



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 09:31 PM UTC

PDB ID : 7XQY / pdb_00007xqy
Title : Crystal structure of T2R-TTL-15 complex
Authors : Lun, T.; ChengYong, W.
Deposited on : 2022-05-09
Resolution : 2.35 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

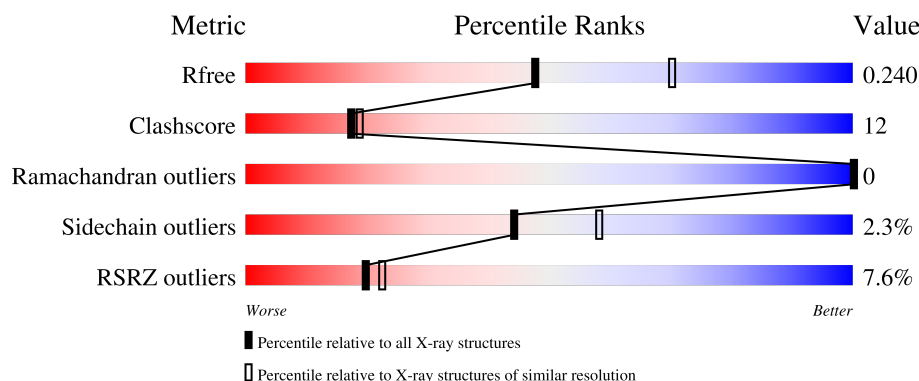
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.35 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1596 (2.36-2.36)
Clashscore	190562	1663 (2.36-2.36)
Ramachandran outliers	187476	1646 (2.36-2.36)
Sidechain outliers	187428	1646 (2.36-2.36)
RSRZ outliers	180081	1598 (2.36-2.36)

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	450	 2% 78% 19% •
1	C	450	 2% 78% 19% •
2	B	445	 3% 71% 24% 5%
2	D	445	 8% 66% 27% • 6%
3	E	143	 6% 70% 16% 14%

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Mol	Chain	Length	Quality of chain
4	F	384	23% 57% 33% • 10%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17991 atoms, of which 0 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	4	0
			3427	2170	580	653	24			
1	C	440	Total	C	N	O	S	0	9	0
			3468	2195	585	663	25			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	3	0
			3356	2111	572	647	26			
2	D	420	Total	C	N	O	S	0	1	0
			3295	2072	558	639	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	2	0
			1026	633	186	202	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63042
E	4	ALA	-	expression tag	UNP P63042

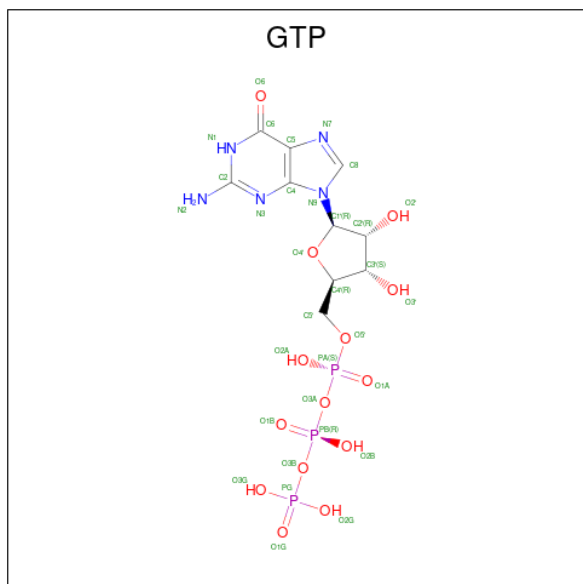
- Molecule 4 is a protein called TTL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	346	Total	C	N	O	S	0	4	0
			2851	1830	487	519	15			

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 (CCD ID: 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 (CCD ID: 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		

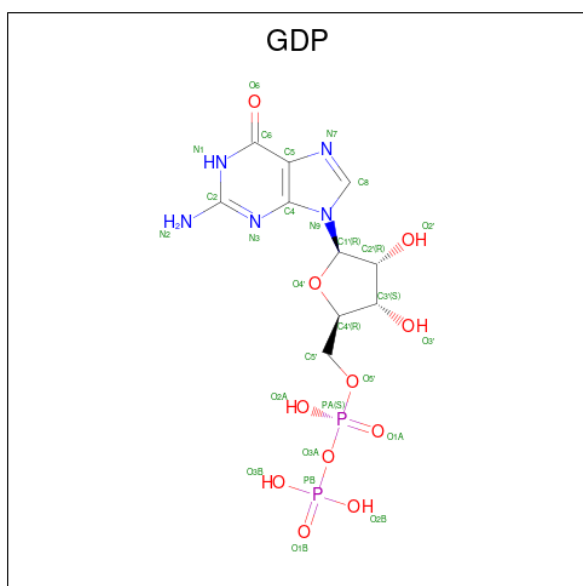
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

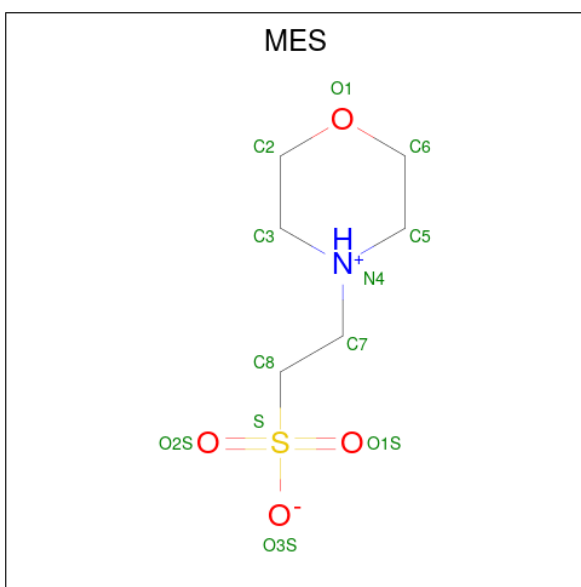
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	1	Total Cl 1 1	0	0

- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



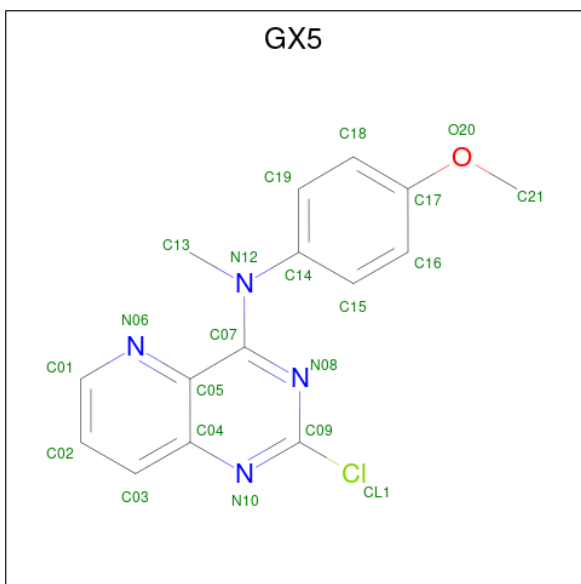
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	B	1	Total C N O P 28 10 5 11 2	0	0
9	D	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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

- Molecule 11 is 2-chloranyl-N-(4-methoxyphenyl)-N-methyl-pyrido[3,2-d]pyrimidin-4-amine (CCD ID: GX5) (formula: C₁₅H₁₃ClN₄O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	Cl	N	O	0	0
			21	15	1	4	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	D	1	Total	C	Cl	N	O	0	0
			21	15	1	4	1		

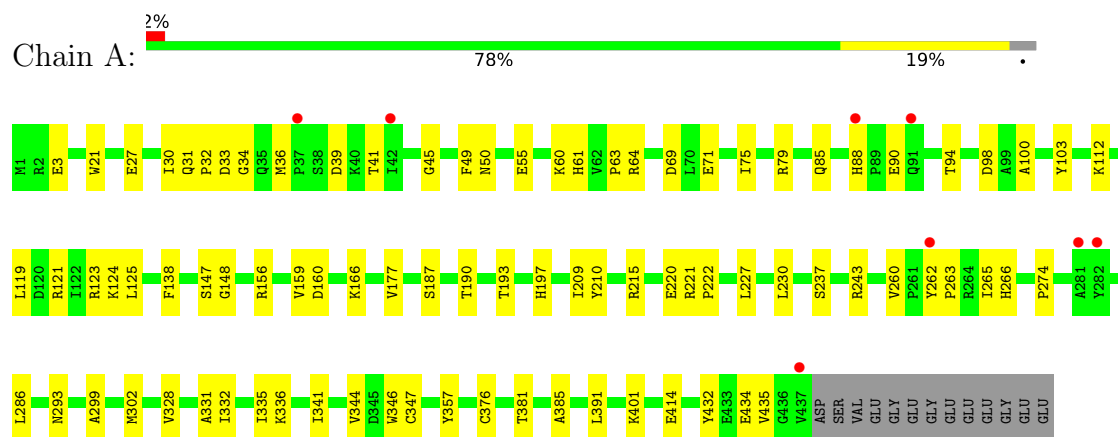
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	76	Total	O	0	0
			76	76		
12	B	59	Total	O	0	0
			59	59		
12	C	163	Total	O	0	0
			163	163		
12	D	28	Total	O	0	0
			28	28		
12	E	17	Total	O	0	0
			17	17		
12	F	33	Total	O	0	0
			33	33		

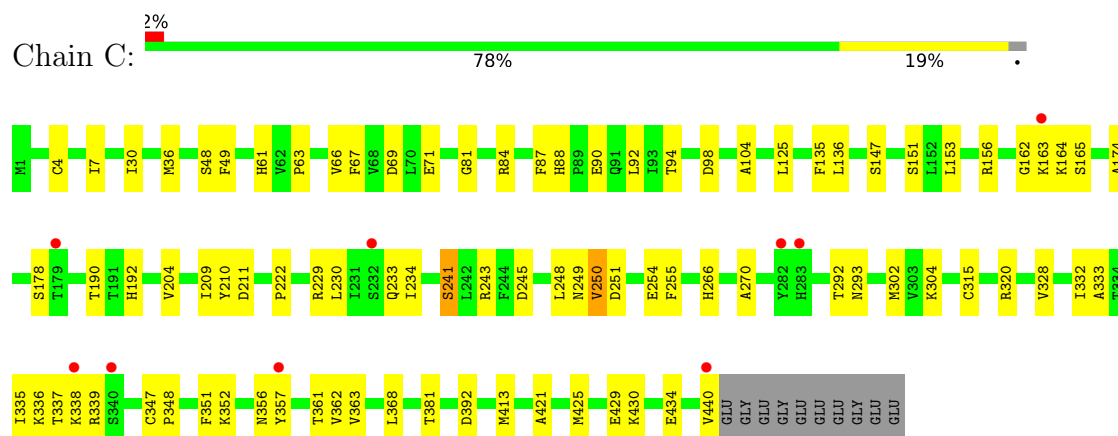
3 Residue-property plots

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

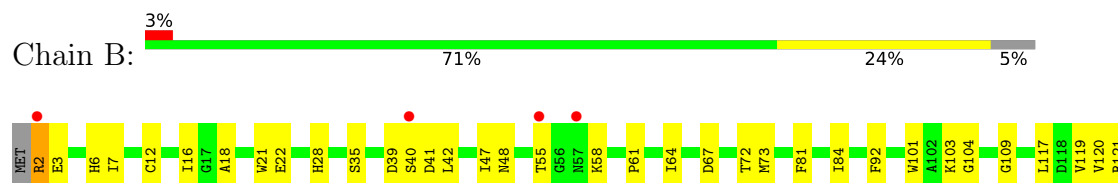
• Molecule 1: Tubulin alpha-1B chain

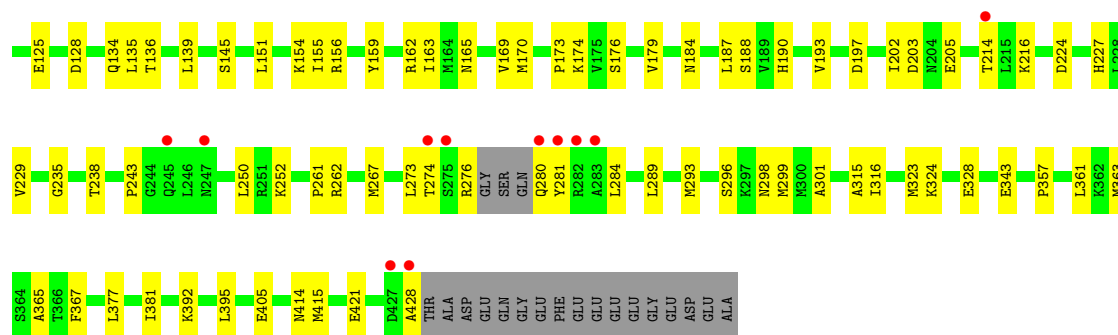


• Molecule 1: Tubulin alpha-1B chain

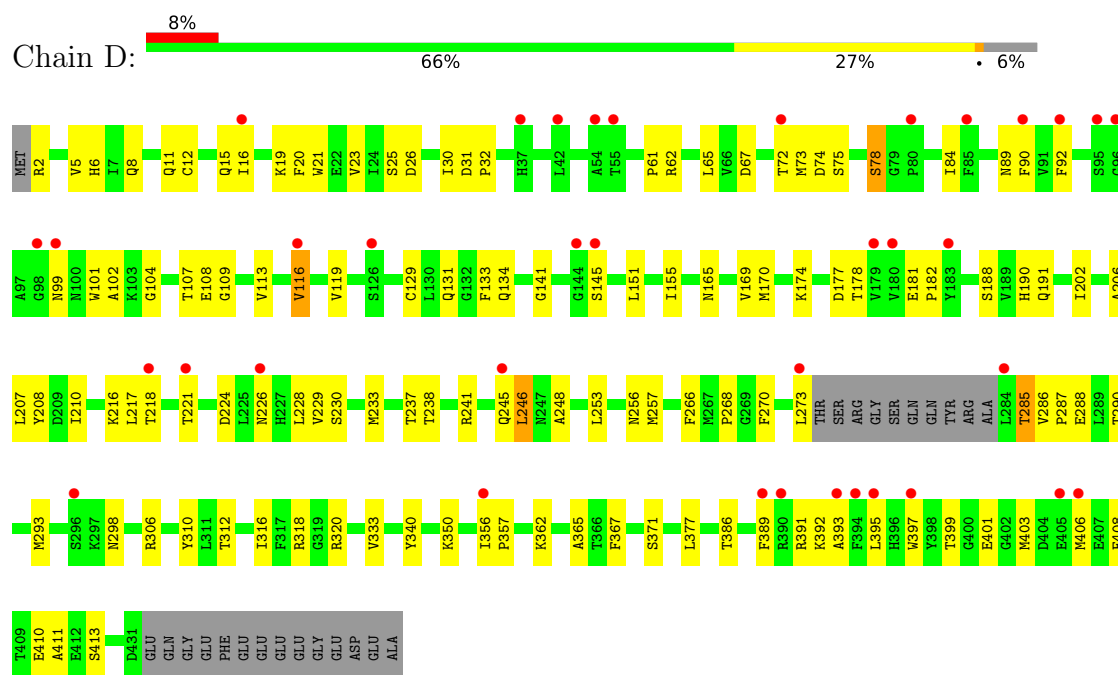


• Molecule 2: Tubulin beta chain

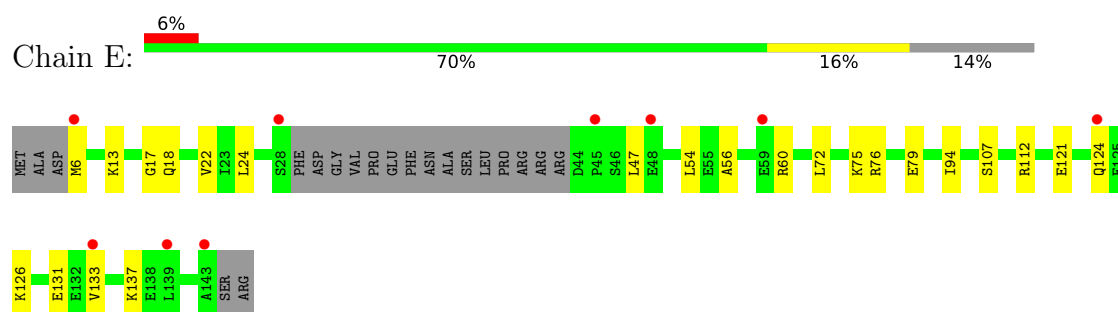




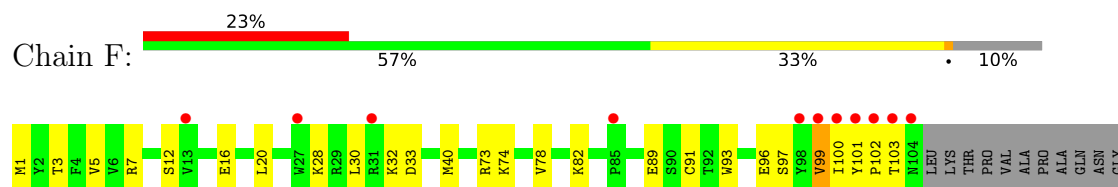
• Molecule 2: Tubulin beta chain



• Molecule 3: Stathmin-4



• Molecule 4: TTL



ILE	ARG	HIS	LEU	ILE	ASN	ASN	THR	ARG	T125	D126	E127	E128	V130	F131	L132	A133	A134	Y135	M136	R137	R138	R139	E140	G141	R142	E143	G144	N145	V146	W147	I148	A149	K150	S151	S152	ALA	GLY	ALA	LYS	GLY	E158	G159	I160	L161	I162	S163	S164	E165	A166	S167	E168	L169	L170	D171	F172	I173	D174	E175																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																										
	Q176	G177	Q178	V179	H180	V181	I182	Q183	K184	Y185	L186	E187	K188	P189	L190	L191	L192	E193	P194	G195	H196	R197	K198	F199	D200	T201	R202	V205	L206	H209	Y214	R217	E218	G219	V220	L221	R222	T223	S224	S225	E226	P227	Y228	N229	S230	A231	N232	F233	Q234	D235	K236	T237	G238	H239	L240	T241																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																												
N242	H243	C244	I245	Q246	K247	E248	Y249	S250	K251	N252	Y253	G254	R255	Y256	E257	N260	F263	F264	Q269	Y270	L271	N272	A274	L275	N276	T277	T278	L279	L284	K288	H289	I290	I291	R292	M296	C297	I298	E299	P300	T304	L307	S311	D318	F319	N320	E324																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																						
I330	E331	V332	N333	G334	A335	C338	A339	Q340	K341	L342	Y343	V353	A362	ASP	THR	GLY	GLN	LYS	THR	SER	GLN	PRO	T372	F375	I376	K377	L378	H379	H380	HIS	HIS	HIS	HIS																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																			

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.42Å 158.33Å 180.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	41.58 – 2.35 41.58 – 2.35	Depositor EDS
% Data completeness (in resolution range)	99.9 (41.58-2.35) 99.8 (41.58-2.35)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.67 (at 2.34Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.199 , 0.236 0.203 , 0.240	Depositor DCC
R_{free} test set	2000 reflections (1.58%)	wwPDB-VP
Wilson B-factor (Å ²)	49.6	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.3	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	0.95	EDS
Total number of atoms	17991	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% 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: GTP, MG, GX5, GDP, MES, CA, CL

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	0.39	0/3517	0.57	0/4776
1	C	0.44	0/3570	0.63	0/4847
2	B	0.42	0/3436	0.61	1/4653 (0.0%)
2	D	0.35	0/3368	0.55	0/4564
3	E	0.39	0/1041	0.57	0/1382
4	F	0.32	0/2927	0.55	1/3955 (0.0%)
All	All	0.39	0/17859	0.58	2/24177 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	227	PRO	CA-N-CD	-7.03	102.15	112.00
2	B	299	MET	CA-CB-CG	-5.90	102.30	114.10

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	3427	0	3341	69	0
1	C	3468	0	3388	61	0
2	B	3356	0	3238	91	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3295	0	3166	108	0
3	E	1026	0	1042	20	0
4	F	2851	0	2826	99	0
5	A	32	0	12	0	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
9	B	28	0	12	1	0
9	D	28	0	11	3	0
10	B	24	0	25	4	0
11	B	21	0	0	0	0
11	D	21	0	0	3	0
12	A	76	0	0	0	0
12	B	59	0	0	4	0
12	C	163	0	0	1	0
12	D	28	0	0	0	0
12	E	17	0	0	1	0
12	F	33	0	0	3	0
All	All	17991	0	17073	432	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 12.

All (432) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:20:PHE:HB2	2:D:233:MET:HE2	1.45	0.97
2:B:235:GLY:O	2:B:238:THR:HG22	1.68	0.93
1:A:31:GLN:HG3	1:A:32:PRO:HD2	1.56	0.88
4:F:82:LYS:NZ	4:F:97:SER:O	2.07	0.87
2:D:102:ALA:HB2	2:D:403:MET:HE3	1.54	0.86
2:D:226:ASN:ND2	9:D:501:GDP:O6	2.09	0.85
1:A:262:TYR:HE1	1:A:346:TRP:CZ2	1.96	0.84
4:F:135:TYR:OH	4:F:165:GLU:HA	1.77	0.84
2:D:102:ALA:HB2	2:D:403:MET:CE	2.09	0.82
1:C:241:SER:HA	1:C:249:ASN:HD21	1.45	0.81
3:E:13:LYS:HB2	3:E:18:GLN:HB3	1.61	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:121:ARG:O	2:B:125:GLU:HG2	1.81	0.80
1:C:209:ILE:HD11	1:C:302:MET:SD	2.24	0.78
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.66	0.77
2:D:221:THR:HG22	2:D:224:ASP:OD2	1.85	0.77
2:B:238:THR:HG21	2:B:316:ILE:HG21	1.66	0.76
2:D:285:THR:HG23	2:D:287:PRO:HD2	1.67	0.76
1:A:31:GLN:HG3	1:A:32:PRO:CD	2.16	0.76
2:D:392:LYS:C	2:D:395:LEU:HD13	2.11	0.75
2:B:280:GLN:HG2	2:B:281:TYR:H	1.50	0.75
1:A:36:MET:HE1	1:A:49:PHE:CE1	2.21	0.75
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.27	0.74
4:F:131:PHE:CE2	4:F:182:ILE:HD11	2.22	0.74
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.69	0.74
2:D:191:GLN:HE22	3:E:126:LYS:HE2	1.53	0.73
2:D:113:VAL:O	2:D:116:VAL:HG13	1.91	0.71
1:A:166:LYS:HE2	1:A:197:HIS:O	1.91	0.70
1:C:250:VAL:HG22	1:C:255:PHE:CE2	2.26	0.70
4:F:170:LEU:H	4:F:170:LEU:HD12	1.55	0.70
4:F:226:GLU:CG	4:F:237:THR:HG22	2.21	0.70
4:F:1:MET:HE2	4:F:28:LYS:HB3	1.73	0.70
2:D:293:MET:HG2	2:D:367:PHE:HB2	1.74	0.69
2:B:238:THR:CG2	2:B:316:ILE:HG21	2.21	0.69
1:C:36:MET:HE3	1:C:61:HIS:CD2	2.27	0.69
1:C:234:ILE:HD13	1:C:302:MET:SD	2.32	0.69
4:F:226:GLU:HG3	4:F:237:THR:HG22	1.75	0.69
3:E:47:LEU:HD12	3:E:47:LEU:O	1.93	0.69
4:F:16:GLU:O	4:F:20:LEU:HG	1.94	0.68
4:F:144:GLY:HA3	4:F:187:GLU:OE1	1.92	0.68
4:F:223:THR:HG21	4:F:257:GLU:OE1	1.92	0.68
2:D:67:ASP:OD2	2:D:72:THR:HG21	1.94	0.67
2:B:35:SER:HB3	2:B:58:LYS:HE2	1.76	0.67
2:B:284:LEU:O	2:B:363:MET:HE1	1.92	0.67
2:B:81:PHE:O	2:B:84:ILE:HG22	1.93	0.67
2:D:12:CYS:SG	2:D:16:ILE:HD12	2.35	0.67
2:D:11:GLN:HG3	2:D:15:GLN:HE22	1.59	0.67
2:D:107:THR:HG22	2:D:108:GLU:N	2.11	0.66
1:A:220:GLU:HG2	2:B:324:LYS:HD2	1.77	0.65
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.32	0.65
2:D:191:GLN:HE22	3:E:126:LYS:CE	2.09	0.65
2:D:246:LEU:HD12	2:D:248:ALA:HB2	1.79	0.64
2:B:392:LYS:HE3	2:B:405:GLU:OE2	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:149:ALA:CB	4:F:182:ILE:HG22	2.28	0.64
1:A:45:GLY:O	1:A:50:ASN:ND2	2.29	0.64
2:D:5:VAL:HG12	2:D:62:ARG:HD3	1.80	0.64
4:F:198:LYS:HG2	4:F:199:PHE:H	1.63	0.64
2:D:11:GLN:HG3	2:D:15:GLN:NE2	2.13	0.63
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.33	0.63
4:F:131:PHE:CD2	4:F:182:ILE:HD11	2.33	0.63
2:D:238:THR:HG21	2:D:318:ARG:HD2	1.79	0.63
4:F:101:TYR:N	4:F:126:ASP:OD2	2.30	0.63
2:B:316:ILE:N	2:B:316:ILE:HD12	2.14	0.62
4:F:277:THR:HG22	4:F:278:THR:H	1.64	0.62
4:F:202:ARG:HB3	4:F:220[B]:VAL:HG12	1.82	0.62
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.81	0.62
4:F:226:GLU:HG3	4:F:237:THR:CG2	2.30	0.62
2:D:116:VAL:HG21	2:D:151:LEU:HD21	1.82	0.62
2:D:73:MET:HG2	2:D:90:PHE:CD1	2.35	0.61
2:D:229:VAL:O	2:D:233:MET:HG3	2.00	0.61
2:B:2:ARG:NE	2:B:48:ASN:OD1	2.31	0.61
1:A:209:ILE:HD11	1:A:302:MET:SD	2.40	0.61
4:F:150:LYS:HG2	4:F:151:SER:N	2.16	0.61
4:F:217:ARG:HG3	4:F:218:GLU:HG2	1.83	0.61
3:E:131:GLU:OE1	3:E:131:GLU:HA	2.00	0.61
1:A:262:TYR:CE1	1:A:346:TRP:CZ2	2.85	0.60
4:F:277:THR:HG22	4:F:278:THR:N	2.15	0.60
1:C:211[A]:ASP:OD2	1:C:304:LYS:NZ	2.35	0.59
4:F:96:GLU:O	4:F:183:GLN:HB2	2.03	0.59
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.02	0.59
2:B:284:LEU:O	2:B:363:MET:CE	2.50	0.59
1:A:147:SER:HB2	1:A:190:THR:HB	1.85	0.59
2:D:141:GLY:HA3	9:D:501:GDP:O3A	2.03	0.59
2:D:391:ARG:HD2	2:D:393:ALA:HB2	1.85	0.58
2:B:73:MET:HE2	2:B:92:PHE:HB3	1.84	0.58
4:F:150:LYS:HG2	4:F:151:SER:H	1.69	0.58
1:C:440:VAL:HG12	1:C:440:VAL:O	2.02	0.58
2:B:48:ASN:H	2:B:48:ASN:ND2	2.02	0.58
2:B:280:GLN:CG	2:B:281:TYR:H	2.17	0.58
1:A:55:GLU:HG2	1:A:61:HIS:CD2	2.38	0.58
2:B:280:GLN:HG2	2:B:281:TYR:N	2.17	0.57
2:D:362:LYS:HD3	2:D:362:LYS:N	2.19	0.57
4:F:225:SER:H	4:F:246:GLN:HE22	1.49	0.57
4:F:226:GLU:HG2	4:F:237:THR:HG22	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:288:LYS:NZ	12:F:403:HOH:O	2.28	0.57
1:A:88:HIS:CE1	1:A:90:GLU:HG2	2.40	0.57
2:D:216:LYS:O	2:D:217:LEU:HD23	2.05	0.57
1:A:27:GLU:OE1	1:A:243:ARG:NH2	2.35	0.56
4:F:127:GLU:O	4:F:130:VAL:HG22	2.06	0.56
2:B:39:ASP:OD1	2:B:40:SER:N	2.38	0.56
2:D:74:ASP:O	2:D:78:SER:OG	2.23	0.56
2:B:296:SER:N	10:B:504:MES:O1S	2.29	0.55
2:B:104:GLY:O	2:B:109:GLY:HA3	2.07	0.55
2:B:170:MET:HE2	2:B:377:LEU:HD21	1.86	0.55
2:D:356:ILE:HD12	2:D:357:PRO:HD2	1.88	0.55
1:A:346:TRP:H	1:A:346:TRP:CD1	2.24	0.55
2:D:285:THR:HG23	2:D:287:PRO:CD	2.36	0.55
1:A:262:TYR:HE1	1:A:346:TRP:CH2	2.25	0.55
2:D:65:LEU:N	2:D:65:LEU:HD12	2.21	0.55
2:B:293:MET:HE2	2:B:367:PHE:HB2	1.87	0.55
3:E:112:ARG:NH2	12:E:201:HOH:O	2.38	0.55
4:F:99:VAL:C	4:F:100:ILE:HD13	2.32	0.55
1:A:265:ILE:O	1:A:265:ILE:HG22	2.06	0.55
1:A:336:LYS:HD3	3:E:24:LEU:HD13	1.89	0.55
4:F:145:ASN:OD1	4:F:147:TRP:NE1	2.40	0.55
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.88	0.54
2:B:273:LEU:HD11	2:B:298:ASN:HA	1.88	0.54
1:C:241:SER:HA	1:C:249:ASN:ND2	2.20	0.54
4:F:5:VAL:HG13	4:F:32:LYS:HA	1.88	0.54
4:F:135:TYR:HH	4:F:165:GLU:HA	1.71	0.54
2:D:5:VAL:HG12	2:D:62:ARG:CD	2.37	0.54
1:A:36:MET:HE3	1:A:39:ASP:HB2	1.90	0.54
1:A:112:LYS:HD2	3:E:54:LEU:HB3	1.89	0.53
2:B:190:HIS:O	2:B:193:VAL:HG12	2.07	0.53
4:F:138:ARG:NH1	4:F:184:LYS:HE3	2.22	0.53
2:B:58:LYS:NZ	12:B:603:HOH:O	2.40	0.53
1:C:250:VAL:HG22	1:C:255:PHE:CZ	2.43	0.53
2:B:261:PRO:HD2	12:B:631:HOH:O	2.09	0.53
2:D:5:VAL:CG2	2:D:133:PHE:CD2	2.91	0.53
4:F:89:GLU:CD	4:F:89:GLU:H	2.16	0.53
1:A:331:ALA:O	1:A:335:ILE:HG13	2.08	0.53
1:A:336:LYS:HE2	1:A:341:ILE:HB	1.89	0.53
2:D:20:PHE:HB2	2:D:233:MET:CE	2.30	0.53
1:A:90:GLU:O	1:A:121:ARG:HD2	2.08	0.53
1:A:401:LYS:NZ	2:B:428:ALA:HB1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:25:SER:HB3	2:D:30:ILE:HG22	1.90	0.53
2:D:206:ALA:O	2:D:210:ILE:HG13	2.09	0.53
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.45	0.52
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.27	0.52
1:A:88:HIS:ND1	1:A:90:GLU:HG2	2.24	0.52
1:A:159:VAL:HG12	1:A:160:ASP:OD1	2.09	0.52
2:D:21:TRP:CE3	2:D:61:PRO:HB3	2.43	0.52
4:F:246:GLN:O	4:F:250:SER:HB2	2.09	0.52
1:C:293[A]:ASN:CG	1:C:339:ARG:HH21	2.17	0.52
2:D:99:ASN:HD22	2:D:178:THR:HG21	1.74	0.52
4:F:264:PHE:HB2	12:F:410:HOH:O	2.09	0.52
2:B:315:ALA:C	2:B:316:ILE:HD12	2.33	0.52
4:F:1:MET:CE	4:F:28:LYS:HB3	2.38	0.52
1:C:36:MET:HE1	1:C:49:PHE:CE1	2.45	0.52
2:D:221:THR:HG23	2:D:224:ASP:H	1.75	0.52
1:A:60:LYS:NZ	1:A:85:GLN:O	2.42	0.52
1:A:75:ILE:O	1:A:79:ARG:HG3	2.09	0.52
2:D:20:PHE:CB	2:D:233:MET:HE2	2.29	0.52
3:E:72:LEU:O	3:E:76:ARG:HG2	2.09	0.51
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.91	0.51
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.40	0.51
2:D:170:MET:HE3	2:D:377:LEU:HD11	1.93	0.51
4:F:78:VAL:HG21	4:F:181:VAL:HG21	1.92	0.51
2:B:224:ASP:OD1	2:B:276:ARG:NH1	2.43	0.51
2:D:285:THR:CG2	2:D:287:PRO:HD2	2.39	0.51
2:B:145:SER:HB2	2:B:188:SER:OG	2.11	0.51
1:C:302:MET:N	1:C:302:MET:HE2	2.26	0.51
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.39	0.51
2:D:257:MET:HE3	2:D:312:THR:OG1	2.10	0.51
1:A:34:GLY:O	1:A:61:HIS:N	2.32	0.51
2:B:203:ASP:HB2	2:B:301:ALA:HA	1.92	0.51
2:D:392:LYS:O	2:D:395:LEU:HD13	2.11	0.51
1:C:174:ALA:O	1:C:178:SER:HB3	2.11	0.51
2:D:5:VAL:HG22	2:D:133:PHE:CD2	2.46	0.51
4:F:3:THR:HB	4:F:30:LEU:HD11	1.93	0.51
2:D:290:THR:HG22	2:D:333:VAL:HG21	1.92	0.51
2:B:73:MET:HE2	2:B:92:PHE:CD1	2.46	0.50
4:F:131:PHE:CE2	4:F:182:ILE:CD1	2.92	0.50
1:C:30:ILE:HG12	1:C:36:MET:HE2	1.93	0.50
4:F:377:LYS:HG2	4:F:379:HIS:ND1	2.26	0.50
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:202:ILE:HG21	2:D:229:VAL:HG22	1.94	0.50
3:E:6:MET:HE3	3:E:22:VAL:HG11	1.94	0.50
4:F:73:ARG:HG2	4:F:73:ARG:HH11	1.77	0.50
4:F:126:ASP:OD1	4:F:128:ARG:HG2	2.11	0.50
1:A:260:VAL:HG11	1:A:266:HIS:HB3	1.94	0.50
2:B:169:VAL:HA	2:B:202:ILE:O	2.12	0.49
2:D:141:GLY:O	2:D:145[A]:SER:OG	2.27	0.49
4:F:99:VAL:O	4:F:100:ILE:HD13	2.12	0.49
1:C:245:ASP:OD1	1:C:245:ASP:N	2.44	0.49
2:D:169:VAL:HA	2:D:202:ILE:O	2.13	0.49
4:F:148:ILE:HG13	4:F:162:ILE:HG12	1.93	0.49
1:C:30:ILE:CG1	1:C:36:MET:HE2	2.43	0.49
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.48	0.49
2:D:226:ASN:ND2	9:D:501:GDP:C6	2.80	0.49
1:C:104:ALA:HB2	1:C:413:MET:SD	2.52	0.49
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.43	0.49
4:F:198:LYS:HG2	4:F:199:PHE:N	2.28	0.49
4:F:32:LYS:HE3	4:F:33:ASP:OD1	2.13	0.49
1:A:221:ARG:HG3	2:B:323:MET:CG	2.43	0.48
2:B:28:HIS:ND1	2:B:47:ILE:HD13	2.28	0.48
2:B:267:MET:HG3	2:B:301:ALA:HB3	1.93	0.48
2:D:293:MET:SD	2:D:365:ALA:HB1	2.52	0.48
4:F:263:PHE:CE2	4:F:341:LYS:HD3	2.48	0.48
4:F:333:ASN:ND2	4:F:335:ALA:H	2.11	0.48
2:B:2:ARG:NH1	2:B:128:ASP:OD2	2.47	0.48
2:D:246:LEU:CD1	2:D:248:ALA:HB2	2.41	0.48
1:A:293:ASN:HA	1:A:335:ILE:HD13	1.95	0.48
2:B:67:ASP:O	2:B:92:PHE:HA	2.14	0.48
1:C:320:ARG:HA	1:C:356:ASN:O	2.12	0.48
4:F:284:LEU:HD12	4:F:284:LEU:HA	1.63	0.48
1:A:344:VAL:HG21	1:A:346:TRP:CZ2	2.48	0.48
2:D:181:GLU:HB2	2:D:182:PRO:HD3	1.94	0.48
1:A:221:ARG:HG3	2:B:323:MET:HG3	1.94	0.48
4:F:279:LEU:HD13	4:F:284:LEU:HD22	1.95	0.48
4:F:99:VAL:HG12	4:F:127:GLU:OE1	2.14	0.48
4:F:223:THR:HG22	4:F:260:ASN:O	2.13	0.48
2:B:197:ASP:OD1	10:B:503:MES:H72	2.13	0.48
2:D:389:PHE:CE1	2:D:408:PHE:HB3	2.48	0.48
4:F:318:ASP:OD2	4:F:331:GLU:HG2	2.14	0.47
2:D:207:LEU:HD22	2:D:228:LEU:HB2	1.97	0.47
4:F:225:SER:OG	4:F:260:ASN:OD1	2.33	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:61:PRO:CD	2:B:84:ILE:HG12	2.45	0.47
1:C:48:SER:HB3	1:C:243:ARG:O	2.14	0.47
2:D:2:ARG:HD2	2:D:2:ARG:HA	1.47	0.47
2:B:7:ILE:O	2:B:135:LEU:HA	2.14	0.47
2:B:139:LEU:HA	2:B:145:SER:HB3	1.96	0.47
1:C:333:ALA:O	1:C:337:THR:HG23	2.15	0.47
1:C:361:THR:HG22	1:C:362:VAL:N	2.28	0.47
3:E:47:LEU:HD12	3:E:47:LEU:C	2.40	0.47
4:F:338:CYS:HB3	4:F:343:TYR:CE1	2.50	0.47
2:B:227:HIS:NE2	2:B:274:THR:HG23	2.30	0.47
2:D:266:PHE:O	2:D:268:PRO:HD3	2.15	0.47
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.97	0.47
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.49	0.47
2:B:16[B]:ILE:HD13	2:B:229:VAL:HG11	1.97	0.47
2:B:103:LYS:NZ	12:B:605:HOH:O	2.43	0.47
4:F:128:ARG:HD3	4:F:170:LEU:HD23	1.98	0.47
2:B:159:TYR:HB3	2:B:162:ARG:HG2	1.97	0.46
2:D:73:MET:HG2	2:D:90:PHE:CE1	2.50	0.46
4:F:206:LEU:HD23	4:F:353:VAL:CG2	2.45	0.46
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.50	0.46
2:D:2:ARG:N	2:D:131:GLN:HG3	2.30	0.46
2:D:67:ASP:O	2:D:92:PHE:HA	2.16	0.46
2:D:101:TRP:HD1	2:D:145[A]:SER:HB2	1.81	0.46
2:D:102:ALA:CB	2:D:403:MET:CE	2.90	0.46
2:D:238:THR:OG1	2:D:316:ILE:HG21	2.15	0.46
2:D:395:LEU:O	2:D:399:THR:HG22	2.14	0.46
4:F:140:GLU:C	4:F:142:ARG:H	2.23	0.46
4:F:158:GLU:C	4:F:160:ILE:HD12	2.40	0.46
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.50	0.46
2:D:233:MET:HE3	2:D:233:MET:HB3	1.76	0.46
1:C:248:LEU:CD1	1:C:357:TYR:OH	2.64	0.46
1:C:430:LYS:O	1:C:434:GLU:HG3	2.15	0.46
2:D:397:TRP:CD1	2:D:397:TRP:H	2.33	0.46
2:B:40:SER:OG	2:B:41:ASP:N	2.48	0.46
1:A:414:GLU:OE2	3:E:60:ARG:CZ	2.64	0.46
2:B:2:ARG:CB	2:B:2:ARG:HH11	2.29	0.46
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.51	0.46
2:B:357:PRO:HB2	2:B:361:LEU:O	2.16	0.46
4:F:103:THR:HG22	4:F:174:ASP:HB3	1.98	0.46
4:F:233:PHE:HE1	4:F:239:HIS:CE1	2.34	0.46
1:A:262:TYR:CE1	1:A:346:TRP:CH2	3.03	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:56:ALA:HB1	3:E:60:ARG:HH12	1.81	0.46
4:F:91:CYS:SG	4:F:93:TRP:CE2	3.08	0.46
4:F:333:ASN:HD21	4:F:335:ALA:C	2.24	0.46
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.33	0.45
2:D:89:ASN:HA	2:D:119:VAL:HG11	1.98	0.45
2:D:174:LYS:HG2	2:D:208:TYR:CD1	2.51	0.45
2:D:257:MET:HE3	2:D:257:MET:HB3	1.82	0.45
2:D:395:LEU:HD12	2:D:395:LEU:N	2.31	0.45
2:B:117:LEU:HD11	2:B:154:LYS:HB3	1.99	0.45
2:D:285:THR:HG22	2:D:288:GLU:CD	2.41	0.45
2:D:134:GLN:HA	2:D:165:ASN:O	2.16	0.45
2:D:391:ARG:CD	2:D:393:ALA:HB2	2.47	0.45
1:A:88:HIS:ND1	1:A:90:GLU:CG	2.80	0.45
2:B:101:TRP:CE3	2:B:187:LEU:HD13	2.52	0.45
1:A:119:LEU:HD11	1:A:156:ARG:HB3	1.98	0.45
2:B:173:PRO:HA	2:B:176:SER:HB2	1.99	0.45
1:C:69:ASP:O	1:C:94:THR:HA	2.17	0.45
4:F:167:SER:O	4:F:171:ASP:HB2	2.16	0.45
2:D:19:LYS:HA	2:D:19:LYS:HD3	1.81	0.45
2:D:73:MET:HG2	2:D:90:PHE:HD1	1.79	0.45
1:A:30:ILE:HG12	1:A:36:MET:HB2	1.99	0.45
1:A:293:ASN:HA	1:A:335:ILE:CD1	2.47	0.45
1:A:346:TRP:CZ3	1:A:347:CYS:SG	3.09	0.45
2:B:2:ARG:HH11	2:B:2:ARG:CG	2.30	0.45
2:B:216:LYS:HA	2:B:216:LYS:HD3	1.67	0.45
1:C:147:SER:HB2	1:C:190:THR:HB	1.99	0.45
1:C:229:ARG:CD	1:C:363:VAL:HG21	2.47	0.45
2:B:324:LYS:HE3	2:B:328:GLU:OE2	2.17	0.45
1:C:204:VAL:HG13	1:C:302:MET:HG3	1.98	0.45
4:F:74:LYS:NZ	4:F:150:LYS:HD3	2.32	0.45
2:D:104:GLY:O	2:D:109:GLY:HA3	2.16	0.44
2:D:293:MET:CG	2:D:367:PHE:HB2	2.46	0.44
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.47	0.44
2:D:210:ILE:HD13	2:D:273:LEU:CD1	2.48	0.44
2:D:306:ARG:HG2	2:D:340:TYR:CZ	2.52	0.44
2:D:12:CYS:SG	2:D:16:ILE:CD1	3.05	0.44
2:D:23:VAL:HG21	2:D:230:SER:OG	2.16	0.44
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.47	0.44
4:F:163:SER:OG	4:F:164:SER:N	2.50	0.44
4:F:197:ARG:NH2	4:F:257:GLU:OE2	2.46	0.44
3:E:60:ARG:HG3	3:E:60:ARG:HH11	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:340:GLN:NE2	12:F:401:HOH:O	2.24	0.44
2:D:285:THR:CG2	2:D:288:GLU:H	2.31	0.44
4:F:160:ILE:HD12	4:F:160:ILE:N	2.33	0.44
2:B:289:LEU:HG	2:B:365:ALA:HB2	2.00	0.44
4:F:304:THR:HG21	4:F:311:SER:HB2	1.99	0.44
1:A:21:TRP:CH2	1:A:63:PRO:HB3	2.52	0.44
2:B:151:LEU:O	2:B:155:ILE:HG13	2.18	0.44
1:C:66:VAL:HG23	1:C:125:LEU:HD12	2.00	0.44
1:C:81:GLY:O	1:C:84:ARG:NH1	2.47	0.44
1:C:328:VAL:O	1:C:332:ILE:HG13	2.17	0.44
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.99	0.43
1:C:302:MET:HE2	1:C:302:MET:CA	2.47	0.43
4:F:7:ARG:CD	4:F:40:MET:HE2	2.48	0.43
1:A:123:ARG:HG3	1:A:123:ARG:HH11	1.83	0.43
2:B:64:ILE:HG12	2:B:119:VAL:HG12	2.00	0.43
2:B:170:MET:HE3	2:B:170:MET:HB3	1.52	0.43
2:B:273:LEU:HD23	2:B:273:LEU:HA	1.66	0.43
2:D:286:VAL:HB	2:D:287:PRO:HD3	2.00	0.43
1:C:233:GLN:HG3	1:C:368:LEU:HD22	2.00	0.43
1:A:33:ASP:O	1:A:60:LYS:HD2	2.18	0.43
1:A:100:ALA:HA	2:B:252:LYS:HG3	1.99	0.43
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.01	0.43
2:B:134:GLN:HA	2:B:165:ASN:O	2.19	0.43
4:F:100:ILE:HD12	4:F:128:ARG:HB3	2.00	0.43
4:F:269:GLN:HE21	4:F:273:ASP:CG	2.27	0.43
4:F:292:ARG:NH1	4:F:380:HIS:HB3	2.34	0.43
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.53	0.43
2:B:174:LYS:HD2	2:B:205:GLU:HG3	2.00	0.43
2:B:381:ILE:CG2	2:B:415:MET:HE1	2.49	0.43
2:B:179:VAL:HG12	1:C:348:PRO:HG2	2.01	0.43
2:B:262:ARG:NH2	2:B:421[A]:GLU:OE2	2.51	0.43
2:D:253:LEU:HD13	11:D:502:GX5:C09	2.49	0.43
2:D:397:TRP:CD1	2:D:397:TRP:N	2.87	0.43
1:C:135:PHE:O	1:C:136:LEU:HD23	2.18	0.43
4:F:235:ASP:O	4:F:235:ASP:CG	2.62	0.43
1:A:385:ALA:HB2	1:A:432:TYR:CG	2.54	0.43
2:D:190:HIS:ND1	2:D:411:ALA:HA	2.34	0.43
2:D:237:THR:O	2:D:241:ARG:HG3	2.19	0.43
4:F:198:LYS:HE3	4:F:239:HIS:O	2.19	0.43
4:F:247:LYS:NZ	4:F:253:TYR:OH	2.52	0.43
1:A:274:PRO:HB3	1:A:286:LEU:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:328:VAL:O	1:A:332:ILE:HG13	2.19	0.42
2:B:162:ARG:O	10:B:503:MES:H52	2.19	0.42
2:D:238:THR:HG21	2:D:318:ARG:CD	2.48	0.42
2:D:377:LEU:C	2:D:377:LEU:HD23	2.44	0.42
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.01	0.42
2:D:350:LYS:HG2	11:D:502:GX5:C21	2.50	0.42
3:E:75:LYS:O	3:E:79:GLU:HG3	2.19	0.42
1:C:156:ARG:NH1	12:C:617:HOH:O	2.49	0.42
2:D:151:LEU:O	2:D:155:ILE:HG13	2.20	0.42
2:D:170:MET:HB2	2:D:170:MET:HE2	1.71	0.42
2:D:270:PHE:O	2:D:298:ASN:HB3	2.19	0.42
1:C:164:LYS:HE2	1:C:164:LYS:HB2	1.83	0.42
1:C:425:MET:HE3	1:C:425:MET:HB3	1.66	0.42
2:D:256:ASN:HB3	11:D:502:GX5:C17	2.49	0.42
4:F:89:GLU:CD	4:F:89:GLU:N	2.77	0.42
1:A:36:MET:HE1	1:A:49:PHE:CZ	2.55	0.42
1:C:67:PHE:HB2	1:C:92:LEU:HD23	2.00	0.42
4:F:209:HIS:HA	4:F:311:SER:O	2.19	0.42
1:A:215:ARG:NH2	1:A:299:ALA:HB1	2.35	0.42
2:D:5:VAL:CG2	2:D:133:PHE:HD2	2.31	0.42
2:D:101:TRP:CE3	2:D:403:MET:HE1	2.55	0.42
2:D:191:GLN:HE22	3:E:126:LYS:NZ	2.17	0.42
1:A:237:SER:OG	1:A:376:CYS:HB3	2.19	0.42
1:C:392:ASP:OD2	1:C:429:GLU:OE2	2.37	0.42
4:F:244:CYS:SG	4:F:245:ILE:N	2.92	0.42
2:B:2:ARG:HD2	2:B:3:GLU:CD	2.45	0.42
1:C:192:HIS:CG	1:C:421:ALA:HA	2.55	0.42
2:B:28:HIS:HD1	2:B:47:ILE:HD13	1.84	0.42
4:F:271:LEU:CD2	4:F:275[B]:LEU:HD12	2.49	0.42
2:B:48:ASN:H	2:B:48:ASN:HD22	1.64	0.41
1:C:36:MET:HE1	1:C:49:PHE:CD1	2.55	0.41
2:D:207:LEU:HD11	2:D:229:VAL:CG2	2.50	0.41
3:E:121:GLU:HA	3:E:124:GLN:OE1	2.19	0.41
4:F:149:ALA:HB1	4:F:182:ILE:HG22	1.99	0.41
1:A:401:LYS:HZ1	2:B:428:ALA:HB1	1.83	0.41
2:B:2:ARG:NH1	2:B:2:ARG:CG	2.83	0.41
2:B:316:ILE:N	2:B:316:ILE:CD1	2.83	0.41
2:B:395:LEU:HD23	2:B:395:LEU:HA	1.87	0.41
1:C:48:SER:HB3	1:C:243:ARG:C	2.46	0.41
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.51	0.41
2:D:401:GLU:O	3:E:137:LYS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:163:ILE:HG21	2:B:250:LEU:HB3	2.02	0.41
2:B:395:LEU:HD13	2:B:405:GLU:HG2	2.03	0.41
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.84	0.41
1:C:254:GLU:HG2	1:C:352:LYS:HE2	2.02	0.41
2:D:310:TYR:CD1	2:D:371:SER:HB2	2.55	0.41
2:D:320:ARG:HH11	2:D:320:ARG:HG3	1.86	0.41
4:F:131:PHE:CD1	4:F:131:PHE:C	2.96	0.41
1:A:263:PRO:O	1:A:266:HIS:HD2	2.04	0.41
2:B:12:CYS:HB2	9:B:501:GDP:C8	2.56	0.41
4:F:73:ARG:HH11	4:F:73:ARG:CG	2.33	0.41
4:F:166:ALA:O	4:F:170:LEU:HD12	2.20	0.41
1:A:69:ASP:O	1:A:94:THR:HA	2.21	0.41
1:A:434:GLU:HG3	1:A:435:VAL:N	2.35	0.41
2:B:16[A]:ILE:HD11	2:B:136:THR:HB	2.02	0.41
2:B:156:ARG:HD2	10:B:503:MES:O1	2.20	0.41
2:B:343:GLU:H	2:B:343:GLU:CD	2.26	0.41
2:D:393:ALA:O	2:D:395:LEU:HD12	2.20	0.41
4:F:102:PRO:HG2	4:F:177:GLY:C	2.46	0.41
4:F:271:LEU:HD23	4:F:275[B]:LEU:HD12	2.03	0.41
2:B:42:LEU:HD23	2:B:243:PRO:HG2	2.02	0.41
2:B:101:TRP:HB2	2:B:184:ASN:OD1	2.21	0.41
2:B:61:PRO:HD3	2:B:84:ILE:HG12	2.03	0.41
2:B:190:HIS:CE1	2:B:414:ASN:HD22	2.38	0.41
2:D:2:ARG:HB2	2:D:129:CYS:O	2.20	0.41
4:F:198:LYS:HE3	4:F:239:HIS:HA	2.02	0.41
1:A:31:GLN:HB3	1:A:33:ASP:OD1	2.21	0.41
1:A:125:LEU:HD23	1:A:125:LEU:HA	1.82	0.41
2:B:64:ILE:HD13	2:B:120:VAL:HG22	2.03	0.41
1:C:7:ILE:HG21	1:C:153:LEU:HD21	2.03	0.41
1:C:266:HIS:CD2	1:C:266:HIS:O	2.74	0.41
1:C:270:ALA:O	1:C:302:MET:HB2	2.21	0.41
4:F:93:TRP:CD2	4:F:290:ILE:HG12	2.56	0.41
2:B:72:THR:N	12:B:602:HOH:O	2.54	0.41
2:B:381:ILE:HG22	2:B:415:MET:HE1	2.02	0.41
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.56	0.41
2:D:170:MET:HG2	2:D:377:LEU:HD21	2.03	0.41
4:F:149:ALA:HB2	4:F:182:ILE:HG22	2.00	0.41
4:F:242:ASN:OD1	4:F:242:ASN:N	2.54	0.41
1:C:30:ILE:HD11	1:C:36:MET:HE2	2.02	0.40
1:C:248:LEU:HD11	1:C:357:TYR:OH	2.22	0.40
4:F:166:ALA:HA	4:F:169:LEU:HD12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:PHE:CD1	1:A:138:PHE:N	2.89	0.40
2:B:18:ALA:O	2:B:22:GLU:HG3	2.21	0.40
2:D:406:MET:O	2:D:410:GLU:HG3	2.22	0.40
4:F:217:ARG:HG3	4:F:218:GLU:N	2.36	0.40
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.56	0.40
1:C:250:VAL:CG2	1:C:255:PHE:CE2	3.02	0.40
4:F:229:ASN:OD1	4:F:231:ALA:HB3	2.21	0.40
4:F:298:ILE:C	4:F:300:PRO:HD2	2.46	0.40
1:C:351:PHE:N	1:C:351:PHE:CD1	2.88	0.40
2:D:392:LYS:C	2:D:395:LEU:CD1	2.90	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	439/450 (98%)	424 (97%)	15 (3%)	0	100	100
1	C	446/450 (99%)	431 (97%)	15 (3%)	0	100	100
2	B	423/445 (95%)	412 (97%)	11 (3%)	0	100	100
2	D	416/445 (94%)	395 (95%)	21 (5%)	0	100	100
3	E	121/143 (85%)	120 (99%)	1 (1%)	0	100	100
4	F	342/384 (89%)	322 (94%)	20 (6%)	0	100	100
All	All	2187/2317 (94%)	2104 (96%)	83 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	371/378 (98%)	366 (99%)	5 (1%)	61	76
1	C	379/378 (100%)	364 (96%)	15 (4%)	28	37
2	B	369/383 (96%)	366 (99%)	3 (1%)	73	84
2	D	362/383 (94%)	348 (96%)	14 (4%)	28	39
3	E	112/127 (88%)	110 (98%)	2 (2%)	51	66
4	F	314/342 (92%)	303 (96%)	11 (4%)	32	42
All	All	1907/1991 (96%)	1857 (97%)	50 (3%)	44	54

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	THR
1	A	177	VAL
1	A	193[A]	THR
1	A	193[B]	THR
1	A	381	THR
2	B	2	ARG
2	B	55	THR
2	B	214	THR
1	C	151[A]	SER
1	C	151[B]	SER
1	C	163	LYS
1	C	165[A]	SER
1	C	165[B]	SER
1	C	241	SER
1	C	250	VAL
1	C	251	ASP
1	C	315[A]	CYS
1	C	315[B]	CYS
1	C	336	LYS
1	C	338	LYS
1	C	347[A]	CYS
1	C	347[B]	CYS

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Mol	Chain	Res	Type
1	C	381	THR
2	D	8	GLN
2	D	26	ASP
2	D	75	SER
2	D	78	SER
2	D	84	ILE
2	D	116	VAL
2	D	177	ASP
2	D	188	SER
2	D	218	THR
2	D	245	GLN
2	D	246	LEU
2	D	285	THR
2	D	386	THR
2	D	413	SER
3	E	107	SER
3	E	133	VAL
4	F	12	SER
4	F	99	VAL
4	F	183	GLN
4	F	240	LEU
4	F	255[A]	ARG
4	F	255[B]	ARG
4	F	279	LEU
4	F	296[A]	MET
4	F	296[B]	MET
4	F	307	LEU
4	F	324	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	258	ASN
1	A	393	HIS
2	B	165	ASN
2	B	247	ASN
2	B	375	GLN
1	C	15	GLN
1	C	249	ASN
1	C	256	GLN
1	C	358	GLN

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Mol	Chain	Res	Type
2	D	15	GLN
2	D	94	GLN
2	D	99	ASN
2	D	329	GLN
2	D	335	ASN
3	E	92	ASN
3	E	103	GLN
4	F	183	GLN
4	F	234	GLN
4	F	246	GLN
4	F	260	ASN
4	F	269	GLN
4	F	310	GLN
4	F	333	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 6 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
9	GDP	D	501	-	29,30,30	1.13	4 (13%)	45,47,47	2.52	12 (26%)
10	MES	B	503	-	12,12,12	2.05	1 (8%)	15,16,16	2.18	4 (26%)
9	GDP	B	501	6	29,30,30	1.26	4 (13%)	45,47,47	1.65	7 (15%)
5	GTP	A	501	6	33,34,34	0.95	3 (9%)	50,54,54	1.50	9 (18%)
11	GX5	B	505	-	23,23,23	1.33	3 (13%)	27,32,32	2.17	8 (29%)
5	GTP	C	501	6	33,34,34	0.84	1 (3%)	50,54,54	1.56	8 (16%)
11	GX5	D	502	-	23,23,23	1.40	3 (13%)	27,32,32	2.60	8 (29%)
10	MES	B	504	-	12,12,12	2.82	1 (8%)	15,16,16	1.52	3 (20%)

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
9	GDP	D	501	-	-	3/16/32/32	0/3/3/3
10	MES	B	503	-	-	5/6/14/14	0/1/1/1
9	GDP	B	501	6	-	5/16/32/32	0/3/3/3
5	GTP	A	501	6	-	9/22/38/38	0/3/3/3
11	GX5	B	505	-	-	2/10/10/10	0/3/3/3
5	GTP	C	501	6	-	9/22/38/38	0/3/3/3
11	GX5	D	502	-	-	2/10/10/10	0/3/3/3
10	MES	B	504	-	-	3/6/14/14	0/1/1/1

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	504	MES	C8-S	-9.63	1.64	1.77
10	B	503	MES	C8-S	-6.78	1.68	1.77
11	D	502	GX5	C09-N10	3.81	1.33	1.30
11	B	505	GX5	C09-N10	3.43	1.33	1.30
9	B	501	GDP	C5-C4	3.19	1.47	1.38
9	D	501	GDP	C5-C4	3.02	1.47	1.38
11	D	502	GX5	C07-N12	2.68	1.45	1.39
11	B	505	GX5	C07-N12	2.56	1.44	1.39
5	A	501	GTP	PA-O3A	2.53	1.62	1.59
9	B	501	GDP	C6-N1	-2.49	1.34	1.38
11	B	505	GX5	C05-C04	-2.48	1.38	1.42
9	B	501	GDP	C5-N7	-2.48	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	501	GDP	PA-O3A	2.46	1.62	1.59
11	D	502	GX5	C14-N12	2.23	1.47	1.42
9	B	501	GDP	C4-N9	-2.20	1.32	1.38
9	D	501	GDP	C2-N3	2.19	1.38	1.33
9	D	501	GDP	C5-N7	-2.17	1.34	1.39
5	C	501	GTP	C2-N3	2.02	1.38	1.33
5	A	501	GTP	PB-O3B	2.02	1.61	1.59
5	A	501	GTP	C2-N3	2.00	1.38	1.33

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	502	GX5	N10-C09-N08	-9.85	120.81	130.58
9	D	501	GDP	C5-C4-N3	-8.49	114.87	128.39
11	B	505	GX5	N10-C09-N08	-8.08	122.56	130.58
9	D	501	GDP	C2-N3-C4	6.29	123.14	112.30
9	D	501	GDP	N9-C4-N3	6.29	138.53	125.95
10	B	503	MES	C5-N4-C3	6.20	122.20	108.84
9	D	501	GDP	C2-N1-C6	-6.09	114.07	125.11
11	D	502	GX5	CL1-C09-N10	5.02	119.88	115.72
9	B	501	GDP	C5-C4-N3	-5.02	120.40	128.39
5	C	501	GTP	C5-C4-N3	-4.38	121.42	128.39
5	A	501	GTP	C2-N3-C4	4.33	119.76	112.30
9	D	501	GDP	O6-C6-C5	-4.27	115.27	126.53
9	B	501	GDP	C2-N3-C4	4.08	119.33	112.30
9	B	501	GDP	N9-C4-N3	3.86	133.67	125.95
11	D	502	GX5	C09-N08-C07	3.85	122.40	111.13
5	C	501	GTP	C2-N3-C4	3.79	118.83	112.30
5	A	501	GTP	C5-C4-N3	-3.78	122.37	128.39
11	B	505	GX5	CL1-C09-N10	3.52	118.63	115.72
9	D	501	GDP	C5-C6-N1	3.51	122.18	113.25
9	B	501	GDP	C6-C5-N7	3.50	136.66	130.29
5	C	501	GTP	N9-C8-N7	-3.33	107.23	113.40
11	B	505	GX5	C09-N08-C07	3.32	120.86	111.13
9	B	501	GDP	O2B-PB-O3A	3.29	115.67	104.64
5	C	501	GTP	C8-N7-C5	3.27	110.09	104.26
11	D	502	GX5	C01-N06-C05	3.08	120.94	117.31
10	B	503	MES	O3S-S-C8	3.02	111.91	106.00
9	D	501	GDP	C4-C5-N7	-3.00	105.91	110.67
5	A	501	GTP	N9-C8-N7	-2.96	107.92	113.40
11	D	502	GX5	CL1-C09-N08	2.94	119.32	115.17
11	B	505	GX5	C01-N06-C05	2.90	120.72	117.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	504	MES	C5-N4-C3	2.81	114.89	108.84
5	C	501	GTP	O3B-PB-O1B	2.71	118.87	110.70
10	B	503	MES	C7-N4-C5	2.63	118.26	111.24
5	C	501	GTP	C2-N1-C6	-2.60	120.40	125.11
5	A	501	GTP	C8-N7-C5	2.59	108.88	104.26
11	B	505	GX5	CL1-C09-N08	2.58	118.81	115.17
5	C	501	GTP	N9-C4-N3	2.58	131.11	125.95
9	D	501	GDP	C6-C5-N7	2.50	134.84	130.29
9	B	501	GDP	C4-C5-N7	-2.48	106.73	110.67
9	D	501	GDP	C8-N7-C5	2.46	108.63	104.26
11	B	505	GX5	C02-C03-C04	-2.45	116.74	120.09
5	C	501	GTP	C4-C5-N7	-2.41	106.85	110.67
9	D	501	GDP	N2-C2-N3	-2.39	115.00	119.67
9	D	501	GDP	O4'-C1'-C2'	-2.34	101.60	106.62
11	D	502	GX5	C02-C03-C04	-2.33	116.91	120.09
11	D	502	GX5	N08-C07-N12	2.30	118.50	116.09
5	A	501	GTP	N2-C2-N1	2.27	121.55	116.76
11	B	505	GX5	N08-C07-N12	2.24	118.44	116.09
5	A	501	GTP	C2-N1-C6	-2.24	121.05	125.11
5	A	501	GTP	C4-C5-N7	-2.22	107.16	110.67
11	D	502	GX5	C02-C01-N06	-2.21	120.72	123.97
9	D	501	GDP	O2A-PA-O3A	2.21	113.24	107.27
10	B	503	MES	C7-N4-C3	2.19	117.09	111.24
9	B	501	GDP	O6-C6-C5	-2.15	120.86	126.53
11	B	505	GX5	C02-C01-N06	-2.12	120.85	123.97
5	A	501	GTP	C6-C5-N7	2.10	134.12	130.29
5	A	501	GTP	O6-C6-C5	-2.04	121.15	126.53
10	B	504	MES	C7-N4-C5	-2.02	105.85	111.24
10	B	504	MES	O1-C6-C5	-2.01	107.44	111.77

There are no chirality outliers.

All (38) torsion outliers are listed below:

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

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Mol	Chain	Res	Type	Atoms
9	B	501	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A
10	B	503	MES	C8-C7-N4-C5
10	B	503	MES	C7-C8-S-O1S
10	B	503	MES	C7-C8-S-O2S
10	B	503	MES	C7-C8-S-O3S
11	D	502	GX5	C18-C17-O20-C21
11	D	502	GX5	C16-C17-O20-C21
11	B	505	GX5	C18-C17-O20-C21
11	B	505	GX5	C16-C17-O20-C21
10	B	503	MES	C8-C7-N4-C3
10	B	504	MES	C8-C7-N4-C3
10	B	504	MES	C8-C7-N4-C5
5	A	501	GTP	PB-O3B-PG-O1G
9	B	501	GDP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
10	B	504	MES	C7-C8-S-O1S
5	C	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A
9	B	501	GDP	PB-O3A-PA-O1A
5	A	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3A-PA-O1A

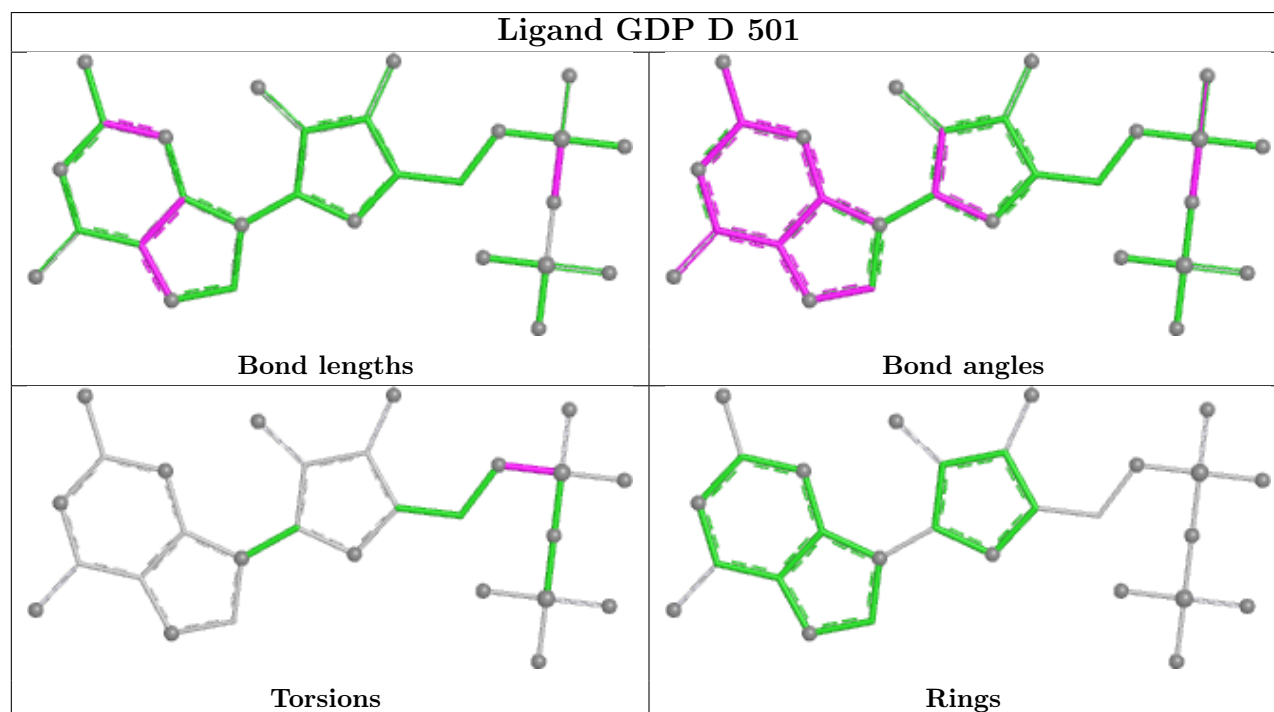
There are no ring outliers.

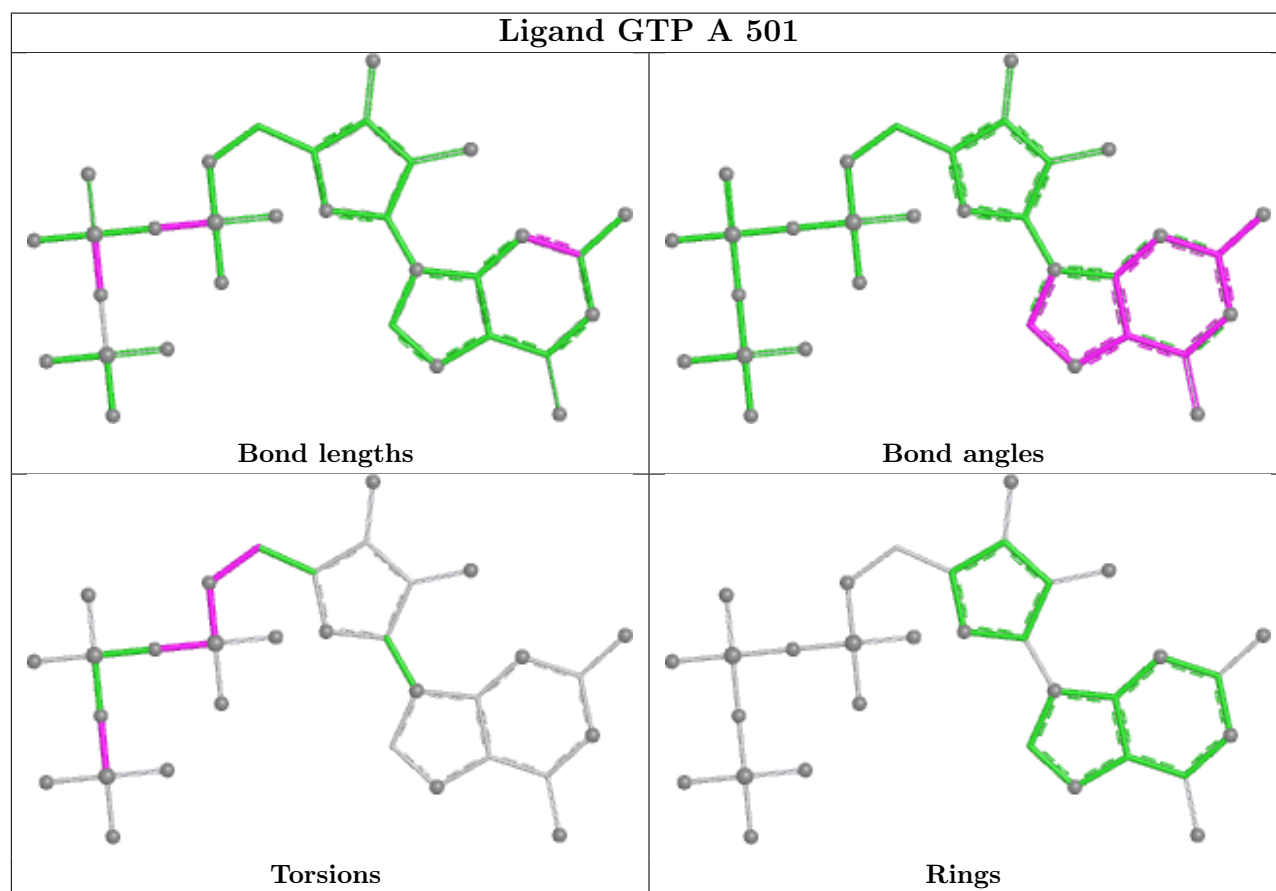
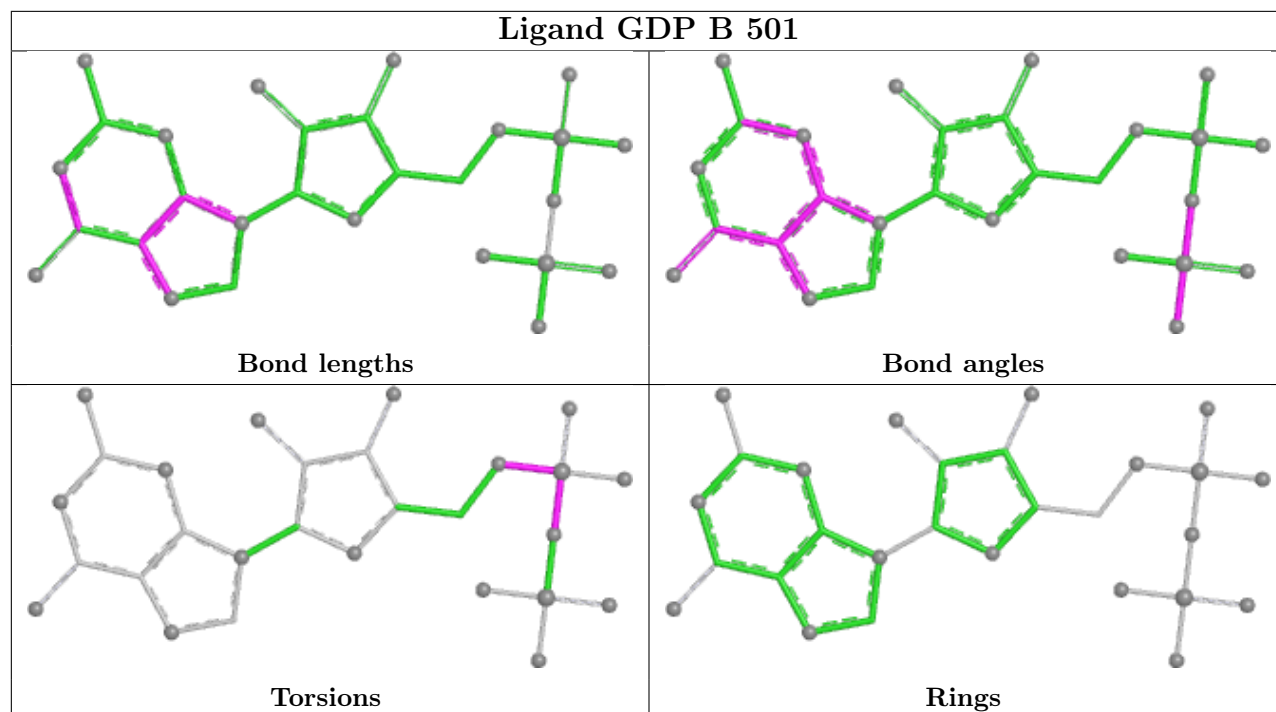
5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	501	GDP	3	0
10	B	503	MES	3	0
9	B	501	GDP	1	0
11	D	502	GX5	3	0
10	B	504	MES	1	0

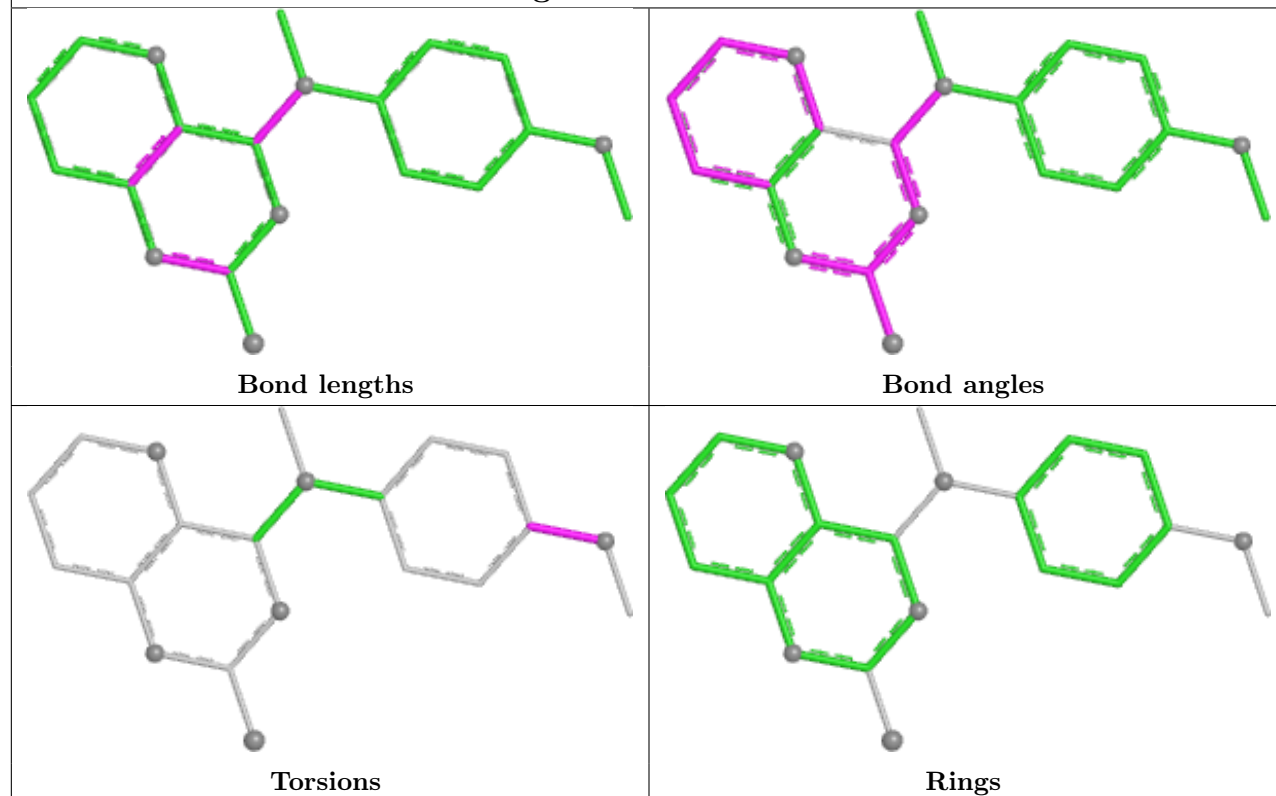
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

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.

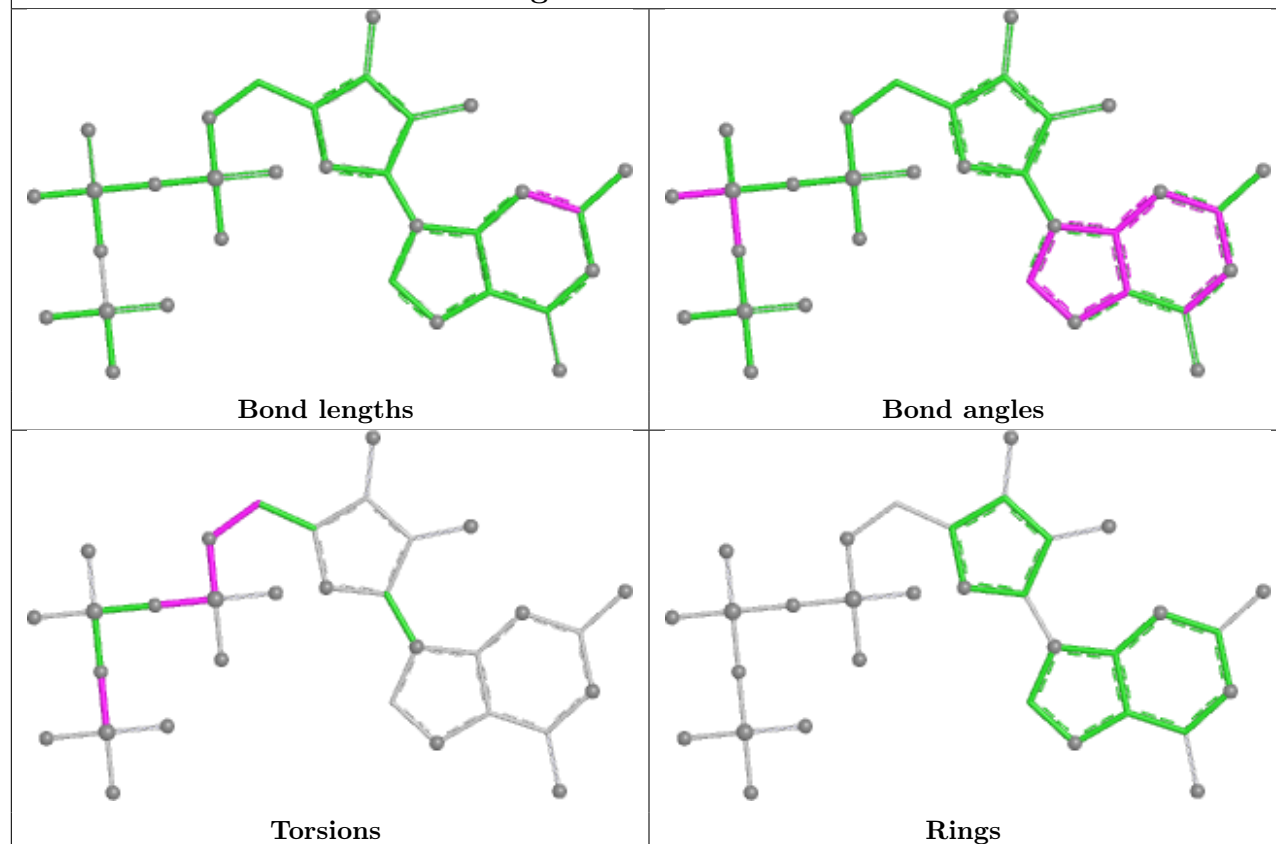


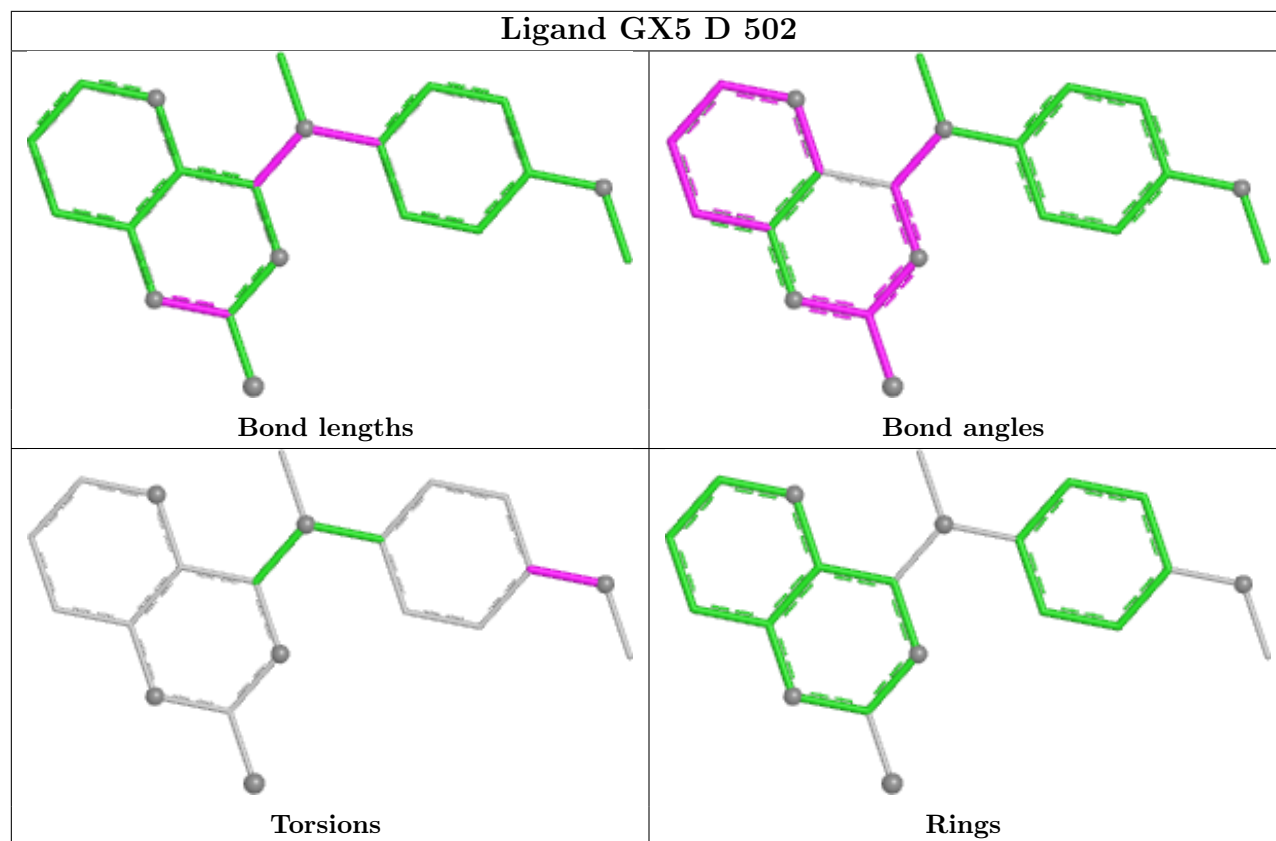


Ligand GX5 B 505



Ligand GTP C 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	0.18	8 (1%) 67 72	31, 52, 75, 89	4 (0%)
1	C	440/450 (97%)	-0.20	9 (2%) 65 70	26, 43, 63, 79	8 (1%)
2	B	424/445 (95%)	0.23	15 (3%) 47 53	24, 51, 81, 114	3 (0%)
2	D	420/445 (94%)	0.83	37 (8%) 15 18	37, 69, 97, 115	1 (0%)
3	E	123/143 (86%)	0.81	9 (7%) 21 24	30, 65, 100, 126	2 (1%)
4	F	346/384 (90%)	1.21	88 (25%) 1 1	32, 73, 137, 156	4 (1%)
All	All	2190/2317 (94%)	0.44	166 (7%) 20 22	24, 56, 101, 156	22 (1%)

All (166) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	245	ILE	7.1
4	F	160	ILE	5.7
2	B	428	ALA	4.9
4	F	240	LEU	4.8
4	F	169	LEU	4.7
4	F	249	TYR	4.1
4	F	136	ASN	4.0
4	F	125	THR	4.0
2	B	283	ALA	3.9
3	E	143	ALA	3.9
4	F	186	LEU	3.9
2	B	57	ASN	3.9
4	F	98	TYR	3.8
2	B	55	THR	3.8
4	F	162	ILE	3.8
2	D	55	THR	3.7
4	F	132	LEU	3.7
4	F	141	GLY	3.7
2	B	274	THR	3.5

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Mol	Chain	Res	Type	RSRZ
4	F	181	VAL	3.5
4	F	362	ALA	3.5
4	F	225	SER	3.5
1	A	437	VAL	3.5
4	F	135	TYR	3.5
4	F	182	ILE	3.5
4	F	161	LEU	3.4
2	D	394	PHE	3.4
2	D	284	LEU	3.4
4	F	99	VAL	3.4
4	F	149	ALA	3.3
4	F	104	ASN	3.3
2	B	282	ARG	3.3
4	F	233	PHE	3.3
4	F	130	VAL	3.3
4	F	152	SER	3.3
4	F	253	TYR	3.3
4	F	159	GLY	3.2
2	D	16	ILE	3.2
2	B	281	TYR	3.2
1	A	262	TYR	3.1
4	F	166	ALA	3.1
4	F	101	TYR	3.1
2	D	96	GLY	3.1
1	C	440	VAL	3.1
4	F	179	VAL	3.0
1	A	88	HIS	3.0
2	B	214	THR	3.0
4	F	372	THR	3.0
2	B	275	SER	3.0
3	E	139	LEU	2.9
2	D	99	ASN	2.9
4	F	158	GLU	2.9
4	F	100	ILE	2.9
4	F	241	THR	2.8
4	F	150	LYS	2.8
4	F	170	LEU	2.8
4	F	191	LEU	2.8
2	D	389	PHE	2.8
4	F	172	PHE	2.8
2	D	72	THR	2.8
2	D	218	THR	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	397	TRP	2.8
4	F	199	PHE	2.8
4	F	320	MET	2.7
4	F	231	ALA	2.7
1	C	163	LYS	2.7
2	D	179	VAL	2.7
4	F	228	TYR	2.6
4	F	236	LYS	2.6
4	F	256	TYR	2.6
4	F	139	ARG	2.6
2	D	92	PHE	2.6
2	D	180	VAL	2.6
4	F	102	PRO	2.6
4	F	148	ILE	2.6
4	F	198	LYS	2.6
4	F	103	THR	2.6
4	F	163	SER	2.6
2	B	247	ASN	2.5
1	A	42	ILE	2.5
1	C	357	TYR	2.5
4	F	275[A]	LEU	2.5
4	F	168	GLU	2.5
2	B	427	ASP	2.5
3	E	59	GLU	2.5
1	A	282	TYR	2.5
4	F	144	GLY	2.5
4	F	244	CYS	2.4
4	F	331	GLU	2.4
2	D	116	VAL	2.4
2	D	406	MET	2.4
2	B	245	GLN	2.4
4	F	176	GLN	2.4
4	F	146	VAL	2.4
4	F	173	ILE	2.4
1	A	91	GLN	2.4
3	E	45	PRO	2.4
2	D	98	GLY	2.4
1	C	340	SER	2.4
4	F	239	HIS	2.4
4	F	128	ARG	2.4
4	F	255[A]	ARG	2.4
2	D	54	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
2	D	393	ALA	2.4
4	F	167	SER	2.4
2	D	395	LEU	2.4
4	F	230	SER	2.3
2	D	85	PHE	2.3
1	A	37	PRO	2.3
2	D	296	SER	2.3
3	E	48	GLU	2.3
4	F	27	TRP	2.3
4	F	379	HIS	2.3
2	D	356	ILE	2.3
2	D	80	PRO	2.3
4	F	165	GLU	2.3
4	F	192	LEU	2.2
4	F	196	HIS	2.2
2	D	42	LEU	2.2
2	D	144	GLY	2.2
1	A	281	ALA	2.2
1	C	179	THR	2.2
2	B	2	ARG	2.2
4	F	227	PRO	2.2
2	B	40	SER	2.2
2	D	95	SER	2.2
2	D	226	ASN	2.2
4	F	126	ASP	2.2
1	C	338	LYS	2.2
2	B	280	GLN	2.2
4	F	234	GLN	2.2
4	F	243	HIS	2.2
3	E	28	SER	2.2
4	F	13	VAL	2.1
1	C	283	HIS	2.1
2	D	245	GLN	2.1
4	F	133	ALA	2.1
4	F	223	THR	2.1
2	D	390	ARG	2.1
3	E	6	MET	2.1
4	F	251	LYS	2.1
4	F	85	PRO	2.1
4	F	334	GLY	2.1
2	D	126	SER	2.1
2	D	405	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	282	TYR	2.1
4	F	235	ASP	2.1
4	F	180	HIS	2.1
3	E	133	VAL	2.1
2	D	90	PHE	2.1
4	F	131	PHE	2.1
4	F	263	PHE	2.1
1	C	232	SER	2.1
2	D	273	LEU	2.1
4	F	229	ASN	2.1
4	F	147	TRP	2.1
2	D	145[A]	SER	2.0
4	F	189	PRO	2.0
2	D	183	TYR	2.0
2	D	221	THR	2.0
4	F	164	SER	2.0
2	D	37	HIS	2.0
3	E	124	GLN	2.0
4	F	31	ARG	2.0
4	F	194	PRO	2.0
4	F	330	ILE	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	CL	A	504	1/1	0.85	0.12	87,87,87,87	0
9	GDP	D	501	28/28	0.87	0.14	57,65,77,80	0

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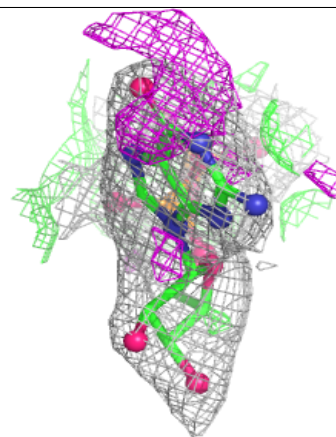
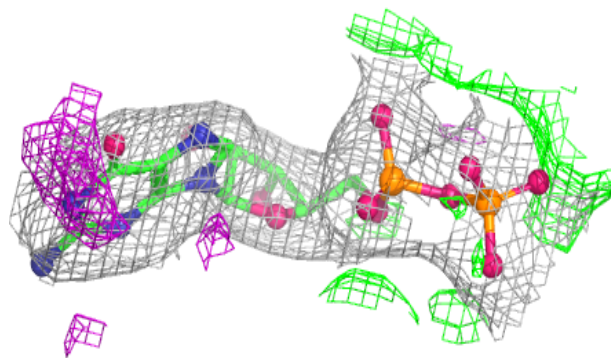
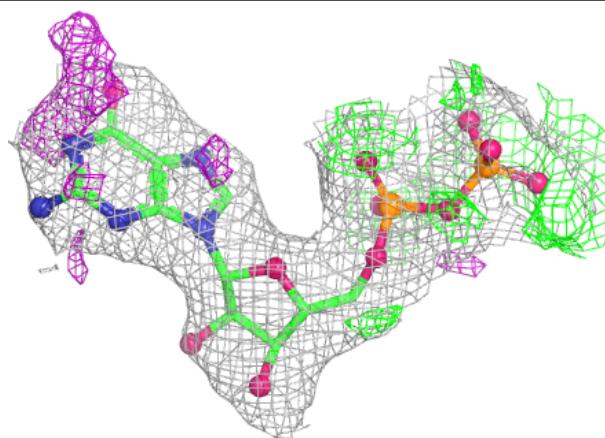
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	MES	B	504	12/12	0.87	0.13	71,72,84,97	0
10	MES	B	503	12/12	0.93	0.10	47,61,74,74	0
11	GX5	D	502	21/21	0.93	0.13	39,51,64,124	0
11	GX5	B	505	21/21	0.97	0.08	37,40,46,70	0
5	GTP	C	501	32/32	0.98	0.05	32,37,42,42	0
6	MG	B	502	1/1	0.98	0.05	42,42,42,42	0
7	CA	A	503	1/1	0.98	0.04	75,75,75,75	0
5	GTP	A	501	32/32	0.98	0.06	36,42,47,48	0
9	GDP	B	501	28/28	0.98	0.05	36,41,44,45	0
6	MG	A	502	1/1	0.99	0.07	41,41,41,41	0
7	CA	C	503	1/1	0.99	0.03	52,52,52,52	0
6	MG	C	502	1/1	0.99	0.09	40,40,40,40	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.

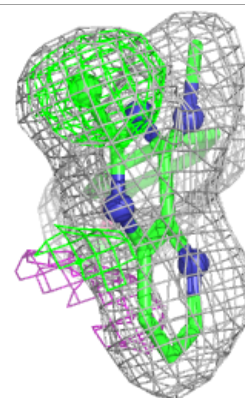
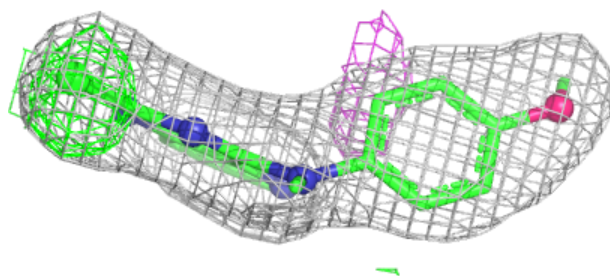
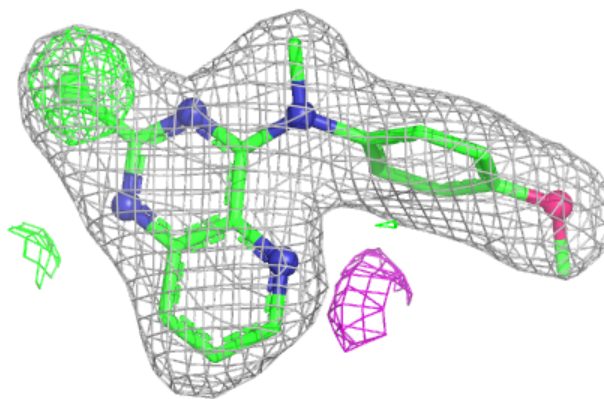
Electron density around GDP D 501:

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

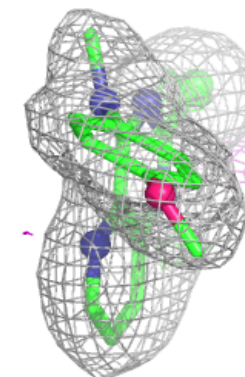
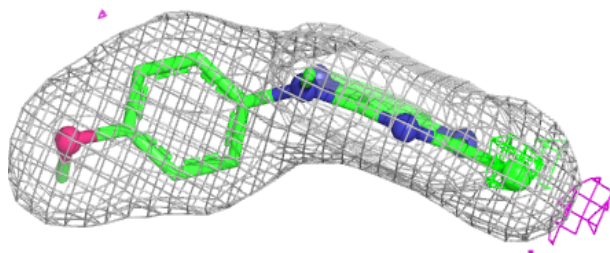
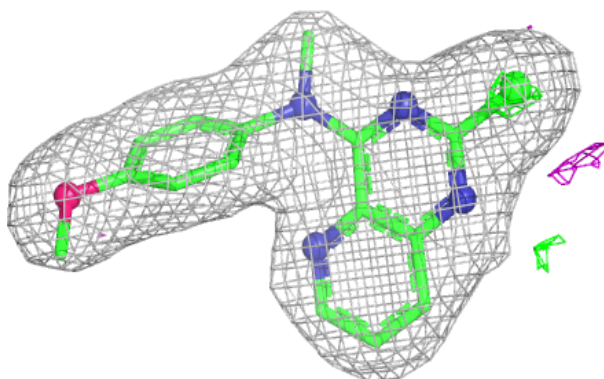


Electron density around GX5 D 502:

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

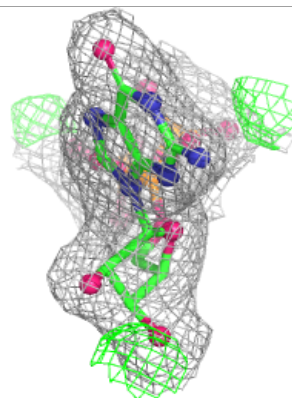
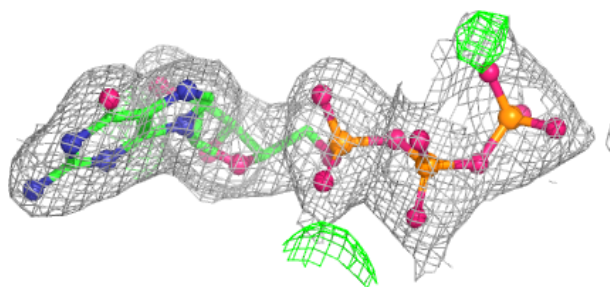
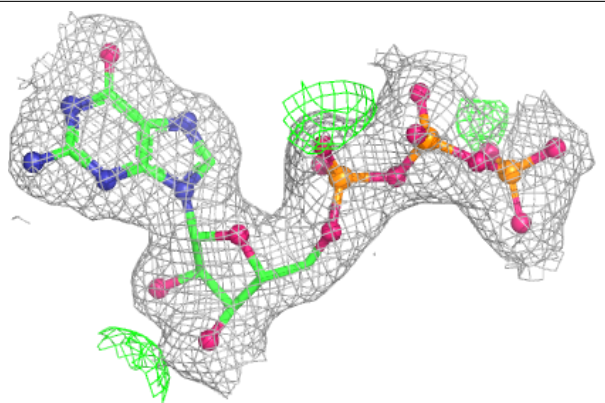
**Electron density around GX5 B 505:**

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

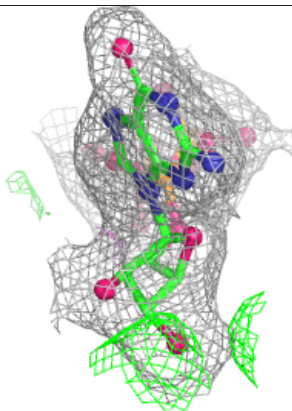
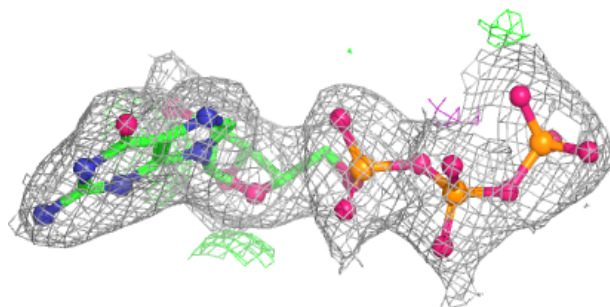
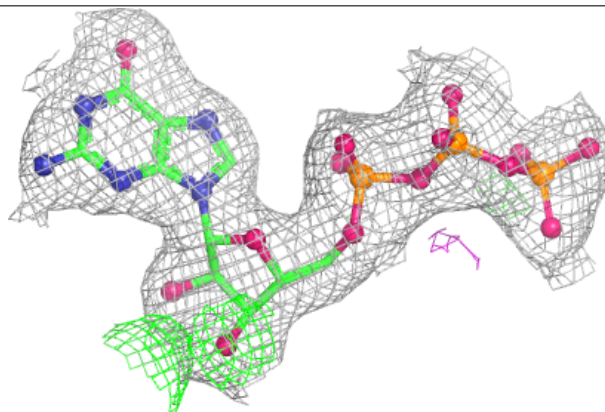


Electron density around GTP C 501:

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

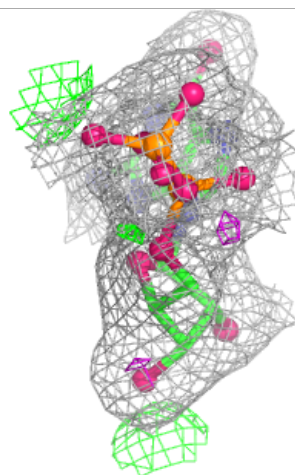
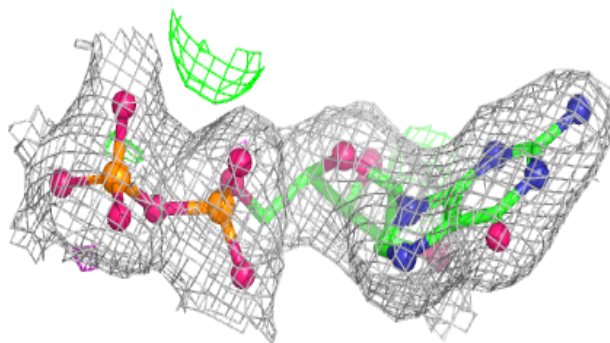
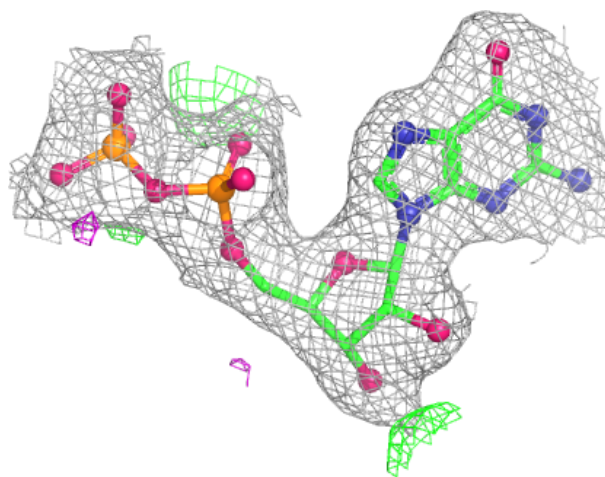
**Electron density around GTP A 501:**

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



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.