



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 21, 2021 – 12:54 PM EDT

PDB ID : 5S4U
Title : Tubulin-Z30620520-complex
Authors : Muehlethaler, T.; Gioia, D.; Prota, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.
Deposited on : 2020-11-08
Resolution : 2.39 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.20
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.20

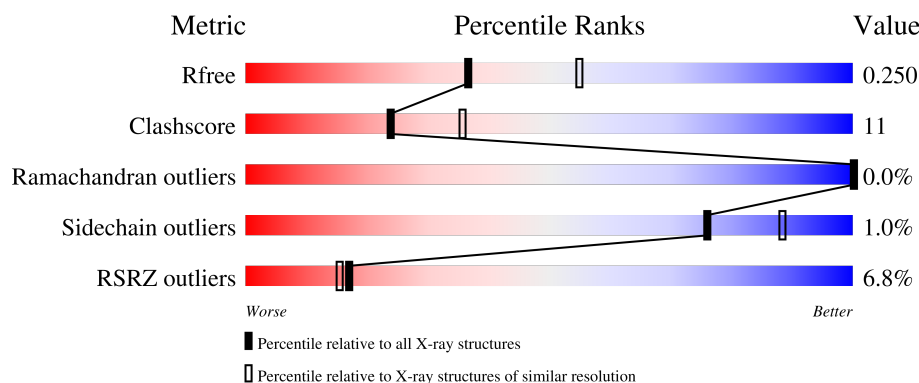
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	451	<div> <div>4%</div> <div>73% 24% . .</div> </div>
1	C	451	<div> <div>2%</div> <div>76% 21% .</div> </div>
2	B	445	<div> <div>5%</div> <div>70% 25% .</div> </div>
2	D	445	<div> <div>6%</div> <div>72% 24% .</div> </div>
3	E	143	<div> <div>6%</div> <div>73% 13% 14%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	384	<div><div></div><div>17%</div><div>69%</div><div>22%</div><div>8%</div></div>

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17989 atoms, of which 17 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3424	2167	582	653	22			
1	C	440	Total	C	N	O	S	0	1	0
			3443	2178	585	657	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	425	Total	C	N	O	S	2	1	0
			3359	2109	577	646	27			
2	D	428	Total	C	N	O	S	5	0	0
			3353	2104	572	650	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	0	0
			1014	625	183	201	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63043
E	4	ALA	-	expression tag	UNP P63043

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	352	Total	C	N	O	S	0	0	0
			2877	1843	495	525	14			

There are 6 discrepancies between the modelled and reference sequences:

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

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



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

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

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

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

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

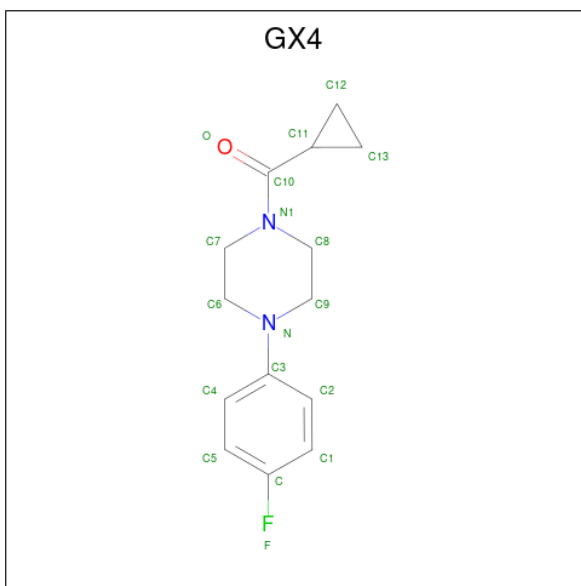
- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).





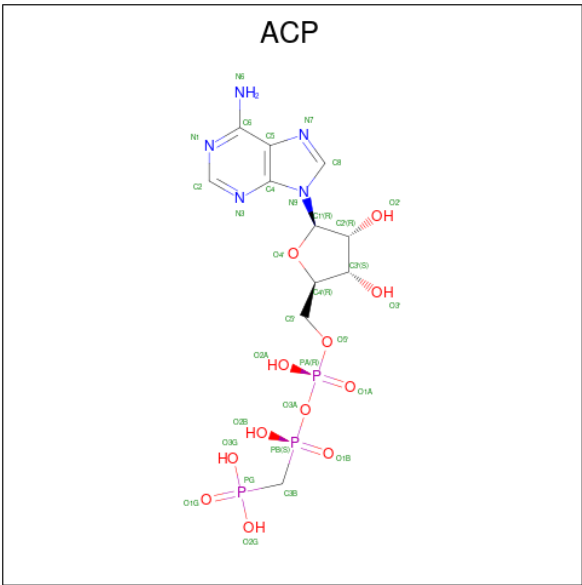
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is cyclopropyl-[4-(4-fluorophenyl)piperazin-1-yl]methanone (three-letter code: GX4) (formula: $C_{14}H_{17}FN_2O$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	F	H	N	O	0
			35	14	1	17	2	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	N	O	P	0	0
			31	11	5	12	3		

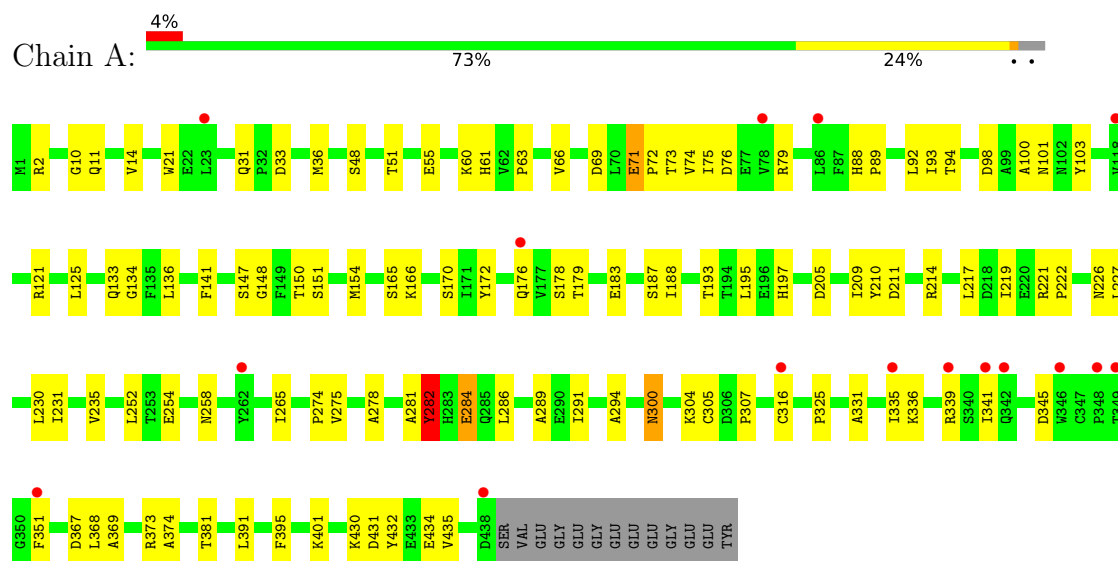
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	58	Total	O	0	0
			58	58		
12	B	62	Total	O	0	0
			62	62		
12	C	156	Total	O	0	0
			156	156		
12	D	19	Total	O	0	0
			19	19		
12	E	9	Total	O	0	0
			9	9		
12	F	8	Total	O	0	0
			8	8		

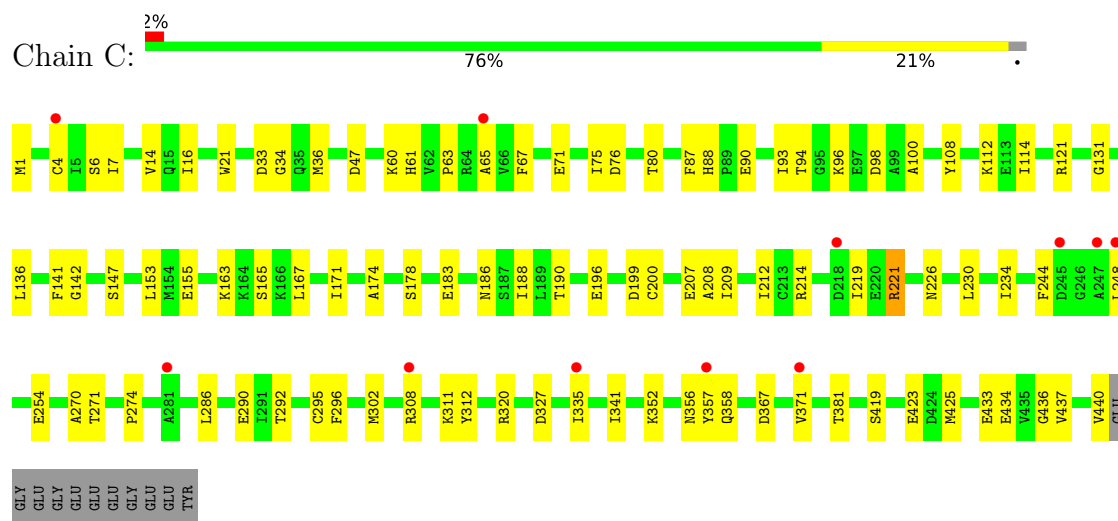
3 Residue-property plots [i](#)

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

- Molecule 1: Tubulin alpha-1B chain

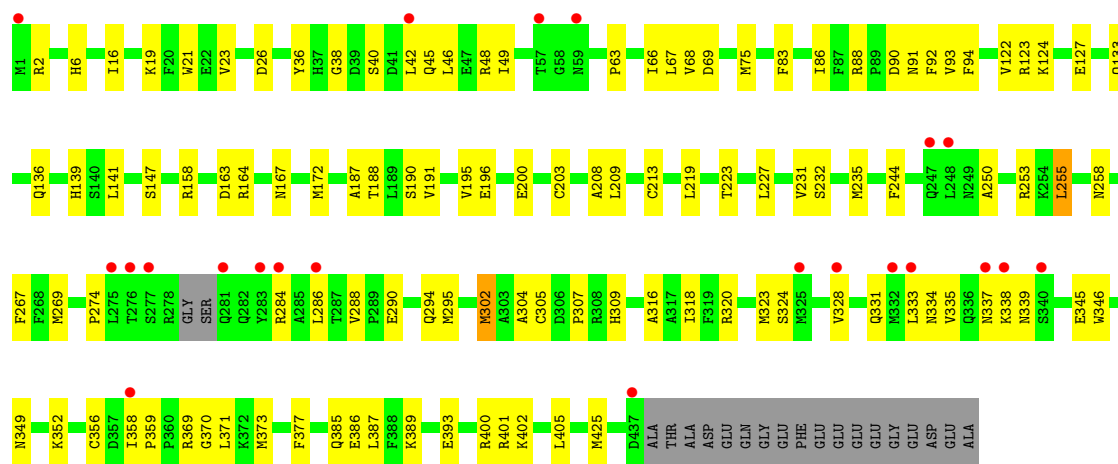


- Molecule 1: Tubulin alpha-1B chain

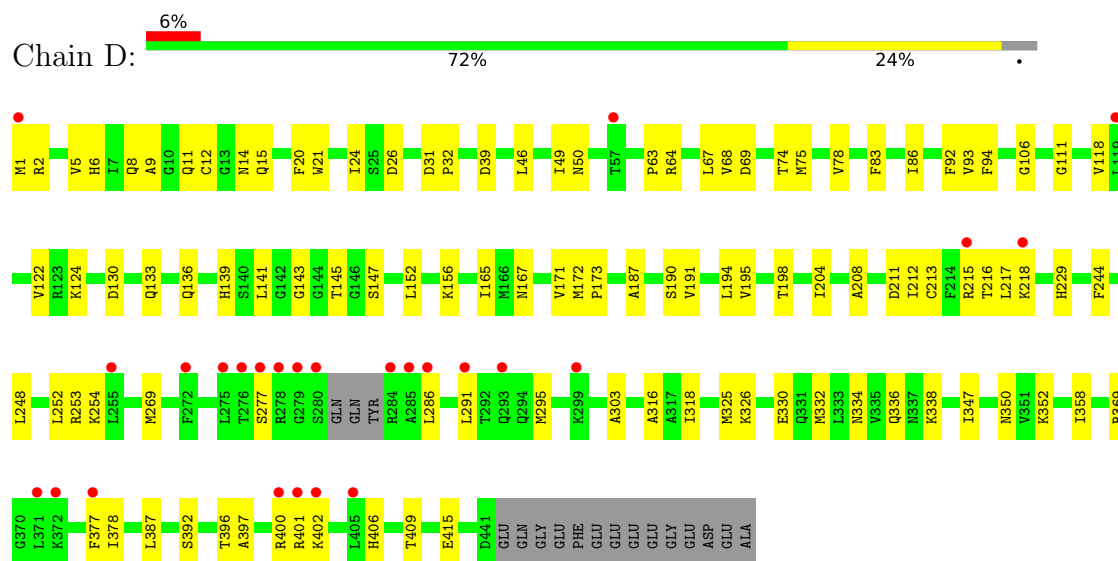


- Molecule 2: Tubulin beta-2B chain

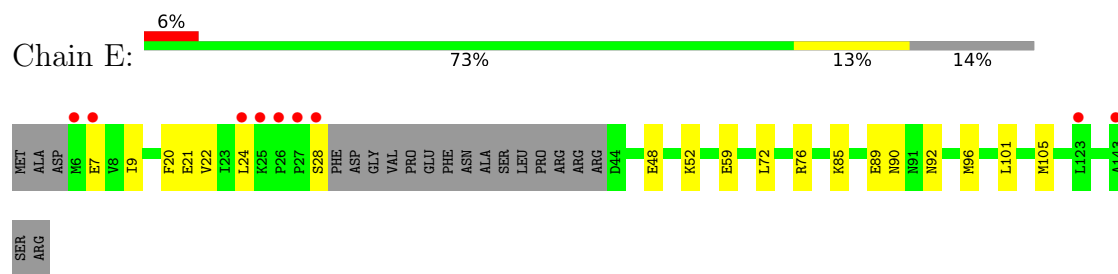




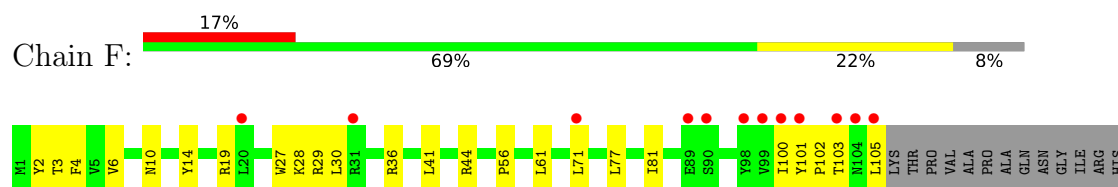
• Molecule 2: Tubulin beta-2B chain

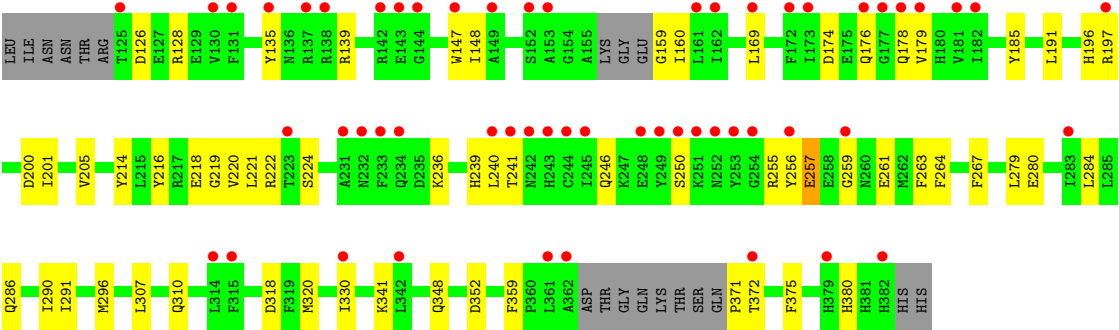


• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-Tyrosine Ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.88Å 158.88Å 178.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	62.56 – 2.39 90.48 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.8 (62.56-2.39) 99.8 (90.48-2.39)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.21 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.211 , 0.252 0.211 , 0.250	Depositor DCC
R_{free} test set	5848 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å ²)	62.0	Xtriage
Anisotropy	0.392	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 51.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17989	wwPDB-VP
Average B, all atoms (Å ²)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.49% 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: MG, MES, ACP, GTP, GX4, CA, GDP

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.25	0/3502	0.42	0/4754
1	C	0.26	0/3521	0.42	0/4780
2	B	0.25	0/3433	0.42	0/4647
2	D	0.25	0/3426	0.41	0/4640
3	E	0.24	0/1022	0.34	0/1356
4	F	0.24	0/2944	0.39	0/3978
All	All	0.25	0/17848	0.41	0/24155

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3424	0	3334	79	0
1	C	3443	0	3352	73	0
2	B	3359	0	3235	88	0
2	D	3353	0	3229	76	0
3	E	1014	0	1029	16	0
4	F	2877	0	2839	68	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	1	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	4	0
9	B	12	0	12	5	0
10	B	18	17	0	1	0
11	F	31	0	14	4	0
12	A	58	0	0	1	1
12	B	62	0	0	0	0
12	C	156	0	0	5	1
12	D	19	0	0	1	0
12	E	9	0	0	1	0
12	F	8	0	0	0	0
All	All	17972	17	17092	385	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 11.

All (385) 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:221:ARG:HG3	2:D:325:MET:HG2	1.46	0.97
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.47	0.93
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.57	0.87
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.55	0.86
4:F:241:THR:HG1	11:F:401:ACP:HO3'	1.16	0.86
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.59	0.84
1:C:209:ILE:HD11	1:C:302:MET:HE3	1.59	0.84
2:D:217:LEU:HA	2:D:277:SER:HB3	1.59	0.81
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.63	0.81
2:B:284:ARG:NH2	2:B:290:GLU:OE2	2.14	0.80
2:B:2:ARG:HB2	2:B:133:GLN:HG3	1.66	0.77
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.00	0.77
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:337:ASN:OD1	4:F:36:ARG:HD3	1.86	0.75
2:B:147:SER:HG	2:B:190:SER:HG	1.34	0.75
2:B:253[A]:ARG:NH1	9:B:504:MES:O3S	2.19	0.75
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.17	0.73
1:C:270:ALA:O	1:C:302:MET:HG2	1.87	0.73
2:B:2:ARG:HB2	2:B:133:GLN:CG	2.20	0.72
2:B:333:LEU:O	2:B:337:ASN:ND2	2.23	0.72
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.72	0.71
2:D:136:GLN:HA	2:D:167:ASN:O	1.90	0.71
2:B:209:LEU:CD2	2:B:302:MET:HG2	2.21	0.70
2:D:1:MET:HG3	2:D:50:ASN:HD22	1.55	0.70
1:C:434:GLU:OE1	12:C:601:HOH:O	2.09	0.70
4:F:318:ASP:OD2	11:F:401:ACP:O2G	2.10	0.70
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.57	0.69
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.75	0.69
1:C:47:ASP:OD2	12:C:602:HOH:O	2.09	0.69
2:B:83:PHE:O	2:B:86:ILE:HG22	1.94	0.68
1:C:76:ASP:O	1:C:80:THR:HG22	1.94	0.67
4:F:371:PRO:HA	4:F:372:THR:O	1.94	0.67
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.25	0.67
2:D:83:PHE:O	2:D:86:ILE:HG22	1.95	0.67
4:F:102:PRO:HG2	4:F:105:LEU:CD1	2.25	0.66
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.36	0.66
1:A:166:LYS:HE2	1:A:197:HIS:O	1.96	0.65
1:C:327:ASP:OD2	12:C:603:HOH:O	2.14	0.65
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.79	0.65
2:D:145:THR:HB	8:D:501:GDP:O2B	1.96	0.64
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.80	0.64
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.79	0.64
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.30	0.64
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.33	0.63
2:B:69:ASP:O	2:B:94:PHE:HA	1.98	0.63
1:C:271:THR:HG21	1:C:295:CYS:O	1.97	0.63
4:F:200:ASP:OD1	4:F:222:ARG:HB2	1.98	0.63
2:B:187:ALA:O	2:B:191:VAL:HG23	1.99	0.63
4:F:320:MET:HG3	4:F:330:ILE:HD11	1.81	0.62
1:A:351:PHE:HE1	3:E:24:LEU:HD11	1.63	0.62
4:F:246:GLN:O	4:F:250:SER:HB3	1.99	0.62
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.81	0.62
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.34	0.62
1:C:214:ARG:HG2	1:C:219:ILE:O	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.35	0.62
2:B:88:ARG:HH11	2:B:90:ASP:HB2	1.65	0.62
1:C:286:LEU:HA	1:C:290:GLU:OE1	2.00	0.61
2:D:1:MET:HG3	2:D:50:ASN:HB2	1.80	0.61
2:B:253[A]:ARG:NH1	9:B:504:MES:S	2.71	0.61
4:F:148:ILE:HD11	4:F:160:ILE:HG21	1.82	0.61
2:B:136:GLN:HA	2:B:167:ASN:O	2.01	0.61
1:C:209:ILE:HD11	1:C:302:MET:CE	2.30	0.60
2:B:253[A]:ARG:NH1	9:B:504:MES:O1S	2.30	0.60
1:C:163:LYS:HG3	3:E:90:ASN:OD1	2.00	0.60
2:B:209:LEU:HD23	2:B:302:MET:HG2	1.84	0.59
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.38	0.59
2:D:397:ALA:O	2:D:401:ARG:NH1	2.35	0.59
4:F:201:ILE:HG12	4:F:221:LEU:HG	1.84	0.59
2:B:209:LEU:HD21	2:B:302:MET:HG2	1.83	0.59
2:B:123:ARG:O	2:B:127:GLU:HG3	2.03	0.59
1:C:165:SER:HA	1:C:199:ASP:OD2	2.02	0.59
1:A:431:ASP:O	1:A:435:VAL:HG23	2.02	0.59
1:C:320:ARG:HA	1:C:356:ASN:O	2.01	0.59
1:A:214:ARG:HG2	1:A:219:ILE:O	2.02	0.59
8:D:501:GDP:O1A	12:D:601:HOH:O	2.17	0.58
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.35	0.58
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.68	0.58
2:B:370:GLY:O	2:B:371:LEU:HD23	2.03	0.58
1:C:186:ASN:O	1:C:190:THR:HG22	2.03	0.58
4:F:371:PRO:CA	4:F:372:THR:HB	2.33	0.58
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.86	0.58
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.39	0.58
2:B:244:PHE:CD1	2:B:358:ILE:HD12	2.39	0.57
4:F:286:GLN:O	4:F:290:ILE:HG13	2.05	0.57
2:D:1:MET:CE	2:D:50:ASN:HB2	2.33	0.57
4:F:236:LYS:HB3	4:F:240:LEU:CD1	2.31	0.57
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.05	0.57
2:B:316:ALA:HB1	10:B:505:GX4:C4	2.35	0.56
2:D:1:MET:HG3	2:D:50:ASN:CB	2.35	0.56
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.32	0.56
2:D:332:MET:O	2:D:336:GLN:HG3	2.06	0.56
4:F:159:GLY:C	4:F:160:ILE:HD12	2.26	0.56
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.88	0.56
1:C:308:ARG:HD2	12:C:707:HOH:O	2.06	0.56
2:D:152:LEU:O	2:D:156:LYS:HG2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:LYS:HB3	2:B:405:LEU:HD12	1.88	0.55
3:E:72:LEU:O	3:E:76:ARG:HG2	2.06	0.55
4:F:371:PRO:HA	4:F:372:THR:C	2.25	0.55
1:A:141:PHE:HB3	1:A:187:SER:OG	2.07	0.55
2:D:69:ASP:O	2:D:94:PHE:HA	2.06	0.55
1:A:176:GLN:CG	4:F:56:PRO:HB3	2.36	0.55
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.88	0.55
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.40	0.55
1:C:93:ILE:CD1	1:C:121:ARG:HG3	2.32	0.55
1:A:187:SER:CB	1:A:391:LEU:HD21	2.37	0.55
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.42	0.55
2:B:42:LEU:H	2:B:42:LEU:HD12	1.72	0.55
2:D:2:ARG:HB2	2:D:133:GLN:HE21	1.72	0.55
1:C:178:SER:OG	2:D:352:LYS:NZ	2.39	0.54
1:A:176:GLN:HG3	4:F:56:PRO:HB3	1.89	0.54
4:F:371:PRO:HA	4:F:372:THR:HB	1.88	0.54
4:F:10:ASN:CB	4:F:44:ARG:HH22	2.17	0.54
1:C:108:TYR:O	1:C:112:LYS:HG2	2.07	0.54
2:B:19:LYS:O	2:B:23:VAL:HG23	2.08	0.54
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.09	0.53
1:A:101:ASN:HD22	2:B:258:ASN:HD21	1.56	0.53
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.23	0.53
1:C:433:GLU:O	1:C:437:VAL:HG23	2.08	0.53
2:D:141:LEU:HD12	2:D:172:MET:SD	2.48	0.53
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.44	0.53
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.23	0.53
2:B:26:ASP:OD1	2:B:369:ARG:NH2	2.41	0.53
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.89	0.53
1:A:2:ARG:HB2	1:A:133:GLN:HE21	1.72	0.53
2:B:158:ARG:NH1	2:B:196:GLU:O	2.41	0.53
3:E:85:LYS:NZ	12:E:201:HOH:O	2.38	0.53
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.90	0.53
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.91	0.53
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.90	0.52
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.44	0.52
4:F:2:TYR:CE1	4:F:359:PHE:HB3	2.44	0.52
2:B:269:MET:HE1	2:B:307:PRO:HG3	1.91	0.52
1:A:66:VAL:HG23	1:A:125:LEU:HD12	1.92	0.52
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.73	0.52
3:E:85:LYS:O	3:E:89:GLU:HG3	2.10	0.52
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.44	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.44	0.52
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.90	0.52
2:B:389:LYS:O	2:B:393:GLU:HG3	2.09	0.52
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.45	0.52
2:D:208:ALA:O	2:D:212:ILE:HG13	2.10	0.52
2:D:11:GLN:HG3	2:D:74:THR:OG1	2.10	0.52
2:B:141:LEU:HD12	2:B:172:MET:SD	2.50	0.51
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.91	0.51
1:A:136:LEU:HD21	1:A:252:LEU:HD21	1.91	0.51
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.46	0.51
2:D:2:ARG:CB	2:D:133:GLN:HE21	2.23	0.51
1:C:234:ILE:HG12	1:C:302:MET:HE2	1.92	0.51
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.46	0.51
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.28	0.51
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.93	0.51
1:C:34:GLY:HA3	1:C:60:LYS:HG3	1.93	0.51
2:B:124:LYS:HD3	2:B:124:LYS:C	2.31	0.51
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.44	0.51
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.46	0.51
1:C:1:MET:HE3	1:C:131:GLY:HA3	1.93	0.51
2:B:318:ILE:N	2:B:318:ILE:HD12	2.26	0.50
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.93	0.50
2:D:46:LEU:HA	2:D:49:ILE:HB	1.94	0.50
2:D:171:VAL:HA	2:D:204:ILE:O	2.12	0.50
2:D:326:LYS:O	2:D:330:GLU:HG3	2.12	0.50
4:F:71:LEU:HD12	4:F:77:LEU:HD13	1.93	0.50
1:A:231:ILE:O	1:A:235:VAL:HG23	2.12	0.50
4:F:101:TYR:CD2	4:F:179:VAL:HG22	2.47	0.50
4:F:19:ARG:HD2	4:F:19:ARG:O	2.12	0.50
4:F:320:MET:CG	4:F:330:ILE:HD11	2.42	0.50
2:D:8:GLN:NE2	2:D:14:ASN:HA	2.27	0.50
2:D:124:LYS:C	2:D:124:LYS:HD3	2.32	0.50
2:B:323:MET:HB3	2:B:373:MET:HE2	1.94	0.50
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.47	0.50
2:D:74:THR:O	2:D:78:VAL:HG23	2.11	0.49
2:B:250:ALA:HB3	2:B:255:LEU:HD13	1.94	0.49
4:F:4:PHE:CZ	4:F:29:ARG:HB2	2.47	0.49
1:C:14:VAL:HG13	1:C:67:PHE:CD2	2.48	0.49
1:C:208:ALA:O	1:C:212:ILE:HG13	2.13	0.49
2:D:118:VAL:O	2:D:122:VAL:HG23	2.12	0.49
4:F:185:TYR:OH	4:F:239:HIS:HB3	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:67:LEU:N	2:D:67:LEU:HD12	2.27	0.49
1:A:141:PHE:O	1:A:147:SER:HB3	2.13	0.49
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.28	0.49
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.95	0.49
1:C:419:SER:O	1:C:423:GLU:HG3	2.12	0.49
1:C:142:GLY:HA3	1:C:183:GLU:OE1	2.13	0.48
2:D:318:ILE:N	2:D:318:ILE:HD12	2.28	0.48
2:B:385:GLN:OE1	2:B:389:LYS:HE3	2.14	0.48
4:F:61:LEU:HD12	4:F:310:GLN:O	2.14	0.48
2:B:305:CYS:O	2:B:307:PRO:HD3	2.12	0.48
2:D:316:ALA:HB3	2:D:378:ILE:HB	1.96	0.48
2:D:392:SER:O	2:D:396:THR:HG22	2.13	0.48
1:A:284:GLU:CD	1:A:284:GLU:H	2.15	0.48
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.95	0.48
2:B:40:SER:OG	2:B:42:LEU:HD13	2.14	0.48
2:D:1:MET:HE2	2:D:50:ASN:HB2	1.93	0.48
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.94	0.48
1:C:75:ILE:HD12	1:C:94:THR:HG22	1.96	0.48
3:E:48:GLU:HG2	3:E:52:LYS:HE3	1.95	0.48
1:A:275:VAL:HG13	1:A:368:LEU:CD2	2.44	0.48
2:B:359:PRO:HB2	2:B:371:LEU:O	2.13	0.48
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.29	0.48
1:A:335:ILE:HG23	1:A:339:ARG:CG	2.37	0.47
2:D:286:LEU:HD21	2:D:291:LEU:HD13	1.96	0.47
1:C:33:ASP:O	1:C:60:LYS:HE2	2.14	0.47
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.96	0.47
1:A:294:ALA:O	1:A:300:ASN:ND2	2.46	0.47
2:B:274:PRO:HB3	2:B:286:LEU:CD2	2.42	0.47
2:B:191:VAL:O	2:B:195:VAL:HG23	2.14	0.47
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.50	0.47
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.15	0.47
3:E:7:GLU:O	3:E:22:VAL:HA	2.14	0.47
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.44	0.47
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.49	0.47
2:B:213:CYS:HB3	2:B:219:LEU:HD12	1.95	0.47
2:B:323:MET:HB3	2:B:373:MET:CE	2.44	0.47
2:B:402:LYS:CB	2:B:405:LEU:HD12	2.45	0.47
1:C:226:ASN:ND2	1:C:367:ASP:OD2	2.47	0.47
1:C:311:LYS:HD2	1:C:436:GLY:O	2.15	0.47
2:D:402:LYS:HE2	2:D:415:GLU:OE1	2.14	0.47
2:B:334:ASN:OD1	2:B:338:LYS:HD3	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.49	0.47
2:B:345:GLU:OE1	2:B:345:GLU:N	2.38	0.47
4:F:191:LEU:HD12	4:F:196:HIS:CE1	2.49	0.47
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.50	0.46
2:D:1:MET:HG3	2:D:50:ASN:ND2	2.27	0.46
4:F:241:THR:OG1	11:F:401:ACP:O3'	2.02	0.46
4:F:259:GLY:O	4:F:261:GLU:HG3	2.15	0.46
1:A:336:LYS:HD2	1:A:341:ILE:HD12	1.97	0.46
3:E:48:GLU:CG	3:E:52:LYS:HE3	2.45	0.46
4:F:197:ARG:HB2	4:F:224:SER:O	2.15	0.46
2:D:215:ARG:O	2:D:218:LYS:HE3	2.16	0.46
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.97	0.46
2:B:320:ARG:HA	2:B:356:CYS:O	2.15	0.46
1:A:103:TYR:CE2	1:A:148:GLY:HA2	2.51	0.46
2:B:335:VAL:O	2:B:339:ASN:ND2	2.48	0.46
2:B:324:SER:O	2:B:328:VAL:HG23	2.16	0.46
1:A:188:ILE:HD12	1:A:395:PHE:HB2	1.98	0.46
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.50	0.46
1:C:6:SER:O	1:C:65:ALA:HA	2.15	0.46
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.97	0.45
2:D:75:MET:HE3	2:D:92:PHE:CD2	2.52	0.45
1:A:289:ALA:HA	1:A:331:ALA:CB	2.46	0.45
2:D:67:LEU:HD22	2:D:92:PHE:CE2	2.51	0.45
2:D:406:HIS:HA	2:D:409:THR:OG1	2.17	0.45
2:D:248:LEU:HD11	2:D:352:LYS:HB3	1.99	0.45
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.52	0.45
1:C:174:ALA:O	1:C:178:SER:HB3	2.17	0.45
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.57	0.45
1:C:271:THR:HG21	1:C:295:CYS:HA	1.99	0.45
1:C:75:ILE:HB	1:C:94:THR:HG21	1.99	0.45
1:C:254:GLU:HG2	1:C:352:LYS:CE	2.45	0.45
4:F:280:GLU:OE1	4:F:284:LEU:HD23	2.16	0.45
1:C:271:THR:CG2	1:C:295:CYS:HA	2.47	0.45
2:B:250:ALA:CB	2:B:255:LEU:HD13	2.47	0.45
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.47	0.45
4:F:176:GLN:HB3	4:F:178:GLN:NE2	2.32	0.45
2:B:231:VAL:O	2:B:235:MET:HG3	2.17	0.45
4:F:160:ILE:HD12	4:F:160:ILE:N	2.32	0.45
1:A:66:VAL:HG23	1:A:125:LEU:CD1	2.47	0.44
1:A:69:ASP:O	1:A:94:THR:HA	2.17	0.44
4:F:296:MET:SD	4:F:380:HIS:HB2	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:LEU:N	2:B:67:LEU:HD12	2.32	0.44
4:F:341:LYS:HG2	4:F:341:LYS:O	2.17	0.44
1:C:274:PRO:HG2	1:C:371:VAL:HG11	1.99	0.44
2:D:191:VAL:O	2:D:195:VAL:HG23	2.18	0.44
4:F:101:TYR:N	4:F:126:ASP:OD1	2.40	0.44
1:A:31:GLN:HB2	1:A:33:ASP:OD1	2.18	0.44
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.35	0.44
2:B:288:VAL:HG12	2:B:331:GLN:HG3	2.00	0.44
2:B:349:ASN:O	2:B:352:LYS:HE2	2.17	0.44
2:D:20:PHE:CZ	2:D:24:ILE:HD13	2.52	0.44
1:A:188:ILE:HD12	1:A:395:PHE:CD2	2.53	0.44
2:B:66:ILE:HD12	2:B:122:VAL:HG22	2.00	0.44
1:C:234:ILE:HD12	1:C:234:ILE:H	1.83	0.44
1:A:11:GLN:HG3	1:A:74:VAL:HG21	2.00	0.44
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.99	0.44
2:B:38:GLY:HA3	2:B:45:GLN:OE1	2.17	0.44
2:B:68:VAL:HA	2:B:93:VAL:O	2.18	0.44
1:A:10:GLY:O	1:A:14:VAL:HG23	2.18	0.44
1:A:345:ASP:HB3	3:E:28:SER:HB2	1.98	0.44
2:B:295:MET:HG3	2:B:377:PHE:HB2	1.99	0.44
1:A:75:ILE:HB	1:A:94:THR:CG2	2.48	0.43
2:B:42:LEU:HD12	2:B:42:LEU:N	2.33	0.43
1:C:96:LYS:NZ	2:D:130:ASP:OD1	2.49	0.43
2:D:147:SER:HB2	2:D:190:SER:OG	2.17	0.43
4:F:240:LEU:HD12	4:F:240:LEU:N	2.33	0.43
2:D:8:GLN:HE21	2:D:14:ASN:HA	1.83	0.43
1:A:100:ALA:CB	2:B:253[B]:ARG:HG2	2.49	0.43
2:D:106:GLY:O	2:D:111:GLY:HA3	2.19	0.43
1:C:75:ILE:HB	1:C:94:THR:CG2	2.48	0.43
2:B:167:ASN:OD1	2:B:200:GLU:HB2	2.19	0.43
2:B:250:ALA:HB3	2:B:255:LEU:CD1	2.48	0.43
1:C:230:LEU:O	1:C:234:ILE:HD12	2.18	0.43
1:C:296:PHE:CD1	1:C:335:ILE:HD13	2.54	0.43
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.00	0.43
2:D:211:ASP:O	2:D:215:ARG:HB2	2.19	0.43
3:E:101:LEU:O	3:E:105:MET:HG2	2.19	0.43
4:F:3:THR:HA	4:F:28:LYS:O	2.18	0.43
1:A:79:ARG:HG2	1:A:92:LEU:HD12	2.00	0.43
2:D:5:VAL:HG22	2:D:64:ARG:HD3	2.01	0.43
2:B:295:MET:CG	2:B:377:PHE:HB2	2.49	0.43
4:F:267:PHE:CE2	4:F:279:LEU:HD13	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:THR:O	1:A:154:MET:HG2	2.19	0.42
2:B:46:LEU:HA	2:B:49:ILE:HB	1.99	0.42
2:B:163:ASP:O	2:B:253[A]:ARG:NH2	2.49	0.42
9:B:504:MES:H51	9:B:504:MES:H81	1.56	0.42
2:D:9:ALA:HA	2:D:68:VAL:O	2.18	0.42
1:A:274:PRO:HD2	1:A:374:ALA:HB2	2.01	0.42
1:C:141:PHE:O	1:C:147:SER:HB3	2.20	0.42
1:C:292:THR:HG22	1:C:335:ILE:HD12	2.01	0.42
3:E:9:ILE:HG13	3:E:21:GLU:HB3	2.01	0.42
1:C:16:ILE:CD1	1:C:171:ILE:HD11	2.50	0.42
1:C:196:GLU:HG2	12:C:662:HOH:O	2.19	0.42
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.49	0.42
2:D:173:PRO:HG3	2:D:187:ALA:HB2	2.02	0.42
1:A:151:SER:HB2	1:A:193:THR:OG1	2.20	0.42
1:A:179:THR:HA	2:B:352:LYS:HD2	2.01	0.42
1:A:291:ILE:HD13	1:A:373:ARG:HG3	2.01	0.42
1:A:305:CYS:O	1:A:307:PRO:HD3	2.19	0.42
2:B:188:THR:HA	2:B:425:MET:CE	2.49	0.42
4:F:6:VAL:HG22	4:F:41:LEU:HD12	2.01	0.42
4:F:19:ARG:HD2	4:F:19:ARG:C	2.40	0.42
1:C:312:TYR:CE1	1:C:341:ILE:HG23	2.55	0.42
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.49	0.42
2:B:164:ARG:O	9:B:504:MES:H31	2.19	0.42
1:C:98:ASP:HB2	5:C:501:GTP:O2G	2.19	0.42
2:D:75:MET:HE3	2:D:92:PHE:HD2	1.84	0.42
1:A:325:PRO:HB3	3:E:20:PHE:CE1	2.55	0.42
2:B:290:GLU:O	2:B:294:GLN:HG3	2.20	0.42
2:B:188:THR:HA	2:B:425:MET:HE2	2.02	0.41
2:B:223:THR:O	2:B:227:LEU:HD13	2.20	0.41
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.01	0.41
4:F:135:TYR:OH	4:F:139:ARG:NH2	2.53	0.41
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.55	0.41
2:B:309:HIS:ND1	2:B:386:GLU:OE2	2.53	0.41
4:F:103:THR:HG23	4:F:128:ARG:NH2	2.36	0.41
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.55	0.41
1:A:55:GLU:HA	1:A:60:LYS:O	2.20	0.41
2:B:163:ASP:O	2:B:253[B]:ARG:NH1	2.53	0.41
2:D:68:VAL:HA	2:D:93:VAL:O	2.21	0.41
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.49	0.41
4:F:255:ARG:HD3	4:F:256:TYR:CZ	2.55	0.41
1:A:281:ALA:O	1:A:282:TYR:HD2	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:100:ALA:HB2	2:D:253:ARG:HD2	2.01	0.41
1:C:174:ALA:HB1	1:C:207:GLU:HB2	2.02	0.41
1:C:270:ALA:C	1:C:302:MET:HG2	2.41	0.41
2:D:172:MET:HG3	2:D:387:LEU:HD11	2.02	0.41
4:F:205:VAL:HG21	4:F:291:ILE:HG21	2.02	0.41
11:F:401:ACP:O3G	11:F:401:ACP:O1B	2.37	0.41
1:C:93:ILE:HG22	1:C:114:ILE:HD11	2.02	0.41
4:F:100:ILE:HD12	4:F:128:ARG:HA	2.03	0.41
1:A:74:VAL:HB	12:A:610:HOH:O	2.20	0.41
1:A:289:ALA:HA	1:A:331:ALA:HB1	2.02	0.41
1:C:100:ALA:HA	2:D:254:LYS:HG3	2.02	0.41
2:D:212:ILE:O	2:D:216:THR:HB	2.20	0.41
4:F:2:TYR:HB2	4:F:27:TRP:CD2	2.55	0.41
4:F:3:THR:HB	4:F:30:LEU:HD11	2.03	0.41
4:F:77:LEU:O	4:F:81:ILE:HG13	2.21	0.41
2:B:88:ARG:HD3	2:B:91:ASN:OD1	2.21	0.41
1:C:440:VAL:HG12	1:C:440:VAL:O	2.21	0.41
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.21	0.41
2:D:248:LEU:HD21	2:D:352:LYS:HB3	2.03	0.41
4:F:100:ILE:CD1	4:F:128:ARG:HA	2.51	0.41
4:F:371:PRO:N	4:F:372:THR:HB	2.35	0.41
1:A:2:ARG:HB2	1:A:133:GLN:NE2	2.35	0.41
1:A:48:SER:O	1:A:51:THR:HG23	2.21	0.41
1:A:71:GLU:HG2	1:A:72:PRO:N	2.35	0.41
1:A:134:GLY:HA3	1:A:165:SER:O	2.21	0.41
1:C:209:ILE:HG23	1:C:230:LEU:HD23	2.03	0.41
2:D:11:GLN:O	2:D:15:GLN:HG2	2.20	0.41
1:A:103:TYR:CD2	1:A:148:GLY:HA2	2.56	0.41
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.86	0.41
2:B:400:ARG:HG3	2:B:401:ARG:HG2	2.03	0.41
3:E:59:GLU:OE1	3:E:59:GLU:HA	2.21	0.41
1:A:93:ILE:HD11	1:A:121:ARG:HG3	2.03	0.40
1:C:155:GLU:HB3	3:E:101:LEU:HD22	2.03	0.40
1:A:195:LEU:HD12	1:A:195:LEU:HA	1.94	0.40
2:D:26:ASP:OD2	2:D:369:ARG:HD2	2.21	0.40
4:F:307:LEU:HD12	4:F:307:LEU:HA	1.94	0.40
1:A:178:SER:OG	1:A:183:GLU:OE1	2.31	0.40
4:F:220:VAL:HG12	4:F:263:PHE:CE1	2.55	0.40
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.03	0.40
1:A:430:LYS:HE2	1:A:434:GLU:OE2	2.21	0.40
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:92:ASN:O	3:E:96:MET:HG2	2.21	0.40
1:A:286:LEU:O	1:A:373:ARG:NH1	2.49	0.40
2:D:194:LEU:HD22	2:D:198:THR:HG21	2.03	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:A:648:HOH:O	12:C:707:HOH:O[3_555]	1.94	0.26

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	436/451 (97%)	425 (98%)	10 (2%)	1 (0%)	47	62
1	C	439/451 (97%)	430 (98%)	9 (2%)	0	100	100
2	B	422/445 (95%)	407 (96%)	15 (4%)	0	100	100
2	D	424/445 (95%)	411 (97%)	13 (3%)	0	100	100
3	E	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
4	F	344/384 (90%)	332 (96%)	12 (4%)	0	100	100
All	All	2184/2319 (94%)	2123 (97%)	60 (3%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	TYR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	369/379 (97%)	362 (98%)	7 (2%)	57	75
1	C	372/379 (98%)	369 (99%)	3 (1%)	81	91
2	B	368/383 (96%)	363 (99%)	5 (1%)	67	82
2	D	368/383 (96%)	365 (99%)	3 (1%)	81	91
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	315/342 (92%)	314 (100%)	1 (0%)	92	97
All	All	1902/1993 (95%)	1883 (99%)	19 (1%)	76	88

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

Mol	Chain	Res	Type
1	A	71	GLU
1	A	221	ARG
1	A	282	TYR
1	A	284	GLU
1	A	300	ASN
1	A	316	CYS
1	A	381	THR
2	B	48	ARG
2	B	139	HIS
2	B	232	SER
2	B	255	LEU
2	B	302	MET
1	C	71	GLU
1	C	221	ARG
1	C	381	THR
2	D	39	ASP
2	D	139	HIS
2	D	229	HIS
4	F	257	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	101	ASN
1	A	300	ASN
1	A	301	GLN
2	B	282	GLN
1	C	133	GLN
1	C	300	ASN
1	C	356	ASN
1	C	372	GLN
2	D	50	ASN
2	D	133	GLN
4	F	178	GLN
4	F	269	GLN
4	F	348	GLN
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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 16 ligands modelled in this entry, 9 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	GDP	D	501	6	24,30,30	1.18	2 (8%)	31,47,47	1.96	8 (25%)
9	MES	B	504	-	12,12,12	2.21	1 (8%)	14,16,16	2.07	5 (35%)
11	ACP	F	401	6	27,33,33	1.39	5 (18%)	32,52,52	1.50	4 (12%)
5	GTP	A	501	6	26,34,34	1.00	1 (3%)	33,54,54	1.72	7 (21%)
5	GTP	C	501	6	26,34,34	0.97	1 (3%)	33,54,54	1.62	6 (18%)
10	GX4	B	505	-	20,20,20	1.15	1 (5%)	28,28,28	1.08	3 (10%)
8	GDP	B	501	6	24,30,30	1.15	2 (8%)	31,47,47	1.89	7 (22%)

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	GDP	D	501	6	-	3/12/32/32	0/3/3/3
9	MES	B	504	-	-	4/6/14/14	0/1/1/1
11	ACP	F	401	6	-	12/15/38/38	0/3/3/3
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3
5	GTP	C	501	6	-	7/18/38/38	0/3/3/3
10	GX4	B	505	-	-	4/12/24/24	0/3/3/3
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.38	1.67	1.77
8	D	501	GDP	C6-C5	4.11	1.48	1.41
8	B	501	GDP	C6-C5	3.93	1.48	1.41
5	A	501	GTP	C6-N1	3.19	1.38	1.33
5	C	501	GTP	C6-N1	3.03	1.38	1.33
10	B	505	GX4	C10-N1	3.01	1.39	1.34
11	F	401	ACP	PG-O2G	2.98	1.61	1.54
11	F	401	ACP	PG-O3G	2.98	1.61	1.54
11	F	401	ACP	PB-O3A	2.77	1.61	1.58
11	F	401	ACP	C5-C4	2.47	1.47	1.40
8	B	501	GDP	C5-C4	2.45	1.47	1.40
8	D	501	GDP	C5-C4	2.44	1.47	1.40
11	F	401	ACP	PB-O2B	2.24	1.61	1.56

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	N3-C2-N1	-5.37	120.06	127.22
5	C	501	GTP	N3-C2-N1	-5.05	120.49	127.22
8	D	501	GDP	C2-N3-C4	4.82	120.87	115.36
8	B	501	GDP	C2-N3-C4	4.73	120.76	115.36
5	A	501	GTP	C2-N3-C4	4.39	120.37	115.36
8	B	501	GDP	C6-C5-C4	-4.24	116.75	120.80
11	F	401	ACP	PA-O3A-PB	-4.21	119.20	132.56
8	D	501	GDP	C6-N1-C2	4.11	122.46	115.93
8	B	501	GDP	C6-N1-C2	4.10	122.45	115.93
8	D	501	GDP	C5-C6-N1	-4.04	117.90	123.43
9	B	504	MES	O1S-S-C8	3.92	111.63	106.92
8	D	501	GDP	C6-C5-C4	-3.79	117.18	120.80
8	B	501	GDP	C5-C6-N1	-3.78	118.26	123.43
9	B	504	MES	C5-N4-C3	3.76	117.30	108.83
5	C	501	GTP	C2-N3-C4	3.76	119.65	115.36
11	F	401	ACP	C3'-C2'-C1'	3.52	106.27	100.98
8	D	501	GDP	PA-O3A-PB	-3.41	121.13	132.83
8	B	501	GDP	N3-C2-N1	-3.40	122.69	127.22
8	D	501	GDP	N3-C2-N1	-3.30	122.82	127.22
11	F	401	ACP	N3-C2-N1	-3.19	123.69	128.68
5	C	501	GTP	C5-C6-N1	-3.15	119.12	123.43
5	A	501	GTP	C5-C6-N1	-2.97	119.37	123.43
9	B	504	MES	C6-C5-N4	-2.91	105.69	110.10
10	B	505	GX4	C7-C6-N	2.80	116.14	110.70
5	C	501	GTP	PA-O3A-PB	-2.78	123.29	132.83
8	D	501	GDP	C4-C5-N7	-2.76	106.53	109.40
8	B	501	GDP	PA-O3A-PB	-2.70	123.55	132.83
5	C	501	GTP	C6-N1-C2	2.65	120.15	115.93
10	B	505	GX4	C9-N-C6	2.63	117.32	111.52
5	A	501	GTP	PA-O3A-PB	-2.61	123.86	132.83
11	F	401	ACP	C4-C5-N7	-2.56	106.73	109.40
5	A	501	GTP	C6-N1-C2	2.53	119.95	115.93
8	B	501	GDP	C4-C5-N7	-2.48	106.81	109.40
9	B	504	MES	O3S-S-C8	2.39	109.64	105.77
8	D	501	GDP	C3'-C2'-C1'	2.39	104.57	100.98
10	B	505	GX4	C8-N1-C7	2.33	117.10	112.62
9	B	504	MES	C7-N4-C5	2.29	117.08	111.23
5	A	501	GTP	N2-C2-N1	2.27	120.79	117.25
5	A	501	GTP	PB-O3B-PG	-2.27	125.03	132.83
5	C	501	GTP	PB-O3B-PG	-2.02	125.91	132.83

There are no chirality outliers.

All (40) torsion outliers are listed below:

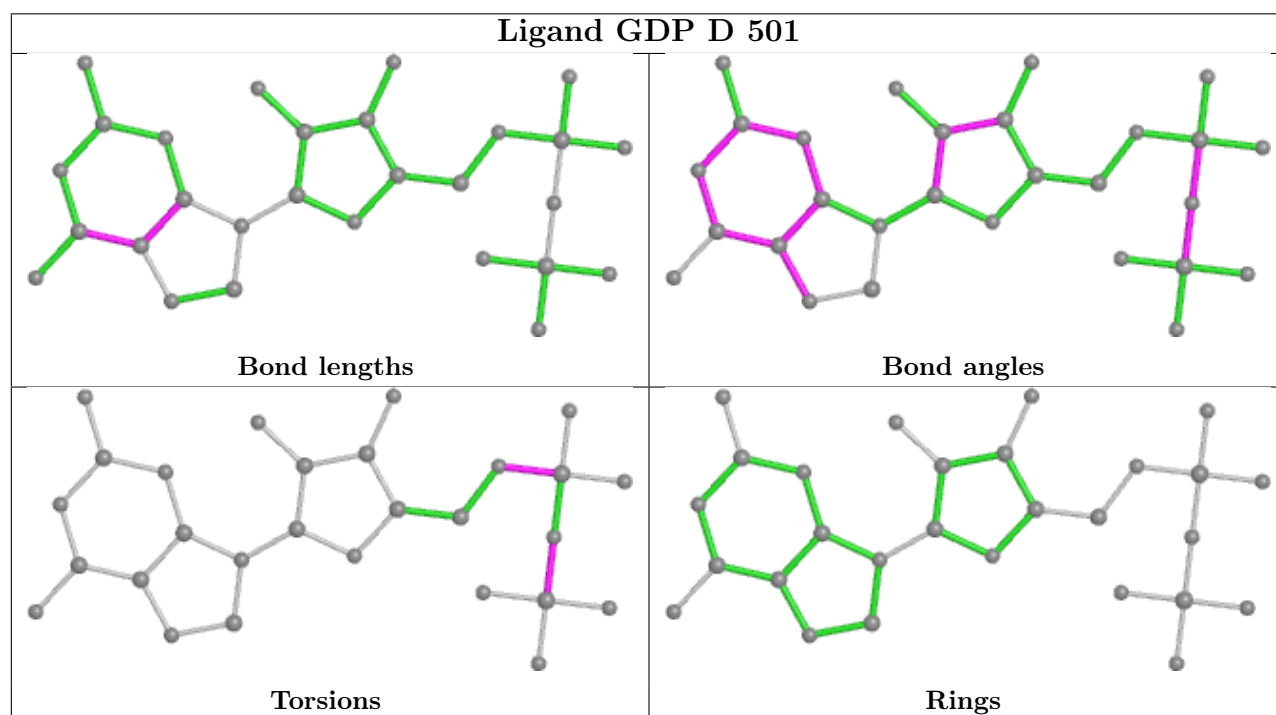
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
9	B	504	MES	C8-C7-N4-C5
9	B	504	MES	C7-C8-S-O2S
9	B	504	MES	C7-C8-S-O3S
10	B	505	GX4	N1-C10-C11-C12
10	B	505	GX4	O-C10-C11-C12
11	F	401	ACP	PB-C3B-PG-O1G
11	F	401	ACP	PB-C3B-PG-O2G
11	F	401	ACP	PB-C3B-PG-O3G
11	F	401	ACP	PG-C3B-PB-O1B
11	F	401	ACP	PG-C3B-PB-O3A
11	F	401	ACP	C5'-O5'-PA-O1A
11	F	401	ACP	C3'-C4'-C5'-O5'
11	F	401	ACP	O4'-C4'-C5'-O5'
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O2G
11	F	401	ACP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O2A
11	F	401	ACP	C5'-O5'-PA-O2A
9	B	504	MES	C7-C8-S-O1S
10	B	505	GX4	C2-C3-N-C6
11	F	401	ACP	PG-C3B-PB-O2B
10	B	505	GX4	C4-C3-N-C6
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
8	D	501	GDP	PA-O3A-PB-O2B
11	F	401	ACP	PB-O3A-PA-O2A
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A

There are no ring outliers.

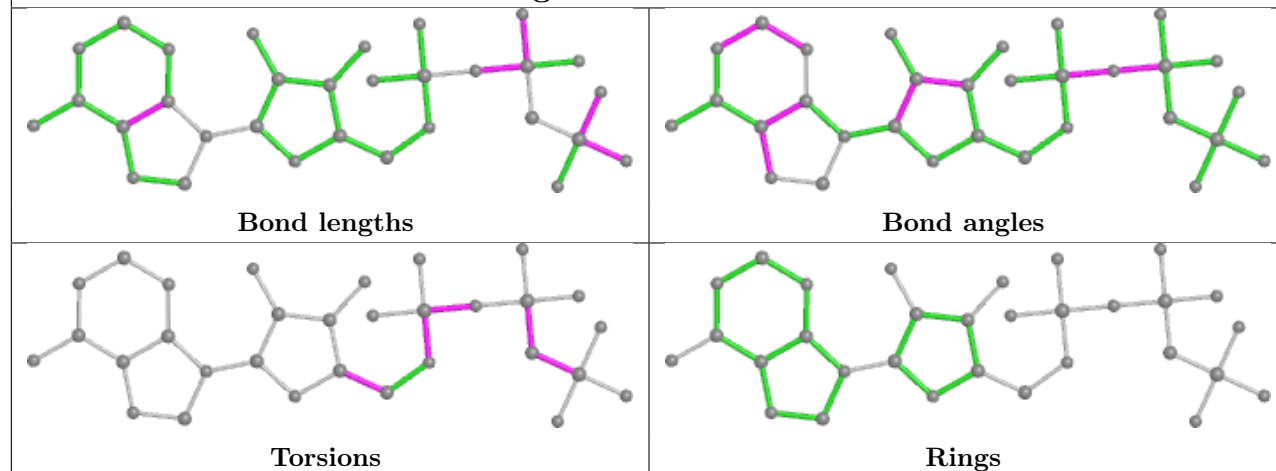
6 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	4	0
9	B	504	MES	5	0
11	F	401	ACP	4	0
5	A	501	GTP	1	0
5	C	501	GTP	1	0
10	B	505	GX4	1	0

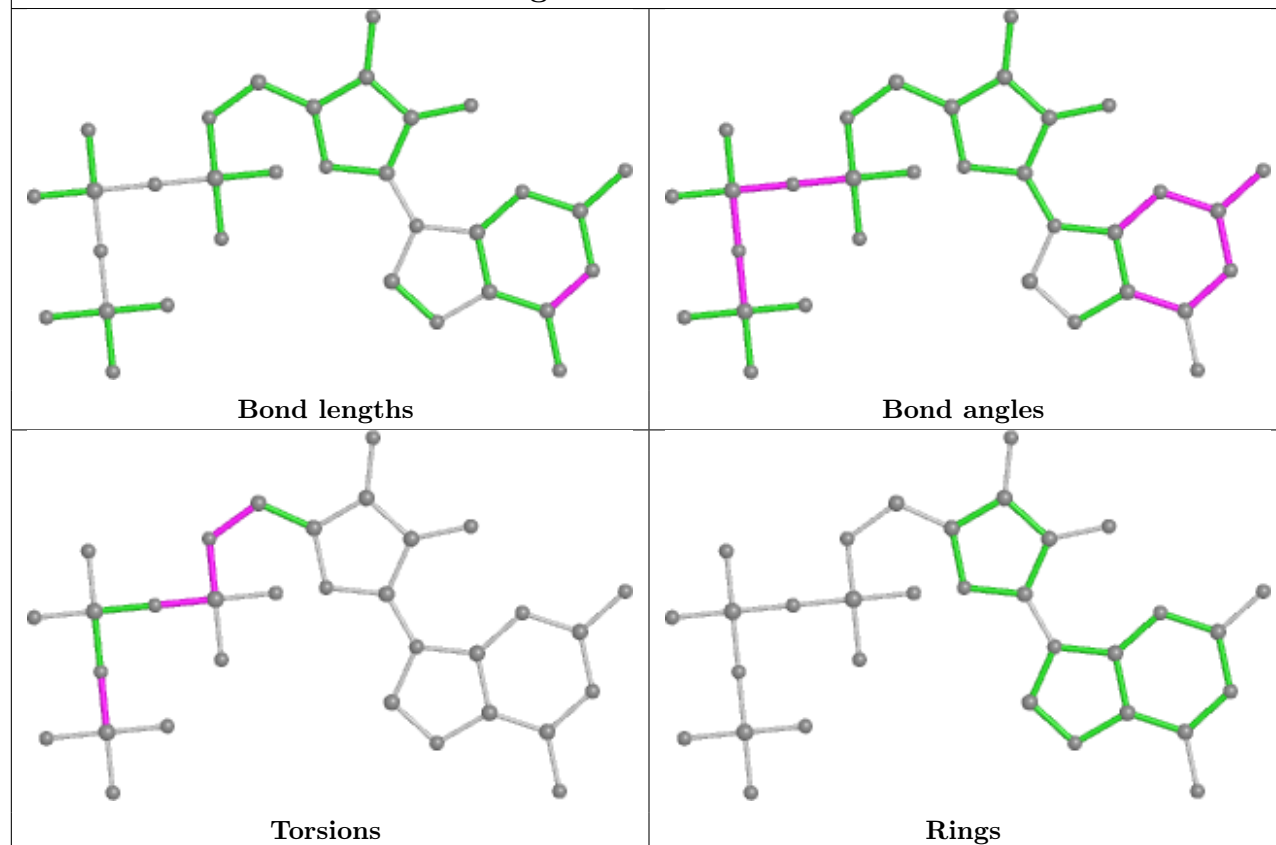
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



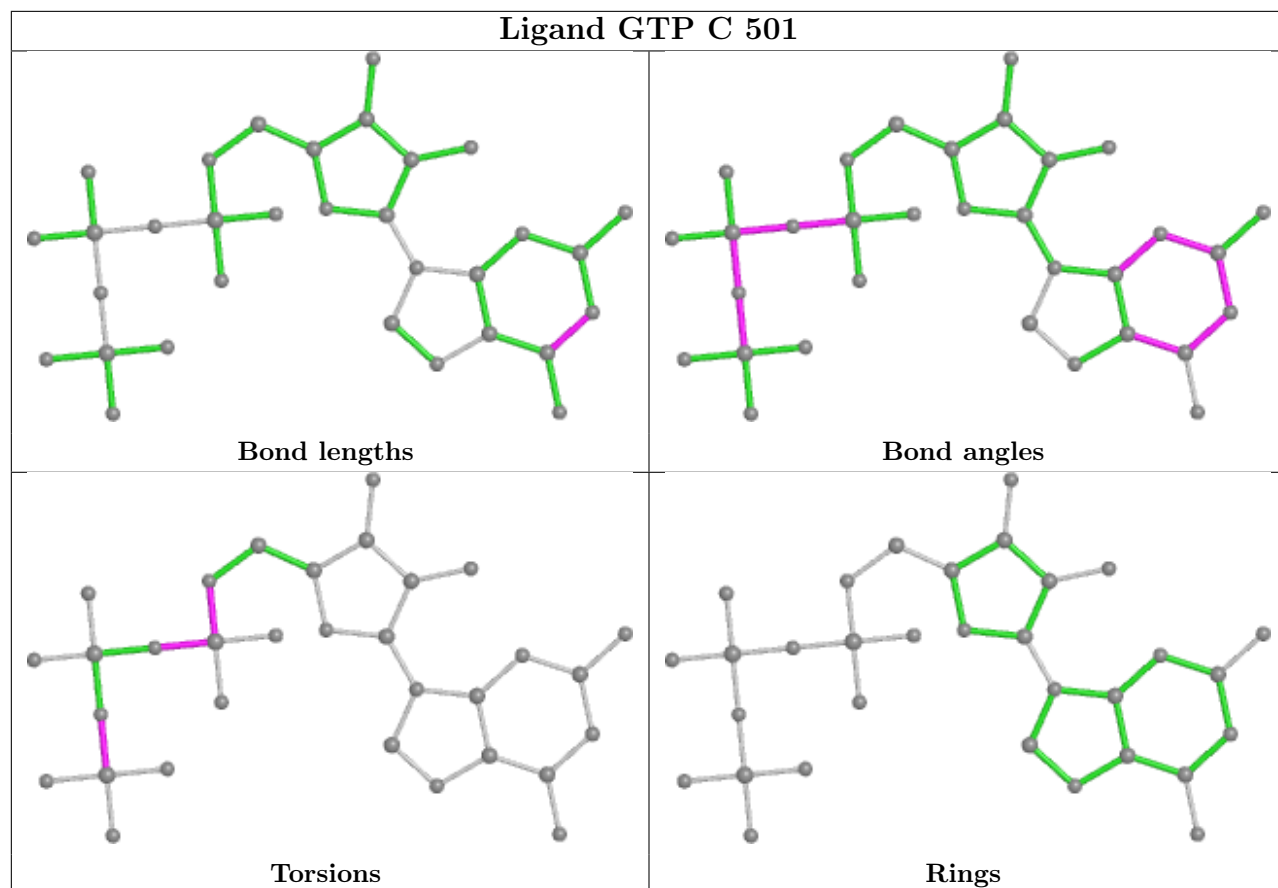
Ligand ACP F 401



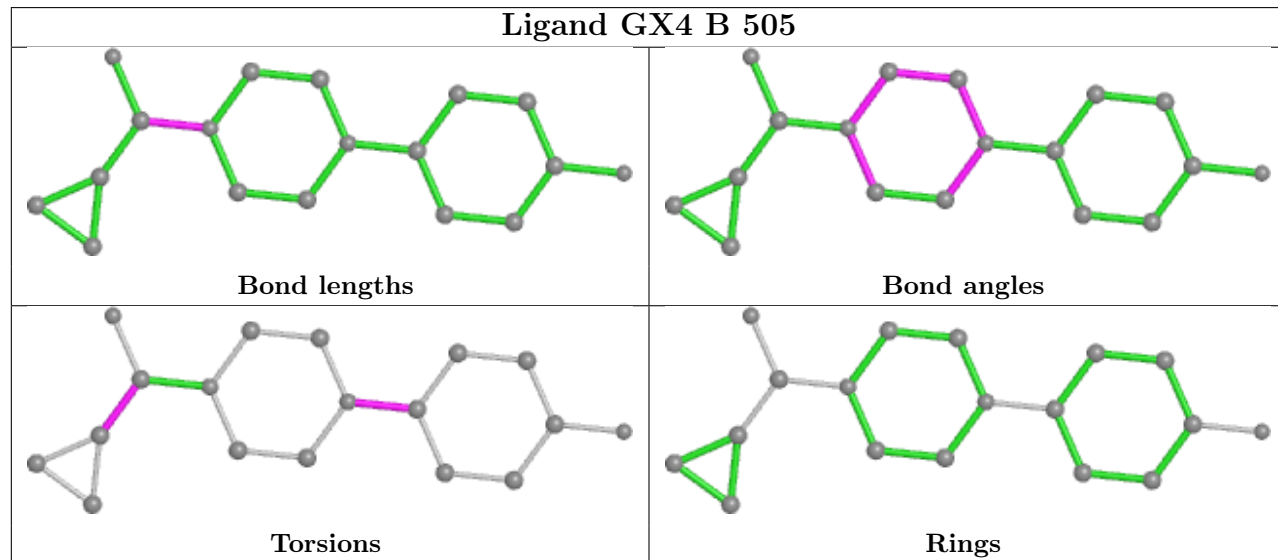
Ligand GTP A 501

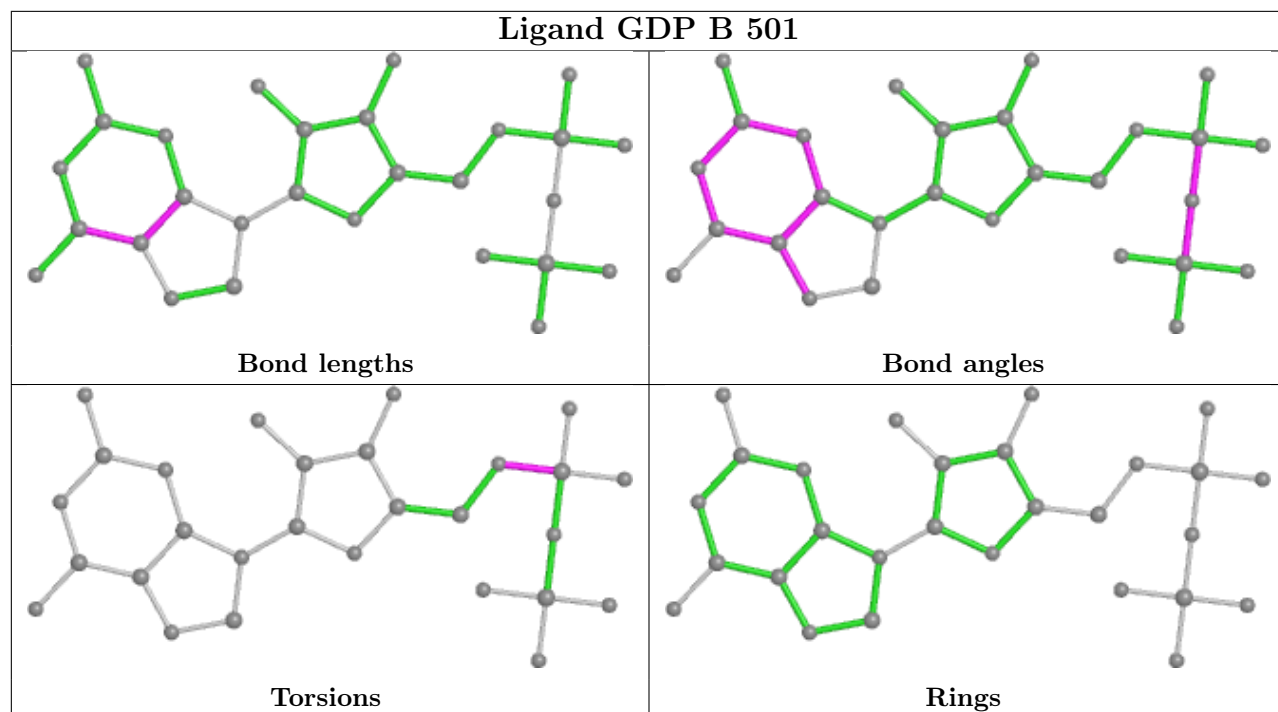


Ligand GTP C 501



Ligand GX4 B 505





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	438/451 (97%)	0.50	16 (3%)	41 41	53, 72, 109, 184	0
1	C	440/451 (97%)	0.64	11 (2%)	57 55	47, 61, 84, 122	0
2	B	425/445 (95%)	0.66	22 (5%)	27 26	49, 69, 119, 159	2 (0%)
2	D	428/445 (96%)	0.59	26 (6%)	21 20	56, 79, 113, 155	4 (0%)
3	E	123/143 (86%)	0.93	9 (7%)	15 13	59, 84, 123, 156	0
4	F	352/384 (91%)	1.18	67 (19%)	1 1	69, 99, 161, 187	0
All	All	2206/2319 (95%)	0.71	151 (6%)	17 15	47, 75, 130, 187	6 (0%)

All (151) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	89	GLU	9.8
2	D	276	THR	9.4
4	F	240	LEU	7.8
3	E	24	LEU	7.4
3	E	26	PRO	7.2
4	F	173	ILE	7.1
3	E	27	PRO	6.6
2	D	278	ARG	6.6
2	B	284	ARG	6.4
4	F	90	SER	6.1
2	B	281	GLN	5.9
4	F	169	LEU	5.9
4	F	177	GLY	5.9
2	B	276	THR	5.8
1	A	349	THR	5.8
3	E	25	LYS	5.6
2	B	333	LEU	5.6
1	A	438	ASP	5.6
2	D	277	SER	5.0

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Mol	Chain	Res	Type	RSRZ
4	F	249	TYR	4.8
4	F	103	THR	4.8
2	D	279	GLY	4.7
4	F	105	LEU	4.7
4	F	253	TYR	4.6
1	A	351	PHE	4.6
4	F	232	ASN	4.5
4	F	248	GLU	4.4
4	F	153	ALA	4.4
3	E	6	MET	4.2
4	F	182	ILE	4.1
4	F	330	ILE	4.1
3	E	143	ALA	4.0
4	F	137	ARG	4.0
4	F	143	GLU	4.0
2	B	1	MET	4.0
4	F	149	ALA	3.9
3	E	28	SER	3.9
2	B	283	TYR	3.9
4	F	130	VAL	3.9
2	D	280	SER	3.9
2	D	285	ALA	3.8
4	F	223	THR	3.8
2	B	337	ASN	3.8
4	F	101	TYR	3.8
4	F	251	LYS	3.7
2	D	401	ARG	3.7
1	A	341	ILE	3.7
4	F	142	ARG	3.6
4	F	234	GLN	3.6
2	B	247	GLN	3.6
4	F	99	VAL	3.6
4	F	147	TRP	3.6
4	F	152	SER	3.5
1	A	339	ARG	3.5
4	F	233	PHE	3.4
2	B	275	LEU	3.4
1	A	262	TYR	3.4
4	F	243	HIS	3.4
4	F	244	CYS	3.3
4	F	254	GLY	3.3
2	D	215	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	346	TRP	3.3
4	F	181	VAL	3.3
4	F	71	LEU	3.2
4	F	172	PHE	3.2
4	F	231	ALA	3.1
4	F	245	ILE	3.1
2	D	299	LYS	3.1
2	B	340	SER	3.1
4	F	138	ARG	3.0
2	B	57	THR	3.0
2	D	284	ARG	3.0
4	F	104	ASN	3.0
4	F	98	TYR	3.0
2	D	275	LEU	3.0
4	F	100	ILE	3.0
2	B	358	ILE	2.9
4	F	250	SER	2.9
4	F	20	LEU	2.9
4	F	361	LEU	2.9
4	F	242	ASN	2.9
4	F	135	TYR	2.9
1	A	78	VAL	2.8
2	B	325	MET	2.8
2	D	286	LEU	2.8
1	C	308	ARG	2.8
2	D	405	LEU	2.7
4	F	241	THR	2.7
2	D	402	LYS	2.7
4	F	372	THR	2.7
1	A	335	ILE	2.6
2	D	293	GLN	2.6
2	D	400	ARG	2.6
4	F	31	ARG	2.6
4	F	252	ASN	2.6
2	B	286	LEU	2.6
2	B	328	VAL	2.6
4	F	178	GLN	2.6
4	F	259	GLY	2.6
4	F	315	PHE	2.6
4	F	197	ARG	2.5
2	B	277	SER	2.5
4	F	144	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
3	E	123	LEU	2.5
4	F	256	TYR	2.5
1	C	335	ILE	2.5
4	F	131	PHE	2.5
4	F	382	HIS	2.4
1	A	348	PRO	2.4
1	C	218	ASP	2.4
2	D	372	LYS	2.4
1	A	176	GLN	2.4
2	D	57	THR	2.4
3	E	7	GLU	2.4
4	F	283	ILE	2.4
2	B	332	MET	2.4
2	D	1	MET	2.3
1	C	248	LEU	2.3
2	B	42	LEU	2.3
4	F	314	LEU	2.3
1	C	371	VAL	2.3
2	D	255	LEU	2.3
1	C	4[A]	CYS	2.3
4	F	179	VAL	2.3
2	B	437	ASP	2.3
1	A	342	GLN	2.3
2	B	248	LEU	2.2
2	D	272	PHE	2.2
1	C	65	ALA	2.2
4	F	162	ILE	2.2
4	F	379	HIS	2.2
2	D	119	LEU	2.2
4	F	161	LEU	2.2
1	C	245	ASP	2.2
4	F	362	ALA	2.2
2	D	377	PHE	2.2
1	C	281	ALA	2.1
1	A	118	VAL	2.1
1	C	247	ALA	2.1
2	D	218	LYS	2.1
4	F	176	GLN	2.1
4	F	125	THR	2.1
1	A	23	LEU	2.0
1	A	86	LEU	2.0
1	A	316	CYS	2.0

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Mol	Chain	Res	Type	RSRZ
4	F	342	LEU	2.0
2	B	59	ASN	2.0
1	C	357	TYR	2.0
2	D	291	LEU	2.0
2	D	371	LEU	2.0
2	B	338	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

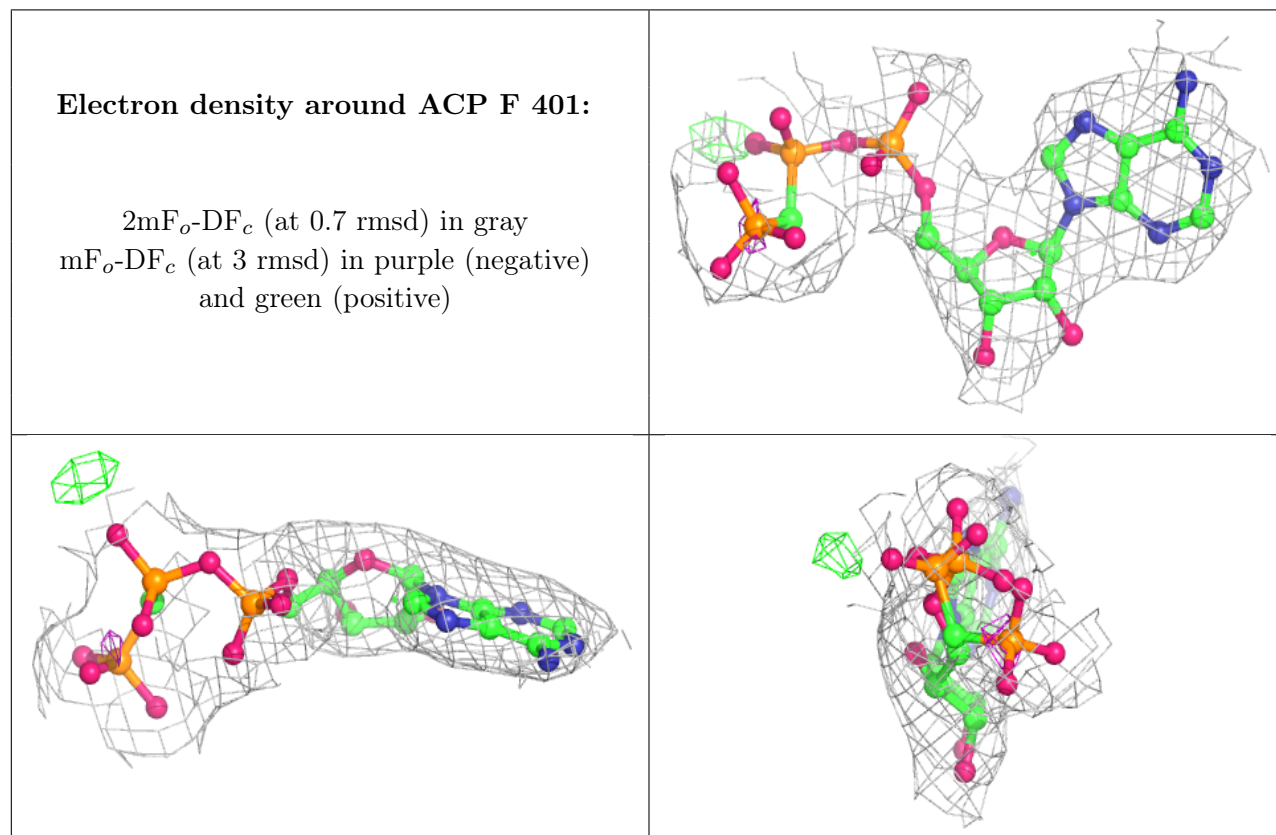
There are no monosaccharides in this entry.

6.4 Ligands [i](#)

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

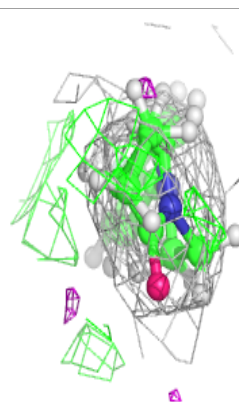
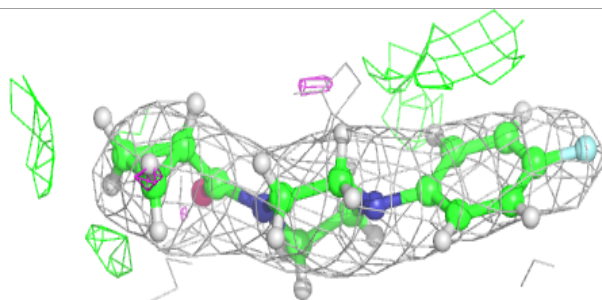
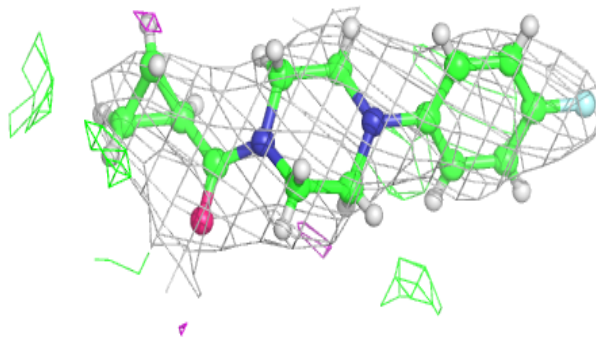
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	CA	B	503	1/1	0.69	0.19	101,101,101,101	0
11	ACP	F	401	31/31	0.84	0.14	101,113,121,126	0
7	CA	A	504	1/1	0.87	0.14	99,99,99,99	0
6	MG	D	502	1/1	0.90	0.17	82,82,82,82	0
10	GX4	B	505	18/18	0.93	0.23	74,81,96,97	0
9	MES	B	504	12/12	0.93	0.16	75,79,89,93	0
6	MG	F	402	1/1	0.95	0.07	99,99,99,99	0
8	GDP	D	501	28/28	0.96	0.15	67,75,85,91	0
6	MG	B	502	1/1	0.96	0.14	50,50,50,50	0
7	CA	A	503	1/1	0.97	0.09	98,98,98,98	0
6	MG	A	502	1/1	0.98	0.14	51,51,51,51	0
5	GTP	A	501	32/32	0.98	0.14	48,55,58,61	0
6	MG	C	502	1/1	0.98	0.15	56,56,56,56	0
5	GTP	C	501	32/32	0.98	0.18	47,52,56,59	0
7	CA	C	503	1/1	0.99	0.13	78,78,78,78	0
8	GDP	B	501	28/28	0.99	0.18	46,53,57,59	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.

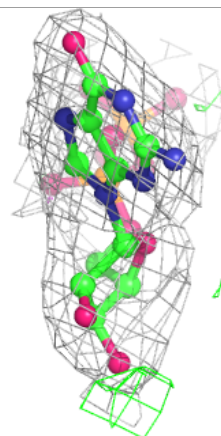
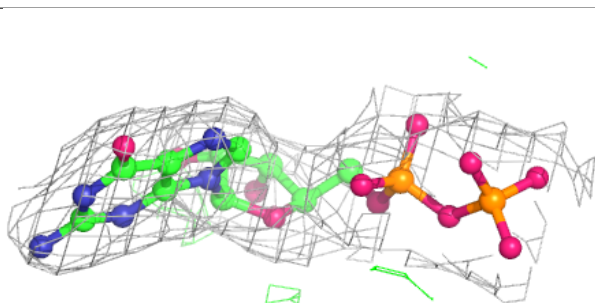
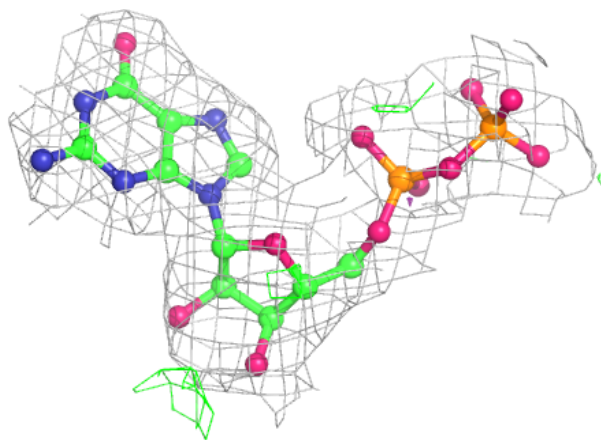


Electron density around GX4 B 505:

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

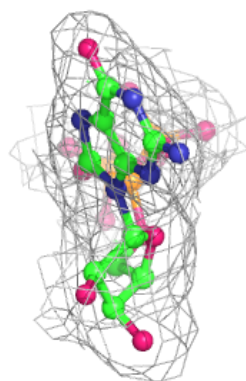
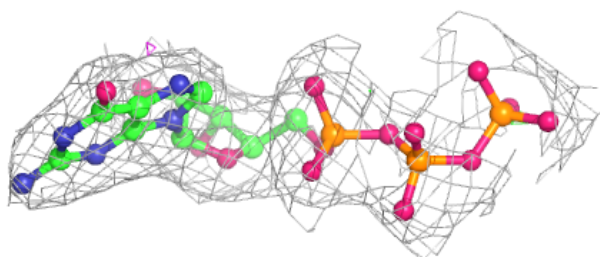
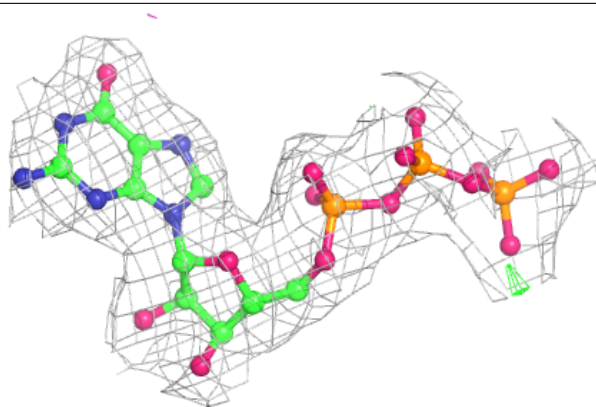
**Electron density around GDP D 501:**

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

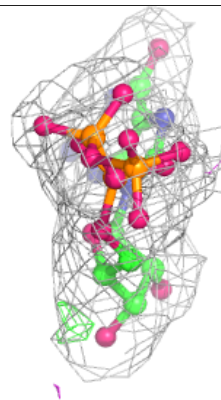
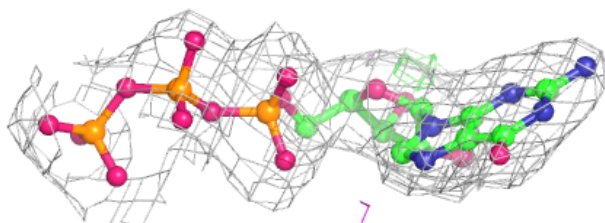
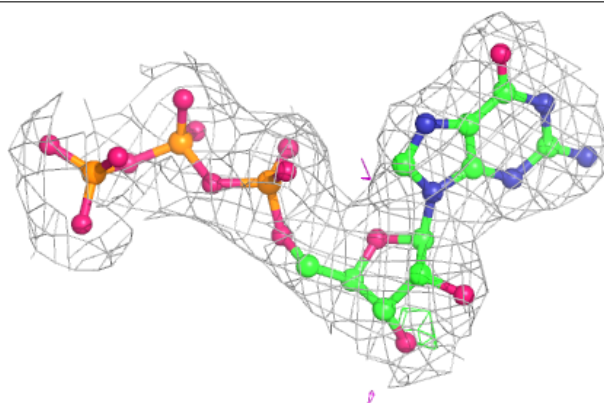


Electron density around GTP A 501:

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

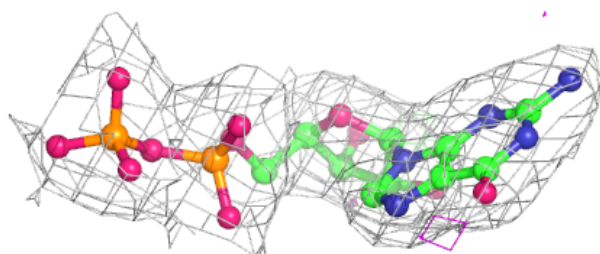
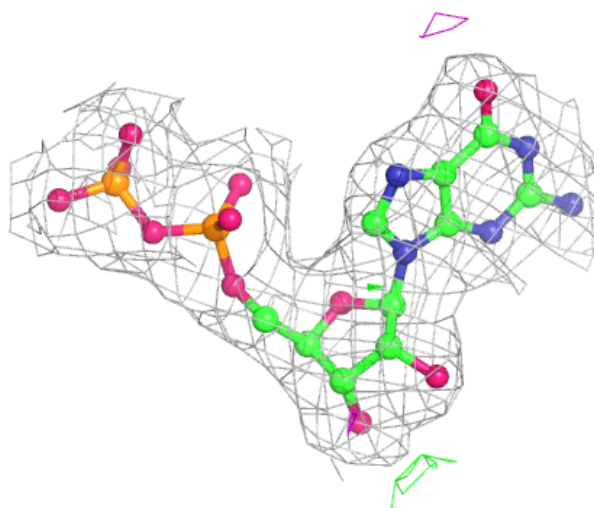
**Electron density around GTP C 501:**

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



Electron density around GDP B 501:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.