Full wwPDB X-ray Structure Validation Report (i)

Mar 14, 2026 – 08:40 PM UTC

PDB ID	:	8JJC / pdb_00008jjc
Title	:	Tubulin-Y62
Authors	:	Yang, J.
Deposited on	:	2023-05-30
Resolution	:	2.76 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 (i) 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 (i)) were used in the production of this report:

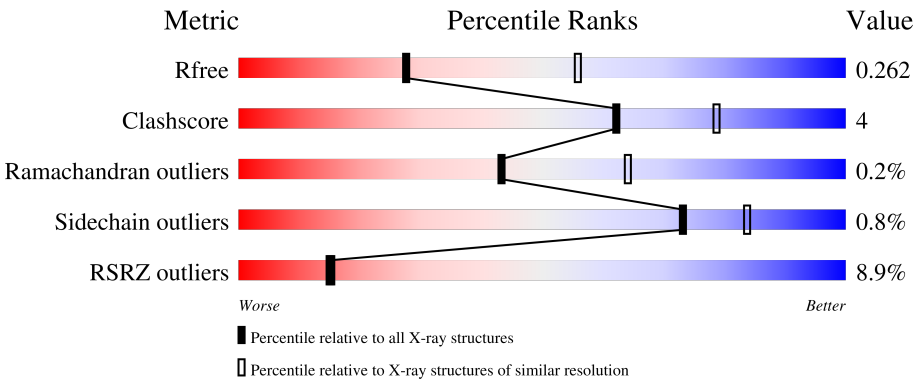
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

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 2.76 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}	180053	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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 <=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	4% 89% 8% •
1	C	451	3% 89% 9% •
2	B	431	6% 88% 10% •
2	D	431	9% 85% 13% •
3	E	189	8% 61% • 35%

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Mol	Chain	Length	Quality of chain
4	F	380	22% 81% 10% • 8%

2 Entry composition (i)

There are 13 unique types of molecules in this entry. The entry contains 33734 atoms, of which 16410 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	438	6653	2146	3260	576	648	23	0	2	0
1	C	440	6779	2183	3331	584	658	23	0	5	0

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
2	B	425	6414	2078	3111	562	638	25	0	1	0
2	D	423	6361	2059	3090	556	632	24	0	0	0

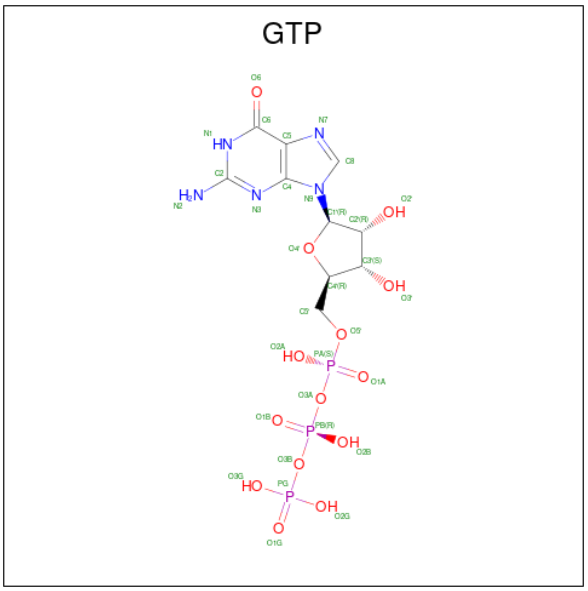
- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
3	E	123	1988	614	995	183	191	5	0	2	0

- Molecule 4 is a protein called TTL.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
4	F	349	5225	1726	2533	462	490	14	0	0	0

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
5	A	1	42	10	10	5	14	3	42	0
			Total	C	H	N	O	P		
5	C	1	42	10	10	5	14	3	42	0
			Total	C	H	N	O	P		
5	D	1	42	10	10	5	14	3	42	0

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

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

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	A	2	2	2	2	0

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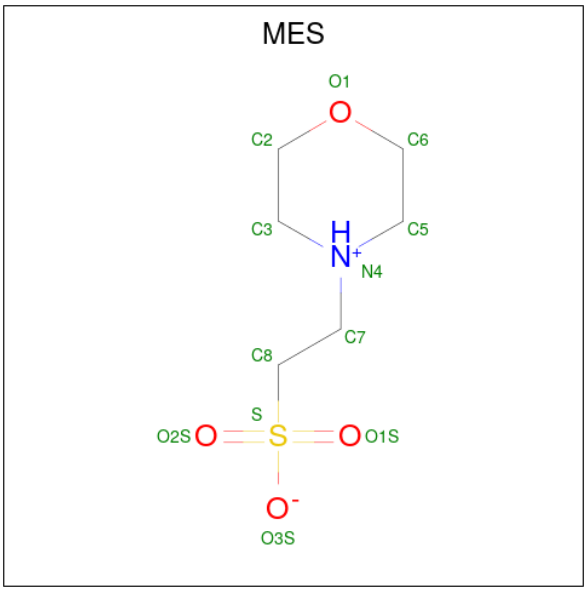
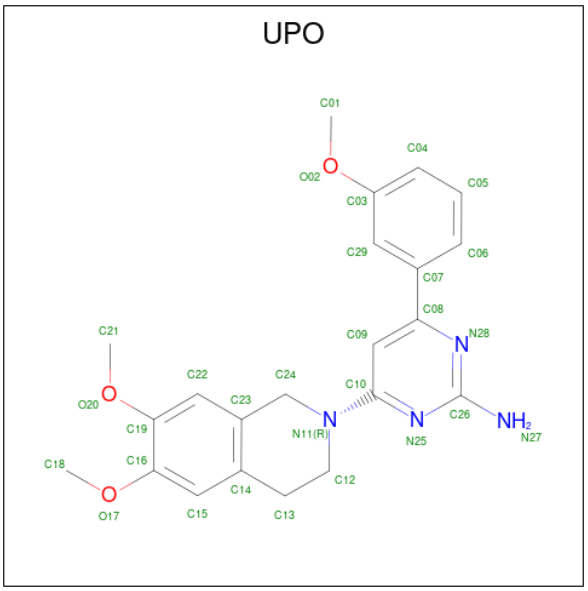
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	B	2	2	2	2	0
7	C	1	1	1	1	0
7	D	1	1	1	1	0

- Molecule 8 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



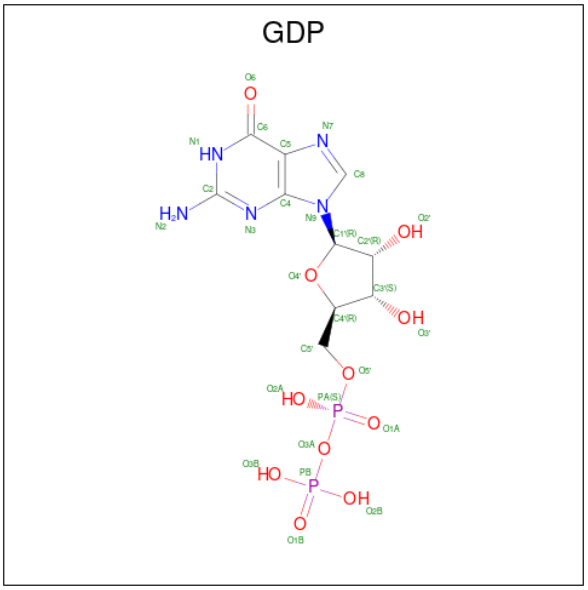
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	S		
8	B	1	24	6	12	1	4	1	24	0

- Molecule 9 is 4-(6,7-dimethoxy-3,4-dihydro-1 {H}-isoquinolin-2-yl)-6-(3-methoxyphenyl)pyrimidin-2-amine (CCD ID: UPO) (formula: $C_{22}H_{24}N_4O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	H	N	O		
9	B	1	53	22	24	4	3	0	0

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

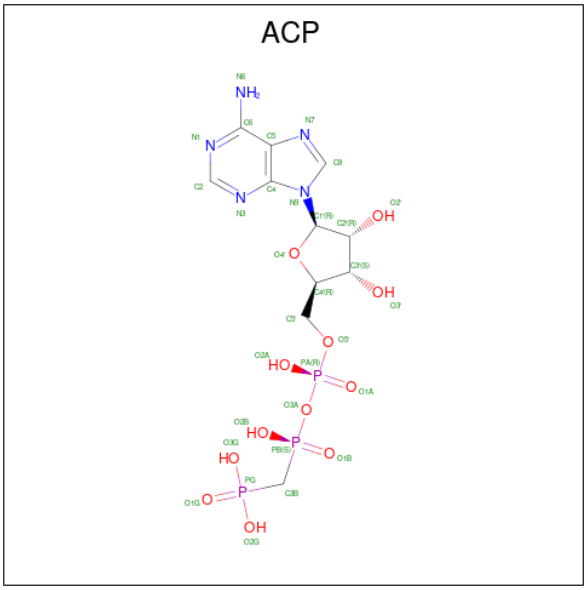


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
10	B	1	38	10	10	5	11	2	38	0

- Molecule 11 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
11	D	1	1	1	1	0

- 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
			Total	C	H	N	O	P		
12	F	1	45	11	14	5	12	3	45	0

- Molecule 13 is water.

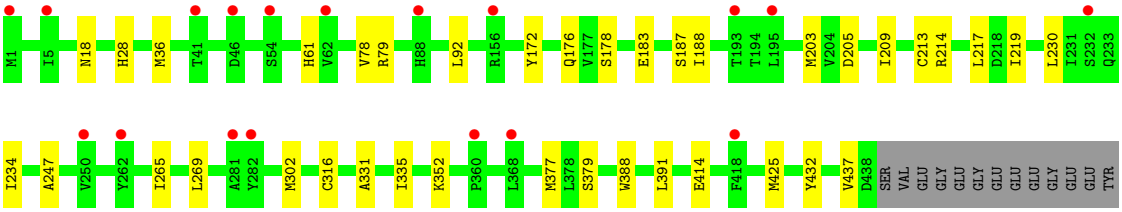
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
13	A	1	1	1	0	0
13	B	2	2	2	0	0
13	C	9	9	9	0	0
13	D	1	1	1	0	0
13	F	3	3	3	0	0

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.

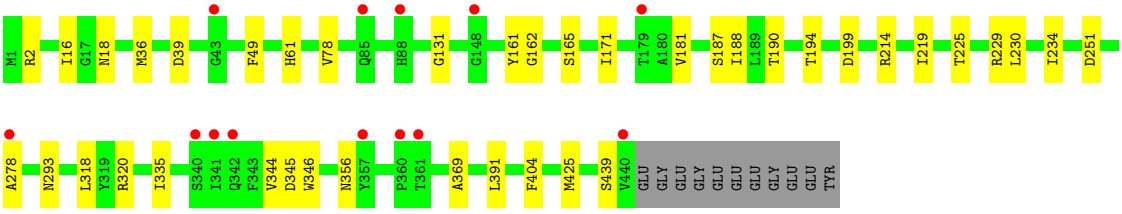
• Molecule 1: Tubulin alpha-1B chain

Chain A:



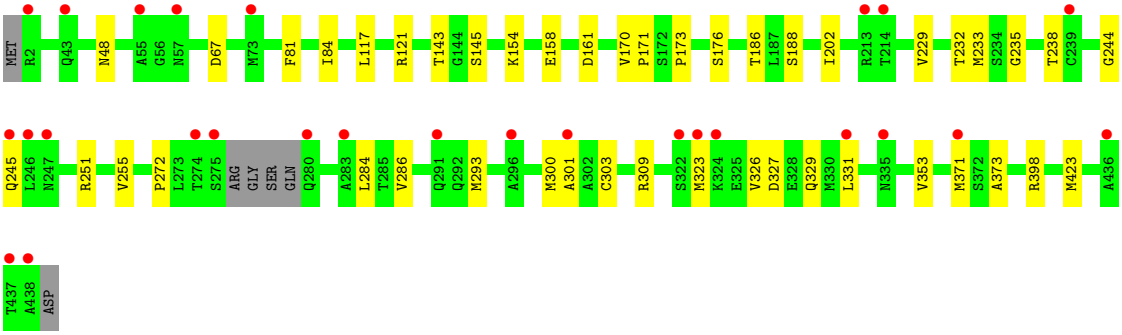
• Molecule 1: Tubulin alpha-1B chain

Chain C:



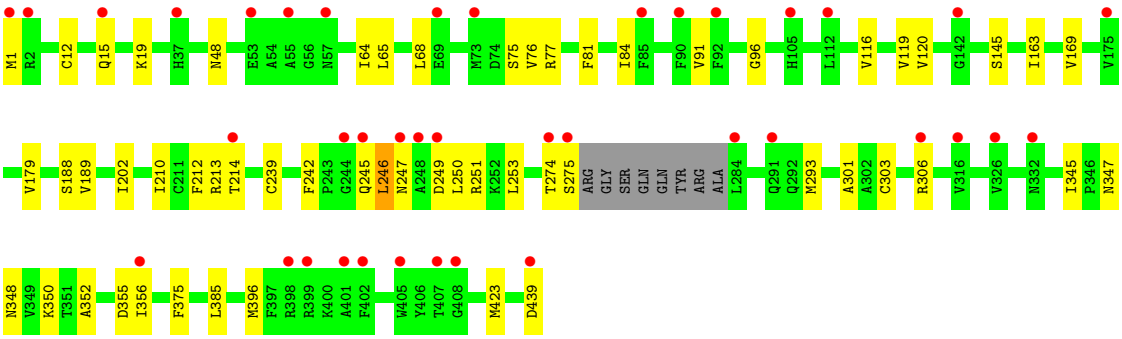
• Molecule 2: Tubulin beta chain

Chain B:



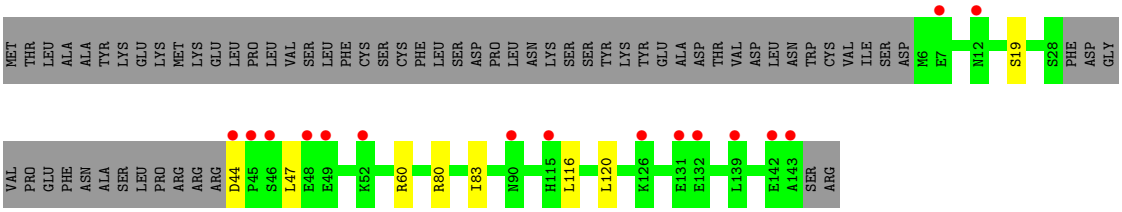
• Molecule 2: Tubulin beta chain

Chain D:



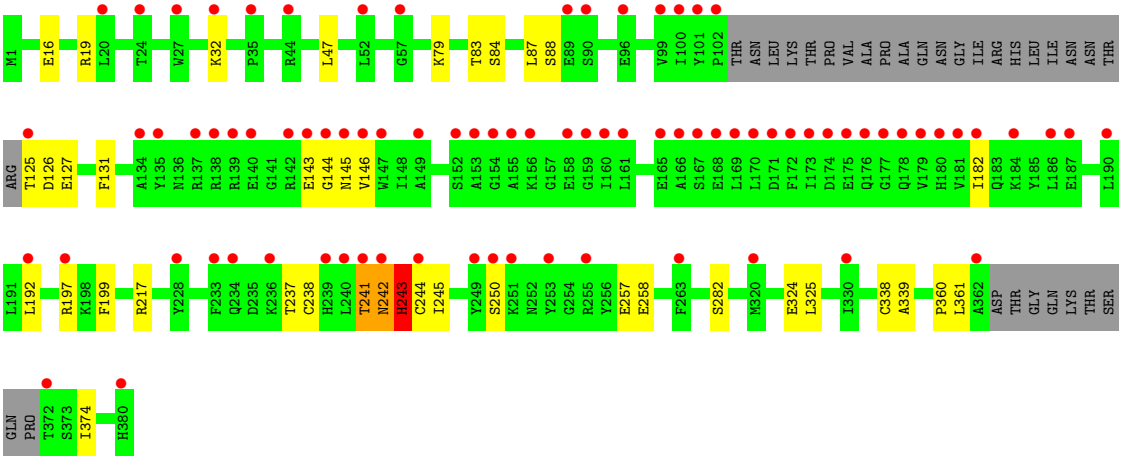
- Molecule 3: Stathmin-4

Chain E:



- Molecule 4: TTL

Chain F:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.49Å 157.00Å 180.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.74 – 2.76 47.74 – 2.76	Depositor EDS
% Data completeness (in resolution range)	99.3 (47.74-2.76) 99.3 (47.74-2.76)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.24 (at 2.77Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.235 , 0.264 0.240 , 0.262	Depositor DCC
R_{free} test set	1143 reflections (1.49%)	wwPDB-VP
Wilson B-factor (Å^2)	70.6	Xtriage
Anisotropy	0.107	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 42.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	33734	wwPDB-VP
Average B, all atoms (Å^2)	75.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: MG, MES, GDP, CL, GTP, ACP, CA, UPO

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	0.17	0/3473	0.39	0/4723
1	C	0.18	0/3539	0.38	0/4810
2	B	0.17	0/3380	0.38	0/4588
2	D	0.17	0/3343	0.39	0/4537
3	E	0.17	0/1004	0.30	0/1336
4	F	0.15	0/2754	0.32	0/3741
All	All	0.17	0/17493	0.37	0/23735

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	3393	3260	3271	24	0
1	C	3448	3331	3344	27	0
2	B	3303	3111	3141	26	0
2	D	3271	3090	3130	33	1
3	E	993	995	998	5	0
4	F	2692	2533	2545	27	1
5	A	32	10	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	10	12	0	0
5	D	32	10	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
8	B	12	12	12	0	0
9	B	29	24	0	0	0
10	B	28	10	12	0	0
11	D	1	0	0	0	0
12	F	31	14	14	0	0
13	A	1	0	0	0	0
13	B	2	0	0	0	0
13	C	9	0	0	0	0
13	D	1	0	0	1	0
13	F	3	0	0	0	0
All	All	17324	16410	16503	139	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 4.

All (139) 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:C:36:MET:HE3	1:C:39:ASP:HB2	1.62	0.79
3:E:116:LEU:O	3:E:120:LEU:HD12	1.88	0.72
2:B:293:MET:HE3	2:B:373:ALA:HB1	1.74	0.69
2:D:145:SER:OG	2:D:188:SER:OG	2.07	0.67
2:B:229:VAL:HG12	2:B:233:MET:HE2	1.78	0.66
2:B:235:GLY:O	2:B:238:THR:HG22	1.94	0.66
1:A:178:SER:OG	1:A:183:GLU:OE2	2.17	0.63
1:A:187:SER:CB	1:A:391:LEU:HD21	2.31	0.60
2:D:91:VAL:HG11	2:D:116:VAL:HG22	1.83	0.60
2:B:145:SER:OG	2:B:188:SER:OG	2.19	0.60
4:F:241:THR:O	4:F:241:THR:OG1	2.19	0.60
1:C:278:ALA:HA	1:C:369:ALA:HB2	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:81:PHE:O	2:B:84:ILE:HG22	2.02	0.59
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.84	0.59
4:F:79:LYS:O	4:F:83:THR:OG1	2.13	0.59
2:B:293:MET:CE	2:B:373:ALA:HB1	2.32	0.59
2:B:284:LEU:O	2:B:371:MET:HE3	2.02	0.59
4:F:243:HIS:C	4:F:243:HIS:HD1	2.11	0.59
4:F:237:THR:OG1	4:F:250:SER:OG	2.19	0.58
4:F:217:ARG:NH2	4:F:374:ILE:HG22	2.18	0.58
2:B:398:ARG:NH1	1:C:439:SER:OG	2.37	0.57
2:B:117:LEU:HD21	2:B:154:LYS:HB3	1.86	0.56
2:D:246:LEU:HD22	2:D:352:ALA:HB2	1.87	0.56
2:B:161:ASP:O	2:B:251:ARG:NH2	2.39	0.56
2:D:347:ASN:O	2:D:350:LYS:NZ	2.39	0.56
1:A:188:ILE:HG23	1:A:425:MET:HG3	1.87	0.55
1:C:36:MET:HE1	1:C:49:PHE:CE2	2.41	0.55
1:A:209:ILE:HD11	1:A:302:MET:HE3	1.87	0.54
2:D:48:ASN:N	2:D:48:ASN:OD1	2.40	0.54
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.43	0.53
1:C:2:ARG:HA	1:C:131:GLY:O	2.08	0.53
1:C:293:ASN:OD1	1:C:335:ILE:HD11	2.09	0.53
1:A:203:MET:HE1	1:A:388:TRP:CZ2	2.45	0.52
1:C:187:SER:CB	1:C:391:LEU:HD21	2.40	0.52
4:F:192:LEU:HD11	4:F:199:PHE:CD2	2.44	0.52
1:A:188:ILE:HD12	1:A:425:MET:HG3	1.92	0.51
2:D:91:VAL:HG11	2:D:116:VAL:CG2	2.40	0.51
4:F:143:GLU:O	4:F:145:ASN:N	2.43	0.51
2:B:202:ILE:HD13	2:B:229:VAL:HG13	1.92	0.51
2:D:247:ASN:HB3	2:D:253:LEU:HB2	1.93	0.51
1:A:414:GLU:OE2	3:E:60:ARG:NH1	2.44	0.51
2:B:272:PRO:HB3	2:B:284:LEU:HD22	1.91	0.51
4:F:237:THR:HG1	4:F:250:SER:HG	1.52	0.50
1:C:18:ASN:HD21	1:C:78:VAL:HG22	1.76	0.50
2:D:301:ALA:O	2:D:303:CYS:N	2.45	0.50
2:D:163:ILE:HD11	2:D:251:ARG:HB2	1.93	0.49
1:C:230:LEU:O	1:C:234:ILE:HD12	2.13	0.49
2:D:81:PHE:O	2:D:84:ILE:HG22	2.11	0.49
4:F:131:PHE:CE1	4:F:182:ILE:HG21	2.48	0.49
1:C:225:THR:O	1:C:229:ARG:HG3	2.12	0.49
2:D:274:THR:O	2:D:275:SER:CB	2.60	0.49
1:A:230:LEU:O	1:A:234:ILE:HD12	2.13	0.49
2:B:323:MET:O	2:B:326:VAL:HG22	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:239:CYS:HB3	2:D:247:ASN:O	2.12	0.49
2:B:121:ARG:NH1	2:B:158:GLU:OE1	2.45	0.49
1:C:190:THR:O	1:C:194:THR:HG23	2.12	0.48
2:D:439:ASP:OD1	13:D:601:HOH:O	2.20	0.48
2:D:189:VAL:HG11	2:D:423:MET:HE2	1.94	0.48
4:F:242:ASN:N	4:F:242:ASN:OD1	2.44	0.48
1:C:36:MET:HE1	1:C:49:PHE:CZ	2.48	0.48
2:D:65:LEU:HD12	2:D:65:LEU:N	2.29	0.48
2:D:116:VAL:O	2:D:119:VAL:HG12	2.14	0.48
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.77	0.48
1:C:16:ILE:CD1	1:C:171:ILE:HD11	2.43	0.48
3:E:47:LEU:C	3:E:47:LEU:HD23	2.39	0.48
3:E:80:ARG:HA	3:E:83:ILE:HG22	1.96	0.47
2:B:323:MET:HE3	2:B:353:VAL:HG21	1.96	0.47
2:D:210:ILE:O	2:D:214:THR:OG1	2.30	0.47
1:A:28:HIS:O	1:A:36:MET:HE3	2.15	0.47
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.49	0.47
2:D:385:LEU:C	2:D:385:LEU:HD23	2.39	0.47
4:F:243:HIS:C	4:F:243:HIS:ND1	2.71	0.47
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.97	0.47
1:C:318:LEU:HD12	1:C:318:LEU:N	2.29	0.47
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.51	0.46
4:F:197:ARG:NH2	4:F:257:GLU:OE2	2.49	0.46
2:D:179:VAL:O	2:D:396:MET:HE1	2.16	0.46
4:F:360:PRO:C	4:F:361:LEU:HD12	2.40	0.46
2:D:249:ASP:OD1	2:D:250:LEU:N	2.49	0.46
2:D:345:ILE:HG22	2:D:348:ASN:HB3	1.98	0.46
2:D:15:GLN:O	2:D:19:LYS:HG2	2.15	0.46
2:B:327:ASP:O	2:B:331:LEU:HG	2.16	0.46
1:C:181[A]:VAL:HG21	1:C:404:PHE:CZ	2.51	0.46
1:C:214:ARG:HG2	1:C:219:ILE:O	2.16	0.45
1:C:188:ILE:HG23	1:C:425:MET:HG3	1.98	0.45
4:F:192:LEU:H	4:F:192:LEU:HD12	1.80	0.45
2:B:244:GLY:O	2:B:245:GLN:C	2.59	0.45
2:B:67:ASP:HA	2:B:143:THR:HG21	1.99	0.45
2:D:65:LEU:CD2	2:D:76:VAL:HG11	2.47	0.45
4:F:126:ASP:OD1	4:F:127:GLU:N	2.50	0.45
2:B:301:ALA:O	2:B:303:CYS:N	2.46	0.45
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.99	0.45
1:C:36:MET:HE2	1:C:61:HIS:CD2	2.52	0.44
2:D:212:PHE:CD2	2:D:212:PHE:C	2.95	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:87:LEU:O	4:F:88:SER:OG	2.25	0.44
1:A:79:ARG:HG2	1:A:92:LEU:HD12	1.98	0.44
2:B:232:THR:OG1	2:B:300:MET:HE3	2.18	0.44
2:D:242:PHE:CD1	2:D:356:ILE:CD1	3.00	0.44
1:A:316:CYS:HA	1:A:352:LYS:O	2.18	0.44
1:C:36:MET:HE2	1:C:61:HIS:NE2	2.32	0.44
2:D:12:CYS:SG	2:D:169:VAL:HG21	2.58	0.44
2:D:68:LEU:O	2:D:96:GLY:N	2.51	0.44
4:F:32:LYS:HD2	4:F:32:LYS:H	1.83	0.44
4:F:244:CYS:SG	4:F:245:ILE:N	2.91	0.43
1:C:165:SER:HA	1:C:199:ASP:OD2	2.19	0.43
2:D:246:LEU:HD11	2:D:350:LYS:HB3	2.00	0.43
1:A:247:ALA:HB3	3:E:19:SER:OG	2.19	0.43
1:A:377:MET:HE3	1:A:379:SER:OG	2.18	0.43
2:B:286:VAL:HG13	2:B:326:VAL:HG12	2.01	0.43
2:D:64:ILE:HD13	2:D:120:VAL:HG22	2.01	0.43
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.01	0.43
1:A:214:ARG:HB3	1:A:219:ILE:O	2.18	0.43
1:C:161:TYR:O	1:C:162:GLY:C	2.62	0.43
2:D:245:GLN:O	2:D:246:LEU:O	2.36	0.43
4:F:125:THR:OG1	4:F:126:ASP:N	2.52	0.43
4:F:192:LEU:HD12	4:F:192:LEU:N	2.35	0.42
1:C:345:ASP:OD2	1:C:439:SER:N	2.49	0.42
1:A:213:CYS:O	1:A:217:LEU:HB2	2.20	0.42
4:F:338:CYS:SG	4:F:339:ALA:N	2.93	0.42
4:F:131:PHE:CZ	4:F:182:ILE:HG21	2.54	0.42
1:C:320:ARG:HA	1:C:356:ASN:O	2.20	0.42
2:D:169:VAL:HA	2:D:202:ILE:O	2.20	0.42
2:B:173:PRO:HA	2:B:176:SER:HB2	2.02	0.41
2:D:1:MET:N	2:D:48:ASN:ND2	2.68	0.41
2:D:293:MET:CG	2:D:375:PHE:HB2	2.51	0.41
2:B:170:VAL:HG13	2:B:171:PRO:HD2	2.02	0.41
2:B:251:ARG:O	2:B:255:VAL:HG23	2.21	0.41
2:B:48:ASN:OD1	2:B:48:ASN:N	2.53	0.41
1:A:331:ALA:O	1:A:335:ILE:HG12	2.21	0.41
4:F:84:SER:O	4:F:88:SER:N	2.51	0.41
1:A:203:MET:HE1	1:A:388:TRP:CH2	2.55	0.41
1:A:234:ILE:HD12	1:A:234:ILE:H	1.86	0.41
4:F:238:CYS:O	4:F:238:CYS:SG	2.79	0.41
1:C:181[B]:VAL:HG21	1:C:404:PHE:CZ	2.56	0.40
1:A:269:LEU:N	1:A:379:SER:O	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:ILE:HD13	1:C:171:ILE:HD11	2.03	0.40
2:B:186:THR:HG23	2:B:423:MET:HE2	2.03	0.40
4:F:16:GLU:OE2	4:F:19:ARG:NH2	2.55	0.40
4:F:47:LEU:C	4:F:47:LEU:HD23	2.46	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)
2:D:213:ARG:HH22	4:F:324:GLU:OE1[3_545]	1.56	0.04

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	438/451 (97%)	429 (98%)	9 (2%)	0	100	100
1	C	443/451 (98%)	432 (98%)	11 (2%)	0	100	100
2	B	422/431 (98%)	409 (97%)	13 (3%)	0	100	100
2	D	419/431 (97%)	405 (97%)	13 (3%)	1 (0%)	43	64
3	E	121/189 (64%)	120 (99%)	1 (1%)	0	100	100
4	F	343/380 (90%)	326 (95%)	14 (4%)	3 (1%)	14	28
All	All	2186/2333 (94%)	2121 (97%)	61 (3%)	4 (0%)	43	64

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	246	LEU
4	F	144	GLY
4	F	243	HIS
4	F	258	GLU

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	362/379 (96%)	360 (99%)	2 (1%)	78	88
1	C	372/379 (98%)	371 (100%)	1 (0%)	86	93
2	B	355/370 (96%)	353 (99%)	2 (1%)	78	88
2	D	353/370 (95%)	349 (99%)	4 (1%)	65	79
3	E	104/171 (61%)	103 (99%)	1 (1%)	68	81
4	F	273/338 (81%)	269 (98%)	4 (2%)	57	74
All	All	1819/2007 (91%)	1805 (99%)	14 (1%)	73	84

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	176	GLN
1	A	437	VAL
2	B	309	ARG
2	B	329	GLN
1	C	251	ASP
2	D	75	SER
2	D	77	ARG
2	D	306	ARG
2	D	355	ASP
3	E	44	ASP
4	F	146	VAL
4	F	241	THR
4	F	242	ASN
4	F	243	HIS

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

Mol	Chain	Res	Type
1	A	102	ASN
1	A	358	GLN
2	B	8	GLN

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Mol	Chain	Res	Type
2	B	14	ASN
2	B	134	GLN
2	B	227	HIS
2	B	292	GLN
2	B	298	ASN
1	C	85	GLN
1	C	300	ASN
1	C	356	ASN
2	D	383	GLN
2	D	404	HIS
4	F	136	ASN
4	F	183	GLN
4	F	252	ASN
4	F	380	HIS

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 19 ligands modelled in this entry, 12 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
8	MES	B	502	-	12,12,12	2.30	1 (8%)	15,16,16	1.65	1 (6%)
5	GTP	D	503	6	33,34,34	0.94	1 (3%)	50,54,54	1.58	8 (16%)
9	UPO	B	505	-	32,32,32	1.66	7 (21%)	44,45,45	1.74	8 (18%)
12	ACP	F	402	6	31,33,33	1.62	7 (22%)	47,52,52	1.92	12 (25%)
5	GTP	C	501	6	33,34,34	0.95	1 (3%)	50,54,54	1.63	8 (16%)
10	GDP	B	506	6	29,30,30	1.15	3 (10%)	45,47,47	1.74	7 (15%)
5	GTP	A	501	6	33,34,34	0.92	1 (3%)	50,54,54	1.57	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
8	MES	B	502	-	-	1/6/14/14	0/1/1/1
5	GTP	D	503	6	-	4/22/38/38	0/3/3/3
9	UPO	B	505	-	-	4/14/23/23	0/4/4/4
12	ACP	F	402	6	-	6/19/38/38	0/3/3/3
5	GTP	C	501	6	-	7/22/38/38	0/3/3/3
10	GDP	B	506	6	-	0/16/32/32	0/3/3/3
5	GTP	A	501	6	-	4/22/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	502	MES	C8-S	-7.70	1.66	1.77
9	B	505	UPO	C10-N11	5.30	1.49	1.37
12	F	402	ACP	C5-C4	4.65	1.47	1.39
9	B	505	UPO	C12-N11	3.44	1.52	1.46
10	B	506	GDP	C5-C4	3.08	1.47	1.38
9	B	505	UPO	C26-N25	3.04	1.40	1.35
12	F	402	ACP	PG-O3G	2.92	1.61	1.55
12	F	402	ACP	PG-O2G	2.90	1.61	1.55
12	F	402	ACP	C5-C6	2.68	1.48	1.41
9	B	505	UPO	C12-C13	2.58	1.56	1.51
12	F	402	ACP	PB-O3A	2.43	1.61	1.58
9	B	505	UPO	C10-N25	2.39	1.37	1.34
10	B	506	GDP	C6-N1	-2.38	1.34	1.38
12	F	402	ACP	C8-N7	2.32	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	402	ACP	C5-N7	-2.31	1.34	1.39
5	A	501	GTP	C2-N3	2.23	1.38	1.33
5	C	501	GTP	C2-N3	2.19	1.38	1.33
5	D	503	GTP	C2-N3	2.15	1.38	1.33
9	B	505	UPO	C26-N28	2.14	1.39	1.35
10	B	506	GDP	C5-N7	-2.13	1.34	1.39
9	B	505	UPO	C26-N27	2.03	1.38	1.33

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	F	402	ACP	C5-C4-N3	-5.90	118.59	126.72
10	B	506	GDP	C5-C4-N3	-5.85	119.08	128.39
5	C	501	GTP	C5-C4-N3	-5.27	120.00	128.39
5	A	501	GTP	C5-C4-N3	-5.14	120.21	128.39
9	B	505	UPO	N25-C10-N11	5.10	123.00	116.56
5	D	503	GTP	C5-C4-N3	-5.10	120.27	128.39
9	B	505	UPO	C09-C10-N11	-4.91	116.42	122.35
5	C	501	GTP	C2-N3-C4	4.86	120.67	112.30
10	B	506	GDP	C2-N3-C4	4.85	120.65	112.30
12	F	402	ACP	N3-C4-N9	4.83	135.39	127.17
5	D	503	GTP	C2-N3-C4	4.58	120.18	112.30
5	A	501	GTP	C2-N3-C4	4.57	120.17	112.30
10	B	506	GDP	N9-C4-N3	4.37	134.70	125.95
8	B	502	MES	C5-N4-C3	4.36	118.23	108.84
12	F	402	ACP	PB-O3A-PA	-3.93	119.55	132.37
12	F	402	ACP	C2-N3-C4	3.88	121.32	111.83
12	F	402	ACP	N3-C2-N1	-3.70	122.99	128.58
9	B	505	UPO	C12-C13-C14	3.60	117.56	111.34
5	A	501	GTP	N9-C4-N3	3.45	132.86	125.95
5	C	501	GTP	N9-C4-N3	3.36	132.67	125.95
12	F	402	ACP	C4-C5-N7	-3.34	106.76	110.58
9	B	505	UPO	C08-N28-C26	-3.30	114.40	116.35
10	B	506	GDP	C6-C5-N7	3.24	136.18	130.29
5	D	503	GTP	N9-C4-N3	3.21	132.37	125.95
9	B	505	UPO	C21-O20-C19	-3.09	112.98	117.51
9	B	505	UPO	O20-C19-C16	3.05	119.54	115.40
5	D	503	GTP	C2-N1-C6	-2.97	119.72	125.11
5	C	501	GTP	C2-N1-C6	-2.95	119.75	125.11
12	F	402	ACP	C4-N9-C8	2.92	108.81	105.74
5	A	501	GTP	C2-N1-C6	-2.89	119.87	125.11
12	F	402	ACP	C5-N7-C8	2.65	107.61	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	D	503	GTP	C8-N7-C5	2.56	108.81	104.26
5	D	503	GTP	N9-C8-N7	-2.55	108.68	113.40
12	F	402	ACP	C3'-C2'-C1'	2.54	106.26	101.46
5	C	501	GTP	C5-C6-N1	2.53	119.70	113.25
5	C	501	GTP	N9-C8-N7	-2.53	108.71	113.40
5	A	501	GTP	N9-C8-N7	-2.51	108.75	113.40
10	B	506	GDP	C4-C5-N7	-2.50	106.70	110.67
5	C	501	GTP	C8-N7-C5	2.50	108.72	104.26
5	A	501	GTP	C5-C6-N1	2.47	119.53	113.25
5	D	503	GTP	C5-C6-N1	2.44	119.45	113.25
5	A	501	GTP	O6-C6-C5	-2.41	120.18	126.53
5	A	501	GTP	C8-N7-C5	2.41	108.55	104.26
5	D	503	GTP	O6-C6-C5	-2.40	120.19	126.53
5	C	501	GTP	O6-C6-C5	-2.40	120.20	126.53
12	F	402	ACP	N9-C8-N7	-2.21	110.80	113.94
9	B	505	UPO	N27-C26-N28	-2.11	114.05	117.22
10	B	506	GDP	O6-C6-C5	-2.11	120.97	126.53
10	B	506	GDP	C2'-C3'-C4'	2.10	106.66	102.61
9	B	505	UPO	C26-N25-C10	-2.07	114.97	116.61
12	F	402	ACP	C2-N1-C6	2.05	122.11	118.73
12	F	402	ACP	C6-C5-N7	2.04	136.03	132.09

There are no chirality outliers.

All (26) 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-O2A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O2A
12	F	402	ACP	PG-C3B-PB-O1B
12	F	402	ACP	PG-C3B-PB-O3A
12	F	402	ACP	C5'-O5'-PA-O1A
12	F	402	ACP	C5'-O5'-PA-O2A
12	F	402	ACP	C5'-O5'-PA-O3A
9	B	505	UPO	C29-C03-O02-C01
9	B	505	UPO	C04-C03-O02-C01
9	B	505	UPO	C22-C19-O20-C21
9	B	505	UPO	C16-C19-O20-C21
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A

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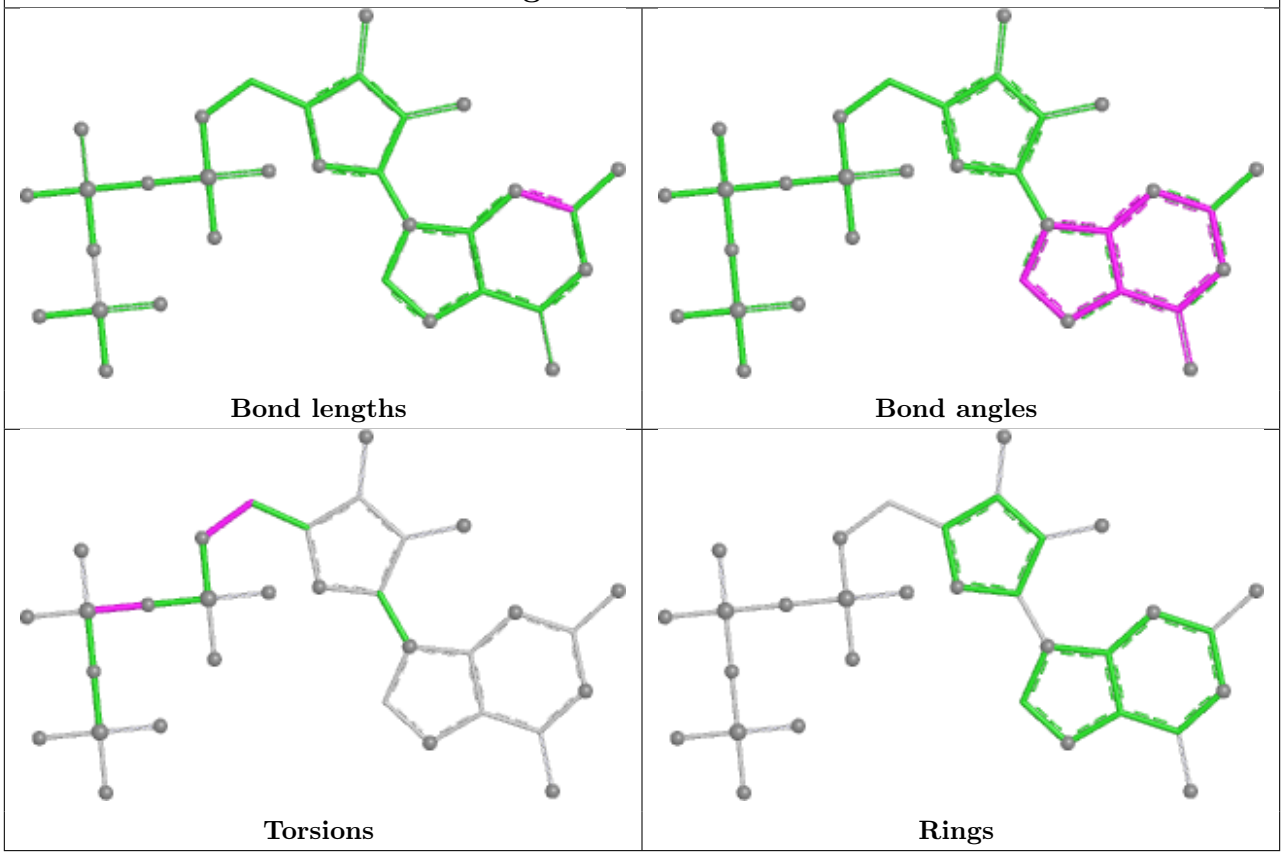
Mol	Chain	Res	Type	Atoms
5	D	503	GTP	PA-O3A-PB-O3B
5	D	503	GTP	C4'-C5'-O5'-PA
12	F	402	ACP	PG-C3B-PB-O2B
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	C4'-C5'-O5'-PA
8	B	502	MES	C8-C7-N4-C3
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	D	503	GTP	PA-O3A-PB-O1B
5	D	503	GTP	PA-O3A-PB-O2B

There are no ring outliers.

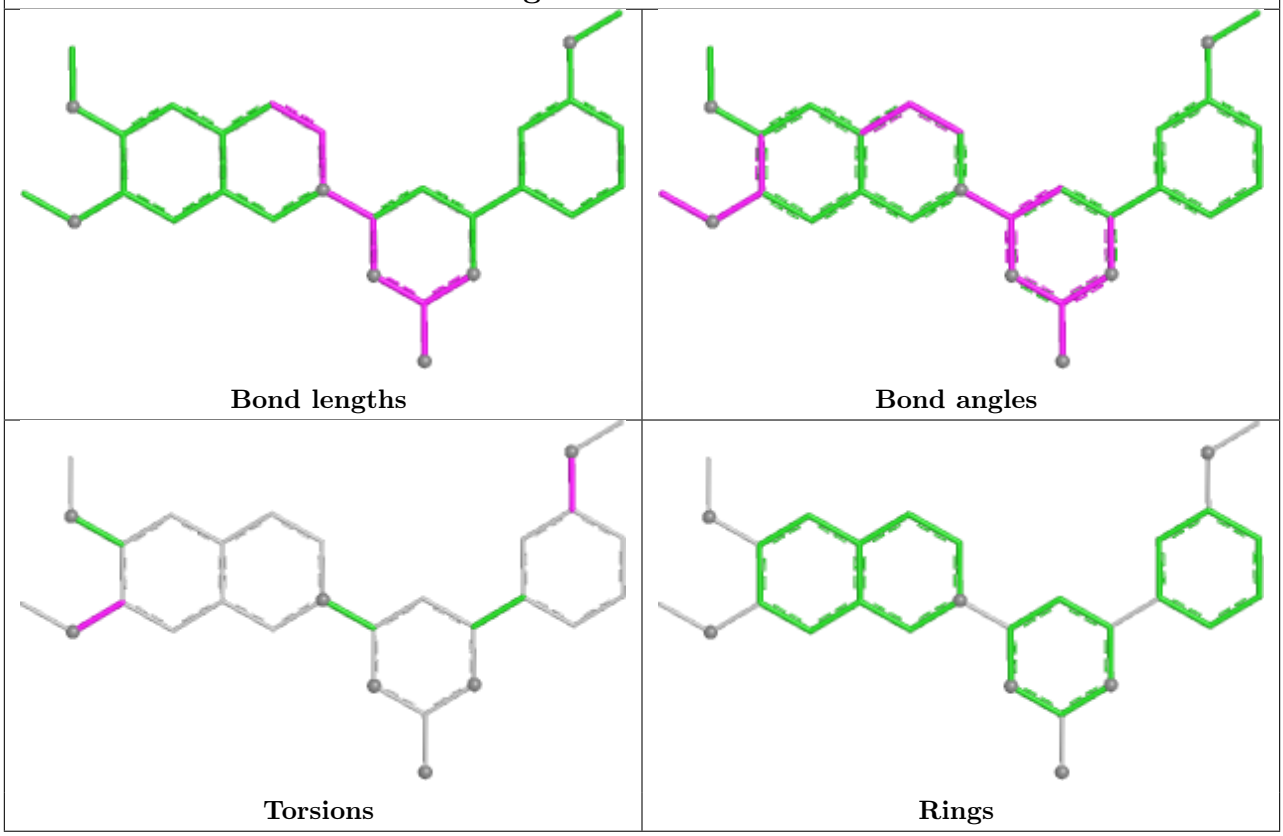
No monomer is involved in short contacts.

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 then 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.

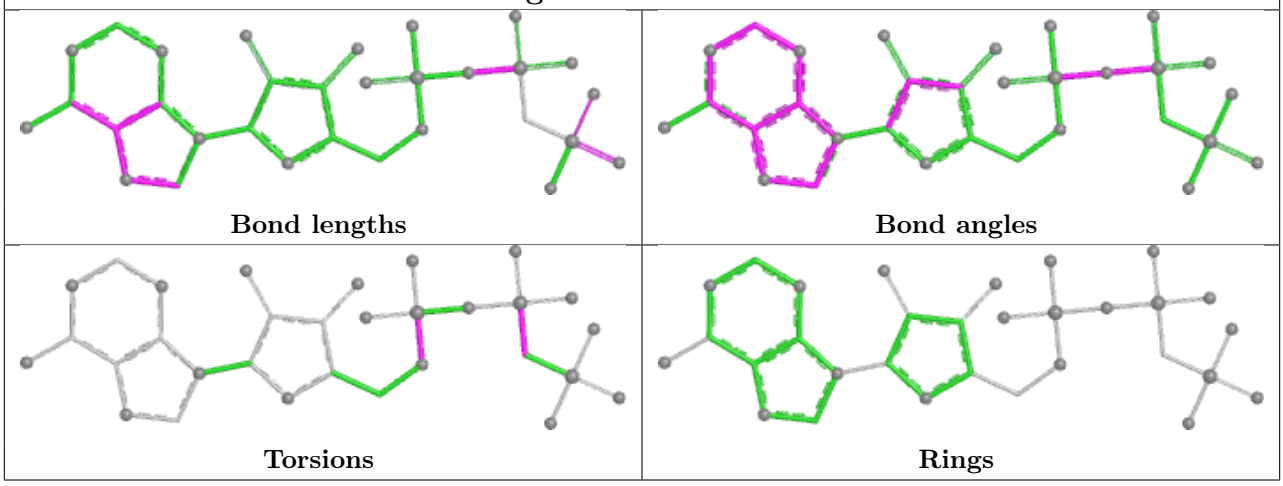
Ligand GTP D 503



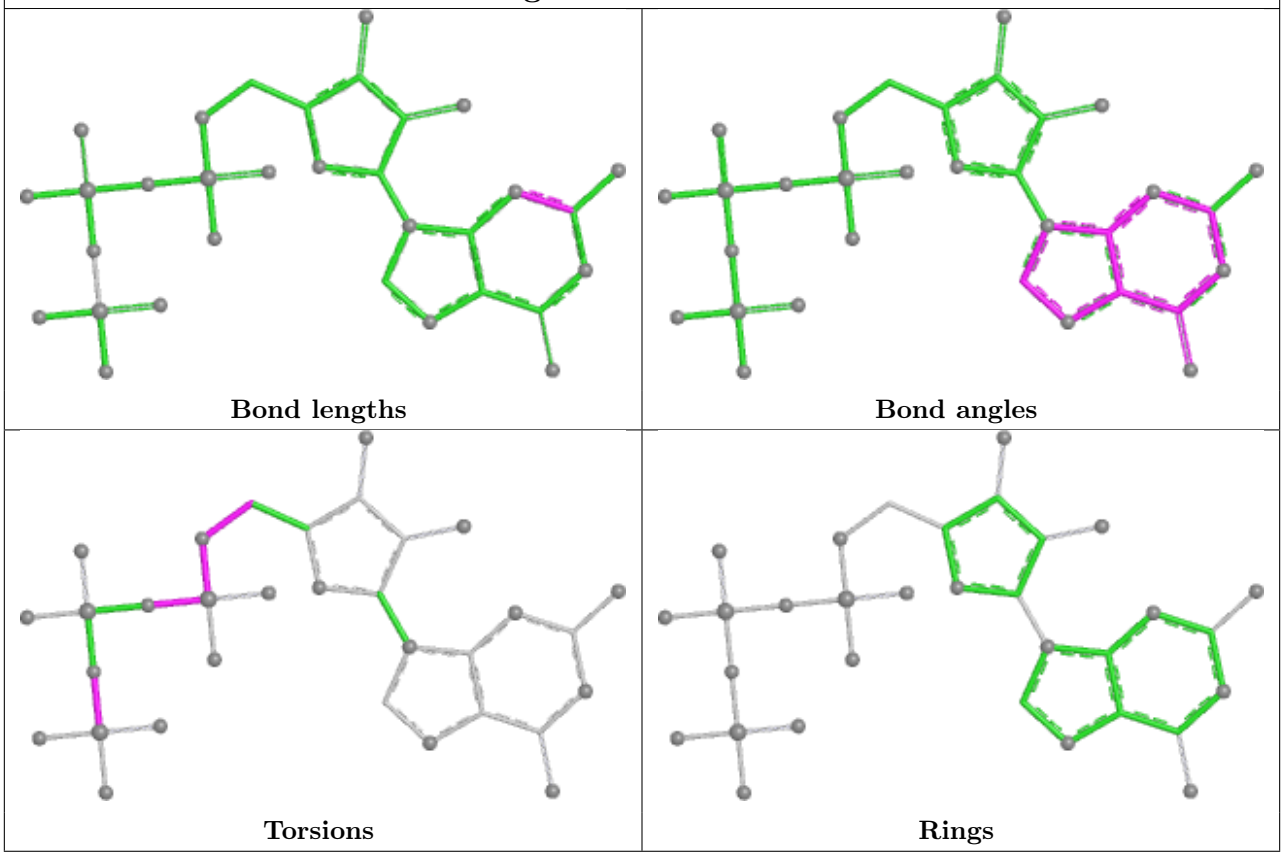
Ligand UPO B 505



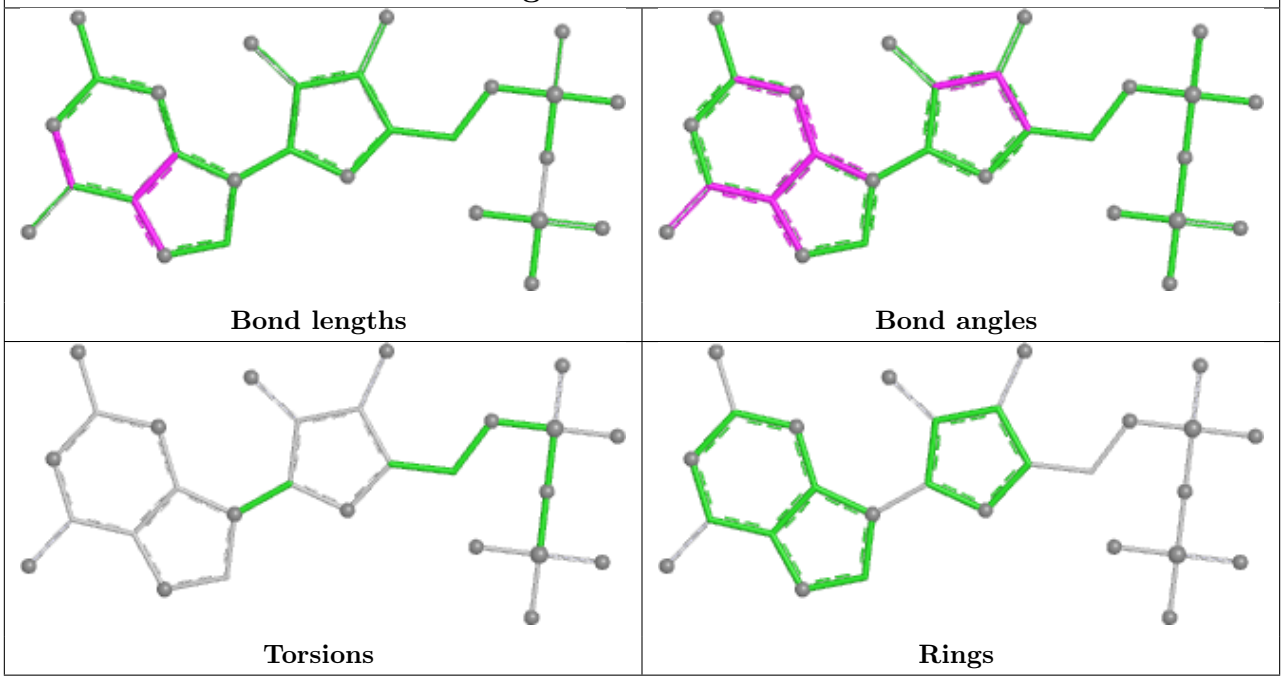
Ligand ACP F 402



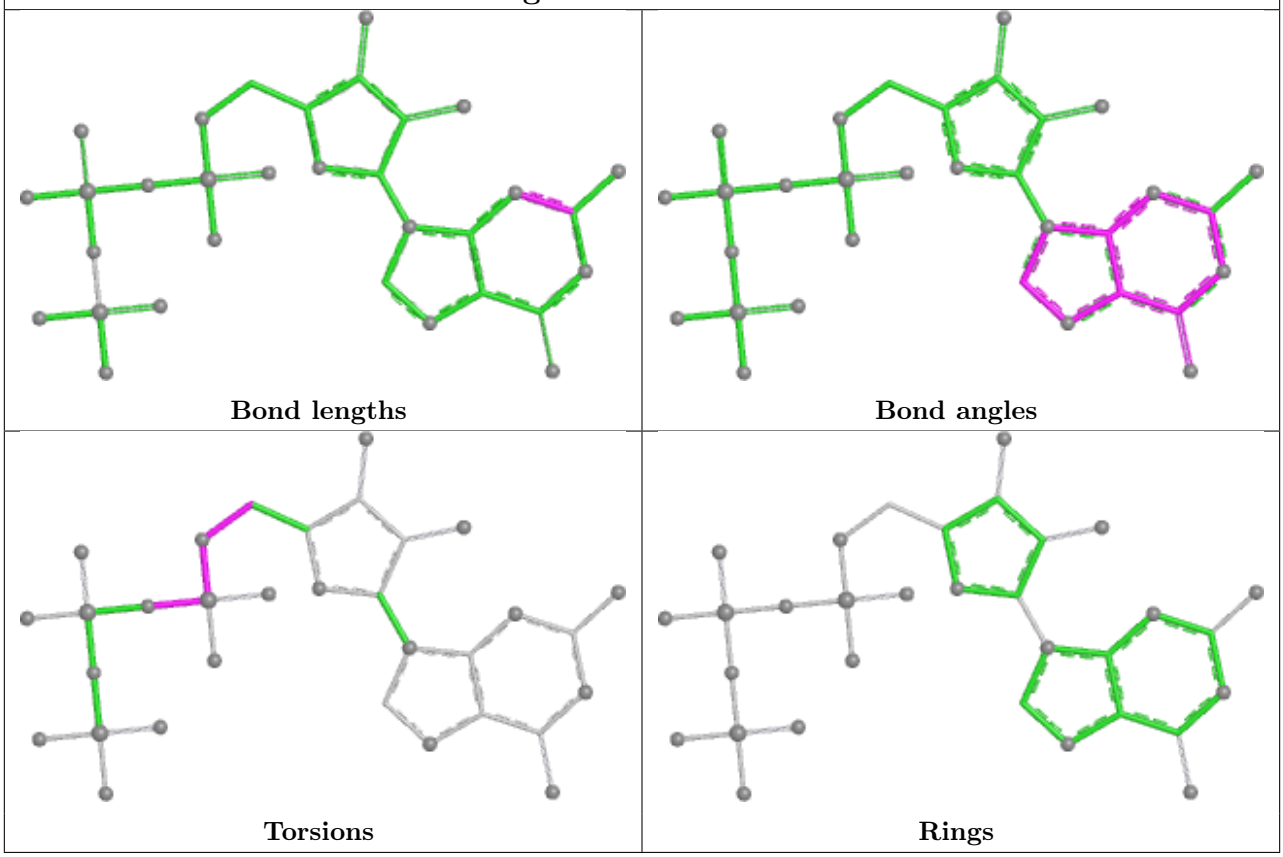
Ligand GTP C 501



Ligand GDP B 506



Ligand GTP A 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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%)	0.53	18 (4%)	41	39	33, 69, 88, 107	2 (0%)
1	C	440/451 (97%)	0.20	13 (2%)	52	50	28, 59, 76, 94	5 (1%)
2	B	425/431 (98%)	0.63	27 (6%)	25	25	37, 69, 98, 112	1 (0%)
2	D	423/431 (98%)	0.80	39 (9%)	14	14	58, 82, 101, 113	0
3	E	123/189 (65%)	0.87	16 (13%)	7	6	35, 80, 113, 126	2 (1%)
4	F	349/380 (91%)	1.31	82 (23%)	2	2	65, 93, 140, 151	0
All	All	2198/2333 (94%)	0.68	195 (8%)	15	15	28, 73, 113, 151	10 (0%)

All (195) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	135	TYR	5.8
4	F	169	LEU	5.5
2	B	438	ALA	5.0
2	B	247	ASN	4.9
4	F	165	GLU	4.9
1	A	282	TYR	4.7
4	F	176	GLN	4.7
3	E	143	ALA	4.5
4	F	170	LEU	4.5
4	F	140	GLU	4.4
4	F	172	PHE	4.3
4	F	240	LEU	4.2
2	B	280	GLN	4.2
2	D	275	SER	4.2
4	F	159	GLY	4.2
4	F	145	ASN	4.1
3	E	142	GLU	4.0
2	D	57	ASN	4.0
4	F	249	TYR	3.9

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Mol	Chain	Res	Type	RSRZ
4	F	160	ILE	3.9
2	D	92	PHE	3.8
4	F	146	VAL	3.8
4	F	152	SER	3.8
4	F	171	ASP	3.8
4	F	175	GLU	3.8
2	D	1	MET	3.8
1	C	440	VAL	3.8
4	F	158	GLU	3.7
4	F	173	ILE	3.7
4	F	174	ASP	3.7
4	F	255	ARG	3.6
4	F	233	PHE	3.6
4	F	241	THR	3.5
2	D	73	MET	3.5
2	D	244	GLY	3.5
1	A	156	ARG	3.5
2	B	246	LEU	3.5
4	F	236	LYS	3.4
2	B	55	ALA	3.4
4	F	186	LEU	3.3
4	F	168	GLU	3.3
2	B	323	MET	3.3
2	B	214	THR	3.3
2	B	331	LEU	3.3
4	F	156	LYS	3.2
4	F	181	VAL	3.2
1	A	46	ASP	3.2
4	F	138	ARG	3.2
2	B	213	ARG	3.1
4	F	187	GLU	3.1
2	B	245	GLN	3.1
1	A	1	MET	3.1
4	F	99	VAL	3.1
2	B	324	LYS	3.1
2	D	85	PHE	3.1
4	F	89	GLU	3.1
4	F	178	GLN	3.0
4	F	52	LEU	3.0
3	E	45	PRO	3.0
2	D	245	GLN	3.0
4	F	161	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
4	F	96	GLU	3.0
4	F	102	PRO	3.0
4	F	320	MET	3.0
2	D	55	ALA	3.0
2	D	274	THR	2.9
4	F	179	VAL	2.9
3	E	132	GLU	2.9
4	F	139	ARG	2.9
4	F	100	ILE	2.9
4	F	143	GLU	2.8
1	A	54	SER	2.8
2	D	175	VAL	2.8
4	F	362	ALA	2.8
1	C	340	SER	2.8
2	D	69	GLU	2.8
2	D	405	TRP	2.8
2	D	402	PHE	2.8
1	A	62	VAL	2.7
4	F	137	ARG	2.7
4	F	180	HIS	2.7
1	C	179	THR	2.7
4	F	142	ARG	2.7
4	F	149	ALA	2.7
4	F	372	THR	2.7
4	F	182	ILE	2.7
3	E	49	GLU	2.7
4	F	24	THR	2.7
2	D	249	ASP	2.7
4	F	253	TYR	2.6
3	E	46	SER	2.6
4	F	27	TRP	2.6
2	B	57	ASN	2.6
2	B	274	THR	2.6
2	D	284	LEU	2.6
1	C	360	PRO	2.6
3	E	12[A]	ASN	2.6
4	F	155	ALA	2.6
1	A	88	HIS	2.5
2	B	43	GLN	2.5
1	A	41	THR	2.5
2	D	247	ASN	2.5
3	E	52	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	360	PRO	2.5
1	C	85	GLN	2.5
2	D	407	THR	2.5
2	B	275	SER	2.5
4	F	147	TRP	2.5
3	E	48	GLU	2.5
4	F	144	GLY	2.5
4	F	228	TYR	2.5
3	E	7	GLU	2.4
4	F	35	PRO	2.4
2	B	296	ALA	2.4
4	F	192	LEU	2.4
4	F	44	ARG	2.4
1	C	361	THR	2.4
4	F	239	HIS	2.4
4	F	167	SER	2.4
2	D	316	VAL	2.4
2	B	436	ALA	2.4
4	F	153	ALA	2.4
2	B	2	ARG	2.4
4	F	263	PHE	2.4
3	E	126	LYS	2.3
2	D	15	GLN	2.3
2	D	142	GLY	2.3
2	D	398	ARG	2.3
1	A	418	PHE	2.3
2	D	356	ILE	2.3
2	B	291	GLN	2.3
2	D	291	GLN	2.3
1	A	250	VAL	2.3
2	D	326	VAL	2.3
2	B	437	THR	2.3
2	B	335	ASN	2.3
4	F	90	SER	2.3
4	F	197	ARG	2.3
1	C	148	GLY	2.3
2	D	248	ALA	2.2
1	C	88[A]	HIS	2.2
4	F	20	LEU	2.2
4	F	134	ALA	2.2
4	F	184	LYS	2.2
4	F	251	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
4	F	242	ASN	2.2
4	F	250	SER	2.2
4	F	166	ALA	2.2
2	B	73	MET	2.2
2	D	105	HIS	2.2
2	D	401	ALA	2.2
4	F	125	THR	2.2
2	D	332	ASN	2.2
1	C	342	GLN	2.2
1	A	195	LEU	2.2
1	C	341	ILE	2.2
4	F	32	LYS	2.1
4	F	177	GLY	2.1
1	A	5	ILE	2.1
2	D	439	ASP	2.1
3	E	115	HIS	2.1
2	D	90	PHE	2.1
3	E	131	GLU	2.1
2	D	214	THR	2.1
3	E	139	LEU	2.1
4	F	101	TYR	2.1
4	F	190	LEU	2.1
1	C	43	GLY	2.1
2	D	408	GLY	2.1
2	D	37	HIS	2.1
4	F	330	ILE	2.1
1	A	232	SER	2.1
2	B	283	ALA	2.1
3	E	90	ASN	2.1
4	F	244	CYS	2.1
4	F	57	GLY	2.1
4	F	154	GLY	2.1
4	F	380	HIS	2.1
3	E	44	ASP	2.1
1	C	278	ALA	2.1
1	A	368	LEU	2.1
2	D	112	LEU	2.1
2	B	239	CYS	2.1
1	A	262	TYR	2.1
2	D	306	ARG	2.0
1	A	281	ALA	2.0
2	B	301	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	322	SER	2.0
2	D	2	ARG	2.0
2	D	399	ARG	2.0
2	D	53	GLU	2.0
1	A	193	THR	2.0
2	B	371	MET	2.0
4	F	234	GLN	2.0
1	C	357	TYR	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 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(Å^2)	Q<0.9
5	GTP	A	501	32/32	-	-	52,53,64,67	42
5	GTP	C	501	32/32	-	-	45,48,58,64	42
5	GTP	D	503	32/32	-	-	72,78,91,91	42
6	MG	A	502	1/1	-	-	57,57,57,57	1
6	MG	B	501	1/1	-	-	56,56,56,56	1
6	MG	C	502	1/1	-	-	50,50,50,50	1
6	MG	D	501	1/1	-	-	85,85,85,85	1
6	MG	F	401	1/1	-	-	93,93,93,93	1
7	CA	A	503	1/1	-	-	77,77,77,77	1
7	CA	A	504	1/1	-	-	64,64,64,64	1
7	CA	B	503	1/1	-	-	67,67,67,67	1
7	CA	B	504	1/1	-	-	69,69,69,69	1
7	CA	C	503	1/1	-	-	63,63,63,63	1
7	CA	D	502	1/1	-	-	76,76,76,76	1
8	MES	B	502	12/12	-	-	56,59,69,69	24

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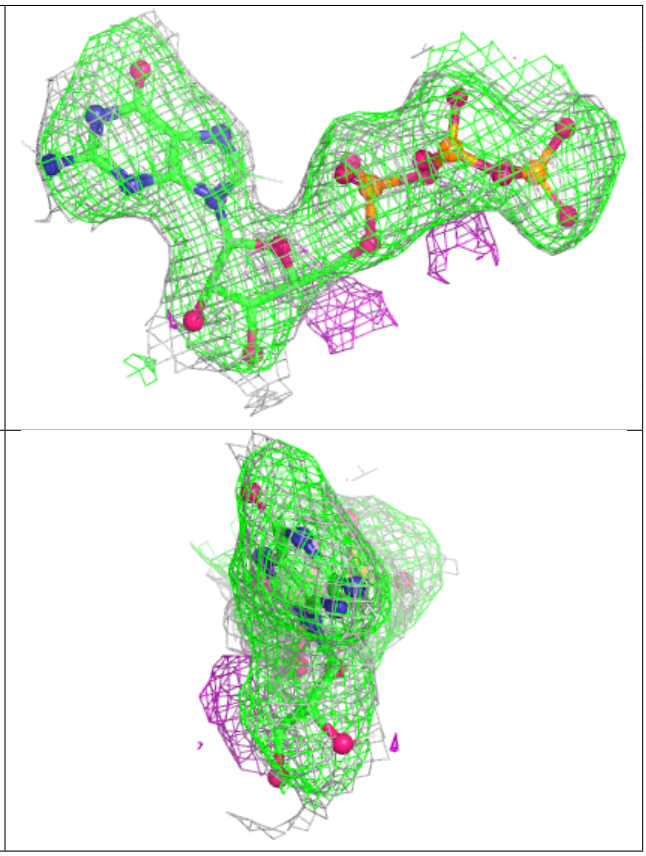
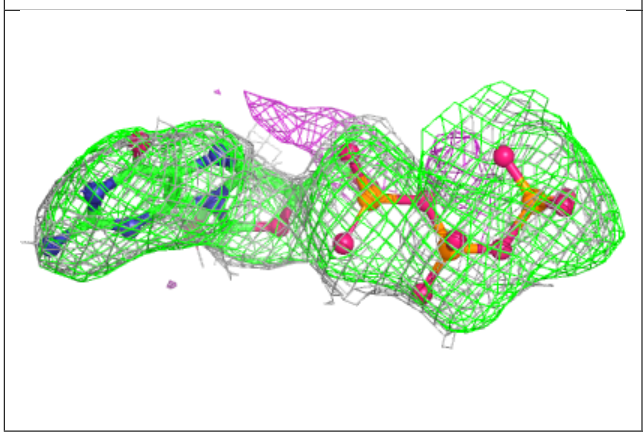
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
9	UPO	B	505	29/29	0.88	0.17	58,75,94,96	0
10	GDP	B	506	28/28	-	-	49,53,64,65	38
11	CL	D	504	1/1	-	-	66,66,66,66	1
12	ACP	F	402	31/31	-	-	89,100,121,125	45

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:

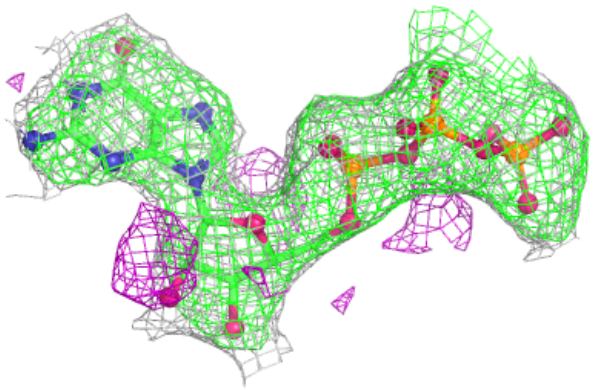
2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

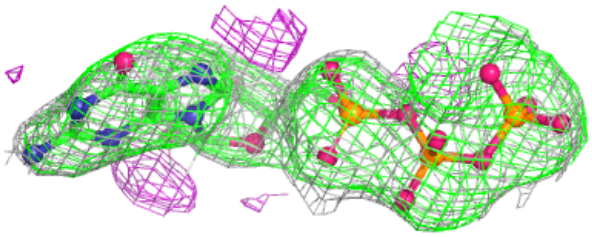


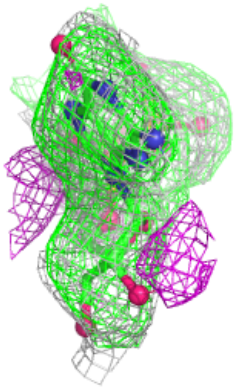


Electron density around GTP C 501:

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

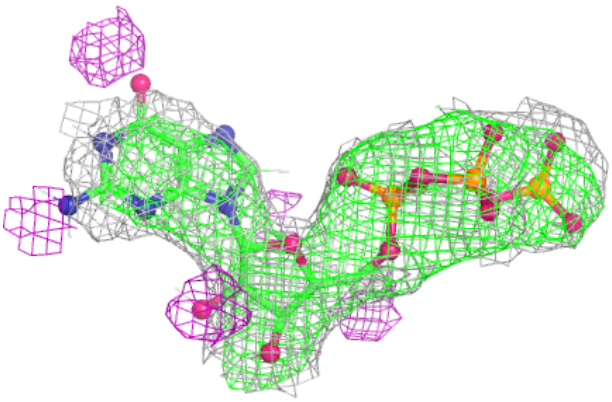


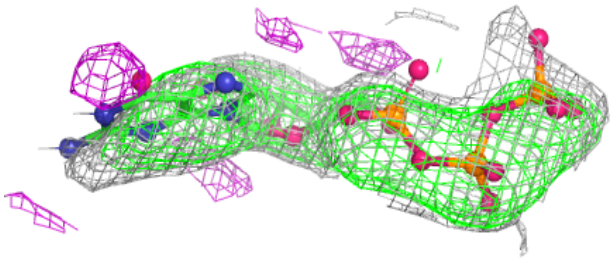


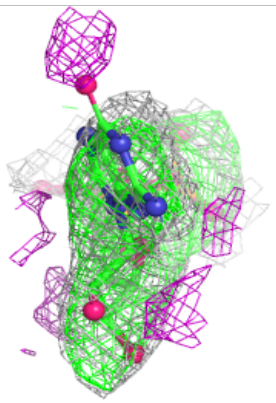


Electron density around GTP D 503:

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

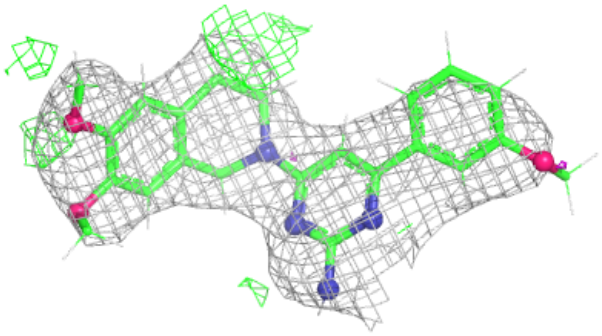


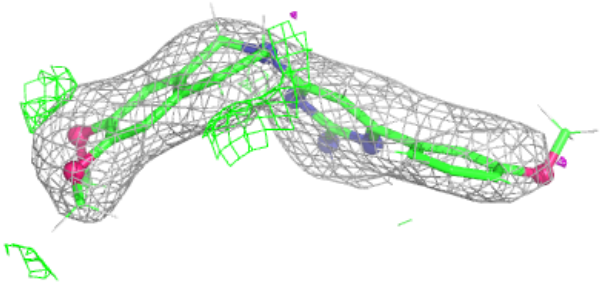


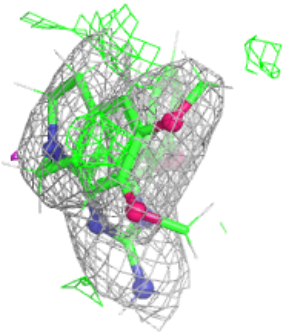


Electron density around UPO B 505:

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

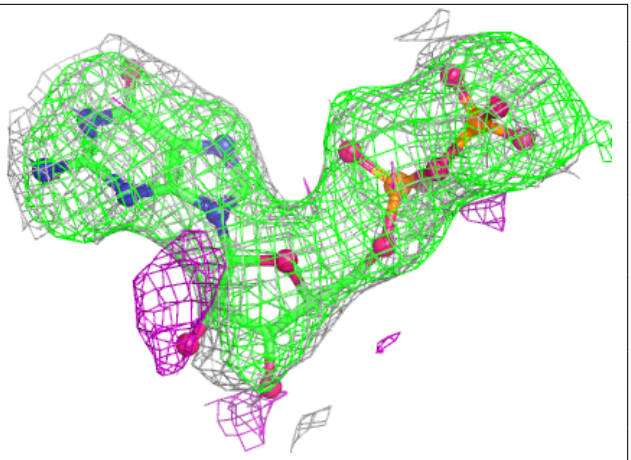


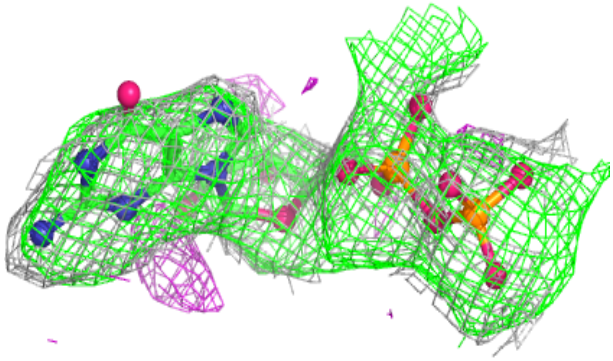


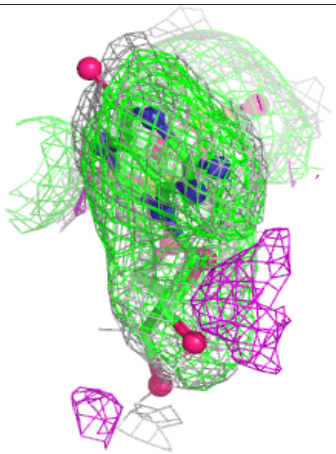


Electron density around GDP B 506:

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

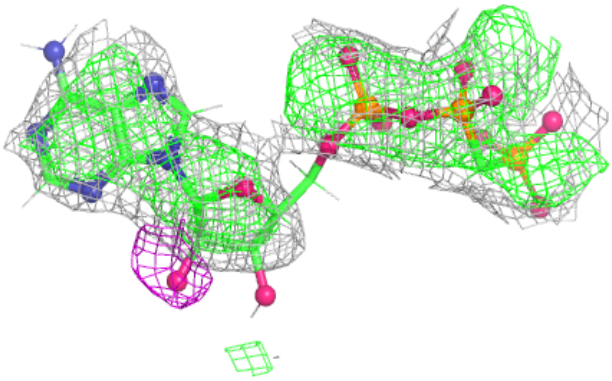


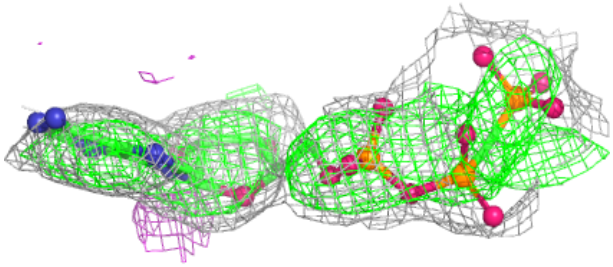


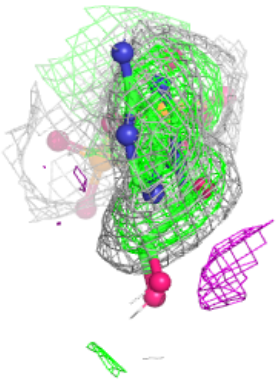


Electron density around ACP F 402:

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







6.5 Other polymers (i)

There are no such residues in this entry.