



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:50 PM UTC

PDB ID : 7CPD / pdb_00007cpd
Title : Crystal structure of T2R-TTL-(+)-6-Br-JP18 complex
Authors : Jiang, H.; Luo, C.
Deposited on : 2020-08-06
Resolution : 2.51 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

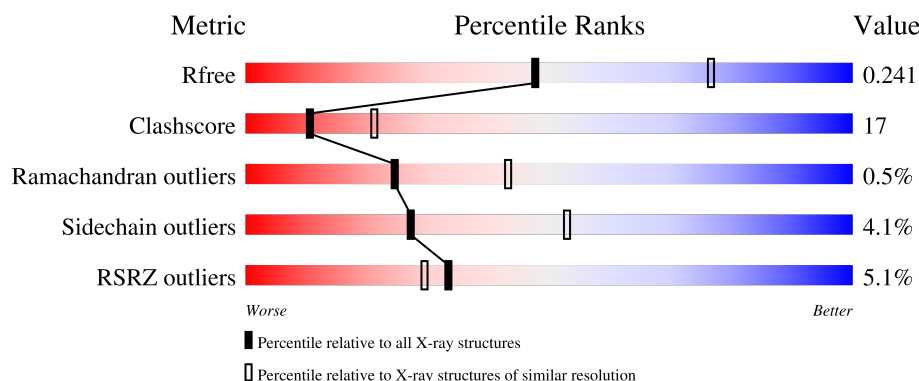
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.51 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.



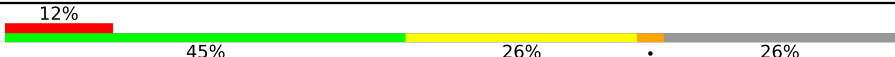
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	451	2% 71% 25% ..
1	C	451	2% 77% 20% ..
2	B	445	% 65% 28% • 6%
2	D	445	6% 59% 33% • 5%
3	E	189	4% 41% 19% • 36%

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Mol	Chain	Length	Quality of chain
4	F	378	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
11	GOL	C	501	-	-	X	-

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17559 atoms, of which 105 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	11	0
			3456	2197	580	654	25			
1	C	440	Total	C	N	O	S	0	10	0
			3484	2206	587	667	24			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	417	Total	C	N	O	S	1	10	0
			3337	2105	562	644	26			
2	D	421	Total	C	N	O	S	0	4	0
			3321	2092	561	640	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	121	Total	C	N	O	S	0	3	0
			1016	628	183	199	6			

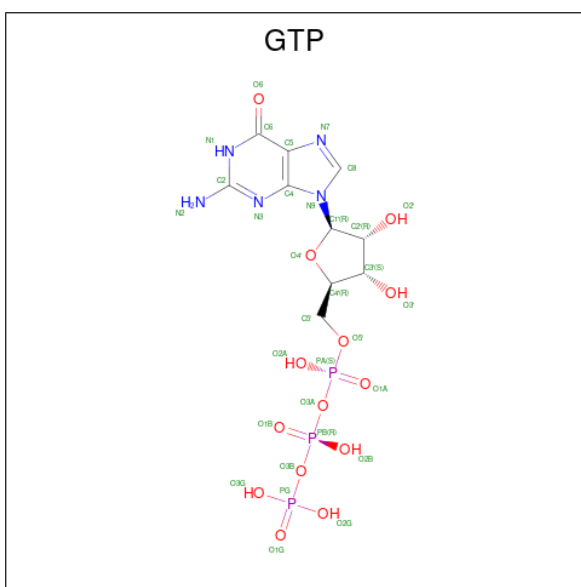
There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	-19	SER	ALA	conflict	UNP Q9H169

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	280	Total	C	N	O	S	0	5	0
			2310	1503	383	412	12			

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: C₁₀H₁₆N₅O₁₄P₃).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total 44	C 10	H 12	N 5	O 14	P 3	0	0
5	C	1	Total 44	C 10	H 12	N 5	O 14	P 3	0	0

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

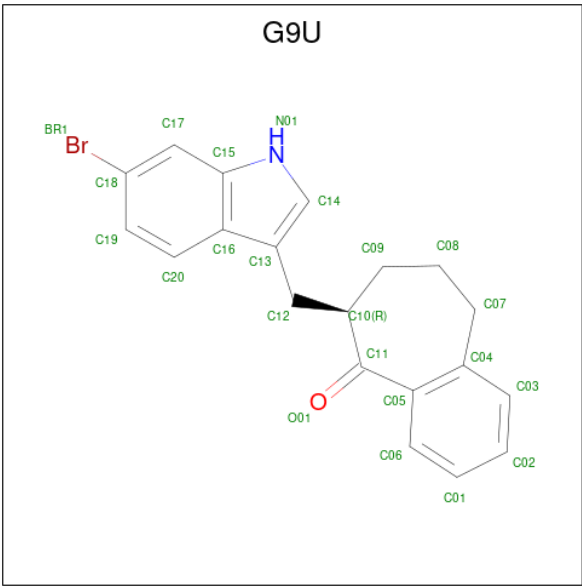
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total Mg 1 1	0	0
6	B	1	Total Mg 1 1	0	0
6	C	1	Total Mg 1 1	0	0

- 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	B	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

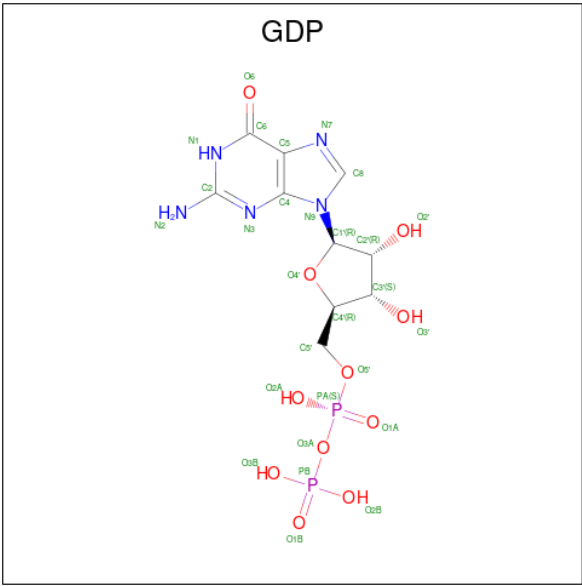
- Molecule 8 is (6R)-6-[(6-bromanyl-1H-indol-3-yl)methyl]-6,7,8,9-tetrahydrobenzo[7]annulen-5-one (CCD ID: G9U) (formula: C₂₀H₁₈BrNO) (labeled as "Ligand of Interest" by

depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	Br	C	H	N	O		
8	B	1	41	1	20	18	1	1	0	0
8	D	1	41	1	20	18	1	1	0	0

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



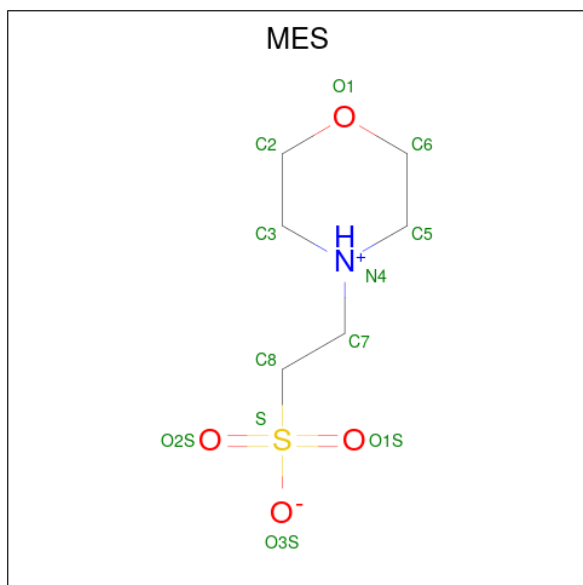
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
			Total	C	H	N	O	P		
9	B	1	40	10	12	5	11	2	0	0

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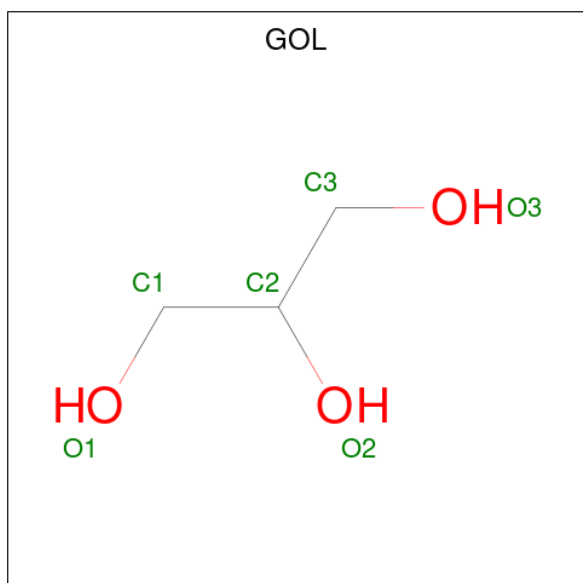
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	D	1	Total	C	H	N	O	P	
			40	10	12	5	11	2	

- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	H	N	O	S	
			25	6	13	1	4	1	

- Molecule 11 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	C	1	Total	C	H	O	0	0
			14	3	8	3		

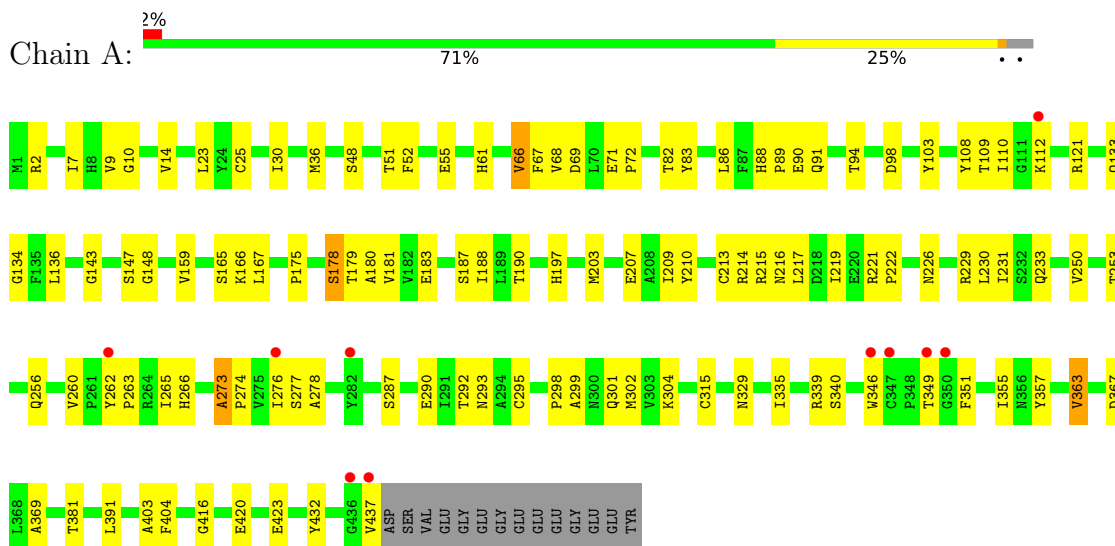
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	72	Total	O	0	0
			72	72		
12	B	56	Total	O	0	0
			56	56		
12	C	148	Total	O	0	0
			148	148		
12	D	21	Total	O	0	0
			21	21		
12	E	16	Total	O	0	0
			16	16		
12	F	27	Total	O	0	0
			27	27		

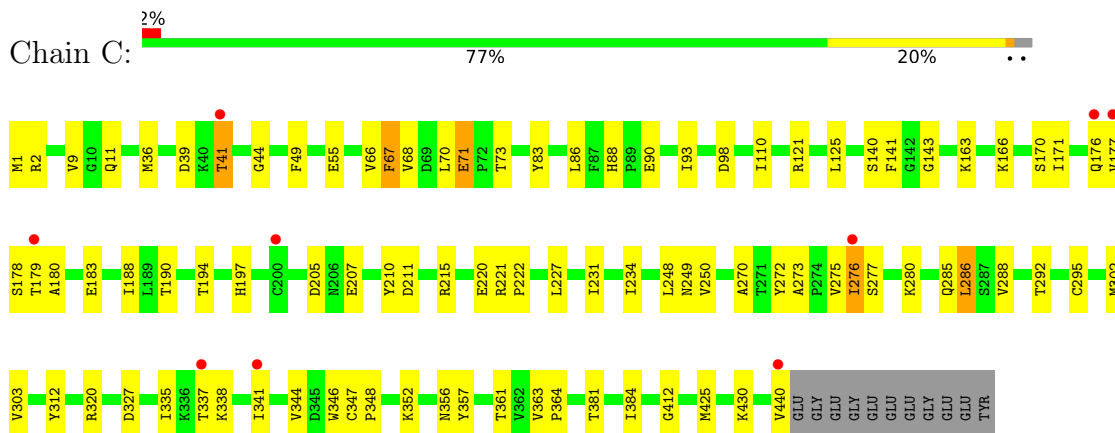
3 Residue-property plots [i](#)

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

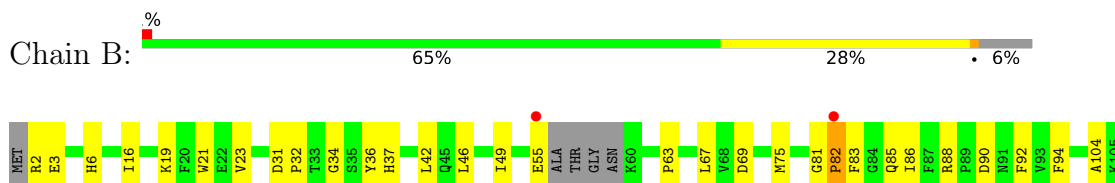
• Molecule 1: Tubulin alpha-1B chain

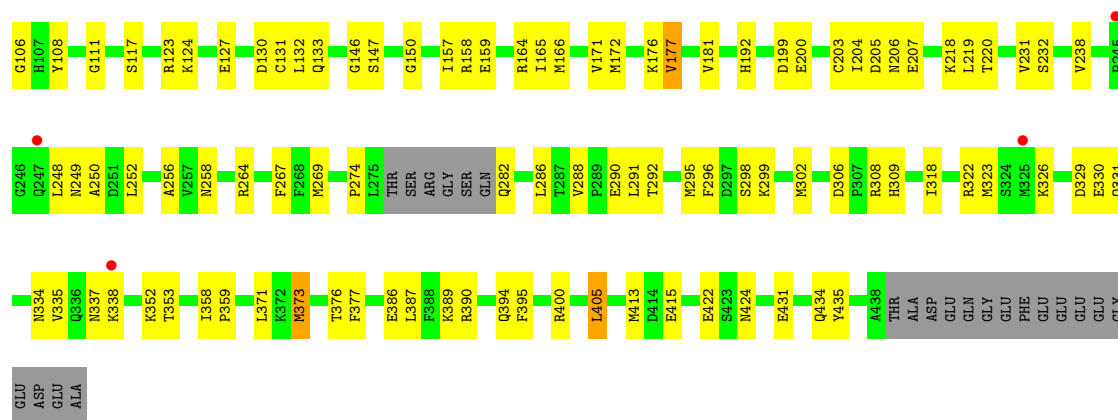


• Molecule 1: Tubulin alpha-1B chain

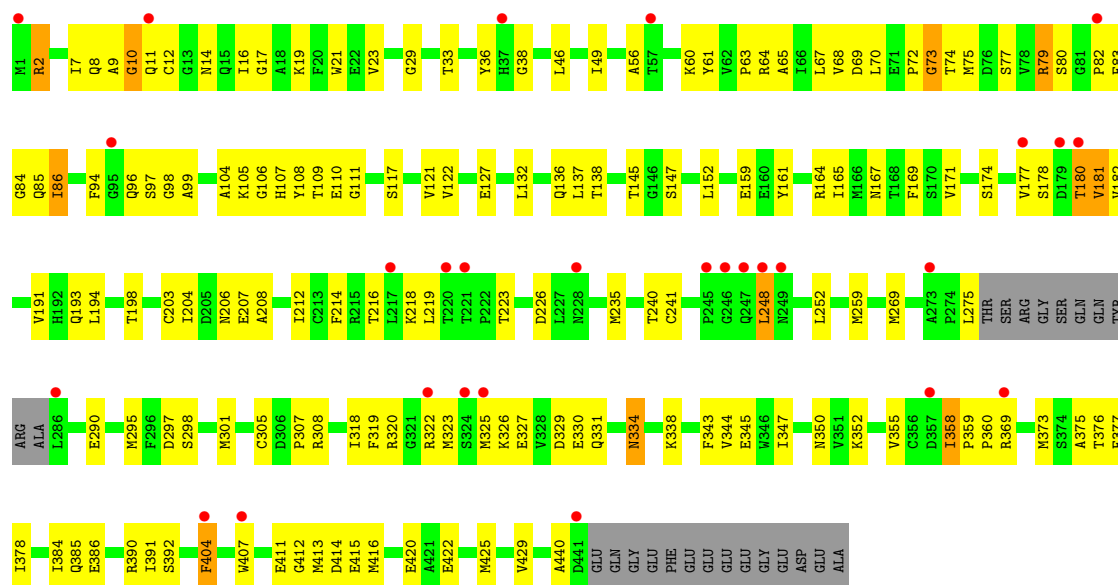


• Molecule 2: Tubulin beta-2B chain

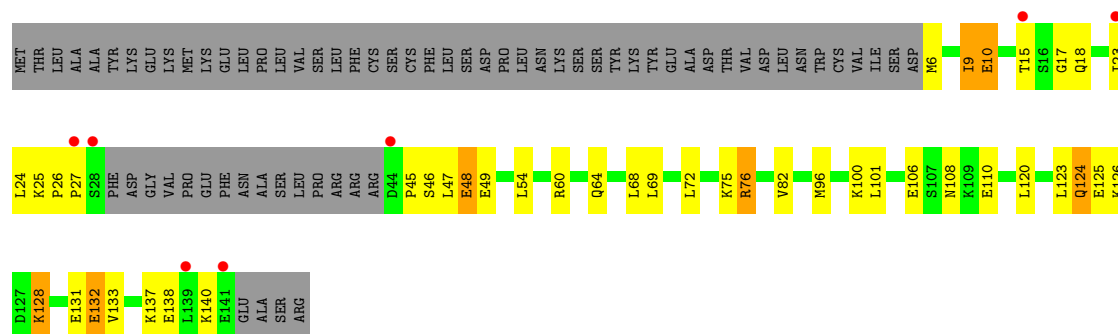




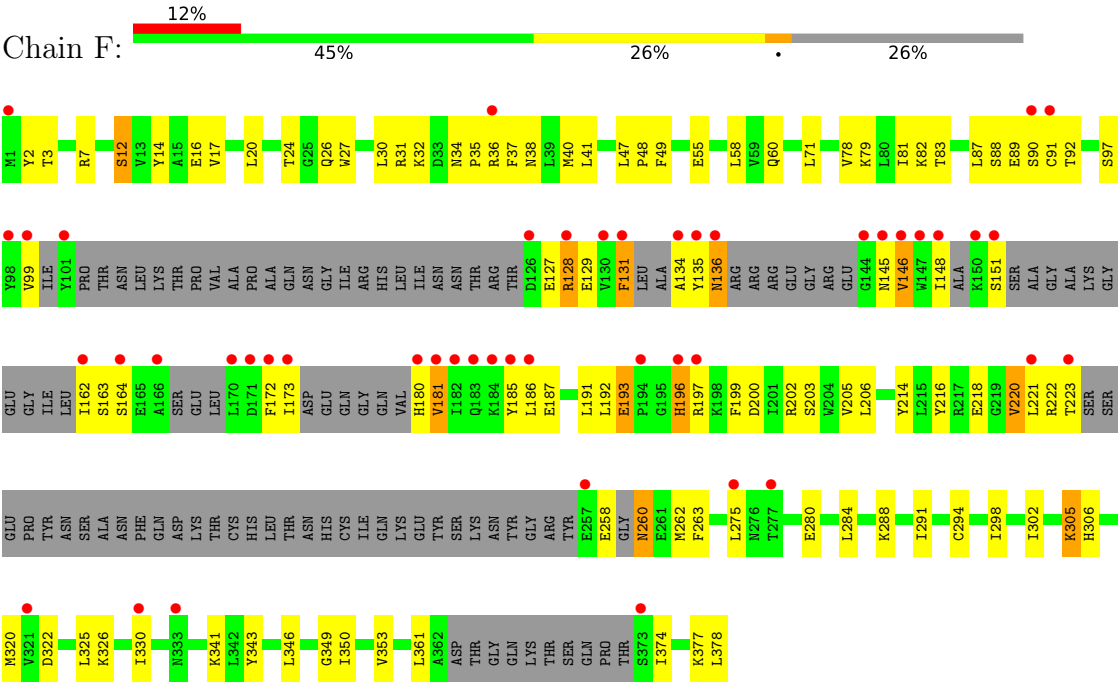
• Molecule 2: Tubulin beta-2B chain



• Molecule 3: Stathmin-4



• Molecule 4: Tubulin tyrosine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.78Å 156.55Å 182.59Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.89 – 2.51 49.89 – 2.51	Depositor EDS
% Data completeness (in resolution range)	97.0 (49.89-2.51) 97.0 (49.89-2.51)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.62 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.10.1_2155	Depositor
R, R_{free}	0.183 , 0.240 0.187 , 0.241	Depositor DCC
R_{free} test set	5064 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.102	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 51.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17559	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 2.61% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GTP, GOL, GDP, G9U, CA, MG, 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	0.38	0/3567	0.55	1/4846 (0.0%)
1	C	0.48	1/3589 (0.0%)	0.63	3/4874 (0.1%)
2	B	0.41	0/3437	0.57	0/4653
2	D	0.35	0/3406	0.52	2/4615 (0.0%)
3	E	0.35	0/1033	0.50	0/1370
4	F	0.38	0/2367	0.56	2/3184 (0.1%)
All	All	0.40	1/17399 (0.0%)	0.57	8/23542 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	273	ALA	C-O	-6.68	1.17	1.24

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	273	ALA	C-N-CD	7.82	137.80	120.60
4	F	193	GLU	C-N-CD	6.80	135.56	120.60
1	C	275	VAL	CA-C-N	-5.46	112.15	121.97
1	C	275	VAL	C-N-CA	-5.46	112.15	121.97
4	F	185	TYR	N-CA-C	-5.40	102.29	110.28
1	C	272	TYR	N-CA-C	5.13	117.76	109.40
2	D	10	GLY	CA-C-N	5.12	127.60	120.63
2	D	10	GLY	C-N-CA	5.12	127.60	120.63

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	3456	0	3395	101	0
1	C	3484	0	3407	96	0
2	B	3337	0	3232	112	0
2	D	3321	0	3212	134	0
3	E	1016	0	1041	48	0
4	F	2310	0	2316	109	0
5	A	32	12	12	1	0
5	C	32	12	12	2	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	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	23	18	0	1	0
8	D	23	18	0	1	0
9	B	28	12	12	0	0
9	D	28	12	12	1	0
10	B	12	13	13	4	0
11	C	6	8	8	5	0
12	A	72	0	0	3	0
12	B	56	0	0	3	0
12	C	148	0	0	5	0
12	D	21	0	0	0	0
12	E	16	0	0	2	0
12	F	27	0	0	2	0
All	All	17454	105	16672	567	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 17.

All (567) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:ILE:HD11	1:C:280:LYS:CB	1.49	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:276:ILE:CD1	1:C:280:LYS:HB2	1.69	1.21
1:C:276:ILE:HG13	1:C:280:LYS:NZ	1.59	1.14
4:F:200:ASP:HB3	4:F:320:MET:HE2	1.31	1.12
2:D:105:LYS:HD2	2:D:110:GLU:HG3	1.31	1.10
1:C:276:ILE:HG13	1:C:280:LYS:CE	1.82	1.08
1:C:276:ILE:HG12	1:C:277:SER:N	1.57	1.07
1:C:276:ILE:HG12	1:C:277:SER:H	0.89	1.04
1:C:276:ILE:CG1	1:C:277:SER:H	1.77	0.98
1:C:276:ILE:CG1	1:C:280:LYS:NZ	2.29	0.94
4:F:3:THR:HG23	4:F:38:ASN:H	1.33	0.92
1:C:276:ILE:HG13	1:C:280:LYS:HZ1	1.20	0.92
1:C:276:ILE:HG13	1:C:280:LYS:HE2	1.49	0.92
2:B:123:ARG:O	2:B:127:GLU:HG2	1.70	0.91
1:C:270:ALA:HB3	1:C:302:MET:HE2	1.49	0.90
2:D:83:PHE:O	2:D:86:ILE:HG22	1.71	0.90
4:F:199:PHE:HB2	4:F:221:LEU:HD21	1.52	0.90
1:C:276:ILE:CG1	1:C:280:LYS:HZ1	1.86	0.88
1:A:209[A]:ILE:HG23	1:A:230:LEU:HD23	1.55	0.87
1:C:286:LEU:H	1:C:286:LEU:HD12	1.38	0.87
4:F:31:ARG:HD3	4:F:32:LYS:H	1.40	0.86
2:B:83:PHE:O	2:B:86:ILE:HG22	1.75	0.85
2:D:105:LYS:HD3	2:D:109:THR:HG1	1.44	0.81
1:A:112:LYS:HD3	3:E:54:LEU:HD22	1.63	0.81
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.64	0.79
4:F:151:SER:HB2	4:F:180:HIS:HA	1.64	0.79
1:A:112:LYS:HE2	3:E:54:LEU:HD13	1.64	0.79
1:C:276:ILE:HD11	1:C:280:LYS:HB2	0.83	0.79
2:D:323:MET:HB3	2:D:373:MET:HE3	1.66	0.78
2:B:337:ASN:ND2	4:F:58:LEU:HD21	1.98	0.78
2:D:105:LYS:CD	2:D:110:GLU:HG3	2.12	0.77
1:A:108:TYR:O	1:A:112:LYS:HG2	1.85	0.76
2:D:105:LYS:HD3	2:D:109:THR:OG1	1.83	0.76
4:F:199:PHE:HB3	4:F:223:THR:HG22	1.65	0.76
1:C:320:ARG:HD3	12:C:616:HOH:O	1.85	0.76
4:F:320:MET:HG2	4:F:330:ILE:HD11	1.66	0.76
2:D:171:VAL:CG1	2:D:206:ASN:HD21	1.98	0.76
2:D:223:THR:HG22	2:D:226:ASP:OD2	1.86	0.75
4:F:199:PHE:CB	4:F:221:LEU:HD21	2.15	0.75
4:F:128:ARG:O	4:F:131:PHE:HB3	1.87	0.75
2:B:306:ASP:HB3	2:B:309:HIS:CD2	2.21	0.75
4:F:199:PHE:HB2	4:F:221:LEU:CD2	2.15	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:217:LEU:CB	1:A:219:ILE:HD12	2.18	0.74
1:A:209[A]:ILE:HD11	1:A:302[A]:MET:SD	2.28	0.74
1:A:217:LEU:HB3	1:A:219:ILE:HD12	1.69	0.74
4:F:3:THR:HG23	4:F:38:ASN:N	2.02	0.74
4:F:31:ARG:HD3	4:F:32:LYS:N	2.03	0.74
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.23	0.73
1:C:276:ILE:CG1	1:C:280:LYS:HE2	2.17	0.73
2:D:193:GLN:OE1	3:E:126:LYS:NZ	2.22	0.73
2:B:42:LEU:HD22	2:B:358:ILE:HD11	1.70	0.73
2:B:159:GLU:HB2	3:E:72:LEU:HD23	1.69	0.72
2:D:75:MET:CE	2:D:94:PHE:HB3	2.19	0.72
2:D:69:ASP:CB	2:D:75:MET:HE2	2.18	0.72
1:A:229:ARG:CZ	1:A:363:VAL:HG11	2.19	0.72
2:D:223:THR:HG23	2:D:226:ASP:H	1.53	0.72
2:B:176:LYS:HD2	2:B:207:GLU:HG3	1.70	0.72
1:C:292:THR:O	1:C:295[B]:CYS:HB2	1.91	0.71
1:C:276:ILE:HD11	1:C:280:LYS:HB3	1.65	0.71
4:F:31:ARG:HH11	4:F:32:LYS:HG3	1.55	0.71
2:B:334:ASN:CG	2:B:338:LYS:HE2	2.17	0.70
1:C:248:LEU:HD12	1:C:357:TYR:OH	1.92	0.70
4:F:131:PHE:O	4:F:134:ALA:N	2.26	0.69
1:C:276:ILE:CD1	1:C:280:LYS:CB	2.46	0.69
2:D:241:CYS:SG	2:D:318:ILE:HD12	2.33	0.68
2:D:174:SER:O	2:D:178:SER:HB2	1.93	0.68
4:F:346:LEU:O	4:F:350:ILE:HG13	1.93	0.68
1:A:209[B]:ILE:CD1	1:A:231:ILE:HD11	2.24	0.68
4:F:47:LEU:HD23	4:F:48:PRO:HD2	1.75	0.67
2:D:269[A]:MET:HE2	2:D:305:CYS:HB2	1.77	0.67
4:F:99:VAL:HA	4:F:181:VAL:HG12	1.76	0.67
3:E:6:MET:N	12:E:202:HOH:O	2.27	0.67
2:D:75:MET:HE1	2:D:94:PHE:HB3	1.76	0.67
4:F:24:THR:HG22	4:F:26:GLN:HG3	1.76	0.67
1:C:194[B]:THR:HG21	12:C:612:HOH:O	1.95	0.67
1:A:136[A]:LEU:HD23	1:A:167:LEU:HB2	1.77	0.66
2:B:326:LYS:O	2:B:330:GLU:HG3	1.96	0.66
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.10	0.66
2:B:334:ASN:O	2:B:338:LYS:HD2	1.96	0.66
4:F:341:LYS:HD2	4:F:341:LYS:O	1.96	0.66
2:D:79:ARG:O	2:D:84:GLY:HA3	1.97	0.65
1:C:288:VAL:HG23	11:C:501:GOL:H31	1.79	0.65
2:B:334:ASN:ND2	2:B:338:LYS:HE2	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ALA:O	1:C:183:GLU:HG3	1.97	0.65
4:F:136:ASN:C	4:F:145:ASN:OD1	2.40	0.65
2:D:207:GLU:CB	2:D:390:ARG:HH12	2.10	0.65
2:D:69:ASP:HB3	2:D:75:MET:HE2	1.77	0.65
2:D:136:GLN:HA	2:D:167:ASN:O	1.96	0.64
4:F:192:LEU:HD22	4:F:262:MET:HE1	1.77	0.64
1:C:288:VAL:HB	11:C:501:GOL:H11	1.79	0.64
2:D:416:MET:O	2:D:420:GLU:HG3	1.96	0.64
2:D:318:ILE:HG23	2:D:376:THR:HB	1.78	0.64
1:C:276:ILE:CG1	1:C:280:LYS:CE	2.67	0.64
2:D:105:LYS:HE2	2:D:411:GLU:OE2	1.98	0.63
2:D:12:CYS:HB2	9:D:502:GDP:C8	2.32	0.63
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.31	0.63
3:E:125:GLU:OE1	3:E:128:LYS:NZ	2.29	0.63
1:C:276:ILE:CD1	1:C:280:LYS:HE2	2.29	0.63
4:F:199:PHE:CB	4:F:223:THR:HG22	2.28	0.63
1:A:276:ILE:HG22	1:A:277:SER:N	2.13	0.62
1:A:112:LYS:HZ1	3:E:54:LEU:CD1	2.12	0.62
1:A:83:TYR:CD1	1:A:86:LEU:HD22	2.34	0.62
4:F:146:VAL:CG1	4:F:187:GLU:OE2	2.48	0.62
2:D:358:ILE:O	2:D:358:ILE:HG13	1.97	0.62
1:A:215:ARG:HG2	1:A:216:ASN:OD1	1.99	0.62
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.34	0.62
4:F:199:PHE:CG	4:F:221:LEU:HD21	2.34	0.61
2:D:369:ARG:HD3	2:D:369:ARG:N	2.15	0.61
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.83	0.61
4:F:146:VAL:HG12	4:F:187:GLU:OE2	2.00	0.61
3:E:120:LEU:O	3:E:124:GLN:HG2	2.00	0.61
3:E:60:ARG:O	3:E:64:GLN:HG3	2.00	0.60
1:A:9:VAL:HG22	1:A:68[B]:VAL:CG1	2.30	0.60
1:C:176:GLN:HE22	1:C:207:GLU:HG3	1.66	0.60
2:D:171:VAL:CG1	2:D:206:ASN:ND2	2.64	0.60
2:D:171:VAL:HG12	2:D:206:ASN:HD21	1.67	0.60
2:D:180:THR:HG22	2:D:181:VAL:N	2.15	0.60
2:D:269[A]:MET:CE	2:D:305:CYS:HB2	2.31	0.60
2:B:36:TYR:CZ	2:B:46:LEU:HD11	2.36	0.60
1:A:88:HIS:O	1:A:91:GLN:HG2	2.01	0.60
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.36	0.60
2:D:107:HIS:O	2:D:152:LEU:HD22	2.00	0.60
2:D:85:GLN:OE1	2:D:85:GLN:N	2.30	0.60
1:C:276:ILE:CG1	1:C:280:LYS:HB2	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:3:THR:HG22	4:F:38:ASN:OD1	2.02	0.60
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.83	0.60
1:C:288:VAL:H	11:C:501:GOL:H31	1.66	0.60
1:A:329:ASN:O	3:E:6:MET:HE1	2.02	0.60
2:B:248:LEU:HD23	2:B:249:ASN:H	1.67	0.59
4:F:12:SER:HB2	4:F:343:TYR:CE1	2.38	0.59
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.37	0.59
1:A:7:ILE:HG12	1:A:66[B]:VAL:CG1	2.33	0.59
2:D:323:MET:HB3	2:D:373:MET:CE	2.33	0.59
4:F:320:MET:CG	4:F:330:ILE:HD11	2.32	0.59
2:D:63:PRO:O	2:D:65:ALA:N	2.35	0.59
2:D:345:GLU:CG	2:D:440:ALA:HB2	2.33	0.59
4:F:99:VAL:HG12	4:F:127:GLU:OE1	2.01	0.59
1:A:14:VAL:HG13	1:A:67:PHE:HD2	1.68	0.59
1:A:112:LYS:CE	3:E:54:LEU:HD13	2.31	0.59
12:A:633:HOH:O	3:E:15:THR:HB	2.02	0.59
1:A:83:TYR:HD1	1:A:86:LEU:HD22	1.67	0.59
2:D:326:LYS:O	2:D:330:GLU:HG3	2.02	0.59
4:F:87:LEU:O	4:F:91:CYS:HB3	2.02	0.59
1:A:346:TRP:H	1:A:346:TRP:CD1	2.20	0.59
2:B:248:LEU:HD23	2:B:249:ASN:N	2.18	0.59
2:B:323:MET:HB3	2:B:373:MET:HE1	1.85	0.58
1:A:88:HIS:ND1	1:A:90:GLU:HG2	2.18	0.58
3:E:9:ILE:HG22	3:E:10:GLU:H	1.67	0.58
4:F:31:ARG:NH1	4:F:32:LYS:HG3	2.17	0.58
2:D:86:ILE:O	2:D:86:ILE:HD12	2.02	0.58
2:D:69:ASP:HB3	2:D:75:MET:CE	2.33	0.58
2:B:337:ASN:OD1	4:F:36:ARG:NH2	2.30	0.58
4:F:260:ASN:N	4:F:260:ASN:HD22	2.01	0.58
4:F:280:GLU:HA	4:F:284[B]:LEU:HB2	1.86	0.58
2:D:345:GLU:HG3	2:D:440:ALA:HB2	1.85	0.58
3:E:25:LYS:HD3	3:E:26:PRO:O	2.04	0.58
4:F:203:SER:HA	12:F:412:HOH:O	2.03	0.57
4:F:78:VAL:CG1	4:F:82:LYS:HE2	2.34	0.57
1:C:41:THR:O	1:C:41:THR:OG1	2.22	0.57
2:D:69:ASP:HB2	2:D:75:MET:HE2	1.86	0.57
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.40	0.57
2:D:414:ASP:OD1	2:D:415:GLU:N	2.38	0.57
2:D:203:CYS:SG	2:D:384[B]:ILE:HD11	2.45	0.57
3:E:76:ARG:O	3:E:76:ARG:HD3	2.05	0.57
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.35	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:6:MET:HG3	3:E:24:LEU:HD23	1.86	0.57
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.40	0.56
2:D:240:THR:HB	2:D:318:ILE:CD1	2.35	0.56
1:A:166:LYS:HE2	1:A:197:HIS:O	2.05	0.56
1:C:1:MET:O	1:C:2:ARG:HB2	2.05	0.56
1:C:337:THR:OG1	1:C:338:LYS:HD2	2.05	0.56
2:D:207:GLU:OE1	2:D:390:ARG:NH1	2.38	0.56
4:F:151:SER:CB	4:F:180:HIS:HA	2.33	0.56
1:A:112:LYS:CD	3:E:54:LEU:HD22	2.33	0.56
1:A:215:ARG:NH1	12:A:607:HOH:O	2.39	0.56
2:D:208:ALA:O	2:D:212:ILE:HG13	2.05	0.56
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.86	0.56
1:A:217:LEU:HB2	1:A:219:ILE:HD12	1.87	0.56
12:B:631:HOH:O	3:E:75:LYS:HD2	2.06	0.56
2:D:33:THR:O	2:D:60:LYS:HD2	2.06	0.56
3:E:106:GLU:O	3:E:110:GLU:HG3	2.06	0.56
1:A:147:SER:HB2	1:A:190:THR:HB	1.88	0.56
1:C:166:LYS:HE2	1:C:197:HIS:O	2.06	0.56
2:B:295:MET:CG	2:B:377:PHE:HB2	2.36	0.55
1:C:1:MET:HB3	1:C:2:ARG:NH2	2.20	0.55
1:A:175:PRO:HA	1:A:178:SER:HB2	1.87	0.55
1:A:276:ILE:HG22	1:A:277:SER:H	1.71	0.55
2:B:181:VAL:HG12	1:C:348:PRO:HG2	1.89	0.55
2:D:334:ASN:ND2	2:D:338:LYS:HE2	2.19	0.55
4:F:131:PHE:C	4:F:131:PHE:HD1	2.14	0.55
2:D:82:PRO:O	2:D:83:PHE:HB2	2.06	0.55
2:B:298:SER:OG	2:B:308:ARG:NH1	2.40	0.55
1:C:286:LEU:H	1:C:286:LEU:CD1	2.15	0.55
2:D:240:THR:HB	2:D:318:ILE:HD13	1.88	0.55
4:F:47:LEU:HD23	4:F:48:PRO:CD	2.37	0.55
4:F:298:ILE:HD12	4:F:302:ILE:HD13	1.89	0.55
2:B:218:LYS:C	2:B:219:LEU:HD23	2.32	0.55
2:D:132:LEU:HB3	2:D:164:ARG:NH1	2.22	0.55
1:C:36:MET:HE1	1:C:49:PHE:CE2	2.42	0.55
1:C:71:GLU:OE1	1:C:73:THR:HB	2.07	0.55
1:C:363:VAL:HG13	1:C:364:PRO:HD2	1.88	0.55
2:B:132:LEU:HB3	2:B:164:ARG:NH1	2.22	0.55
4:F:31:ARG:HA	4:F:31:ARG:NE	2.22	0.55
1:C:286:LEU:HD12	1:C:286:LEU:N	2.16	0.54
4:F:131:PHE:C	4:F:131:PHE:CD1	2.85	0.54
2:B:274:PRO:HB3	2:B:286:LEU:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:TYR:CZ	3:E:17:GLY:HA2	2.42	0.54
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.41	0.54
4:F:199:PHE:CD1	4:F:221:LEU:HD21	2.42	0.54
2:B:106:GLY:O	2:B:111:GLY:HA3	2.08	0.54
2:D:36:TYR:CE2	2:D:46:LEU:HD11	2.43	0.54
2:D:180:THR:HG22	2:D:181:VAL:H	1.73	0.54
4:F:191:LEU:N	4:F:191:LEU:HD22	2.23	0.54
1:A:229:ARG:NH2	1:A:363:VAL:HG11	2.22	0.54
2:D:36:TYR:CE1	2:D:38:GLY:HA3	2.43	0.54
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.43	0.54
2:D:8:GLN:NE2	2:D:14:ASN:HA	2.21	0.54
2:D:212:ILE:HG23	2:D:275:LEU:HD13	1.90	0.54
4:F:16:GLU:O	4:F:20:LEU:HG	2.08	0.54
3:E:132:GLU:N	3:E:132:GLU:OE1	2.40	0.53
4:F:220:VAL:HG23	4:F:263:PHE:CE2	2.43	0.53
1:C:66:VAL:HG23	1:C:125:LEU:HD11	1.91	0.53
1:C:179:THR:O	8:D:501:G9U:N01	2.41	0.53
4:F:349:GLY:O	4:F:353[A]:VAL:HG22	2.09	0.53
4:F:214:TYR:CE2	4:F:353[B]:VAL:HG11	2.42	0.53
2:B:159:GLU:CB	3:E:72:LEU:HD23	2.37	0.53
3:E:9:ILE:HD11	3:E:23:ILE:HD12	1.88	0.53
4:F:146:VAL:HG11	4:F:187:GLU:HG2	1.90	0.53
1:A:287:SER:OG	1:A:290:GLU:HG3	2.09	0.53
2:B:205:ASP:OD1	2:B:207:GLU:N	2.40	0.53
1:A:209[B]:ILE:HD12	1:A:231:ILE:HD11	1.89	0.53
2:D:412:GLY:HA3	3:E:133:VAL:O	2.08	0.53
1:C:412:GLY:HA3	3:E:108[A]:ASN:ND2	2.24	0.53
1:A:298:PRO:HA	1:A:301:GLN:CD	2.34	0.52
2:B:295:MET:HG2	2:B:377:PHE:HB2	1.92	0.52
2:B:63:PRO:HD3	2:B:86:ILE:HG13	1.92	0.52
1:C:141:PHE:CE2	1:C:170:SER:HB3	2.45	0.52
2:D:106:GLY:O	2:D:111:GLY:HA3	2.10	0.52
1:A:10:GLY:O	1:A:14:VAL:HG23	2.09	0.52
2:B:192:HIS:NE2	2:B:424[A]:ASN:OD1	2.42	0.52
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.45	0.52
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.92	0.51
2:B:104:ALA:HB2	2:B:413:MET:SD	2.50	0.51
3:E:128:LYS:O	3:E:131:GLU:HG3	2.10	0.51
1:A:72:PRO:HA	1:A:94:THR:HG21	1.93	0.51
1:A:112:LYS:HZ1	3:E:54:LEU:HD11	1.75	0.51
2:D:194:LEU:HD22	2:D:198:THR:HG21	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:215:ARG:NH1	1:A:299:ALA:HB1	2.25	0.51
1:A:262:TYR:CE2	1:A:346:TRP:CH2	2.99	0.51
1:A:9:VAL:HA	1:A:68[B]:VAL:HG13	1.93	0.51
4:F:193:GLU:OE1	4:F:196:HIS:ND1	2.44	0.51
4:F:202:ARG:HB2	4:F:222:ARG:NH1	2.26	0.51
4:F:305:LYS:HD2	4:F:306:HIS:ND1	2.25	0.51
2:B:67:LEU:N	2:B:67:LEU:HD12	2.26	0.51
1:C:41:THR:HB	1:C:44:GLY:O	2.11	0.51
2:B:69:ASP:O	2:B:94:PHE:HA	2.10	0.51
2:B:331:GLN:O	2:B:334:ASN:HB3	2.11	0.51
4:F:361:LEU:HD11	12:F:401:HOH:O	2.10	0.51
1:A:159:VAL:HG11	3:E:47:LEU:HB2	1.93	0.51
1:A:217:LEU:HB3	1:A:219:ILE:CD1	2.38	0.51
2:D:327:GLU:O	2:D:331:GLN:HG2	2.11	0.50
2:D:108:TYR:CG	3:E:133:VAL:HG11	2.45	0.50
1:A:214:ARG:HG2	1:A:219:ILE:O	2.12	0.50
1:C:277:SER:H	1:C:280:LYS:NZ	2.09	0.50
2:D:46:LEU:HA	2:D:49:ILE:HB	1.94	0.50
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.93	0.50
2:D:180:THR:HG21	2:D:182:VAL:HG22	1.93	0.50
4:F:288:LYS:HG2	4:F:378[B]:LEU:HD21	1.93	0.50
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.77	0.50
2:B:286:LEU:HD22	2:B:290:GLU:HB3	1.94	0.50
2:D:7:ILE:O	2:D:137:LEU:HA	2.10	0.50
4:F:78:VAL:HG13	4:F:82:LYS:HE2	1.93	0.50
2:D:171:VAL:HA	2:D:204:ILE:O	2.11	0.50
2:D:295:MET:CG	2:D:377:PHE:HB2	2.41	0.50
2:D:2:ARG:HH11	2:D:2:ARG:HG2	1.77	0.50
4:F:47:LEU:HD13	4:F:49:PHE:CZ	2.47	0.50
1:C:276:ILE:HG12	1:C:280:LYS:NZ	2.20	0.50
2:D:358:ILE:O	2:D:358:ILE:CG1	2.60	0.50
2:B:274:PRO:HB3	2:B:286:LEU:CD1	2.42	0.50
2:B:286:LEU:HD22	2:B:290:GLU:CB	2.42	0.49
4:F:24:THR:CG2	4:F:26:GLN:HG3	2.42	0.49
1:C:276:ILE:HD11	1:C:280:LYS:CA	2.36	0.49
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.43	0.49
2:D:105:LYS:HE2	2:D:411:GLU:CD	2.37	0.49
2:D:207:GLU:HB3	2:D:390:ARG:HH12	1.75	0.49
4:F:3:THR:HG23	4:F:37:PHE:HA	1.95	0.49
1:A:14:VAL:HG13	1:A:67:PHE:CD2	2.47	0.49
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.43	0.49
2:D:56:ALA:HB3	2:D:60:LYS:HB2	1.95	0.49
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.46	0.49
2:B:199:ASP:OD1	10:B:505:MES:H32	2.13	0.49
1:C:176:GLN:NE2	1:C:207:GLU:HG3	2.27	0.49
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.95	0.49
1:A:7:ILE:HG12	1:A:66[B]:VAL:HG12	1.94	0.49
1:A:143:GLY:N	5:A:501:GTP:H5'	2.28	0.49
1:A:207:GLU:OE2	1:A:304:LYS:HD2	2.13	0.49
2:B:352:LYS:HG3	2:B:353:THR:N	2.28	0.49
1:C:277:SER:H	1:C:280:LYS:HZ3	1.59	0.48
2:B:292:THR:HA	2:B:295:MET:HE2	1.94	0.48
2:B:390:ARG:HD3	12:B:608:HOH:O	2.11	0.48
1:C:347:CYS:HB2	1:C:348:PRO:HD2	1.96	0.48
3:E:138:GLU:C	3:E:140:LYS:H	2.21	0.48
1:C:143:GLY:N	5:C:502:GTP:H5'	2.29	0.48
4:F:3:THR:CG2	4:F:37:PHE:HA	2.44	0.48
2:B:291:LEU:HD23	2:B:291:LEU:HA	1.59	0.48
2:D:214:PHE:O	2:D:218:LYS:HA	2.13	0.48
2:B:19:LYS:HB3	2:B:232:SER:OG	2.13	0.48
2:B:42:LEU:H	2:B:42:LEU:HD12	1.78	0.48
1:C:55:GLU:OE1	12:C:601:HOH:O	2.20	0.48
1:C:270:ALA:HB3	1:C:302:MET:CE	2.35	0.48
1:C:363:VAL:CG1	1:C:364:PRO:HD2	2.43	0.48
2:D:75:MET:HE3	2:D:94:PHE:HB3	1.92	0.48
4:F:92:THR:O	4:F:326:LYS:NZ	2.41	0.48
1:A:110:ILE:O	1:A:110:ILE:HG22	2.14	0.48
2:B:3:GLU:OE1	2:B:130:ASP:N	2.45	0.48
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.95	0.48
2:D:11:GLN:HA	2:D:74:THR:HG21	1.95	0.48
2:B:282:GLN:HG3	2:B:282:GLN:O	2.12	0.48
3:E:46:SER:OG	3:E:48:GLU:HG3	2.14	0.48
4:F:192:LEU:HD22	4:F:262:MET:CE	2.42	0.48
1:A:180:ALA:O	1:A:183:GLU:HG3	2.14	0.47
1:C:70:LEU:HD13	1:C:110:ILE:CG2	2.44	0.47
1:A:112:LYS:CE	3:E:54:LEU:HD22	2.44	0.47
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.96	0.47
2:B:219:LEU:HD23	2:B:219:LEU:N	2.28	0.47
2:D:169:PHE:CE2	2:D:235:MET:HG2	2.49	0.47
2:D:404:PHE:HE2	2:D:407:TRP:CE2	2.31	0.47
2:B:16[B]:ILE:HG21	2:B:231:VAL:HG11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:349:GLY:HA3	4:F:374:ILE:HD11	1.95	0.47
2:B:157:ILE:HG21	2:B:166:MET:HE1	1.95	0.47
2:B:358:ILE:N	2:B:358:ILE:HD12	2.30	0.47
2:D:29:GLY:O	2:D:36:TYR:HD1	1.97	0.47
1:A:90:GLU:HB2	1:A:121:ARG:NH1	2.30	0.47
2:B:282:GLN:HG2	2:B:371:LEU:HD23	1.95	0.47
2:D:207:GLU:HB2	2:D:390:ARG:HH12	1.79	0.47
2:B:250:ALA:HA	8:B:501:G9U:O01	2.15	0.47
2:D:109:THR:OG1	2:D:110:GLU:N	2.47	0.47
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.97	0.47
2:B:359:PRO:HB2	2:B:371:LEU:O	2.14	0.47
2:D:19:LYS:O	2:D:23:VAL:HG23	2.15	0.47
4:F:163:SER:OG	4:F:164:SER:N	2.48	0.47
2:B:34:GLY:HA2	2:B:86:ILE:CD1	2.44	0.47
2:B:177:VAL:HG13	2:B:206:ASN:HB3	1.97	0.47
2:D:2:ARG:HH11	2:D:2:ARG:CG	2.28	0.47
2:D:104:ALA:HB2	2:D:413:MET:SD	2.55	0.47
2:D:297:ASP:OD1	2:D:298:SER:N	2.47	0.47
2:B:192:HIS:ND1	2:B:424[B]:ASN:ND2	2.61	0.47
1:C:66:VAL:HG12	1:C:68[A]:VAL:HG23	1.97	0.47
4:F:206:LEU:HD23	4:F:353[A]:VAL:CG2	2.45	0.47
2:B:21:TRP:CH2	2:B:63:PRO:HB3	2.49	0.46
2:D:191:VAL:HG11	2:D:425:MET:HG3	1.97	0.46
4:F:89:GLU:O	4:F:90:SER:HB3	2.14	0.46
1:A:273:ALA:HA	1:A:274:PRO:HA	1.71	0.46
4:F:186:LEU:O	4:F:186:LEU:HG	2.15	0.46
1:A:98:ASP:C	1:A:98:ASP:OD1	2.58	0.46
1:C:234:ILE:HG21	1:C:302:MET:SD	2.55	0.46
2:D:301:MET:HE3	2:D:307:PRO:HG3	1.96	0.46
1:A:112:LYS:HZ1	3:E:54:LEU:HD13	1.78	0.46
1:C:227:LEU:O	1:C:231:ILE:HG13	2.16	0.46
2:B:46:LEU:HA	2:B:49:ILE:HB	1.97	0.46
2:B:306:ASP:HB3	2:B:309:HIS:CG	2.50	0.46
1:C:66:VAL:HG23	1:C:125:LEU:CD1	2.45	0.46
4:F:2:TYR:HB2	4:F:27:TRP:CD2	2.51	0.46
4:F:361:LEU:HD12	4:F:361:LEU:N	2.29	0.46
2:B:146:GLY:O	2:B:150:GLY:HA3	2.16	0.46
4:F:135:TYR:CG	4:F:135:TYR:O	2.69	0.46
2:B:295:MET:HE3	2:B:296:PHE:CE2	2.51	0.46
1:C:1:MET:HE2	1:C:1:MET:HB2	1.81	0.46
3:E:26:PRO:HB2	3:E:27:PRO:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ARG:HA	2:B:131:CYS:O	2.16	0.46
2:B:19:LYS:HA	2:B:19:LYS:HD3	1.83	0.46
2:B:88:ARG:HH12	2:B:90:ASP:HB2	1.79	0.46
2:B:322:ARG:O	2:B:322:ARG:CG	2.64	0.46
2:B:400:ARG:HE	2:B:400:ARG:HB3	1.53	0.46
2:D:259:MET:HE2	2:D:378:ILE:HG22	1.98	0.46
2:D:308:ARG:HG3	2:D:308:ARG:HH11	1.81	0.46
2:B:322:ARG:O	2:B:322:ARG:HG3	2.15	0.46
3:E:48:GLU:HG3	3:E:49:GLU:N	2.31	0.46
2:B:288:VAL:O	2:B:292:THR:HG23	2.16	0.45
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.99	0.45
2:D:171:VAL:HG12	2:D:206:ASN:ND2	2.31	0.45
2:D:320:ARG:NH2	2:D:358:ILE:HD11	2.32	0.45
1:A:209[A]:ILE:CD1	1:A:302[A]:MET:SD	3.00	0.45
2:B:323:MET:HE2	2:B:373:MET:CE	2.47	0.45
1:C:276:ILE:CG1	1:C:280:LYS:HZ3	2.25	0.45
4:F:7:ARG:HD3	4:F:40:MET:HE3	1.98	0.45
3:E:125:GLU:OE1	3:E:125:GLU:HA	2.15	0.45
4:F:71:LEU:HD11	4:F:294:CYS:HB3	1.97	0.45
1:A:9:VAL:HG22	1:A:68[B]:VAL:HG11	1.97	0.45
2:D:322:ARG:HB3	2:D:322:ARG:NH2	2.32	0.45
1:A:263:PRO:O	1:A:266:HIS:ND1	2.43	0.45
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.57	0.45
2:D:305:CYS:HA	2:D:386:GLU:OE2	2.17	0.45
4:F:148:ILE:HD12	4:F:162:ILE:HG13	1.98	0.45
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.51	0.45
4:F:322:ASP:C	4:F:322:ASP:OD1	2.60	0.45
2:D:9:ALA:HA	2:D:68:VAL:O	2.17	0.45
2:D:16:ILE:HG13	2:D:17:GLY:N	2.32	0.45
2:D:323:MET:HE2	2:D:373:MET:HE3	1.99	0.45
1:A:2:ARG:O	1:A:133:GLN:NE2	2.39	0.45
1:A:180:ALA:HA	2:B:258:ASN:OD1	2.16	0.45
2:B:108:TYR:CD2	3:E:82:VAL:HG11	2.51	0.45
2:D:180:THR:CG2	2:D:181:VAL:N	2.78	0.45
3:E:137:LYS:O	3:E:137:LYS:HG2	2.17	0.45
4:F:91:CYS:O	4:F:92:THR:OG1	2.24	0.45
1:A:416:GLY:O	1:A:420[B]:GLU:HG3	2.17	0.45
4:F:3:THR:OG1	4:F:30:LEU:CD2	2.65	0.45
4:F:135:TYR:O	4:F:135:TYR:CD2	2.70	0.45
1:A:292:THR:O	1:A:295:CYS:HB2	2.17	0.44
2:B:81:GLY:O	2:B:82:PRO:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:325:MET:CE	2:D:355:VAL:HG21	2.47	0.44
4:F:146:VAL:CG1	4:F:187:GLU:HG2	2.47	0.44
4:F:202:ARG:HB3	4:F:220:VAL:HG12	1.98	0.44
2:B:334:ASN:CG	2:B:338:LYS:CE	2.90	0.44
2:D:10:GLY:O	2:D:14:ASN:ND2	2.47	0.44
1:A:256:GLN:H	1:A:256:GLN:HG3	1.58	0.44
3:E:9:ILE:HD11	3:E:23:ILE:CD1	2.47	0.44
1:A:23:LEU:HD21	1:A:233:GLN:NE2	2.32	0.44
2:B:2:ARG:HB3	2:B:133:GLN:HG3	1.99	0.44
1:C:221:ARG:NH2	2:D:329:ASP:OD2	2.50	0.44
1:C:250:VAL:HG11	1:C:352:LYS:HE3	2.00	0.44
2:D:97:SER:HB2	2:D:110:GLU:OE2	2.17	0.44
1:A:48:SER:O	1:A:51[A]:THR:HG23	2.18	0.44
1:C:39:ASP:OD2	1:C:41:THR:OG1	2.36	0.44
2:D:109:THR:HG21	2:D:411:GLU:OE1	2.17	0.44
2:D:240:THR:CG2	2:D:318:ILE:HD11	2.47	0.44
4:F:81:ILE:HG12	4:F:87:LEU:HD13	2.00	0.44
4:F:200:ASP:HB3	4:F:320:MET:CE	2.23	0.44
1:A:69:ASP:O	1:A:94:THR:HA	2.18	0.44
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.36	0.44
1:C:320:ARG:HA	1:C:356:ASN:O	2.17	0.44
4:F:173:ILE:HD12	4:F:173:ILE:N	2.32	0.44
2:B:88:ARG:NH1	2:B:124:LYS:HE3	2.33	0.44
2:D:248:LEU:HD11	2:D:352:LYS:HE3	2.00	0.44
3:E:68:LEU:HD12	3:E:72:LEU:HD13	1.99	0.44
1:A:179:THR:HA	2:B:352:LYS:NZ	2.33	0.44
2:B:199:ASP:OD1	10:B:505:MES:H72	2.18	0.44
2:D:159:GLU:HG3	3:E:123:LEU:HB3	2.00	0.43
1:A:276:ILE:CG2	1:A:277:SER:N	2.80	0.43
1:C:83:TYR:HD2	1:C:86:LEU:HD22	1.83	0.43
1:A:278:ALA:HA	1:A:369:ALA:HB2	2.00	0.43
1:C:220:GLU:HG2	2:D:326:LYS:HD3	1.99	0.43
1:C:440:VAL:O	12:C:602:HOH:O	2.21	0.43
4:F:214:TYR:CE2	4:F:353[B]:VAL:CG1	3.01	0.43
2:B:200:GLU:OE2	2:B:256:ALA:HB2	2.18	0.43
2:B:395:PHE:CE1	2:B:422:GLU:HB2	2.53	0.43
2:D:308:ARG:HG3	2:D:308:ARG:NH1	2.33	0.43
4:F:14:TYR:HA	4:F:17:VAL:HB	2.00	0.43
4:F:162:ILE:HD12	4:F:162:ILE:N	2.34	0.43
4:F:214:TYR:OH	4:F:377:LYS:NZ	2.51	0.43
4:F:275[B]:LEU:HD13	4:F:325:LEU:HD11	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:GLU:OE2	12:A:601:HOH:O	2.21	0.43
2:B:358:ILE:HD12	2:B:358:ILE:H	1.83	0.43
2:D:358:ILE:HD12	2:D:359:PRO:O	2.19	0.43
3:E:45:PRO:HA	3:E:49:GLU:OE1	2.18	0.43
2:B:165:ILE:HG21	2:B:252:LEU:HB3	2.00	0.43
2:D:323:MET:SD	2:D:373:MET:HE3	2.58	0.43
2:D:161:TYR:HB3	2:D:164:ARG:CG	2.48	0.43
2:D:223:THR:HG23	2:D:226:ASP:N	2.28	0.43
3:E:69:LEU:O	12:E:201:HOH:O	2.21	0.43
2:B:205:ASP:OD1	2:B:205:ASP:C	2.61	0.43
1:A:213:CYS:O	1:A:217:LEU:HB2	2.17	0.43
1:C:288:VAL:CG2	11:C:501:GOL:H31	2.48	0.43
2:D:70:LEU:O	2:D:98:GLY:N	2.49	0.43
2:D:180:THR:CG2	2:D:181:VAL:H	2.28	0.43
4:F:151:SER:HB3	4:F:180:HIS:CG	2.53	0.43
4:F:305:LYS:HD2	4:F:306:HIS:CE1	2.54	0.43
1:C:41:THR:OG1	1:C:55:GLU:OE2	2.37	0.43
1:C:71:GLU:HG2	1:C:98:ASP:HB3	2.01	0.43
1:C:93:ILE:HD11	1:C:121:ARG:HG3	2.01	0.43
1:C:205:ASP:HB2	1:C:303:VAL:HA	2.01	0.43
1:C:11:GLN:HB3	5:C:502:GTP:O1A	2.19	0.42
1:C:286:LEU:CD1	1:C:286:LEU:N	2.81	0.42
2:D:16:ILE:HD11	2:D:138:THR:HB	1.99	0.42
4:F:24:THR:HG21	4:F:361:LEU:CD2	2.49	0.42
4:F:172:PHE:HD1	4:F:172:PHE:O	2.02	0.42
2:B:85:GLN:HA	2:B:85:GLN:NE2	2.33	0.42
2:B:269:MET:HE3	2:B:269:MET:HB3	1.84	0.42
2:B:318:ILE:HG13	2:B:376:THR:HB	1.99	0.42
1:C:9:VAL:HG22	1:C:68[B]:VAL:CG1	2.49	0.42
1:C:177:VAL:HG23	12:C:654:HOH:O	2.18	0.42
1:C:249:ASN:OD1	1:C:356:ASN:OD1	2.37	0.42
2:B:337:ASN:ND2	4:F:36:ARG:HB3	2.35	0.42
1:C:211[A]:ASP:HB3	1:C:215:ARG:NH2	2.34	0.42
2:B:199:ASP:OD2	10:B:505:MES:H52	2.20	0.42
2:B:264:ARG:NH2	2:B:431[A]:GLU:OE2	2.51	0.42
2:B:16[B]:ILE:HD13	2:B:231:VAL:HG11	2.02	0.42
1:C:140:SER:HA	1:C:171:ILE:HB	2.01	0.42
2:D:425:MET:HB3	2:D:425:MET:HE2	1.71	0.42
2:B:108:TYR:CG	3:E:82:VAL:HG11	2.54	0.42
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.54	0.42
4:F:82:LYS:NZ	4:F:97:SER:O	2.41	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:HIS:CD2	2:B:424[A]:ASN:OD1	2.73	0.42
4:F:24:THR:HG22	4:F:26:GLN:CB	2.50	0.42
2:B:309:HIS:CD2	2:B:386:GLU:OE1	2.73	0.42
2:D:61:TYR:O	2:D:86:ILE:HD11	2.20	0.42
2:D:295:MET:SD	2:D:375:ALA:HB1	2.60	0.42
4:F:206:LEU:HD23	4:F:353[A]:VAL:HG21	2.01	0.42
1:A:134:GLY:HA3	1:A:165:SER:O	2.20	0.42
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.55	0.42
1:A:221:ARG:CZ	2:B:329:ASP:OD2	2.68	0.42
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.85	0.42
2:D:295:MET:HE1	2:D:319:PHE:CZ	2.54	0.42
3:E:47:LEU:HD12	3:E:47:LEU:O	2.19	0.42
1:A:25:CYS:HB3	1:A:30:ILE:O	2.20	0.41
1:A:136[A]:LEU:CD2	1:A:167:LEU:HB2	2.49	0.41
1:A:260:VAL:HG11	1:A:266:HIS:HB3	2.02	0.41
2:B:405:LEU:CD2	2:B:415:GLU:HG2	2.49	0.41
2:D:72:PRO:O	2:D:73:GLY:C	2.63	0.41
2:D:121:VAL:O	2:D:122:VAL:C	2.63	0.41
2:D:345:GLU:HG2	2:D:440:ALA:HB2	2.01	0.41
4:F:221:LEU:C	4:F:221:LEU:HD23	2.45	0.41
1:C:39:ASP:OD1	1:C:41:THR:OG1	2.37	0.41
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.56	0.41
1:C:276:ILE:HG12	1:C:280:LYS:HZ3	1.83	0.41
1:A:403:ALA:O	1:A:404:PHE:HB2	2.21	0.41
1:A:276:ILE:CG2	1:A:277:SER:H	2.34	0.41
2:B:394:GLN:OE1	12:B:601:HOH:O	2.22	0.41
1:C:276:ILE:CG1	1:C:277:SER:N	2.41	0.41
2:D:2:ARG:CG	2:D:2:ARG:NH1	2.84	0.41
2:B:158:ARG:CZ	10:B:505:MES:H21	2.51	0.41
1:C:285:GLN:H	1:C:285:GLN:HG2	1.65	0.41
2:D:36:TYR:CD2	2:D:46:LEU:HD11	2.55	0.41
1:A:88:HIS:CE1	1:A:90:GLU:HG2	2.56	0.41
2:B:2:ARG:HB3	2:B:133:GLN:NE2	2.35	0.41
1:C:67:PHE:CD1	1:C:67:PHE:N	2.87	0.41
2:D:345:GLU:HG3	2:D:440:ALA:CB	2.49	0.41
4:F:24:THR:HG22	4:F:26:GLN:CG	2.45	0.41
1:A:363:VAL:O	1:A:363:VAL:HG12	2.20	0.41
2:B:63:PRO:CD	2:B:86:ILE:HG13	2.50	0.41
2:B:434:GLN:HG3	2:B:435:TYR:N	2.36	0.41
2:D:70:LEU:HG	2:D:145:THR:HG23	2.01	0.41
2:D:318:ILE:CG2	2:D:376:THR:HB	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:ARG:NE	2:B:329:ASP:OD2	2.54	0.41
1:A:315[A]:CYS:HG	1:A:351:PHE:HE2	1.65	0.41
1:A:315[A]:CYS:SG	1:A:351:PHE:CE2	3.13	0.41
1:A:349:THR:HG22	3:E:24:LEU:HB2	2.01	0.41
1:C:302:MET:HB3	1:C:302:MET:HE3	1.82	0.41
2:D:67:LEU:N	2:D:67:LEU:HD12	2.35	0.41
2:D:96:GLN:HA	2:D:96:GLN:OE1	2.19	0.41
2:D:343:PHE:O	2:D:344:VAL:C	2.64	0.41
1:A:88:HIS:O	1:A:89:PRO:C	2.64	0.40
2:B:31:ASP:OD2	2:B:37:HIS:CD2	2.74	0.40
1:C:221:ARG:O	1:C:221:ARG:HG3	2.21	0.40
2:D:169:PHE:CD2	2:D:235:MET:HG2	2.55	0.40
4:F:34:ASN:OD1	4:F:35:PRO:HD2	2.21	0.40
1:A:112:LYS:N	1:A:112:LYS:HD2	2.36	0.40
1:A:203:MET:HE3	1:A:203:MET:HB3	1.90	0.40
4:F:38:ASN:O	4:F:60:GLN:HA	2.21	0.40
4:F:55:GLU:OE1	4:F:55:GLU:HA	2.20	0.40
4:F:127:GLU:O	4:F:128:ARG:C	2.64	0.40
1:A:103:TYR:CE2	1:A:148:GLY:HA2	2.56	0.40
2:B:171:VAL:HA	2:B:204:ILE:O	2.22	0.40
1:C:327:ASP:HB3	11:C:501:GOL:H11	2.04	0.40
4:F:12:SER:HB2	4:F:343:TYR:CZ	2.56	0.40
4:F:79:LYS:O	4:F:83:THR:HG22	2.22	0.40
1:A:262:TYR:CE2	1:A:346:TRP:CZ2	3.10	0.40
1:A:293:ASN:CA	1:A:335:ILE:HD11	2.52	0.40
1:A:355:ILE:O	3:E:17:GLY:HA3	2.22	0.40
2:B:318:ILE:CG1	2:B:376:THR:HB	2.52	0.40
1:A:51[B]:THR:HG22	1:A:52:PHE:CD1	2.57	0.40
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.56	0.40
2:B:248:LEU:HD12	2:B:352:LYS:CE	2.52	0.40
2:D:320:ARG:HD3	2:D:360:PRO:HD3	2.04	0.40
4:F:196:HIS:ND1	4:F:196:HIS:N	2.68	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	446/451 (99%)	425 (95%)	20 (4%)	1 (0%)	43 63
1	C	448/451 (99%)	436 (97%)	10 (2%)	2 (0%)	30 49
2	B	421/445 (95%)	406 (96%)	14 (3%)	1 (0%)	43 63
2	D	421/445 (95%)	399 (95%)	17 (4%)	5 (1%)	10 20
3	E	120/189 (64%)	116 (97%)	3 (2%)	1 (1%)	16 31
4	F	261/378 (69%)	246 (94%)	14 (5%)	1 (0%)	30 49
All	All	2117/2359 (90%)	2028 (96%)	78 (4%)	11 (0%)	24 43

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	64	ARG
1	A	109	THR
2	D	177	VAL
2	D	181	VAL
1	C	41	THR
2	D	180	THR
4	F	88	SER
3	E	10	GLU
1	C	178	SER
2	D	73	GLY
2	B	82	PRO

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	377/379 (100%)	365 (97%)	12 (3%)	34 62
1	C	381/379 (100%)	371 (97%)	10 (3%)	40 68
2	B	371/383 (97%)	358 (96%)	13 (4%)	32 58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	D	366/383 (96%)	348 (95%)	18 (5%)	22	45
3	E	112/171 (66%)	102 (91%)	10 (9%)	9	20
4	F	255/336 (76%)	242 (95%)	13 (5%)	21	43
All	All	1862/2031 (92%)	1786 (96%)	76 (4%)	27	53

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66[A]	VAL
1	A	66[B]	VAL
1	A	82	THR
1	A	178	SER
1	A	181	VAL
1	A	188	ILE
1	A	253	THR
1	A	340	SER
1	A	363	VAL
1	A	381	THR
1	A	423	GLU
1	A	437	VAL
2	B	55	GLU
2	B	117	SER
2	B	147[A]	SER
2	B	147[B]	SER
2	B	177	VAL
2	B	220	THR
2	B	238	VAL
2	B	299	LYS
2	B	302	MET
2	B	335	VAL
2	B	373	MET
2	B	389	LYS
2	B	405	LEU
1	C	67	PHE
1	C	71	GLU
1	C	163	LYS
1	C	190	THR
1	C	276	ILE
1	C	286	LEU
1	C	361	THR
1	C	381	THR

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Mol	Chain	Res	Type
1	C	384	ILE
1	C	430	LYS
2	D	2	ARG
2	D	77	SER
2	D	79	ARG
2	D	80	SER
2	D	86	ILE
2	D	117	SER
2	D	127	GLU
2	D	147	SER
2	D	216	THR
2	D	219	LEU
2	D	248	LEU
2	D	290	GLU
2	D	334	ASN
2	D	358	ILE
2	D	391	ILE
2	D	392	SER
2	D	404	PHE
2	D	422	GLU
3	E	9	ILE
3	E	18	GLN
3	E	48	GLU
3	E	76	ARG
3	E	96	MET
3	E	100	LYS
3	E	101	LEU
3	E	124	GLN
3	E	128	LYS
3	E	132	GLU
4	F	12	SER
4	F	128	ARG
4	F	129	GLU
4	F	131	PHE
4	F	136	ASN
4	F	146	VAL
4	F	181	VAL
4	F	196	HIS
4	F	197	ARG
4	F	220	VAL
4	F	258	GLU
4	F	260	ASN

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Mol	Chain	Res	Type
4	F	305	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	101	ASN
1	A	285	GLN
1	A	393	HIS
2	B	8	GLN
2	B	14	ASN
2	B	15	GLN
2	B	37	HIS
2	B	136	GLN
2	B	309	HIS
1	C	256	GLN
1	C	283	HIS
1	C	309	HIS
1	C	356	ASN
1	C	393	HIS
2	D	206	ASN
2	D	331	GLN
2	D	334	ASN
3	E	12	ASN
3	E	51	GLN
4	F	45	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

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	B	504	6	29,30,30	2.41	12 (41%)	45,47,47	1.79	11 (24%)
9	GDP	D	502	-	29,30,30	1.16	3 (10%)	45,47,47	1.84	7 (15%)
5	GTP	A	501	6	33,34,34	2.28	14 (42%)	50,54,54	1.98	12 (24%)
11	GOL	C	501	-	5,5,5	0.40	0	5,5,5	0.32	0
8	G9U	B	501	-	26,26,26	1.42	3 (11%)	32,37,37	0.63	0
5	GTP	C	502	6	33,34,34	2.37	14 (42%)	50,54,54	1.88	16 (32%)
10	MES	B	505	-	12,12,12	1.55	3 (25%)	15,16,16	2.11	5 (33%)
8	G9U	D	501	-	26,26,26	1.20	3 (11%)	32,37,37	0.81	1 (3%)

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	B	504	6	-	6/16/32/32	0/3/3/3
9	GDP	D	502	-	-	6/16/32/32	0/3/3/3
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3
11	GOL	C	501	-	-	2/4/4/4	-
8	G9U	B	501	-	-	1/4/18/18	0/4/4/4
5	GTP	C	502	6	-	5/22/38/38	0/3/3/3
10	MES	B	505	-	-	4/6/14/14	0/1/1/1
8	G9U	D	501	-	-	1/4/18/18	0/4/4/4

All (52) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	GDP	C6-N1	-5.09	1.29	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	501	GTP	C6-N1	-5.07	1.29	1.38
5	C	502	GTP	C6-N1	-4.71	1.30	1.38
5	A	501	GTP	C5-N7	-4.20	1.30	1.39
5	C	502	GTP	PG-O2G	-4.05	1.39	1.54
9	B	504	GDP	C5-N7	-3.95	1.31	1.39
9	B	504	GDP	PB-O2B	-3.93	1.40	1.54
9	B	504	GDP	C4-N9	-3.88	1.28	1.38
5	C	502	GTP	PB-O1B	-3.85	1.37	1.50
5	C	502	GTP	C4-N9	-3.80	1.28	1.38
5	C	502	GTP	C5-N7	-3.77	1.31	1.39
8	B	501	G9U	C10-C11	3.72	1.54	1.51
5	A	501	GTP	C4-N9	-3.60	1.28	1.38
5	C	502	GTP	PA-O2A	-3.40	1.39	1.55
9	B	504	GDP	PB-O3B	-3.40	1.42	1.54
8	D	501	G9U	O01-C11	3.40	1.26	1.22
8	B	501	G9U	O01-C11	3.40	1.26	1.22
9	B	504	GDP	C8-N9	-3.39	1.29	1.37
5	C	502	GTP	C8-N9	-3.37	1.30	1.37
10	B	505	MES	C8-S	3.28	1.82	1.77
9	B	504	GDP	PB-O1B	-3.26	1.40	1.50
5	A	501	GTP	PG-O2G	-3.19	1.43	1.54
5	A	501	GTP	C8-N9	-3.17	1.30	1.37
9	B	504	GDP	PA-O1A	-3.14	1.39	1.50
9	D	502	GDP	C5-C4	3.12	1.47	1.38
5	C	502	GTP	PG-O3G	-3.08	1.43	1.54
5	C	502	GTP	PG-O1G	-3.07	1.40	1.50
5	A	501	GTP	PB-O2B	-2.98	1.41	1.55
5	A	501	GTP	PG-O1G	-2.91	1.41	1.50
5	A	501	GTP	C2-N1	-2.88	1.30	1.37
8	B	501	G9U	BR1-C18	2.79	1.95	1.90
5	A	501	GTP	O4'-C4'	-2.78	1.38	1.45
9	B	504	GDP	C2-N1	-2.73	1.31	1.37
9	B	504	GDP	PA-O2A	-2.70	1.42	1.55
5	C	502	GTP	PA-O1A	-2.67	1.41	1.50
5	A	501	GTP	PA-O2A	-2.61	1.43	1.55
5	C	502	GTP	C2-N1	-2.57	1.31	1.37
5	C	502	GTP	O4'-C4'	-2.51	1.39	1.45
9	B	504	GDP	O6-C6	-2.49	1.18	1.23
10	B	505	MES	O2S-S	2.44	1.52	1.45
5	A	501	GTP	PA-O1A	-2.41	1.42	1.50
5	A	501	GTP	O6-C6	-2.38	1.19	1.23
9	D	502	GDP	C6-N1	-2.38	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	501	G9U	BR1-C18	2.38	1.95	1.90
8	D	501	G9U	C10-C11	2.32	1.53	1.51
5	A	501	GTP	PG-O3G	-2.30	1.46	1.54
5	C	502	GTP	PB-O2B	-2.29	1.44	1.55
9	B	504	GDP	O4'-C4'	-2.28	1.39	1.45
10	B	505	MES	O1S-S	2.24	1.51	1.45
5	A	501	GTP	C2'-C3'	-2.09	1.47	1.53
9	D	502	GDP	C5-N7	-2.03	1.35	1.39
5	C	502	GTP	PA-O3A	-2.02	1.57	1.59

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	502	GDP	C5-C4-N3	-6.23	118.48	128.39
5	A	501	GTP	C5-C4-N3	-5.74	119.25	128.39
9	D	502	GDP	C2-N3-C4	5.08	121.05	112.30
5	A	501	GTP	O3G-PG-O2G	5.00	126.55	107.80
9	B	504	GDP	C5-C4-N3	-4.97	120.47	128.39
5	A	501	GTP	N9-C4-N3	4.84	135.62	125.95
9	D	502	GDP	N9-C4-N3	4.65	135.25	125.95
5	C	502	GTP	C5-C4-N3	-4.47	121.28	128.39
5	C	502	GTP	N9-C4-N3	4.36	134.67	125.95
5	A	501	GTP	C2-N3-C4	4.18	119.49	112.30
10	B	505	MES	O2S-S-O1S	-4.02	100.74	113.82
9	B	504	GDP	N9-C4-N3	3.94	133.84	125.95
9	B	504	GDP	C2-N3-C4	3.90	119.02	112.30
5	C	502	GTP	C2-N3-C4	3.87	118.96	112.30
10	B	505	MES	C2-C3-N4	3.77	115.85	110.12
9	B	504	GDP	C6-C5-N7	3.63	136.90	130.29
5	C	502	GTP	C6-C5-N7	3.58	136.81	130.29
9	D	502	GDP	C6-C5-N7	3.25	136.20	130.29
5	C	502	GTP	O3G-PG-O2G	3.14	119.57	107.80
10	B	505	MES	O2S-S-C8	3.07	111.37	106.73
9	B	504	GDP	C2'-C1'-N9	3.06	121.78	113.25
9	B	504	GDP	O4'-C1'-N9	-2.95	101.67	108.36
5	C	502	GTP	O5'-C5'-C4'	2.92	118.93	108.99
5	A	501	GTP	O2B-PB-O3B	-2.91	99.41	107.27
5	A	501	GTP	C6-C5-N7	2.90	135.56	130.29
5	A	501	GTP	O6-C6-C5	-2.81	119.11	126.53
5	C	502	GTP	O3A-PB-O1B	-2.81	102.25	110.70
5	A	501	GTP	O5'-PA-O1A	-2.80	97.84	108.94
5	A	501	GTP	O2G-PG-O3B	-2.79	95.29	104.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	B	505	MES	O1-C6-C5	-2.69	105.99	111.77
5	C	502	GTP	PA-O5'-C5'	2.67	136.67	121.35
9	D	502	GDP	C4-C5-N7	-2.63	106.50	110.67
9	B	504	GDP	C4-C5-N7	-2.60	106.55	110.67
5	C	502	GTP	C8-N9-C4	2.58	110.87	106.03
5	C	502	GTP	O2B-PB-O3A	2.58	114.25	107.27
9	D	502	GDP	C3'-C2'-C1'	2.55	106.30	101.46
8	D	501	G9U	O01-C11-C05	2.50	122.96	119.97
9	B	504	GDP	O6-C6-C5	-2.47	120.01	126.53
10	B	505	MES	O1-C2-C3	2.45	117.05	111.77
5	C	502	GTP	O3B-PB-O1B	-2.39	103.51	110.70
5	C	502	GTP	C6-C5-C4	-2.35	115.29	118.83
5	C	502	GTP	O5'-PA-O1A	-2.35	99.62	108.94
9	B	504	GDP	C2-N1-C6	-2.19	121.13	125.11
9	D	502	GDP	O6-C6-C5	-2.13	120.91	126.53
5	C	502	GTP	O2B-PB-O1B	2.12	122.32	112.44
9	B	504	GDP	C8-N9-C4	2.11	109.99	106.03
5	A	501	GTP	C2-N1-C6	-2.10	121.31	125.11
5	A	501	GTP	C5-C6-N1	2.07	118.53	113.25
5	C	502	GTP	C5-C6-N1	2.07	118.52	113.25
5	A	501	GTP	C4-C5-N7	-2.07	107.39	110.67
5	C	502	GTP	O6-C6-C5	-2.02	121.20	126.53
9	B	504	GDP	C5-C6-N1	2.02	118.39	113.25

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	502	GTP	O4'-C4'-C5'-O5'
8	D	501	G9U	C09-C10-C12-C13
9	B	504	GDP	C5'-O5'-PA-O3A
9	B	504	GDP	C5'-O5'-PA-O1A
9	B	504	GDP	C5'-O5'-PA-O2A
9	D	502	GDP	C5'-O5'-PA-O3A
9	D	502	GDP	C5'-O5'-PA-O2A
10	B	505	MES	C8-C7-N4-C5
10	B	505	MES	C7-C8-S-O3S
5	A	501	GTP	O4'-C4'-C5'-O5'
5	C	502	GTP	C3'-C4'-C5'-O5'
11	C	501	GOL	O1-C1-C2-C3

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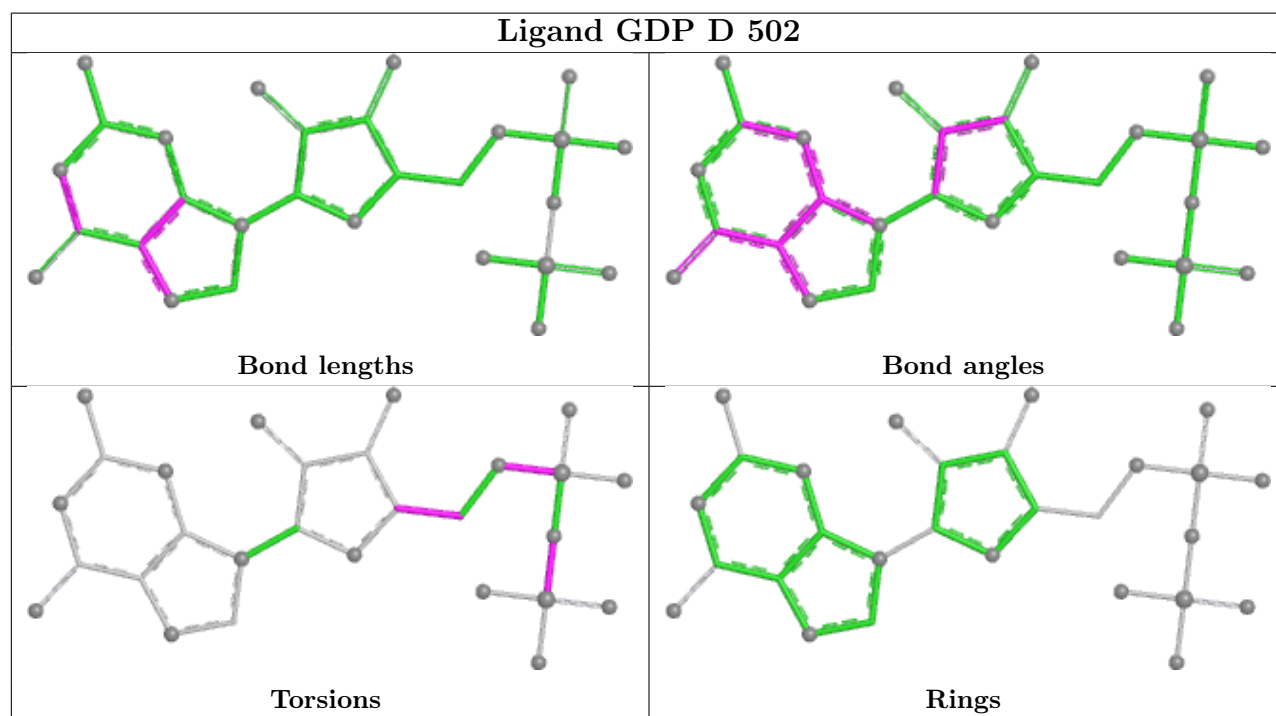
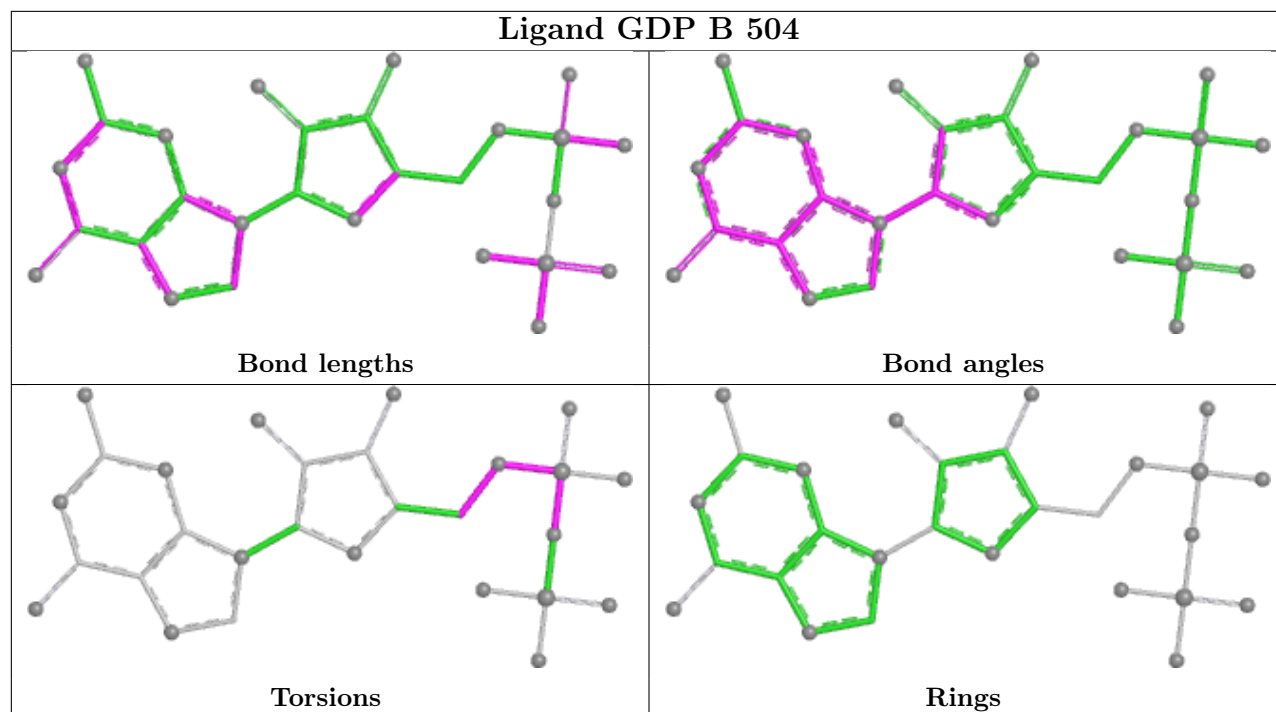
Mol	Chain	Res	Type	Atoms
11	C	501	GOL	O1-C1-C2-O2
5	A	501	GTP	C3'-C4'-C5'-O5'
10	B	505	MES	C7-C8-S-O1S
10	B	505	MES	C7-C8-S-O2S
8	B	501	G9U	C09-C10-C12-C13
9	D	502	GDP	C3'-C4'-C5'-O5'
5	C	502	GTP	C4'-C5'-O5'-PA
9	D	502	GDP	C5'-O5'-PA-O1A
5	A	501	GTP	C4'-C5'-O5'-PA
9	D	502	GDP	O4'-C4'-C5'-O5'
5	C	502	GTP	PG-O3B-PB-O1B
9	B	504	GDP	C4'-C5'-O5'-PA
5	C	502	GTP	PG-O3B-PB-O2B
5	A	501	GTP	PB-O3B-PG-O1G
9	D	502	GDP	PA-O3A-PB-O2B
9	B	504	GDP	PB-O3A-PA-O1A
9	B	504	GDP	PB-O3A-PA-O2A

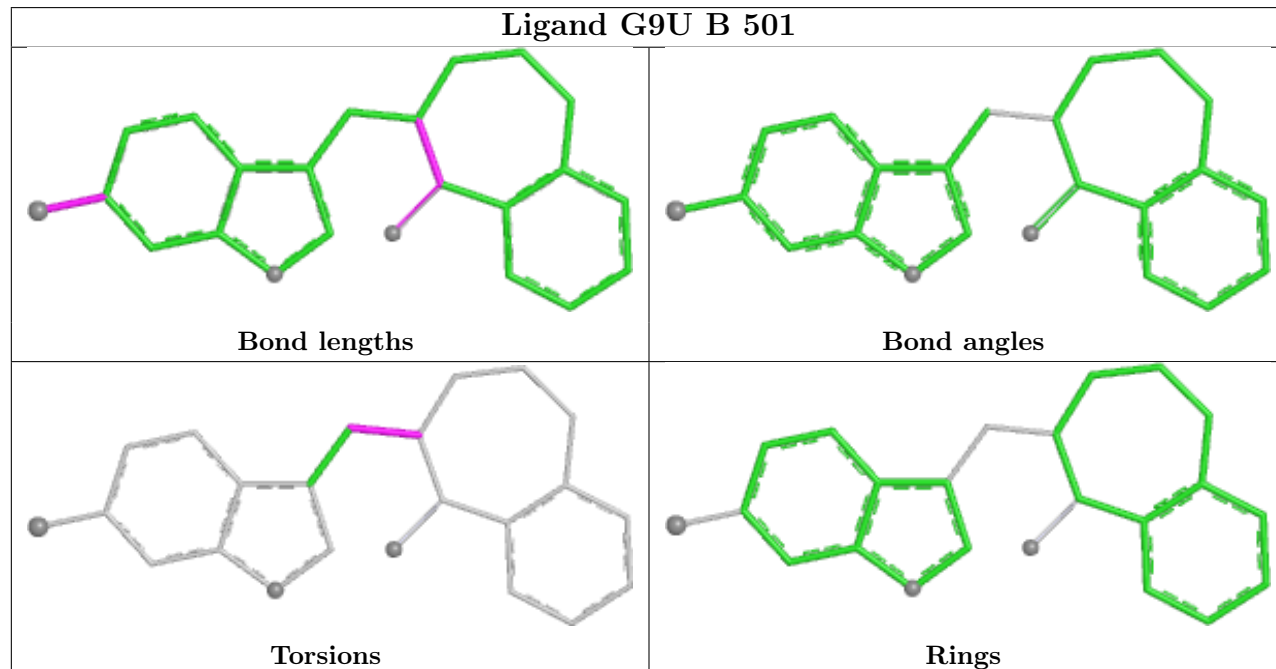
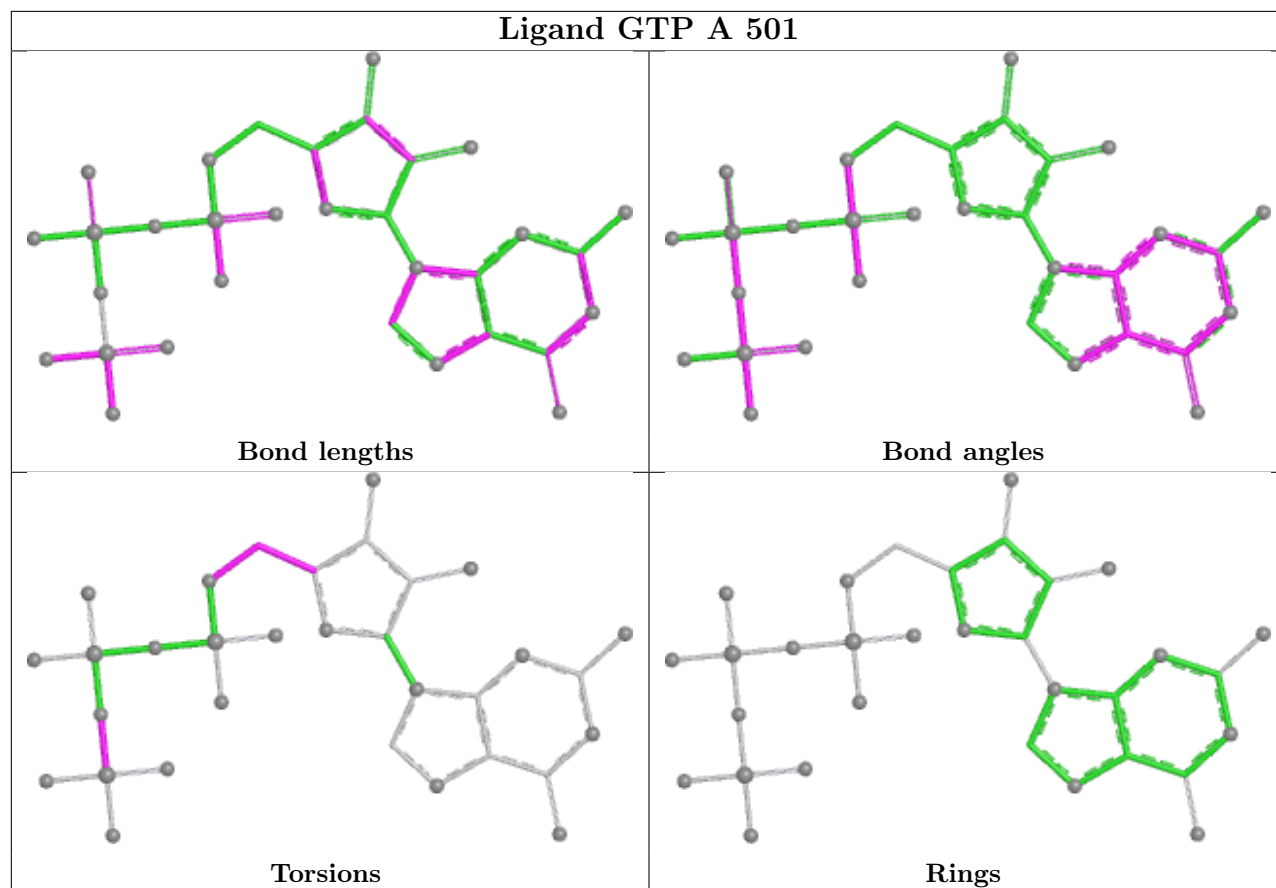
There are no ring outliers.

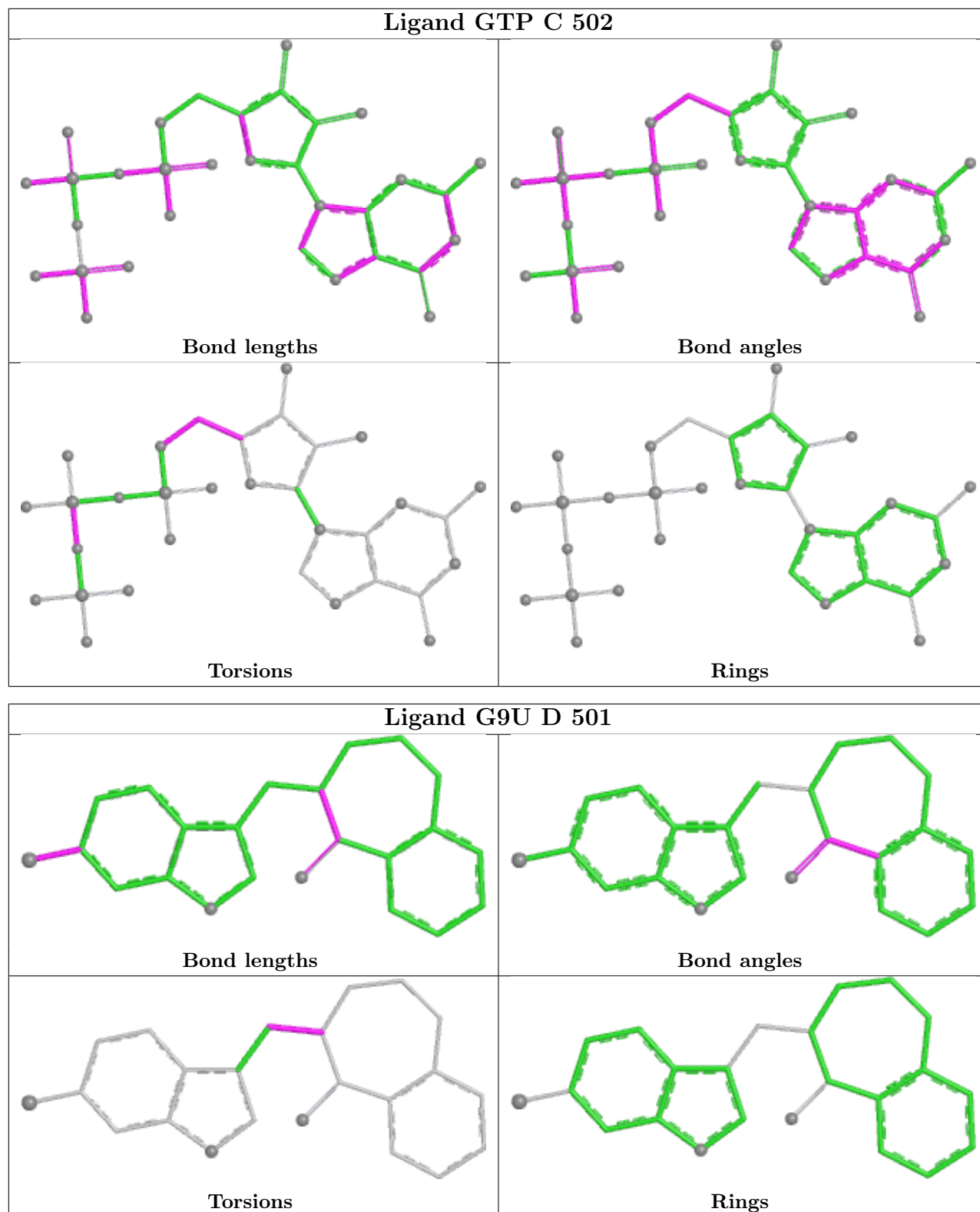
7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	502	GDP	1	0
5	A	501	GTP	1	0
11	C	501	GOL	5	0
8	B	501	G9U	1	0
5	C	502	GTP	2	0
10	B	505	MES	4	0
8	D	501	G9U	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.







5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	437/451 (96%)	0.02	10 (2%) 61 57	21, 47, 73, 84	11 (2%)
1	C	440/451 (97%)	-0.28	9 (2%) 65 61	15, 33, 56, 74	10 (2%)
2	B	417/445 (93%)	-0.13	6 (1%) 73 70	13, 38, 70, 86	11 (2%)
2	D	421/445 (94%)	0.48	28 (6%) 24 21	27, 57, 84, 102	5 (1%)
3	E	121/189 (64%)	0.48	7 (5%) 29 25	19, 56, 86, 112	3 (2%)
4	F	280/378 (74%)	0.98	47 (16%) 4 3	31, 65, 107, 120	5 (1%)
All	All	2116/2359 (89%)	0.17	107 (5%) 33 29	13, 47, 83, 120	45 (2%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	166	ALA	5.8
1	C	276	ILE	5.5
4	F	134	ALA	5.4
4	F	172	PHE	5.2
4	F	99	VAL	5.1
4	F	150	LYS	5.0
4	F	173	ILE	4.9
4	F	148	ILE	4.8
2	D	1	MET	4.8
4	F	147	TRP	4.6
4	F	135	TYR	4.6
4	F	101	TYR	4.5
4	F	257	GLU	4.3
2	D	57	THR	4.3
2	D	179	ASP	4.2
2	D	177	VAL	4.1
2	D	404	PHE	4.1
2	D	369	ARG	4.0
4	F	131	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	200	CYS	4.0
1	A	437	VAL	4.0
1	A	276	ILE	3.9
4	F	196	HIS	3.9
4	F	170	LEU	3.8
4	F	90	SER	3.6
4	F	162	ILE	3.6
4	F	180	HIS	3.5
2	B	247	GLN	3.5
1	A	262	TYR	3.4
4	F	128	ARG	3.4
4	F	194	PRO	3.4
2	D	247	GLN	3.3
4	F	182	ILE	3.3
4	F	181	VAL	3.2
3	E	28	SER	3.2
4	F	130	VAL	3.1
4	F	223	THR	3.0
4	F	151	SER	3.0
4	F	333	ASN	3.0
1	A	347	CYS	3.0
4	F	184	LYS	3.0
4	F	185	TYR	3.0
4	F	144	GLY	2.8
2	D	82	PRO	2.7
1	C	179	THR	2.7
2	D	325	MET	2.7
1	C	176	GLN	2.7
2	D	11	GLN	2.7
2	D	246	GLY	2.7
1	A	112	LYS	2.6
4	F	186	LEU	2.6
1	C	41	THR	2.6
2	D	228	ASN	2.6
2	D	37	HIS	2.6
3	E	44	ASP	2.6
2	B	82	PRO	2.6
4	F	146	VAL	2.6
4	F	183	GLN	2.6
1	A	346	TRP	2.5
2	B	325	MET	2.5
3	E	141	GLU	2.5

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Mol	Chain	Res	Type	RSRZ
4	F	136	ASN	2.5
2	D	180	THR	2.5
2	D	249	ASN	2.5
2	D	221[A]	THR	2.5
2	D	407	TRP	2.4
4	F	197	ARG	2.4
1	C	440	VAL	2.4
4	F	330	ILE	2.4
4	F	221	LEU	2.4
1	A	350	GLY	2.4
2	D	441	ASP	2.4
2	D	324	SER	2.3
3	E	15	THR	2.3
4	F	164	SER	2.3
1	C	337	THR	2.3
1	A	282	TYR	2.3
1	A	436	GLY	2.2
2	B	338	LYS	2.2
4	F	98	TYR	2.2
2	D	220	THR	2.2
4	F	275[A]	LEU	2.2
4	F	36	ARG	2.2
2	D	217	LEU	2.2
4	F	91	CYS	2.2
2	D	357	ASP	2.2
1	C	177	VAL	2.1
4	F	1	MET	2.1
2	D	286	LEU	2.1
2	D	273	ALA	2.1
4	F	145	ASN	2.1
3	E	27	PRO	2.1
4	F	321	VAL	2.1
4	F	277	THR	2.1
3	E	23	ILE	2.1
4	F	126	ASP	2.1
4	F	171	ASP	2.1
2	B	55	GLU	2.1
1	C	341	ILE	2.1
2	B	245	PRO	2.1
1	A	349	THR	2.0
2	D	322	ARG	2.0
2	D	248	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
3	E	139	LEU	2.0
2	D	95	GLY	2.0
2	D	245	PRO	2.0
4	F	373	SER	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](#)

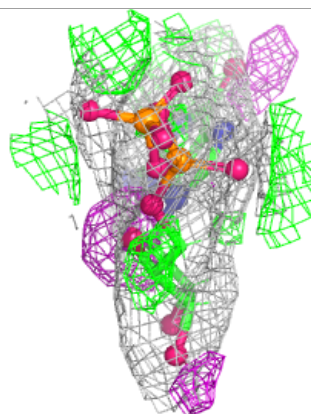
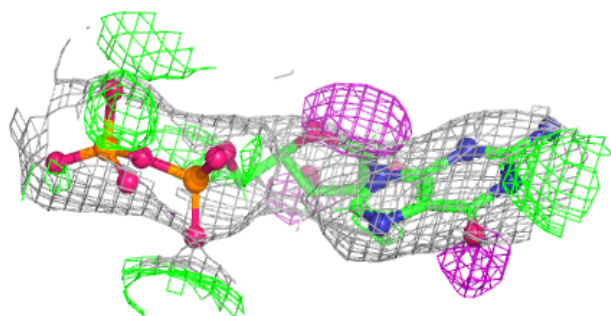
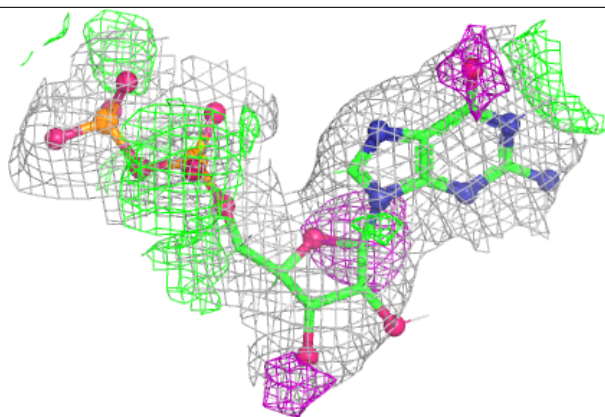
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	502	28/28	0.85	0.15	52,64,82,93	0
11	GOL	C	501	6/6	0.87	0.16	65,80,92,96	0
8	G9U	D	501	23/23	0.89	0.16	42,61,83,121	0
7	CA	B	503	1/1	0.91	0.15	129,129,129,129	0
6	MG	B	502	1/1	0.91	0.14	30,30,30,30	0
7	CA	C	504	1/1	0.95	0.07	96,96,96,96	0
9	GDP	B	504	28/28	0.95	0.09	17,27,49,63	0
5	GTP	A	501	32/32	0.97	0.06	27,34,45,50	0
10	MES	B	505	12/12	0.97	0.07	30,48,58,63	0
8	G9U	B	501	23/23	0.97	0.09	39,54,64,72	0
5	GTP	C	502	32/32	0.98	0.06	24,29,38,41	0
6	MG	C	503	1/1	0.98	0.03	26,26,26,26	0
6	MG	A	502	1/1	0.99	0.05	44,44,44,44	0
7	CA	A	503	1/1	0.99	0.05	73,73,73,73	0

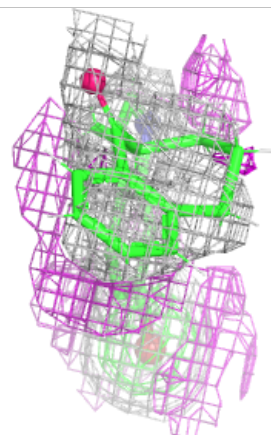
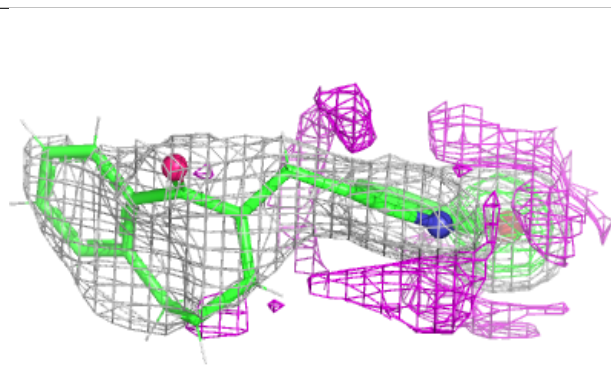
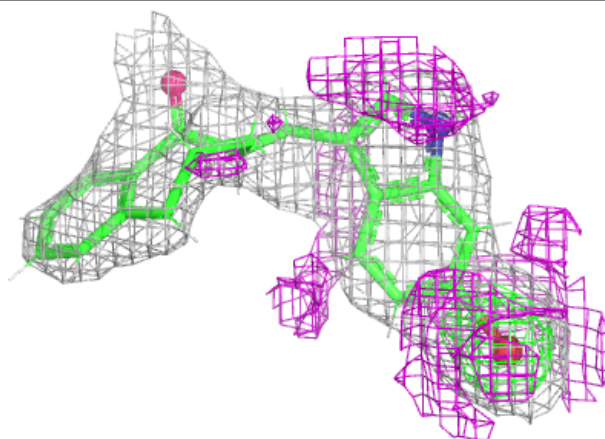
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP D 502:

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

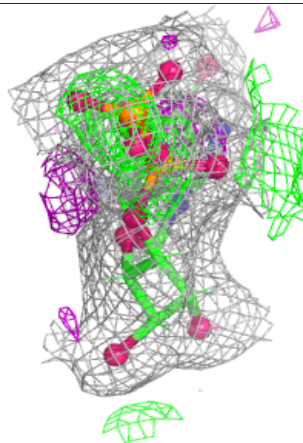
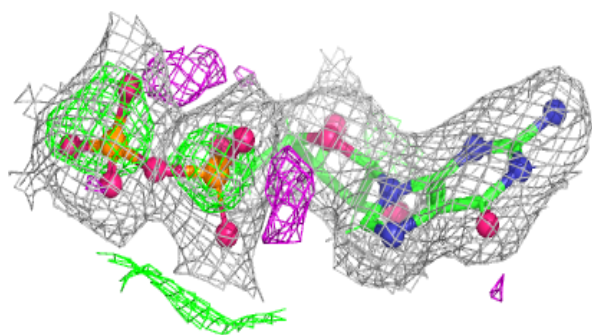
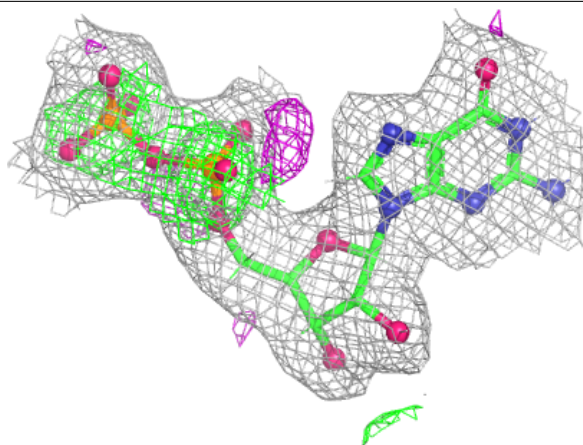
**Electron density around G9U D 501:**

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



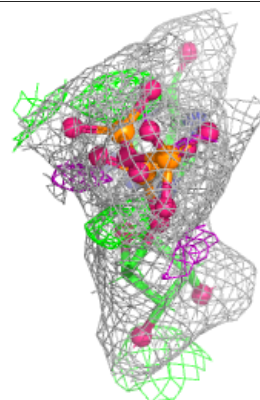
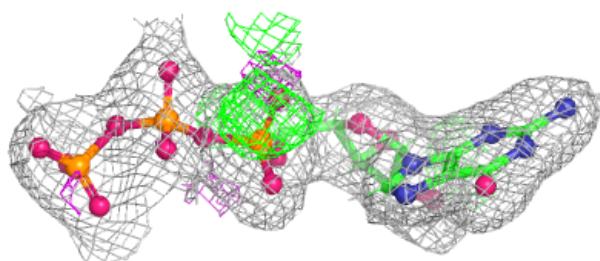
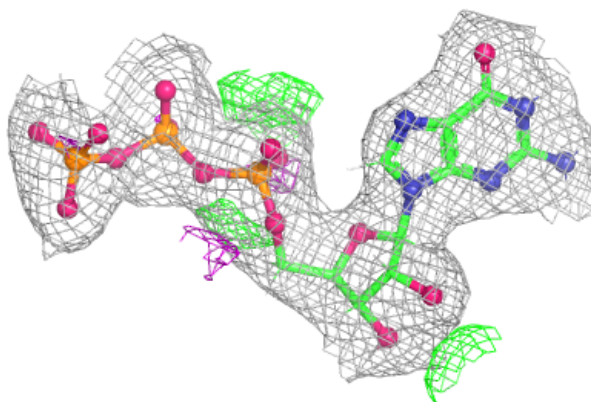
Electron density around GDP B 504:

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

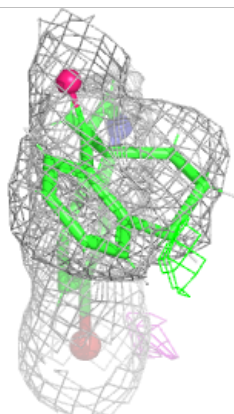
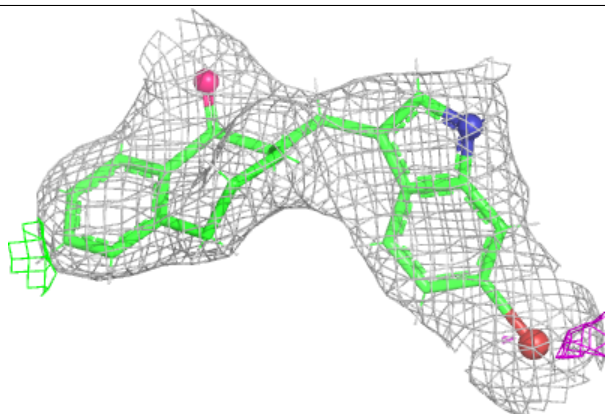


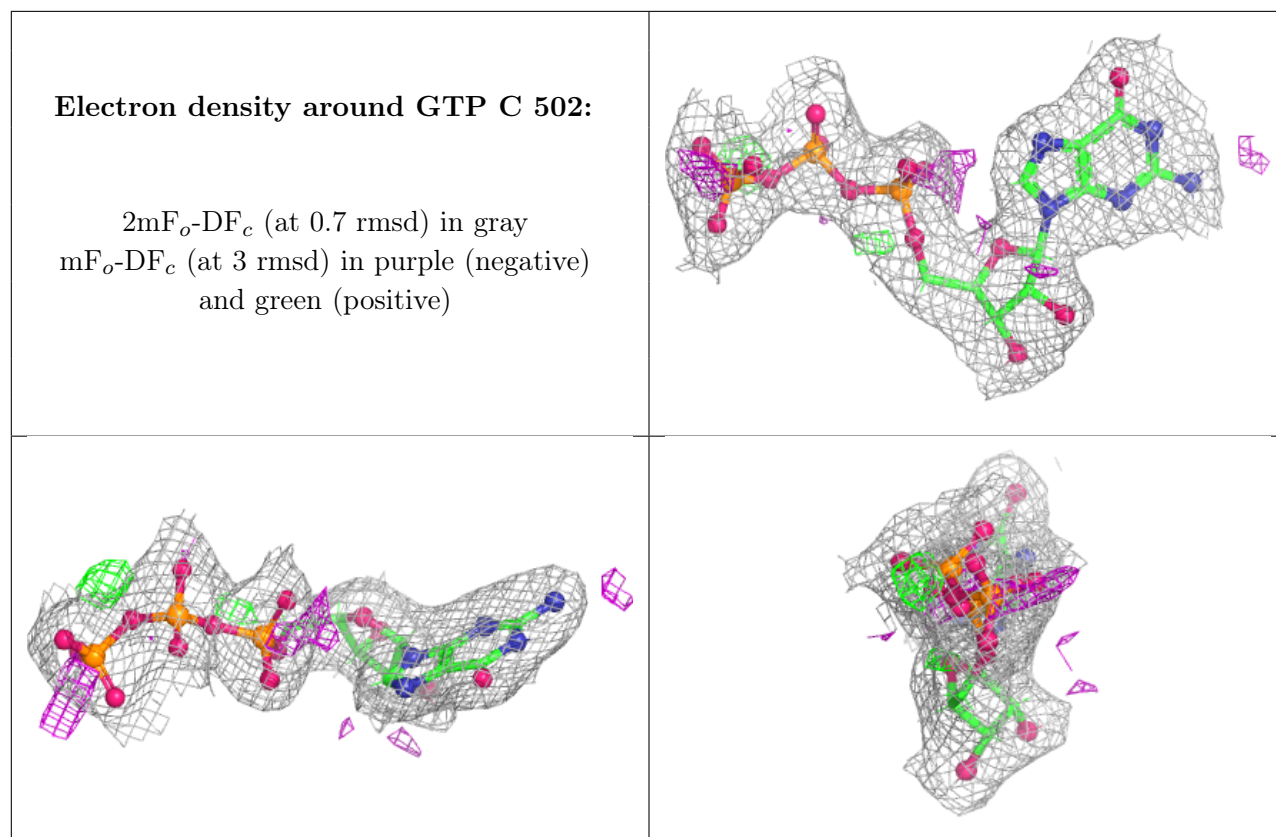
Electron density around GTP A 501:

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

**Electron density around G9U 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.