



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 20, 2025 – 01:17 pm BST

PDB ID : 9H34 / pdb_00009h34
Title : T2R-TTL-PROTAC1 complex
Authors : Maiocchi, A.; Abel, A.-C.; Steinmetz, M.O.; Passarella, D.; Protà, A.E.
Deposited on : 2024-10-15
Resolution : 2.30 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 : 1.8.4, CSD as541be (2020)
Xtriage (Phenix) : 2.0
EDS : 3.0
buster-report : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

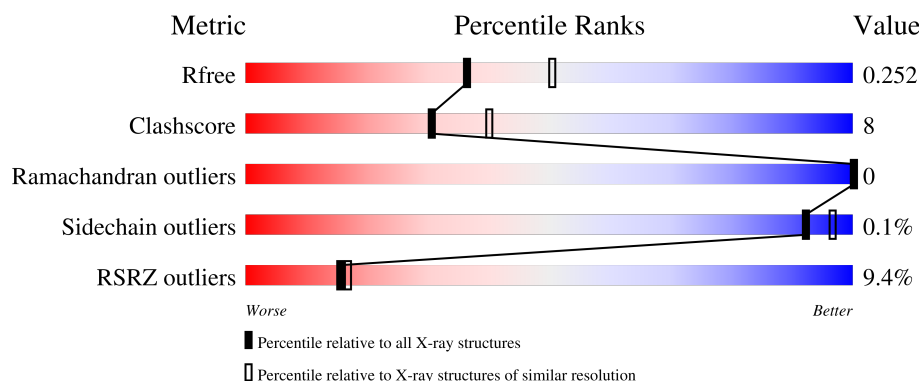
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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}	164625	5963 (2.30-2.30)
Clashscore	180529	6698 (2.30-2.30)
Ramachandran outliers	177936	6640 (2.30-2.30)
Sidechain outliers	177891	6640 (2.30-2.30)
RSRZ outliers	164620	5963 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	451	<div> <div>3%</div> <div>81%</div> <div>15%</div> <div>.</div> </div>
1	C	451	<div> <div>4%</div> <div>80%</div> <div>17%</div> <div>.</div> </div>
2	B	445	<div> <div>6%</div> <div>77%</div> <div>18%</div> <div>5%</div> </div>
2	D	445	<div> <div>12%</div> <div>68%</div> <div>27%</div> <div>.</div> </div>
3	E	143	<div> <div>14%</div> <div>76%</div> <div>10%</div> <div>14%</div> </div>

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Mol	Chain	Length	Quality of chain
4	F	384	<div><div></div><div>21%</div><div>74%</div><div>15%</div><div>10%</div></div>

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17898 atoms, of which 65 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	436	Total	C	N	O	S	0	0	0
			3407	2155	580	650	22			
1	C	440	Total	C	N	O	S	0	1	0
			3443	2178	585	657	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	1	0
			3345	2102	572	644	27			
2	D	426	Total	C	N	O	S	0	0	0
			3342	2098	570	647	27			

- Molecule 3 is a protein called Stathmin-4.

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

There are 2 discrepancies between the modelled and reference sequences:

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

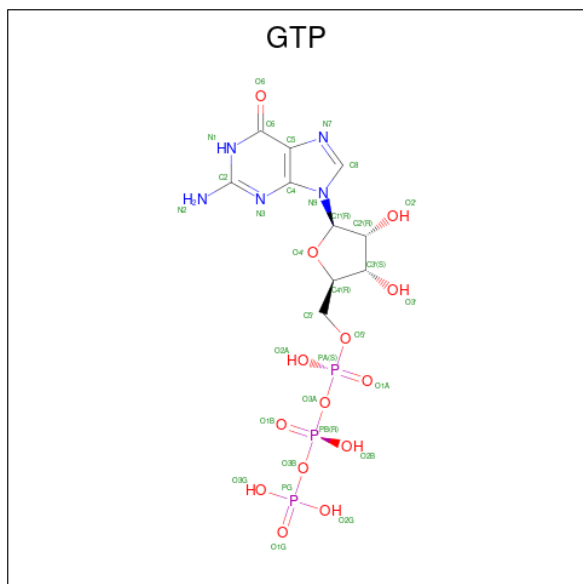
- Molecule 4 is a protein called Tubulin-tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	345	Total	C	N	O	S	0	0	0
			2822	1809	485	514	14			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP A0A8V0Z8P0
F	380	HIS	-	expression tag	UNP A0A8V0Z8P0
F	381	HIS	-	expression tag	UNP A0A8V0Z8P0
F	382	HIS	-	expression tag	UNP A0A8V0Z8P0
F	383	HIS	-	expression tag	UNP A0A8V0Z8P0
F	384	HIS	-	expression tag	UNP A0A8V0Z8P0

- 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 32	C 10	N 5	O 14	P 3	0	0
5	C	1	Total 32	C 10	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	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		
6	C	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

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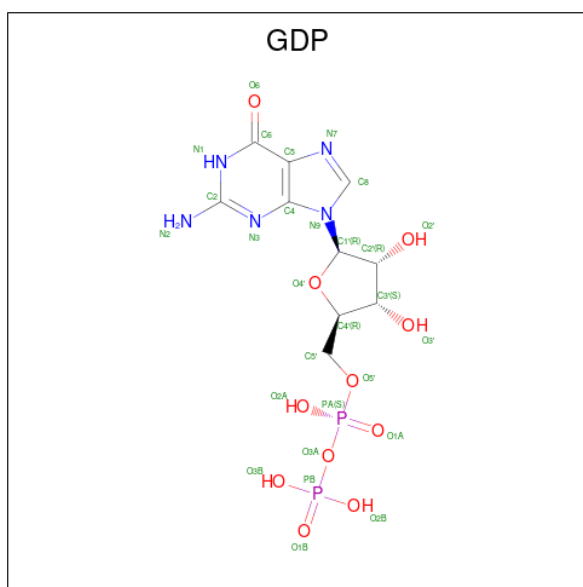
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	F	1	Total	Mg	0	0
			1	1		

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

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

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



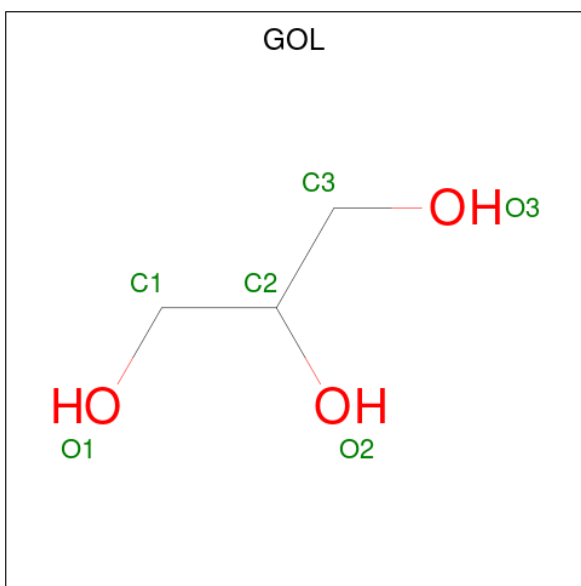
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total 28	C 10	N 5	O 11	P 2	0	0
8	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: C₆H₁₃NO₄S).



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

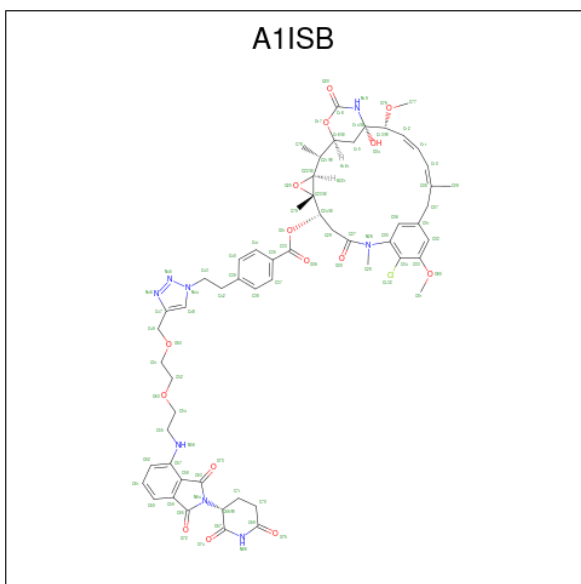
- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			6	3	3		
10	C	1	Total	C	O	0	0
			6	3	3		

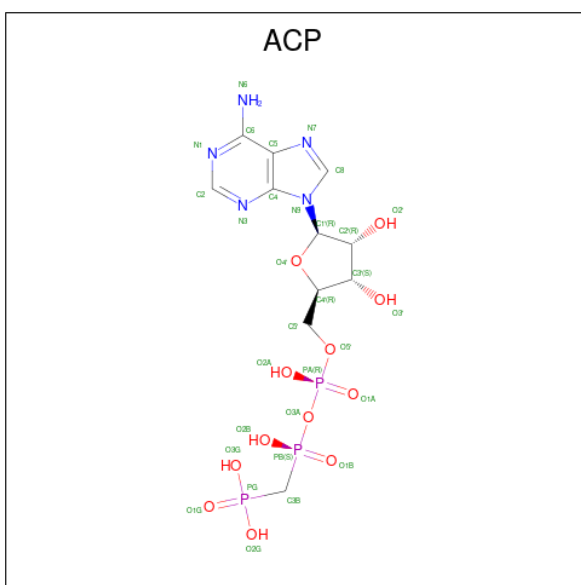
- Molecule 11 is (1S,2R,3S,5S,6S,16E,18E,20R,21S)-11-chloro-21-hydroxy-12,20-dimethoxy-2,

5,9,16-tetramethyl-8,23-dioxo-4,24-dioxo-9,22-diazatetracyclo[19.3.1.1 10,14 .0 3,5]hexacosa-10(26),11,13,16,18-pentaen-6-yl 4-{2-[4-({2-[2-({2-[(3R)-2,6-dioxopiperidin-3-yl]-1,3-dioxo-2,3-dihydro-1H-isoindol-4-yl}amino)ethoxy]ethoxy}methyl)-1H-1,2,3-triazol-1-yl]ethyl}benzoate (CCD ID: A1ISB) (formula: C₅₇H₆₅ClN₈O₁₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
11	D	1	Total	C	Cl	H	N	O	0	0
			146	57	1	65	8	15		

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
12	F	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

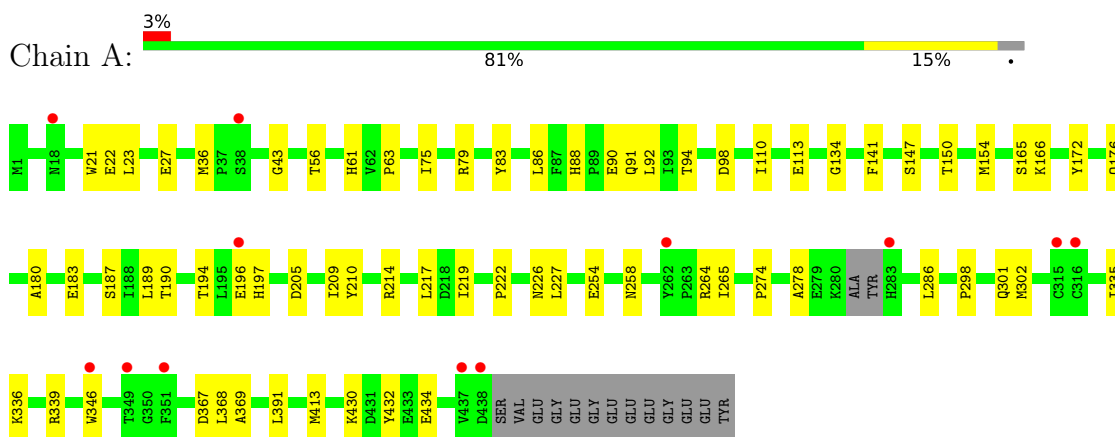
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	39	Total	O	0	0
			39	39		
13	B	49	Total	O	0	0
			49	49		
13	C	85	Total	O	0	0
			85	85		
13	D	14	Total	O	0	0
			14	14		
13	E	5	Total	O	0	0
			5	5		
13	F	3	Total	O	0	0
			3	3		

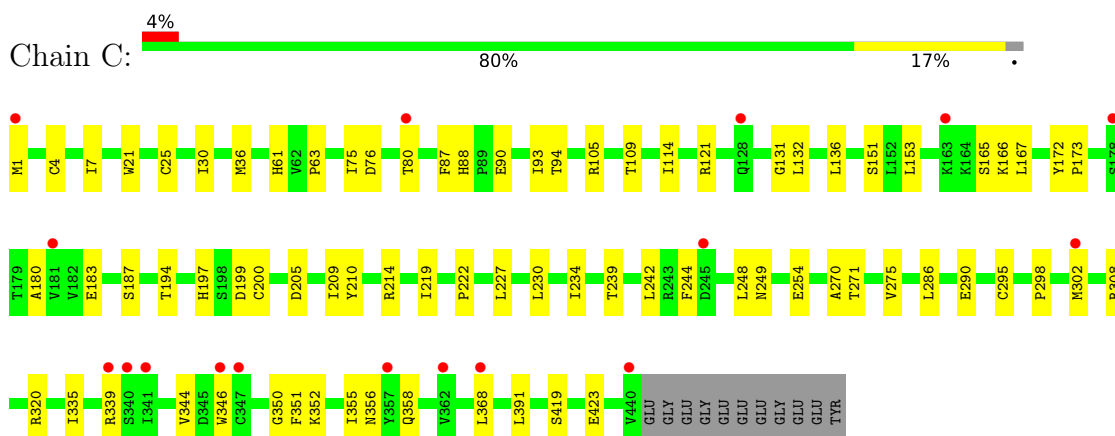
3 Residue-property plots [i](#)

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.

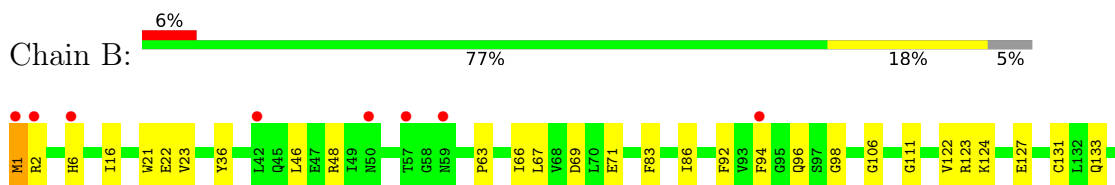
- Molecule 1: Tubulin alpha-1B chain

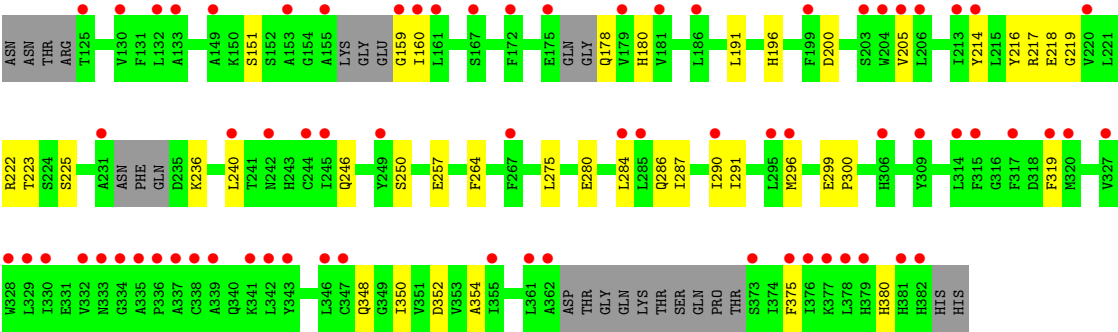


- Molecule 1: Tubulin alpha-1B chain



- Molecule 2: Tubulin beta-2B chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.37Å 156.42Å 181.93Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.72 – 2.30 49.72 – 2.30	Depositor EDS
% Data completeness (in resolution range)	100.0 (49.72-2.30) 100.0 (49.72-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.21.1_5286	Depositor
R, R_{free}	0.233 , 0.252 0.233 , 0.252	Depositor DCC
R_{free} test set	6627 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	67.7	Xtriage
Anisotropy	0.236	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 49.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17898	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.60% 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: GOL, MES, ACP, A1ISB, MG, GDP, GTP, 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	0.07	0/3483	0.22	0/4726
1	C	0.08	0/3521	0.24	0/4780
2	B	0.07	0/3419	0.22	0/4629
2	D	0.06	0/3415	0.19	0/4625
3	E	0.06	0/1022	0.15	0/1356
4	F	0.05	0/2885	0.19	0/3895
All	All	0.07	0/17745	0.21	0/24011

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3407	0	3319	49	0
1	C	3443	0	3352	51	0
2	B	3345	0	3227	59	0
2	D	3342	0	3222	83	0
3	E	1014	0	1029	11	0
4	F	2822	0	2788	38	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	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
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	2	0
9	B	12	0	13	2	0
10	B	6	0	8	0	0
10	C	6	0	8	3	0
11	D	81	65	0	1	0
12	F	31	0	14	0	0
13	A	39	0	0	1	0
13	B	49	0	0	0	0
13	C	85	0	0	0	0
13	D	14	0	0	2	0
13	E	5	0	0	0	0
13	F	3	0	0	0	0
All	All	17833	65	17028	284	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (284) 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)
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.44	0.98
2:B:176:LYS:HD2	2:B:207:GLU:HG3	1.50	0.93
1:C:350:GLY:HA2	10:C:504:GOL:H12	1.54	0.88
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.67	0.77
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.70	0.73
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.69	0.73
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.72	0.72
2:B:2:ARG:HB3	2:B:133:GLN:CG	2.20	0.71
2:B:83:PHE:O	2:B:86:ILE:HG22	1.92	0.70
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.08	0.69
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.75	0.68
2:D:1:MET:HE2	2:D:50:ASN:HB2	1.75	0.67
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.30	0.67
2:D:176:LYS:HD2	2:D:207:GLU:HG3	1.76	0.66
1:A:166:LYS:HE2	1:A:197:HIS:O	1.95	0.66
1:C:350:GLY:CA	10:C:504:GOL:H12	2.24	0.66
2:D:177:VAL:HG21	2:D:206:ASN:HB3	1.76	0.66
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.76	0.66
1:C:76:ASP:O	1:C:80:THR:HG22	1.97	0.65
4:F:10:ASN:HB2	4:F:44:ARG:HH22	1.61	0.65
2:D:217:LEU:HA	2:D:277:SER:HB3	1.79	0.64
2:D:136:GLN:HA	2:D:167:ASN:O	1.98	0.64
2:D:83:PHE:O	2:D:86:ILE:HG22	1.98	0.64
2:B:253[A]:ARG:NH1	9:B:504:MES:O1S	2.21	0.64
2:B:96:GLN:HB3	1:C:1:MET:HE2	1.78	0.64
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.80	0.64
2:D:147:SER:HB2	2:D:190:SER:OG	1.97	0.63
2:B:48:ARG:NH2	2:B:241:CYS:O	2.31	0.62
4:F:246:GLN:O	4:F:250:SER:HB3	1.99	0.62
2:B:248:LEU:HD21	2:B:352:LYS:HB3	1.82	0.62
2:B:270:PRO:HG2	2:B:302:MET:HB2	1.80	0.62
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.40	0.62
3:E:75:LYS:NZ	3:E:79:GLU:OE2	2.29	0.62
2:D:2:ARG:NH2	13:D:601:HOH:O	2.32	0.62
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.81	0.61
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.81	0.61
1:C:180:ALA:O	1:C:183:GLU:HG3	2.01	0.61
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.35	0.61
1:C:209:ILE:HD11	1:C:302:MET:CE	2.31	0.61
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.84	0.60
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.84	0.59
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.66	0.59
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.84	0.59
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.84	0.59
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.85	0.58
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.86	0.58
1:C:320:ARG:HA	1:C:356:ASN:O	2.04	0.58
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.39	0.58
1:A:430:LYS:O	1:A:434:GLU:HG3	2.03	0.58
2:D:145:THR:HB	8:D:501:GDP:O2B	2.04	0.58
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2:ARG:HA	2:B:131:CYS:O	2.05	0.57
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.40	0.57
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.40	0.57
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.37	0.57
2:D:109:THR:HG21	3:E:137:LYS:NZ	2.20	0.56
2:D:385:GLN:HB2	2:D:429:VAL:HG13	1.86	0.56
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.05	0.56
2:B:69:ASP:O	2:B:94:PHE:HA	2.05	0.56
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.21	0.56
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.36	0.56
2:B:136:GLN:HA	2:B:167:ASN:O	2.06	0.55
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.87	0.55
2:D:112:ALA:O	2:D:115:VAL:HG12	2.07	0.55
1:A:187:SER:CB	1:A:391:LEU:HD21	2.37	0.55
2:B:2:ARG:HB3	2:B:133:GLN:HG2	1.87	0.55
2:B:187:ALA:O	2:B:191:VAL:HG23	2.07	0.55
4:F:159:GLY:C	4:F:160:ILE:HD12	2.31	0.55
2:D:234:THR:OG1	2:D:302:MET:HE3	2.06	0.54
1:A:110:ILE:O	1:A:113:GLU:HG2	2.06	0.54
2:D:109:THR:HG21	3:E:137:LYS:HZ2	1.70	0.54
2:D:180:THR:HA	11:D:503:A1ISB:O30	2.08	0.54
2:D:397:ALA:O	2:D:401:ARG:NH1	2.41	0.54
1:A:172:TYR:HB3	1:A:205:ASP:HA	1.89	0.54
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.43	0.53
1:C:239:THR:HA	1:C:242:LEU:HD23	1.89	0.53
2:D:104:ALA:HB2	2:D:413:MET:SD	2.49	0.53
2:D:105:LYS:O	2:D:110:GLU:N	2.38	0.53
2:D:109:THR:O	2:D:113:GLU:HG2	2.09	0.53
2:D:409:THR:O	3:E:140:LYS:NZ	2.42	0.53
1:C:254:GLU:HG2	1:C:352:LYS:CE	2.38	0.53
2:D:290:GLU:O	2:D:294:GLN:HG3	2.09	0.53
3:E:11:LEU:HD11	3:E:18:GLN:HE21	1.74	0.53
2:B:123:ARG:O	2:B:127:GLU:HG3	2.09	0.52
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.91	0.52
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.91	0.52
2:D:392:SER:HB2	2:D:425:MET:HE3	1.92	0.52
1:C:187:SER:HB3	1:C:391:LEU:HD21	1.92	0.52
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.44	0.52
2:D:21:TRP:CE3	2:D:24:ILE:HD11	2.45	0.52
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.28	0.52
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:143:GLY:O	2:D:147:SER:OG	2.26	0.51
1:A:278:ALA:HA	1:A:369:ALA:HB2	1.91	0.51
2:D:31:ASP:OD1	2:D:35:SER:N	2.35	0.51
2:B:169:PHE:HE2	2:B:238:VAL:HG21	1.75	0.51
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.91	0.51
1:C:271:THR:HG21	1:C:295:CYS:O	2.10	0.50
2:D:178:SER:HB3	2:D:183:GLU:OE2	2.11	0.50
4:F:225:SER:OG	4:F:250:SER:OG	2.27	0.50
2:B:71:GLU:HG3	2:B:98:GLY:HA2	1.92	0.50
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.94	0.50
1:A:88:HIS:CE1	1:A:91:GLN:HG3	2.46	0.50
1:C:166:LYS:HE2	1:C:197:HIS:O	2.12	0.50
1:C:286:LEU:HA	1:C:290:GLU:OE1	2.12	0.50
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.51	0.50
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.47	0.50
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.47	0.50
4:F:43:GLU:OE1	4:F:43:GLU:N	2.30	0.50
2:D:181:VAL:HG22	2:D:398:MET:SD	2.51	0.49
1:C:419:SER:O	1:C:423:GLU:HG3	2.12	0.49
2:D:318:ILE:N	2:D:318:ILE:HD12	2.27	0.49
2:B:253[A]:ARG:NH1	9:B:504:MES:S	2.85	0.49
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.94	0.49
2:B:124:LYS:HD3	2:B:124:LYS:C	2.38	0.49
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.45	0.49
2:B:2:ARG:NE	2:B:133:GLN:HG2	2.28	0.49
2:D:141:LEU:HA	2:D:147:SER:HB3	1.95	0.48
4:F:217:ARG:HG3	4:F:218:GLU:HG2	1.95	0.48
2:B:141:LEU:HD12	2:B:172:MET:SD	2.53	0.48
4:F:280:GLU:OE1	4:F:284:LEU:HD23	2.13	0.48
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.44	0.48
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.48	0.48
1:A:298:PRO:HA	1:A:301:GLN:CD	2.39	0.48
1:C:21:TRP:CE3	1:C:63:PRO:HB3	2.49	0.48
1:A:209:ILE:HD11	1:A:302:MET:SD	2.53	0.48
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.96	0.47
2:D:124:LYS:C	2:D:124:LYS:HD3	2.39	0.47
2:D:183:GLU:N	2:D:184:PRO:HD2	2.29	0.47
2:D:21:TRP:CZ2	2:D:65:ALA:HB2	2.49	0.47
2:D:123:ARG:O	2:D:127:GLU:HG3	2.13	0.47
1:A:214:ARG:HG2	1:A:219:ILE:O	2.14	0.47
2:D:9:ALA:HA	2:D:68:VAL:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:99:ALA:O	2:D:105:LYS:HD3	2.14	0.47
2:D:414:ASP:N	2:D:414:ASP:OD1	2.47	0.47
4:F:16:GLU:OE2	4:F:19:ARG:NH2	2.45	0.47
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.96	0.47
1:C:275:VAL:HG13	1:C:368:LEU:HD21	1.96	0.47
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.45	0.47
2:D:174:SER:OG	2:D:207:GLU:HB2	2.14	0.47
4:F:287:ILE:HG23	4:F:319:PHE:CE2	2.49	0.47
1:A:141:PHE:O	1:A:147:SER:HB3	2.14	0.47
2:B:106:GLY:O	2:B:111:GLY:HA3	2.14	0.47
4:F:286:GLN:O	4:F:290:ILE:HG13	2.16	0.46
2:B:204:ILE:HD13	2:B:231:VAL:HG13	1.97	0.46
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.98	0.46
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.50	0.46
1:C:270:ALA:O	1:C:302:MET:HG2	2.15	0.46
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.33	0.46
1:C:165:SER:HA	1:C:199:ASP:OD2	2.15	0.46
2:D:387:LEU:HD23	2:D:387:LEU:C	2.41	0.46
4:F:160:ILE:HD12	4:F:160:ILE:N	2.31	0.46
1:A:79:ARG:HG2	1:A:92:LEU:HD12	1.98	0.46
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.50	0.46
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.49	0.46
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.96	0.46
2:D:316:ALA:HB3	2:D:378:ILE:HB	1.97	0.46
2:D:332:MET:O	2:D:336:GLN:HG3	2.16	0.46
1:A:83:TYR:HB3	1:A:86:LEU:HD12	1.98	0.46
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.98	0.46
1:C:214:ARG:HG2	1:C:219:ILE:O	2.16	0.46
1:A:264:ARG:HB2	13:A:603:HOH:O	2.16	0.46
2:B:318:ILE:N	2:B:318:ILE:HD12	2.31	0.46
1:C:25:CYS:HB3	1:C:30:ILE:O	2.16	0.46
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.80	0.46
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.51	0.46
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.17	0.45
3:E:60:ARG:O	3:E:64:GLN:HG3	2.14	0.45
1:C:234:ILE:HG12	1:C:302:MET:SD	2.56	0.45
4:F:223:THR:OG1	4:F:257:GLU:OE2	2.28	0.45
2:D:69:ASP:O	2:D:94:PHE:HA	2.16	0.45
1:C:351:PHE:H	10:C:504:GOL:H31	1.80	0.45
2:D:102:ASN:HB3	2:D:105:LYS:HG3	1.99	0.45
2:D:274:PRO:HB3	2:D:286:LEU:HD22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:317:ALA:C	2:B:318:ILE:HD12	2.42	0.45
1:A:88:HIS:HD1	1:A:90:GLU:HB2	1.80	0.45
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.99	0.45
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.98	0.45
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.17	0.45
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.52	0.45
2:D:46:LEU:HA	2:D:49:ILE:HB	2.00	0.44
1:A:180:ALA:O	1:A:183:GLU:HG3	2.17	0.44
1:C:187:SER:CB	1:C:391:LEU:HD21	2.48	0.44
4:F:350:ILE:O	4:F:354:ALA:HB3	2.17	0.44
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.53	0.44
2:B:347:ILE:HG22	2:B:350:ASN:HB3	1.99	0.44
2:D:385:GLN:O	2:D:389:LYS:HG3	2.17	0.44
2:B:147:SER:OG	2:B:190:SER:OG	2.23	0.44
2:D:21:TRP:CE3	2:D:63:PRO:HB3	2.52	0.44
2:D:105:LYS:HE3	2:D:110:GLU:HG3	1.99	0.44
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.98	0.44
2:B:174:SER:OG	2:B:207:GLU:HB2	2.18	0.44
2:D:19:LYS:O	2:D:23:VAL:HG23	2.18	0.44
2:B:169:PHE:CE2	2:B:238:VAL:HG21	2.53	0.43
2:D:48:ARG:NH2	13:D:603:HOH:O	2.50	0.43
4:F:87:LEU:O	4:F:88:SER:OG	2.28	0.43
2:B:431:GLU:O	2:B:434:GLN:HG2	2.18	0.43
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.53	0.43
2:D:18:ALA:O	2:D:22:GLU:HG3	2.18	0.43
2:B:66:ILE:HD12	2:B:122:VAL:HG22	2.00	0.43
2:B:295:MET:HE3	2:B:296:PHE:CE2	2.54	0.43
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.31	0.43
1:A:150:THR:O	1:A:154:MET:HG2	2.18	0.43
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.54	0.43
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.53	0.43
1:C:151:SER:HA	1:C:194:THR:HG22	2.00	0.43
2:D:23:VAL:HG21	2:D:232:SER:HB2	2.00	0.43
3:E:101:LEU:O	3:E:105:MET:HG2	2.18	0.43
2:D:15:GLN:O	2:D:19:LYS:HG2	2.19	0.43
2:D:152:LEU:O	2:D:156:LYS:HG2	2.17	0.43
2:D:171:VAL:HA	2:D:204:ILE:O	2.19	0.43
4:F:191:LEU:HD12	4:F:196:HIS:CE1	2.53	0.43
4:F:296:MET:SD	4:F:380:HIS:HB2	2.58	0.43
2:D:194:LEU:HD22	2:D:198:THR:HG21	2.00	0.43
1:C:173:PRO:HB3	1:C:183:GLU:OE1	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:10:GLY:O	2:D:14:ASN:ND2	2.36	0.43
3:E:137:LYS:O	3:E:140:LYS:HG2	2.19	0.43
1:A:346:TRP:CD1	1:A:346:TRP:H	2.36	0.43
2:B:22:GLU:HG3	2:B:83:PHE:CE1	2.53	0.43
3:E:72:LEU:O	3:E:76:ARG:HG2	2.19	0.43
1:A:22:GLU:HG3	1:A:83:TYR:CE2	2.54	0.43
1:A:176:GLN:NE2	4:F:56:PRO:HB3	2.34	0.43
2:B:2:ARG:HB3	2:B:133:GLN:HG3	1.97	0.42
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.54	0.42
2:B:1:MET:SD	2:B:1:MET:N	2.71	0.42
1:C:131:GLY:O	1:C:132:LEU:C	2.62	0.42
2:D:115:VAL:HG23	2:D:153:LEU:HD23	2.01	0.42
1:A:88:HIS:ND1	1:A:90:GLU:HB2	2.35	0.42
1:C:93:ILE:CG2	1:C:114:ILE:HD11	2.45	0.42
1:A:43:GLY:HA2	1:A:56:THR:O	2.19	0.42
2:D:191:VAL:O	2:D:195:VAL:HG23	2.19	0.42
2:D:298:SER:HB3	2:D:307:PRO:HD2	2.02	0.42
2:D:346:TRP:CE3	2:D:347:ILE:HG13	2.55	0.42
1:A:194:THR:O	1:A:194:THR:HG22	2.19	0.42
1:C:234:ILE:HD12	1:C:234:ILE:N	2.34	0.42
4:F:102:PRO:HD2	4:F:105:LEU:HD22	2.01	0.42
4:F:178:GLN:N	4:F:178:GLN:OE1	2.53	0.42
2:B:207:GLU:OE1	2:B:390:ARG:NH1	2.53	0.42
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.20	0.42
1:C:172:TYR:HB3	1:C:205:ASP:HA	2.01	0.42
2:D:67:LEU:N	2:D:67:LEU:HD12	2.35	0.42
4:F:214:TYR:HB3	4:F:375:PHE:HB3	2.01	0.42
2:D:32:PRO:HB3	2:D:82:PRO:O	2.20	0.42
1:C:248:LEU:HD13	1:C:355:ILE:HD12	2.02	0.42
4:F:70:LYS:HA	4:F:76:SER:HB3	2.01	0.42
1:A:88:HIS:CE1	1:A:90:GLU:HB2	2.55	0.41
1:A:265:ILE:HD12	1:A:432:TYR:CE2	2.55	0.41
2:B:387:LEU:C	2:B:387:LEU:HD23	2.45	0.41
1:A:180:ALA:HA	2:B:258:ASN:OD1	2.20	0.41
4:F:81:ILE:HA	4:F:87:LEU:HD12	2.03	0.41
1:C:244:PHE:CD1	1:C:358:GLN:HG2	2.55	0.41
1:A:23:LEU:O	1:A:27:GLU:HG3	2.21	0.41
1:A:134:GLY:HA3	1:A:165:SER:O	2.21	0.41
1:A:147:SER:HB2	1:A:190:THR:HB	2.02	0.41
2:D:75:MET:SD	2:D:94:PHE:HB3	2.60	0.41
4:F:20:LEU:O	4:F:24:THR:HG23	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:332:MET:O	2:D:335:VAL:HG12	2.20	0.41
4:F:10:ASN:CB	4:F:44:ARG:HH22	2.30	0.41
2:B:248:LEU:HD21	2:B:352:LYS:CB	2.47	0.41
2:B:248:LEU:CD2	2:B:352:LYS:HB3	2.48	0.41
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.56	0.41
1:C:75:ILE:HD12	1:C:94:THR:HG22	2.01	0.41
2:D:187:ALA:O	2:D:191:VAL:HG23	2.21	0.41
2:B:67:LEU:N	2:B:67:LEU:HD12	2.36	0.41
2:D:48:ARG:HH12	2:D:250:ALA:HB1	1.86	0.41
2:D:165:ILE:HA	2:D:199:ASP:OD2	2.21	0.41
4:F:275:LEU:N	4:F:275:LEU:HD22	2.36	0.41
1:A:189:LEU:CD2	1:A:413:MET:HE1	2.51	0.41
2:B:158:ARG:NH1	2:B:196:GLU:O	2.54	0.41
2:B:308:ARG:HA	2:B:342:TYR:CE1	2.56	0.41
1:C:105:ARG:HA	1:C:109:THR:HB	2.03	0.40
2:D:317:ALA:C	2:D:318:ILE:HD12	2.47	0.40
4:F:299:GLU:HB3	4:F:300:PRO:HD3	2.02	0.40
1:A:79:ARG:HG2	1:A:92:LEU:CD1	2.51	0.40
2:B:199:ASP:C	2:B:200:GLU:HG3	2.45	0.40
2:B:234:THR:O	2:B:238:VAL:HG13	2.21	0.40
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.56	0.40
2:D:416:MET:O	2:D:420:GLU:HG3	2.21	0.40
4:F:151:SER:HB3	4:F:180:HIS:CG	2.56	0.40
4:F:178:GLN:HG2	4:F:180:HIS:CE1	2.56	0.40
2:B:205:ASP:OD2	2:B:390:ARG:NH1	2.50	0.40
1:A:196:GLU:HA	1:A:196:GLU:OE1	2.21	0.40
3:E:92:ASN:O	3:E:96:MET:HG2	2.20	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	432/451 (96%)	428 (99%)	4 (1%)	0	100	100
1	C	439/451 (97%)	432 (98%)	7 (2%)	0	100	100
2	B	420/445 (94%)	417 (99%)	3 (1%)	0	100	100
2	D	422/445 (95%)	420 (100%)	2 (0%)	0	100	100
3	E	119/143 (83%)	119 (100%)	0	0	100	100
4	F	333/384 (87%)	329 (99%)	4 (1%)	0	100	100
All	All	2165/2319 (93%)	2145 (99%)	20 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	368/379 (97%)	368 (100%)	0	100	100
1	C	372/379 (98%)	372 (100%)	0	100	100
2	B	368/383 (96%)	367 (100%)	1 (0%)	91	96
2	D	367/383 (96%)	367 (100%)	0	100	100
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	309/342 (90%)	309 (100%)	0	100	100
All	All	1894/1993 (95%)	1893 (100%)	1 (0%)	92	97

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	1	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	393	HIS

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Mol	Chain	Res	Type
2	B	8	GLN
2	B	14	ASN
2	B	101	ASN
2	B	136	GLN
2	B	193	GLN
2	B	349	ASN
2	B	434	GLN
1	C	393	HIS
2	D	6	HIS
2	D	15	GLN
2	D	50	ASN
2	D	136	GLN
2	D	300	ASN
3	E	12	ASN
3	E	18	GLN
3	E	92	ASN
3	E	103	GLN
3	E	115	HIS
3	E	136	ASN
4	F	180	HIS
4	F	196	HIS
4	F	269	GLN
4	F	306	HIS
4	F	333	ASN
4	F	348	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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 18 ligands modelled in this entry, 9 are monoatomic - leaving 9 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$
5	GTP	C	501	6	26,34,34	1.12	2 (7%)	32,54,54	1.43	5 (15%)
8	GDP	B	501	6	24,30,30	0.95	1 (4%)	30,47,47	1.13	3 (10%)
5	GTP	A	501	6	26,34,34	1.12	2 (7%)	32,54,54	1.46	6 (18%)
9	MES	B	504	-	12,12,12	1.14	1 (8%)	14,16,16	0.91	1 (7%)
10	GOL	C	504	-	5,5,5	0.33	0	5,5,5	0.34	0
11	A1ISB	D	503	-	87,89,89	3.54	28 (32%)	108,130,130	1.89	24 (22%)
12	ACP	F	401	6	27,33,33	2.29	3 (11%)	32,52,52	1.17	4 (12%)
8	GDP	D	501	6	24,30,30	0.95	1 (4%)	30,47,47	1.29	4 (13%)
10	GOL	B	505	-	5,5,5	0.33	0	5,5,5	0.29	0

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
5	GTP	C	501	6	-	8/18/38/38	0/3/3/3
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	A	501	6	-	8/18/38/38	0/3/3/3
9	MES	B	504	-	-	0/6/14/14	0/1/1/1
10	GOL	C	504	-	-	0/4/4/4	-
11	A1ISB	D	503	-	-	14/67/125/125	0/7/9/9
12	ACP	F	401	6	-	6/15/38/38	0/3/3/3
8	GDP	D	501	6	-	2/12/32/32	0/3/3/3
10	GOL	B	505	-	-	0/4/4/4	-

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	503	A1ISB	O20-C18	15.92	1.51	1.21
12	F	401	ACP	PB-O3A	10.76	1.70	1.58
11	D	503	A1ISB	O72-C65	9.56	1.41	1.22
11	D	503	A1ISB	O73-C63	9.34	1.40	1.22
11	D	503	A1ISB	O17-C16	8.40	1.57	1.46
11	D	503	A1ISB	O75-C69	8.25	1.40	1.23
11	D	503	A1ISB	O74-C67	7.78	1.38	1.23
11	D	503	A1ISB	C67-N68	7.78	1.50	1.37
11	D	503	A1ISB	O76-C13	7.65	1.57	1.43
11	D	503	A1ISB	C27-N26	7.04	1.49	1.35
11	D	503	A1ISB	C69-N68	6.89	1.49	1.37
11	D	503	A1ISB	O31-C24	-4.88	1.38	1.46
11	D	503	A1ISB	C07-C01	4.56	1.59	1.51
11	D	503	A1ISB	C05-N26	4.36	1.49	1.44
5	A	501	GTP	C5-C6	-3.96	1.39	1.47
5	C	501	GTP	C5-C6	-3.93	1.39	1.47
11	D	503	A1ISB	O31-C33	3.75	1.42	1.34
11	D	503	A1ISB	C57-N56	3.07	1.45	1.37
9	B	504	MES	C8-S	3.05	1.81	1.77
11	D	503	A1ISB	C48-N44	-2.98	1.32	1.35
11	D	503	A1ISB	C60-C59	2.98	1.44	1.39
11	D	503	A1ISB	C63-N64	-2.93	1.34	1.40
11	D	503	A1ISB	C14-N19	-2.84	1.42	1.46
11	D	503	A1ISB	O80-C03	2.82	1.41	1.37
11	D	503	A1ISB	C29-C27	2.69	1.56	1.51
11	D	503	A1ISB	C59-C65	-2.62	1.44	1.48
11	D	503	A1ISB	C07-C08	2.59	1.54	1.51
11	D	503	A1ISB	C66-N64	2.48	1.51	1.46
8	D	501	GDP	C6-N1	-2.41	1.34	1.37
8	B	501	GDP	C6-N1	-2.34	1.34	1.37
11	D	503	A1ISB	O17-C18	-2.34	1.31	1.35
11	D	503	A1ISB	C65-N64	-2.23	1.35	1.40
11	D	503	A1ISB	C58-C63	-2.21	1.45	1.49
12	F	401	ACP	PB-O2B	-2.20	1.51	1.56
11	D	503	A1ISB	C48-C47	2.17	1.39	1.36
5	A	501	GTP	C2-N3	2.16	1.38	1.33
12	F	401	ACP	C8-N7	-2.15	1.30	1.34
5	C	501	GTP	C2-N3	2.11	1.38	1.33

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	503	A1ISB	O25-C23-C24	7.65	129.28	115.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	503	A1ISB	C69-N68-C67	-6.78	117.17	126.61
11	D	503	A1ISB	C70-C69-N68	4.64	121.86	116.65
11	D	503	A1ISB	O31-C33-C35	4.12	118.57	111.92
11	D	503	A1ISB	C57-C58-C63	4.03	134.88	129.21
11	D	503	A1ISB	C59-C58-C57	-3.98	119.17	121.91
11	D	503	A1ISB	O80-C03-C04	3.59	119.79	115.53
8	D	501	GDP	PA-O3A-PB	-3.51	120.77	132.83
11	D	503	A1ISB	O25-C23-C79	-3.36	109.34	114.17
12	F	401	ACP	O1G-PG-C3B	-3.36	104.00	111.24
5	A	501	GTP	PA-O3A-PB	-3.26	121.63	132.83
5	A	501	GTP	C5-C6-N1	3.13	119.49	113.95
11	D	503	A1ISB	C78-C21-C22	-3.11	105.82	112.55
5	C	501	GTP	C5-C6-N1	3.09	119.41	113.95
11	D	503	A1ISB	O73-C63-C58	-3.08	124.70	129.09
8	D	501	GDP	C3'-C2'-C1'	3.05	105.58	100.98
5	C	501	GTP	PA-O3A-PB	-3.04	122.39	132.83
5	C	501	GTP	C8-N7-C5	3.04	108.78	102.99
5	A	501	GTP	C8-N7-C5	2.99	108.68	102.99
11	D	503	A1ISB	C16-O17-C18	-2.98	113.44	121.06
11	D	503	A1ISB	C79-C23-C22	-2.98	114.29	121.05
11	D	503	A1ISB	C58-C63-N64	2.96	109.36	105.82
5	C	501	GTP	PB-O3B-PG	-2.95	122.69	132.83
8	B	501	GDP	PA-O3A-PB	-2.89	122.91	132.83
12	F	401	ACP	O2B-PB-O1B	2.88	119.69	110.07
5	A	501	GTP	PB-O3B-PG	-2.79	123.27	132.83
5	A	501	GTP	C2-N1-C6	-2.76	120.01	125.10
11	D	503	A1ISB	C59-C65-N64	2.74	108.94	105.96
5	C	501	GTP	C2-N1-C6	-2.72	120.09	125.10
11	D	503	A1ISB	C71-C66-N64	-2.67	107.37	113.85
9	B	504	MES	O2S-S-C8	-2.42	104.00	106.92
11	D	503	A1ISB	O17-C16-C21	2.40	110.75	105.76
12	F	401	ACP	PB-O3A-PA	-2.37	125.04	132.56
11	D	503	A1ISB	C29-C27-N26	2.34	121.53	118.89
8	D	501	GDP	C8-N7-C5	2.33	107.43	102.99
11	D	503	A1ISB	O80-C03-C02	-2.32	120.13	124.12
8	B	501	GDP	C5-C6-N1	2.30	118.01	113.95
8	B	501	GDP	C8-N7-C5	2.30	107.36	102.99
8	D	501	GDP	C5-C6-N1	2.27	117.95	113.95
11	D	503	A1ISB	C48-C47-N46	-2.22	108.05	111.34
11	D	503	A1ISB	C65-N64-C63	-2.20	109.00	111.53
11	D	503	A1ISB	C06-C05-C04	-2.18	119.76	122.53
5	A	501	GTP	O6-C6-C5	-2.15	120.17	124.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	401	ACP	O3G-PG-O2G	2.09	114.18	108.08
11	D	503	A1ISB	C28-N26-C05	2.06	119.59	116.72
11	D	503	A1ISB	C59-C58-C63	-2.04	105.95	108.15
11	D	503	A1ISB	C81-O80-C03	-2.04	114.45	117.53

There are no chirality outliers.

All (41) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
11	D	503	A1ISB	C12-C13-O76-C77
11	D	503	A1ISB	C04-C03-O80-C81
11	D	503	A1ISB	C54-C55-N56-C57
11	D	503	A1ISB	C58-C57-N56-C55
12	F	401	ACP	PB-C3B-PG-O1G
12	F	401	ACP	PB-C3B-PG-O2G
12	F	401	ACP	PB-C3B-PG-O3G
12	F	401	ACP	C5'-O5'-PA-O1A
12	F	401	ACP	C5'-O5'-PA-O3A
11	D	503	A1ISB	C62-C57-N56-C55
11	D	503	A1ISB	C02-C03-O80-C81
11	D	503	A1ISB	O31-C33-C35-C37
11	D	503	A1ISB	O31-C33-C35-C41
11	D	503	A1ISB	O36-C33-C35-C37
5	C	501	GTP	PB-O3B-PG-O1G
11	D	503	A1ISB	O36-C33-C35-C41
5	A	501	GTP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O2A
11	D	503	A1ISB	O36-C33-O31-C24
11	D	503	A1ISB	C55-C54-O53-C52
11	D	503	A1ISB	C15-C16-C21-C78
5	C	501	GTP	PB-O3A-PA-O2A
11	D	503	A1ISB	C35-C33-O31-C24
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G

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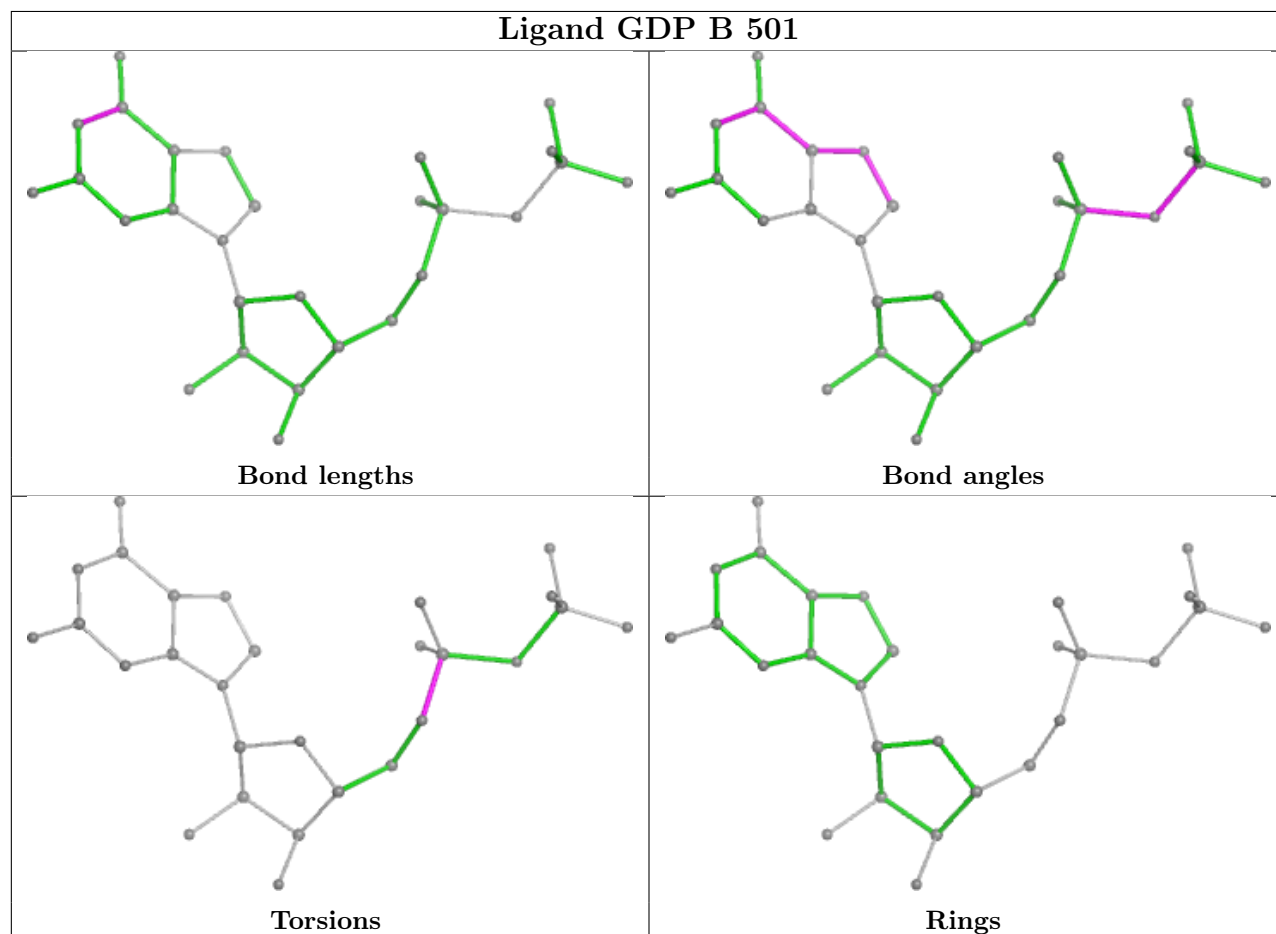
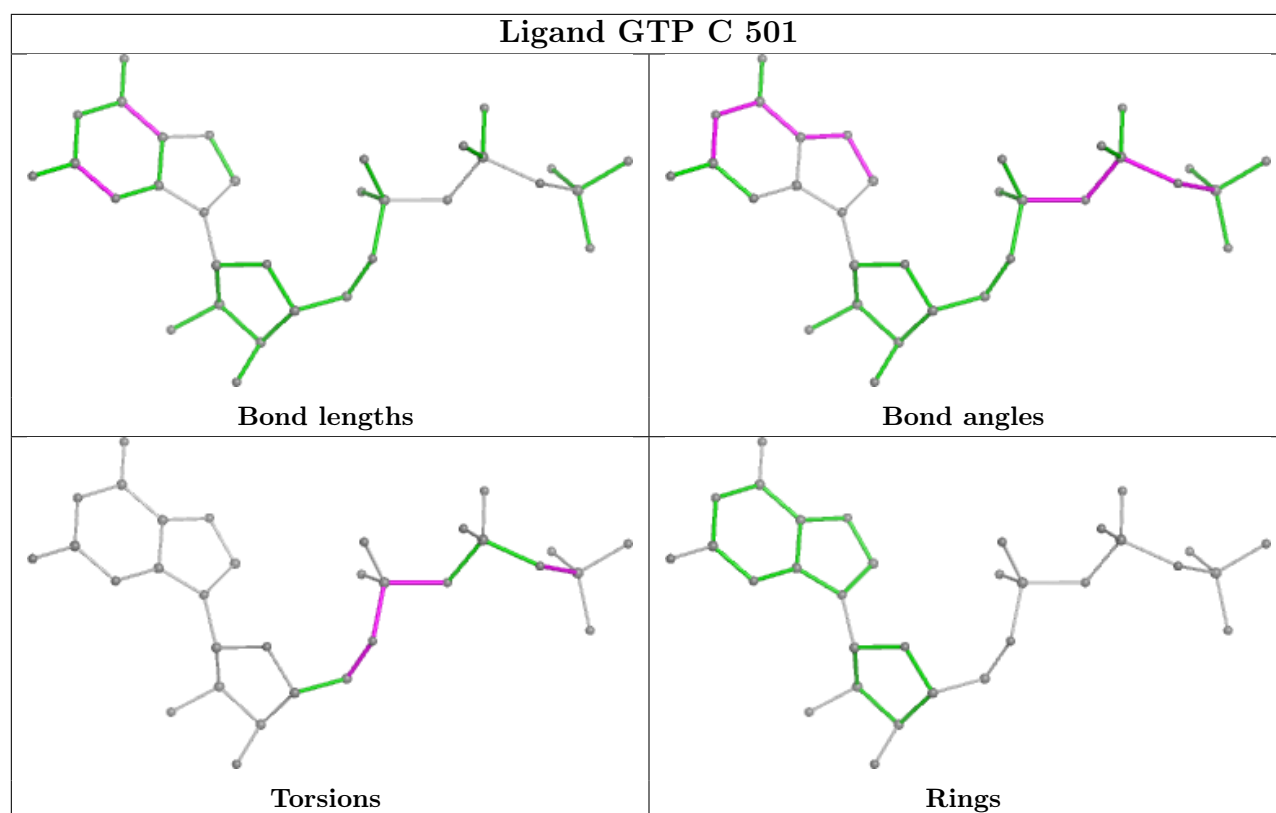
Mol	Chain	Res	Type	Atoms
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O2A
12	F	401	ACP	C5'-O5'-PA-O2A

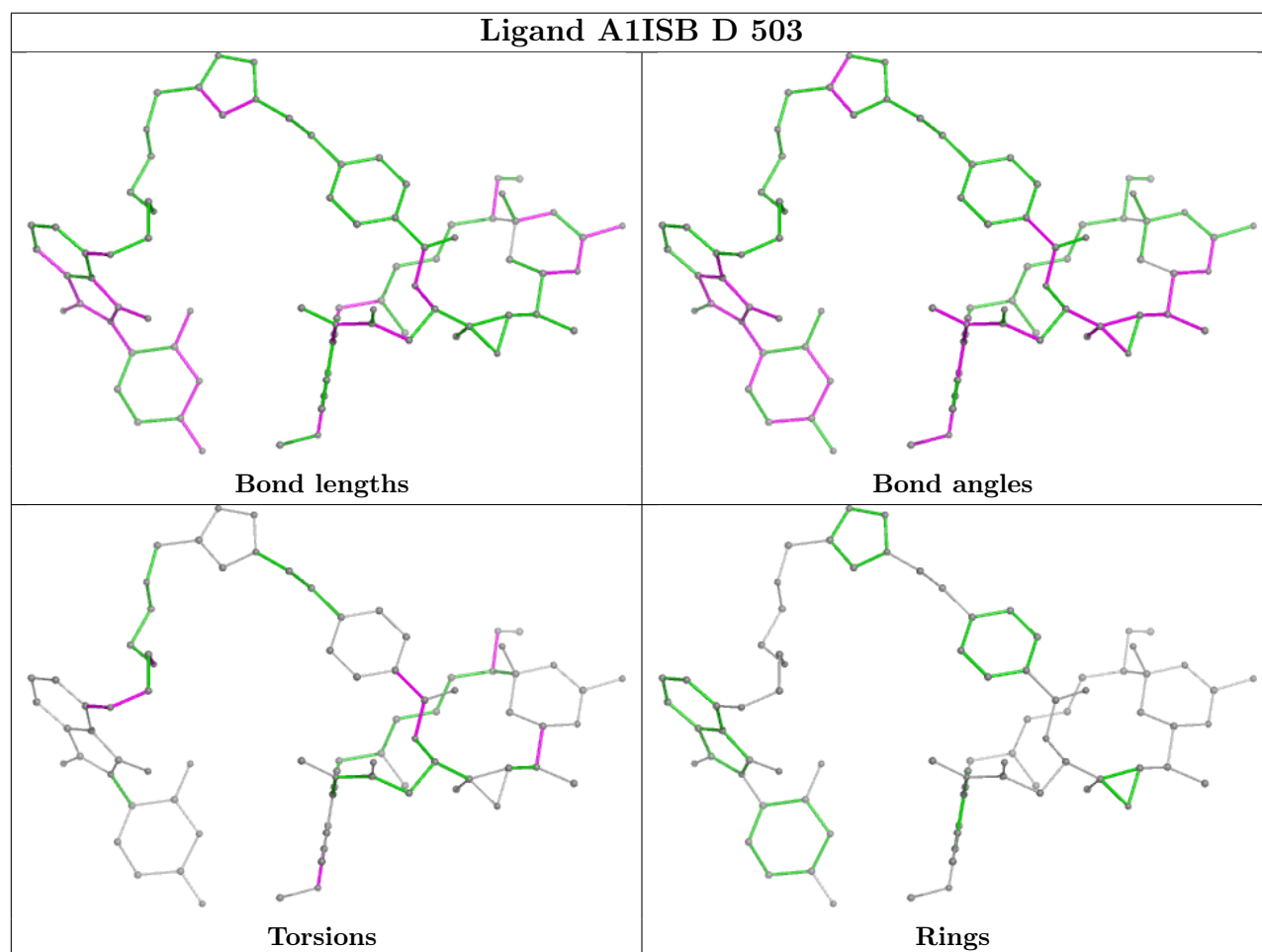
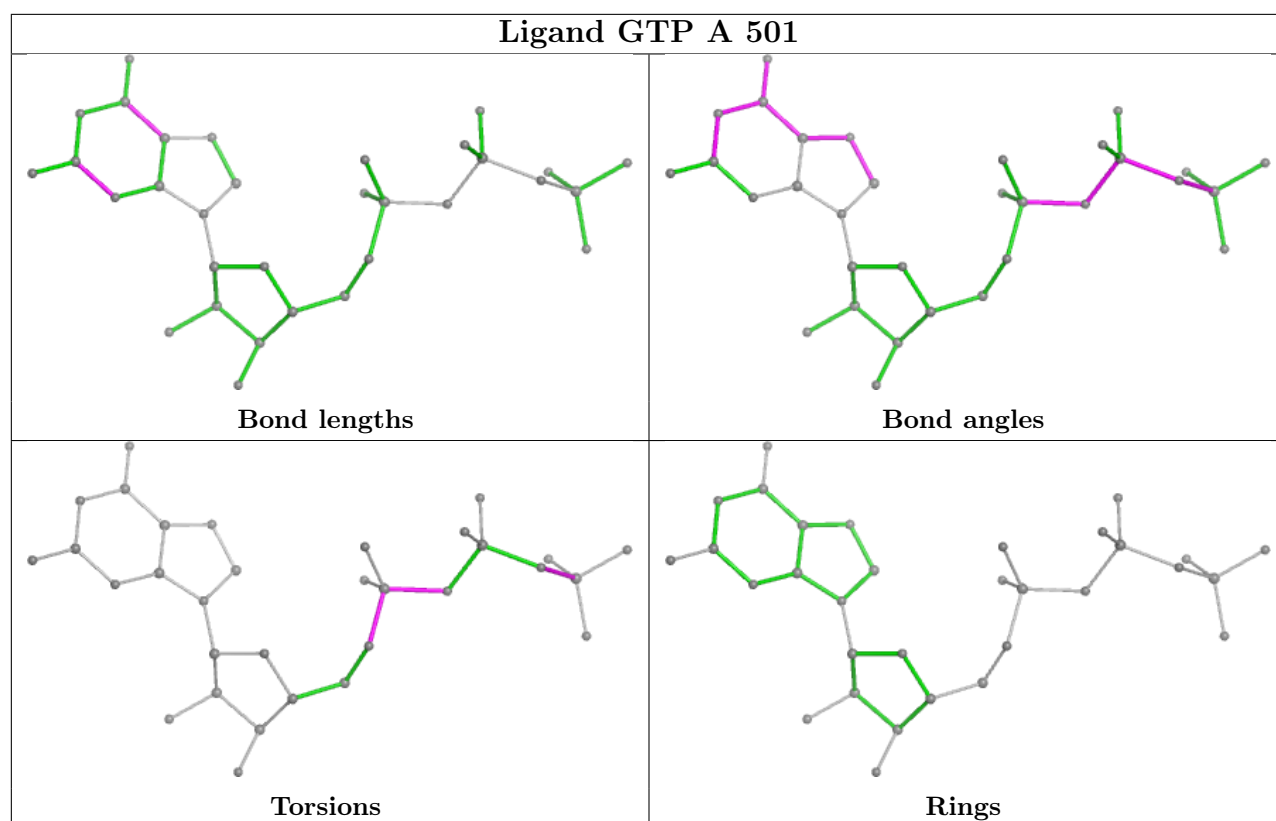
There are no ring outliers.

5 monomers are involved in 9 short contacts:

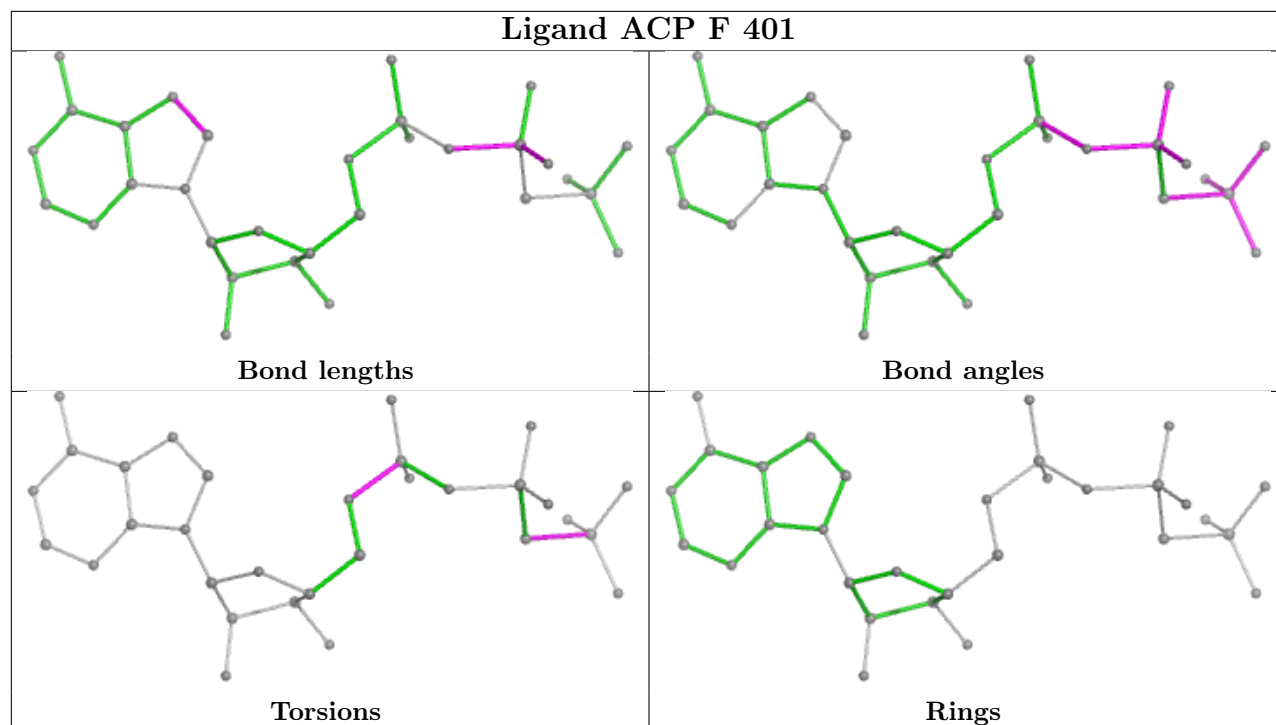
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	501	GTP	1	0
9	B	504	MES	2	0
10	C	504	GOL	3	0
11	D	503	A1ISB	1	0
8	D	501	GDP	2	0

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

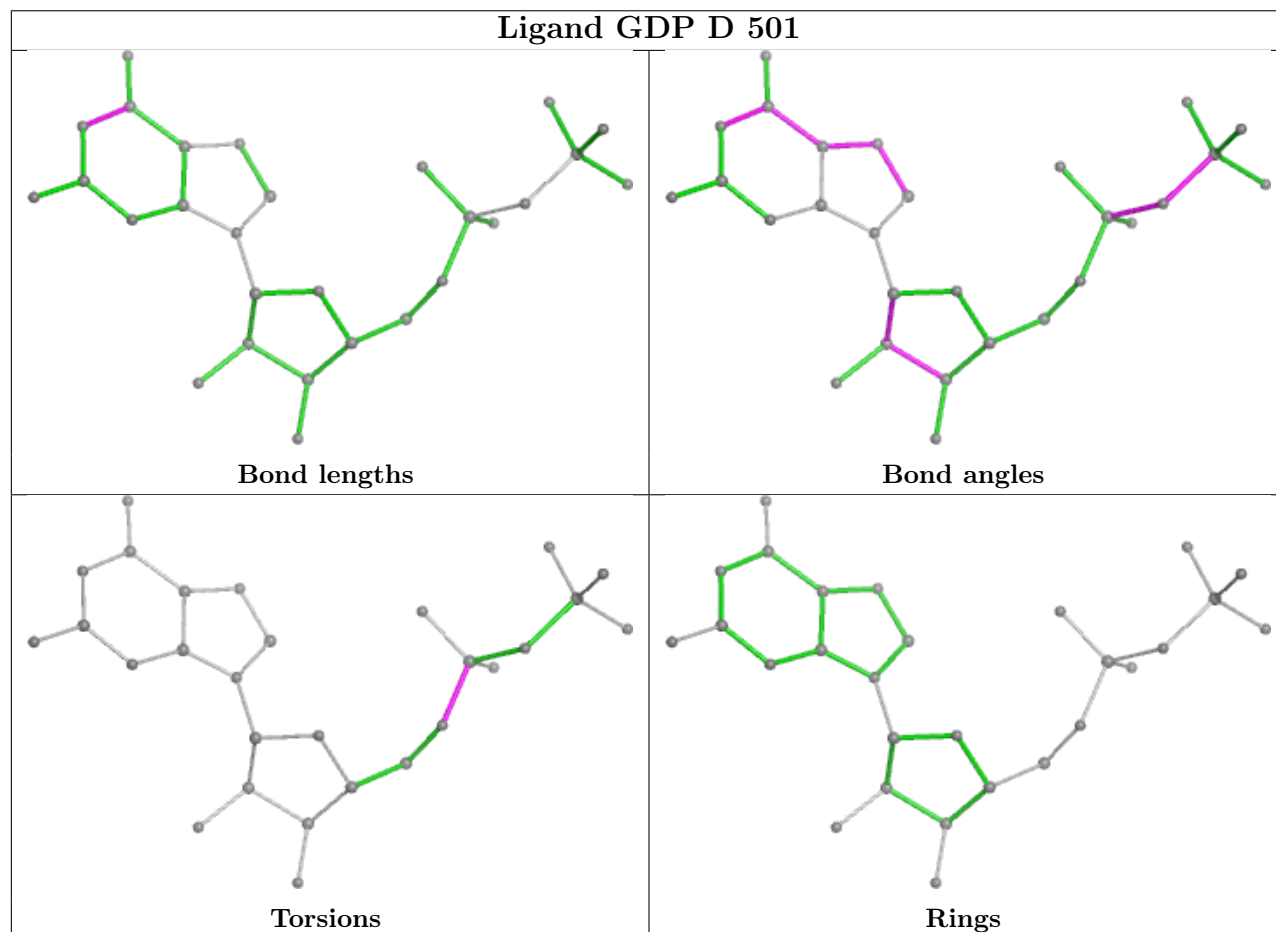




Ligand ACP F 401



Ligand GDP D 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	436/451 (96%)	0.47	12 (2%) 55 56	60, 81, 107, 125	0
1	C	440/451 (97%)	0.55	17 (3%) 44 45	30, 69, 84, 103	1 (0%)
2	B	423/445 (95%)	0.67	27 (6%) 27 28	34, 75, 103, 123	1 (0%)
2	D	426/445 (95%)	1.02	52 (12%) 10 11	67, 97, 128, 146	0
3	E	123/143 (86%)	1.20	20 (16%) 5 6	73, 100, 131, 141	0
4	F	345/384 (89%)	1.32	79 (22%) 2 3	61, 118, 165, 219	0
All	All	2193/2319 (94%)	0.81	207 (9%) 15 17	30, 84, 134, 219	2 (0%)

All (207) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	279	GLY	6.1
4	F	155	ALA	5.7
2	D	277	SER	5.6
2	B	1	MET	5.4
3	E	143	ALA	5.2
4	F	330	ILE	5.1
4	F	159	GLY	4.5
4	F	319	PHE	4.4
4	F	376	ILE	4.4
4	F	362	ALA	4.2
2	D	276	THR	4.0
4	F	231	ALA	4.0
2	D	172	MET	3.9
4	F	179	VAL	3.9
2	D	42	LEU	3.9
1	C	340	SER	3.8
1	C	341	ILE	3.8
3	E	6	MET	3.8
4	F	105	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
2	B	276	THR	3.7
1	A	283	HIS	3.7
4	F	320	MET	3.6
4	F	338	CYS	3.6
1	A	351	PHE	3.6
3	E	23	ILE	3.6
4	F	332	VAL	3.6
4	F	378	LEU	3.6
1	C	440	VAL	3.5
1	C	302	MET	3.5
2	D	1	MET	3.5
2	B	57	THR	3.5
2	B	435	TYR	3.4
4	F	317	PHE	3.3
4	F	334	GLY	3.3
2	D	275	LEU	3.3
2	B	284	ARG	3.2
2	B	425	MET	3.2
3	E	8	VAL	3.2
1	C	163	LYS	3.2
4	F	335	ALA	3.2
4	F	381	HIS	3.2
1	A	316	CYS	3.2
3	E	102	ALA	3.1
2	B	437	ASP	3.1
2	D	161	TYR	3.1
2	D	285	ALA	3.1
2	B	275	LEU	3.0
4	F	205	VAL	3.0
4	F	186	LEU	3.0
3	E	27	PRO	3.0
2	B	283	TYR	3.0
2	D	378	ILE	3.0
4	F	296	MET	3.0
2	D	311	ARG	3.0
2	D	66	ILE	2.9
4	F	343	TYR	2.9
2	B	325	MET	2.9
4	F	240	LEU	2.9
4	F	377	LYS	2.9
3	E	7	GLU	2.9
4	F	204	TRP	2.8

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Mol	Chain	Res	Type	RSRZ
3	E	20	PHE	2.8
3	E	45	PRO	2.8
2	D	167	ASN	2.8
2	B	277	SER	2.8
4	F	336	PRO	2.8
4	F	220	VAL	2.8
4	F	328	TRP	2.8
4	F	132	LEU	2.8
2	D	340	SER	2.8
2	D	319	PHE	2.8
4	F	295	LEU	2.8
2	D	334	ASN	2.8
1	C	357	TYR	2.7
2	D	305	CYS	2.7
1	C	80	THR	2.7
2	B	347	ILE	2.7
4	F	355	ILE	2.7
1	A	438	ASP	2.7
1	C	362	VAL	2.7
4	F	149	ALA	2.7
4	F	382	HIS	2.7
2	B	172	MET	2.7
3	E	28	SER	2.7
4	F	375	PHE	2.7
2	B	248	LEU	2.7
4	F	181	VAL	2.7
3	E	24	LEU	2.6
3	E	139	LEU	2.6
4	F	329	LEU	2.6
2	D	298	SER	2.6
2	D	247	GLN	2.6
1	A	437	VAL	2.6
2	D	421	ALA	2.6
4	F	337	ALA	2.6
4	F	206	LEU	2.6
2	B	59	ASN	2.6
2	D	278	ARG	2.6
2	B	286	LEU	2.6
2	D	57	THR	2.6
2	D	342	TYR	2.6
4	F	249	TYR	2.6
4	F	245	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	1	MET	2.5
2	D	323	MET	2.5
4	F	339	ALA	2.5
2	D	248	LEU	2.5
1	A	18	ASN	2.5
2	D	212	ILE	2.5
4	F	160	ILE	2.5
2	D	177	VAL	2.5
2	D	351	VAL	2.5
4	F	125	THR	2.5
2	D	37	HIS	2.5
2	D	406	HIS	2.5
4	F	306	HIS	2.5
2	B	400	ARG	2.5
4	F	153	ALA	2.5
4	F	172	PHE	2.5
4	F	315	PHE	2.5
3	E	11	LEU	2.5
4	F	284	LEU	2.5
4	F	379	HIS	2.5
2	D	189	LEU	2.4
4	F	342	LEU	2.4
2	D	184	PRO	2.4
2	B	203	CYS	2.4
2	B	42	LEU	2.4
4	F	285	LEU	2.4
3	E	15	THR	2.4
2	D	122	VAL	2.4
2	D	325	MET	2.4
4	F	347	CYS	2.4
1	A	349	THR	2.3
2	B	346	TRP	2.3
4	F	267	PHE	2.3
4	F	341	LYS	2.3
2	D	128	SER	2.3
3	E	22	VAL	2.3
2	D	130	ASP	2.3
2	B	167	ASN	2.3
4	F	346	LEU	2.3
1	C	181	VAL	2.3
4	F	130	VAL	2.3
2	D	343	PHE	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	308	ARG	2.3
4	F	213	ILE	2.3
3	E	90	ASN	2.3
4	F	161	LEU	2.3
4	F	327	VAL	2.3
1	A	315	CYS	2.3
4	F	72	CYS	2.3
2	D	345	GLU	2.2
4	F	104	ASN	2.2
2	B	2	ARG	2.2
3	E	105	MET	2.2
4	F	175	GLU	2.2
4	F	214	TYR	2.2
3	E	84	GLN	2.2
1	A	346	TRP	2.2
4	F	89	GLU	2.2
4	F	290	ILE	2.2
4	F	309	TYR	2.2
1	C	128	GLN	2.2
4	F	13	VAL	2.2
1	A	196	GLU	2.1
1	C	178	SER	2.1
1	C	347	CYS	2.1
1	C	346	TRP	2.1
2	D	141	LEU	2.1
2	B	6	HIS	2.1
2	D	185	TYR	2.1
4	F	75	ALA	2.1
2	D	372	LYS	2.1
1	C	339	ARG	2.1
1	C	368	LEU	2.1
4	F	242	ASN	2.1
4	F	361	LEU	2.1
2	D	307	PRO	2.1
3	E	103	GLN	2.1
2	D	403	ALA	2.1
4	F	199	PHE	2.1
2	D	441	ASP	2.1
1	A	38	SER	2.1
4	F	203	SER	2.1
2	B	50	ASN	2.1
4	F	314	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	262	TYR	2.1
2	D	377	PHE	2.1
1	C	245	ASP	2.1
2	D	50	ASN	2.1
4	F	35	PRO	2.1
4	F	333	ASN	2.1
2	B	220	THR	2.1
4	F	133	ALA	2.1
2	D	118	VAL	2.0
2	B	94	PHE	2.0
3	E	47	LEU	2.0
4	F	244	CYS	2.0
2	B	431	GLU	2.0
2	D	160	GLU	2.0
4	F	93	TRP	2.0
2	D	121	VAL	2.0
2	D	192	HIS	2.0
4	F	167	SER	2.0
4	F	373	SER	2.0
2	D	286	LEU	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
11	A1ISB	D	503	81/81	0.60	0.18	96,125,146,156	0
10	GOL	C	504	6/6	0.80	0.18	91,93,97,98	0
6	MG	F	402	1/1	0.85	0.10	116,116,116,116	0

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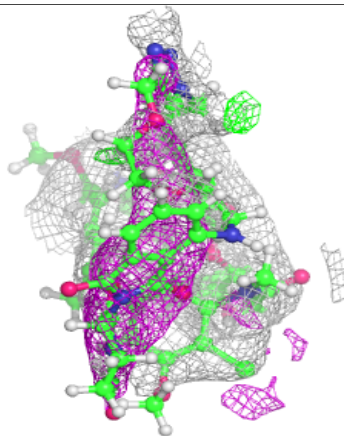
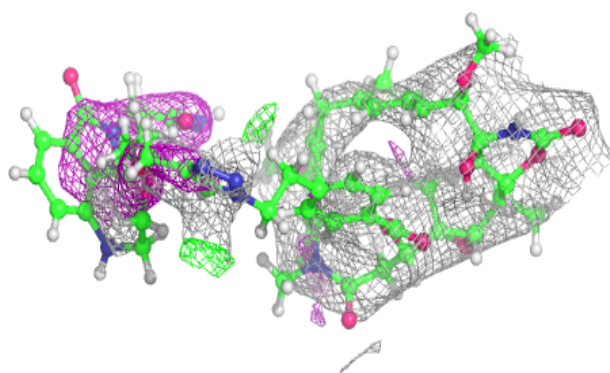
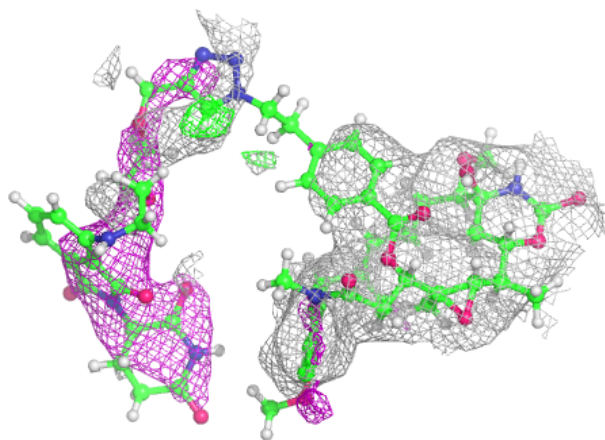
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
10	GOL	B	505	6/6	0.85	0.14	50,55,57,60	0
12	ACP	F	401	31/31	0.87	0.11	124,131,136,141	0
6	MG	D	502	1/1	0.89	0.11	117,117,117,117	0
8	GDP	D	501	28/28	0.91	0.12	91,103,113,115	0
5	GTP	C	501	32/32	0.92	0.20	89,98,120,133	0
9	MES	B	504	12/12	0.92	0.13	51,57,61,61	0
7	CA	A	504	1/1	0.92	0.15	65,65,65,65	0
5	GTP	A	501	32/32	0.93	0.18	69,90,159,178	0
7	CA	B	503	1/1	0.93	0.18	57,57,57,57	0
8	GDP	B	501	28/28	0.96	0.08	52,57,64,67	0
7	CA	A	503	1/1	0.97	0.10	69,69,69,69	0
6	MG	A	502	1/1	0.97	0.06	69,69,69,69	0
6	MG	B	502	1/1	0.98	0.14	52,52,52,52	0
7	CA	C	503	1/1	0.98	0.04	93,93,93,93	0
6	MG	C	502	1/1	0.98	0.09	94,94,94,94	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.

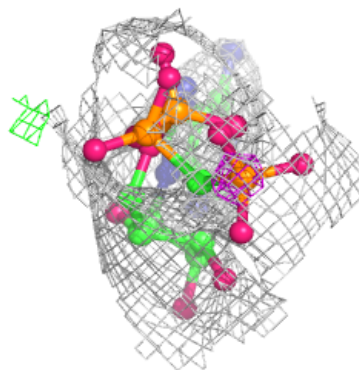
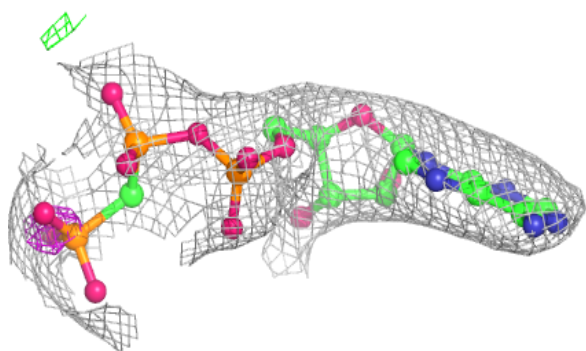
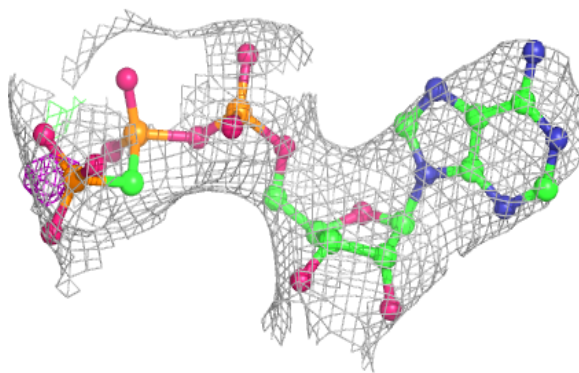
Electron density around A1ISB D 503:

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

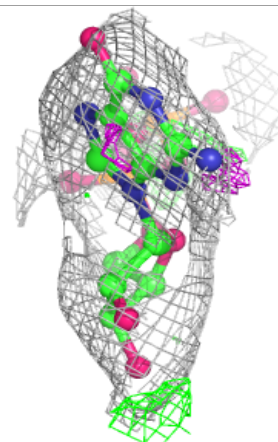
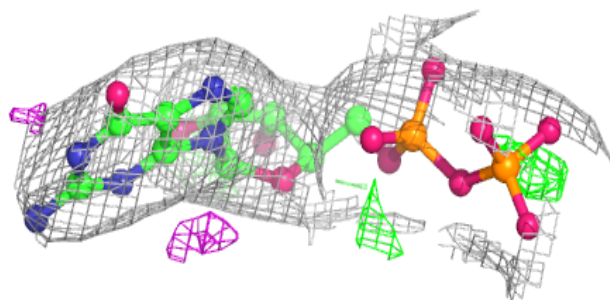
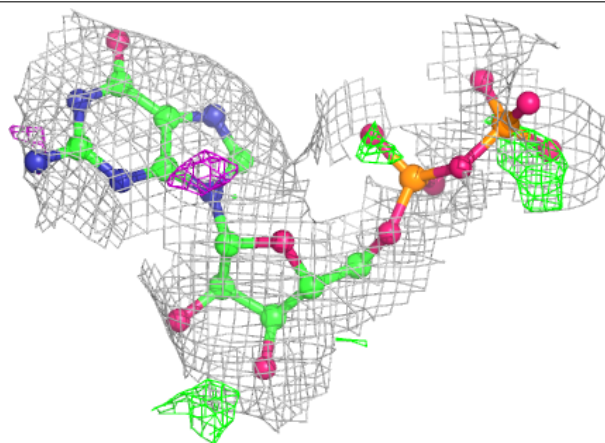


Electron density around ACP F 401:

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

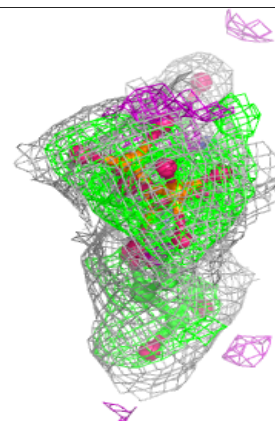
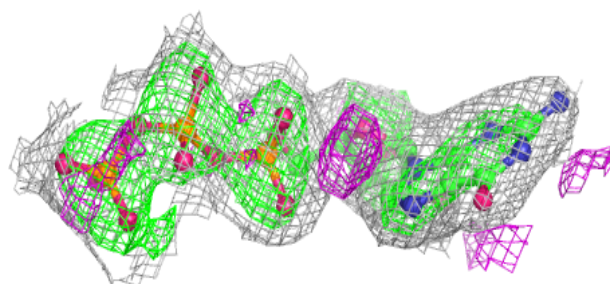
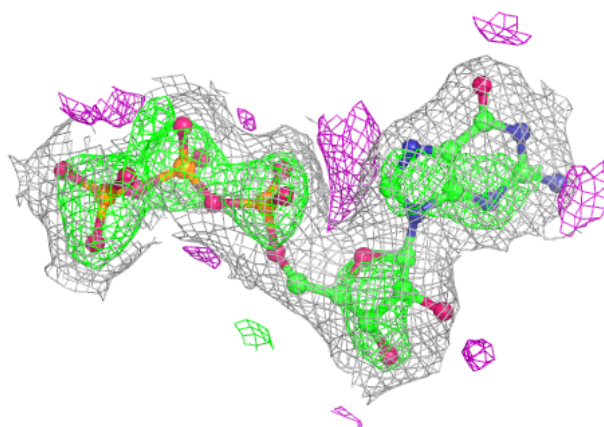
**Electron density around GDP D 501:**

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



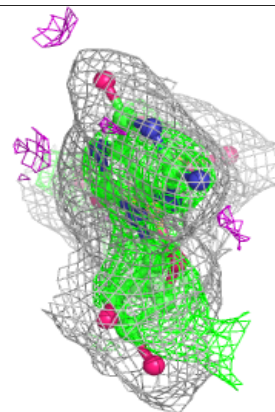
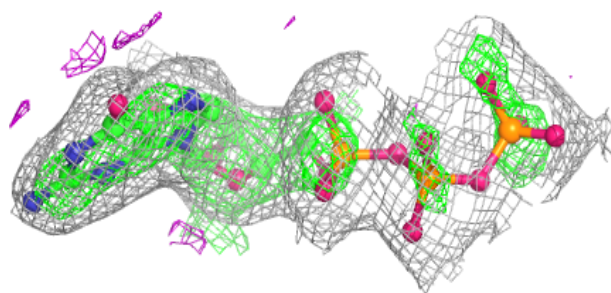
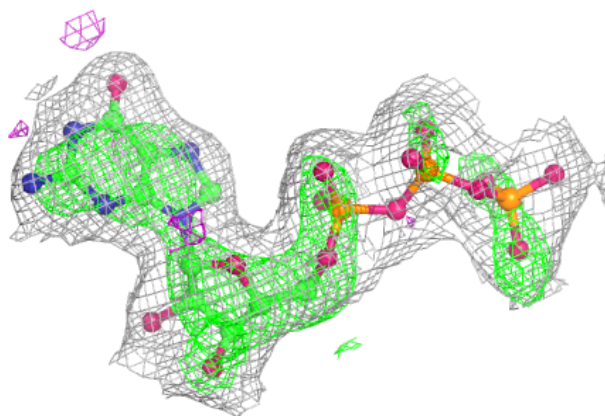
Electron density around GTP C 501:

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



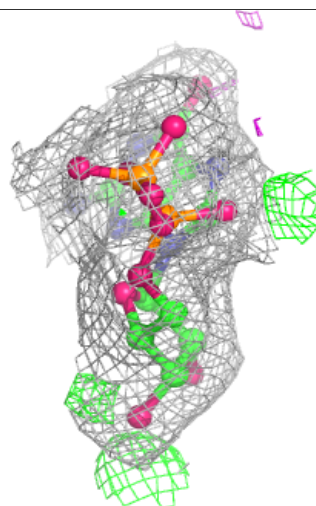
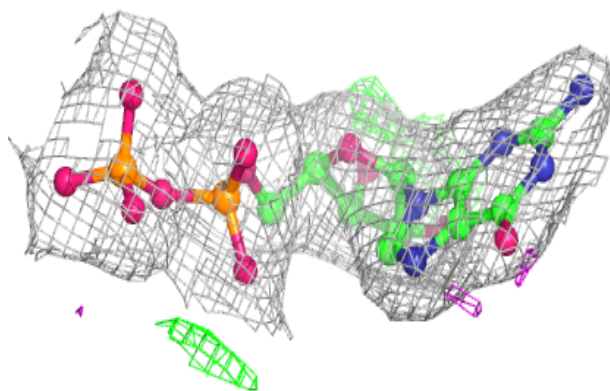
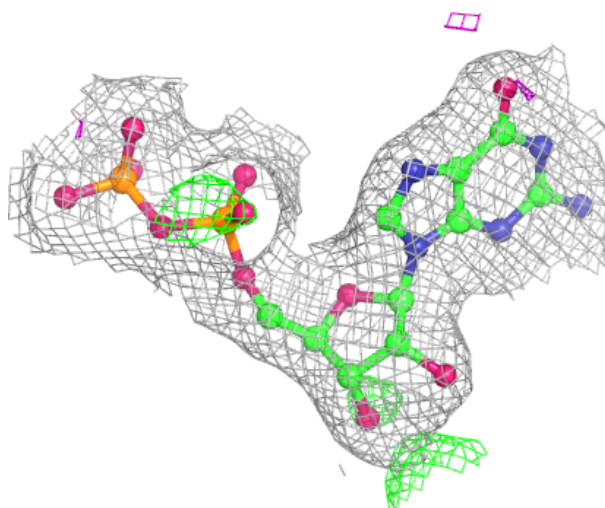
Electron density around GTP A 501:

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



Electron density around GDP B 501:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.