD3	2.13	0.83
2:B:42:LEU:HD22	2:B:243:PRO:HG2	1.59	0.82
2:B:1:MET:HE1	2:B:251:ARG:HD2	1.61	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:263:PHE:HE2	4:F:341:LYS:HD3	1.44	0.82
1:A:166:LYS:HE2	1:A:197:HIS:O	1.80	0.81
2:B:332:ASN:OD1	2:B:336:LYS:HE3	1.81	0.81
2:D:134:GLN:HA	2:D:165:ASN:O	1.80	0.80
2:B:317:PHE:CE1	2:B:330:MET:HE2	2.16	0.80
4:F:199:PHE:CD1	4:F:221:LEU:HG	2.16	0.80
1:A:97:GLU:HB2	2:B:1:MET:HG3	1.65	0.79
2:D:406:MET:HA	2:D:406:MET:HE2	1.65	0.77
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.67	0.77
1:C:147:SER:HB2	1:C:190:THR:OG1	1.85	0.77
1:C:381:THR:HG22	1:C:383:ALA:H	1.49	0.77
2:B:1:MET:HB3	2:B:131:GLN:CB	2.14	0.76
2:D:290:THR:HG22	2:D:333:VAL:HG21	1.67	0.76
2:B:232:THR:OG1	2:B:300:MET:HE2	1.86	0.76
3:E:120:LEU:O	3:E:124:GLN:HG2	1.86	0.75
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.68	0.75
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.67	0.74
1:C:71:GLU:HB2	1:C:98:ASP:HB3	1.70	0.74
1:A:163:LYS:HE2	1:A:164:LYS:HZ3	1.54	0.73
4:F:13:VAL:O	4:F:17:VAL:HG23	1.89	0.73
1:C:1:MET:HB3	1:C:130:THR:OG1	1.89	0.72
4:F:199:PHE:CE1	4:F:221:LEU:CD2	2.74	0.70
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.72	0.70
1:C:230:LEU:O	1:C:234:ILE:HD12	1.91	0.70
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.73	0.70
2:D:239:CYS:HB2	10:D:503:W4F:C18	2.22	0.69
2:B:170:MET:HG3	2:B:377:LEU:HD11	1.75	0.69
4:F:31:ARG:HH21	4:F:32:LYS:HG3	1.57	0.69
2:B:42:LEU:CD2	2:B:243:PRO:HG2	2.23	0.68
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.74	0.68
4:F:199:PHE:CE1	4:F:221:LEU:CG	2.77	0.68
2:D:73:MET:HB3	2:D:77:ARG:NH2	2.08	0.68
4:F:16:GLU:O	4:F:20:LEU:HG	1.92	0.68
4:F:100:ILE:HD11	4:F:128:ARG:HA	1.76	0.68
2:B:73:MET:HE3	2:B:90:PHE:HD2	1.59	0.67
2:D:65:LEU:HD22	2:D:90:PHE:CE2	2.31	0.66
1:A:247:ALA:HB3	3:E:19:SER:OG	1.95	0.66
2:D:284:LEU:HD23	2:D:288:GLU:HB2	1.78	0.66
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.77	0.66
2:B:317:PHE:HE1	2:B:330:MET:HE2	1.60	0.66
4:F:82:LYS:NZ	4:F:97:SER:O	2.28	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:395:LEU:HD21	2:B:405:GLU:HG2	1.78	0.66
2:B:134:GLN:HA	2:B:165:ASN:O	1.94	0.65
4:F:16:GLU:OE2	4:F:20:LEU:HD21	1.98	0.64
1:C:278:ALA:HA	1:C:369:ALA:HB2	1.80	0.64
4:F:199:PHE:CD1	4:F:221:LEU:CG	2.80	0.64
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.33	0.64
1:A:1:MET:HE2	1:A:50:ASN:CB	2.28	0.64
2:B:392:LYS:HD3	2:B:405:GLU:OE2	1.98	0.64
1:A:230:LEU:O	1:A:234:ILE:HD12	1.99	0.63
2:D:30:ILE:HG13	2:D:30:ILE:O	1.98	0.63
4:F:73:ARG:HB2	4:F:76:SER:OG	1.98	0.63
4:F:191:LEU:HA	4:F:197:ARG:O	1.99	0.63
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.35	0.62
1:A:413:MET:HE2	1:A:418:PHE:CE2	2.35	0.62
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.81	0.62
1:A:1:MET:HE2	1:A:50:ASN:HB3	1.81	0.62
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.36	0.61
1:C:30:ILE:HD11	1:C:36:MET:HE2	1.83	0.61
4:F:199:PHE:CD1	4:F:221:LEU:HD23	2.35	0.61
4:F:78:VAL:HG13	4:F:82:LYS:HZ2	1.63	0.61
2:B:317:PHE:CZ	2:B:330:MET:HE2	2.35	0.61
4:F:8:ASP:OD2	4:F:11:SER:HB2	2.01	0.61
1:A:181:VAL:O	1:A:398:MET:HE1	2.01	0.60
1:C:209:ILE:HG22	1:C:227:LEU:CD2	2.31	0.60
4:F:199:PHE:HE1	4:F:221:LEU:CD2	2.14	0.60
2:D:32:PRO:HA	2:D:81:PHE:CD2	2.36	0.60
1:C:30:ILE:CG1	1:C:36:MET:HE2	2.31	0.60
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.36	0.60
2:B:324:LYS:O	2:B:328:GLU:HG3	2.02	0.60
1:C:252:LEU:HD12	1:C:252:LEU:O	2.02	0.60
4:F:292:ARG:O	4:F:296:MET:HG2	2.02	0.60
4:F:192:LEU:CD2	4:F:262:MET:HE1	2.28	0.59
2:B:179:VAL:HG22	1:C:258:ASN:OD1	2.02	0.59
4:F:199:PHE:CD1	4:F:221:LEU:CD2	2.86	0.59
2:B:36:TYR:CD2	2:B:44:LEU:HD21	2.37	0.58
2:D:406:MET:HE2	2:D:406:MET:CA	2.31	0.58
2:D:299:MET:HA	2:D:299:MET:HE2	1.86	0.58
1:A:156:ARG:CG	1:A:156:ARG:HH21	2.16	0.58
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.37	0.58
1:C:36:MET:HE3	1:C:61:HIS:CD2	2.37	0.58
2:D:29:GLY:O	2:D:36:TYR:CD1	2.56	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:SER:CB	1:A:391:LEU:HD21	2.33	0.58
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.85	0.58
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.85	0.58
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.19	0.57
1:A:251:ASP:OD2	1:A:253:THR:HB	2.05	0.57
2:D:81:PHE:O	2:D:84:ILE:HG22	2.05	0.57
4:F:298:ILE:HD12	4:F:302:ILE:HD13	1.87	0.57
2:B:229:VAL:HG12	2:B:233:MET:HE2	1.86	0.56
2:D:221:THR:HG23	2:D:224:ASP:H	1.69	0.56
2:B:67:ASP:O	2:B:92:PHE:HA	2.06	0.56
2:B:324:LYS:HE2	2:B:328:GLU:OE2	2.06	0.56
2:D:295:ASP:OD2	2:D:297:LYS:HE3	2.06	0.56
2:B:345:ILE:HG22	2:B:348:ASN:HB3	1.87	0.56
1:C:280:LYS:O	1:C:284:GLU:HG3	2.06	0.56
2:D:22:GLU:OE2	2:D:80:PRO:HG2	2.05	0.56
2:D:294:PHE:O	2:D:306:ARG:NH2	2.37	0.56
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.41	0.56
2:B:73:MET:HE3	2:B:90:PHE:CD2	2.40	0.56
4:F:101:TYR:HD1	4:F:126:ASP:HB2	1.71	0.55
2:B:172:SER:OG	2:B:205:GLU:CG	2.55	0.55
1:A:9:VAL:HG22	1:A:68:VAL:CG1	2.37	0.55
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.41	0.55
2:D:319:GLY:HA2	2:D:357:PRO:HG3	1.89	0.55
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.89	0.54
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.25	0.54
2:B:170:MET:HB2	2:B:203:ASP:HA	1.90	0.54
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.71	0.54
2:D:208:TYR:HE2	2:D:220:PRO:HD3	1.72	0.54
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.38	0.54
1:A:419:SER:O	1:A:423:GLU:HG3	2.08	0.54
1:C:207:GLU:OE1	1:C:304:LYS:HE2	2.08	0.54
4:F:199:PHE:C	4:F:199:PHE:CD2	2.85	0.54
1:A:390:ARG:HD2	4:F:54:HIS:CD2	2.43	0.54
2:D:287:PRO:HA	2:D:329:GLN:HG3	1.90	0.54
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.91	0.53
4:F:81:ILE:HA	4:F:87:LEU:HD12	1.89	0.53
2:B:273:LEU:HD11	2:B:298:ASN:HA	1.89	0.53
2:B:316:ILE:CG2	2:B:366:THR:HB	2.38	0.53
2:D:284:LEU:HD23	2:D:288:GLU:CB	2.38	0.53
4:F:14:TYR:HA	4:F:17:VAL:HG23	1.90	0.53
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:406:MET:HA	2:D:406:MET:CE	2.35	0.53
2:D:7:ILE:O	2:D:135:LEU:HA	2.08	0.53
1:A:119:LEU:CD1	1:A:156:ARG:HG2	2.34	0.53
1:A:163:LYS:HE2	1:A:164:LYS:NZ	2.22	0.53
4:F:274:ALA:C	4:F:275:LEU:HD12	2.34	0.53
4:F:191:LEU:HD22	4:F:197:ARG:O	2.08	0.53
2:D:267:MET:HB2	2:D:301:ALA:HB3	1.91	0.53
2:D:345:ILE:HG22	2:D:348:ASN:HB3	1.90	0.52
3:E:116:LEU:HD23	3:E:119:MET:CE	2.40	0.52
2:B:20:PHE:HB2	2:B:233:MET:CE	2.40	0.52
1:A:207:GLU:OE2	1:A:304:LYS:HD2	2.09	0.52
2:D:42:LEU:HD22	2:D:243:PRO:HG2	1.92	0.52
1:C:1:MET:O	1:C:2:ARG:HB2	2.09	0.52
1:A:28:HIS:HB3	1:A:36:MET:HE3	1.92	0.52
2:D:343:GLU:HG2	2:D:430:ALA:HB2	1.92	0.52
4:F:324:GLU:O	4:F:324:GLU:HG3	2.10	0.52
2:B:169:VAL:HA	2:B:202:ILE:O	2.10	0.52
4:F:199:PHE:HE1	4:F:221:LEU:CG	2.23	0.51
1:C:71:GLU:HG2	1:C:72:PRO:CD	2.39	0.51
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.93	0.51
2:B:145:SER:HG	2:B:188:SER:HG	1.56	0.51
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.46	0.51
2:D:68:LEU:H	2:D:143:THR:HG21	1.76	0.51
2:D:174:LYS:HB3	2:D:208:TYR:CD1	2.45	0.51
2:B:81:PHE:O	2:B:84:ILE:HG22	2.10	0.51
2:B:314:ALA:HB1	10:B:503:W4F:C16	2.40	0.51
4:F:69:ASP:OD1	4:F:69:ASP:N	2.44	0.51
4:F:199:PHE:HE1	4:F:221:LEU:HD21	1.75	0.51
4:F:326:LYS:HE2	4:F:328:TRP:CZ2	2.46	0.51
2:D:61:PRO:HD3	2:D:84:ILE:HG12	1.93	0.50
4:F:24:THR:HG21	4:F:361:LEU:HD13	1.92	0.50
1:A:10:GLY:O	1:A:14:VAL:HG23	2.12	0.50
4:F:326:LYS:HD3	4:F:328:TRP:CZ2	2.47	0.50
2:B:209:ASP:HB3	2:B:213:ARG:HD2	1.94	0.50
2:B:330:MET:O	2:B:334:GLN:HG3	2.11	0.50
2:D:169:VAL:HA	2:D:202:ILE:O	2.11	0.50
2:B:228:LEU:HB3	2:B:300:MET:HE1	1.93	0.50
3:E:58:GLU:HG2	3:E:62:LYS:HE2	1.92	0.50
4:F:213:ILE:HD12	4:F:296:MET:CE	2.42	0.50
1:A:120:ASP:O	1:A:124:LYS:HG2	2.11	0.50
1:C:30:ILE:CD1	1:C:36:MET:HE2	2.42	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.47	0.50
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.94	0.49
1:A:174:ALA:O	1:A:178:SER:HB3	2.12	0.49
2:D:304:ASP:HB3	2:D:307:HIS:ND1	2.27	0.49
2:D:7:ILE:O	2:D:135:LEU:HD12	2.12	0.49
1:C:34:GLY:HA3	1:C:60:LYS:HG3	1.93	0.49
1:C:285:GLN:OE1	1:C:285:GLN:HA	2.11	0.49
2:D:32:PRO:HA	2:D:81:PHE:CE2	2.47	0.49
3:E:58:GLU:HG3	3:E:61:ARG:NH2	2.28	0.49
4:F:192:LEU:HD22	4:F:262:MET:CE	2.35	0.49
1:A:1:MET:HE2	1:A:50:ASN:HB2	1.93	0.49
1:C:166:LYS:HE2	1:C:197:HIS:O	2.12	0.49
2:D:73:MET:CB	2:D:77:ARG:HH21	2.16	0.49
2:D:290:THR:CG2	2:D:333:VAL:HG21	2.40	0.49
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.48	0.49
2:B:76:VAL:O	2:B:82:GLY:HA3	2.13	0.49
2:D:65:LEU:N	2:D:65:LEU:HD12	2.28	0.49
2:B:7:ILE:O	2:B:135:LEU:HA	2.13	0.49
2:B:172:SER:OG	2:B:205:GLU:HG2	2.12	0.49
2:D:5:VAL:HB	2:D:133:PHE:CD1	2.48	0.49
4:F:40:MET:HE2	4:F:42:GLY:HA3	1.95	0.49
2:D:70:PRO:HG3	2:D:93:GLY:O	2.13	0.48
1:A:12:ALA:HB3	1:A:140:SER:HB3	1.94	0.48
2:B:22:GLU:HG2	2:B:81:PHE:CD1	2.49	0.48
2:D:64:ILE:HD13	2:D:120:VAL:HG22	1.96	0.48
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.48	0.48
1:A:357:TYR:CZ	3:E:17:GLY:HA2	2.48	0.48
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.94	0.48
2:B:304:ASP:HB3	2:B:307:HIS:ND1	2.29	0.48
2:B:20:PHE:HB2	2:B:233:MET:HE3	1.95	0.48
2:B:104:GLY:O	2:B:109:GLY:HA3	2.14	0.48
2:D:285:THR:OG1	2:D:288:GLU:HG3	2.13	0.48
2:D:386:THR:O	2:D:390:ARG:HG2	2.14	0.48
1:A:12:ALA:CB	1:A:140:SER:HB3	2.44	0.47
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.49	0.47
2:B:73:MET:SD	2:B:92:PHE:HB3	2.54	0.47
2:B:172:SER:OG	2:B:205:GLU:HG3	2.14	0.47
1:C:180:ALA:HB1	2:D:256:ASN:OD1	2.14	0.47
1:C:140:SER:HA	1:C:171:ILE:HB	1.96	0.47
2:D:29:GLY:O	2:D:36:TYR:HD1	1.98	0.47
1:C:71:GLU:CB	1:C:98:ASP:HB3	2.40	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:14:TYR:HA	4:F:17:VAL:CG2	2.44	0.47
1:A:90:GLU:O	1:A:121:ARG:HD2	2.13	0.47
1:A:156:ARG:CG	1:A:156:ARG:NH2	2.73	0.47
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.49	0.47
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.45	0.47
1:A:233:GLN:HG3	1:A:368:LEU:HD12	1.97	0.47
1:C:293:ASN:CG	1:C:339:ARG:HH21	2.23	0.47
2:D:139:LEU:HD12	2:D:170:MET:SD	2.54	0.47
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.45	0.47
4:F:131:PHE:CD1	4:F:182:ILE:HG21	2.50	0.47
1:C:320:ARG:HA	1:C:356:ASN:O	2.15	0.47
4:F:185:TYR:OH	4:F:239:HIS:CD2	2.68	0.47
1:A:70:LEU:HG	1:A:145:THR:HG23	1.96	0.47
4:F:361:LEU:O	4:F:362:ALA:C	2.58	0.46
2:D:170:MET:HB2	2:D:203:ASP:HA	1.98	0.46
1:A:195:LEU:HD12	1:A:266:HIS:CE1	2.50	0.46
4:F:31:ARG:HE	4:F:32:LYS:H	1.63	0.46
2:B:235:GLY:HA3	2:B:366:THR:OG1	2.16	0.46
4:F:189:PRO:HA	4:F:322:ASP:HA	1.97	0.46
1:A:72:PRO:HD3	1:A:95:GLY:O	2.14	0.46
2:B:296:SER:HA	2:B:299:MET:HG2	1.97	0.46
2:D:145:SER:OG	2:D:188:SER:OG	2.24	0.46
1:A:21:TRP:CH2	1:A:63:PRO:HB3	2.50	0.46
1:C:274:PRO:HG3	1:C:286:LEU:HD13	1.97	0.46
1:A:28:HIS:O	1:A:36:MET:HE3	2.15	0.46
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.50	0.46
2:B:262:ARG:HE	2:B:421:GLU:CD	2.24	0.46
4:F:24:THR:HG21	4:F:361:LEU:CD1	2.46	0.46
4:F:131:PHE:CE1	4:F:182:ILE:HG21	2.51	0.46
4:F:199:PHE:HD1	4:F:221:LEU:CG	2.29	0.46
1:C:162:GLY:CA	3:E:94:ILE:HD11	2.44	0.46
2:D:215:LEU:C	2:D:217:LEU:HD12	2.41	0.46
2:D:218:THR:O	2:D:218:THR:HG23	2.16	0.46
1:C:18:ASN:HD21	1:C:78:VAL:HG22	1.81	0.45
4:F:3:THR:HB	4:F:30:LEU:HD11	1.98	0.45
2:B:102:ALA:HB2	2:B:403:MET:SD	2.56	0.45
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.98	0.45
4:F:79:LYS:O	4:F:83:THR:OG1	2.26	0.45
2:B:154:LYS:HE3	3:E:76:ARG:CZ	2.46	0.45
1:A:71:GLU:HB3	1:A:98:ASP:HB3	1.98	0.45
2:B:73:MET:CE	2:B:90:PHE:HB3	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:PRO:HA	2:B:176:SER:HB2	1.97	0.45
3:E:136:ASN:HD22	3:E:136:ASN:C	2.19	0.45
1:A:395:PHE:CD1	1:A:422:ARG:HD3	2.52	0.45
1:A:346:TRP:CZ3	1:A:347:CYS:SG	3.10	0.45
2:B:20:PHE:CZ	2:B:24:ILE:HD13	2.52	0.45
2:D:363:MET:HE2	2:D:363:MET:HB3	1.80	0.45
2:D:221:THR:HG22	2:D:224:ASP:OD2	2.16	0.45
1:A:55:GLU:HG2	1:A:61:HIS:CD2	2.52	0.45
2:B:316:ILE:HG23	2:B:366:THR:HB	1.98	0.45
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.99	0.45
1:A:134:GLY:HA3	1:A:165:SER:O	2.16	0.45
2:B:219:THR:HG21	1:C:326:LYS:HA	1.99	0.45
1:C:163:LYS:HA	1:C:163:LYS:HD3	1.57	0.45
1:C:165:SER:HA	1:C:199:ASP:OD2	2.16	0.45
3:E:58:GLU:O	3:E:62:LYS:HG2	2.17	0.45
1:A:209:ILE:HD11	1:A:302:MET:SD	2.57	0.44
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.46	0.44
1:A:358:GLN:NE2	13:A:601:HOH:O	2.50	0.44
1:C:419:SER:O	1:C:423:GLU:HG3	2.16	0.44
2:B:101:TRP:CE3	2:B:187:LEU:HD13	2.51	0.44
1:C:409:VAL:HA	1:C:413:MET:O	2.18	0.44
1:A:297:GLU:OE2	1:A:339:ARG:NH2	2.35	0.44
1:C:1:MET:O	13:C:601:HOH:O	2.21	0.44
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.52	0.44
4:F:93:TRP:HB2	4:F:290:ILE:HD11	1.98	0.44
4:F:377:LYS:HD3	4:F:379:HIS:NE2	2.32	0.44
4:F:100:ILE:CD1	4:F:128:ARG:HA	2.46	0.44
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.53	0.44
1:C:6:SER:O	1:C:65:ALA:HA	2.18	0.44
2:D:19:LYS:O	2:D:23:VAL:HG23	2.18	0.44
2:B:189:VAL:O	2:B:193:VAL:HG23	2.17	0.44
2:D:324:LYS:HG2	2:D:328:GLU:OE2	2.18	0.44
1:C:205:ASP:HB2	1:C:303:VAL:HA	2.00	0.44
2:D:126:SER:O	2:D:126:SER:OG	2.21	0.44
1:C:36:MET:HE1	1:C:49:PHE:CD1	2.53	0.43
1:C:107:HIS:O	1:C:152:LEU:HD22	2.18	0.43
4:F:4:PHE:HA	4:F:39:LEU:O	2.18	0.43
1:A:65:ALA:O	1:A:91:GLN:NE2	2.39	0.43
2:B:284:LEU:HD21	2:B:292:GLN:OE1	2.18	0.43
2:B:19:LYS:O	2:B:23:VAL:HG23	2.19	0.43
2:B:65:LEU:N	2:B:65:LEU:HD12	2.33	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:TYR:CD1	1:A:148:GLY:HA2	2.53	0.43
1:A:192:HIS:CG	1:A:421:ALA:HA	2.53	0.43
3:E:70:LYS:HE3	3:E:70:LYS:HB2	1.79	0.43
4:F:26:GLN:CD	4:F:361:LEU:HD22	2.43	0.43
4:F:182:ILE:HD13	4:F:182:ILE:HA	1.65	0.43
1:C:93:ILE:CG2	1:C:114:ILE:HD11	2.47	0.43
4:F:324:GLU:OE1	4:F:324:GLU:HA	2.19	0.43
1:A:291:ILE:HD13	1:A:373:ARG:HG3	2.01	0.43
1:A:298:PRO:HA	1:A:301:GLN:CD	2.43	0.43
2:B:70:PRO:HG3	2:B:93:GLY:O	2.19	0.43
2:D:383:GLU:O	2:D:386:THR:HG22	2.19	0.43
2:D:387:ALA:HA	2:D:390:ARG:NE	2.34	0.43
4:F:146:VAL:HG11	4:F:233:PHE:CZ	2.54	0.43
2:B:7:ILE:O	2:B:135:LEU:HD12	2.19	0.42
1:C:104:ALA:HB2	1:C:413:MET:SD	2.59	0.42
2:D:32:PRO:O	2:D:84:ILE:HB	2.18	0.42
4:F:18:SER:HA	4:F:21:LEU:HD12	2.01	0.42
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.54	0.42
1:C:151:SER:HB2	1:C:193:THR:CG2	2.50	0.42
2:D:377:LEU:C	2:D:377:LEU:HD23	2.44	0.42
1:A:156:ARG:HG2	1:A:156:ARG:NH2	2.33	0.42
2:B:101:TRP:NE1	2:B:146:GLY:HA2	2.35	0.42
1:C:196:GLU:HG2	1:C:197:HIS:CD2	2.55	0.42
2:D:182:PRO:CG	2:D:388:MET:HE1	2.48	0.42
3:E:116:LEU:O	3:E:120:LEU:HG	2.19	0.42
1:A:346:TRP:CD1	1:A:346:TRP:H	2.36	0.42
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.49	0.42
1:C:1:MET:HB2	1:C:131:GLY:HA3	2.00	0.42
2:D:86:ARG:NH2	2:D:88:ASP:OD2	2.51	0.42
2:D:170:MET:HG3	2:D:377:LEU:HD11	2.01	0.42
4:F:146:VAL:O	4:F:184:LYS:HD2	2.20	0.42
2:B:35:SER:OG	2:B:58:LYS:HE2	2.20	0.42
2:D:107:THR:O	2:D:111:GLU:HG3	2.19	0.42
4:F:296:MET:CE	4:F:380:HIS:CG	3.03	0.42
1:C:66:VAL:HG23	1:C:125:LEU:HD11	2.01	0.42
1:A:225:THR:O	1:A:229:ARG:HG3	2.18	0.42
2:D:101:TRP:NE1	2:D:146:GLY:HA2	2.35	0.42
4:F:213:ILE:HD12	4:F:296:MET:HE2	2.00	0.42
1:C:150:THR:O	1:C:154:MET:HG2	2.20	0.42
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.55	0.42
1:A:316:CYS:HA	1:A:352:LYS:O	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:154:LYS:HE3	3:E:76:ARG:NE	2.35	0.42
2:B:112:LEU:HD23	2:B:147:MET:HE1	2.02	0.42
2:B:5:VAL:HB	2:B:133:PHE:CD1	2.56	0.41
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.56	0.41
2:D:65:LEU:CD2	2:D:76:VAL:HG11	2.50	0.41
2:D:317:PHE:O	2:D:353:VAL:HA	2.20	0.41
2:D:209:ASP:HB3	2:D:213:ARG:HD3	2.02	0.41
2:D:102:ALA:HB2	2:D:403:MET:SD	2.60	0.41
3:E:116:LEU:HD23	3:E:119:MET:HE3	2.02	0.41
1:C:16:ILE:HD13	1:C:171:ILE:HD11	2.01	0.41
4:F:284:LEU:HA	4:F:284:LEU:HD12	1.78	0.41
2:B:286:VAL:HB	2:B:287:PRO:HD3	2.03	0.41
3:E:25:LYS:HG3	3:E:26:PRO:HD2	2.03	0.41
10:B:503:W4F:O2	10:B:503:W4F:C10	2.68	0.41
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.39	0.41
4:F:199:PHE:HD1	4:F:221:LEU:HD23	1.81	0.41
1:C:174:ALA:HB2	1:C:207:GLU:N	2.36	0.41
2:D:193:VAL:HG11	2:D:414:ASN:ND2	2.36	0.41
4:F:143:GLU:OE1	4:F:143:GLU:HA	2.20	0.41
2:B:290:THR:HG22	2:B:333:VAL:HG21	2.02	0.41
2:D:251:ARG:O	2:D:255:VAL:HG23	2.21	0.41
4:F:185:TYR:OH	4:F:198:LYS:NZ	2.54	0.41
2:B:112:LEU:HG	2:B:112:LEU:O	2.20	0.41
1:C:36:MET:HE1	1:C:49:PHE:CE1	2.55	0.41
2:D:151:LEU:O	2:D:155:ILE:HG13	2.21	0.41
3:E:119:MET:HA	3:E:122:ARG:CZ	2.50	0.41
4:F:191:LEU:CD2	4:F:197:ARG:O	2.68	0.41
4:F:214:TYR:HB3	4:F:375:PHE:HB3	2.02	0.41
1:A:398:MET:HE2	2:B:346:PRO:HD2	2.03	0.41
2:B:377:LEU:C	2:B:377:LEU:HD23	2.45	0.41
3:E:119:MET:HA	3:E:122:ARG:NH2	2.36	0.41
2:B:21:TRP:CE3	2:B:61:PRO:HB3	2.56	0.40
2:B:293:MET:CE	2:B:365:ALA:HB1	2.50	0.40
1:C:7:ILE:HG21	1:C:153:LEU:CD2	2.51	0.40
2:D:249:ASP:OD1	2:D:251:ARG:N	2.54	0.40
2:D:299:MET:HE2	2:D:299:MET:CA	2.49	0.40
4:F:13:VAL:HG21	4:F:336:PRO:O	2.21	0.40
4:F:234:GLN:OE1	4:F:234:GLN:CA	2.69	0.40
1:A:344:VAL:HG21	1:A:346:TRP:CE2	2.56	0.40
1:C:139:HIS:CD2	1:C:150:THR:HG21	2.56	0.40
1:A:9:VAL:HA	1:A:68:VAL:HG13	2.02	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:34:GLY:O	2:D:58:LYS:HA	2.22	0.40
1:A:9:VAL:HG22	1:A:68:VAL:HG11	2.03	0.40
1:A:241:SER:HB2	1:A:249:ASN:O	2.21	0.40
1:C:338:LYS:HE2	1:C:338:LYS:HB2	1.94	0.40
2:D:286:VAL:HB	2:D:287:PRO:HD3	2.03	0.40
2:B:61:PRO:HD3	2:B:84:ILE:HG12	2.03	0.40
1:C:46:ASP:OD1	1:C:46:ASP:N	2.55	0.40
1:C:209:ILE:CG2	1:C:227:LEU:HD22	2.43	0.40
1:C:271:THR:HG23	1:C:300:ASN:C	2.47	0.40
4:F:81:ILE:HG12	4:F:87:LEU:HD13	2.02	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:291:GLN:NE2	4:F:90:SER:OG[4_455]	2.02	0.18
2:D:291:GLN:OE1	4:F:90:SER:OG[4_455]	2.13	0.07

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/451 (96%)	426 (98%)	9 (2%)	0	100	100
1	C	438/451 (97%)	429 (98%)	9 (2%)	0	100	100
2	B	426/445 (96%)	415 (97%)	11 (3%)	0	100	100
2	D	417/445 (94%)	407 (98%)	10 (2%)	0	100	100
3	E	117/189 (62%)	114 (97%)	3 (3%)	0	100	100
4	F	324/380 (85%)	316 (98%)	8 (2%)	0	100	100
All	All	2157/2361 (91%)	2107 (98%)	50 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	365/379 (96%)	363 (100%)	2 (0%)	81	92
1	C	369/379 (97%)	367 (100%)	2 (0%)	81	92
2	B	362/383 (94%)	360 (99%)	2 (1%)	78	91
2	D	357/383 (93%)	350 (98%)	7 (2%)	48	74
3	E	108/171 (63%)	108 (100%)	0	100	100
4	F	294/338 (87%)	288 (98%)	6 (2%)	48	74
All	All	1855/2033 (91%)	1836 (99%)	19 (1%)	68	86

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	156	ARG
1	A	433	GLU
2	B	205	GLU
2	B	361	LEU
1	C	251	ASP
1	C	279	GLU
2	D	30	ILE
2	D	179	VAL
2	D	246	LEU
2	D	284	LEU
2	D	293	MET
2	D	306	ARG
2	D	329	GLN
4	F	103	THR
4	F	182	ILE
4	F	197	ARG
4	F	199	PHE
4	F	230	SER
4	F	234	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	309	HIS
1	A	372	GLN
1	A	393	HIS
2	B	227	HIS
2	B	247	ASN
2	B	329	GLN
2	B	426	GLN
1	C	285	GLN
2	D	292	GLN
3	E	90	ASN
4	F	176	GLN
4	F	183	GLN
4	F	260	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 6 are monoatomic - leaving 9 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
12	ACP	F	401	-	31,33,33	1.65	8 (25%)	47,52,52	1.83	10 (21%)
9	MES	B	502	-	12,12,12	2.33	1 (8%)	15,16,16	1.77	3 (20%)
8	GOL	A	504	-	5,5,5	0.93	0	5,5,5	1.09	0
10	W4F	B	503	-	24,24,24	3.42	21 (87%)	32,32,32	2.32	10 (31%)
11	GDP	B	504	6	29,30,30	1.16	2 (6%)	45,47,47	1.73	6 (13%)
5	GTP	A	501	6	33,34,34	0.99	3 (9%)	50,54,54	1.56	8 (16%)
5	GTP	D	501	6	33,34,34	0.97	1 (3%)	50,54,54	1.58	8 (16%)
10	W4F	D	503	-	24,24,24	3.08	19 (79%)	32,32,32	2.37	11 (34%)
5	GTP	C	501	6	33,34,34	0.98	2 (6%)	50,54,54	1.56	8 (16%)

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
12	ACP	F	401	-	-	6/19/38/38	0/3/3/3
9	MES	B	502	-	-	2/6/14/14	0/1/1/1
8	GOL	A	504	-	-	0/4/4/4	-
10	W4F	B	503	-	-	8/13/13/13	0/2/2/2
11	GDP	B	504	6	-	3/16/32/32	0/3/3/3
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3
5	GTP	D	501	6	-	8/22/38/38	0/3/3/3
10	W4F	D	503	-	-	5/13/13/13	0/2/2/2
5	GTP	C	501	6	-	6/22/38/38	0/3/3/3

All (57) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	502	MES	C8-S	-7.80	1.66	1.77
10	B	503	W4F	O4-C13	-5.53	1.28	1.38
10	D	503	W4F	O4-C13	-4.92	1.29	1.38
10	D	503	W4F	O4-C17	-4.78	1.29	1.42
10	B	503	W4F	O3-C16	-4.77	1.29	1.42
12	F	401	ACP	C5-C4	4.74	1.47	1.39
10	B	503	W4F	C6-C1	-4.50	1.32	1.38
10	B	503	W4F	O4-C17	-4.46	1.30	1.42
10	B	503	W4F	O2-C1	-4.32	1.27	1.36
10	D	503	W4F	O5-C12	-4.25	1.30	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	W4F	C14-C13	-4.23	1.32	1.41
10	D	503	W4F	O5-C18	-4.11	1.31	1.42
10	B	503	W4F	C8-C9	-4.06	1.40	1.51
10	D	503	W4F	O3-C16	-3.95	1.31	1.42
10	D	503	W4F	O1-C10	-3.93	1.31	1.42
10	B	503	W4F	O1-C10	-3.81	1.32	1.42
10	B	503	W4F	O1-C2	-3.77	1.31	1.37
10	D	503	W4F	O1-C2	-3.73	1.31	1.37
10	B	503	W4F	C11-C9	-3.68	1.33	1.39
10	D	503	W4F	C14-C13	-3.60	1.33	1.41
10	B	503	W4F	C7-C5	-3.58	1.41	1.51
10	B	503	W4F	C12-C13	-3.52	1.33	1.41
10	B	503	W4F	C15-C9	-3.25	1.33	1.39
10	D	503	W4F	C12-C13	-3.16	1.34	1.41
11	B	504	GDP	C5-C4	3.14	1.47	1.38
10	D	503	W4F	O2-C1	-3.05	1.30	1.36
10	D	503	W4F	O3-C14	-3.02	1.32	1.37
10	D	503	W4F	C11-C9	-3.00	1.34	1.39
10	D	503	W4F	C4-C5	-2.95	1.33	1.38
10	D	503	W4F	C11-C12	-2.91	1.33	1.38
12	F	401	ACP	PG-O3G	2.90	1.61	1.55
12	F	401	ACP	PG-O2G	2.87	1.61	1.55
10	D	503	W4F	C3-C4	-2.84	1.34	1.38
10	B	503	W4F	C11-C12	-2.83	1.34	1.38
12	F	401	ACP	C5-C6	2.74	1.48	1.41
10	B	503	W4F	C4-C5	-2.72	1.33	1.38
12	F	401	ACP	PB-O3A	2.55	1.61	1.58
10	B	503	W4F	C15-C14	-2.54	1.34	1.38
10	D	503	W4F	C7-C5	-2.53	1.44	1.51
10	B	503	W4F	O3-C14	-2.47	1.33	1.37
10	B	503	W4F	C3-C4	-2.42	1.34	1.38
11	B	504	GDP	C6-N1	-2.39	1.34	1.38
10	B	503	W4F	C3-C2	-2.38	1.34	1.39
10	D	503	W4F	C3-C2	-2.32	1.34	1.39
10	B	503	W4F	O5-C18	-2.29	1.36	1.42
12	F	401	ACP	C8-N7	2.29	1.36	1.31
12	F	401	ACP	C5-N7	-2.25	1.35	1.39
5	A	501	GTP	C2-N3	2.22	1.38	1.33
10	D	503	W4F	C6-C1	-2.20	1.35	1.38
5	D	501	GTP	C2-N3	2.20	1.38	1.33
5	C	501	GTP	C2-N3	2.16	1.38	1.33
10	B	503	W4F	C6-C5	-2.16	1.35	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	D	503	W4F	C6-C5	-2.11	1.35	1.39
12	F	401	ACP	PB-O2B	2.08	1.61	1.56
5	A	501	GTP	PA-O3A	2.05	1.61	1.59
5	C	501	GTP	PA-O3A	2.05	1.61	1.59
5	A	501	GTP	PB-O3A	2.02	1.61	1.59

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	503	W4F	O1-C2-C1	8.35	127.08	114.55
10	D	503	W4F	C18-O5-C12	-6.97	107.29	117.51
11	B	504	GDP	C5-C4-N3	-6.00	118.84	128.39
12	F	401	ACP	C5-C4-N3	-5.80	118.74	126.72
10	D	503	W4F	O1-C2-C1	5.17	122.31	114.55
5	D	501	GTP	C5-C4-N3	-5.02	120.41	128.39
11	B	504	GDP	C2-N3-C4	5.01	120.92	112.30
5	C	501	GTP	C5-C4-N3	-4.96	120.50	128.39
10	B	503	W4F	O1-C2-C3	-4.95	115.95	124.30
5	A	501	GTP	C5-C4-N3	-4.94	120.53	128.39
12	F	401	ACP	N3-C4-N9	4.64	135.06	127.17
5	A	501	GTP	C2-N3-C4	4.62	120.25	112.30
5	D	501	GTP	C2-N3-C4	4.60	120.23	112.30
5	C	501	GTP	C2-N3-C4	4.60	120.22	112.30
11	B	504	GDP	N9-C4-N3	4.36	134.67	125.95
9	B	502	MES	C5-N4-C3	4.15	117.78	108.84
10	D	503	W4F	O5-C12-C11	-3.94	117.30	124.08
10	D	503	W4F	C11-C12-C13	3.72	124.36	120.22
12	F	401	ACP	C2-N3-C4	3.67	120.80	111.83
12	F	401	ACP	PB-O3A-PA	-3.58	120.70	132.37
10	B	503	W4F	C10-O1-C2	3.42	122.53	117.51
12	F	401	ACP	C4-C5-N7	-3.41	106.68	110.58
10	D	503	W4F	C7-C5-C6	3.40	126.25	120.54
11	B	504	GDP	C6-C5-N7	3.37	136.42	130.29
5	D	501	GTP	N9-C4-N3	3.23	132.41	125.95
12	F	401	ACP	N3-C2-N1	-3.19	123.75	128.58
5	C	501	GTP	N9-C4-N3	3.16	132.28	125.95
5	A	501	GTP	N9-C4-N3	3.16	132.28	125.95
10	B	503	W4F	C8-C9-C15	3.06	125.69	120.54
10	D	503	W4F	C14-C13-C12	-3.02	116.62	119.56
10	B	503	W4F	O3-C14-C15	-2.94	119.02	124.08
5	D	501	GTP	C2-N1-C6	-2.91	119.84	125.11
5	C	501	GTP	C2-N1-C6	-2.89	119.88	125.11

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C2-N1-C6	-2.87	119.91	125.11
10	B	503	W4F	O3-C14-C13	2.78	119.90	115.14
9	B	502	MES	C6-C5-N4	-2.71	106.01	110.12
5	A	501	GTP	N9-C8-N7	-2.67	108.44	113.40
5	C	501	GTP	N9-C8-N7	-2.67	108.45	113.40
5	D	501	GTP	N9-C8-N7	-2.66	108.46	113.40
12	F	401	ACP	C4-N9-C8	2.64	108.51	105.74
11	B	504	GDP	C4-C5-N7	-2.62	106.52	110.67
10	D	503	W4F	C8-C9-C15	2.62	124.94	120.54
5	A	501	GTP	C8-N7-C5	2.54	108.78	104.26
5	D	501	GTP	C8-N7-C5	2.53	108.78	104.26
12	F	401	ACP	C5-N7-C8	2.52	107.40	103.45
5	D	501	GTP	C5-C6-N1	2.51	119.65	113.25
5	C	501	GTP	C8-N7-C5	2.51	108.73	104.26
5	A	501	GTP	C5-C6-N1	2.51	119.63	113.25
5	C	501	GTP	C5-C6-N1	2.48	119.57	113.25
10	B	503	W4F	C3-C2-C1	-2.46	116.96	119.87
5	C	501	GTP	O6-C6-C5	-2.46	120.03	126.53
12	F	401	ACP	C3'-C2'-C1'	2.42	106.04	101.46
5	A	501	GTP	O6-C6-C5	-2.41	120.18	126.53
5	D	501	GTP	O6-C6-C5	-2.40	120.19	126.53
10	D	503	W4F	C3-C2-C1	-2.38	117.05	119.87
9	B	502	MES	O1S-S-C8	2.36	110.29	106.73
10	B	503	W4F	C8-C9-C11	-2.36	116.58	120.54
10	B	503	W4F	C8-C7-C5	2.30	121.08	113.23
10	D	503	W4F	C7-C8-C9	2.21	120.76	113.23
10	D	503	W4F	O1-C2-C3	-2.18	120.62	124.30
10	B	503	W4F	C7-C8-C9	2.18	120.64	113.23
10	D	503	W4F	C11-C9-C15	-2.13	116.11	119.01
11	B	504	GDP	O6-C6-C5	-2.09	121.02	126.53
12	F	401	ACP	C6-C5-N7	2.06	136.06	132.09

There are no chirality outliers.

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A

Continued on next page...

Continued from previous page...

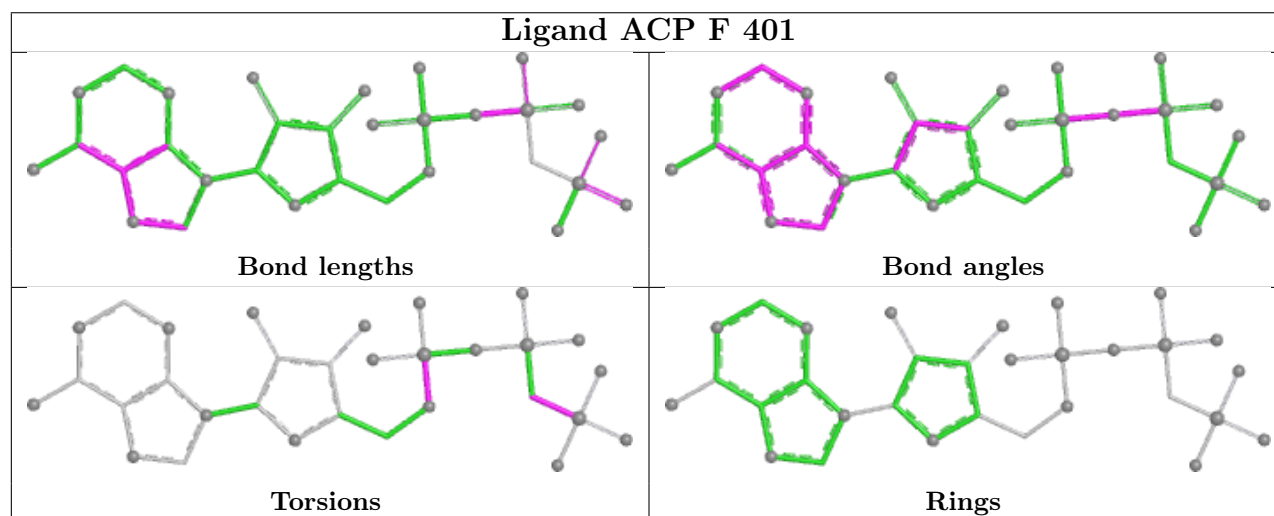
Mol	Chain	Res	Type	Atoms
5	D	501	GTP	C5'-O5'-PA-O1A
9	B	502	MES	C8-C7-N4-C5
11	B	504	GDP	C5'-O5'-PA-O3A
11	B	504	GDP	C5'-O5'-PA-O1A
11	B	504	GDP	C5'-O5'-PA-O2A
12	F	401	ACP	PB-C3B-PG-O1G
12	F	401	ACP	PB-C3B-PG-O2G
12	F	401	ACP	PB-C3B-PG-O3G
12	F	401	ACP	C5'-O5'-PA-O1A
10	B	503	W4F	C1-C2-O1-C10
10	B	503	W4F	C3-C2-O1-C10
10	D	503	W4F	C3-C2-O1-C10
10	B	503	W4F	C15-C14-O3-C16
10	B	503	W4F	C13-C14-O3-C16
10	D	503	W4F	C1-C2-O1-C10
10	D	503	W4F	C11-C12-O5-C18
10	D	503	W4F	C13-C12-O5-C18
9	B	502	MES	C8-C7-N4-C3
5	C	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
5	D	501	GTP	PB-O3A-PA-O2A
5	D	501	GTP	C3'-C4'-C5'-O5'
5	D	501	GTP	C5'-O5'-PA-O3A
5	D	501	GTP	C5'-O5'-PA-O2A
12	F	401	ACP	C5'-O5'-PA-O2A
12	F	401	ACP	C5'-O5'-PA-O3A
5	A	501	GTP	C4'-C5'-O5'-PA
10	B	503	W4F	C7-C8-C9-C15
10	B	503	W4F	C7-C8-C9-C11
5	C	501	GTP	C4'-C5'-O5'-PA
5	D	501	GTP	O4'-C4'-C5'-O5'
10	B	503	W4F	C4-C5-C7-C8
10	B	503	W4F	C6-C5-C7-C8
10	D	503	W4F	C5-C7-C8-C9
5	A	501	GTP	PB-O3B-PG-O2G
5	D	501	GTP	PB-O3A-PA-O1A
5	D	501	GTP	C4'-C5'-O5'-PA

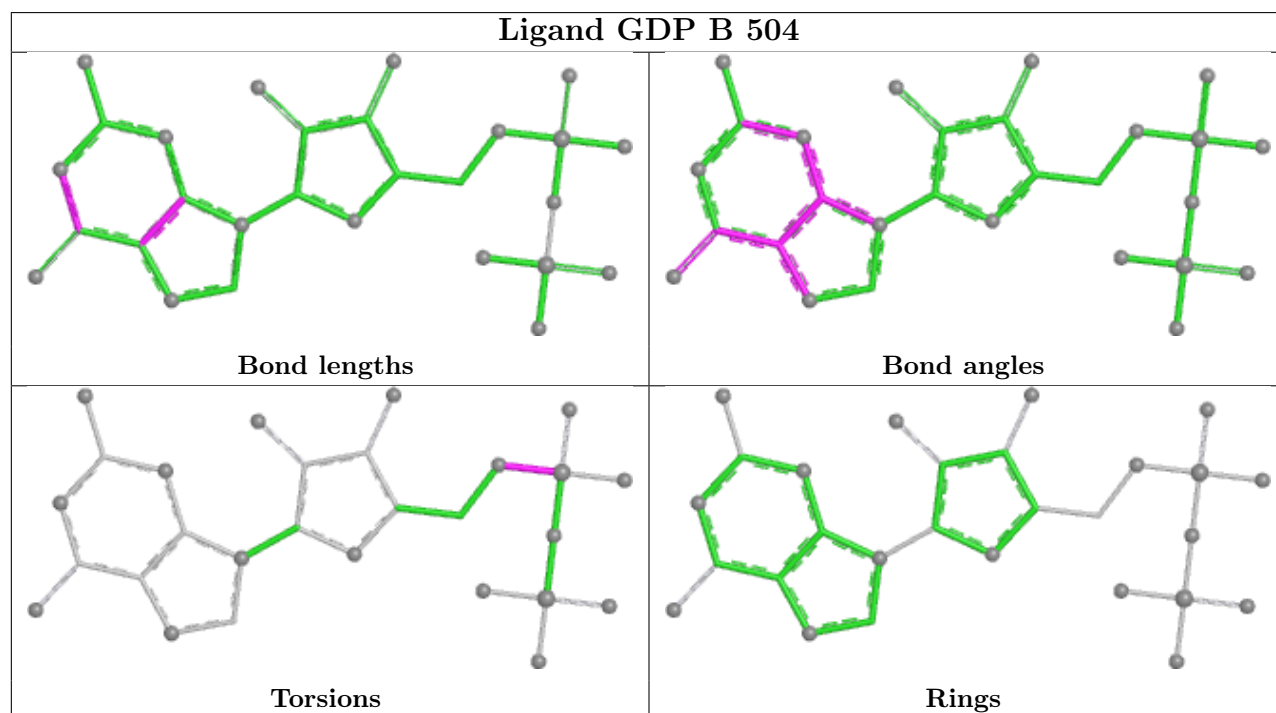
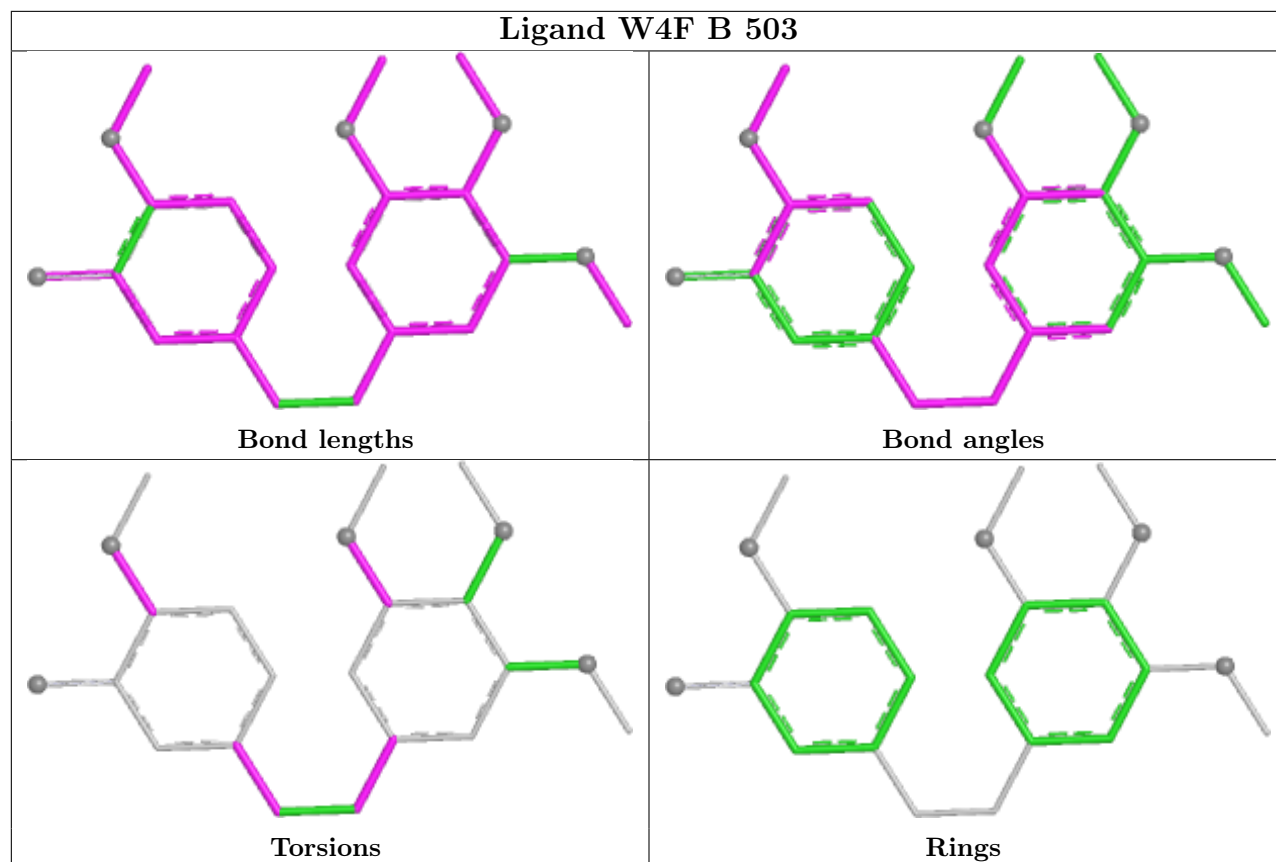
There are no ring outliers.

2 monomers are involved in 3 short contacts:

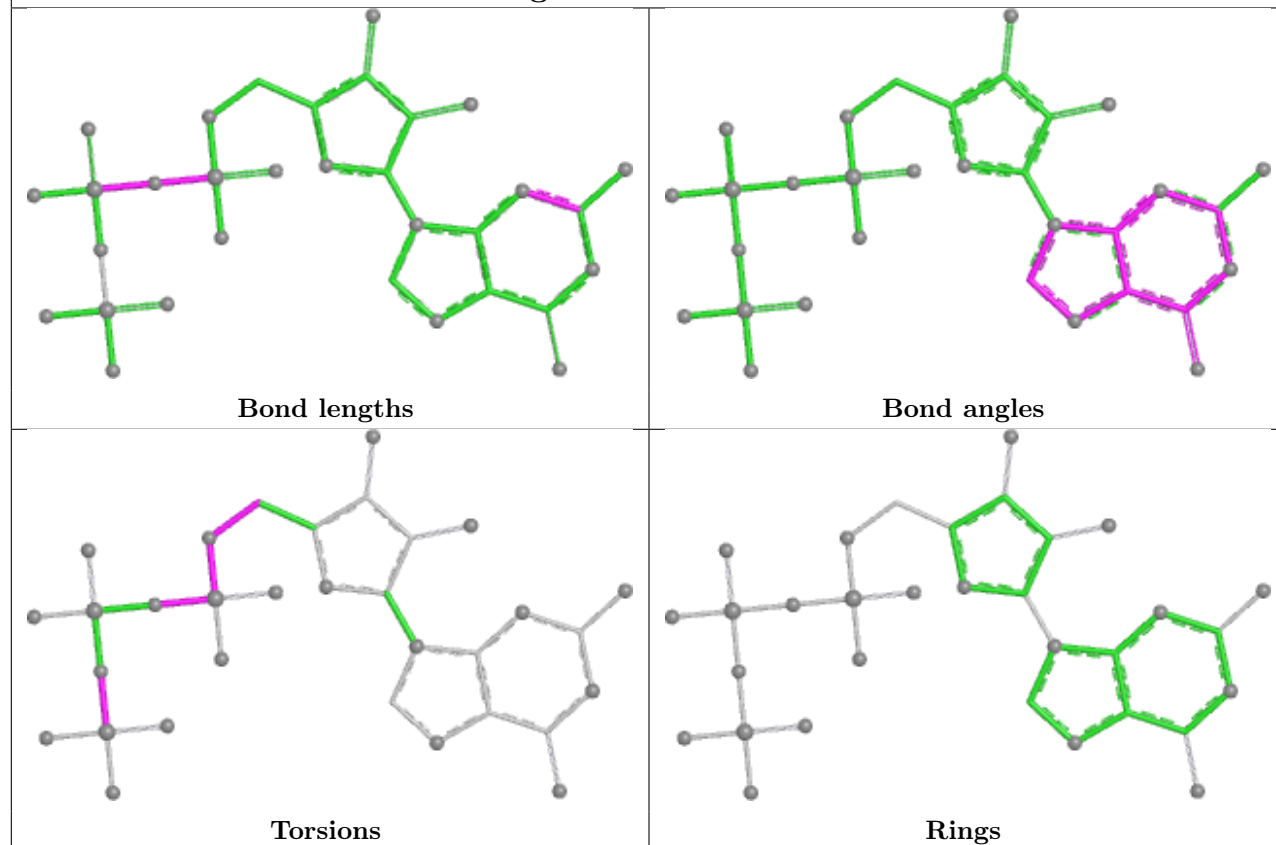
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	503	W4F	2	0
10	D	503	W4F	1	0

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.

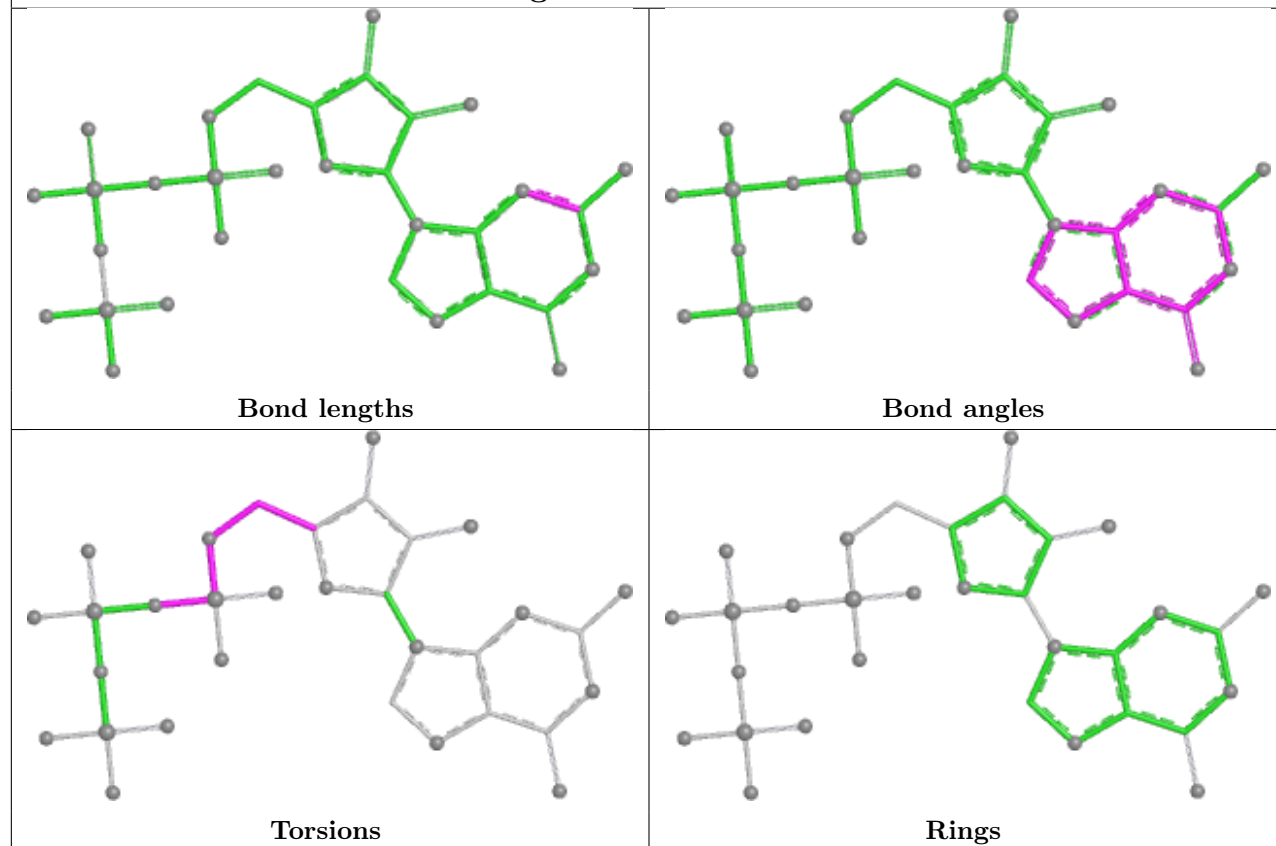




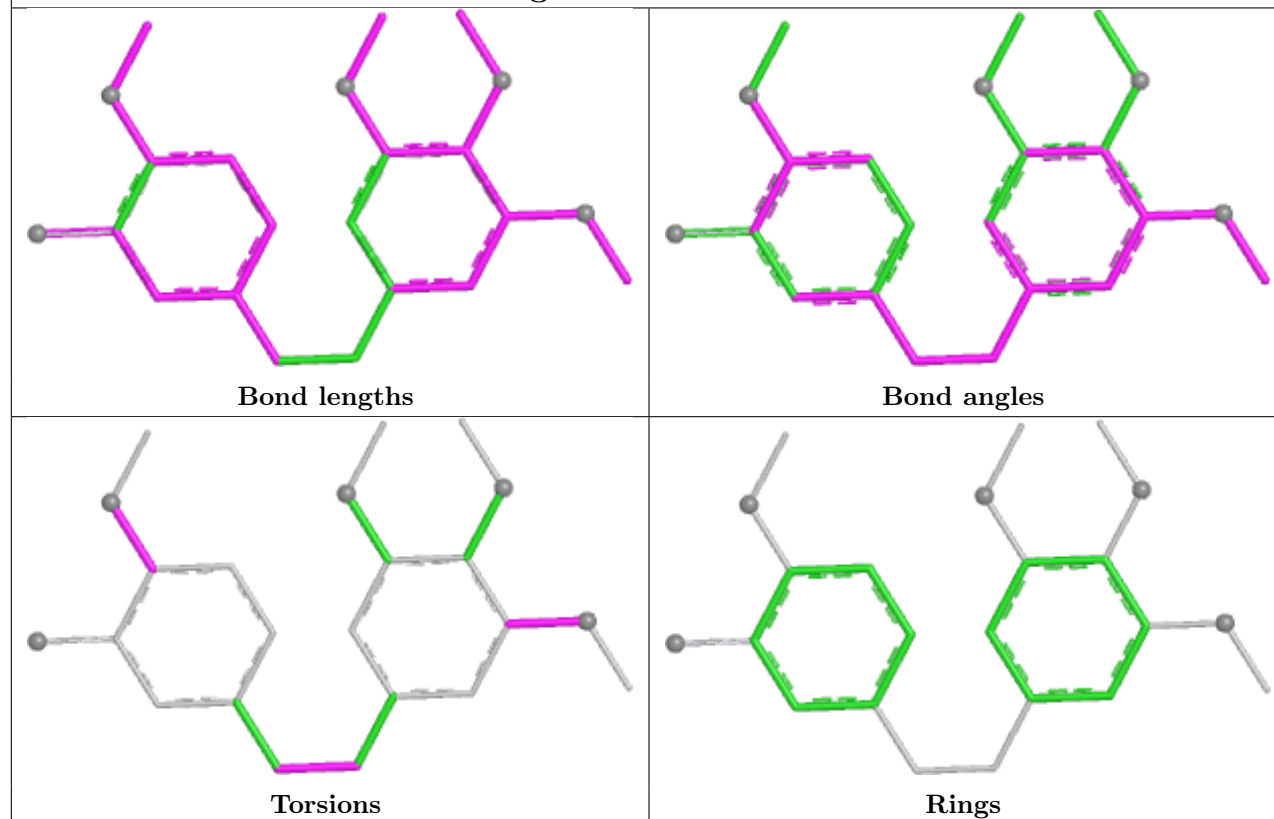
Ligand GTP A 501



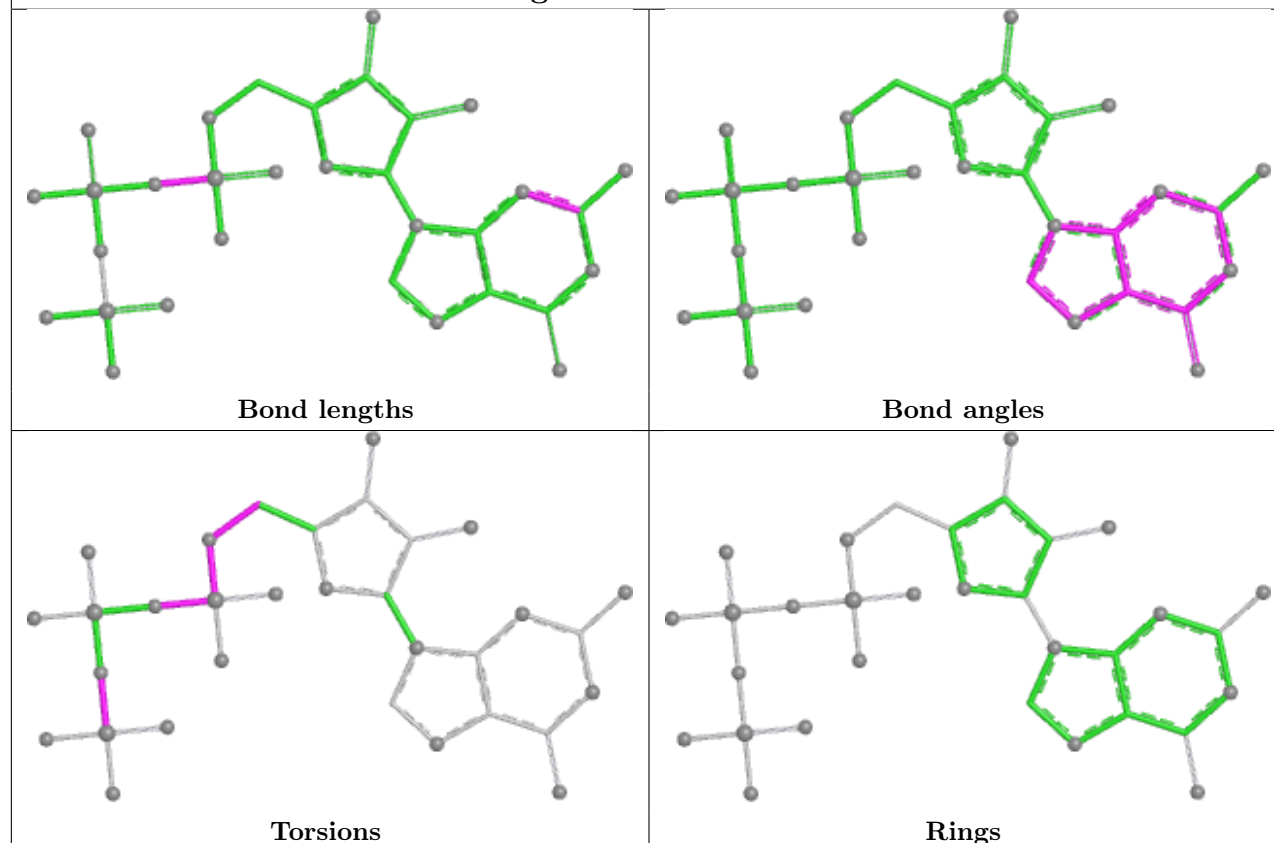
Ligand GTP D 501



Ligand W4F D 503



Ligand GTP C 501



5.7 Other polymers

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	437/451 (96%)	0.23	6 (1%) 73 69	42, 60, 78, 92	0
1	C	440/451 (97%)	0.04	11 (2%) 58 52	36, 51, 71, 85	0
2	B	428/445 (96%)	0.33	13 (3%) 52 47	39, 61, 87, 118	0
2	D	421/445 (94%)	0.66	23 (5%) 30 25	46, 76, 99, 118	0
3	E	121/189 (64%)	0.66	4 (3%) 49 43	52, 73, 102, 122	0
4	F	334/380 (87%)	0.93	40 (11%) 9 7	54, 86, 137, 152	0
All	All	2181/2361 (92%)	0.43	97 (4%) 39 33	36, 65, 105, 152	0

All (97) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	179	THR	8.0
4	F	161	LEU	5.0
2	B	1	MET	5.0
4	F	103	THR	4.9
2	B	72	THR	4.8
4	F	172	PHE	4.8
4	F	362	ALA	4.7
2	D	1	MET	4.3
2	D	101	TRP	4.0
2	B	2	ARG	3.9
4	F	162	ILE	3.9
4	F	170	LEU	3.7
1	C	178	SER	3.7
4	F	372	THR	3.6
1	A	262	TYR	3.6
4	F	149	ALA	3.5
4	F	180	HIS	3.5
1	C	440	VAL	3.5
4	F	181	VAL	3.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
4	F	233	PHE	3.4
2	D	170	MET	3.3
2	B	280	GLN	3.3
4	F	178	GLN	3.3
2	B	177	ASP	3.2
4	F	232	ASN	3.1
4	F	148	ILE	3.1
1	A	346	TRP	3.1
2	D	2	ARG	3.0
2	B	92	PHE	3.0
2	D	6	HIS	2.9
4	F	88	SER	2.9
1	C	340	SER	2.9
4	F	179	VAL	2.9
3	E	28	SER	2.9
2	D	31	ASP	2.8
4	F	128	ARG	2.8
2	D	394	PHE	2.7
4	F	231	ALA	2.7
1	A	282	TYR	2.7
4	F	173	ILE	2.7
1	A	437	VAL	2.7
2	B	175	VAL	2.7
3	E	140	LYS	2.6
1	C	174	ALA	2.6
4	F	166	ALA	2.6
4	F	132	LEU	2.6
2	B	323	MET	2.6
2	D	55	THR	2.5
2	B	55	THR	2.5
1	C	175	PRO	2.5
2	D	81	PHE	2.5
2	D	48	ASN	2.5
4	F	182	ILE	2.5
4	F	177	GLY	2.4
4	F	239	HIS	2.4
3	E	6	MET	2.4
2	D	216	LYS	2.4
1	C	410	GLY	2.4
1	C	342	GLN	2.4
2	B	54	ALA	2.4
4	F	237	THR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	96	GLY	2.3
2	D	141	GLY	2.3
2	D	54	ALA	2.3
4	F	169	LEU	2.3
4	F	131	PHE	2.3
2	D	219	THR	2.2
4	F	167	SER	2.2
1	C	142	GLY	2.2
2	D	140	GLY	2.2
4	F	146	VAL	2.2
2	D	212	PHE	2.2
4	F	196	HIS	2.2
1	A	283	HIS	2.2
3	E	135	LYS	2.2
2	D	218	THR	2.2
4	F	228	TYR	2.2
2	D	15	GLN	2.2
2	B	128	ASP	2.2
1	C	341	ILE	2.1
4	F	199	PHE	2.1
2	B	42	LEU	2.1
4	F	253	TYR	2.1
4	F	130	VAL	2.1
2	D	245	GLN	2.1
4	F	21	LEU	2.1
4	F	57	GLY	2.1
4	F	224	SER	2.1
4	F	89	GLU	2.1
2	D	70	PRO	2.1
2	D	273	LEU	2.0
1	C	293	ASN	2.0
4	F	245	ILE	2.0
2	B	245	GLN	2.0
2	D	395	LEU	2.0
1	A	68	VAL	2.0
4	F	98	TYR	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

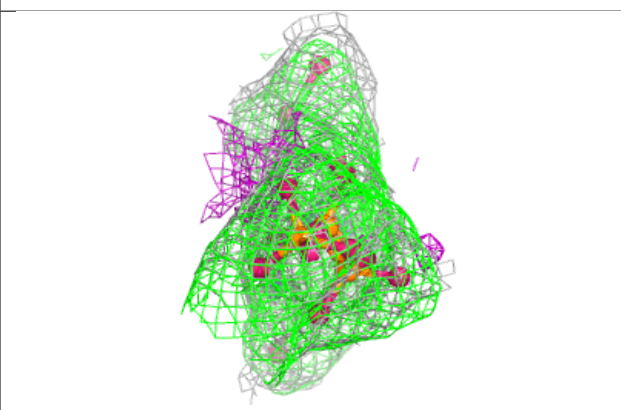
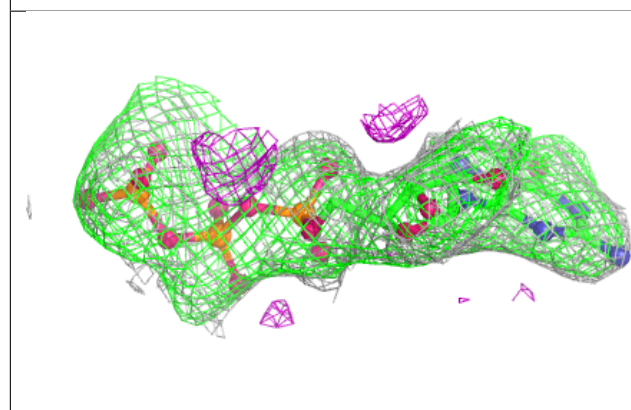
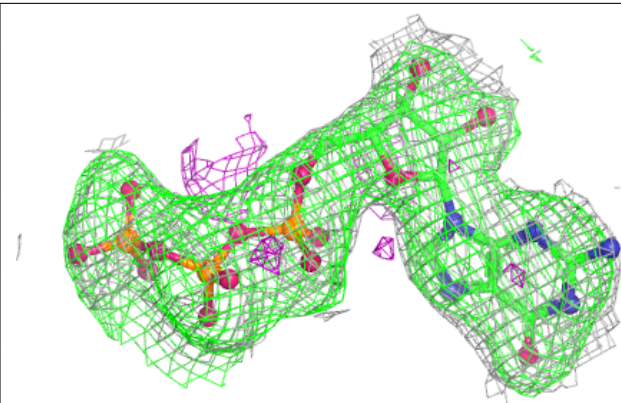
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GTP	A	501	32/32	-	-	51,52,57,58	32
5	GTP	C	501	32/32	-	-	43,46,54,55	32
5	GTP	D	501	32/32	-	-	74,78,82,83	32
6	MG	A	502	1/1	-	-	56,56,56,56	1
6	MG	B	501	1/1	-	-	59,59,59,59	1
6	MG	C	502	1/1	-	-	46,46,46,46	1
6	MG	D	502	1/1	-	-	83,83,83,83	1
7	CA	A	503	1/1	-	-	76,76,76,76	1
7	CA	C	503	1/1	-	-	65,65,65,65	1
8	GOL	A	504	6/6	-	-	52,52,53,53	6
9	MES	B	502	12/12	-	-	56,59,62,62	12
10	W4F	B	503	23/23	0.92	0.09	50,65,78,81	0
10	W4F	D	503	23/23	0.92	0.10	46,72,90,99	0
11	GDP	B	504	28/28	-	-	47,53,57,57	28
12	ACP	F	401	31/31	-	-	89,100,103,104	31

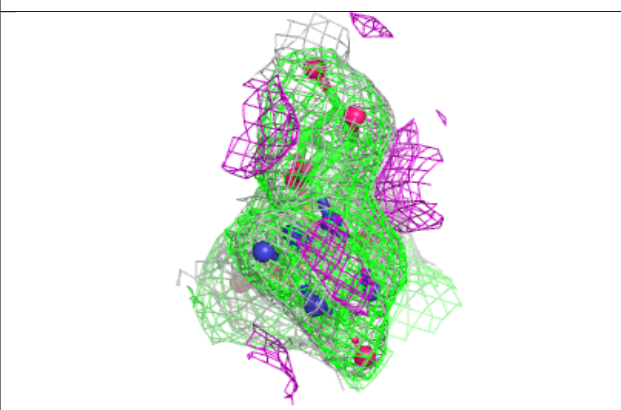
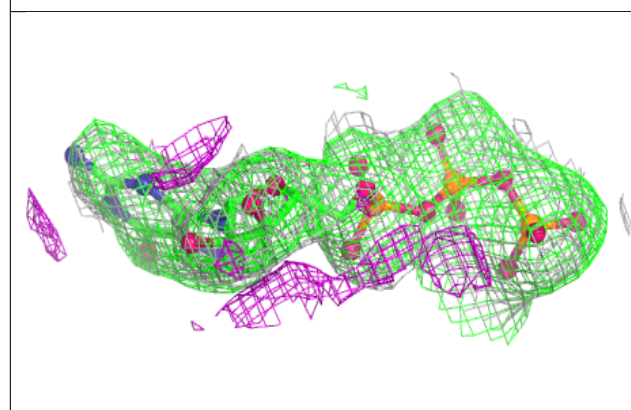
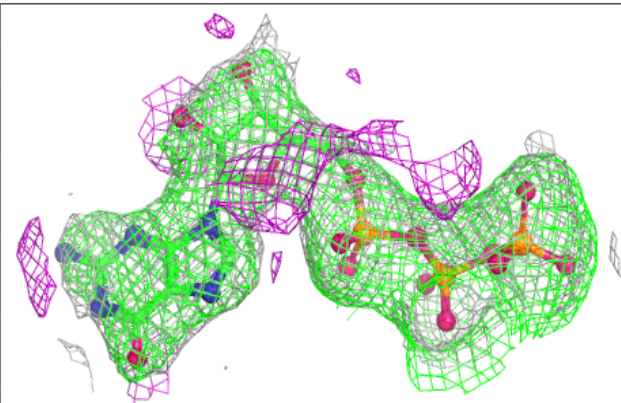
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 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)

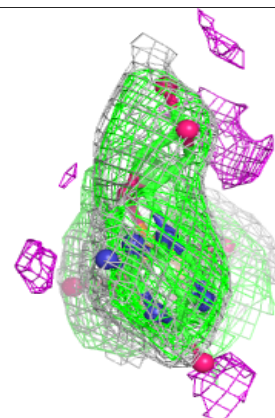
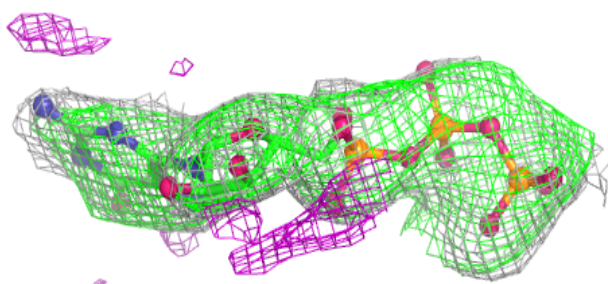
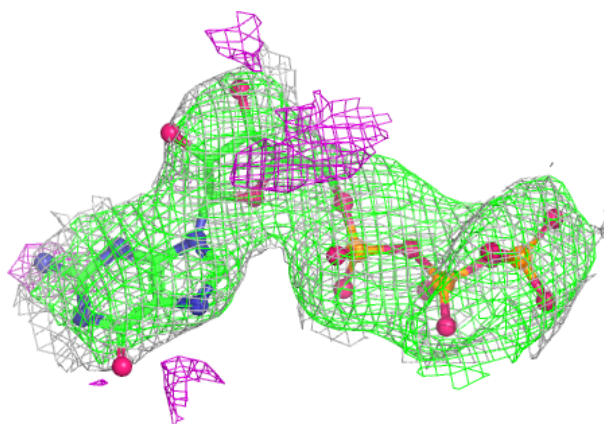
**Electron density around GTP C 501:**

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

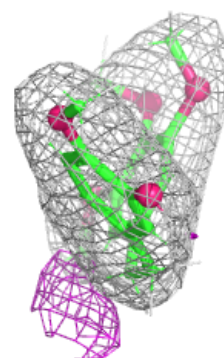
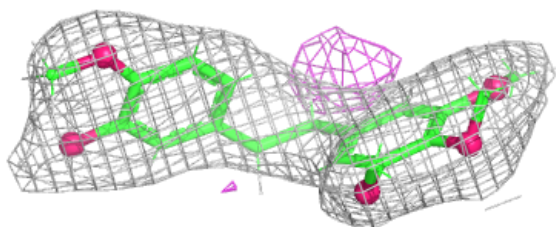
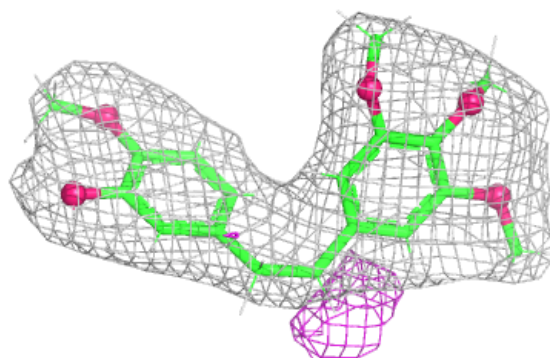


Electron density around GTP D 501:

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

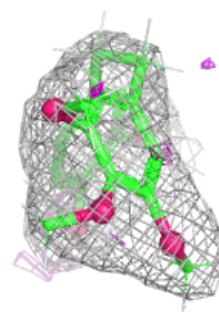
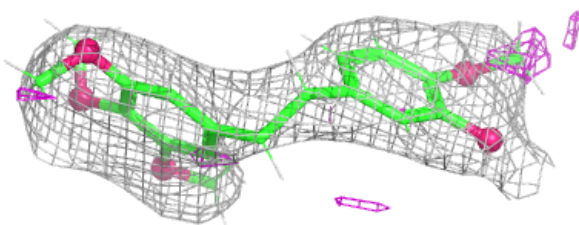
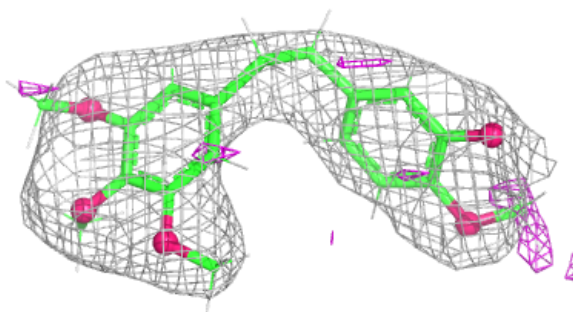
**Electron density around W4F B 503:**

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



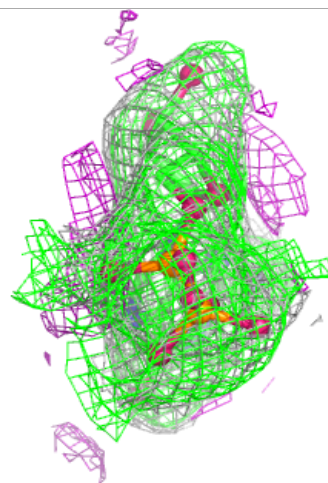
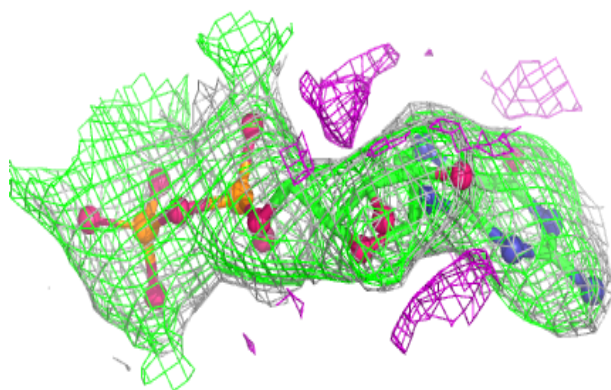
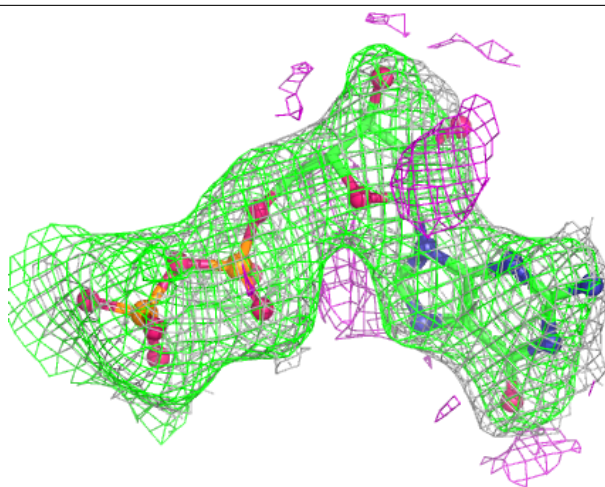
Electron density around W4F D 503:

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



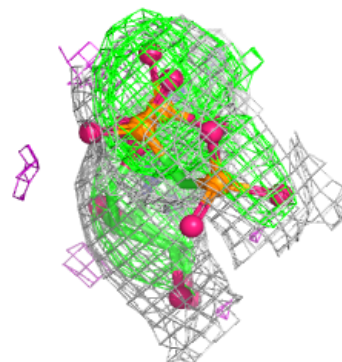
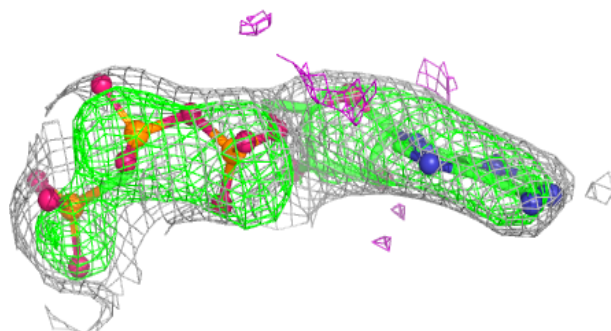
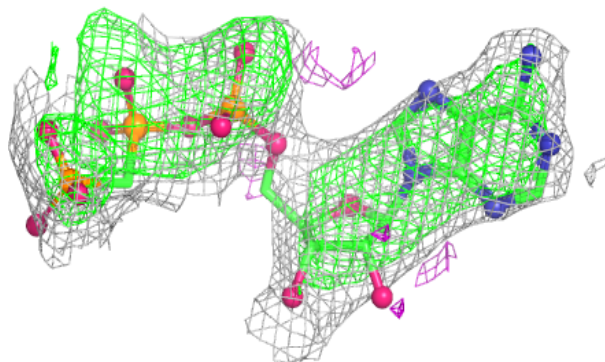
Electron density around GDP B 504:

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



Electron density around ACP F 401:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.