



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 12:05 pm BST

PDB ID : 6BRF
Title : Tubulin-RB3_SLD-TTL in complex with heterocyclic pyrimidine compound 4b
Authors : Kumar, G.; Wang, Y.; Li, W.; White, S.W.
Deposited on : 2017-11-30
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

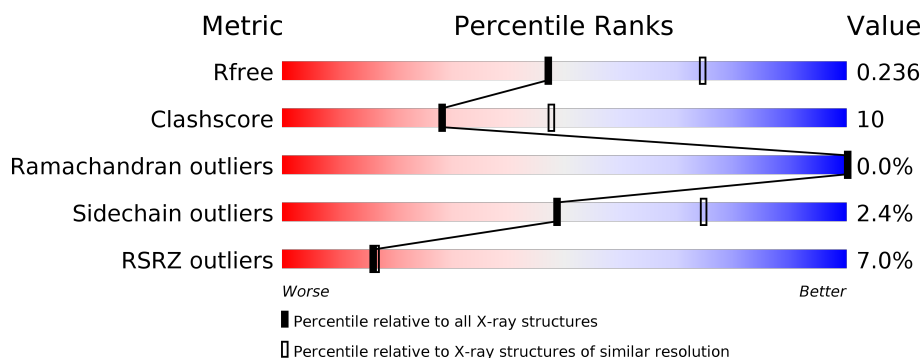
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	450	<div> <div>2%</div> <div>81% 15% ..</div> </div>
1	C	450	<div> <div>83% 15% .</div> </div>
2	B	445	<div> <div>3%</div> <div>78% 17% ..</div> </div>
2	D	445	<div> <div>9%</div> <div>66% 27% . 5%</div> </div>
3	E	143	<div> <div>4%</div> <div>67% 15% . 15%</div> </div>
4	F	384	<div> <div>23%</div> <div>59% 25% . 14%</div> </div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17963 atoms, of which 14 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
			3416	2163	581	650	22			
1	C	440	Total	C	N	O	S	0	0	0
			3437	2175	584	656	22			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	427	Total	C	N	O	S	0	0	0
			3361	2110	576	649	26			
2	D	421	Total	C	N	O	S	0	0	0
			3309	2080	562	640	27			

- 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
			1000	617	181	197	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	expression tag	UNP Q9H169
E	4	ALA	-	expression tag	UNP Q9H169

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	332	Total	C	N	O	S	0	0	0
			2724	1749	468	493	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

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



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

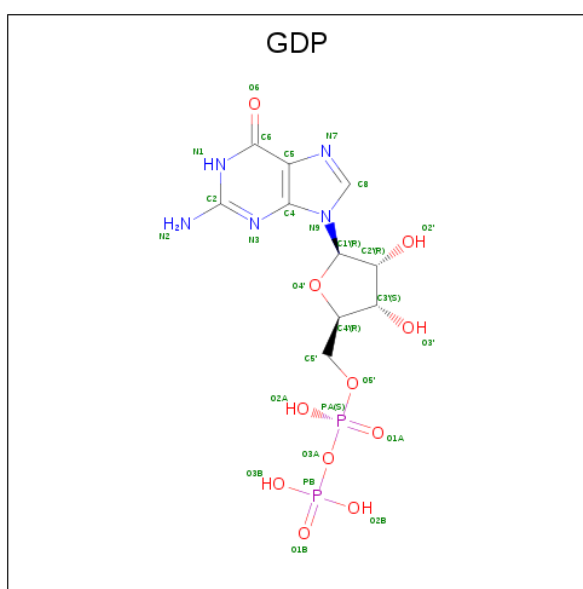
- Molecule 6 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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



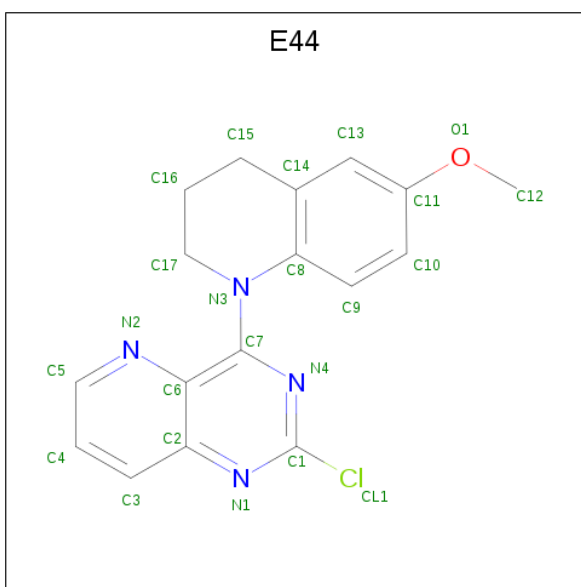
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N O P 28 10 5 11 2	0	0
8	D	1	Total C N O P 28 10 5 11 2	0	0

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



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

- Molecule 10 is 2-chloro-4-(6-methoxy-3,4-dihydroquinolin-1(2H)-yl)pyrido[3,2-d]pyrimidine (three-letter code: E44) (formula: C₁₇H₁₅ClN₄O) (labeled as "Ligand of Interest" by author).



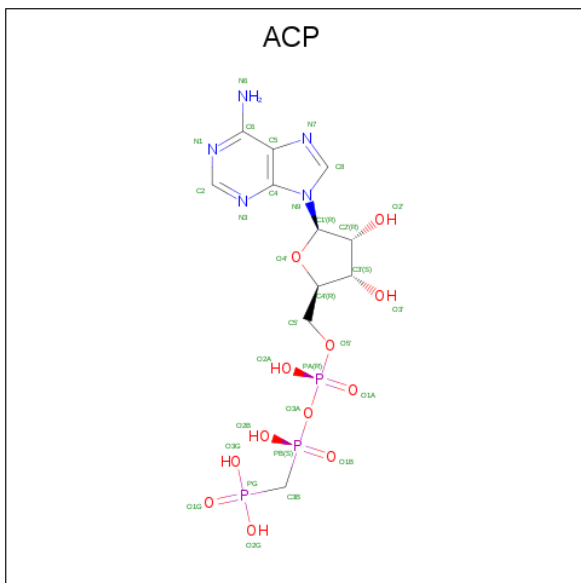
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	Cl	N	O	0	0
			23	17	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	D	1	Total	C	Cl	N	O	0	0
			23	17	1	4	1		

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



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	F	1	Total	C	H	N	O	P	0	0
			45	11	14	5	12	3		

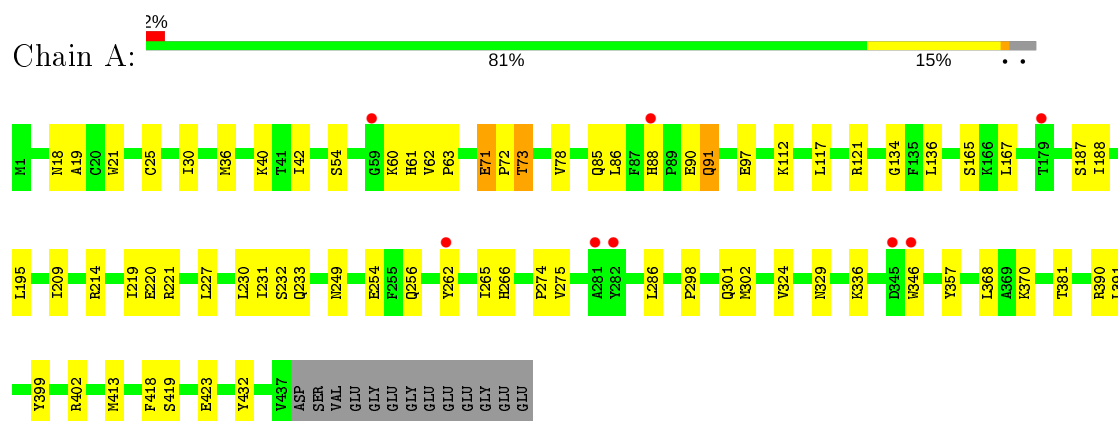
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	102	Total	O	0	0
			102	102		
12	B	99	Total	O	0	0
			99	99		
12	C	191	Total	O	0	0
			191	191		
12	D	37	Total	O	0	0
			37	37		
12	E	22	Total	O	0	0
			22	22		
12	F	24	Total	O	0	0
			24	24		

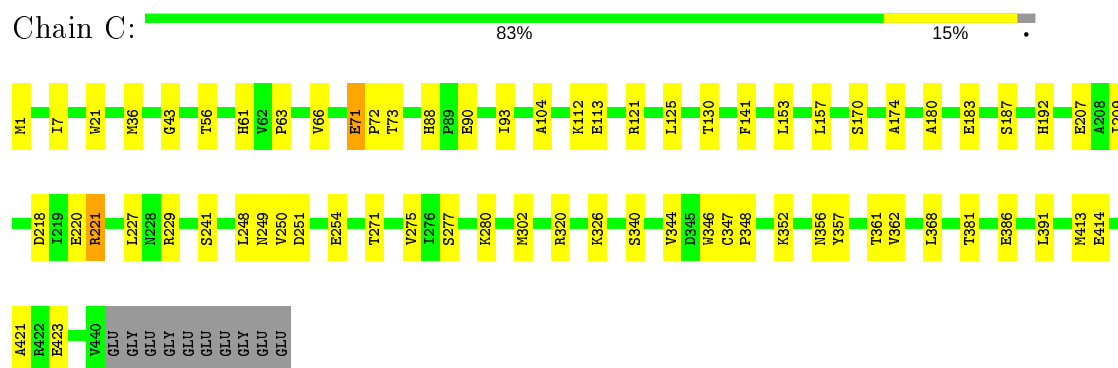
3 Residue-property plots [i](#)

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

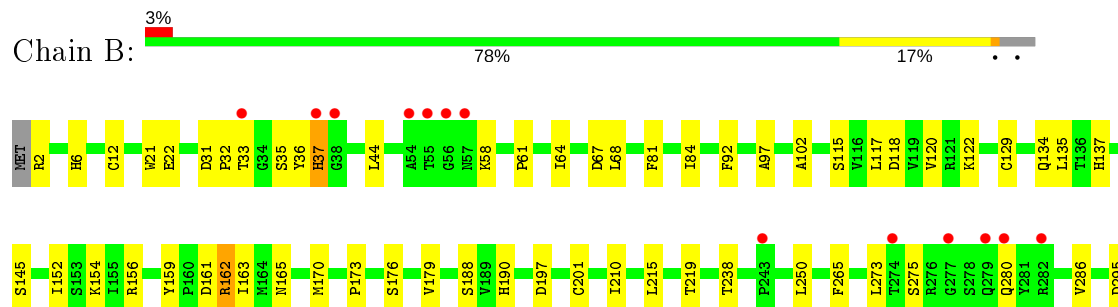
• Molecule 1: Tubulin alpha-1B chain



• Molecule 1: Tubulin alpha-1B chain

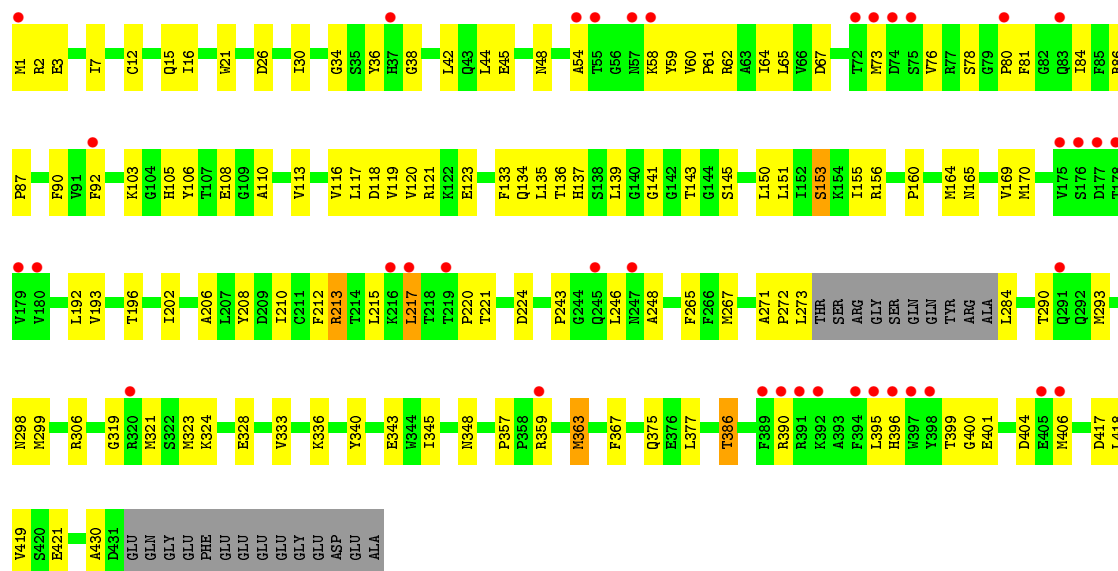


• Molecule 2: Tubulin beta-2B chain

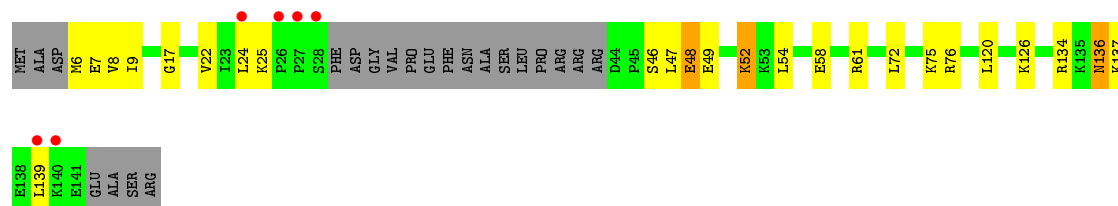




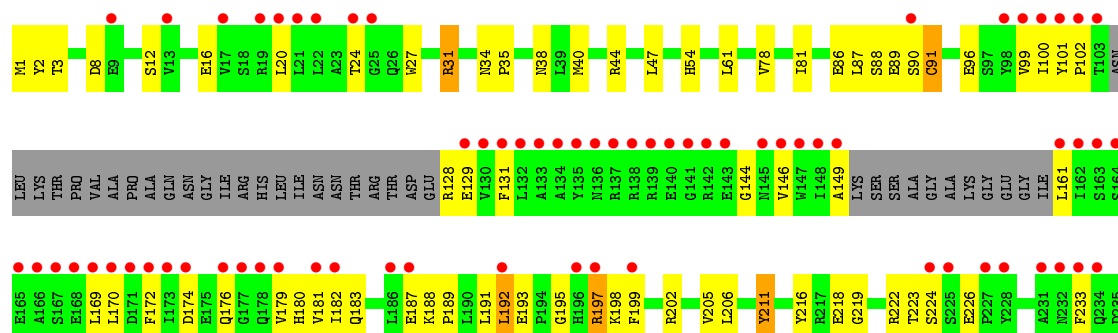
• Molecule 2: Tubulin beta-2B chain

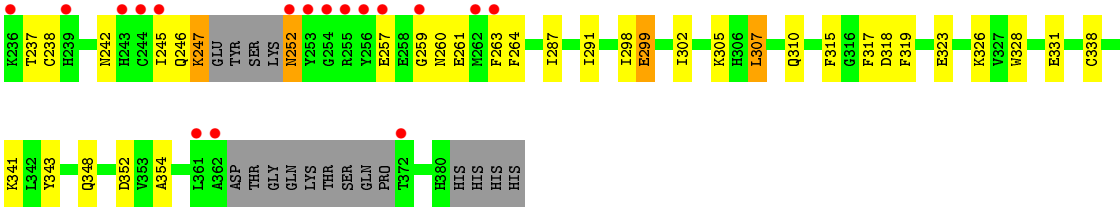


• Molecule 3: Stathmin-4



• Molecule 4: Tubulin tyrosine ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.13Å 157.75Å 181.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.78 – 2.50 49.78 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.8 (49.78-2.50) 98.8 (49.78-2.50)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.06 (at 2.51Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.187 , 0.237 0.187 , 0.236	Depositor DCC
R_{free} test set	5208 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å ²)	36.8	Xtriage
Anisotropy	0.017	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 46.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17963	wwPDB-VP
Average B, all atoms (Å ²)	52.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, E44, CA, GTP, ACP, MES

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	0.34	0/3494	0.52	0/4743
1	C	0.38	0/3515	0.55	0/4772
2	B	0.35	0/3436	0.51	0/4654
2	D	0.31	0/3382	0.49	0/4581
3	E	0.31	0/1008	0.42	0/1337
4	F	0.30	0/2786	0.47	0/3764
All	All	0.34	0/17621	0.51	0/23851

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	3416	0	3331	53	0
1	C	3437	0	3348	45	0
2	B	3361	0	3238	54	0
2	D	3309	0	3189	100	0
3	E	1000	0	1018	24	0
4	F	2724	0	2690	76	0
5	A	32	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	F	1	0	0	0	0
8	B	28	0	12	1	0
8	D	28	0	12	4	0
9	B	24	0	24	5	0
10	B	23	0	0	1	0
10	D	23	0	0	0	0
11	F	31	14	13	0	0
12	A	102	0	0	3	0
12	B	99	0	0	2	0
12	C	191	0	0	6	0
12	D	37	0	0	4	0
12	E	22	0	0	1	0
12	F	24	0	0	0	0
All	All	17949	14	16899	336	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 10.

All (336) 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:71:GLU:OE2	1:C:73:THR:HB	1.67	0.94
4:F:226:GLU:HG3	4:F:237:THR:HG23	1.59	0.84
2:D:60:VAL:HG11	2:D:86:ARG:HG3	1.61	0.83
4:F:223:THR:HG21	4:F:257:GLU:OE2	1.82	0.79
4:F:211:TYR:CE2	4:F:299:GLU:HG3	2.16	0.79
2:B:170:MET:HG3	2:B:377:LEU:HD21	1.63	0.79
1:A:117:LEU:HD11	1:A:121:ARG:NH1	1.99	0.77
2:D:290:THR:HG22	2:D:333:VAL:HG21	1.67	0.75
1:C:218:ASP:OD1	1:C:280:LYS:NZ	2.19	0.75
4:F:169:LEU:HD12	4:F:170:LEU:HD12	1.69	0.74
4:F:31:ARG:HD3	4:F:31:ARG:H	1.53	0.73
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.70	0.73
2:D:170:MET:HG3	2:D:377:LEU:HD11	1.70	0.73
2:D:134:GLN:HA	2:D:165:ASN:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:136:ASN:HA	3:E:139:LEU:HD12	1.69	0.73
3:E:6:MET:HE2	3:E:24:LEU:HD22	1.71	0.71
4:F:78:VAL:HG21	4:F:181:VAL:HG11	1.73	0.71
1:A:88:HIS:O	1:A:91:GLN:HG3	1.91	0.71
2:D:153:SER:OG	3:E:126:LYS:HE2	1.91	0.70
1:A:71:GLU:OE2	12:A:601:HOH:O	2.09	0.69
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.74	0.69
2:D:73:MET:SD	2:D:90:PHE:HB3	2.33	0.68
2:B:316:ILE:HG23	2:B:366:THR:HB	1.74	0.68
1:A:97:GLU:OE2	12:A:602:HOH:O	2.12	0.68
2:B:336:LYS:NZ	4:F:1:MET:O	2.26	0.68
2:B:336:LYS:HE2	2:B:336:LYS:HA	1.76	0.68
2:D:1:MET:HG2	2:D:48:ASN:HD22	1.59	0.67
4:F:226:GLU:HG3	4:F:237:THR:CG2	2.25	0.67
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.29	0.67
2:B:134:GLN:HA	2:B:165:ASN:O	1.95	0.66
1:C:271:THR:HG23	12:C:680:HOH:O	1.93	0.66
2:B:118:ASP:O	2:B:122:LYS:HG2	1.95	0.66
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.77	0.66
2:D:1:MET:CE	2:D:48:ASN:HB2	2.27	0.65
2:D:15:GLN:NE2	8:D:501:GDP:O6	2.29	0.65
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.32	0.65
2:D:1:MET:HE2	2:D:48:ASN:HB2	1.78	0.65
1:A:88:HIS:HE1	1:A:90:GLU:HG3	1.62	0.65
3:E:6:MET:O	12:E:201:HOH:O	2.14	0.65
1:A:88:HIS:N	1:A:91:GLN:OE1	2.25	0.64
3:E:8:VAL:O	3:E:9:ILE:HD13	1.96	0.64
1:C:71:GLU:HG2	1:C:72:PRO:HD2	1.80	0.64
2:D:73:MET:HG3	2:D:90:PHE:HD2	1.63	0.63
4:F:195:GLY:HA3	4:F:197:ARG:HD2	1.78	0.63
2:D:65:LEU:CD2	2:D:76:VAL:HG11	2.29	0.63
1:A:419:SER:O	1:A:423:GLU:HG2	1.98	0.63
4:F:205:VAL:HG11	4:F:291:ILE:HD13	1.80	0.63
4:F:169:LEU:CD1	4:F:170:LEU:HD12	2.28	0.63
4:F:211:TYR:CD2	4:F:299:GLU:HG3	2.34	0.63
12:B:665:HOH:O	3:E:75:LYS:HD2	1.99	0.62
1:A:88:HIS:CE1	1:A:90:GLU:HG3	2.34	0.62
2:D:246:LEU:HD13	2:D:248:ALA:HB2	1.80	0.62
2:D:336:LYS:NZ	12:D:602:HOH:O	2.32	0.62
2:D:141:GLY:HA3	8:D:501:GDP:O3A	1.99	0.62
1:A:18:ASN:HD21	1:A:78:VAL:HG22	1.65	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:246:GLN:OE1	4:F:260:ASN:ND2	2.33	0.62
4:F:81:ILE:O	4:F:88:SER:HB2	1.99	0.62
2:B:145:SER:HG	2:B:188:SER:HG	1.48	0.61
2:D:80:PRO:O	2:D:81:PHE:HB2	2.00	0.61
2:D:290:THR:CG2	2:D:333:VAL:HG21	2.30	0.61
4:F:86:GLU:N	4:F:86:GLU:OE1	2.24	0.61
2:D:2:ARG:NH1	12:D:603:HOH:O	2.33	0.61
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.00	0.61
2:D:103:LYS:HD3	2:D:108:GLU:OE1	2.01	0.61
2:B:2:ARG:NH1	2:B:129:CYS:SG	2.73	0.60
2:D:106:TYR:O	3:E:134:ARG:NH1	2.28	0.60
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.83	0.60
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.82	0.60
4:F:189:PRO:HG2	4:F:191:LEU:HD21	1.83	0.60
4:F:8:ASP:OD1	4:F:44:ARG:HG3	2.01	0.60
4:F:247:LYS:N	4:F:247:LYS:HD2	2.16	0.60
1:A:220:GLU:HG2	2:B:324:LYS:HD3	1.84	0.60
2:D:1:MET:HB2	2:D:3:GLU:OE1	2.01	0.59
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.38	0.59
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.20	0.59
4:F:192:LEU:HD11	4:F:199:PHE:CD1	2.37	0.59
2:D:170:MET:CE	2:D:377:LEU:HD21	2.33	0.59
4:F:169:LEU:HD12	4:F:170:LEU:N	2.18	0.59
1:A:249:ASN:N	1:A:254:GLU:OE2	2.35	0.59
1:C:220:GLU:OE2	2:D:324:LYS:HD3	2.02	0.59
4:F:192:LEU:H	4:F:192:LEU:HD12	1.68	0.59
1:A:329:ASN:OD1	3:E:22:VAL:HG11	2.03	0.59
4:F:99:VAL:O	4:F:100:ILE:HD13	2.02	0.59
4:F:191:LEU:HA	4:F:197:ARG:O	2.02	0.59
2:D:272:PRO:HB3	2:D:284:LEU:HD21	1.84	0.59
2:D:73:MET:CG	2:D:90:PHE:HD2	2.16	0.59
4:F:31:ARG:HD3	4:F:31:ARG:N	2.17	0.59
2:D:143:THR:HB	8:D:501:GDP:O1B	2.03	0.58
4:F:149:ALA:HB3	4:F:161:LEU:HB3	1.85	0.58
2:B:67:ASP:O	2:B:92:PHE:HA	2.04	0.58
3:E:48:GLU:O	3:E:52:LYS:HE2	2.03	0.58
1:C:250:VAL:HG11	1:C:352:LYS:HE3	1.85	0.58
1:A:209:ILE:HD11	1:A:302:MET:SD	2.43	0.57
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.34	0.57
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.37	0.57
3:E:8:VAL:C	3:E:9:ILE:HD13	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:33:THR:CG2	2:B:58:LYS:HE3	2.35	0.57
4:F:247:LYS:H	4:F:247:LYS:HD2	1.70	0.57
4:F:188:LYS:HG2	4:F:323:GLU:CD	2.25	0.57
2:D:34:GLY:HA2	2:D:84:ILE:HD11	1.86	0.57
2:D:118:ASP:OD1	2:D:121:ARG:NH1	2.39	0.56
2:D:267:MET:HE1	2:D:299:MET:HG3	1.88	0.55
1:C:71:GLU:HG2	1:C:72:PRO:CD	2.35	0.55
4:F:223:THR:HG22	4:F:260:ASN:O	2.07	0.55
2:D:169:VAL:HA	2:D:202:ILE:O	2.06	0.55
4:F:226:GLU:OE1	4:F:252:ASN:HB3	2.06	0.55
4:F:197:ARG:HB3	4:F:224:SER:O	2.07	0.55
4:F:326:LYS:HE2	4:F:328:TRP:CZ2	2.42	0.55
1:A:214:ARG:HG2	1:A:219:ILE:O	2.08	0.54
1:A:262:TYR:CE2	1:A:346:TRP:CZ2	2.96	0.54
2:D:401:GLU:HA	3:E:137:LYS:HG3	1.90	0.54
1:C:1:MET:HB3	1:C:130:THR:OG1	2.08	0.54
1:C:71:GLU:HG2	1:C:72:PRO:N	2.23	0.53
2:D:155:ILE:HG21	2:D:164:MET:HE1	1.89	0.53
1:C:386:GLU:OE2	12:C:601:HOH:O	2.19	0.53
2:D:133:PHE:CE1	2:D:155:ILE:HD11	2.44	0.53
2:D:170:MET:HE2	2:D:377:LEU:HD21	1.89	0.53
2:D:116:VAL:CG1	2:D:151:LEU:HD11	2.39	0.53
2:D:156:ARG:NH2	12:D:601:HOH:O	2.27	0.53
3:E:47:LEU:HD12	3:E:47:LEU:O	2.08	0.53
4:F:242:ASN:HB2	4:F:245:ILE:HB	1.91	0.53
1:A:117:LEU:HD11	1:A:121:ARG:HH11	1.73	0.53
2:B:219:THR:HG21	1:C:326:LYS:HA	1.91	0.53
2:B:81:PHE:O	2:B:84:ILE:HG22	2.08	0.53
2:D:73:MET:HE3	2:D:92:PHE:HB3	1.90	0.53
2:B:238:THR:HG21	2:B:316:ILE:HD11	1.91	0.53
1:A:71:GLU:HG2	1:A:72:PRO:N	2.23	0.52
2:B:159:TYR:HB3	2:B:162:ARG:HG2	1.90	0.52
2:D:271:ALA:HB2	2:D:298:ASN:HD22	1.75	0.52
3:E:58:GLU:HG3	3:E:61:ARG:HH21	1.75	0.52
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.39	0.52
4:F:247:LYS:O	4:F:247:LYS:HG2	2.09	0.52
4:F:172:PHE:O	4:F:176:GLN:HG2	2.09	0.52
2:B:201:CYS:SG	2:B:265:PHE:HB3	2.49	0.52
1:C:43:GLY:HA2	1:C:56:THR:O	2.09	0.52
4:F:338:CYS:HB3	4:F:343:TYR:CE2	2.45	0.52
2:B:161:ASP:OD1	2:B:162:ARG:HD3	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:48:GLU:HG3	3:E:49:GLU:N	2.24	0.52
1:C:320:ARG:HA	1:C:356:ASN:O	2.10	0.52
2:D:396:HIS:HA	2:D:399:THR:HG22	1.90	0.52
1:A:71:GLU:OE1	1:A:73:THR:OG1	2.25	0.51
2:D:81:PHE:O	2:D:84:ILE:HG22	2.11	0.51
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.93	0.51
2:D:208:TYR:CE1	2:D:220:PRO:HD2	2.45	0.51
2:D:221:THR:HG23	2:D:224:ASP:H	1.75	0.51
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.46	0.51
4:F:149:ALA:O	4:F:180:HIS:ND1	2.43	0.51
1:A:54:SER:OG	1:A:62:VAL:HG22	2.11	0.50
1:A:357:TYR:CZ	3:E:17:GLY:HA2	2.46	0.50
1:A:40:LYS:O	1:A:42:ILE:HD12	2.10	0.50
3:E:46:SER:OG	3:E:49:GLU:HG3	2.11	0.50
2:B:197:ASP:OD1	9:B:502:MES:H62	2.11	0.50
1:A:221:ARG:NE	2:B:327:ASP:OD2	2.45	0.50
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.46	0.50
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.46	0.50
4:F:16:GLU:O	4:F:20:LEU:HG	2.11	0.50
2:D:343:GLU:HG3	2:D:430:ALA:HB2	1.94	0.50
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.47	0.50
2:B:377:LEU:HD12	2:B:377:LEU:O	2.12	0.50
2:D:16:ILE:HD11	2:D:136:THR:HB	1.94	0.50
4:F:205:VAL:CG2	4:F:315:PHE:HB2	2.42	0.49
2:B:280:GLN:O	2:B:280:GLN:HG3	2.12	0.49
2:D:319:GLY:HA2	2:D:357:PRO:HG3	1.94	0.49
3:E:7:GLU:CD	3:E:9:ILE:HD11	2.32	0.49
2:B:156:ARG:HD2	9:B:502:MES:H22	1.94	0.49
2:D:215:LEU:HB3	2:D:217:LEU:HD12	1.94	0.49
4:F:202:ARG:NE	4:F:318:ASP:OD1	2.35	0.49
2:D:36:TYR:CD2	2:D:44:LEU:HD11	2.48	0.49
2:D:404:ASP:OD1	2:D:406:MET:HB2	2.13	0.49
1:A:187:SER:CB	1:A:391:LEU:HD21	2.42	0.49
2:D:7:ILE:O	2:D:135:LEU:HD12	2.13	0.49
2:D:116:VAL:HG11	2:D:151:LEU:HD11	1.94	0.48
2:D:139:LEU:HA	2:D:145:SER:HB3	1.95	0.48
1:C:180:ALA:O	1:C:183:GLU:HG3	2.14	0.48
1:C:229:ARG:HD2	12:C:642:HOH:O	2.13	0.48
2:D:1:MET:HG2	2:D:48:ASN:ND2	2.24	0.48
2:D:293:MET:CG	2:D:367:PHE:HB2	2.43	0.48
1:A:195:LEU:HD12	1:A:266:HIS:CE1	2.48	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:173:PRO:HA	2:B:176:SER:HB2	1.96	0.48
2:D:110:ALA:O	2:D:113:VAL:HG12	2.14	0.48
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.48	0.48
1:C:340:SER:HA	12:C:638:HOH:O	2.14	0.48
2:D:246:LEU:CD1	2:D:248:ALA:HB2	2.44	0.48
1:C:220:GLU:CG	2:D:324:LYS:HD3	2.44	0.48
2:D:30:ILE:HD13	2:D:59:TYR:HB2	1.96	0.48
1:A:25:CYS:HB3	1:A:30:ILE:O	2.13	0.48
2:D:306:ARG:HG2	2:D:340:TYR:CZ	2.49	0.48
1:A:60:LYS:NZ	1:A:85:GLN:O	2.47	0.47
2:B:22:GLU:HG2	2:B:81:PHE:CD1	2.49	0.47
2:B:12:CYS:HB2	8:B:501:GDP:C8	2.49	0.47
3:E:72:LEU:O	3:E:76:ARG:HG2	2.14	0.47
4:F:102:PRO:CB	4:F:174:ASP:HA	2.43	0.47
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.49	0.47
2:D:400:GLY:O	3:E:137:LYS:HG3	2.14	0.47
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.97	0.47
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.97	0.47
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.50	0.47
2:D:26:ASP:OD1	2:D:359:ARG:NH2	2.48	0.47
2:D:375:GLN:HB2	2:D:419:VAL:HG13	1.95	0.47
2:D:73:MET:CE	2:D:92:PHE:HB3	2.44	0.47
4:F:224:SER:HA	4:F:246:GLN:NE2	2.29	0.47
2:B:295:ASP:HA	9:B:503:MES:O3S	2.14	0.47
2:D:62:ARG:HG3	2:D:123:GLU:OE1	2.15	0.47
2:B:324:LYS:O	2:B:328:GLU:HG3	2.14	0.47
2:D:343:GLU:CG	2:D:430:ALA:HB2	2.45	0.47
4:F:224:SER:HA	4:F:246:GLN:HE22	1.80	0.47
2:B:386:THR:O	2:B:390:ARG:HG2	2.15	0.47
2:D:192:LEU:HD22	2:D:196:THR:HG21	1.97	0.46
2:D:293:MET:HG3	2:D:367:PHE:HB2	1.96	0.46
2:D:386:THR:O	2:D:390:ARG:HG2	2.14	0.46
2:B:36:TYR:CD2	2:B:44:LEU:HD11	2.50	0.46
2:D:105:HIS:O	2:D:150:LEU:HD22	2.16	0.46
4:F:40:MET:CE	4:F:47:LEU:HG	2.45	0.46
1:C:277:SER:OG	1:C:280:LYS:HE2	2.15	0.46
2:D:345:ILE:HG22	2:D:348:ASN:HB3	1.97	0.46
2:D:395:LEU:O	2:D:399:THR:HG22	2.15	0.46
1:A:413:MET:HE1	1:A:418:PHE:CE1	2.50	0.46
9:B:503:MES:H81	9:B:503:MES:H51	1.50	0.46
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:206:ALA:O	2:D:210:ILE:HG13	2.15	0.46
2:D:324:LYS:O	2:D:328:GLU:HG3	2.15	0.46
4:F:144:GLY:HA3	4:F:187:GLU:OE1	2.16	0.46
4:F:20:LEU:O	4:F:24:THR:HG23	2.15	0.46
4:F:169:LEU:O	4:F:172:PHE:HB3	2.16	0.46
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.45	0.46
3:E:58:GLU:HG3	3:E:61:ARG:NH2	2.31	0.46
4:F:195:GLY:C	4:F:197:ARG:HG3	2.36	0.46
1:A:370:LYS:HE3	1:A:370:LYS:HB2	1.62	0.46
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.46	0.46
2:B:405:GLU:HG3	12:B:685:HOH:O	2.15	0.46
1:C:104:ALA:HB2	1:C:413:MET:SD	2.56	0.46
2:B:135:LEU:CD2	2:B:152:ILE:HD11	2.46	0.46
2:B:301:ALA:O	2:B:303:CYS:N	2.49	0.46
2:D:45:GLU:OE1	2:D:243:PRO:HG3	2.15	0.46
2:D:417:ASP:O	2:D:421:GLU:HG3	2.16	0.46
2:D:7:ILE:O	2:D:135:LEU:HA	2.16	0.46
4:F:87:LEU:O	4:F:91:CYS:HB2	2.16	0.46
1:A:413:MET:CE	1:A:418:PHE:CE1	2.99	0.45
2:D:155:ILE:CG2	2:D:164:MET:HE1	2.46	0.45
2:D:87:PRO:HD2	12:D:627:HOH:O	2.15	0.45
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.50	0.45
2:D:7:ILE:HD13	2:D:151:LEU:HD21	1.98	0.45
4:F:206:LEU:HD21	4:F:354:ALA:HB2	1.99	0.45
2:B:102:ALA:HB2	2:B:403:MET:SD	2.56	0.45
2:B:215:LEU:HD13	2:B:275:SER:HA	1.97	0.45
1:C:209:ILE:HD11	1:C:302:MET:SD	2.56	0.45
4:F:181:VAL:HG12	4:F:182:ILE:N	2.32	0.45
1:C:423:GLU:HG2	12:C:785:HOH:O	2.16	0.45
2:D:1:MET:HE3	2:D:48:ASN:HB2	1.99	0.45
2:B:190:HIS:ND1	2:B:414:ASN:ND2	2.64	0.45
4:F:100:ILE:HD12	4:F:128:ARG:HB2	1.99	0.45
2:B:31:ASP:OD1	2:B:33:THR:HB	2.16	0.45
1:A:19:ALA:CB	1:A:232:SER:OG	2.65	0.45
4:F:298:ILE:HD12	4:F:302:ILE:HD13	1.99	0.45
2:B:286:VAL:HB	2:B:325:GLU:HG2	1.98	0.44
4:F:101:TYR:CD1	4:F:179:VAL:HG22	2.53	0.44
2:B:68:LEU:HD12	2:B:97:ALA:HB2	1.98	0.44
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.83	0.44
2:D:396:HIS:HA	2:D:399:THR:CG2	2.48	0.44
4:F:259:GLY:O	4:F:261:GLU:HG3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:PRO:HA	1:A:301:GLN:CD	2.37	0.44
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.99	0.44
2:B:36:TYR:C	2:B:37:HIS:HD1	2.19	0.44
10:B:505:E44:N2	10:B:505:E44:C9	2.80	0.44
2:D:67:ASP:O	2:D:92:PHE:HA	2.18	0.44
1:A:324:VAL:HG22	12:A:604:HOH:O	2.16	0.44
2:B:117:LEU:HD11	2:B:154:LYS:HB3	2.00	0.44
2:D:64:ILE:HG12	2:D:119:VAL:HG12	1.99	0.44
1:C:153:LEU:O	1:C:157:LEU:HG	2.18	0.43
1:C:241:SER:HA	1:C:249:ASN:OD1	2.18	0.43
4:F:101:TYR:HD1	4:F:179:VAL:HG22	1.83	0.43
1:A:274:PRO:HB3	1:A:286:LEU:HD12	2.00	0.43
1:A:112:LYS:HD2	3:E:54:LEU:HB3	2.00	0.43
1:A:227:LEU:O	1:A:231:ILE:HG13	2.18	0.43
4:F:307:LEU:HD23	4:F:307:LEU:HA	1.83	0.43
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.53	0.43
2:D:170:MET:HE3	2:D:377:LEU:HD21	1.99	0.43
2:B:33:THR:HG22	2:B:35:SER:H	1.84	0.43
4:F:2:TYR:HB2	4:F:27:TRP:CD2	2.53	0.43
4:F:40:MET:HE1	4:F:47:LEU:HG	1.99	0.43
1:A:136:LEU:HD22	1:A:167:LEU:HB2	2.01	0.43
2:D:193:VAL:HG22	2:D:265:PHE:CE2	2.54	0.43
2:D:193:VAL:HG21	2:D:418:LEU:HD22	2.01	0.43
2:B:21:TRP:CH2	2:B:61:PRO:HB3	2.53	0.43
2:B:64:ILE:HD13	2:B:120:VAL:HG22	2.01	0.43
2:D:321:MET:HB3	2:D:363:MET:HE1	2.01	0.43
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.54	0.42
2:D:116:VAL:O	2:D:120:VAL:HG23	2.19	0.42
4:F:96:GLU:O	4:F:183:GLN:HB2	2.18	0.42
4:F:102:PRO:HB3	4:F:174:ASP:HA	2.01	0.42
1:C:275:VAL:HG13	1:C:368:LEU:CD2	2.48	0.42
2:D:208:TYR:HE1	2:D:220:PRO:HD2	1.83	0.42
2:B:296:SER:N	9:B:503:MES:O3S	2.44	0.42
2:D:54:ALA:HB3	2:D:58:LYS:O	2.20	0.42
4:F:193:GLU:OE1	4:F:193:GLU:HA	2.20	0.42
2:B:161:ASP:C	2:B:162:ARG:HD2	2.40	0.42
2:B:210:ILE:HG23	2:B:273:LEU:HD13	2.01	0.42
2:D:155:ILE:CG2	2:D:164:MET:CE	2.97	0.42
1:C:221:ARG:HG3	2:D:323:MET:SD	2.60	0.42
1:A:42:ILE:N	1:A:42:ILE:HD12	2.35	0.42
1:C:361:THR:HG22	1:C:362:VAL:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.54	0.42
1:A:18:ASN:ND2	1:A:78:VAL:HG22	2.34	0.42
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.54	0.42
4:F:205:VAL:HG22	4:F:315:PHE:HB2	2.00	0.42
1:A:336:LYS:HD2	1:A:336:LYS:HA	1.82	0.41
2:D:160:PRO:HG3	3:E:120:LEU:HD21	2.01	0.41
2:D:212:PHE:HD1	2:D:213:ARG:HD2	1.85	0.41
2:D:36:TYR:CE1	2:D:38:GLY:HA3	2.55	0.41
2:D:193:VAL:CG2	2:D:418:LEU:HD22	2.50	0.41
4:F:146:VAL:HG21	4:F:233:PHE:CZ	2.54	0.41
1:C:192:HIS:CG	1:C:421:ALA:HA	2.55	0.41
1:C:414:GLU:HB3	12:C:752:HOH:O	2.19	0.41
4:F:34:ASN:OD1	4:F:35:PRO:HD2	2.19	0.41
1:A:275:VAL:HG13	1:A:368:LEU:HD21	2.02	0.41
1:A:134:GLY:HA3	1:A:165:SER:O	2.20	0.41
1:A:399:TYR:O	1:A:402:ARG:NH1	2.52	0.41
4:F:131:PHE:C	4:F:131:PHE:CD2	2.92	0.41
3:E:24:LEU:C	3:E:25:LYS:HG3	2.42	0.41
4:F:205:VAL:HG21	4:F:317:PHE:CE1	2.56	0.41
4:F:263:PHE:CE2	4:F:341:LYS:HD3	2.56	0.41
2:B:163:ILE:HG21	2:B:250:LEU:HB3	2.03	0.41
1:A:262:TYR:CE2	1:A:346:TRP:HZ2	2.39	0.41
2:D:21:TRP:CH2	2:D:61:PRO:HB3	2.56	0.41
4:F:326:LYS:HE2	4:F:328:TRP:CH2	2.56	0.41
4:F:3:THR:O	4:F:38:ASN:HB2	2.21	0.40
1:A:63:PRO:HD3	1:A:86:LEU:HG	2.02	0.40
1:A:390:ARG:HD2	4:F:54:HIS:CD2	2.56	0.40
2:D:210:ILE:HG23	2:D:273:LEU:HD13	2.02	0.40
2:B:162:ARG:HD2	2:B:162:ARG:N	2.35	0.40
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.03	0.40
1:C:187:SER:HB3	1:C:391:LEU:HD21	2.03	0.40
4:F:61:LEU:HD12	4:F:310:GLN:HB2	2.03	0.40
2:B:360:GLY:O	2:B:361:LEU:HD23	2.21	0.40
2:D:117:LEU:O	2:D:121:ARG:HG3	2.21	0.40
4:F:305:LYS:HE3	4:F:305:LYS:HB2	1.90	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	435/450 (97%)	425 (98%)	10 (2%)	0	100	100
1	C	438/450 (97%)	427 (98%)	11 (2%)	0	100	100
2	B	425/445 (96%)	418 (98%)	7 (2%)	0	100	100
2	D	417/445 (94%)	409 (98%)	8 (2%)	0	100	100
3	E	117/143 (82%)	116 (99%)	1 (1%)	0	100	100
4	F	322/384 (84%)	306 (95%)	15 (5%)	1 (0%)	41	61
All	All	2154/2317 (93%)	2101 (98%)	52 (2%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	91	CYS

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	368/378 (97%)	362 (98%)	6 (2%)	62	84
1	C	371/378 (98%)	366 (99%)	5 (1%)	69	87
2	B	369/383 (96%)	362 (98%)	7 (2%)	57	80
2	D	364/383 (95%)	356 (98%)	8 (2%)	52	77
3	E	109/127 (86%)	106 (97%)	3 (3%)	43	70
4	F	298/342 (87%)	282 (95%)	16 (5%)	22	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1879/1991 (94%)	1834 (98%)	45 (2%)	49 74

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	73	THR
1	A	91	GLN
1	A	188	ILE
1	A	256	GLN
1	A	381	THR
2	B	37	HIS
2	B	115	SER
2	B	137	HIS
2	B	162	ARG
2	B	316	ILE
2	B	324	LYS
2	B	333	VAL
1	C	71	GLU
1	C	221	ARG
1	C	251	ASP
1	C	347	CYS
1	C	381	THR
2	D	42	LEU
2	D	78	SER
2	D	137	HIS
2	D	153	SER
2	D	213	ARG
2	D	217	LEU
2	D	363	MET
2	D	386	THR
3	E	48	GLU
3	E	52	LYS
3	E	136	ASN
4	F	12	SER
4	F	31	ARG
4	F	89	GLU
4	F	90	SER
4	F	129	GLU
4	F	192	LEU
4	F	197	ARG
4	F	198	LYS

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Mol	Chain	Res	Type
4	F	211	TYR
4	F	222	ARG
4	F	238	CYS
4	F	247	LYS
4	F	252	ASN
4	F	299	GLU
4	F	307	LEU
4	F	331	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
2	B	99	ASN
1	C	356	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 carbohydrates 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
11	ACP	F	402	7	27,33,33	4.72	10 (37%)	32,52,52	2.33	5 (15%)
9	MES	B	502	-	12,12,12	2.02	1 (8%)	14,16,16	2.16	4 (28%)
5	GTP	C	501	7	26,34,34	0.99	1 (3%)	33,54,54	1.89	9 (27%)
8	GDP	B	501	7	24,30,30	1.11	2 (8%)	31,47,47	1.86	7 (22%)
5	GTP	A	501	7	26,34,34	1.10	1 (3%)	33,54,54	1.83	8 (24%)
8	GDP	D	501	-	24,30,30	1.22	2 (8%)	31,47,47	1.91	9 (29%)
10	E44	D	502	-	25,26,26	0.89	2 (8%)	30,37,37	1.30	2 (6%)
10	E44	B	505	-	25,26,26	0.87	2 (8%)	30,37,37	1.32	2 (6%)
9	MES	B	503	-	12,12,12	2.22	1 (8%)	14,16,16	1.91	5 (35%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	ACP	F	402	7	-	3/15/38/38	0/3/3/3
9	MES	B	502	-	-	4/6/14/14	0/1/1/1
5	GTP	C	501	7	-	7/18/38/38	0/3/3/3
8	GDP	B	501	7	-	3/12/32/32	0/3/3/3
5	GTP	A	501	7	-	6/18/38/38	0/3/3/3
8	GDP	D	501	-	-	5/12/32/32	0/3/3/3
10	E44	D	502	-	-	2/5/16/16	0/4/4/4
10	E44	B	505	-	-	2/5/16/16	0/4/4/4
9	MES	B	503	-	-	1/6/14/14	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	F	402	ACP	O4'-C1'	15.13	1.62	1.41
11	F	402	ACP	C2'-C1'	-14.98	1.31	1.53
9	B	503	MES	C8-S	-7.32	1.67	1.77
11	F	402	ACP	PB-O3A	6.97	1.66	1.58
9	B	502	MES	C8-S	-6.69	1.68	1.77
11	F	402	ACP	O4'-C4'	-6.23	1.31	1.45
8	D	501	GDP	C6-C5	4.27	1.48	1.41
5	A	501	GTP	C6-N1	3.65	1.39	1.33
8	B	501	GDP	C6-C5	3.26	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	501	GTP	C6-N1	3.21	1.38	1.33
11	F	402	ACP	C6-N6	3.14	1.45	1.34
10	B	505	E44	C1-N1	3.02	1.32	1.30
11	F	402	ACP	O2'-C2'	2.91	1.49	1.43
10	D	502	E44	C1-N1	2.85	1.32	1.30
11	F	402	ACP	O3'-C3'	-2.82	1.36	1.43
11	F	402	ACP	C5-C4	-2.58	1.34	1.40
11	F	402	ACP	C2-N3	2.54	1.36	1.32
8	D	501	GDP	C5-C4	2.49	1.47	1.40
10	D	502	E44	C7-N3	2.37	1.44	1.39
8	B	501	GDP	C5-C4	2.27	1.46	1.40
10	B	505	E44	C7-N3	2.17	1.44	1.39
11	F	402	ACP	PB-O2B	-2.13	1.51	1.56

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	F	402	ACP	C5-C6-N6	8.63	133.47	120.35
11	F	402	ACP	N6-C6-N1	-5.65	106.84	118.57
5	A	501	GTP	N3-C2-N1	-5.57	119.79	127.22
5	C	501	GTP	N3-C2-N1	-5.34	120.10	127.22
11	F	402	ACP	N3-C2-N1	-5.34	120.34	128.68
8	D	501	GDP	C2-N3-C4	5.25	121.36	115.36
10	B	505	E44	N1-C1-N4	-5.10	125.48	130.62
10	D	502	E44	N1-C1-N4	-4.91	125.67	130.62
8	B	501	GDP	C2-N3-C4	4.53	120.53	115.36
5	A	501	GTP	C2-N3-C4	4.37	120.35	115.36
9	B	502	MES	O3S-S-C8	4.34	112.78	105.77
8	B	501	GDP	C6-C5-C4	-4.31	116.68	120.80
9	B	502	MES	C6-C5-N4	-4.21	103.72	110.10
9	B	503	MES	C5-N4-C3	4.04	117.93	108.83
5	C	501	GTP	C2-N3-C4	4.01	119.94	115.36
8	B	501	GDP	C6-N1-C2	4.01	122.29	115.93
8	D	501	GDP	C5-C6-N1	-3.83	118.19	123.43
8	D	501	GDP	C6-N1-C2	3.83	122.02	115.93
5	C	501	GTP	C5-C6-N1	-3.70	118.38	123.43
11	F	402	ACP	C3'-C2'-C1'	3.67	106.50	100.98
8	B	501	GDP	N3-C2-N1	-3.65	122.36	127.22
8	B	501	GDP	C5-C6-N1	-3.59	118.52	123.43
8	D	501	GDP	C6-C5-C4	-3.46	117.49	120.80
8	D	501	GDP	N3-C2-N1	-3.30	122.82	127.22
9	B	502	MES	C5-N4-C3	3.23	116.10	108.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C5-C6-N1	-3.08	119.22	123.43
5	C	501	GTP	C6-N1-C2	3.06	120.79	115.93
8	D	501	GDP	C4-C5-N7	-2.96	106.31	109.40
10	B	505	E44	C1-N4-C7	2.92	119.71	111.04
10	D	502	E44	C1-N4-C7	2.89	119.60	111.04
9	B	503	MES	C6-C5-N4	-2.86	105.76	110.10
9	B	502	MES	C7-N4-C5	2.77	118.32	111.23
5	A	501	GTP	C6-N1-C2	2.73	120.27	115.93
5	A	501	GTP	PA-O3A-PB	-2.65	123.72	132.83
5	C	501	GTP	O3G-PG-O3B	2.64	113.48	104.64
5	C	501	GTP	N2-C2-N1	2.58	121.26	117.25
5	A	501	GTP	N2-C2-N1	2.50	121.14	117.25
5	C	501	GTP	C4-C5-N7	-2.49	106.81	109.40
11	F	402	ACP	PA-O3A-PB	-2.45	124.80	132.56
5	C	501	GTP	PA-O3A-PB	-2.40	124.57	132.83
9	B	503	MES	O3S-S-C8	2.39	109.63	105.77
8	B	501	GDP	C4-C5-N7	-2.32	106.98	109.40
8	B	501	GDP	PA-O3A-PB	-2.31	124.89	132.83
5	A	501	GTP	O2G-PG-O3B	2.24	112.16	104.64
8	D	501	GDP	O3B-PB-O3A	2.18	111.94	104.64
5	A	501	GTP	PB-O3B-PG	-2.16	125.41	132.83
5	C	501	GTP	PB-O3B-PG	-2.15	125.44	132.83
8	D	501	GDP	C3'-C2'-C1'	2.15	104.21	100.98
9	B	503	MES	C7-N4-C5	2.13	116.69	111.23
9	B	503	MES	O2S-S-C8	2.06	109.39	106.92
8	D	501	GDP	PA-O3A-PB	-2.06	125.77	132.83

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	F	402	ACP	PG-C3B-PB-O1B
11	F	402	ACP	PG-C3B-PB-O2B
11	F	402	ACP	PG-C3B-PB-O3A
9	B	502	MES	C8-C7-N4-C5
9	B	502	MES	C7-C8-S-O1S
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
5	A	501	GTP	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O2A
10	D	502	E44	C6-C7-N3-C17
9	B	503	MES	C8-C7-N4-C5
10	B	505	E44	C6-C7-N3-C17
9	B	502	MES	C7-C8-S-O3S
10	D	502	E44	N4-C7-N3-C17
10	B	505	E44	N4-C7-N3-C17
8	D	501	GDP	PA-O3A-PB-O2B
8	B	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O1A
9	B	502	MES	C7-C8-S-O2S
8	D	501	GDP	PA-O3A-PB-O1B
5	C	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O1G

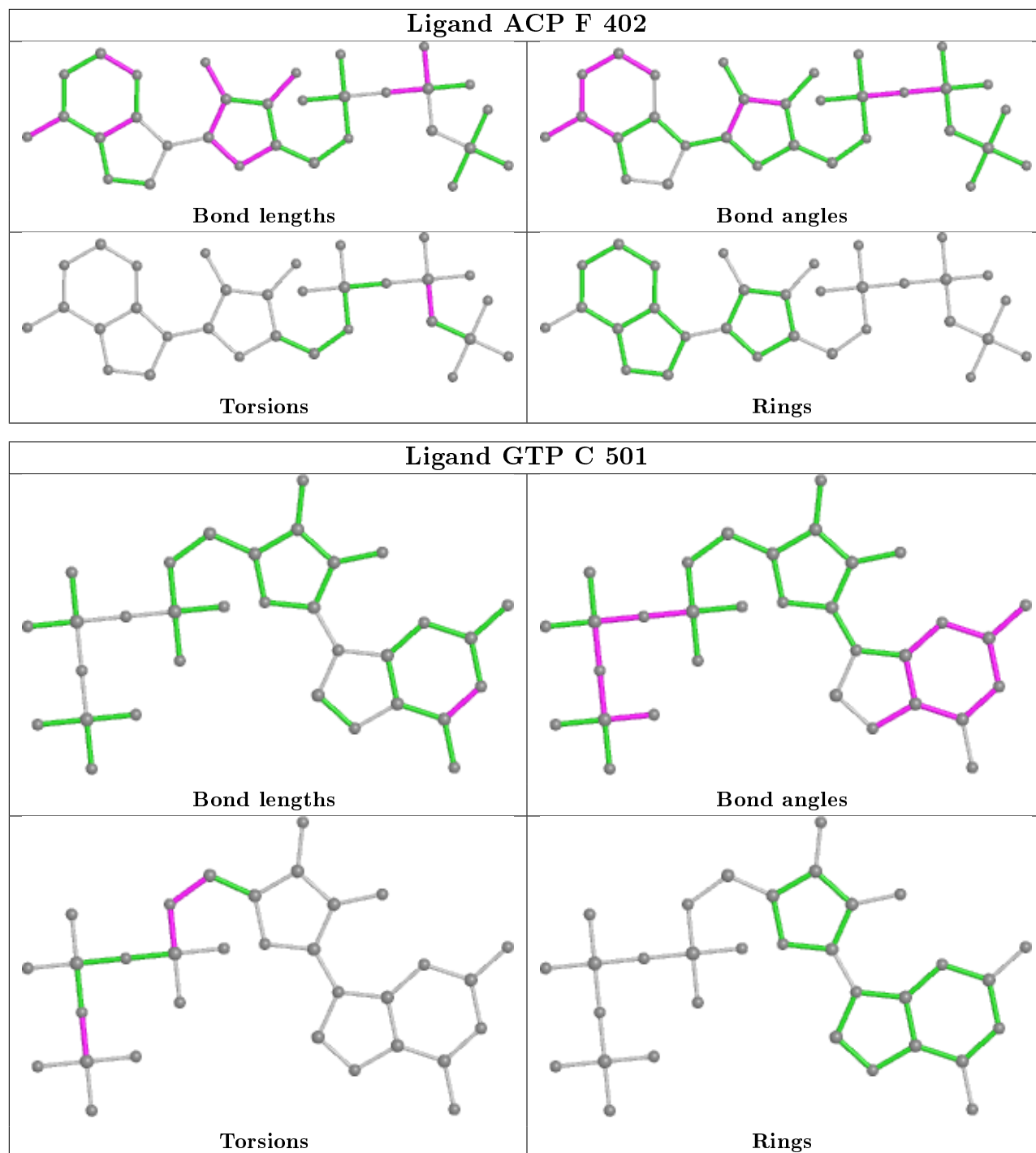
There are no ring outliers.

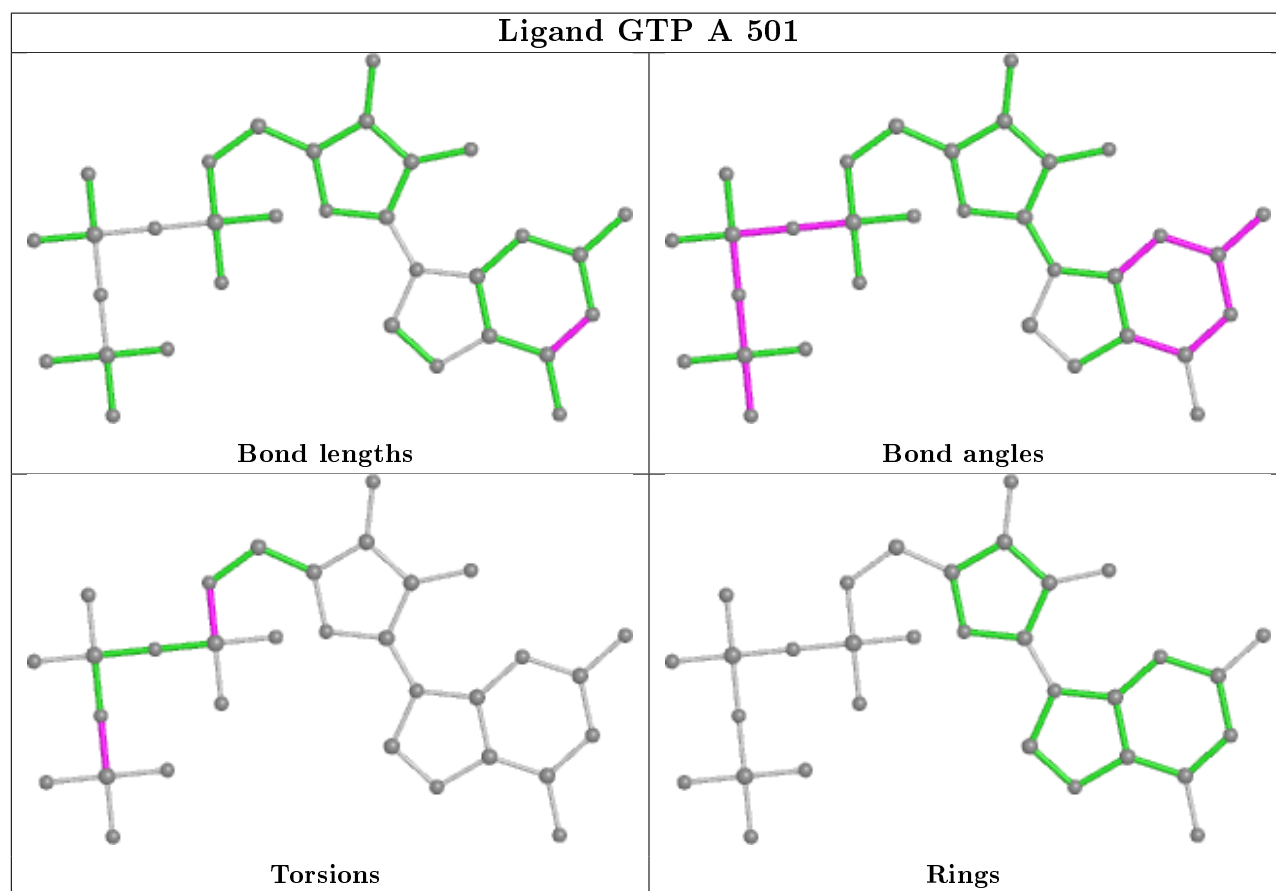
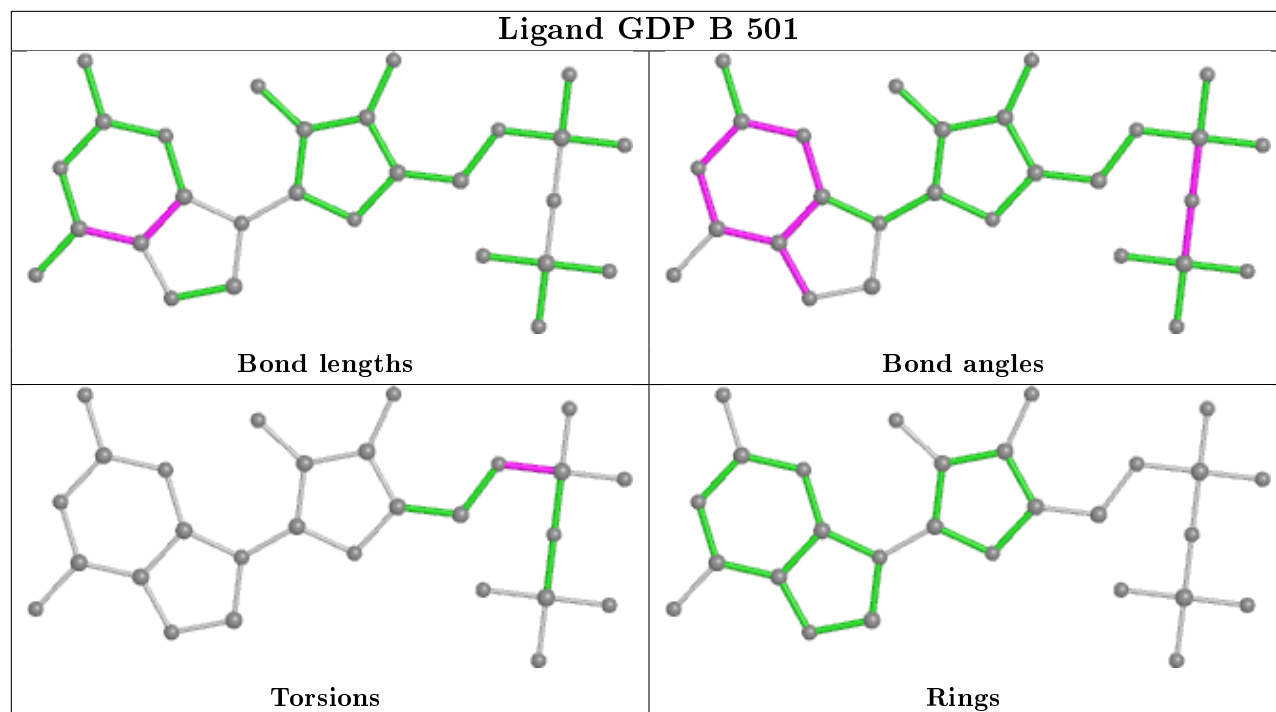
5 monomers are involved in 11 short contacts:

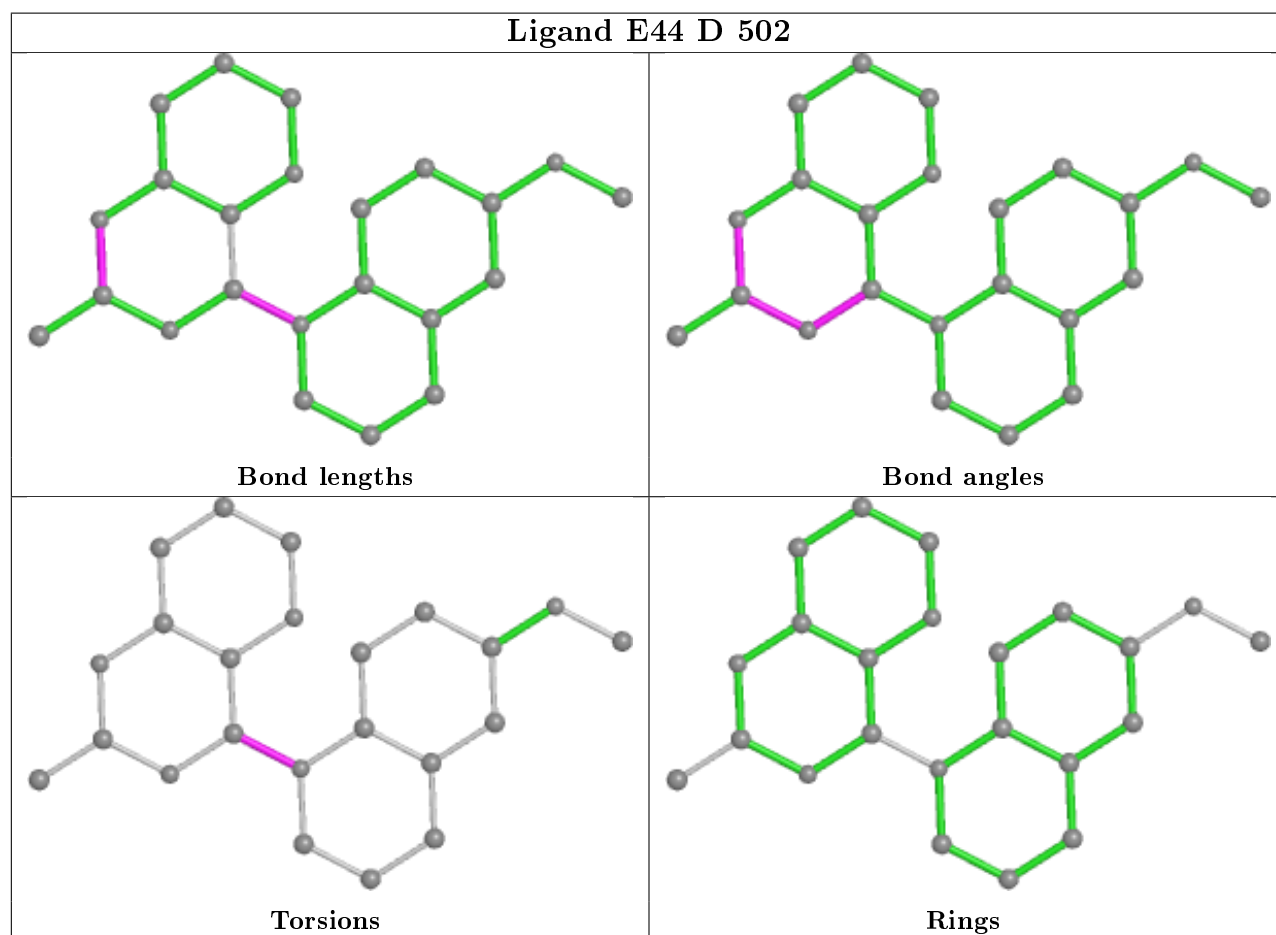
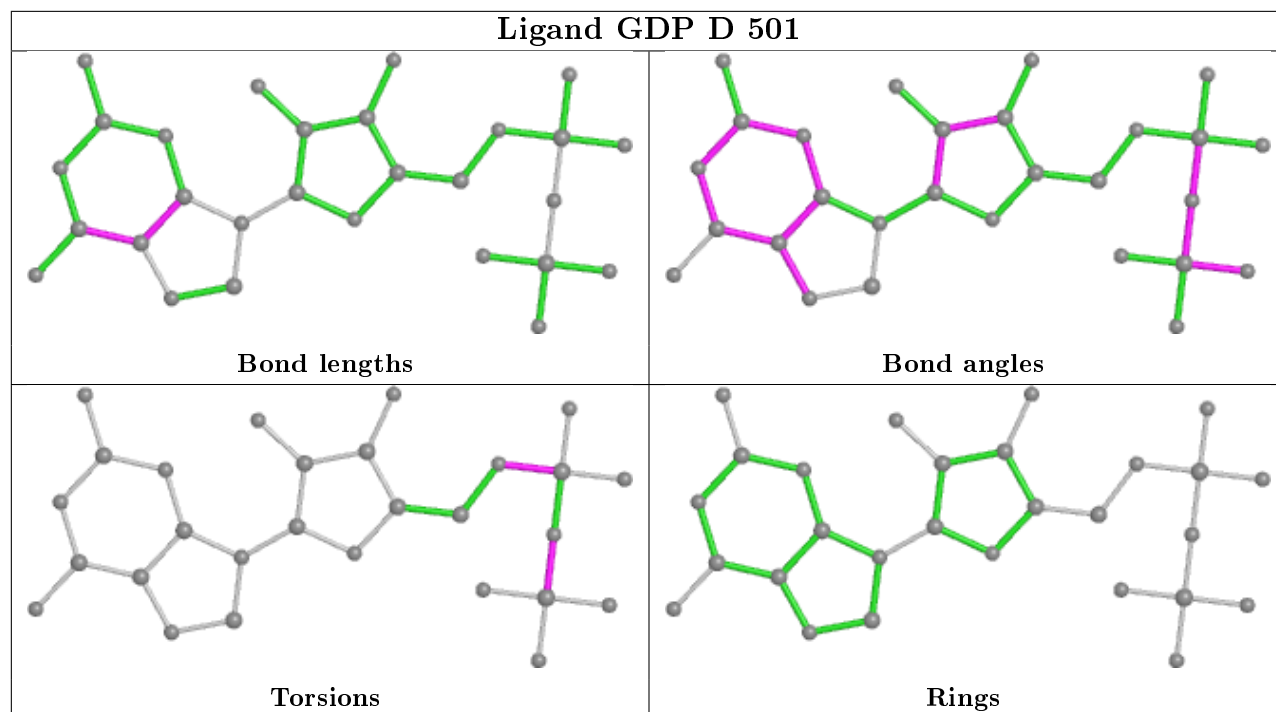
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	502	MES	2	0
8	B	501	GDP	1	0
8	D	501	GDP	4	0
10	B	505	E44	1	0
9	B	503	MES	3	0

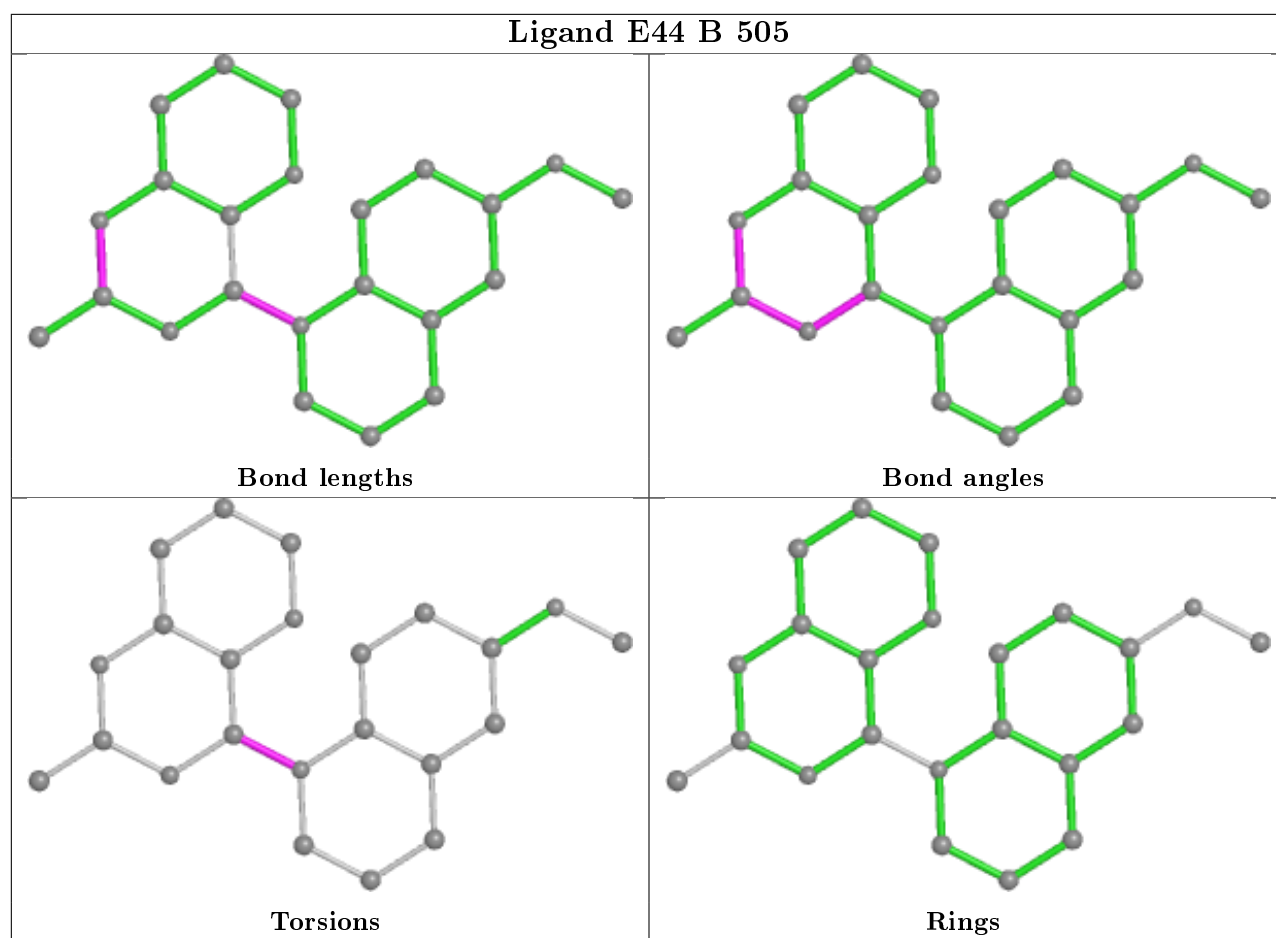
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/450 (97%)	-0.12	8 (1%) 68 71	24, 42, 73, 86	0
1	C	440/450 (97%)	-0.32	0 100 100	19, 31, 59, 84	0
2	B	427/445 (95%)	-0.13	14 (3%) 46 50	20, 39, 77, 126	0
2	D	421/445 (94%)	0.42	38 (9%) 9 9	29, 63, 102, 132	0
3	E	121/143 (84%)	0.16	6 (4%) 28 30	28, 56, 88, 105	0
4	F	332/384 (86%)	0.96	87 (26%) 0 0	30, 69, 130, 149	0
All	All	2178/2317 (94%)	0.12	153 (7%) 16 16	19, 47, 100, 149	0

All (153) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	233	PHE	8.5
4	F	173	ILE	7.6
4	F	134	ALA	6.1
4	F	130	VAL	5.7
4	F	167	SER	5.5
4	F	259	GLY	5.2
4	F	133	ALA	5.0
4	F	132	LEU	5.0
4	F	169	LEU	4.9
4	F	234	GLN	4.9
2	D	37	HIS	4.9
4	F	162	ILE	4.9
2	D	1	MET	4.5
4	F	177	GLY	4.5
4	F	182	ILE	4.5
4	F	231	ALA	4.5
2	B	279	GLN	4.4
2	D	92	PHE	4.4
4	F	253	TYR	4.3

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Mol	Chain	Res	Type	RSRZ
2	D	55	THR	4.3
4	F	244	CYS	4.2
4	F	136	ASN	4.2
4	F	166	ALA	4.2
1	A	262	TYR	4.2
2	D	73	MET	4.1
4	F	103	THR	4.1
2	B	55	THR	4.0
4	F	239	HIS	4.0
2	D	359	ARG	3.9
4	F	178	GLN	3.9
4	F	256	TYR	3.9
4	F	142	ARG	3.9
4	F	236	LYS	3.9
4	F	101	TYR	3.9
4	F	263	PHE	3.8
2	D	397	TRP	3.7
4	F	163	SER	3.7
4	F	170	LEU	3.7
4	F	232	ASN	3.6
3	E	139	LEU	3.6
4	F	171	ASP	3.6
4	F	161	LEU	3.5
2	D	394	PHE	3.5
2	D	80	PRO	3.5
2	D	54	ALA	3.5
4	F	100	ILE	3.4
2	D	180	VAL	3.4
2	D	175	VAL	3.3
4	F	196	HIS	3.3
4	F	165	GLU	3.2
4	F	138	ARG	3.2
4	F	102	PRO	3.2
4	F	372	THR	3.2
4	F	20	LEU	3.2
4	F	139	ARG	3.2
4	F	199	PHE	3.1
4	F	140	GLU	3.1
4	F	252	ASN	3.1
4	F	176	GLN	3.0
3	E	26	PRO	3.0
2	D	395	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
4	F	224	SER	3.0
4	F	149	ALA	3.0
4	F	168	GLU	2.9
2	B	57	ASN	2.9
2	D	390	ARG	2.9
4	F	164	SER	2.9
4	F	21	LEU	2.9
2	D	219	THR	2.9
4	F	129	GLU	2.9
2	B	38	GLY	2.9
2	B	54	ALA	2.9
4	F	135	TYR	2.9
2	D	74	ASP	2.8
4	F	131	PHE	2.8
2	B	277	GLY	2.8
1	A	179	THR	2.8
2	D	72	THR	2.8
2	B	243	PRO	2.8
4	F	24	THR	2.8
4	F	172	PHE	2.8
2	B	33	THR	2.7
2	D	179	VAL	2.7
4	F	181	VAL	2.7
1	A	88	HIS	2.7
4	F	255	ARG	2.7
4	F	148	ILE	2.7
2	D	406	MET	2.7
1	A	346	TRP	2.7
2	B	427	ASP	2.6
2	D	396	HIS	2.6
4	F	145	ASN	2.6
2	B	282	ARG	2.5
4	F	98	TYR	2.5
4	F	362	ALA	2.5
2	D	57	ASN	2.5
2	B	37	HIS	2.5
3	E	140	LYS	2.5
2	D	176	SER	2.5
4	F	137	ARG	2.5
2	D	217	LEU	2.5
2	D	247	ASN	2.5
4	F	25	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
4	F	179	VAL	2.5
3	E	24	LEU	2.4
2	D	398	TYR	2.4
2	D	83	GLN	2.4
4	F	227	PRO	2.4
2	D	405	GLU	2.4
4	F	99	VAL	2.4
4	F	197	ARG	2.4
4	F	174	ASP	2.4
4	F	361	LEU	2.4
4	F	143	GLU	2.3
4	F	147	TRP	2.3
2	D	216	LYS	2.3
1	A	59	GLY	2.3
2	B	56	GLY	2.3
2	D	391	ARG	2.3
4	F	19	ARG	2.3
4	F	257	GLU	2.3
4	F	262	MET	2.3
3	E	27	PRO	2.3
4	F	146	VAL	2.3
2	D	58	LYS	2.3
2	D	245	GLN	2.3
4	F	17	VAL	2.2
2	D	177	ASP	2.2
4	F	225	SER	2.2
4	F	22	LEU	2.2
4	F	13	VAL	2.2
4	F	245	ILE	2.2
4	F	243	HIS	2.2
3	E	28	SER	2.2
4	F	228	TYR	2.2
2	D	291	GLN	2.1
2	D	320	ARG	2.1
4	F	254	GLY	2.1
4	F	9	GLU	2.1
2	D	75	SER	2.1
2	B	280	GLN	2.1
4	F	186	LEU	2.1
4	F	90	SER	2.1
1	A	281	ALA	2.1
1	A	282	TYR	2.1

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Mol	Chain	Res	Type	RSRZ
4	F	141	GLY	2.1
4	F	192	LEU	2.1
2	D	178	THR	2.0
2	D	392	LYS	2.0
1	A	345	ASP	2.0
2	B	274	THR	2.0
2	D	389	PHE	2.0
4	F	187	GLU	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 ⓘ

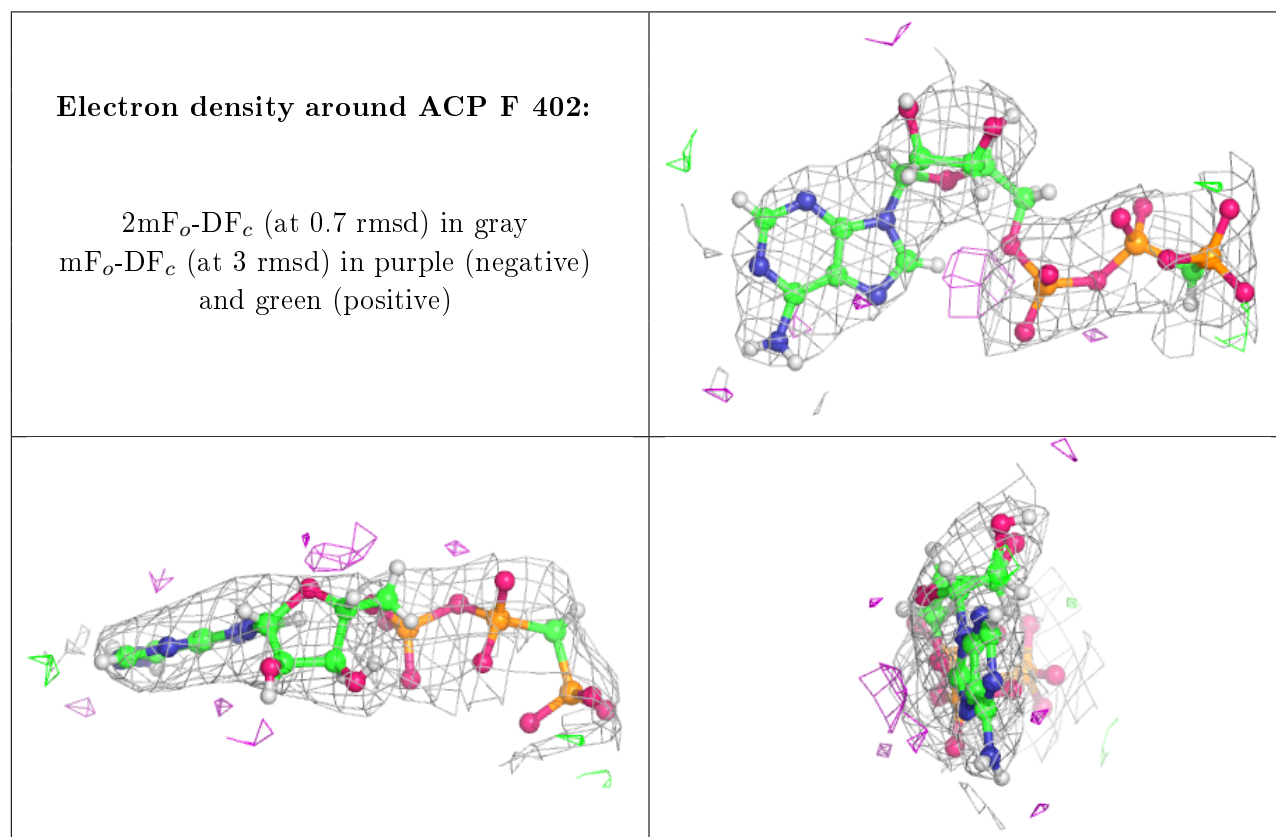
There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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.

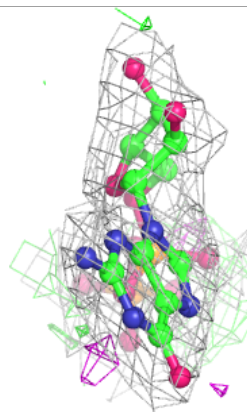
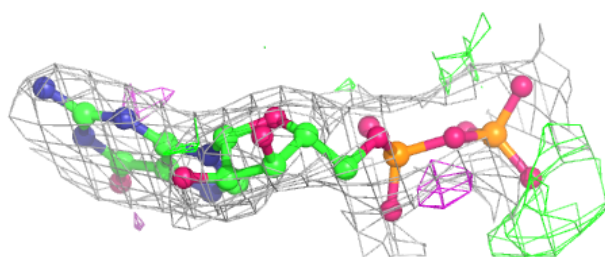
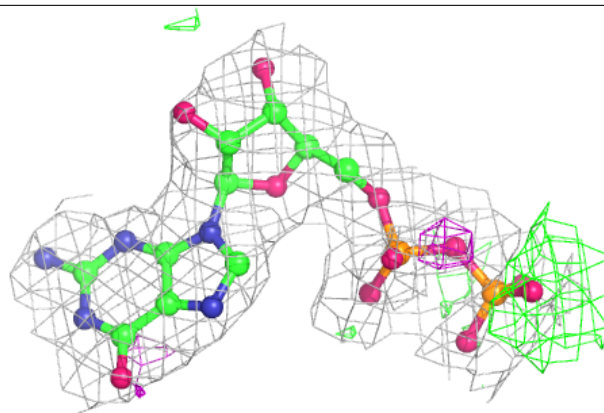
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	MG	F	401	1/1	0.83	0.14	104,104,104,104	0
11	ACP	F	402	31/31	0.88	0.19	79,102,130,151	0
8	GDP	D	501	28/28	0.93	0.13	50,58,65,70	0
9	MES	B	503	12/12	0.96	0.18	69,70,82,82	0
10	E44	D	502	23/23	0.96	0.16	29,35,50,58	0
9	MES	B	502	12/12	0.97	0.13	33,42,55,62	0
7	MG	B	504	1/1	0.97	0.19	26,26,26,26	0
7	MG	A	503	1/1	0.98	0.12	26,26,26,26	0
8	GDP	B	501	28/28	0.98	0.19	17,25,30,37	0
10	E44	B	505	23/23	0.98	0.14	30,36,44,49	0
5	GTP	C	501	32/32	0.99	0.15	24,26,30,31	0
5	GTP	A	501	32/32	0.99	0.19	23,28,32,36	0
6	CA	C	502	1/1	0.99	0.05	41,41,41,41	0
6	CA	A	502	1/1	0.99	0.03	66,66,66,66	0
7	MG	C	503	1/1	0.99	0.10	25,25,25,25	0

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

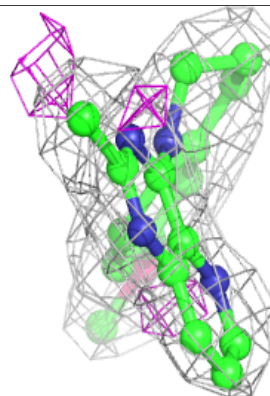
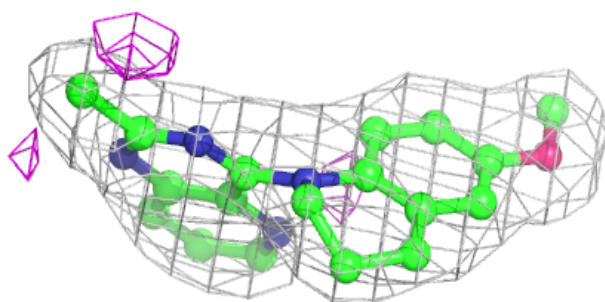
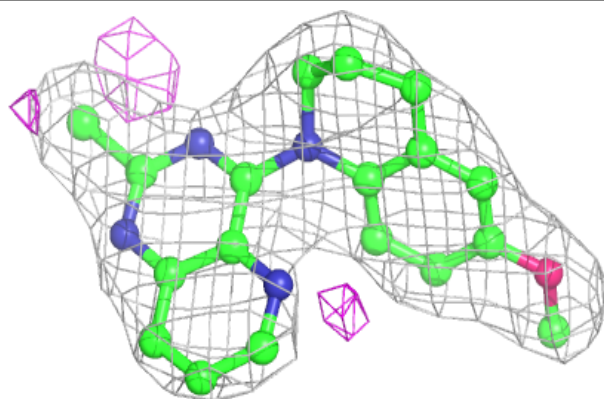


Electron density around GDP D 501:

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

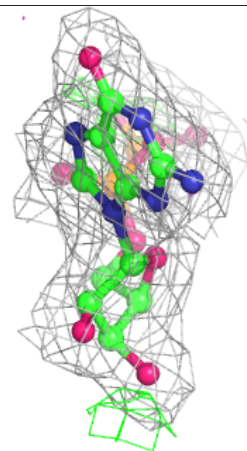
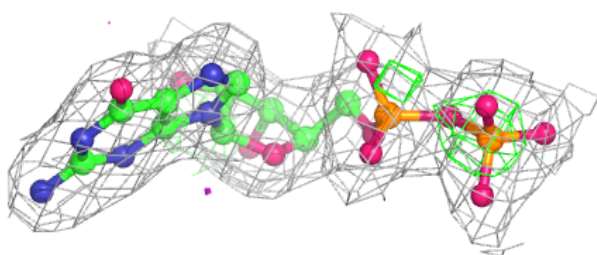
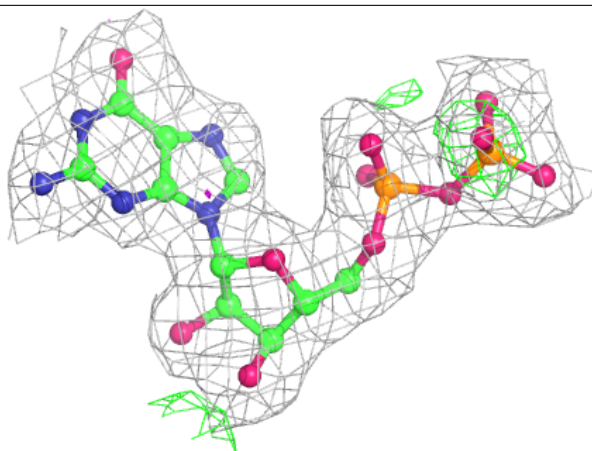
**Electron density around E44 D 502:**

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

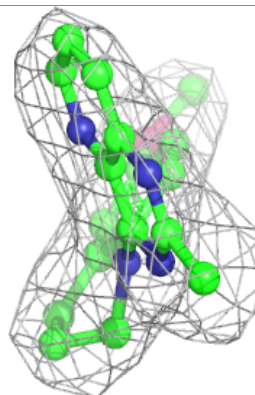
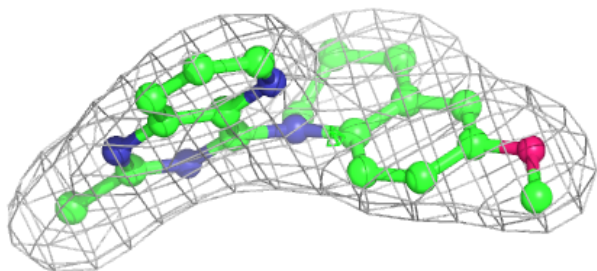
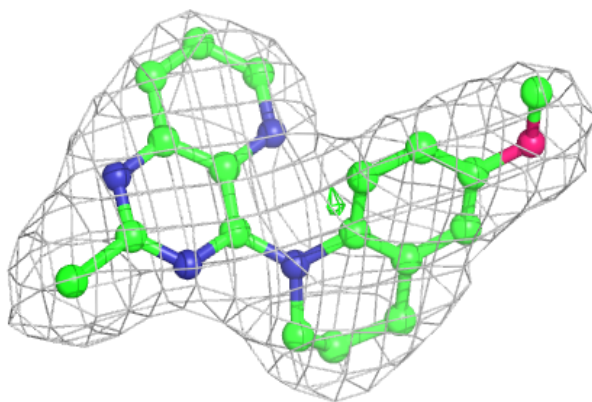


Electron density around GDP B 501:

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

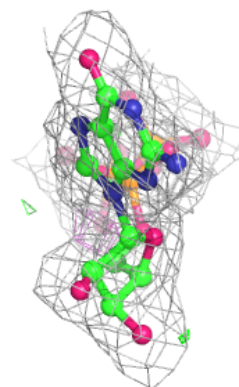
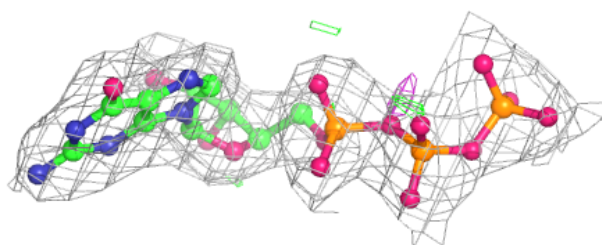
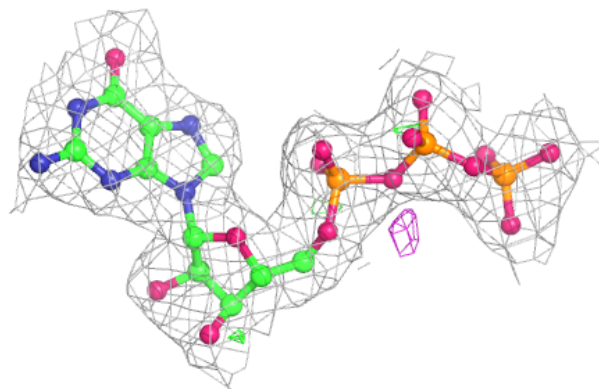
**Electron density around E44 B 505:**

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

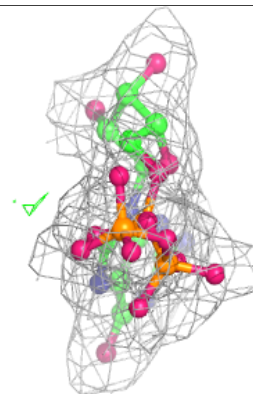
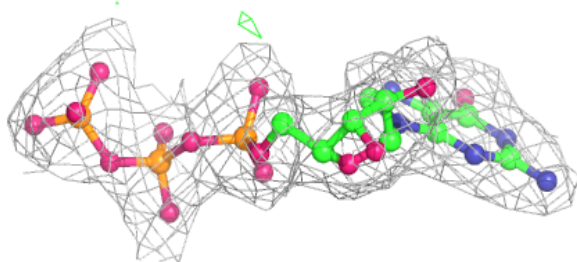
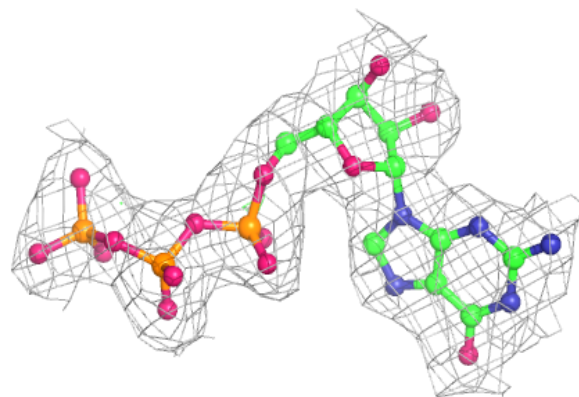


Electron density around GTP C 501:

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

**Electron density around GTP 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)



6.5 Other polymers [i](#)

There are no such residues in this entry.