



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 08:11 PM UTC

PDB ID : 7XR1 / pdb_00007xr1
Title : Crystal structure of T2R-TTL-3a complex
Authors : Lun, T.; Wu, C.Y.
Deposited on : 2022-05-09
Resolution : 2.81 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

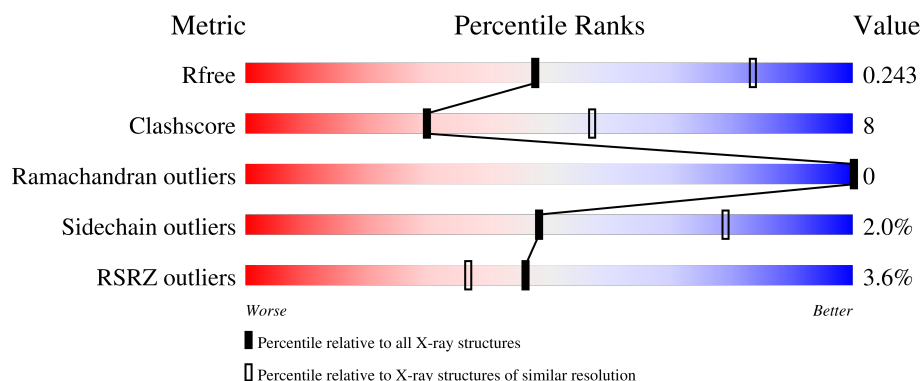
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

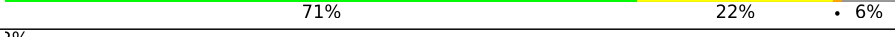
The reported resolution of this entry is 2.81 Å.

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	4591 (2.84-2.80)
Clashscore	190562	5010 (2.84-2.80)
Ramachandran outliers	187476	4916 (2.84-2.80)
Sidechain outliers	187428	4918 (2.84-2.80)
RSRZ outliers	180081	4594 (2.84-2.80)

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	
1	C	450	
2	B	445	
2	D	445	
3	E	143	

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Mol	Chain	Length	Quality of chain
4	F	384	14% 66% 23% • 10%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 17617 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	0	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		

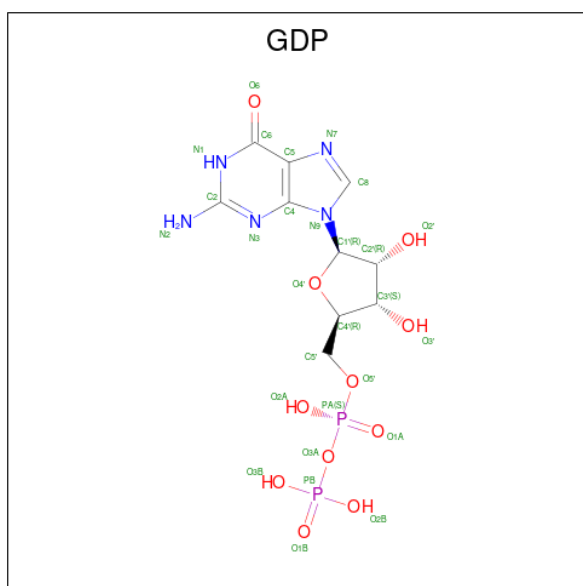
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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

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

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



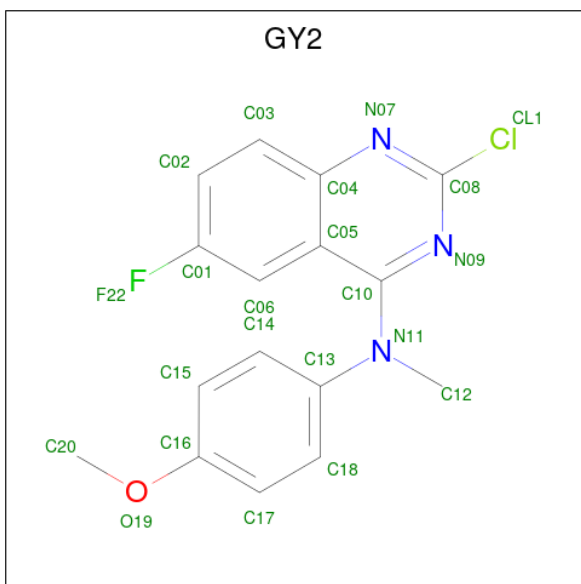
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
9	D	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- 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-6-fluoranyl-N-(4-methoxyphenyl)-N-methyl-quinazolin-4-amine (CCD ID: GY2) (formula: C₁₆H₁₃ClFN₃O) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	B	1	Total	C	Cl	F	N	O	0	0
			22	16	1	1	3	1		

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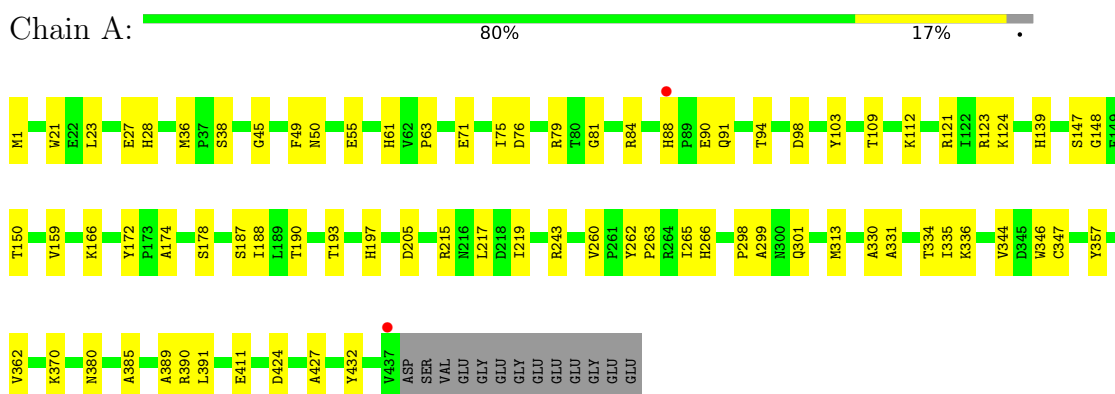
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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	D	1	Total	C	Cl	F	N	O	0	0
			22	16	1	1	3	1		

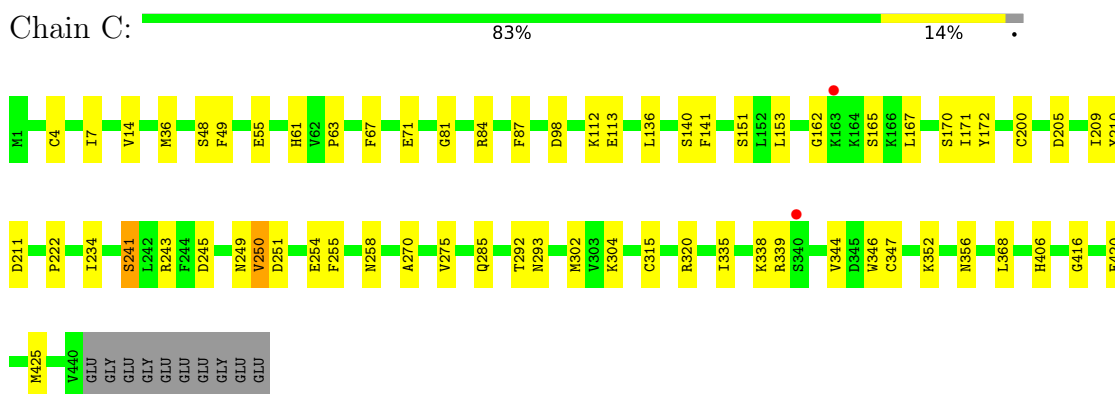
3 Residue-property plots

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.

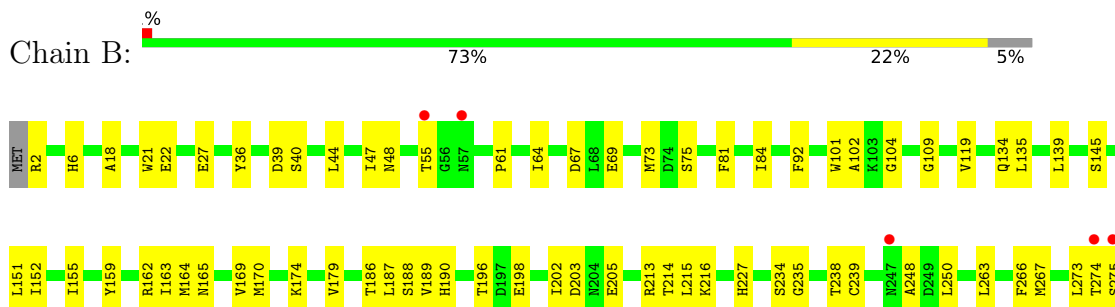
• Molecule 1: Tubulin alpha-1B chain



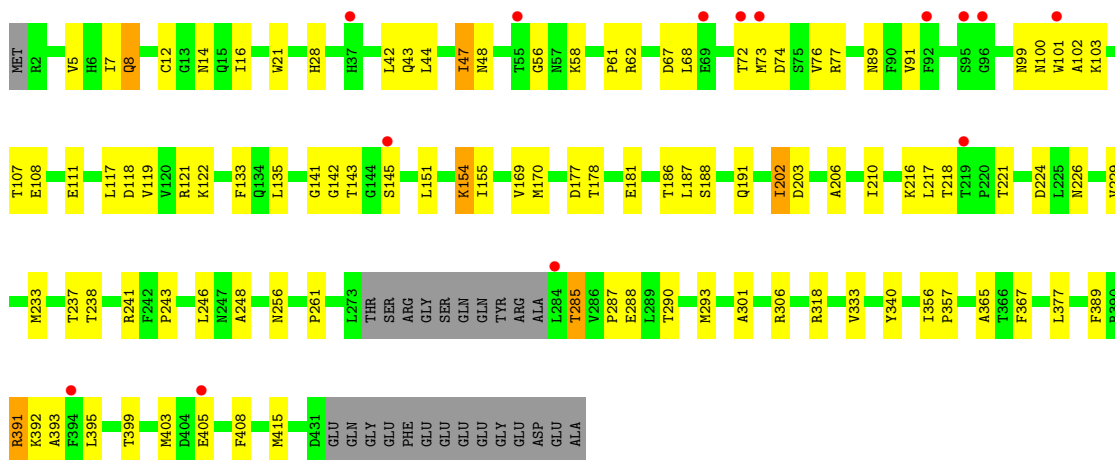
• Molecule 1: Tubulin alpha-1B chain



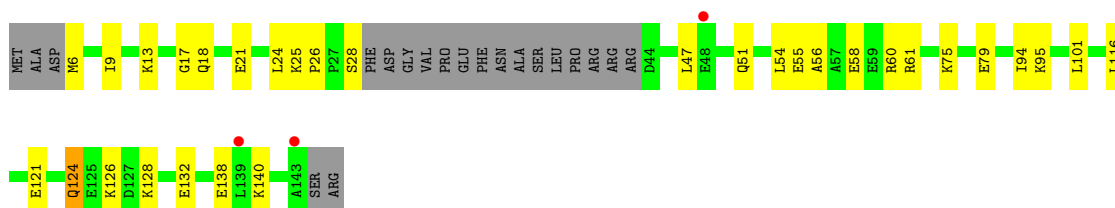
• Molecule 2: Tubulin beta chain



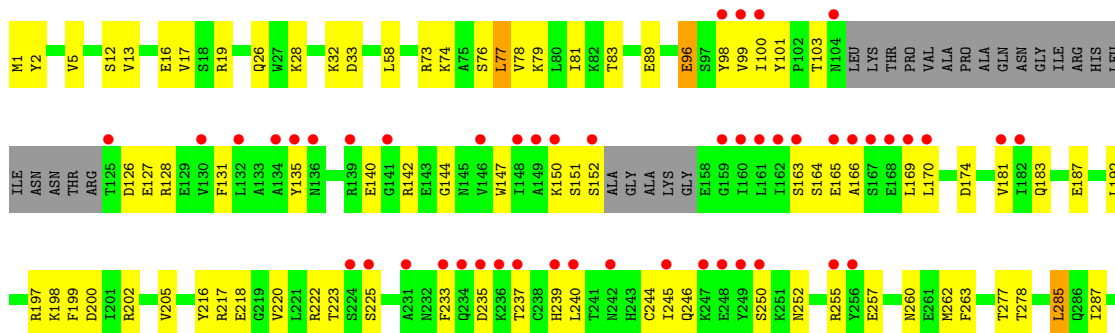
- Molecule 2: Tubulin beta chain

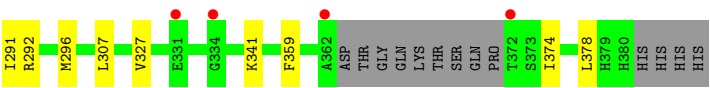


- Molecule 3: Stathmin-4



- Molecule 4: TTL





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.10Å 157.53Å 181.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.35 – 2.81 56.35 – 2.81	Depositor EDS
% Data completeness (in resolution range)	99.8 (56.35-2.81) 99.7 (56.35-2.81)	Depositor EDS
R_{merge}	0.31	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.203 , 0.246 0.202 , 0.243	Depositor DCC
R_{free} test set	2000 reflections (2.71%)	wwPDB-VP
Wilson B-factor (Å ²)	54.3	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	17617	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.65% 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: GY2, CL, GDP, MG, GTP, CA, MES

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.44	0/3517	0.64	0/4776
1	C	0.51	0/3570	0.71	0/4847
2	B	0.52	2/3436 (0.1%)	0.70	6/4653 (0.1%)
2	D	0.45	0/3368	0.65	1/4564 (0.0%)
3	E	0.47	0/1041	0.72	0/1382
4	F	0.38	0/2927	0.60	0/3955
All	All	0.47	2/17859 (0.0%)	0.67	7/24177 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	69	GLU	CA-C	-5.85	1.46	1.52
2	B	69	GLU	C-N	5.59	1.38	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	142	GLY	N-CA-C	8.85	124.10	112.77
2	B	69	GLU	N-CA-C	-5.42	100.75	109.58
2	B	266	PHE	CA-C-N	5.33	128.77	121.74
2	B	266	PHE	C-N-CA	5.33	128.77	121.74
2	B	299	MET	CA-CB-CG	-5.22	103.66	114.10
2	B	69	GLU	CA-C-N	-5.14	114.67	120.89
2	B	69	GLU	C-N-CA	-5.14	114.67	120.89

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3427	0	3341	50	0
1	C	3468	0	3388	39	0
2	B	3356	0	3237	67	0
2	D	3295	0	3166	65	0
3	E	1026	0	1042	22	0
4	F	2851	0	2826	58	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	0	0
9	D	28	0	11	2	0
10	B	24	0	24	1	0
11	B	22	0	0	0	0
11	D	22	0	0	1	0
All	All	17617	0	17071	294	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 8.

All (294) 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)
3:E:13:LYS:HB2	3:E:18:GLN:HB3	1.59	0.84
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.60	0.81
2:D:99:ASN:HD22	2:D:178:THR:HG21	1.46	0.81
2:D:391:ARG:HD2	2:D:393:ALA:HB2	1.65	0.78
4:F:192:LEU:HD22	4:F:262:MET:HE1	1.66	0.78
4:F:32:LYS:HG3	4:F:33:ASP:OD2	1.84	0.77
4:F:73:ARG:HG3	4:F:73:ARG:HH11	1.49	0.76
2:B:73:MET:HE2	2:B:92:PHE:HB3	1.69	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:235:GLY:O	2:B:238:THR:HG22	1.86	0.75
4:F:101:TYR:N	4:F:126:ASP:OD2	2.14	0.75
2:D:100:ASN:HD22	2:D:103:LYS:H	1.32	0.75
4:F:263:PHE:CE2	4:F:341:LYS:HD3	2.24	0.73
4:F:78:VAL:HG21	4:F:181:VAL:HG21	1.72	0.69
2:D:226:ASN:ND2	9:D:501:GDP:O6	2.25	0.69
2:B:280:GLN:HG2	2:B:281:TYR:H	1.59	0.68
1:C:36:MET:HE1	1:C:49:PHE:CE1	2.29	0.68
2:D:100:ASN:HD21	2:D:102:ALA:HB3	1.59	0.68
4:F:135:TYR:OH	4:F:165:GLU:HA	1.94	0.68
1:A:166:LYS:HE2	1:A:197:HIS:O	1.94	0.67
1:A:45:GLY:O	1:A:50:ASN:ND2	2.28	0.66
2:D:238:THR:HG21	2:D:318:ARG:HD2	1.78	0.65
4:F:144:GLY:HA3	4:F:187:GLU:OE1	1.97	0.65
4:F:128:ARG:HE	4:F:170:LEU:HD23	1.61	0.64
2:B:170:MET:HE2	2:B:377:LEU:HD21	1.79	0.63
2:D:102:ALA:HB2	2:D:403:MET:HE3	1.81	0.63
2:B:2:ARG:HD3	2:B:48:ASN:HD22	1.64	0.63
4:F:74:LYS:NZ	4:F:151:SER:O	2.32	0.63
1:C:234:ILE:HD13	1:C:302:MET:SD	2.39	0.63
1:A:90:GLU:O	1:A:121:ARG:HD2	1.99	0.62
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.81	0.62
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.39	0.61
4:F:263:PHE:HE2	4:F:341:LYS:HD3	1.66	0.61
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.81	0.61
2:D:5:VAL:HG12	2:D:62:ARG:HD3	1.83	0.61
2:B:293:MET:HG2	2:B:367:PHE:HB2	1.82	0.60
3:E:47:LEU:O	3:E:51:GLN:HG2	2.00	0.60
1:C:211[A]:ASP:OD2	1:C:304:LYS:NZ	2.33	0.60
1:A:88:HIS:N	1:A:91:GLN:OE1	2.28	0.60
1:A:336:LYS:HD3	3:E:24:LEU:HD13	1.82	0.59
1:A:36:MET:HE1	1:A:49:PHE:CE1	2.38	0.59
2:D:285:THR:HG23	2:D:287:PRO:HD2	1.82	0.59
2:D:145:SER:HB2	2:D:188:SER:OG	2.02	0.59
2:D:356:ILE:HD12	2:D:357:PRO:HD2	1.85	0.59
2:B:389:PHE:O	2:B:392:LYS:HD3	2.03	0.58
2:D:206:ALA:O	2:D:210:ILE:HG13	2.04	0.58
3:E:6:MET:HG3	3:E:24:LEU:HD23	1.86	0.58
4:F:292:ARG:HG3	4:F:378:LEU:HB3	1.85	0.58
1:A:55:GLU:HG2	1:A:61:HIS:CD2	2.38	0.58
2:B:81:PHE:O	2:B:84:ILE:HG22	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:238:THR:CG2	2:B:316:ILE:HG21	2.34	0.57
4:F:5:VAL:HG13	4:F:32:LYS:HA	1.84	0.57
2:B:267:MET:HG3	2:B:301:ALA:HB3	1.86	0.57
2:D:72:THR:O	2:D:76:VAL:HG23	2.04	0.57
1:A:346:TRP:H	1:A:346:TRP:CD1	2.22	0.57
2:B:163:ILE:HG21	2:B:250:LEU:HB3	1.86	0.57
2:D:102:ALA:HB2	2:D:403:MET:CE	2.35	0.57
4:F:16:GLU:HG2	4:F:19:ARG:HH21	1.68	0.57
4:F:13:VAL:O	4:F:17:VAL:HG23	2.05	0.57
1:A:262:TYR:CE2	1:A:346:TRP:CZ2	2.93	0.57
3:E:51:GLN:O	3:E:55:GLU:HG3	2.05	0.57
2:B:190:HIS:CE1	2:B:414:ASN:HD22	2.23	0.56
2:D:117:LEU:HD11	2:D:154:LYS:HG2	1.86	0.56
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.86	0.56
4:F:225:SER:OG	4:F:252:ASN:OD1	2.22	0.56
3:E:140:LYS:HD2	3:E:140:LYS:O	2.06	0.56
1:A:103:TYR:CE2	1:A:148:GLY:HA2	2.41	0.56
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.42	0.55
1:A:147:SER:HB2	1:A:190:THR:HB	1.87	0.55
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.87	0.55
1:C:245:ASP:OD1	1:C:245:ASP:N	2.40	0.55
1:A:215:ARG:NH2	1:A:299:ALA:O	2.40	0.55
2:B:358:PRO:HG2	2:B:361:LEU:HD13	1.88	0.55
3:E:121:GLU:O	3:E:124:GLN:HG3	2.07	0.55
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.89	0.54
1:A:75:ILE:O	1:A:79:ARG:HG3	2.07	0.54
2:B:39:ASP:OD1	2:B:40:SER:N	2.39	0.54
2:D:285:THR:HG22	2:D:288:GLU:CD	2.32	0.54
3:E:25:LYS:NZ	3:E:28:SER:HB2	2.22	0.54
2:B:18:ALA:O	2:B:22:GLU:HG3	2.08	0.54
2:B:165:ASN:HD22	2:B:198:GLU:HG3	1.72	0.54
2:D:107:THR:O	2:D:111:GLU:HG3	2.08	0.54
2:D:246:LEU:CD1	2:D:248:ALA:HB2	2.39	0.53
4:F:197:ARG:NH2	4:F:257:GLU:OE2	2.38	0.53
1:C:81:GLY:O	1:C:84:ARG:HG2	2.09	0.53
4:F:100:ILE:HD12	4:F:128:ARG:HB3	1.90	0.53
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.26	0.53
1:C:36:MET:HE3	1:C:61:HIS:NE2	2.24	0.53
4:F:79:LYS:O	4:F:83:THR:OG1	2.25	0.52
2:B:145:SER:HB2	2:B:188:SER:OG	2.10	0.52
4:F:223:THR:HG21	4:F:257:GLU:OE1	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:12:CYS:SG	2:D:16:ILE:HD12	2.51	0.51
2:D:306:ARG:HG2	2:D:340:TYR:CZ	2.45	0.51
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.10	0.51
2:D:5:VAL:HG12	2:D:62:ARG:CD	2.39	0.51
2:D:21:TRP:CZ3	2:D:61:PRO:HB3	2.46	0.51
2:D:56:GLY:O	2:D:58:LYS:HD3	2.09	0.51
2:B:139:LEU:HA	2:B:145:SER:HB3	1.92	0.51
2:D:221:THR:HG22	2:D:224:ASP:OD2	2.10	0.51
4:F:103:THR:HG22	4:F:174:ASP:HB3	1.92	0.51
2:B:203:ASP:HB2	2:B:301:ALA:HA	1.92	0.51
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.46	0.51
1:C:81:GLY:O	1:C:84:ARG:NH1	2.44	0.51
2:B:301:ALA:O	2:B:303:CYS:N	2.45	0.50
2:D:5:VAL:HG22	2:D:133:PHE:CD2	2.46	0.50
1:C:84:ARG:HG2	1:C:84:ARG:HH11	1.76	0.50
1:A:88:HIS:CD2	1:A:90:GLU:HG2	2.47	0.50
4:F:198:LYS:HG2	4:F:199:PHE:N	2.27	0.50
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.46	0.49
1:A:331:ALA:O	1:A:335:ILE:HG13	2.12	0.49
1:A:344:VAL:HG21	1:A:346:TRP:CZ2	2.47	0.49
1:A:298:PRO:HA	1:A:301:GLN:CD	2.37	0.49
1:A:1:MET:SD	1:A:1:MET:C	2.95	0.49
2:D:68:LEU:HD12	2:D:143:THR:HG23	1.94	0.49
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.48	0.49
2:B:174:LYS:HD2	2:B:205:GLU:HG3	1.95	0.49
2:B:238:THR:HG21	2:B:316:ILE:HG21	1.94	0.49
3:E:56:ALA:HB1	3:E:60:ARG:HH12	1.76	0.49
2:B:294:PHE:CE2	2:B:330:MET:HE1	2.48	0.49
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.48	0.49
4:F:163:SER:OG	4:F:164:SER:N	2.43	0.49
2:D:7:ILE:O	2:D:135:LEU:HD12	2.13	0.49
4:F:150:LYS:HG2	4:F:151:SER:N	2.28	0.49
4:F:246:GLN:OE1	4:F:260:ASN:ND2	2.46	0.49
2:D:395:LEU:O	2:D:399:THR:HG22	2.13	0.48
2:B:104:GLY:O	2:B:109:GLY:HA3	2.13	0.48
4:F:128:ARG:HH21	4:F:170:LEU:HB3	1.79	0.48
2:D:256:ASN:HB3	11:D:502:GY2:C16	2.44	0.48
3:E:95:LYS:HD2	3:E:95:LYS:HA	1.69	0.48
4:F:246:GLN:O	4:F:250:SER:HB3	2.13	0.48
2:B:61:PRO:CD	2:B:84:ILE:HG12	2.43	0.48
2:B:294:PHE:HE2	2:B:330:MET:HE1	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:ILE:HD11	1:C:302:MET:SD	2.53	0.48
2:D:67:ASP:OD2	2:D:72:THR:HG21	2.13	0.48
1:C:140:SER:HA	1:C:171:ILE:HB	1.95	0.48
1:A:112:LYS:HG3	3:E:54:LEU:HD13	1.94	0.48
2:B:61:PRO:HD3	2:B:84:ILE:HG12	1.96	0.48
2:B:273:LEU:HD23	2:B:273:LEU:HA	1.62	0.48
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.49	0.47
2:B:165:ASN:ND2	2:B:198:GLU:HG3	2.29	0.47
2:B:170:MET:HE3	2:B:170:MET:HB3	1.67	0.47
2:D:237:THR:O	2:D:241:ARG:HG3	2.14	0.47
3:E:9:ILE:HG13	3:E:21:GLU:HB3	1.95	0.47
1:C:339:ARG:HH11	1:C:339:ARG:HG2	1.79	0.47
1:A:187:SER:CB	1:A:391:LEU:HD21	2.43	0.47
1:C:250:VAL:HG22	1:C:255:PHE:CZ	2.48	0.47
2:D:389:PHE:CE1	2:D:408:PHE:HB3	2.50	0.47
2:B:186:THR:HA	2:B:415:MET:HE3	1.96	0.47
2:B:289:LEU:HG	2:B:365:ALA:HB2	1.95	0.47
2:D:117:LEU:HD11	2:D:154:LYS:CG	2.43	0.47
1:A:262:TYR:HE2	1:A:346:TRP:CZ2	2.33	0.47
1:A:346:TRP:CZ3	1:A:347:CYS:SG	3.06	0.47
2:D:392:LYS:HZ1	2:D:405:GLU:CD	2.22	0.47
3:E:75:LYS:O	3:E:79:GLU:HG3	2.15	0.47
2:B:67:ASP:O	2:B:92:PHE:HA	2.15	0.47
2:B:162:ARG:O	10:B:503:MES:H52	2.15	0.47
2:D:151:LEU:O	2:D:155:ILE:HG13	2.15	0.47
4:F:1:MET:HE2	4:F:28:LYS:HB3	1.97	0.47
1:C:250:VAL:HG22	1:C:255:PHE:CE2	2.49	0.47
2:B:310:TYR:CE1	2:B:367:PHE:HZ	2.32	0.47
2:B:227:HIS:NE2	2:B:274:THR:HG23	2.30	0.46
2:D:43:GLN:O	2:D:47:ILE:HG23	2.16	0.46
2:D:290:THR:HG22	2:D:333:VAL:HG21	1.96	0.46
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.98	0.46
2:B:263:LEU:HD21	2:B:421[B]:GLU:HB3	1.98	0.46
4:F:73:ARG:HG3	4:F:73:ARG:NH1	2.25	0.46
2:B:215:LEU:HD13	2:B:275:SER:HB2	1.97	0.46
2:D:191:GLN:HE22	3:E:126:LYS:NZ	2.13	0.46
2:D:293:MET:HG2	2:D:367:PHE:HB2	1.98	0.46
1:A:81:GLY:O	1:A:84:ARG:HD3	2.15	0.46
2:B:36:TYR:CE1	2:B:44:LEU:HD21	2.50	0.46
3:E:25:LYS:HD3	3:E:26:PRO:O	2.15	0.46
1:A:330:ALA:O	1:A:334:THR:HG22	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:44:LEU:O	2:D:47:ILE:HG13	2.15	0.46
2:D:74:ASP:HA	2:D:77:ARG:NH1	2.31	0.46
2:D:118:ASP:HA	2:D:121:ARG:NH1	2.30	0.46
2:D:141:GLY:HA3	9:D:501:GDP:O3A	2.16	0.46
4:F:16:GLU:HG2	4:F:19:ARG:NH2	2.31	0.46
2:B:179:VAL:HG22	1:C:258:ASN:OD1	2.16	0.46
2:D:229:VAL:O	2:D:233:MET:HG3	2.16	0.46
2:B:169:VAL:HA	2:B:202:ILE:O	2.15	0.45
2:D:42:LEU:HG	2:D:243:PRO:HG2	1.97	0.45
1:A:76:ASP:HA	1:A:79:ARG:HD2	1.98	0.45
2:B:64:ILE:HG12	2:B:119:VAL:HG12	1.98	0.45
2:B:321:MET:HB3	2:B:363:MET:SD	2.56	0.45
1:A:385:ALA:HB2	1:A:432:TYR:CG	2.51	0.45
1:A:27:GLU:OE1	1:A:243:ARG:NH2	2.45	0.45
1:A:362:VAL:HG21	1:A:370:LYS:HG3	1.98	0.45
3:E:58:GLU:HG3	3:E:61:ARG:NH2	2.32	0.45
1:A:124:LYS:HA	1:A:124:LYS:HD2	1.74	0.45
1:A:123:ARG:HG3	1:A:123:ARG:HH11	1.81	0.45
1:A:260:VAL:HG11	1:A:266:HIS:HB3	1.99	0.45
1:C:167:LEU:HA	1:C:200:CYS:O	2.17	0.45
2:D:170:MET:HE3	2:D:377:LEU:HD11	1.98	0.45
4:F:2:TYR:CZ	4:F:359:PHE:HB3	2.52	0.45
4:F:277:THR:HG22	4:F:278:THR:H	1.83	0.44
2:B:47:ILE:HD12	2:B:47:ILE:HA	1.83	0.44
2:B:216:LYS:HA	2:B:216:LYS:HD3	1.77	0.44
1:C:48:SER:HB3	1:C:243:ARG:O	2.17	0.44
1:C:270:ALA:O	1:C:302:MET:HB2	2.17	0.44
2:B:186:THR:HA	2:B:415:MET:CE	2.47	0.44
2:D:293:MET:SD	2:D:365:ALA:HB1	2.57	0.44
2:B:134:GLN:HA	2:B:165:ASN:O	2.18	0.44
2:B:395:LEU:HD23	2:B:395:LEU:HA	1.88	0.44
4:F:96:GLU:OE1	4:F:98:TYR:OH	2.29	0.44
2:B:159:TYR:HB3	2:B:162:ARG:HG2	2.00	0.44
2:D:101:TRP:CE3	2:D:187:LEU:HD13	2.53	0.44
4:F:32:LYS:HE3	4:F:33:ASP:OD2	2.18	0.44
4:F:166:ALA:HA	4:F:169:LEU:HD12	2.00	0.44
4:F:287:ILE:HG13	4:F:327:VAL:HG11	2.00	0.44
2:B:135:LEU:HD22	2:B:152:ILE:HD11	1.99	0.44
4:F:285:LEU:HA	4:F:285:LEU:HD12	1.85	0.44
2:B:189:VAL:HG11	2:B:415:MET:HG3	2.00	0.43
2:B:421[B]:GLU:O	2:B:424:GLN:HB3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:GLU:HG2	1:C:61:HIS:CD2	2.53	0.43
1:C:84:ARG:HG2	1:C:84:ARG:NH1	2.33	0.43
2:B:280:GLN:CG	2:B:281:TYR:H	2.29	0.43
2:D:21:TRP:CE3	2:D:61:PRO:HB3	2.53	0.43
2:B:293:MET:HE2	2:B:293:MET:HB3	1.77	0.43
2:D:186:THR:HA	2:D:415:MET:HE1	2.00	0.43
2:D:216:LYS:O	2:D:217:LEU:HD23	2.18	0.43
4:F:140:GLU:C	4:F:142:ARG:H	2.26	0.43
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.53	0.43
4:F:1:MET:CE	4:F:28:LYS:HB3	2.49	0.43
4:F:244:CYS:SG	4:F:245:ILE:HG13	2.59	0.43
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.54	0.43
4:F:131:PHE:HE1	4:F:147:TRP:CZ3	2.37	0.42
4:F:150:LYS:HG2	4:F:151:SER:H	1.85	0.42
1:A:174:ALA:O	1:A:178:SER:HB3	2.19	0.42
1:C:14:VAL:HG13	1:C:67:PHE:HD2	1.84	0.42
1:C:320:ARG:HA	1:C:356:ASN:O	2.19	0.42
1:C:416:GLY:O	1:C:420[B]:GLU:HB2	2.19	0.42
1:A:313:MET:HE3	1:A:380:ASN:O	2.19	0.42
2:B:102:ALA:HB2	2:B:403:MET:SD	2.59	0.42
4:F:220[A]:VAL:HG12	4:F:263:PHE:CE1	2.55	0.42
1:A:424:ASP:O	1:A:427:ALA:HB3	2.20	0.42
2:D:28:HIS:HA	2:D:43:GLN:HB3	2.01	0.42
4:F:233:PHE:HE1	4:F:239:HIS:CE1	2.36	0.42
2:B:213:ARG:O	2:B:216:LYS:HE3	2.19	0.42
2:D:122:LYS:HE3	2:D:122:LYS:HB3	1.83	0.42
1:C:293[A]:ASN:ND2	1:C:339:ARG:HH22	2.18	0.42
2:D:203:ASP:HB2	2:D:301:ALA:HA	2.01	0.42
2:B:239:CYS:O	2:B:248:ALA:HB3	2.20	0.42
4:F:74:LYS:NZ	4:F:150:LYS:HD3	2.35	0.42
4:F:77:LEU:O	4:F:81:ILE:HG13	2.19	0.42
1:A:23:LEU:HD12	1:A:23:LEU:HA	1.86	0.42
2:D:169:VAL:HA	2:D:202:ILE:O	2.20	0.42
4:F:99:VAL:HG12	4:F:127:GLU:OE1	2.19	0.42
4:F:307:LEU:HD12	4:F:307:LEU:HA	1.82	0.42
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.48	0.41
2:D:170:MET:HE2	2:D:170:MET:HB2	1.56	0.41
4:F:74:LYS:HZ2	4:F:152:SER:HA	1.85	0.41
4:F:217:ARG:HG3	4:F:218:GLU:HG2	2.03	0.41
1:C:172:TYR:HB3	1:C:205:ASP:HA	2.02	0.41
1:A:217:LEU:HB3	1:A:219:ILE:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:267:MET:HE2	2:B:303:CYS:HB2	2.03	0.41
3:E:128:LYS:O	3:E:132:GLU:HG3	2.20	0.41
3:E:101:LEU:HD12	3:E:101:LEU:HA	1.82	0.41
3:E:128:LYS:HE3	3:E:132:GLU:OE2	2.20	0.41
2:D:8:GLN:NE2	2:D:14:ASN:HA	2.36	0.41
4:F:217:ARG:NH1	4:F:374:ILE:HG22	2.36	0.41
1:A:389:ALA:O	1:A:390:ARG:C	2.64	0.41
2:B:2:ARG:HG3	2:B:2:ARG:NH1	2.36	0.41
2:D:100:ASN:ND2	2:D:102:ALA:HB3	2.32	0.41
4:F:58:LEU:HD23	4:F:58:LEU:HA	1.90	0.41
2:B:250:LEU:HD23	2:B:250:LEU:HA	1.85	0.41
2:B:151:LEU:O	2:B:155:ILE:HG13	2.21	0.41
2:B:164:MET:HG3	2:B:196:THR:HG22	2.03	0.41
1:C:254:GLU:HG2	1:C:352:LYS:HE2	2.02	0.41
1:C:406:HIS:CG	2:D:261:PRO:HD3	2.56	0.41
2:D:221:THR:HG23	2:D:224:ASP:H	1.84	0.41
4:F:89:GLU:H	4:F:89:GLU:CD	2.29	0.41
4:F:99:VAL:C	4:F:100:ILE:HD13	2.45	0.41
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.55	0.41
1:C:241:SER:HA	1:C:249:ASN:OD1	2.21	0.41
2:D:89:ASN:HA	2:D:119:VAL:HG11	2.03	0.41
1:A:79:ARG:NH2	1:A:94:THR:HG23	2.35	0.40
1:A:139:HIS:CD2	1:A:150:THR:HG21	2.56	0.40
2:B:27:GLU:OE2	2:B:234:SER:OG	2.37	0.40
1:C:425:MET:HE3	1:C:425:MET:HB3	1.67	0.40
2:D:178:THR:HB	2:D:181:GLU:HG2	2.04	0.40
1:A:263:PRO:O	1:A:266:HIS:HD2	2.05	0.40
2:D:47:ILE:HD12	2:D:48:ASN:N	2.36	0.40
2:D:73:MET:HE1	2:D:91:VAL:O	2.22	0.40
2:D:107:THR:HG22	2:D:108:GLU:N	2.36	0.40
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.55	0.40
1:A:28:HIS:CE1	1:A:243:ARG:HB3	2.57	0.40
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.52	0.40
3:E:116:LEU:HD23	3:E:116:LEU:HA	1.95	0.40
1:C:7:ILE:HD13	1:C:153:LEU:HD21	2.04	0.40
1:C:141:PHE:CE1	1:C:170:SER:HB3	2.57	0.40
1:A:109:THR:OG1	1:A:411:GLU:OE1	2.36	0.40
2:B:101:TRP:CE3	2:B:187:LEU:HD13	2.56	0.40
2:B:332:ASN:O	2:B:336:LYS:HB2	2.21	0.40
4:F:202:ARG:HB3	4:F:220[A]:VAL:HG22	2.02	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%)	416 (95%)	23 (5%)	0	100	100
1	C	446/450 (99%)	436 (98%)	10 (2%)	0	100	100
2	B	423/445 (95%)	408 (96%)	15 (4%)	0	100	100
2	D	416/445 (94%)	401 (96%)	15 (4%)	0	100	100
3	E	121/143 (85%)	118 (98%)	3 (2%)	0	100	100
4	F	342/384 (89%)	325 (95%)	17 (5%)	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	85
1	C	379/378 (100%)	366 (97%)	13 (3%)	32	66
2	B	369/383 (96%)	366 (99%)	3 (1%)	73	90
2	D	362/383 (94%)	354 (98%)	8 (2%)	45	77
3	E	112/127 (88%)	110 (98%)	2 (2%)	51	80
4	F	314/342 (92%)	300 (96%)	14 (4%)	24	57
All	All	1907/1991 (96%)	1862 (98%)	45 (2%)	48	75

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

Mol	Chain	Res	Type
1	A	38	SER
1	A	159	VAL
1	A	188	ILE
1	A	193[A]	THR
1	A	193[B]	THR
2	B	55	THR
2	B	75	SER
2	B	214	THR
1	C	151[A]	SER
1	C	151[B]	SER
1	C	165[A]	SER
1	C	165[B]	SER
1	C	241	SER
1	C	250	VAL
1	C	251	ASP
1	C	285	GLN
1	C	315[A]	CYS
1	C	315[B]	CYS
1	C	338	LYS
1	C	347[A]	CYS
1	C	347[B]	CYS
2	D	8	GLN
2	D	47	ILE
2	D	154	LYS
2	D	177	ASP
2	D	202	ILE
2	D	218	THR
2	D	285	THR
2	D	391	ARG
3	E	124	GLN
3	E	138	GLU
4	F	12	SER
4	F	26	GLN
4	F	76	SER
4	F	77	LEU
4	F	96	GLU
4	F	183	GLN
4	F	235	ASP
4	F	237	THR
4	F	240	LEU
4	F	255[A]	ARG
4	F	255[B]	ARG

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Mol	Chain	Res	Type
4	F	285	LEU
4	F	296[A]	MET
4	F	296[B]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	256	GLN
1	A	285	GLN
1	A	300	ASN
1	A	309	HIS
1	A	342	GLN
1	A	372	GLN
1	A	393	HIS
2	B	15	GLN
2	B	165	ASN
2	B	247	ASN
2	B	347	ASN
2	B	426	GLN
1	C	256	GLN
2	D	48	ASN
2	D	99	ASN
2	D	100	ASN
2	D	329	GLN
2	D	337	ASN
2	D	347	ASN
2	D	384	GLN
3	E	78	HIS
3	E	103	GLN
4	F	183	GLN
4	F	234	GLN
4	F	269	GLN
4	F	310	GLN
4	F	348	GLN

5.3.3 RNA ⓘ

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$
11	GY2	D	502	-	24,24,24	1.68	4 (16%)	31,34,34	2.98	11 (35%)
10	MES	B	503	-	12,12,12	2.43	1 (8%)	15,16,16	1.93	4 (26%)
9	GDP	D	501	-	29,30,30	1.14	3 (10%)	45,47,47	2.56	12 (26%)
5	GTP	C	501	6	33,34,34	0.89	0	50,54,54	1.56	6 (12%)
9	GDP	B	501	6	29,30,30	1.15	2 (6%)	45,47,47	1.75	7 (15%)
10	MES	B	504	-	12,12,12	2.22	2 (16%)	15,16,16	1.84	4 (26%)
5	GTP	A	501	6	33,34,34	1.03	2 (6%)	50,54,54	1.69	10 (20%)
11	GY2	B	505	-	24,24,24	1.66	5 (20%)	31,34,34	2.59	9 (29%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	GY2	D	502	-	-	0/10/10/10	0/3/3/3
10	MES	B	503	-	-	5/6/14/14	0/1/1/1
9	GDP	D	501	-	-	4/16/32/32	0/3/3/3
5	GTP	C	501	6	-	8/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GDP	B	501	6	-	5/16/32/32	0/3/3/3
10	MES	B	504	-	-	2/6/14/14	0/1/1/1
5	GTP	A	501	6	-	8/22/38/38	0/3/3/3
11	GY2	B	505	-	-	0/10/10/10	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	MES	C8-S	-8.09	1.66	1.77
10	B	504	MES	C8-S	-6.54	1.68	1.77
11	D	502	GY2	C08-N07	4.66	1.33	1.30
11	B	505	GY2	C08-N07	4.66	1.33	1.30
10	B	504	MES	O2S-S	3.45	1.54	1.45
11	D	502	GY2	C05-C04	-3.31	1.37	1.42
9	B	501	GDP	C5-C4	3.17	1.47	1.38
9	D	501	GDP	C5-C4	2.98	1.46	1.38
5	A	501	GTP	PB-O3A	2.83	1.62	1.59
11	B	505	GY2	C10-N11	2.65	1.45	1.39
11	D	502	GY2	C10-N11	2.64	1.45	1.39
11	B	505	GY2	C05-C04	-2.59	1.38	1.42
11	B	505	GY2	C06-C01	2.38	1.39	1.36
11	D	502	GY2	C02-C01	2.36	1.41	1.37
5	A	501	GTP	PA-O3A	2.36	1.62	1.59
9	D	501	GDP	PA-O3A	2.33	1.62	1.59
9	D	501	GDP	C2-N3	2.19	1.38	1.33
9	B	501	GDP	O6-C6	2.09	1.27	1.23
11	B	505	GY2	C13-N11	2.09	1.47	1.42

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	502	GY2	N07-C08-N09	-10.89	119.78	130.58
11	B	505	GY2	N07-C08-N09	-10.03	120.63	130.58
9	D	501	GDP	C5-C4-N3	-8.25	115.26	128.39
11	D	502	GY2	CL1-C08-N07	6.76	121.32	115.72
9	D	501	GDP	C2-N1-C6	-6.30	113.69	125.11
9	D	501	GDP	N9-C4-N3	6.26	138.47	125.95
9	D	501	GDP	C2-N3-C4	6.10	122.81	112.30
9	B	501	GDP	C5-C4-N3	-5.19	120.12	128.39
9	B	501	GDP	C2-N3-C4	4.78	120.53	112.30
9	D	501	GDP	O6-C6-C5	-4.66	114.22	126.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C2-N3-C4	4.47	120.00	112.30
10	B	503	MES	C5-N4-C3	4.41	118.35	108.84
11	B	505	GY2	CL1-C08-N07	4.32	119.30	115.72
11	D	502	GY2	C05-C04-N07	-4.13	118.43	122.80
9	B	501	GDP	C6-C5-N7	4.06	137.68	130.29
10	B	504	MES	C5-N4-C3	3.90	117.25	108.84
5	C	501	GTP	O2B-PB-O3A	3.78	117.48	107.27
9	B	501	GDP	N9-C4-N3	3.77	133.48	125.95
5	A	501	GTP	C5-C4-N3	-3.76	122.41	128.39
5	C	501	GTP	C5-C4-N3	-3.66	122.56	128.39
11	D	502	GY2	C10-C05-C04	3.66	117.90	115.47
11	B	505	GY2	C10-C05-C04	3.64	117.89	115.47
5	A	501	GTP	O2B-PB-O3A	3.61	117.03	107.27
11	B	505	GY2	C08-N09-C10	3.61	121.69	111.13
10	B	503	MES	O3S-S-C8	3.59	113.03	106.00
9	D	501	GDP	C5-C6-N1	3.58	122.37	113.25
5	C	501	GTP	C2-N3-C4	3.54	118.39	112.30
11	B	505	GY2	CL1-C08-N09	3.48	120.06	115.17
11	D	502	GY2	C08-N09-C10	3.47	121.30	111.13
5	A	501	GTP	N2-C2-N1	3.43	124.01	116.76
5	C	501	GTP	N9-C8-N7	-3.41	107.08	113.40
11	D	502	GY2	C02-C01-C06	-3.37	119.39	123.32
5	A	501	GTP	N9-C8-N7	-3.33	107.22	113.40
5	C	501	GTP	C8-N7-C5	3.26	110.06	104.26
11	D	502	GY2	C03-C04-N07	3.25	123.43	118.69
9	D	501	GDP	N2-C2-N3	-3.01	113.79	119.67
11	B	505	GY2	C05-C04-N07	-2.99	119.64	122.80
11	D	502	GY2	C01-C06-C05	2.99	121.11	118.75
10	B	504	MES	C7-N4-C3	2.97	119.16	111.24
9	D	501	GDP	C4-C5-N7	-2.97	105.97	110.67
11	D	502	GY2	F22-C01-C02	2.90	123.19	118.55
11	B	505	GY2	N09-C10-N11	2.86	119.09	116.09
5	A	501	GTP	O6-C6-C5	-2.78	119.19	126.53
9	B	501	GDP	C4-C5-N7	-2.77	106.27	110.67
5	A	501	GTP	C8-N7-C5	2.76	109.17	104.26
5	C	501	GTP	C4-C5-N7	-2.74	106.32	110.67
5	A	501	GTP	C2-N1-C6	-2.71	120.19	125.11
11	D	502	GY2	N09-C10-N11	2.68	118.89	116.09
11	D	502	GY2	CL1-C08-N09	2.65	118.90	115.17
9	D	501	GDP	C8-N7-C5	2.56	108.82	104.26
11	B	505	GY2	C02-C01-C06	-2.54	120.36	123.32
10	B	504	MES	C7-N4-C5	2.54	118.01	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	501	GDP	C6-C5-N7	2.52	134.88	130.29
10	B	503	MES	C7-N4-C5	2.50	117.91	111.24
10	B	504	MES	O2S-S-C8	2.49	110.49	106.73
11	B	505	GY2	C01-C06-C05	2.48	120.70	118.75
9	D	501	GDP	O4'-C1'-C2'	-2.29	101.71	106.62
10	B	503	MES	C7-N4-C3	2.25	117.22	111.24
9	D	501	GDP	O2A-PA-O3A	2.23	113.31	107.27
5	A	501	GTP	C4-C5-N7	-2.13	107.30	110.67
9	B	501	GDP	O2B-PB-O3A	2.10	111.69	104.64
9	B	501	GDP	O3'-C3'-C4'	-2.04	105.21	111.08
5	A	501	GTP	C5-C6-N1	2.01	118.37	113.25

There are no chirality outliers.

All (32) 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	C	501	GTP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O1A
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-O3S
10	B	504	MES	C8-C7-N4-C3
10	B	504	MES	C8-C7-N4-C5
10	B	503	MES	C8-C7-N4-C3
5	C	501	GTP	C3'-C4'-C5'-O5'
5	C	501	GTP	O4'-C4'-C5'-O5'
10	B	503	MES	C7-C8-S-O2S
5	C	501	GTP	PB-O3B-PG-O1G
9	D	501	GDP	PA-O3A-PB-O3B
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O2A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
9	B	501	GDP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O2G

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Mol	Chain	Res	Type	Atoms
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-O1A
9	B	501	GDP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3B-PG-O1G

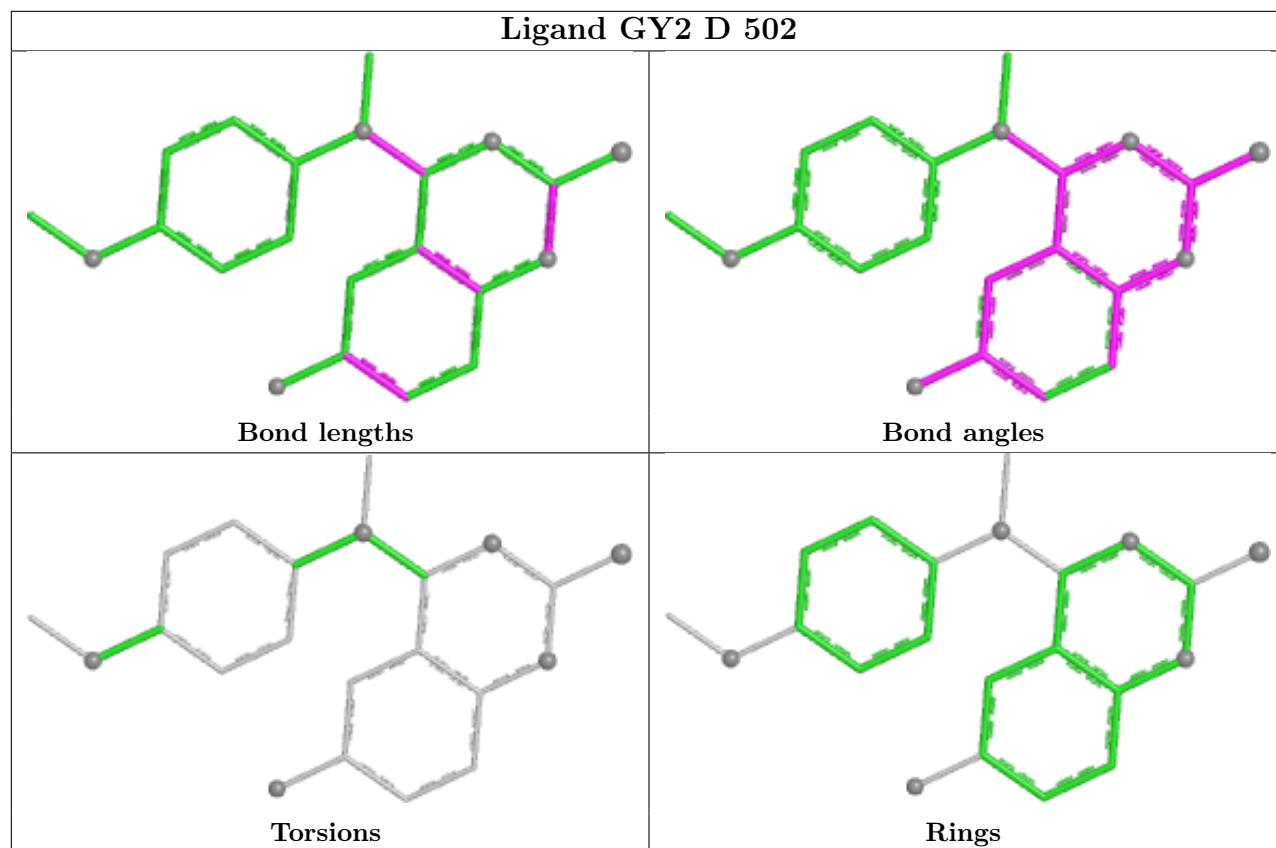
There are no ring outliers.

3 monomers are involved in 4 short contacts:

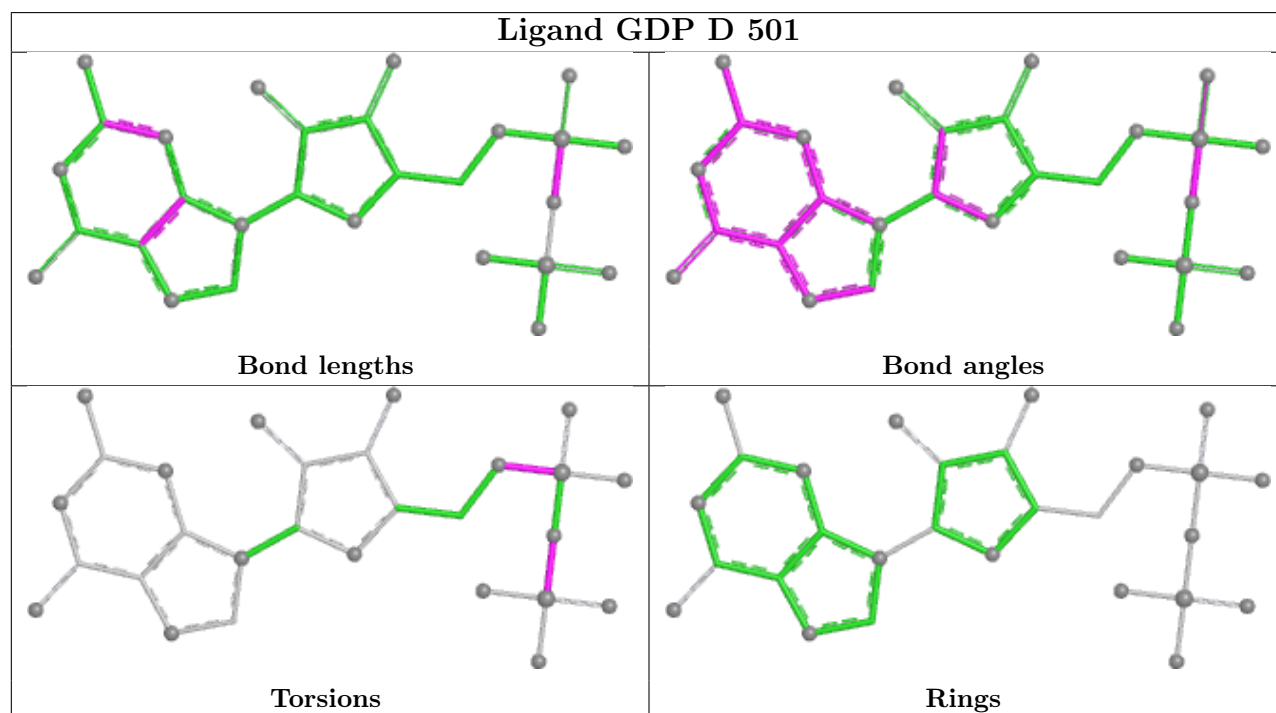
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	D	502	GY2	1	0
10	B	503	MES	1	0
9	D	501	GDP	2	0

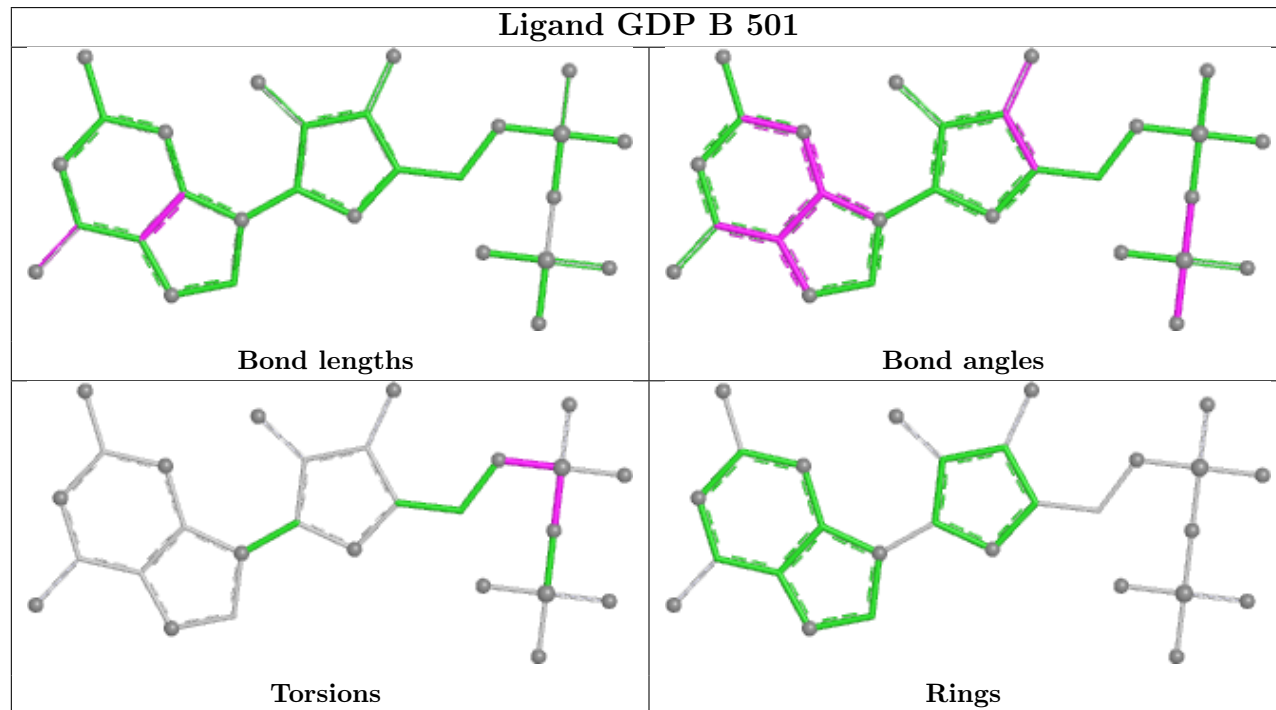
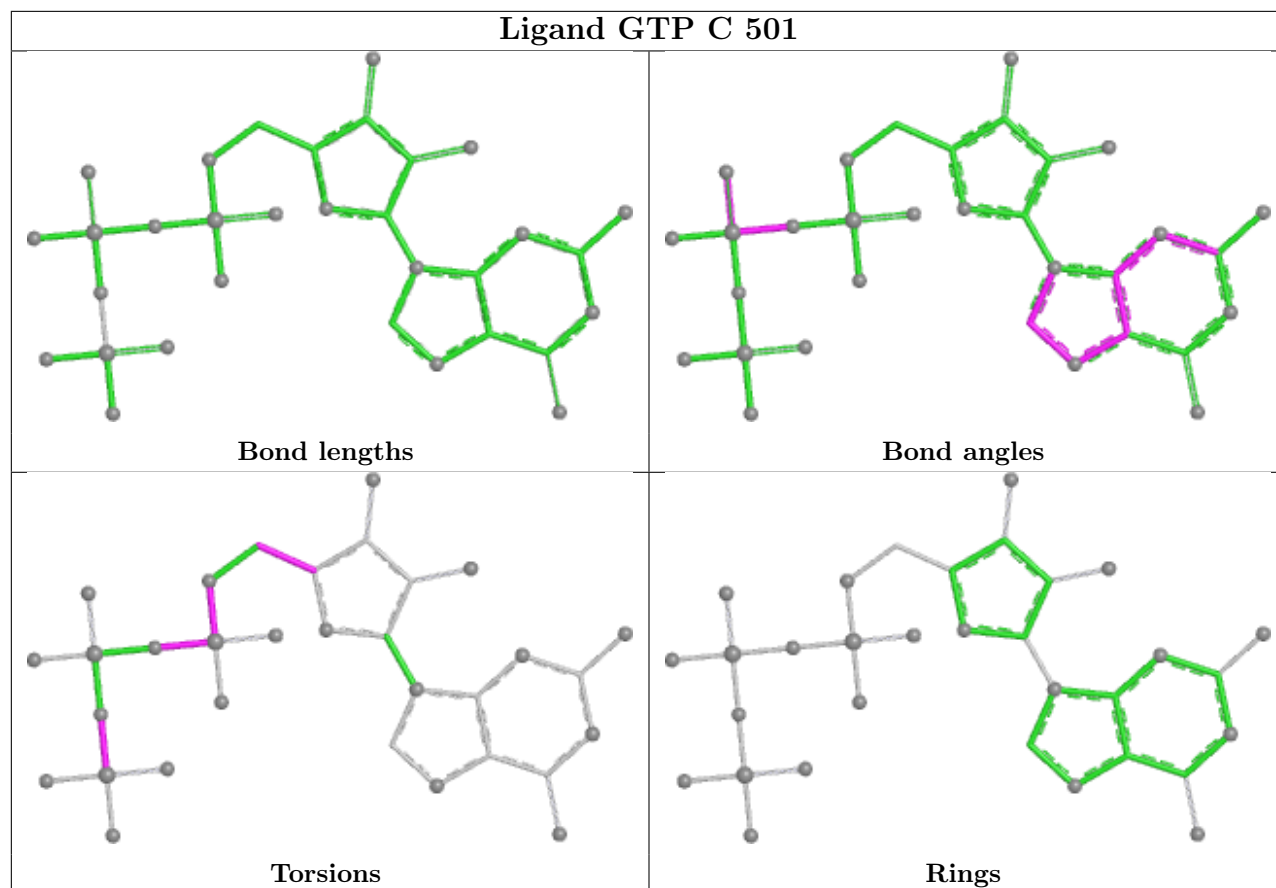
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 GY2 D 502

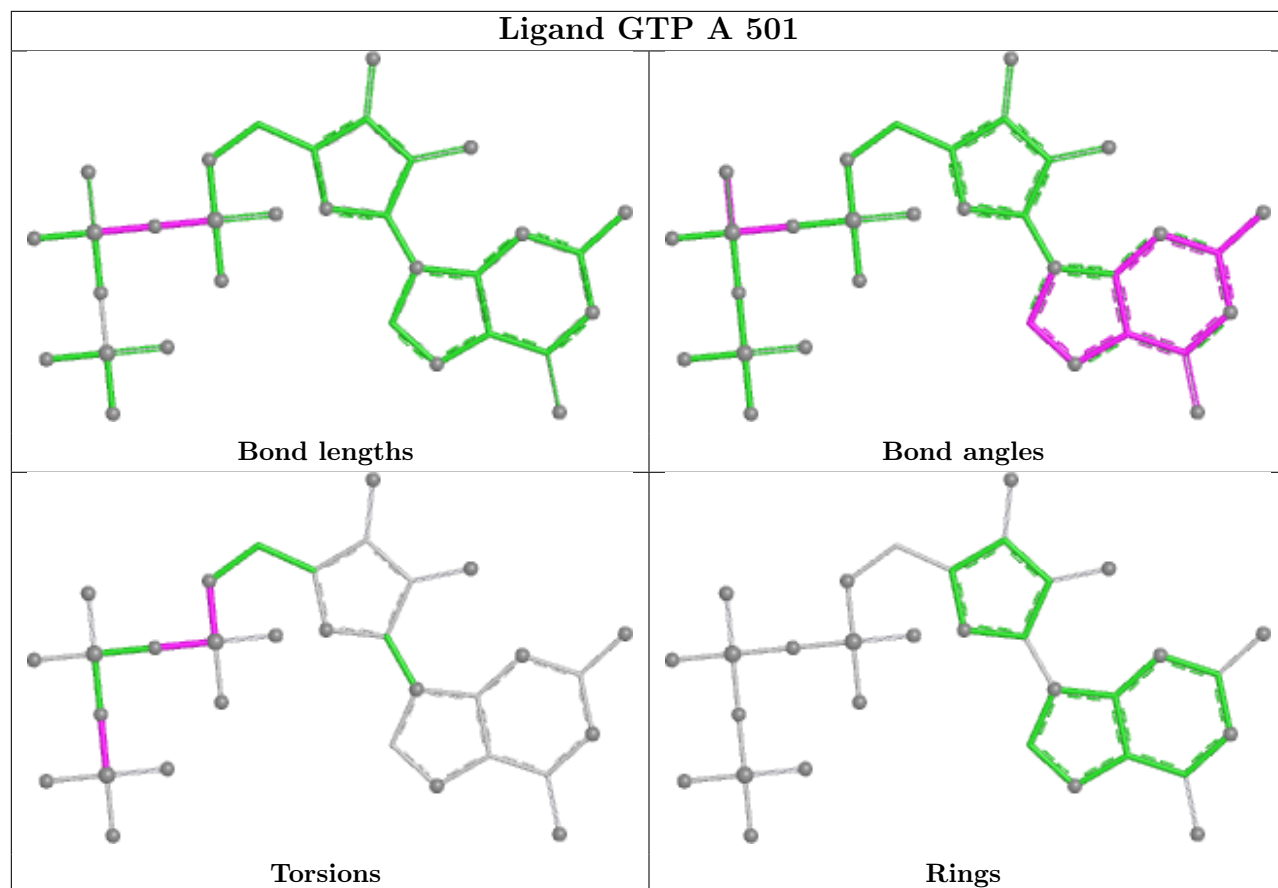


Ligand GDP D 501

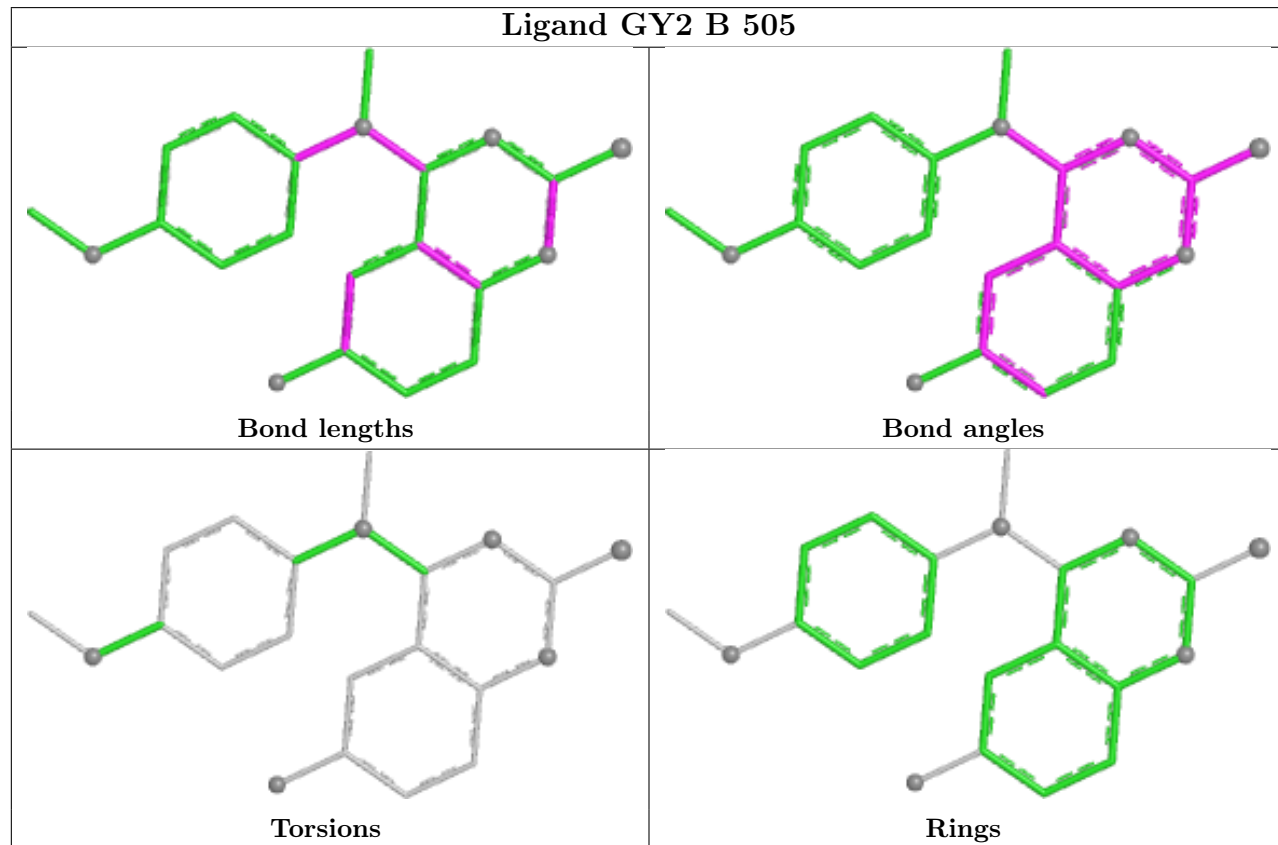




Ligand GTP A 501



Ligand GY2 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	437/450 (97%)	-0.29	2 (0%) 87 82	23, 40, 65, 81	4 (0%)
1	C	440/450 (97%)	-0.52	2 (0%) 87 82	16, 31, 53, 69	8 (1%)
2	B	424/445 (95%)	-0.17	6 (1%) 73 64	19, 40, 71, 104	4 (0%)
2	D	420/445 (94%)	0.30	14 (3%) 49 39	26, 58, 87, 107	1 (0%)
3	E	123/143 (86%)	0.26	3 (2%) 59 49	24, 54, 90, 116	2 (1%)
4	F	346/384 (90%)	0.68	52 (15%) 5 4	25, 63, 127, 145	4 (1%)
All	All	2190/2317 (94%)	-0.01	79 (3%) 46 37	16, 45, 91, 145	23 (1%)

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	169	LEU	5.2
4	F	245	ILE	4.5
4	F	240	LEU	4.1
4	F	125	THR	3.9
4	F	149	ALA	3.9
4	F	160	ILE	3.8
4	F	249	TYR	3.8
2	B	57	ASN	3.7
4	F	150	LYS	3.7
4	F	237	THR	3.6
4	F	181	VAL	3.5
3	E	143	ALA	3.5
4	F	104	ASN	3.4
1	A	88	HIS	3.2
4	F	130	VAL	3.2
4	F	159	GLY	3.2
2	B	275	SER	3.1
2	B	247	ASN	3.0
2	B	428	ALA	3.0

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Mol	Chain	Res	Type	RSRZ
4	F	334	GLY	2.9
4	F	161	LEU	2.9
2	D	145	SER	2.9
4	F	166	ALA	2.9
4	F	162	ILE	2.8
4	F	152	SER	2.8
2	B	55	THR	2.7
4	F	141	GLY	2.7
2	D	73	MET	2.7
4	F	236	LYS	2.7
2	D	95	SER	2.7
2	D	92	PHE	2.7
4	F	182	ILE	2.6
2	D	96	GLY	2.6
4	F	234	GLN	2.6
4	F	233	PHE	2.6
4	F	132	LEU	2.5
4	F	170	LEU	2.5
1	A	437	VAL	2.5
2	D	37	HIS	2.5
2	B	274	THR	2.4
4	F	148	ILE	2.4
4	F	99	VAL	2.4
4	F	250	SER	2.4
2	D	55	THR	2.4
4	F	242	ASN	2.4
4	F	225	SER	2.4
4	F	136	ASN	2.3
3	E	48	GLU	2.3
1	C	340	SER	2.3
2	D	219	THR	2.3
4	F	165	GLU	2.3
4	F	239	HIS	2.3
2	D	72	THR	2.3
4	F	255[A]	ARG	2.3
2	D	69	GLU	2.2
4	F	163	SER	2.2
4	F	331	GLU	2.2
4	F	362	ALA	2.2
2	D	101	TRP	2.2
4	F	167	SER	2.2
2	D	394	PHE	2.2

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Mol	Chain	Res	Type	RSRZ
3	E	139	LEU	2.2
4	F	372	THR	2.2
4	F	247	LYS	2.2
4	F	135	TYR	2.2
4	F	168	GLU	2.2
4	F	134	ALA	2.1
4	F	224	SER	2.1
4	F	139	ARG	2.1
1	C	163	LYS	2.0
2	D	284	LEU	2.0
4	F	100	ILE	2.0
4	F	231	ALA	2.0
4	F	248	GLU	2.0
4	F	98	TYR	2.0
4	F	256	TYR	2.0
2	D	405	GLU	2.0
4	F	235	ASP	2.0
4	F	146	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

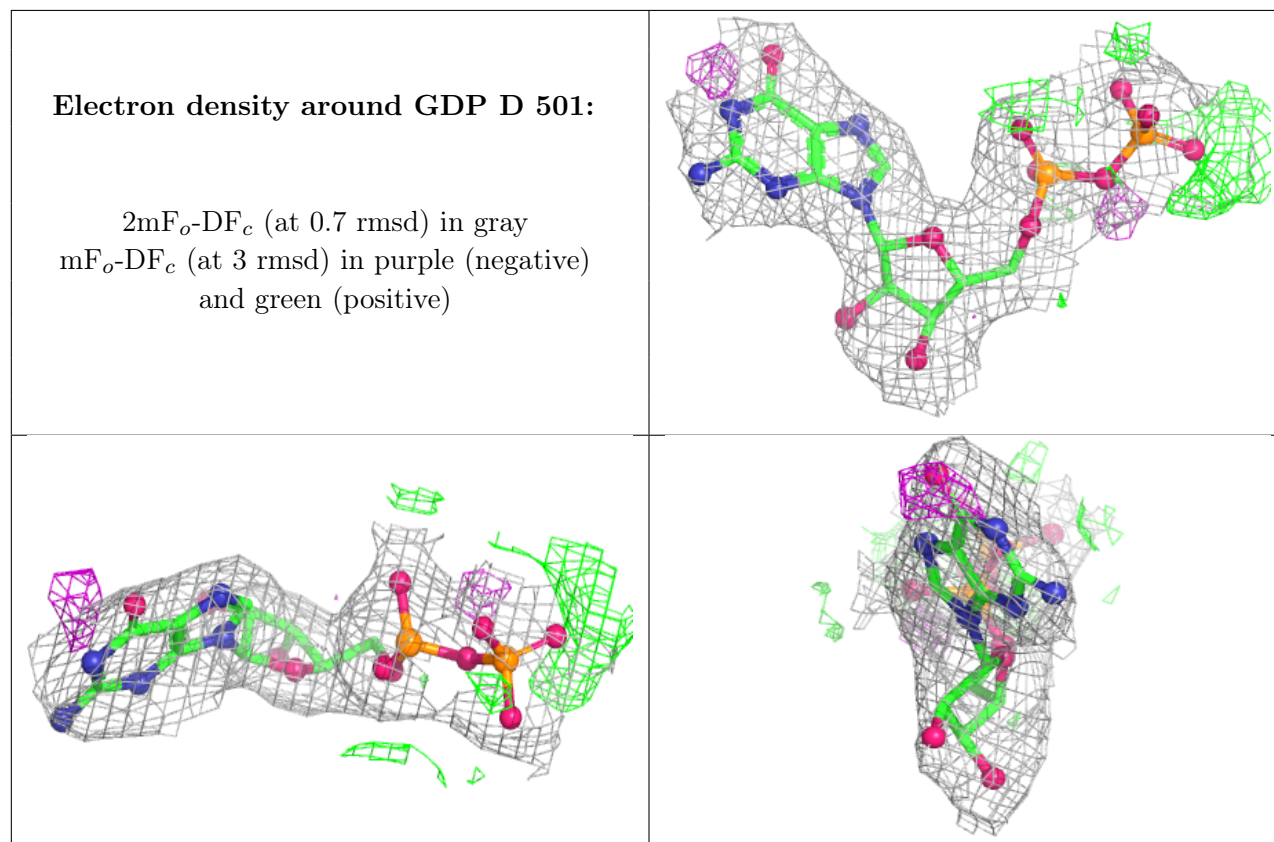
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
9	GDP	D	501	28/28	0.87	0.12	46,57,67,71	0
6	MG	C	502	1/1	0.90	0.30	36,36,36,36	0
10	MES	B	504	12/12	0.90	0.11	52,61,76,79	0
6	MG	A	502	1/1	0.91	0.30	34,34,34,34	0
6	MG	B	502	1/1	0.92	0.22	33,33,33,33	0

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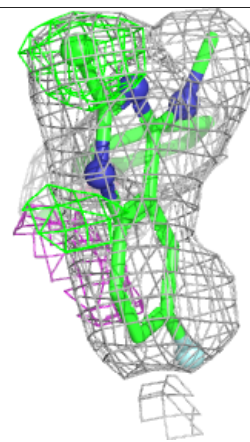
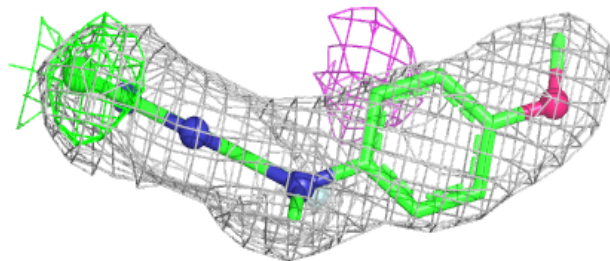
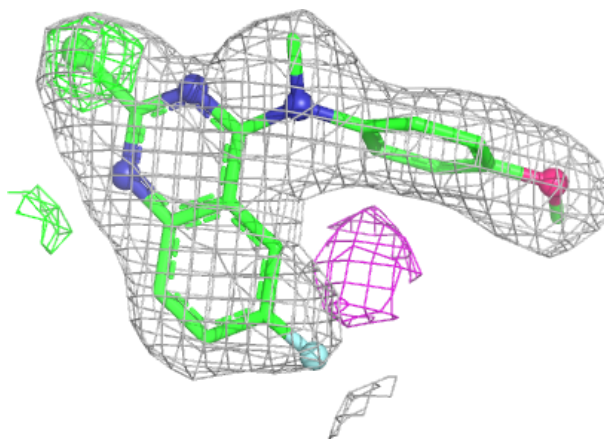
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	CL	A	504	1/1	0.92	0.09	77,77,77,77	0
11	GY2	D	502	22/22	0.92	0.13	28,42,55,188	0
11	GY2	B	505	22/22	0.93	0.12	28,35,45,138	0
10	MES	B	503	12/12	0.96	0.08	31,48,66,72	0
7	CA	C	503	1/1	0.96	0.03	43,43,43,43	0
5	GTP	A	501	32/32	0.97	0.06	24,31,39,43	0
5	GTP	C	501	32/32	0.97	0.06	23,27,31,34	0
9	GDP	B	501	28/28	0.98	0.05	21,28,32,41	0
7	CA	A	503	1/1	0.98	0.04	68,68,68,68	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.



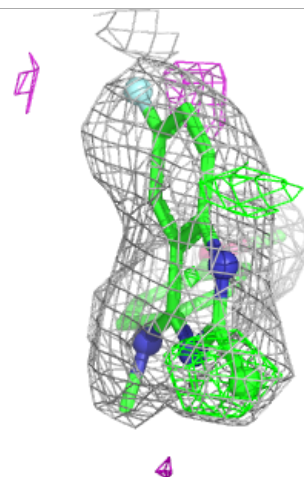
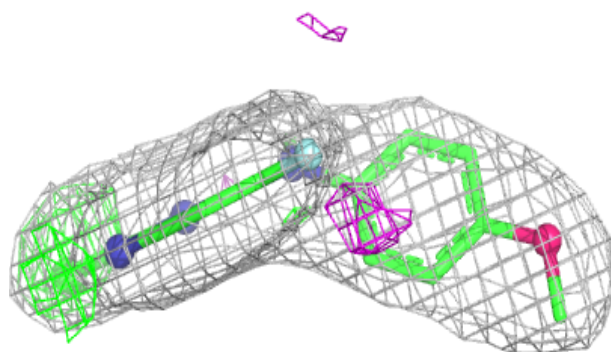
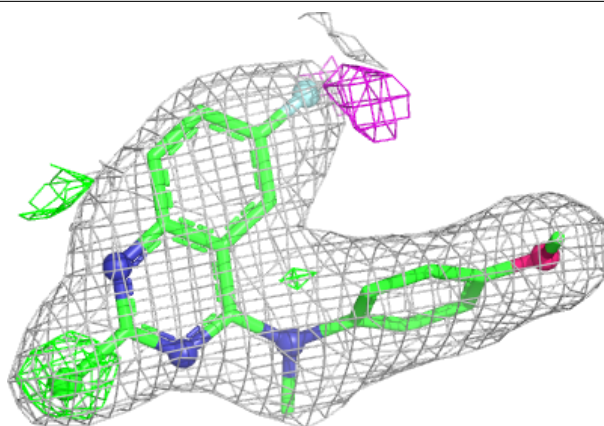
Electron density around GY2 D 502:

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



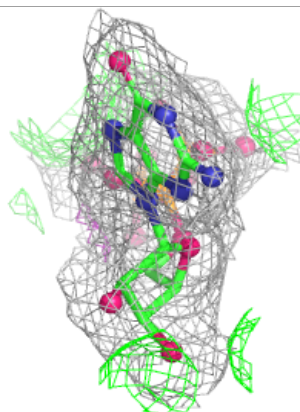
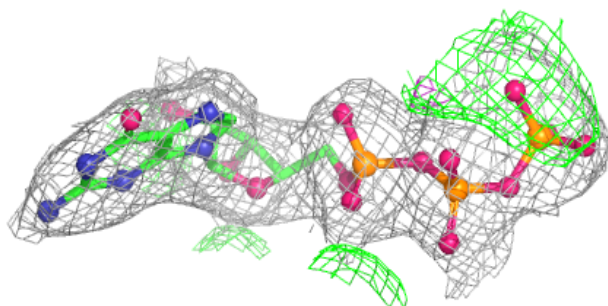
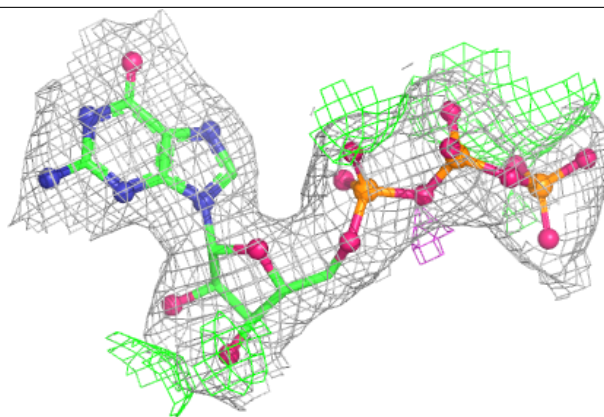
Electron density around GY2 B 505:

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

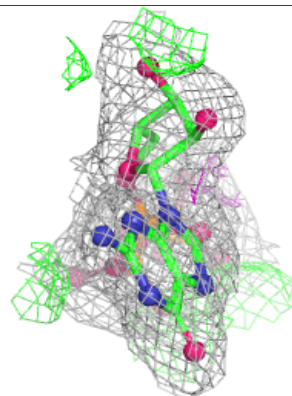
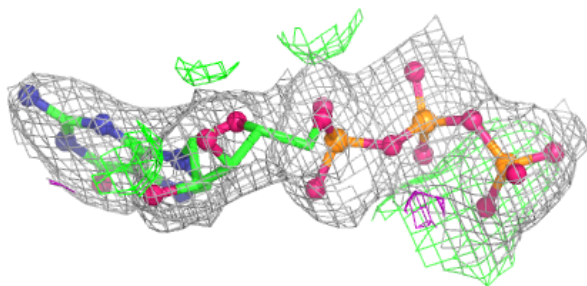
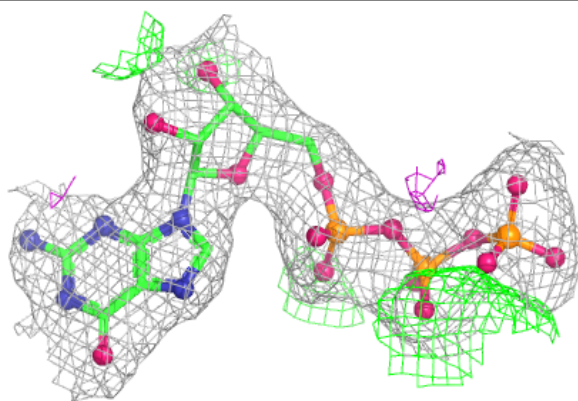


Electron density around GTP A 501:

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

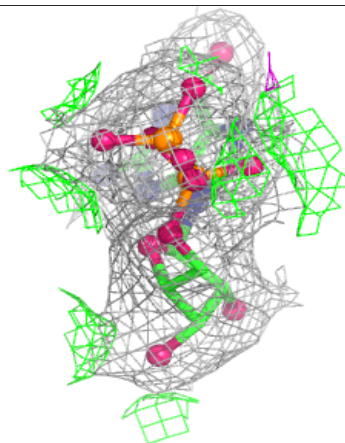
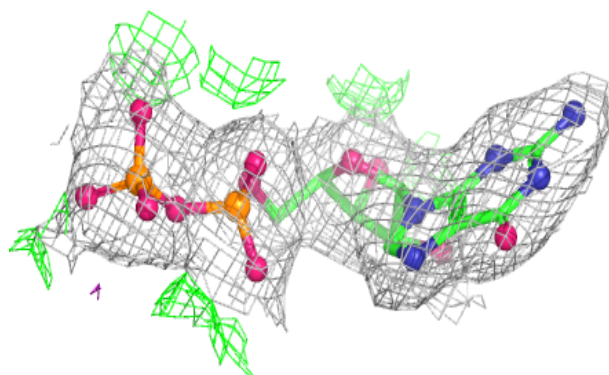
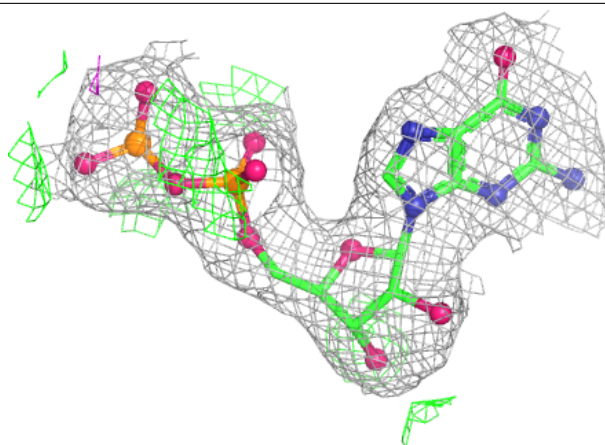
**Electron density around GTP C 501:**

$2mF_o-DF_c$ (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 ⓘ

There are no such residues in this entry.