



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:43 PM UTC

PDB ID : 7DBA / pdb_00007dba
Title : RYX in complex with tubulin
Authors : Wu, C.Y.; Wang, Y.X.
Deposited on : 2020-10-19
Resolution : 2.46 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

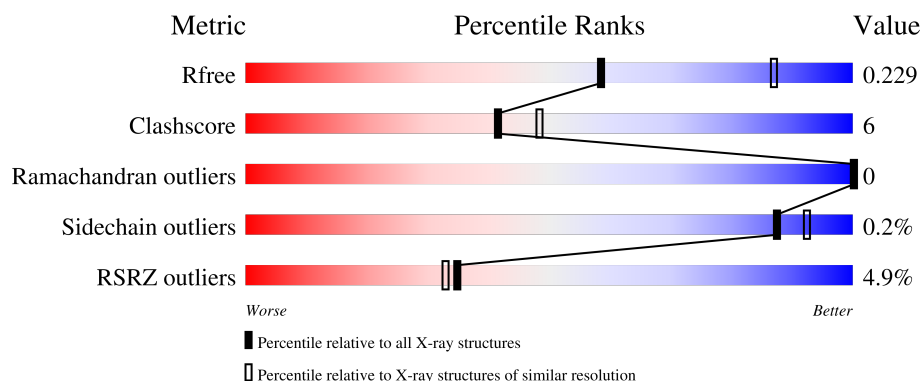
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.46 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	1190 (2.46-2.46)
Clashscore	190562	1229 (2.46-2.46)
Ramachandran outliers	187476	1218 (2.46-2.46)
Sidechain outliers	187428	1218 (2.46-2.46)
RSRZ outliers	180081	1190 (2.46-2.46)

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% 82% 15% .
1	C	451	% 88% 9% .
2	B	445	2% 81% 14% 5%
2	D	445	3% 79% 16% 6%
3	E	143	5% 73% 13% 14%

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Mol	Chain	Length	Quality of chain
4	F	384	17% 71% 21% 8%

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18135 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	11	0
			3479	2203	586	664	26			

- 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	5	0
			3369	2119	576	648	26			
2	D	420	Total	C	N	O	S	0	4	0
			3301	2076	557	641	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	3	0
			1031	637	186	202	6			

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 Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	352	Total	C	N	O	S	0	5	0
			2913	1871	502	525	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		
6	D	1	Total	Mg	0	0
			1	1		

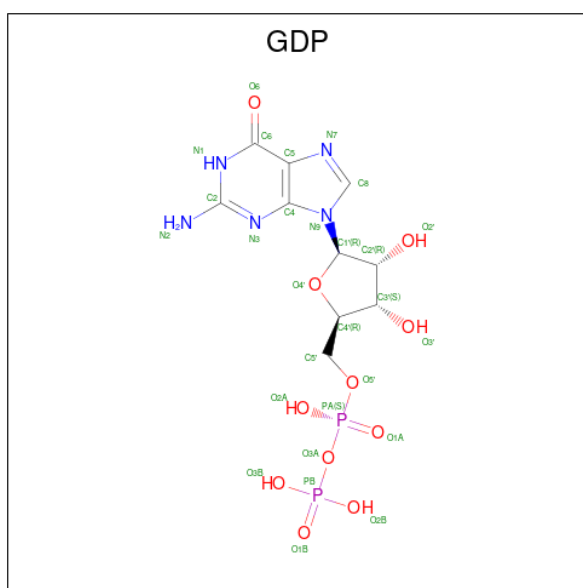
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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		

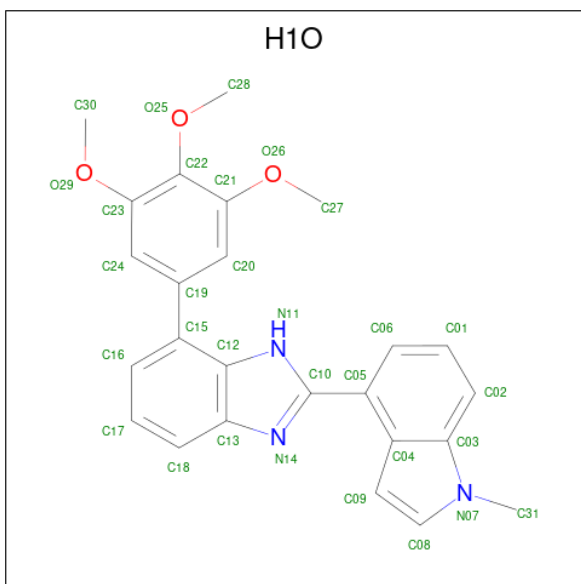
- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).





Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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-(1-methylindol-4-yl)-7-(3,4,5-trimethoxyphenyl)-1 {H}-benzimidazole (CCD ID: H1O) (formula: C₂₅H₂₃N₃O₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			31	25	3	3		

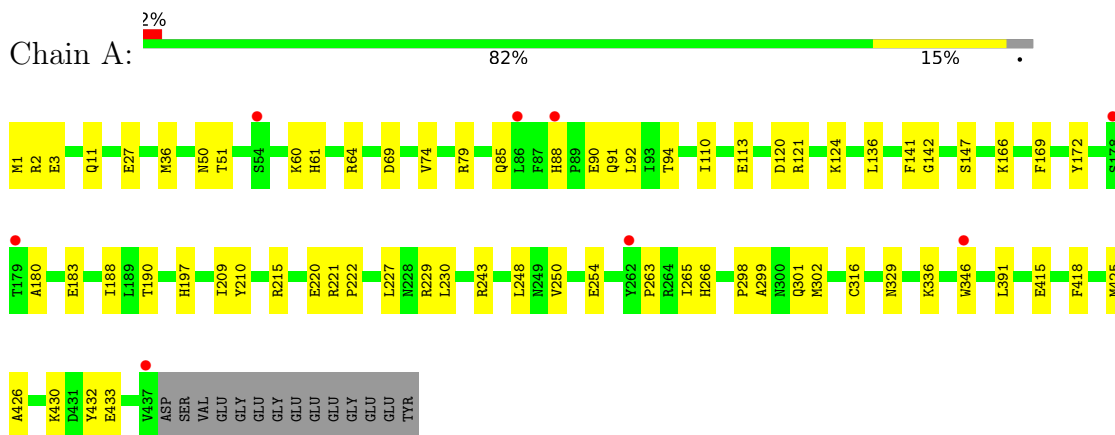
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	89	Total 89	O 89	0	0
12	B	83	Total 83	O 83	0	0
12	C	174	Total 174	O 174	0	0
12	D	41	Total 41	O 41	0	0
12	E	18	Total 18	O 18	0	0
12	F	28	Total 28	O 28	0	0

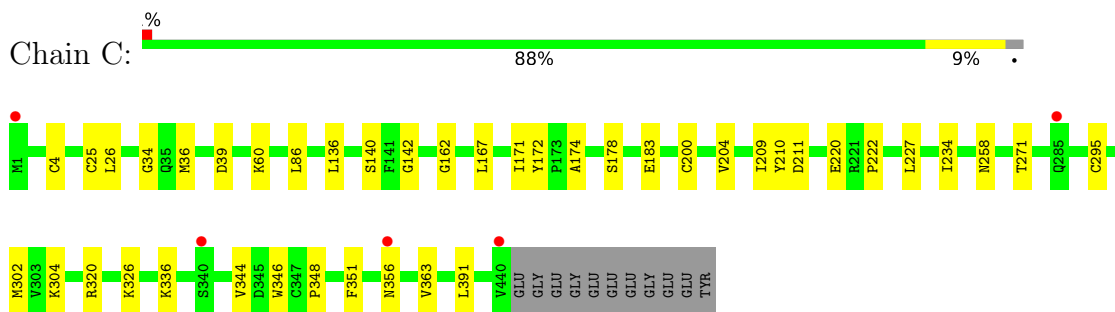
3 Residue-property plots [i](#)

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.

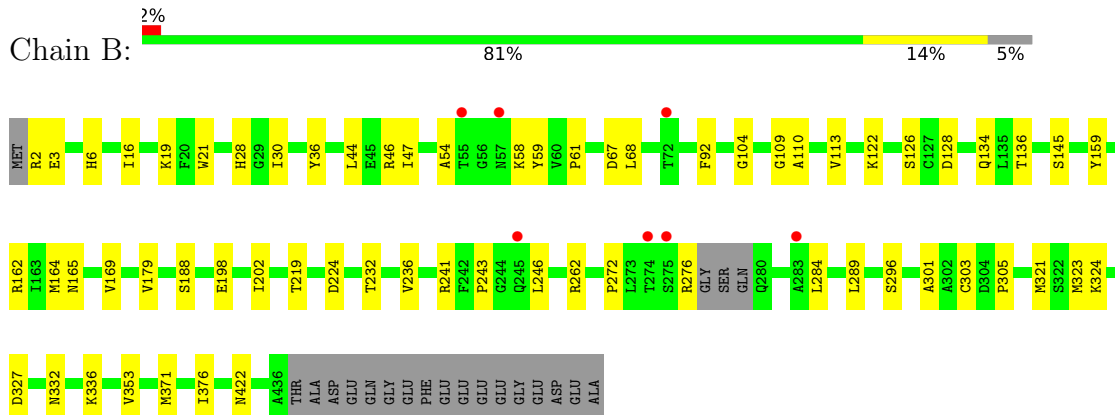
- Molecule 1: Tubulin alpha-1B chain



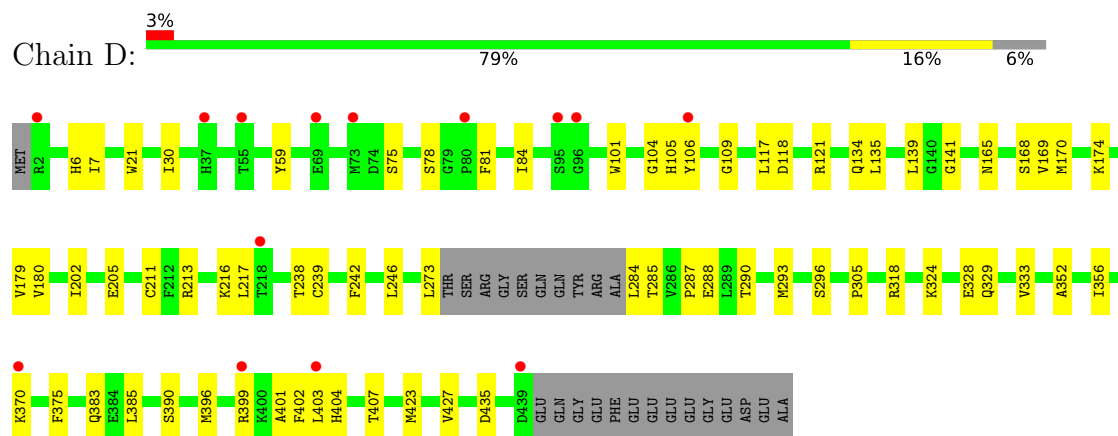
- Molecule 1: Tubulin alpha-1B chain



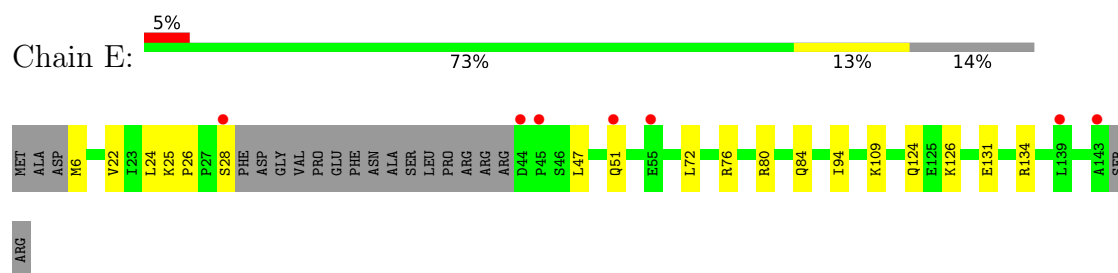
- Molecule 2: Tubulin beta chain



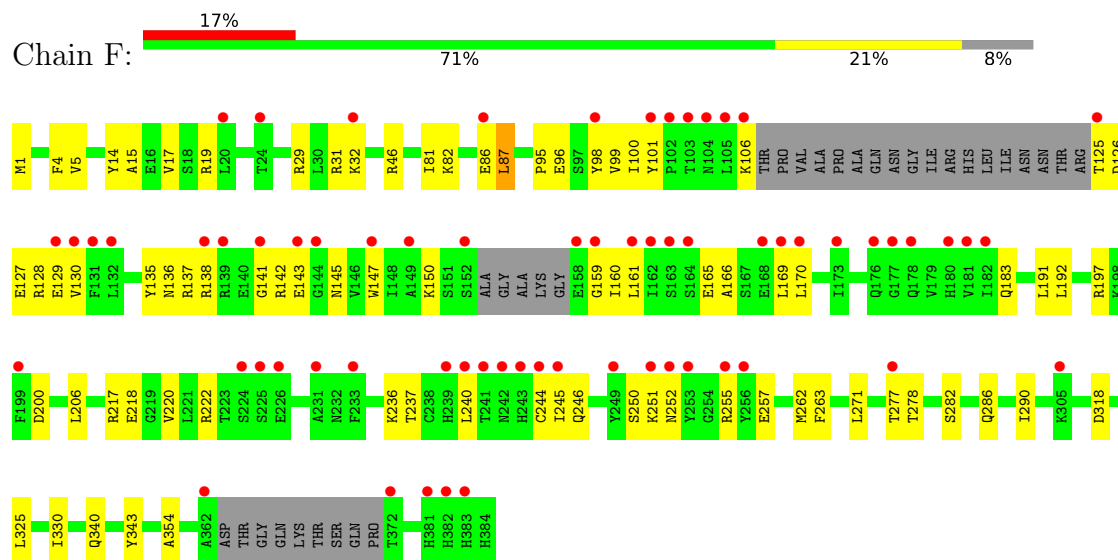
- Molecule 2: Tubulin beta chain



- Molecule 3: Stathmin-4



- Molecule 4: Tubulin tyrosine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.45Å 158.88Å 181.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	31.30 – 2.46 31.30 – 2.46	Depositor EDS
% Data completeness (in resolution range)	99.1 (31.30-2.46) 99.0 (31.30-2.46)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.14 (at 2.45Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.188 , 0.228 0.190 , 0.229	Depositor DCC
R_{free} test set	2000 reflections (1.80%)	wwPDB-VP
Wilson B-factor (Å ²)	43.7	Xtriage
Anisotropy	0.306	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 47.3	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	0.95	EDS
Total number of atoms	18135	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.51% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: H1O, MES, GTP, MG, GDP, CL, CA

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	0.18	0/3517	0.43	0/4776
1	C	0.20	0/3587	0.45	0/4870
2	B	0.21	0/3455	0.44	0/4678
2	D	0.24	0/3383	0.44	0/4586
3	E	0.22	0/1049	0.44	0/1392
4	F	0.23	0/2996	0.53	2/4048 (0.0%)
All	All	0.21	0/17987	0.46	2/24350 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	159	GLY	N-CA-C	5.87	127.09	113.18
4	F	87	LEU	CB-CA-C	5.08	118.69	110.37

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3427	0	3340	47	0
1	C	3479	0	3405	26	0
2	B	3369	0	3257	44	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3301	0	3172	46	0
3	E	1031	0	1051	15	0
4	F	2913	0	2889	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
6	D	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	12	1	0
10	B	24	0	24	0	0
11	B	31	0	0	1	0
12	A	89	0	0	1	0
12	B	83	0	0	2	0
12	C	174	0	0	1	0
12	D	41	0	0	2	0
12	E	18	0	0	3	0
12	F	28	0	0	0	0
All	All	18135	0	17186	224	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 6.

All (224) 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:234:ILE:HG21	1:C:302[B]:MET:SD	2.19	0.83
2:D:399:ARG:HD2	2:D:401:ALA:HB2	1.66	0.77
2:D:105:HIS:HD2	2:D:106:TYR:CE2	2.03	0.76
4:F:86:GLU:O	4:F:87:LEU:HD23	1.86	0.75
1:C:204:VAL:HG22	1:C:302[B]:MET:HE3	1.69	0.75
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.25	0.69
4:F:277:THR:HG21	4:F:282:SER:HB3	1.74	0.69
1:C:211[A]:ASP:OD2	1:C:304:LYS:NZ	2.25	0.69
2:D:239[B]:CYS:SG	12:D:636:HOH:O	2.51	0.69
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.76	0.67
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.26	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:336:LYS:NZ	12:C:601:HOH:O	2.25	0.66
1:A:60:LYS:NZ	1:A:85:GLN:O	2.27	0.66
4:F:137:ARG:NH1	4:F:137:ARG:HB2	2.11	0.66
2:D:404:HIS:HA	2:D:407:THR:HG22	1.79	0.64
2:D:238[B]:THR:HG21	2:D:318:ARG:HD2	1.78	0.64
4:F:217:ARG:HG3	4:F:218:GLU:HG2	1.80	0.63
2:D:324:LYS:O	2:D:328:GLU:HG3	1.99	0.62
3:E:109:LYS:NZ	12:E:202:HOH:O	2.31	0.62
3:E:25:LYS:HG2	3:E:26:PRO:HD2	1.80	0.62
2:D:170:MET:HE2	2:D:385:LEU:HD21	1.81	0.62
1:A:79:ARG:HG2	1:A:92:LEU:HD12	1.81	0.62
2:B:165:ASN:OD1	2:B:198:GLU:HG3	1.99	0.61
4:F:135:TYR:OH	4:F:165:GLU:HA	2.00	0.61
4:F:128:ARG:HD3	4:F:170:LEU:HD23	1.82	0.61
2:B:122:LYS:HG3	12:B:632:HOH:O	2.00	0.61
3:E:80:ARG:NH2	12:E:203:HOH:O	2.33	0.61
1:A:209:ILE:HD11	1:A:302:MET:SD	2.41	0.60
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.41	0.60
4:F:286:GLN:O	4:F:290:ILE:HG13	2.02	0.60
2:D:101:TRP:CZ3	2:D:106:TYR:HE2	2.20	0.60
4:F:192:LEU:HD22	4:F:262:MET:HE1	1.83	0.59
2:B:332:ASN:O	2:B:336:LYS:HB2	2.03	0.59
4:F:251:LYS:HB2	4:F:252:ASN:ND2	2.17	0.59
4:F:31:ARG:NE	4:F:32:LYS:H	2.00	0.59
4:F:161:LEU:HA	4:F:236:LYS:NZ	2.18	0.59
4:F:166:ALA:O	4:F:169:LEU:N	2.36	0.59
2:D:134:GLN:HA	2:D:165:ASN:O	2.03	0.59
4:F:160:ILE:HD12	4:F:240:LEU:HD13	1.86	0.58
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.22	0.58
3:E:124:GLN:OE1	3:E:124:GLN:HA	2.03	0.57
2:D:370:LYS:HE3	2:D:370:LYS:HA	1.87	0.57
2:D:139:LEU:HD21	2:D:168:SER:HB3	1.87	0.56
4:F:5:VAL:HG13	4:F:32:LYS:HA	1.87	0.56
2:D:105:HIS:HD2	2:D:106:TYR:CZ	2.22	0.56
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.88	0.56
1:A:215:ARG:NH2	1:A:299:ALA:HB1	2.21	0.56
2:D:211:CYS:HB3	2:D:217:LEU:HD12	1.88	0.56
2:B:126:SER:OG	2:B:126:SER:O	2.25	0.55
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.88	0.55
3:E:47:LEU:HD11	3:E:51:GLN:NE2	2.22	0.55
4:F:145:ASN:OD1	4:F:147:TRP:NE1	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:141:GLY:O	4:F:142:ARG:HB2	2.06	0.55
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.08	0.55
1:A:426:ALA:O	1:A:430:LYS:HG2	2.07	0.54
1:C:36:MET:SD	1:C:39:ASP:HB2	2.48	0.54
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.43	0.54
2:B:134:GLN:HA	2:B:165:ASN:O	2.07	0.54
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.72	0.54
2:D:329:GLN:O	2:D:333:VAL:HG23	2.08	0.54
1:C:220:GLU:OE2	2:D:324:LYS:NZ	2.41	0.54
4:F:14:TYR:HA	4:F:17:VAL:HB	1.90	0.53
4:F:96:GLU:OE1	4:F:98:TYR:OH	2.26	0.53
4:F:237:THR:O	4:F:246:GLN:NE2	2.41	0.53
2:D:30:ILE:HD13	2:D:59:TYR:HB2	1.90	0.53
3:E:80:ARG:NE	12:E:207:HOH:O	2.41	0.53
4:F:340:GLN:HA	4:F:343:TYR:CD2	2.44	0.53
1:A:141:PHE:O	1:A:147:SER:HB3	2.09	0.52
2:D:105:HIS:CD2	2:D:106:TYR:CE2	2.92	0.52
2:D:404:HIS:HA	2:D:407:THR:CG2	2.40	0.52
2:D:117:LEU:HB3	2:D:121:ARG:NH2	2.24	0.52
4:F:166:ALA:HA	4:F:169:LEU:HD12	1.90	0.52
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.44	0.52
2:D:213:ARG:O	2:D:216:LYS:HE3	2.10	0.52
4:F:99:VAL:O	4:F:100:ILE:HG13	2.09	0.52
2:B:164:MET:HE3	2:B:165:ASN:H	1.75	0.52
2:B:284:LEU:HD23	2:B:289:LEU:HD23	1.91	0.52
2:B:30:ILE:HD13	2:B:59:TYR:HB2	1.90	0.52
2:D:293:MET:HE2	2:D:375:PHE:HB2	1.93	0.51
4:F:220[A]:VAL:HG12	4:F:263:PHE:CE1	2.46	0.51
4:F:277:THR:HG22	4:F:278:THR:H	1.76	0.51
4:F:170:LEU:H	4:F:170:LEU:HD12	1.76	0.51
2:D:118:ASP:OD1	2:D:121:ARG:NH1	2.41	0.51
1:C:140:SER:HA	1:C:171:ILE:HB	1.93	0.50
3:E:131:GLU:HG2	3:E:134:ARG:HH21	1.76	0.50
1:A:1:MET:HE2	1:A:50:ASN:HB3	1.94	0.50
1:A:90:GLU:O	1:A:121:ARG:HD2	2.11	0.50
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.45	0.50
2:B:246:LEU:HG	11:B:505:H1O:C16	2.42	0.50
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.46	0.50
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.46	0.50
2:D:285:THR:HB	2:D:287:PRO:HD2	1.94	0.50
1:A:142:GLY:HA3	1:A:183:GLU:OE2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:67:ASP:O	2:B:92:PHE:HA	2.11	0.50
4:F:31:ARG:HE	4:F:32:LYS:H	1.59	0.49
2:D:296:SER:HB2	2:D:305:PRO:HD2	1.94	0.49
2:B:44:LEU:HA	2:B:47:ILE:HB	1.94	0.49
3:E:72:LEU:O	3:E:76:ARG:HG2	2.12	0.49
2:D:401:ALA:HB1	2:D:402:PHE:CD1	2.48	0.49
4:F:318:ASP:O	4:F:330:ILE:HG12	2.13	0.49
2:B:128:ASP:OD2	2:B:128:ASP:N	2.46	0.48
4:F:15:ALA:O	4:F:19:ARG:HG3	2.13	0.48
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.43	0.48
1:A:250:VAL:HG22	1:A:254:GLU:OE1	2.13	0.48
1:A:263:PRO:O	1:A:266:HIS:HD2	1.96	0.48
2:B:28:HIS:NE2	2:B:241:ARG:HB3	2.29	0.48
2:B:54:ALA:HB3	2:B:58:LYS:HB2	1.96	0.48
1:A:69:ASP:O	1:A:94:THR:HA	2.14	0.47
1:A:329:ASN:O	3:E:6:MET:HE1	2.14	0.47
2:D:179:VAL:O	2:D:396:MET:HE1	2.14	0.47
2:D:246:LEU:HD23	2:D:352:ALA:HB2	1.97	0.47
1:A:229:ARG:NH1	12:A:601:HOH:O	2.21	0.47
2:D:383:GLN:HB2	2:D:427:VAL:HG13	1.95	0.47
4:F:246:GLN:O	4:F:250:SER:HB3	2.14	0.47
2:B:272:PRO:HB3	2:B:284:LEU:HD22	1.97	0.47
2:B:36:TYR:CE2	2:B:44:LEU:HD11	2.50	0.47
1:C:336:LYS:HE2	1:C:351:PHE:CE1	2.49	0.47
2:D:290:THR:HG22	2:D:333:VAL:HG21	1.97	0.47
4:F:82:LYS:NZ	4:F:127:GLU:OE2	2.44	0.47
4:F:128:ARG:HH11	4:F:170:LEU:HD23	1.80	0.47
4:F:125:THR:OG1	4:F:126:ASP:N	2.48	0.47
1:A:110:ILE:O	1:A:113:GLU:HG2	2.14	0.46
2:D:179:VAL:HG13	2:D:180:VAL:HG13	1.97	0.46
4:F:129:GLU:HG2	4:F:130:VAL:N	2.30	0.46
1:A:88:HIS:CD2	1:A:90:GLU:HB2	2.50	0.46
4:F:282:SER:HB2	4:F:325:LEU:HD13	1.96	0.46
1:A:221:ARG:NH1	2:B:327:ASP:OD2	2.48	0.46
2:D:390:SER:HB2	2:D:423:MET:HE3	1.98	0.46
2:D:399:ARG:CD	2:D:401:ALA:HB2	2.39	0.46
2:B:16[A]:ILE:HD11	2:B:136:THR:HB	1.97	0.46
2:B:301:ALA:O	2:B:303:CYS:N	2.46	0.46
2:D:141:GLY:HA3	9:D:501:GDP:O3A	2.16	0.46
2:D:81:PHE:O	2:D:84:ILE:HG22	2.15	0.46
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:126:LYS:HE3	3:E:126:LYS:HB3	1.62	0.46
4:F:191:LEU:HD12	4:F:197:ARG:C	2.41	0.46
1:A:220:GLU:HG2	2:B:324:LYS:HE2	1.98	0.45
2:B:104:GLY:O	2:B:109:GLY:HA3	2.16	0.45
1:A:298:PRO:HA	1:A:301:GLN:CD	2.42	0.45
2:B:262:ARG:HH12	2:B:422[A]:ASN:HD21	1.64	0.45
1:A:188:ILE:HD12	1:A:425:MET:HG3	1.98	0.45
2:B:145:SER:OG	2:B:188:SER:OG	2.26	0.45
2:B:296:SER:HB2	2:B:305:PRO:HD2	1.99	0.45
2:B:224:ASP:OD1	2:B:276:ARG:NH2	2.49	0.45
2:B:232:THR:O	2:B:236:VAL:HG13	2.17	0.45
1:A:166:LYS:HB2	1:A:166:LYS:HE2	1.84	0.45
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.52	0.45
2:D:174:LYS:NZ	2:D:205:GLU:OE2	2.50	0.45
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.52	0.45
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.52	0.45
2:B:19:LYS:HE3	2:B:19:LYS:HB3	1.75	0.44
2:B:179:VAL:HG22	1:C:258:ASN:OD1	2.17	0.44
4:F:101:TYR:N	4:F:126:ASP:OD2	2.49	0.44
1:A:79:ARG:HG2	1:A:92:LEU:CD1	2.48	0.44
1:A:209:ILE:HG22	1:A:227:LEU:HD22	2.00	0.44
2:B:46:ARG:NH2	2:B:243:PRO:HA	2.33	0.44
4:F:161:LEU:HA	4:F:236:LYS:HZ1	1.82	0.44
2:B:159:TYR:HB3	2:B:162[B]:ARG:HG2	1.99	0.44
2:D:104:GLY:O	2:D:109:GLY:HA3	2.17	0.44
2:D:242:PHE:CZ	2:D:356:ILE:HD11	2.52	0.44
1:A:147:SER:HB2	1:A:190:THR:HB	2.00	0.44
1:C:320:ARG:HA	1:C:356:ASN:O	2.18	0.44
2:D:284:LEU:HD12	2:D:288:GLU:HG3	1.99	0.44
4:F:197:ARG:NH2	4:F:257:GLU:OE2	2.49	0.44
2:B:36:TYR:CZ	2:B:44:LEU:HD11	2.52	0.44
1:C:209:ILE:HG22	1:C:227:LEU:HD22	2.00	0.44
4:F:81:ILE:HG12	4:F:87:LEU:HD13	1.98	0.44
1:A:11:GLN:HG3	1:A:74:VAL:HG21	1.99	0.43
1:A:329:ASN:OD1	3:E:22:VAL:HG21	2.18	0.43
2:B:2:ARG:HB3	2:B:3:GLU:H	1.60	0.43
1:C:142:GLY:HA3	1:C:183:GLU:OE2	2.17	0.43
1:A:346:TRP:CD1	1:A:346:TRP:H	2.35	0.43
4:F:99:VAL:O	4:F:127:GLU:HB2	2.18	0.43
2:D:169:VAL:HA	2:D:202:ILE:O	2.18	0.43
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:75:SER:HA	2:D:78:SER:HB2	2.00	0.43
4:F:137:ARG:HB2	4:F:137:ARG:HH11	1.79	0.43
4:F:95:PRO:HB2	4:F:183:GLN:HG3	2.01	0.42
4:F:206:LEU:HD21	4:F:354:ALA:HB2	2.01	0.42
1:C:34:GLY:HA3	1:C:60:LYS:HG3	2.01	0.42
2:D:435:ASP:OD2	12:D:601:HOH:O	2.22	0.42
4:F:251:LYS:HB2	4:F:252:ASN:HD22	1.83	0.42
4:F:143:GLU:H	4:F:143:GLU:CD	2.28	0.42
4:F:150:LYS:HG2	4:F:160:ILE:HG12	2.00	0.42
2:B:323:MET:HG2	2:B:353:VAL:HG21	2.02	0.42
1:C:26:LEU:HD12	1:C:363:VAL:HG12	2.01	0.42
3:E:80:ARG:O	3:E:84:GLN:HG3	2.20	0.42
4:F:244:CYS:SG	4:F:245:ILE:N	2.92	0.42
1:C:174:ALA:O	1:C:178:SER:HB3	2.20	0.42
2:D:273:LEU:HD23	2:D:273:LEU:HA	1.89	0.42
2:B:110:ALA:O	2:B:113:VAL:HG12	2.20	0.42
2:B:169:VAL:HA	2:B:202:ILE:O	2.20	0.42
2:D:403:LEU:O	2:D:403:LEU:HD23	2.19	0.42
4:F:138:ARG:HA	4:F:143:GLU:CD	2.44	0.42
1:A:221:ARG:HD3	2:B:324:LYS:HA	2.02	0.41
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.38	0.41
1:A:433:GLU:OE1	4:F:46:ARG:NH2	2.53	0.41
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.54	0.41
2:B:68:LEU:HD23	2:B:68:LEU:HA	1.93	0.41
4:F:1:MET:HE2	4:F:1:MET:HB3	1.80	0.41
1:C:25:CYS:SG	1:C:86:LEU:HD21	2.60	0.41
2:D:401:ALA:HB1	2:D:402:PHE:HD1	1.85	0.41
2:D:7:ILE:O	2:D:135:LEU:HD12	2.20	0.41
4:F:106:LYS:HA	4:F:106:LYS:HD3	1.87	0.41
1:A:136:LEU:HD23	1:A:169:PHE:HE1	1.85	0.41
1:A:2:ARG:O	1:A:51:THR:HG23	2.21	0.41
2:B:219:THR:HG21	1:C:326:LYS:HA	2.02	0.41
1:C:271:THR:HG21	1:C:295:CYS:O	2.19	0.41
3:E:28:SER:O	3:E:28:SER:OG	2.28	0.41
4:F:318:ASP:HB3	4:F:330:ILE:HD11	2.02	0.41
1:A:248:LEU:HD21	1:A:316[B]:CYS:SG	2.61	0.41
1:A:88:HIS:O	1:A:91:GLN:HG3	2.21	0.41
2:B:219:THR:O	12:B:601:HOH:O	2.22	0.41
1:A:166:LYS:HE2	1:A:197:HIS:O	2.20	0.40
1:C:220:GLU:H	1:C:220:GLU:HG2	1.66	0.40
1:A:180:ALA:HB3	1:A:183:GLU:HG3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:167:LEU:HG	1:C:200:CYS:HB3	2.02	0.40
4:F:138:ARG:HA	4:F:143:GLU:OE1	2.21	0.40
1:A:415:GLU:O	1:A:418:PHE:HB2	2.21	0.40
2:B:236:VAL:HB	2:B:376:ILE:HD11	2.04	0.40
2:B:321:MET:HE2	2:B:371:MET:HG2	2.04	0.40
4:F:4:PHE:CZ	4:F:29:ARG:HB2	2.57	0.40
4:F:136:ASN:C	4:F:138:ARG:N	2.79	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	439/451 (97%)	425 (97%)	14 (3%)	0	100	100
1	C	448/451 (99%)	437 (98%)	11 (2%)	0	100	100
2	B	425/445 (96%)	412 (97%)	13 (3%)	0	100	100
2	D	419/445 (94%)	406 (97%)	13 (3%)	0	100	100
3	E	122/143 (85%)	122 (100%)	0	0	100	100
4	F	349/384 (91%)	333 (95%)	16 (5%)	0	100	100
All	All	2202/2319 (95%)	2135 (97%)	67 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	371/379 (98%)	369 (100%)	2 (0%)	81	87
1	C	381/379 (100%)	381 (100%)	0	100	100
2	B	371/383 (97%)	371 (100%)	0	100	100
2	D	364/383 (95%)	364 (100%)	0	100	100
3	E	113/127 (89%)	113 (100%)	0	100	100
4	F	321/342 (94%)	317 (99%)	4 (1%)	63	74
All	All	1921/1993 (96%)	1915 (100%)	6 (0%)	87	91

All (6) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	120[A]	ASP
1	A	120[B]	ASP
4	F	255[A]	ARG
4	F	255[B]	ARG
4	F	271[A]	LEU
4	F	271[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	50	ASN
1	A	285	GLN
1	A	301	GLN
1	A	393	HIS
2	B	291	GLN
2	B	347	ASN
1	C	85	GLN
1	C	107	HIS
1	C	128	GLN
1	C	356	ASN
2	D	15	GLN
2	D	48	ASN
2	D	57	ASN
2	D	83	GLN
2	D	105	HIS
2	D	195	ASN

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Mol	Chain	Res	Type
2	D	434	GLN
3	E	84	GLN
4	F	45	ASN
4	F	239	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
10	MES	B	504	-	12,12,12	4.56	7 (58%)	15,16,16	2.17	4 (26%)
11	H1O	B	505	-	35,35,35	1.70	7 (20%)	49,51,51	1.46	11 (22%)
9	GDP	B	501	6	29,30,30	1.20	4 (13%)	45,47,47	1.69	7 (15%)
5	GTP	C	501	6	33,34,34	1.04	3 (9%)	50,54,54	1.52	9 (18%)
5	GTP	A	501	6	33,34,34	1.01	3 (9%)	50,54,54	1.52	9 (18%)
10	MES	B	503	-	12,12,12	4.92	7 (58%)	15,16,16	2.58	6 (40%)
9	GDP	D	501	6	29,30,30	1.18	3 (10%)	45,47,47	1.74	8 (17%)

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
10	MES	B	504	-	-	1/6/14/14	0/1/1/1
11	H1O	B	505	-	-	2/14/14/14	0/5/5/5
9	GDP	B	501	6	-	5/16/32/32	0/3/3/3
5	GTP	C	501	6	-	8/22/38/38	0/3/3/3
5	GTP	A	501	6	-	8/22/38/38	0/3/3/3
10	MES	B	503	-	-	1/6/14/14	0/1/1/1
9	GDP	D	501	6	-	3/16/32/32	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	B	503	MES	O1S-S	8.58	1.69	1.45
10	B	504	MES	C7-N4	-8.55	1.28	1.47
10	B	503	MES	O2S-S	7.95	1.67	1.45
10	B	503	MES	C7-N4	-7.86	1.29	1.47
10	B	504	MES	O1S-S	7.58	1.66	1.45
10	B	504	MES	O2S-S	7.32	1.65	1.45
10	B	503	MES	C8-S	6.01	1.86	1.77
10	B	503	MES	O3S-S	5.75	1.68	1.47
11	B	505	H1O	C08-N07	-5.25	1.32	1.37
10	B	504	MES	O3S-S	5.00	1.66	1.47
10	B	504	MES	C8-S	4.47	1.83	1.77
11	B	505	H1O	C04-C03	-3.94	1.37	1.41
11	B	505	H1O	C12-C13	-3.28	1.37	1.40
9	D	501	GDP	C5-C4	3.15	1.47	1.38
11	B	505	H1O	C05-C10	3.09	1.53	1.47
10	B	504	MES	C5-N4	-3.03	1.38	1.46
9	B	501	GDP	C5-C4	3.02	1.47	1.38
5	C	501	GTP	PA-O3A	2.95	1.62	1.59
10	B	503	MES	C3-N4	-2.94	1.38	1.46
10	B	503	MES	C5-N4	-2.72	1.39	1.46
10	B	504	MES	C3-N4	-2.68	1.39	1.46
5	A	501	GTP	PB-O3B	2.60	1.62	1.59
9	B	501	GDP	C6-N1	-2.44	1.34	1.38
9	B	501	GDP	PA-O3A	2.42	1.62	1.59
9	D	501	GDP	C6-N1	-2.20	1.34	1.38
5	C	501	GTP	C2-N3	2.19	1.38	1.33
5	C	501	GTP	PB-O3B	2.18	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	501	GTP	C2-N3	2.15	1.38	1.33
11	B	505	H1O	C15-C19	2.07	1.53	1.49
9	D	501	GDP	C5-N7	-2.06	1.35	1.39
5	A	501	GTP	PA-O3A	2.05	1.61	1.59
11	B	505	H1O	O29-C23	2.02	1.40	1.37
11	B	505	H1O	O26-C21	2.02	1.40	1.37
9	B	501	GDP	C4-N9	-2.01	1.32	1.38

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	501	GDP	C5-C4-N3	-6.03	118.80	128.39
10	B	503	MES	C6-C5-N4	5.76	118.88	110.12
9	B	501	GDP	C5-C4-N3	-5.54	119.57	128.39
10	B	504	MES	C2-C3-N4	4.90	117.57	110.12
10	B	504	MES	C5-N4-C3	4.89	119.37	108.84
9	D	501	GDP	C2-N3-C4	4.87	120.68	112.30
9	B	501	GDP	C2-N3-C4	4.79	120.55	112.30
5	C	501	GTP	C5-C4-N3	-4.64	121.01	128.39
10	B	503	MES	C2-C3-N4	4.63	117.16	110.12
5	A	501	GTP	C5-C4-N3	-4.53	121.18	128.39
9	D	501	GDP	N9-C4-N3	4.53	135.01	125.95
5	A	501	GTP	C2-N3-C4	4.38	119.84	112.30
5	C	501	GTP	C2-N3-C4	4.34	119.77	112.30
10	B	503	MES	C5-N4-C3	4.32	118.15	108.84
9	B	501	GDP	N9-C4-N3	3.94	133.83	125.95
9	B	501	GDP	C6-C5-N7	3.62	136.88	130.29
9	D	501	GDP	C6-C5-N7	3.29	136.28	130.29
11	B	505	H1O	C03-N07-C08	3.02	110.24	108.35
5	C	501	GTP	N9-C4-N3	3.00	131.96	125.95
5	A	501	GTP	N9-C8-N7	-2.99	107.85	113.40
11	B	505	H1O	C12-C13-N14	-2.98	107.88	109.91
10	B	503	MES	O3S-S-C8	2.90	111.69	106.00
5	A	501	GTP	N9-C4-N3	2.90	131.75	125.95
11	B	505	H1O	C02-C03-C04	-2.87	120.02	122.36
5	C	501	GTP	N9-C8-N7	-2.87	108.07	113.40
11	B	505	H1O	O26-C21-C22	2.85	120.02	115.14
11	B	505	H1O	O29-C23-C22	2.82	119.98	115.14
9	B	501	GDP	C4-C5-N7	-2.73	106.34	110.67
5	C	501	GTP	C8-N7-C5	2.71	109.08	104.26
9	D	501	GDP	C4-C5-N7	-2.70	106.40	110.67
5	A	501	GTP	C2-N1-C6	-2.69	120.23	125.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	501	GTP	O2A-PA-O3A	2.63	114.37	107.27
10	B	504	MES	C6-C5-N4	2.58	114.04	110.12
5	C	501	GTP	C2-N1-C6	-2.58	120.44	125.11
5	A	501	GTP	C8-N7-C5	2.57	108.83	104.26
10	B	503	MES	O1S-S-C8	2.55	110.59	106.73
11	B	505	H1O	C30-O29-C23	-2.47	113.88	117.51
11	B	505	H1O	C27-O26-C21	-2.44	113.93	117.51
5	A	501	GTP	O2A-PA-O3A	2.44	113.86	107.27
5	A	501	GTP	C5-C6-N1	2.40	119.36	113.25
10	B	503	MES	C7-N4-C5	2.39	117.60	111.24
11	B	505	H1O	O26-C21-C20	-2.37	119.99	124.08
11	B	505	H1O	O29-C23-C24	-2.34	120.04	124.08
5	A	501	GTP	O6-C6-C5	-2.31	120.44	126.53
5	C	501	GTP	C5-C6-N1	2.27	119.03	113.25
11	B	505	H1O	C13-N14-C10	2.21	107.75	105.17
9	D	501	GDP	O6-C6-C5	-2.21	120.71	126.53
9	D	501	GDP	O2A-PA-O3A	2.15	113.09	107.27
5	C	501	GTP	O6-C6-C5	-2.13	120.92	126.53
9	B	501	GDP	O2B-PB-O3A	2.09	111.66	104.64
9	B	501	GDP	O6-C6-C5	-2.08	121.04	126.53
10	B	504	MES	O2S-S-C8	2.04	109.81	106.73
9	D	501	GDP	C8-N7-C5	2.03	107.88	104.26
11	B	505	H1O	C15-C12-C13	-2.00	120.00	122.48

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O1A
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
5	C	501	GTP	PB-O3B-PG-O1G

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Mol	Chain	Res	Type	Atoms
11	B	505	H1O	C22-C21-O26-C27
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O2A
9	B	501	GDP	PB-O3A-PA-O2A
11	B	505	H1O	C20-C21-O26-C27
10	B	504	MES	C8-C7-N4-C5
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O1A
9	B	501	GDP	PB-O3A-PA-O1A

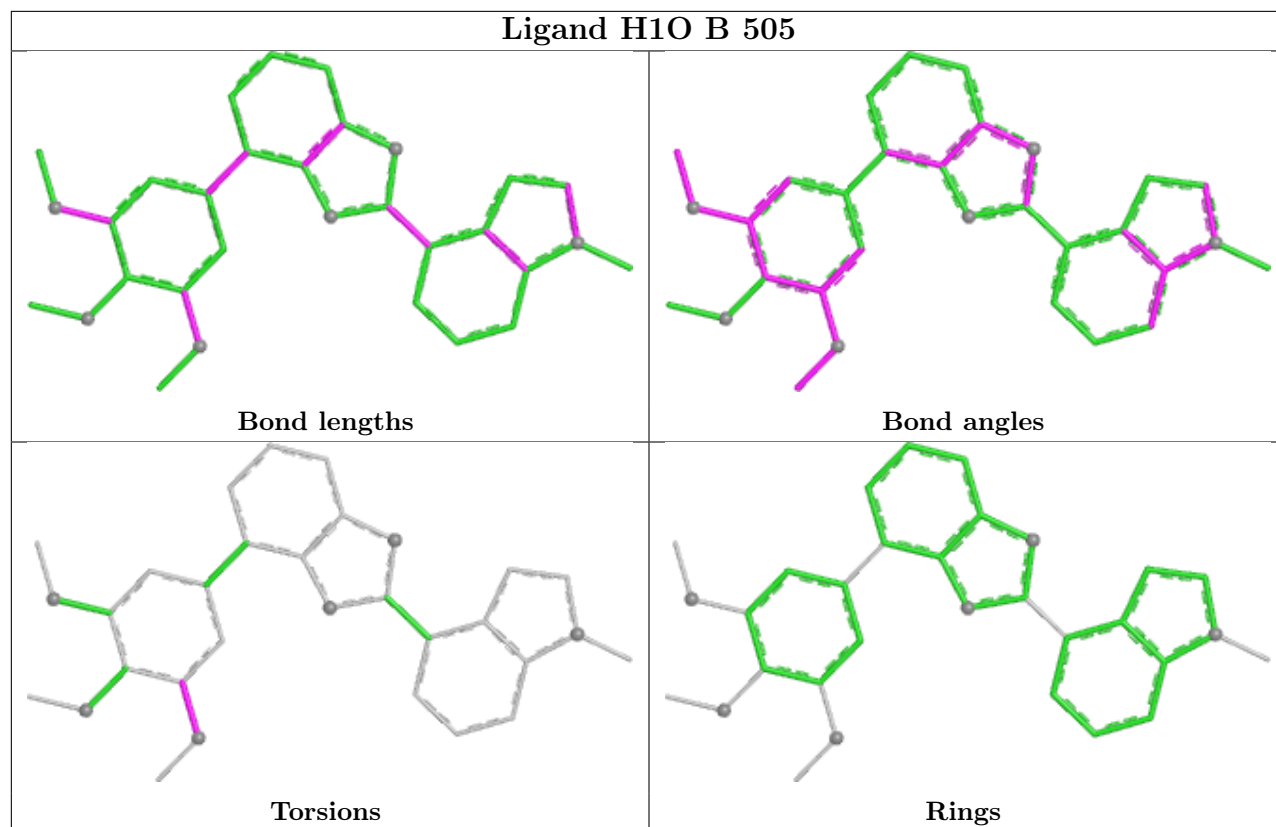
There are no ring outliers.

2 monomers are involved in 2 short contacts:

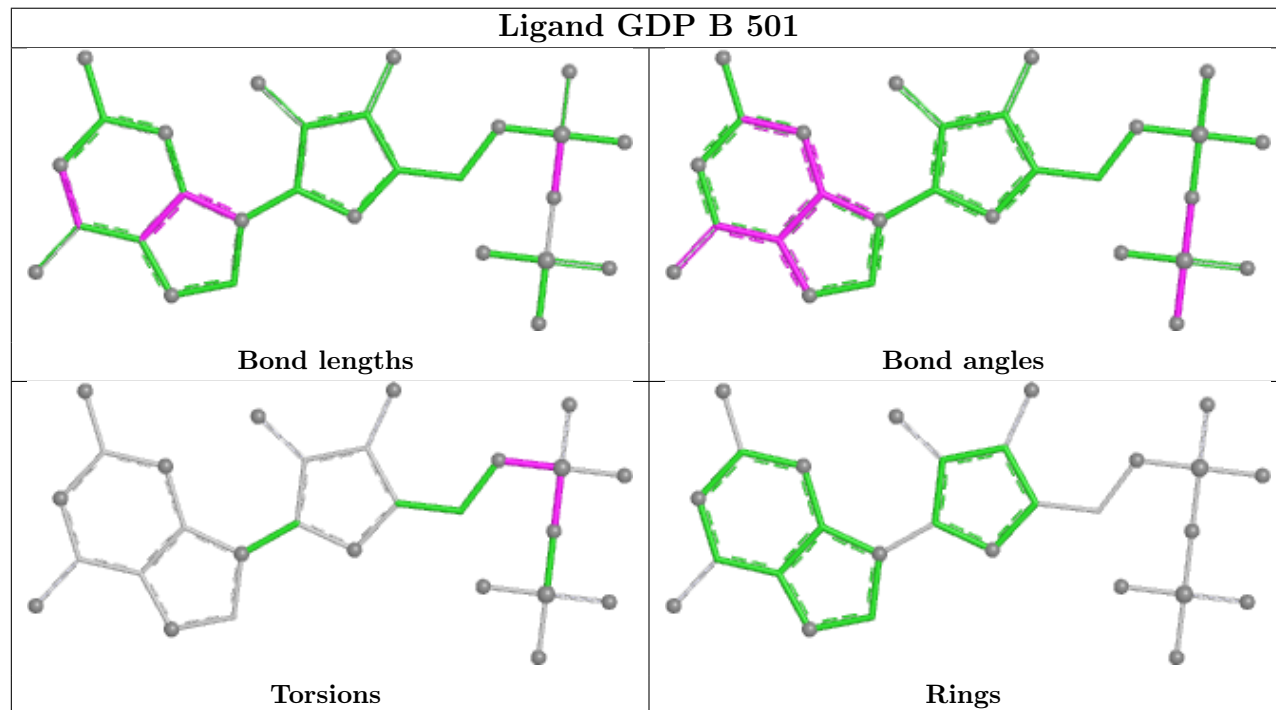
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	505	H1O	1	0
9	D	501	GDP	1	0

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

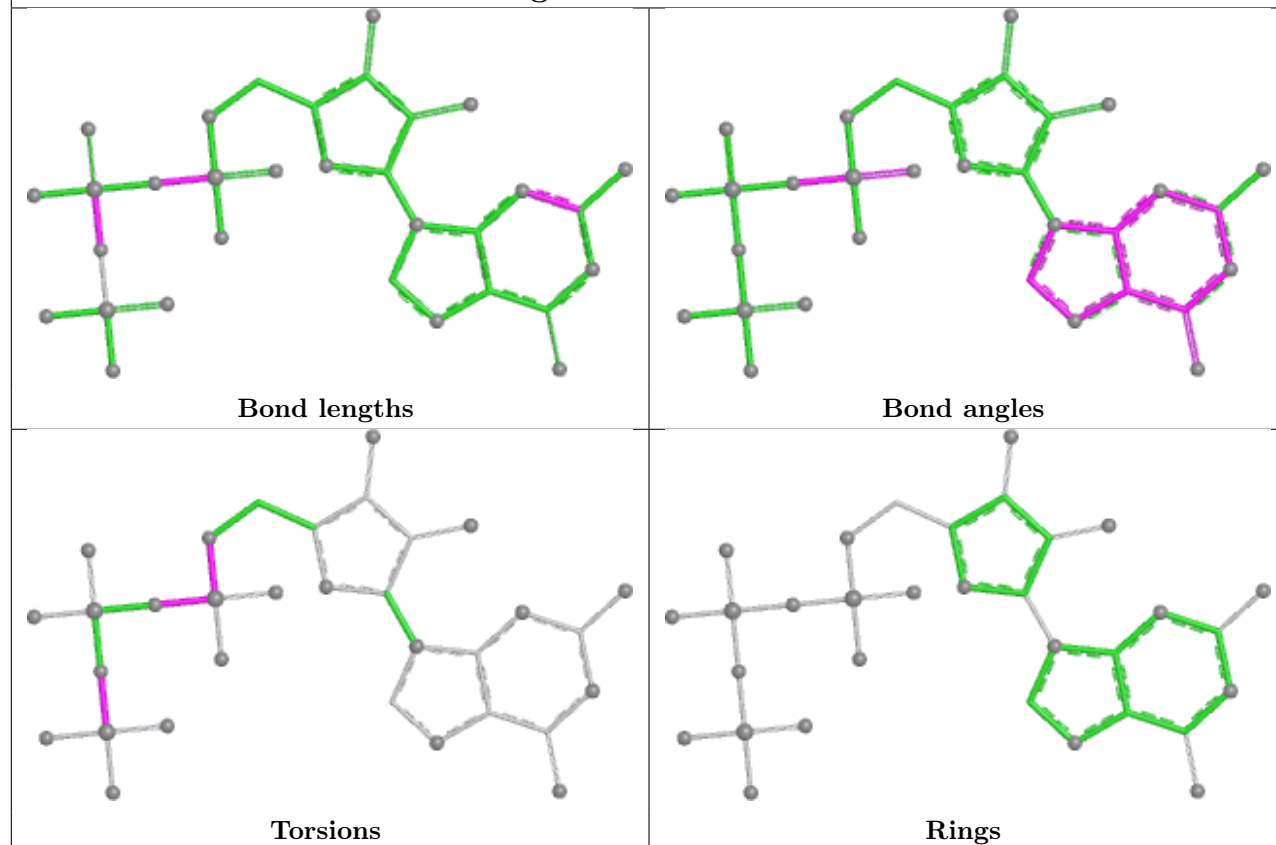
Ligand H1O B 505



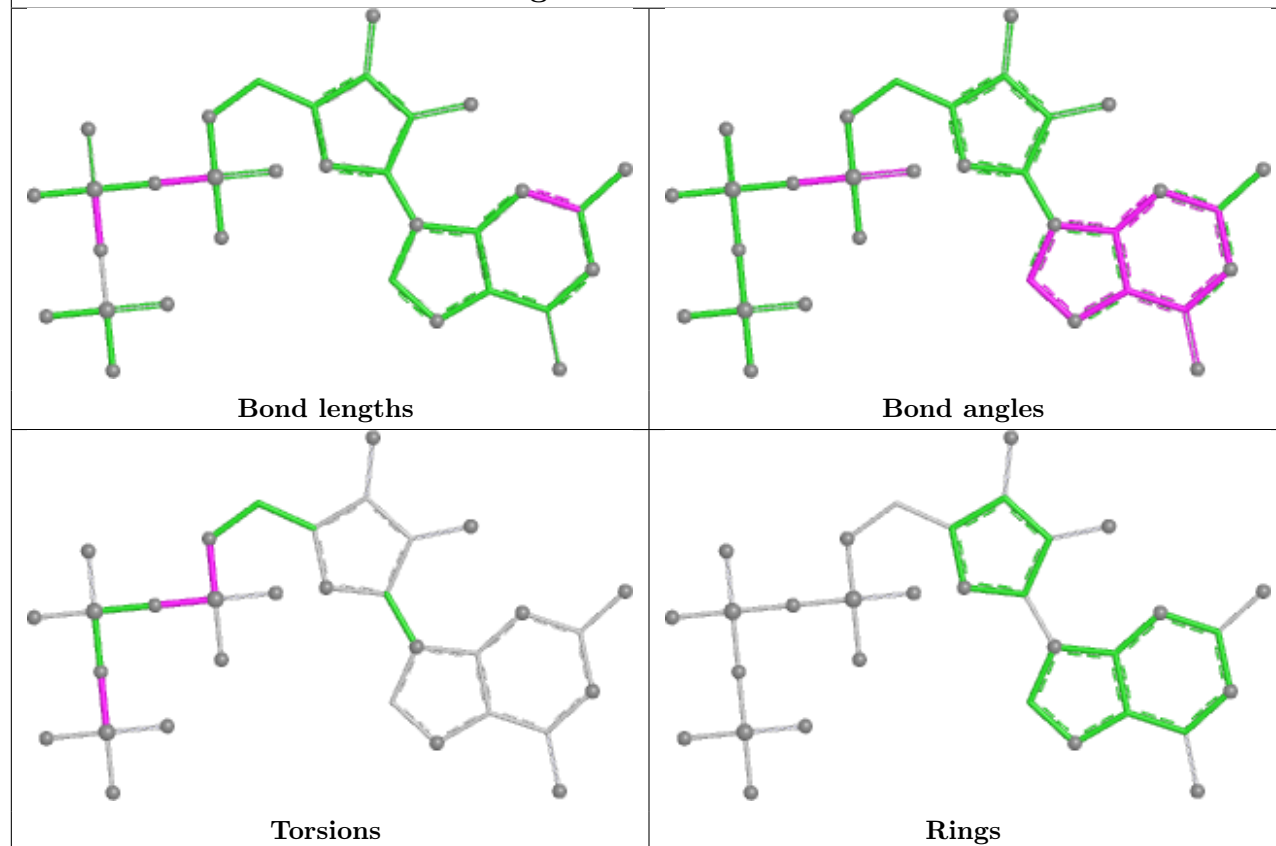
Ligand GDP B 501

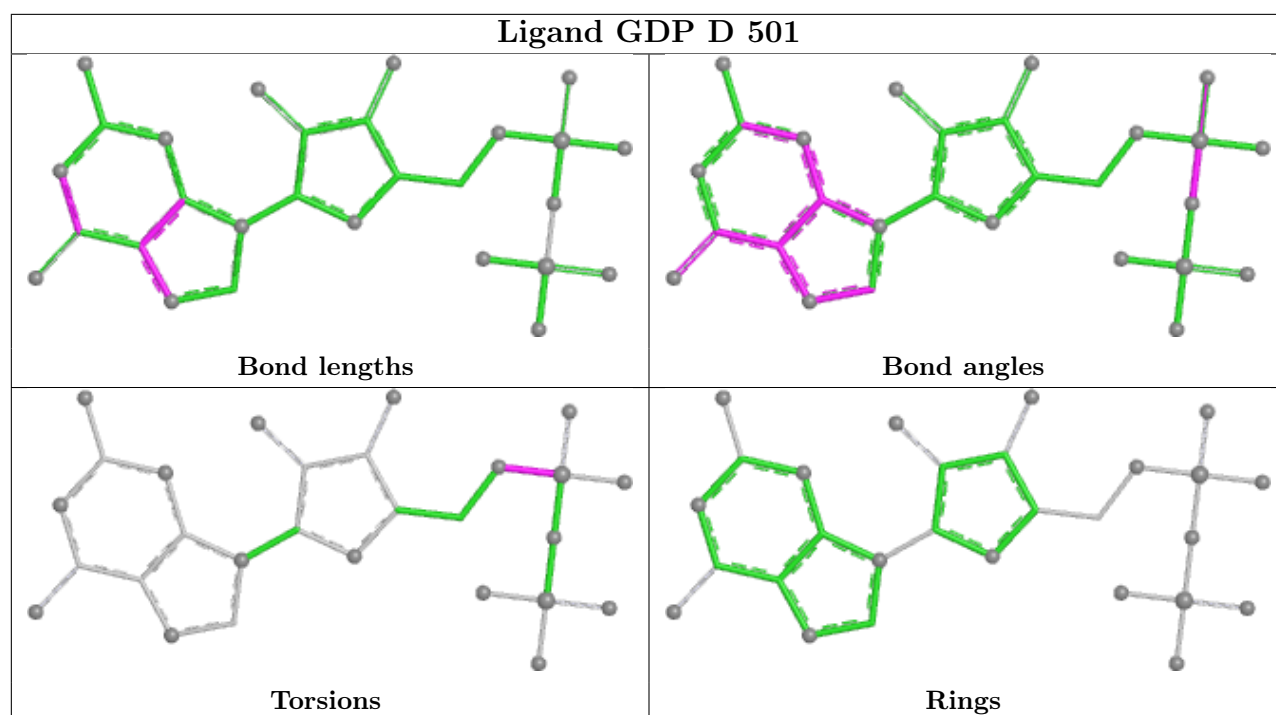


Ligand GTP C 501



Ligand GTP A 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	437/451 (96%)	-0.02	8 (1%) 67 69	25, 45, 71, 88	4 (0%)
1	C	440/451 (97%)	-0.43	5 (1%) 78 79	19, 34, 58, 94	10 (2%)
2	B	424/445 (95%)	-0.04	7 (1%) 69 71	21, 44, 74, 117	6 (1%)
2	D	420/445 (94%)	0.26	14 (3%) 49 50	28, 54, 84, 126	6 (1%)
3	E	123/143 (86%)	0.53	7 (5%) 29 26	24, 57, 92, 125	3 (2%)
4	F	352/384 (91%)	0.98	66 (18%) 3 2	30, 69, 141, 163	5 (1%)
All	All	2196/2319 (94%)	0.14	107 (4%) 35 33	19, 48, 95, 163	34 (1%)

All (107) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	E	143	ALA	5.7
4	F	105	LEU	5.2
4	F	225	SER	4.9
2	D	106	TYR	4.5
2	B	274	THR	4.3
4	F	182	ILE	4.0
4	F	169	LEU	4.0
2	D	55	THR	3.9
4	F	125	THR	3.9
4	F	372	THR	3.9
2	B	57	ASN	3.9
4	F	362	ALA	3.7
4	F	177	GLY	3.6
4	F	152	SER	3.6
4	F	245	ILE	3.6
4	F	249	TYR	3.5
4	F	161	LEU	3.5
1	C	285	GLN	3.3
4	F	103	THR	3.3

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Mol	Chain	Res	Type	RSRZ
4	F	164	SER	3.3
4	F	173	ILE	3.2
1	A	54	SER	3.2
4	F	130	VAL	3.2
4	F	106	LYS	3.1
4	F	132	LEU	3.1
4	F	251	LYS	3.1
4	F	143	GLU	3.1
4	F	253	TYR	3.1
4	F	176	GLN	3.1
3	E	55	GLU	3.1
2	B	275	SER	3.0
4	F	170	LEU	3.0
4	F	240	LEU	3.0
2	D	218	THR	2.9
4	F	181	VAL	2.9
4	F	243	HIS	2.9
4	F	102	PRO	2.9
4	F	101	TYR	2.9
4	F	224	SER	2.8
4	F	277	THR	2.8
1	A	86	LEU	2.8
1	C	340	SER	2.8
4	F	149	ALA	2.8
2	D	96	GLY	2.7
4	F	168	GLU	2.6
1	A	262	TYR	2.6
4	F	141	GLY	2.6
3	E	28	SER	2.6
1	A	437	VAL	2.6
4	F	178	GLN	2.6
4	F	382	HIS	2.6
4	F	255[A]	ARG	2.5
4	F	242	ASN	2.5
2	D	37	HIS	2.5
2	D	69	GLU	2.5
4	F	381	HIS	2.5
4	F	383	HIS	2.5
2	D	2	ARG	2.5
4	F	252	ASN	2.5
4	F	147	TRP	2.5
4	F	158	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
4	F	159	GLY	2.4
4	F	180	HIS	2.4
4	F	138	ARG	2.4
2	B	55	THR	2.4
4	F	144	GLY	2.4
4	F	131	PHE	2.4
4	F	244	CYS	2.4
2	B	283	ALA	2.4
2	D	80	PRO	2.3
1	C	440	VAL	2.3
1	A	346	TRP	2.3
4	F	239	HIS	2.3
2	D	370	LYS	2.3
4	F	305	LYS	2.3
2	D	73	MET	2.3
2	D	439	ASP	2.3
4	F	231	ALA	2.2
4	F	86	GLU	2.2
3	E	45	PRO	2.2
4	F	104	ASN	2.2
4	F	256	TYR	2.2
2	B	72	THR	2.2
4	F	163	SER	2.2
4	F	199	PHE	2.2
4	F	233	PHE	2.2
4	F	98	TYR	2.2
2	D	403	LEU	2.2
4	F	226	GLU	2.2
1	C	1	MET	2.2
2	D	95	SER	2.1
3	E	51	GLN	2.1
1	A	178	SER	2.1
3	E	44	ASP	2.1
4	F	129	GLU	2.1
4	F	32	LYS	2.1
4	F	20	LEU	2.1
4	F	139	ARG	2.1
4	F	24	THR	2.1
3	E	139	LEU	2.0
4	F	162	ILE	2.0
4	F	241	THR	2.0
1	A	88	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
2	B	245	GLN	2.0
2	D	399	ARG	2.0
1	C	356	ASN	2.0
1	A	179	THR	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](#)

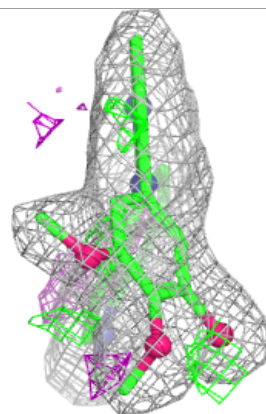
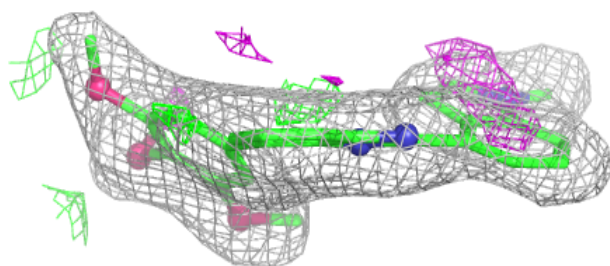
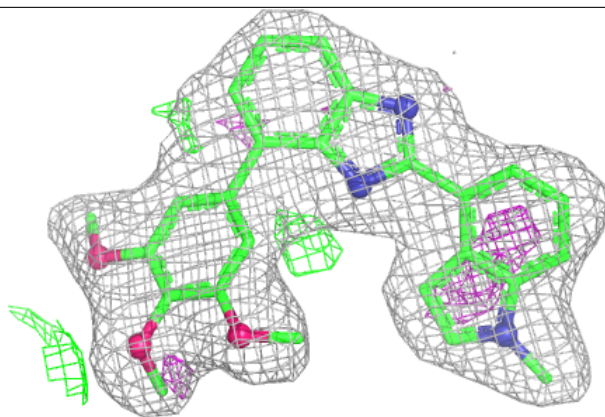
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	D	502	1/1	0.83	0.12	57,57,57,57	0
11	H1O	B	505	31/31	0.89	0.10	30,48,55,58	0
10	MES	B	504	12/12	0.91	0.12	65,73,82,92	0
8	CL	A	504	1/1	0.92	0.12	79,79,79,79	0
9	GDP	D	501	28/28	0.95	0.08	43,50,68,80	0
10	MES	B	503	12/12	0.95	0.09	38,54,60,61	0
5	GTP	A	501	32/32	0.98	0.05	24,37,42,48	0
7	CA	A	503	1/1	0.98	0.05	66,66,66,66	0
7	CA	C	503	1/1	0.98	0.03	49,49,49,49	0
5	GTP	C	501	32/32	0.98	0.05	22,29,34,40	0
6	MG	C	502	1/1	0.99	0.06	31,31,31,31	0
9	GDP	B	501	28/28	0.99	0.05	20,31,40,41	0
6	MG	A	502	1/1	0.99	0.03	32,32,32,32	0
6	MG	B	502	1/1	1.00	0.07	23,23,23,23	0

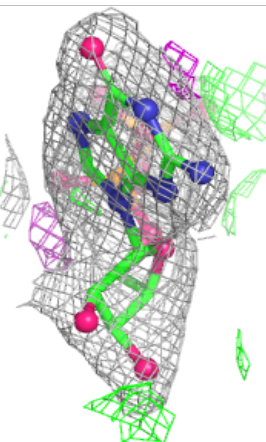
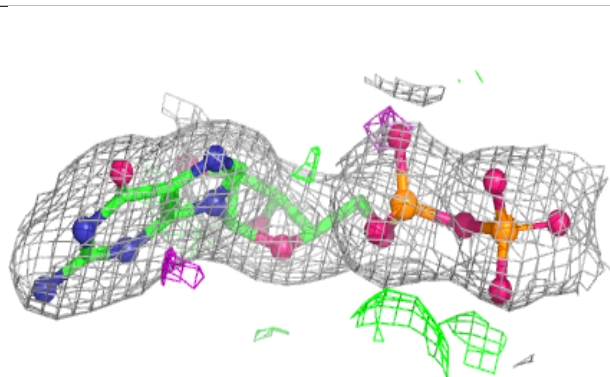
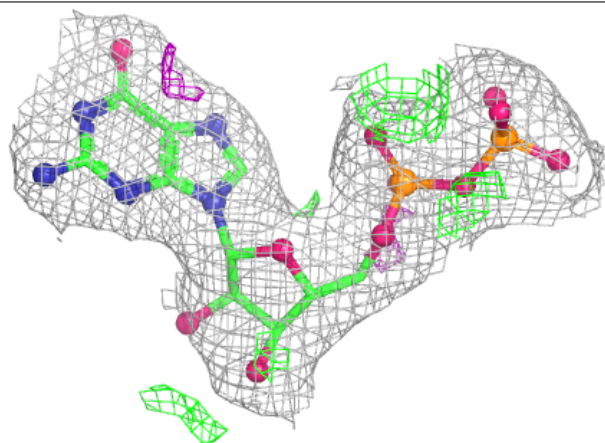
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around H1O B 505:

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

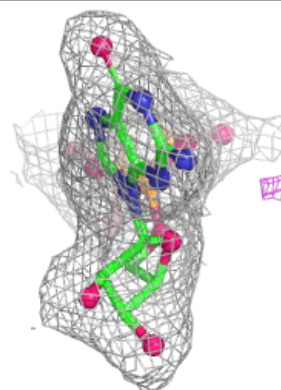
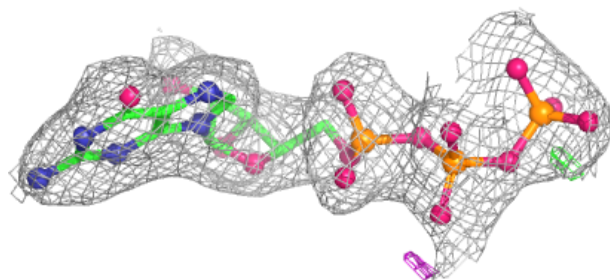
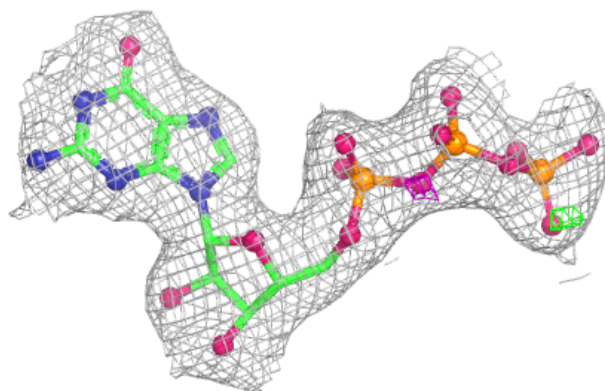
**Electron density around GDP D 501:**

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

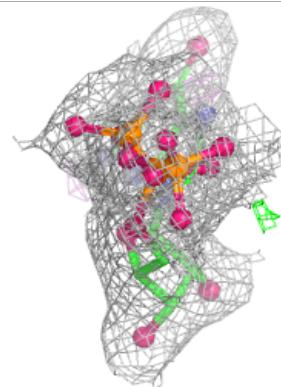
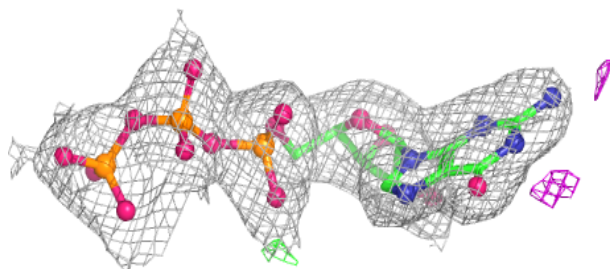
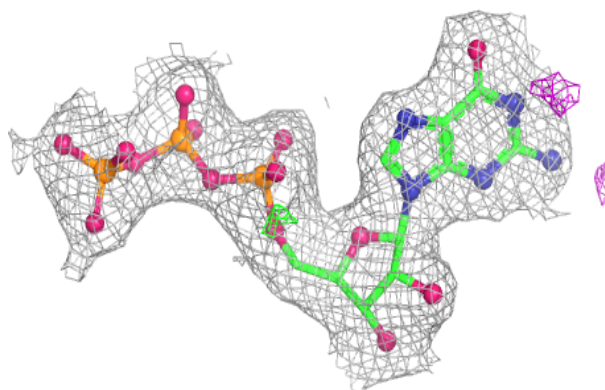


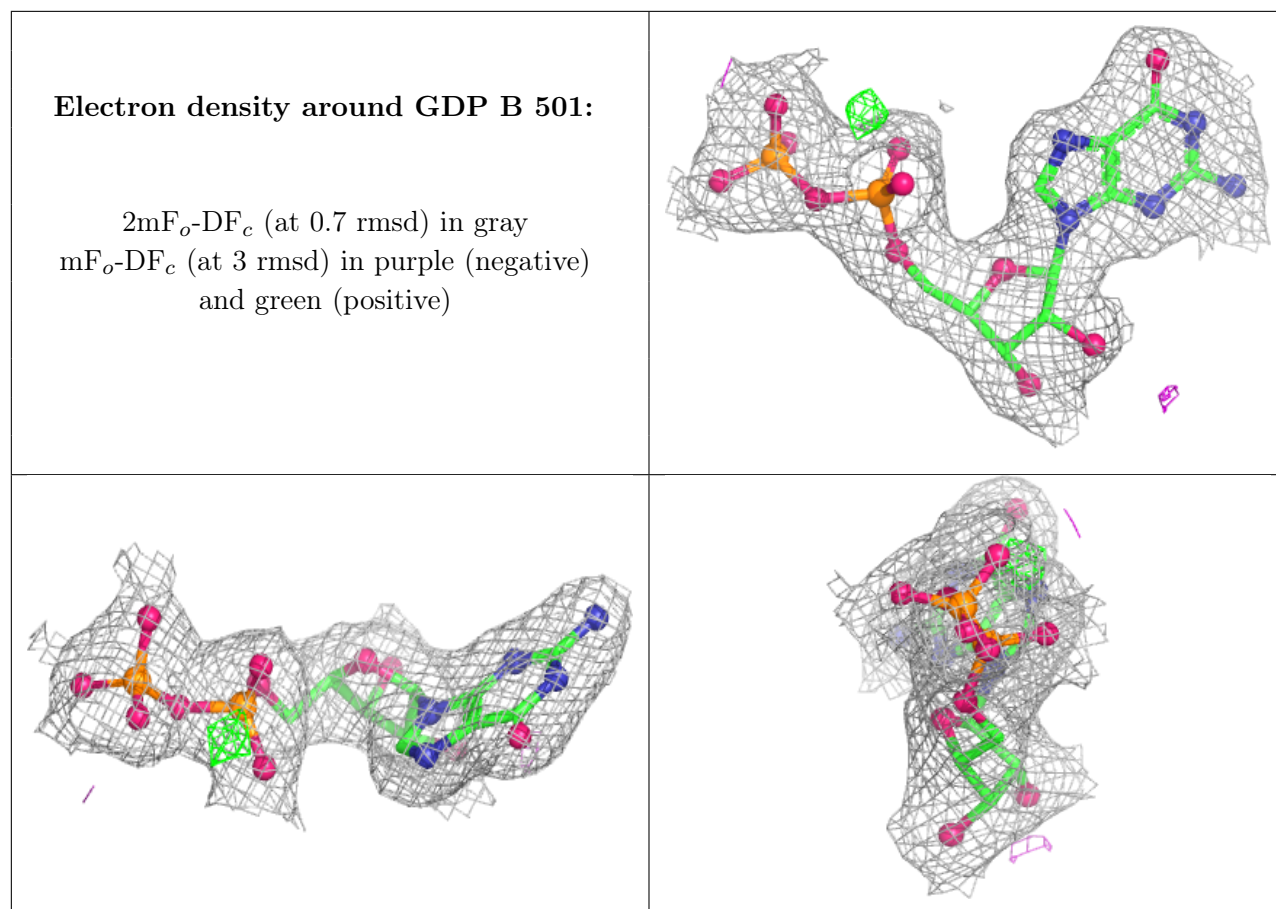
Electron density around GTP A 501:

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

**Electron density around GTP C 501:**

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





6.5 Other polymers ⓘ

There are no such residues in this entry.