



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 08:31 PM UTC

PDB ID : 7CNN / pdb_00007cnn
Title : vinorelbine in complex with tubulin
Authors : Wang, Y.X.; Wu, C.Y.
Deposited on : 2020-08-02
Resolution : 2.50 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

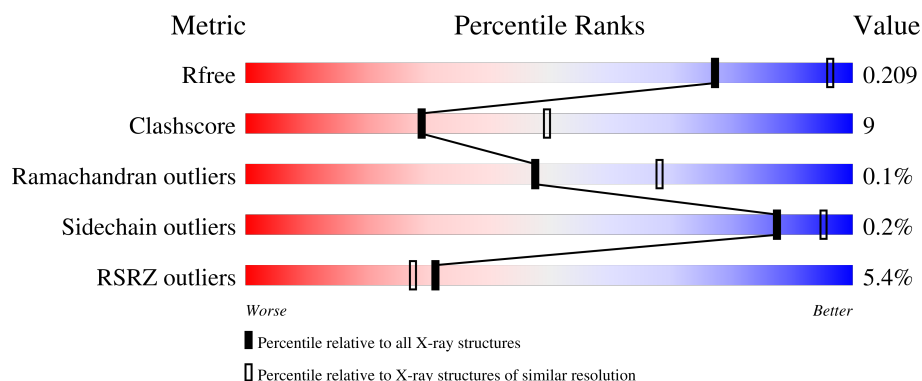
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	
1	C	451	
2	B	445	
2	D	445	
3	E	143	

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Mol	Chain	Length	Quality of chain
4	F	384	

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
10	MES	B	504	-	X	-	-
6	MG	B	506	-	-	-	X
7	CA	B	503	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 18183 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	438	Total	C	N	O	S	0	6	0
			3453	2186	587	656	24			
1	C	440	Total	C	N	O	S	0	8	0
			3463	2192	584	662	25			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	430	Total	C	N	O	S	0	4	0
			3398	2133	582	656	27			
2	D	420	Total	C	N	O	S	0	4	0
			3311	2082	561	641	27			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	122	Total	C	N	O	S	0	4	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

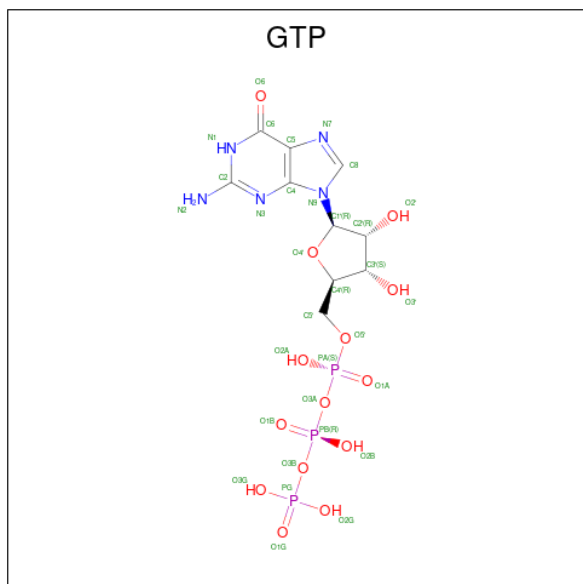
- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	350	Total	C	N	O	S	0	4	0
			2894	1860	496	523	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		
5	D	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	2	Total	Mg	0	0
			2	2		
6	C	1	Total	Mg	0	0
			1	1		

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

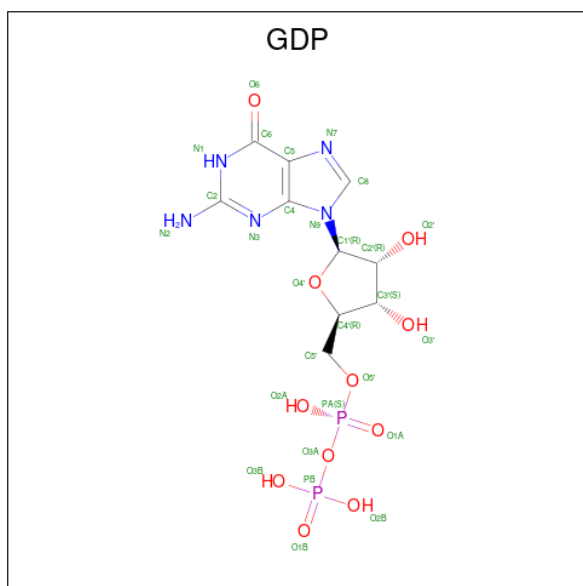
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

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

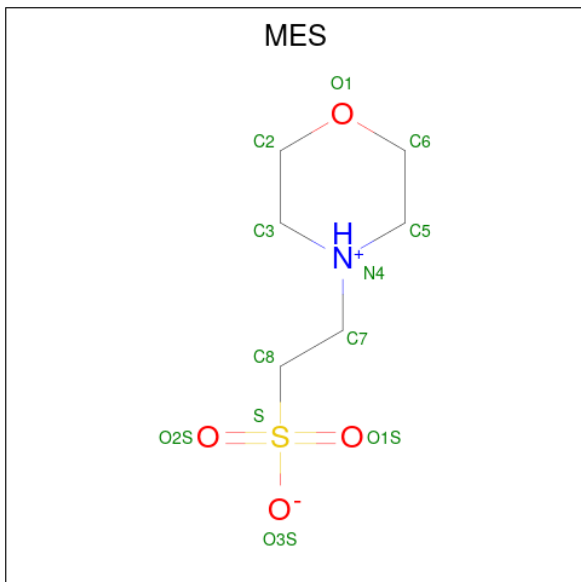
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		

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



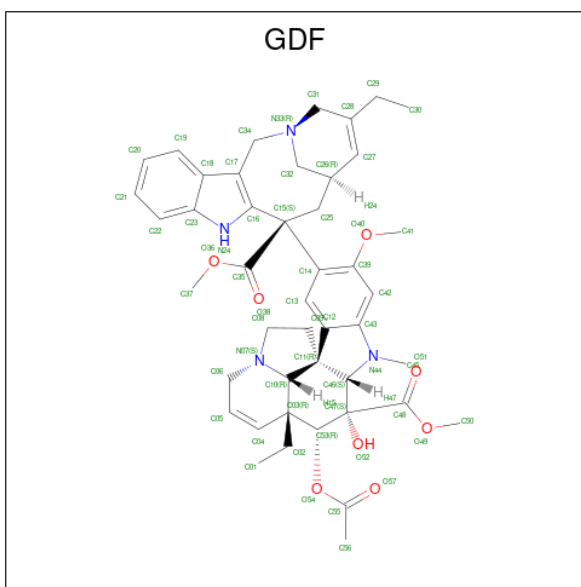
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- 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	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 Vinorelbine (CCD ID: GDF) (formula: $C_{45}H_{54}N_4O_8$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			57	45	4	8		

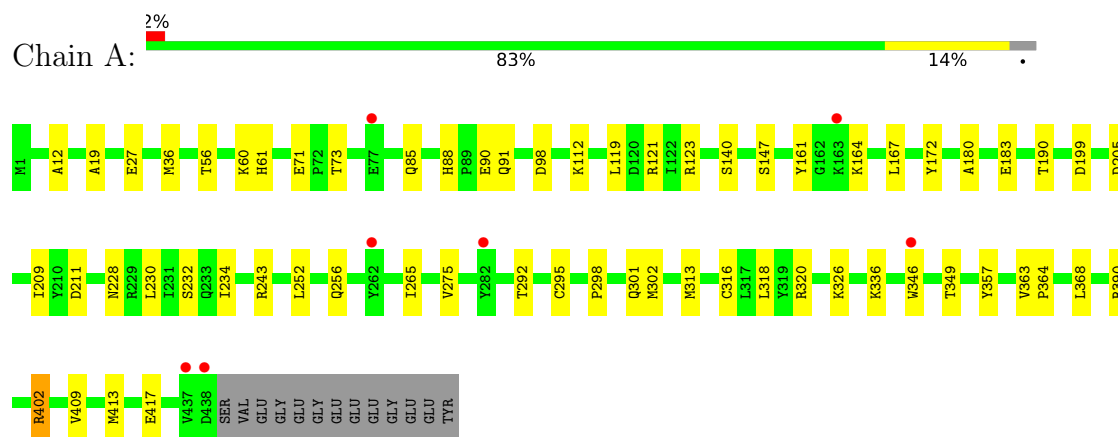
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	91	Total	O	0	0
			91	91		
12	B	87	Total	O	0	0
			87	87		
12	C	154	Total	O	0	0
			154	154		
12	D	34	Total	O	0	0
			34	34		
12	E	18	Total	O	0	0
			18	18		
12	F	34	Total	O	0	0
			34	34		

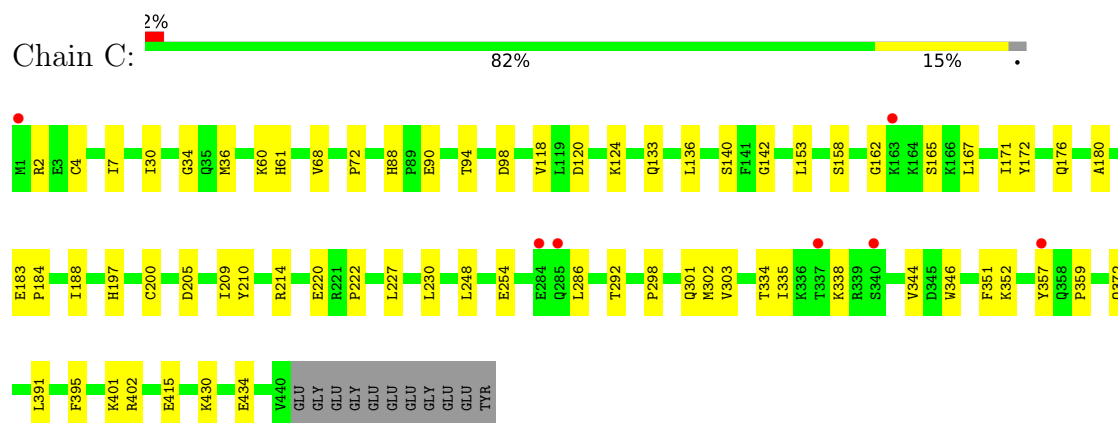
3 Residue-property plots [i](#)

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.

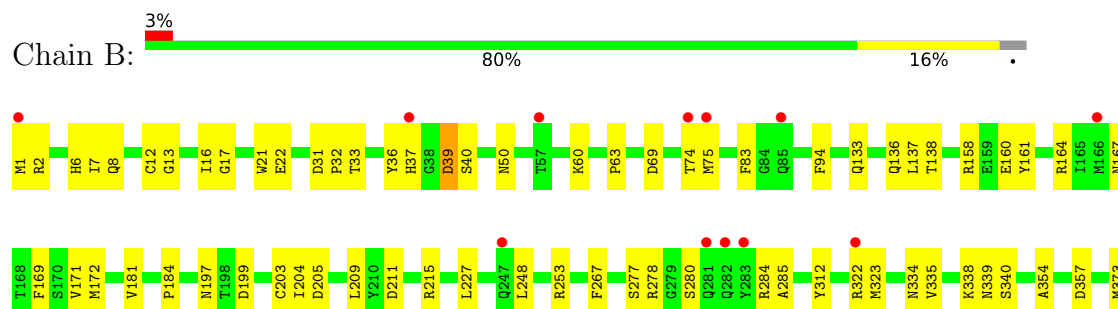
- Molecule 1: Tubulin alpha-1B chain

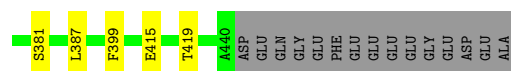


- Molecule 1: Tubulin alpha-1B chain

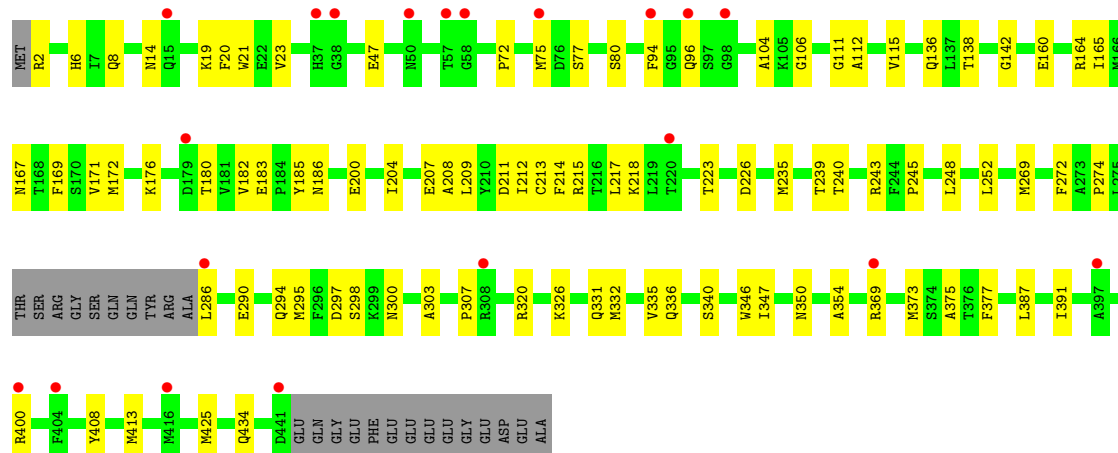
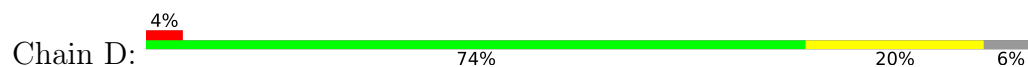


- Molecule 2: Tubulin beta chain

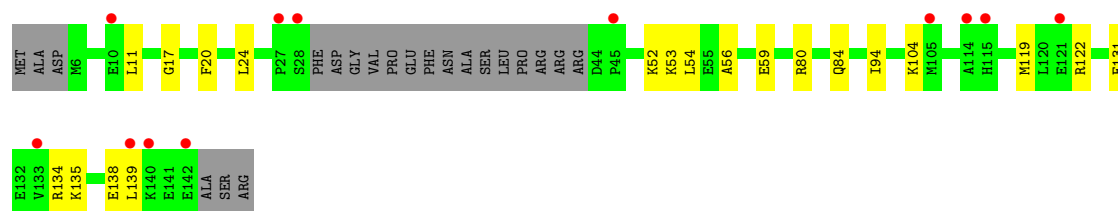




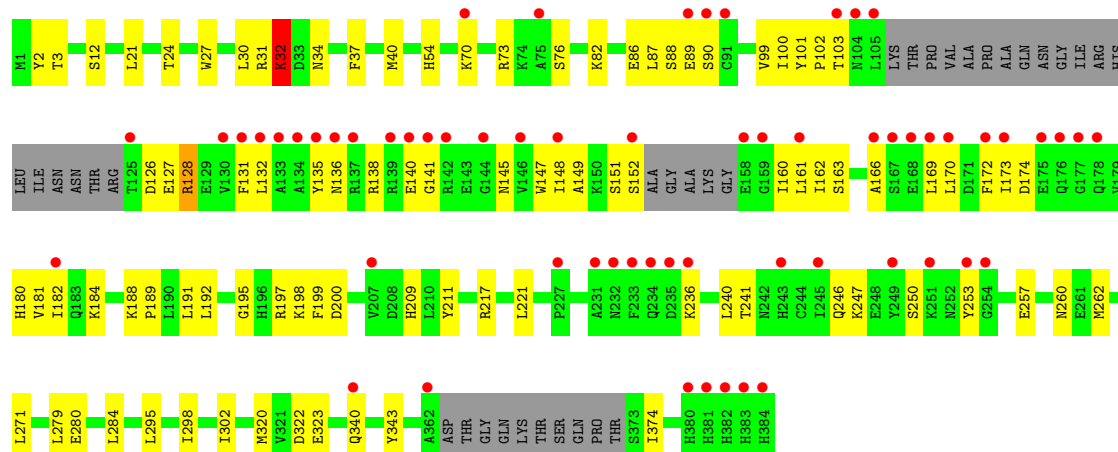
• Molecule 2: Tubulin beta chain



• 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	104.88Å 156.13Å 183.00Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.96 – 2.50 49.96 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.4 (49.96-2.50) 98.5 (49.96-2.50)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.08 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.199 , 0.229 (Not available) , 0.209	Depositor DCC
R_{free} test set	2000 reflections (1.91%)	wwPDB-VP
Wilson B-factor (Å ²)	38.1	Xtriage
Anisotropy	0.087	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 40.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18183	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.89% 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: CA, GDF, GDP, MES, GTP, CL, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.39	0/3549	0.60	1/4817 (0.0%)
1	C	0.53	0/3562	0.66	0/4836
2	B	0.52	0/3485	0.66	0/4720
2	D	0.45	0/3393	0.62	0/4597
3	E	0.47	0/1052	0.60	0/1396
4	F	0.46	0/2974	0.65	2/4018 (0.0%)
All	All	0.48	0/18015	0.64	3/24384 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	128	ARG	NE-CZ-NH1	-7.32	114.19	121.50
4	F	32	LYS	CB-CA-C	-5.57	99.34	110.42
1	A	402	ARG	CG-CD-NE	-5.32	100.31	112.00

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	3453	0	3378	41	0
1	C	3463	0	3382	49	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	3398	0	3284	60	0
2	D	3311	0	3194	61	0
3	E	1031	0	1052	16	0
4	F	2894	0	2867	80	0
5	A	32	0	12	0	0
5	C	32	0	12	1	0
5	D	32	0	12	0	0
6	A	1	0	0	0	0
6	B	2	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	B	1	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	A	1	0	0	0	0
9	B	28	0	12	1	0
10	B	24	0	24	6	0
11	B	57	0	0	5	0
12	A	91	0	0	2	0
12	B	87	0	0	1	0
12	C	154	0	0	2	0
12	D	34	0	0	3	0
12	E	18	0	0	2	0
12	F	34	0	0	2	0
All	All	18183	0	17229	303	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 9.

All (303) 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)
11:B:507:GDF:C03	11:B:507:GDF:C10	1.80	1.57
2:D:104:ALA:HB2	2:D:413:MET:HE2	1.49	0.93
3:E:52:LYS:HZ3	3:E:53:LYS:HE3	1.36	0.91
2:B:399:PHE:CE2	2:B:419:THR:HG22	2.10	0.86
2:B:399:PHE:HE2	2:B:419:THR:HG22	1.37	0.85
2:D:295:MET:HE3	2:D:375:ALA:HB1	1.61	0.80
2:D:408:TYR:HB3	2:D:413:MET:HE3	1.63	0.79
2:D:8:GLN:HE21	2:D:14:ASN:HA	1.52	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:47:GLU:HG2	2:D:245:PRO:HG3	1.71	0.72
2:B:1:MET:HE3	2:B:133:GLN:HB2	1.73	0.70
2:B:172:MET:HE2	2:B:387:LEU:HD21	1.72	0.70
4:F:99:VAL:N	4:F:127:GLU:OE1	2.20	0.70
2:D:8:GLN:NE2	2:D:14:ASN:HA	2.08	0.69
11:B:507:GDF:C10	11:B:507:GDF:C02	2.73	0.65
2:B:277:SER:HB2	2:B:280:SER:HB3	1.80	0.64
4:F:189:PRO:HG2	4:F:191:LEU:HD21	1.79	0.64
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.17	0.63
2:B:253:ARG:NH2	10:B:504:MES:O2S	2.26	0.63
2:D:240[B]:THR:HG21	2:D:320:ARG:HD2	1.81	0.63
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.34	0.62
2:D:295:MET:HG3	2:D:377:PHE:HB2	1.80	0.62
4:F:135:TYR:O	4:F:145:ASN:ND2	2.32	0.62
4:F:195:GLY:HA3	4:F:197:ARG:HD3	1.81	0.62
4:F:31:ARG:HE	4:F:31:ARG:HA	1.65	0.62
4:F:138:ARG:HG3	4:F:138:ARG:HH11	1.65	0.61
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.41	0.61
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.17	0.61
4:F:138:ARG:HG3	4:F:138:ARG:NH1	2.15	0.61
4:F:148:ILE:HG13	4:F:162:ILE:HG13	1.81	0.61
1:C:36:MET:HE3	1:C:61:HIS:CD2	2.36	0.60
1:C:188:ILE:HD13	1:C:395:PHE:HB2	1.83	0.60
4:F:199:PHE:O	4:F:320:MET:HE2	2.02	0.60
4:F:298:ILE:HD12	4:F:302:ILE:HD13	1.84	0.60
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.84	0.60
4:F:128:ARG:O	4:F:131:PHE:HB3	2.02	0.60
4:F:197:ARG:NH2	4:F:257:GLU:OE2	2.35	0.59
11:B:507:GDF:C10	11:B:507:GDF:C53	2.77	0.59
1:A:60:LYS:HZ1	1:A:85:GLN:HG2	1.68	0.59
2:D:176:LYS:NZ	2:D:207:GLU:OE2	2.27	0.59
1:C:188:ILE:CD1	1:C:395:PHE:HB2	2.32	0.59
4:F:246:GLN:OE1	4:F:260:ASN:ND2	2.36	0.59
2:B:415:GLU:HG3	12:B:604:HOH:O	2.03	0.59
4:F:163:SER:HB3	4:F:169:LEU:HD22	1.84	0.58
2:B:1:MET:HG2	2:B:133:GLN:HB3	1.85	0.58
3:E:104:LYS:NZ	12:E:302:HOH:O	2.33	0.58
2:D:142:GLY:O	2:D:186:ASN:ND2	2.25	0.58
4:F:151:SER:HB2	4:F:180:HIS:CE1	2.40	0.57
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.40	0.57
4:F:166:ALA:O	4:F:170:LEU:HB2	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.87	0.56
2:B:172:MET:HG3	2:B:387:LEU:HD21	1.88	0.56
1:C:430:LYS:CE	1:C:434:GLU:OE1	2.54	0.56
2:D:294:GLN:HA	2:D:297:ASP:HB2	1.87	0.56
4:F:103:THR:CG2	4:F:128:ARG:HH22	2.19	0.56
4:F:31:ARG:HA	4:F:31:ARG:NE	2.20	0.56
2:D:136:GLN:HA	2:D:167:ASN:O	2.06	0.56
2:D:290:GLU:O	2:D:294:GLN:HG2	2.06	0.56
1:C:30:ILE:HD11	1:C:36:MET:HE2	1.88	0.56
4:F:86:GLU:OE1	4:F:86:GLU:N	2.37	0.56
4:F:31:ARG:HD3	4:F:32:LYS:H	1.70	0.55
2:B:340[B]:SER:HG	4:F:34:ASN:HD21	1.50	0.55
4:F:209:HIS:ND1	12:F:402:HOH:O	2.32	0.55
2:B:36:TYR:O	2:B:37:HIS:ND1	2.40	0.55
1:C:176:GLN:OE1	1:C:176:GLN:N	2.37	0.55
4:F:103:THR:HG23	4:F:128:ARG:HH22	1.72	0.55
2:D:106:GLY:O	2:D:111:GLY:HA3	2.05	0.55
2:D:164:ARG:HD2	12:D:713:HOH:O	2.07	0.55
2:B:199:ASP:OD1	10:B:504:MES:H32	2.06	0.55
1:C:88:HIS:CE1	1:C:90:GLU:HG3	2.42	0.55
2:D:75:MET:HG3	2:D:94:PHE:HB3	1.89	0.55
2:D:171:VAL:HA	2:D:204:ILE:O	2.07	0.54
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.39	0.54
4:F:148:ILE:HD11	4:F:160:ILE:HG21	1.89	0.54
1:A:19:ALA:HB1	1:A:232:SER:OG	2.08	0.54
2:B:284:ARG:NH1	2:B:285:ALA:O	2.40	0.54
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.25	0.54
4:F:127:GLU:O	4:F:131:PHE:N	2.38	0.54
2:D:2:ARG:HH11	2:D:2:ARG:HB3	1.73	0.53
1:A:112:LYS:HE2	3:E:54:LEU:HB3	1.91	0.53
4:F:192:LEU:HD13	4:F:262:MET:HE1	1.90	0.53
4:F:82:LYS:HE3	4:F:127:GLU:OE2	2.08	0.53
2:B:50[B]:ASN:H	2:B:50[B]:ASN:ND2	2.07	0.53
2:B:138:THR:HG22	2:B:169:PHE:HB2	1.89	0.53
2:D:248:LEU:HD23	2:D:354:ALA:HB2	1.90	0.53
4:F:160:ILE:HG22	4:F:161:LEU:H	1.74	0.53
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.90	0.53
2:B:69:ASP:OD2	2:B:74:THR:OG1	2.21	0.52
2:B:211:ASP:HB3	2:B:215:ARG:HH12	1.74	0.52
1:C:34:GLY:HA3	1:C:60:LYS:HG3	1.91	0.52
4:F:136:ASN:O	4:F:140:GLU:N	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:145:ASN:OD1	4:F:147:TRP:NE1	2.36	0.52
11:B:507:GDF:C03	11:B:507:GDF:C11	2.70	0.52
2:B:322:ARG:NH2	2:B:357:ASP:OD1	2.42	0.52
1:A:326:LYS:HD3	1:A:326:LYS:C	2.35	0.52
1:A:209:ILE:HD11	1:A:302:MET:SD	2.50	0.52
2:D:214:PHE:O	2:D:218:LYS:HA	2.10	0.52
2:B:340[B]:SER:OG	4:F:34:ASN:ND2	2.29	0.51
1:C:120[B]:ASP:OD2	1:C:124:LYS:NZ	2.43	0.51
2:B:335:VAL:HG13	10:B:505:MES:H21	1.92	0.51
3:E:135:LYS:O	3:E:139:LEU:HD13	2.10	0.51
1:A:265:ILE:HG21	1:A:313:MET:HE1	1.93	0.51
3:E:52:LYS:HZ3	3:E:53:LYS:CE	2.18	0.51
4:F:247:LYS:HB3	4:F:253:TYR:CE1	2.46	0.51
4:F:70:LYS:HD2	4:F:76:SER:HB3	1.93	0.51
4:F:140:GLU:HG2	4:F:141:GLY:N	2.26	0.51
2:B:136:GLN:HA	2:B:167:ASN:O	2.11	0.51
2:B:31:ASP:OD1	2:B:33:THR:OG1	2.26	0.50
4:F:101:TYR:HD2	4:F:126:ASP:HB2	1.76	0.50
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.93	0.50
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.92	0.50
2:B:75:MET:HE1	2:B:94:PHE:HB3	1.93	0.50
1:C:188:ILE:HD13	1:C:395:PHE:CB	2.42	0.50
2:B:199:ASP:CG	10:B:504:MES:H32	2.36	0.50
1:C:210:TYR:CE1	1:C:214:ARG:HD2	2.46	0.50
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.47	0.50
4:F:132:LEU:HA	4:F:135:TYR:HB3	1.93	0.50
1:C:286:LEU:H	1:C:286:LEU:HD12	1.77	0.49
1:C:430:LYS:HD3	1:C:434:GLU:CD	2.37	0.49
2:D:19:LYS:O	2:D:23:VAL:HG23	2.12	0.49
2:B:323:MET:HB3	2:B:373:MET:HE1	1.95	0.49
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.78	0.49
3:E:131:GLU:HG2	3:E:134:ARG:HH21	1.77	0.49
4:F:3:THR:HB	4:F:30:LEU:HD11	1.95	0.49
2:B:172:MET:HE2	2:B:387:LEU:CD2	2.40	0.49
2:D:434:GLN:O	12:D:701:HOH:O	2.20	0.49
2:D:331:GLN:O	2:D:335:VAL:HG23	2.12	0.49
3:E:84:GLN:NE2	12:E:305:HOH:O	2.46	0.49
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.95	0.48
1:C:372:GLN:NE2	12:C:603:HOH:O	2.25	0.48
1:C:209:ILE:HD11	1:C:302:MET:HG3	1.95	0.48
1:C:334:THR:HG23	1:C:338:LYS:HD2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:199:PHE:CD2	4:F:221:LEU:HG	2.49	0.48
1:A:27:GLU:OE2	1:A:243:ARG:NH2	2.34	0.48
2:B:334:ASN:HD21	2:B:338:LYS:HE2	1.78	0.48
1:C:430:LYS:HD3	1:C:434:GLU:OE1	2.13	0.48
2:D:72:PRO:HG3	2:D:96:GLN:HA	1.96	0.48
4:F:200:ASP:OD2	4:F:241:THR:OG1	2.29	0.48
4:F:138:ARG:HH12	4:F:184:LYS:HD3	1.79	0.48
2:B:69:ASP:O	2:B:94:PHE:HA	2.14	0.48
1:A:346:TRP:H	1:A:346:TRP:CD1	2.31	0.47
2:D:167:ASN:HD22	2:D:200:GLU:HG3	1.79	0.47
2:D:208:ALA:O	2:D:212:ILE:HG13	2.14	0.47
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.49	0.47
4:F:103:THR:HG23	4:F:128:ARG:HH12	1.79	0.47
2:B:1:MET:HE3	2:B:133:GLN:CB	2.44	0.47
2:B:203:CYS:SG	2:B:267:PHE:HB3	2.54	0.47
1:C:158:SER:OG	1:C:197:HIS:ND1	2.43	0.47
1:A:230:LEU:O	1:A:234:ILE:HD12	2.15	0.47
1:A:292:THR:O	1:A:295:CYS:HB2	2.15	0.47
2:B:12:CYS:HB2	9:B:501:GDP:C8	2.49	0.47
2:D:272:PHE:O	2:D:300:ASN:HB3	2.15	0.47
4:F:88:SER:OG	4:F:90:SER:O	2.33	0.47
2:D:180:THR:HB	2:D:183:GLU:OE1	2.15	0.47
4:F:151:SER:OG	4:F:152:SER:N	2.48	0.47
1:A:167:LEU:HD13	1:A:252:LEU:HD22	1.97	0.47
2:B:75:MET:CE	2:B:94:PHE:HB3	2.45	0.47
4:F:160:ILE:HG22	4:F:161:LEU:N	2.29	0.47
1:C:430:LYS:O	1:C:434:GLU:HG3	2.15	0.47
2:B:22:GLU:HG2	2:B:83:PHE:CD1	2.50	0.46
1:C:401:LYS:HG3	2:D:346:TRP:CE3	2.50	0.46
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.78	0.46
1:C:88:HIS:HE1	1:C:90:GLU:HG3	1.80	0.46
1:C:430:LYS:NZ	1:C:434:GLU:OE1	2.47	0.46
2:D:211:ASP:HB3	2:D:215:ARG:HD2	1.98	0.46
4:F:247:LYS:HE3	4:F:247:LYS:HB2	1.68	0.46
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.16	0.46
1:A:275:VAL:HG13	1:A:368:LEU:HD21	1.98	0.46
1:C:68:VAL:HG21	1:C:118:VAL:HG21	1.98	0.46
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.51	0.45
1:C:142:GLY:HA3	1:C:183:GLU:OE2	2.17	0.45
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.98	0.45
1:A:298:PRO:HA	1:A:301:GLN:CD	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:160:GLU:HG2	2:B:161:TYR:CE1	2.49	0.45
1:A:228:ASN:O	1:A:232:SER:OG	2.31	0.45
2:D:223:THR:HG23	2:D:226:ASP:H	1.81	0.45
2:B:1:MET:HE1	2:B:253:ARG:H	1.81	0.45
2:D:2:ARG:HB3	2:D:2:ARG:NH1	2.31	0.45
2:D:239:THR:O	2:D:243:ARG:HG3	2.17	0.45
4:F:188:LYS:HE2	4:F:323:GLU:OE2	2.17	0.45
4:F:169:LEU:H	4:F:169:LEU:HD23	1.80	0.45
4:F:126:ASP:OD1	4:F:127:GLU:N	2.49	0.45
1:A:147:SER:HB2	1:A:190:THR:HB	1.99	0.45
1:A:199:ASP:HB3	1:A:256:GLN:HG2	1.99	0.45
4:F:149:ALA:HA	4:F:181:VAL:O	2.17	0.45
4:F:169:LEU:O	4:F:172:PHE:HB3	2.16	0.45
1:A:316[B]:CYS:SG	1:A:318:LEU:HD21	2.57	0.45
2:B:158:ARG:NH1	2:B:197:ASN:OD1	2.49	0.45
3:E:56:ALA:O	3:E:59:GLU:HG3	2.16	0.45
3:E:134:ARG:O	3:E:138:GLU:HG3	2.16	0.45
1:A:211:ASP:HB3	12:A:602:HOH:O	2.15	0.45
2:D:298:SER:HB2	2:D:307:PRO:HD2	1.97	0.45
2:D:391:ILE:HG22	2:D:425:MET:HE1	1.99	0.45
2:B:33:THR:O	2:B:60:LYS:HE3	2.17	0.45
2:B:322:ARG:HD2	2:B:322:ARG:HA	1.78	0.44
1:C:2:ARG:HB3	1:C:133:GLN:HB2	1.99	0.44
2:D:215:ARG:O	2:D:218:LYS:HE2	2.17	0.44
2:D:369:ARG:HA	2:D:369:ARG:HD2	1.61	0.44
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.53	0.44
4:F:100:ILE:HD12	4:F:128:ARG:HA	1.98	0.44
4:F:169:LEU:HA	4:F:172:PHE:HB3	1.99	0.44
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.99	0.44
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.52	0.44
2:D:320:ARG:O	2:D:373:MET:HA	2.18	0.44
2:D:167:ASN:ND2	2:D:200:GLU:HG3	2.33	0.44
4:F:12:SER:OG	12:F:401:HOH:O	2.21	0.44
2:D:20:PHE:CD1	2:D:235:MET:HE2	2.53	0.44
4:F:82:LYS:HG2	4:F:89:GLU:CD	2.43	0.44
4:F:211:TYR:OH	4:F:295:LEU:O	2.34	0.44
2:B:181:VAL:O	2:B:184:PRO:HD2	2.18	0.44
2:D:269:MET:HG3	2:D:303:ALA:HB3	2.00	0.44
4:F:340:GLN:HA	4:F:343:TYR:CD2	2.53	0.43
4:F:102:PRO:HA	4:F:174:ASP:OD1	2.18	0.43
4:F:198:LYS:HG2	4:F:199:PHE:H	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:71:GLU:HB3	1:A:98:ASP:HB3	1.99	0.43
1:C:205:ASP:HB2	1:C:303:VAL:HA	1.99	0.43
2:D:332:MET:O	2:D:336:GLN:HG3	2.18	0.43
1:A:336:LYS:HE3	1:A:349:THR:HG21	2.00	0.43
2:B:16:ILE:HG13	2:B:17:GLY:N	2.32	0.43
2:B:36:TYR:OH	2:B:40:SER:O	2.35	0.43
2:B:205:ASP:O	2:B:209:LEU:HG	2.18	0.43
1:C:167:LEU:HG	1:C:200:CYS:HB3	2.00	0.43
3:E:119:MET:HA	3:E:122:ARG:NH2	2.33	0.43
4:F:87:LEU:O	4:F:88:SER:OG	2.29	0.43
1:C:98:ASP:HB2	5:C:501:GTP:O2G	2.19	0.43
1:C:140:SER:HA	1:C:171:ILE:HB	2.01	0.43
1:C:184:PRO:O	1:C:188:ILE:HD12	2.19	0.43
2:D:373:MET:HB3	2:D:373:MET:HE2	1.72	0.43
4:F:173:ILE:HD11	4:F:182:ILE:HD11	2.00	0.43
3:E:11:LEU:HD12	3:E:20:PHE:HB3	2.01	0.43
1:C:220:GLU:HG2	2:D:326:LYS:HD3	2.00	0.43
1:C:359:PRO:HB2	12:C:641:HOH:O	2.19	0.43
2:B:7:ILE:O	2:B:137:LEU:HA	2.18	0.42
2:B:171:VAL:HA	2:B:204:ILE:O	2.20	0.42
2:B:172:MET:HB2	2:B:205:ASP:HA	2.02	0.42
1:C:180:ALA:O	1:C:183:GLU:HG3	2.18	0.42
4:F:247:LYS:HB3	4:F:253:TYR:CZ	2.54	0.42
2:B:339:ASN:HB3	10:B:505:MES:H61	2.00	0.42
2:D:75:MET:HG3	2:D:94:PHE:CG	2.54	0.42
2:D:180:THR:O	2:D:183:GLU:HG3	2.18	0.42
2:B:8:GLN:HB2	2:B:13:GLY:O	2.20	0.42
1:C:205:ASP:CB	1:C:303:VAL:HA	2.50	0.42
4:F:149:ALA:HB2	4:F:169:LEU:HD12	2.02	0.42
4:F:322:ASP:C	4:F:322:ASP:OD1	2.62	0.42
2:B:278:ARG:HE	2:B:278:ARG:HB2	1.59	0.42
1:C:298:PRO:HA	1:C:301:GLN:OE1	2.19	0.42
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.50	0.42
2:D:213:CYS:HA	2:D:217:LEU:HB2	2.02	0.42
1:A:56:THR:OG1	1:A:60:LYS:HB3	2.20	0.42
1:A:90:GLU:HA	1:A:121:ARG:NH1	2.35	0.42
1:A:161:TYR:HB3	1:A:164:LYS:CG	2.50	0.42
1:A:161:TYR:HB3	1:A:164:LYS:HG3	2.02	0.42
1:A:336:LYS:HD3	3:E:24:LEU:HD12	2.02	0.42
2:D:77:SER:O	2:D:80:SER:HB3	2.19	0.42
2:D:112:ALA:O	2:D:115:VAL:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:73:ARG:HG3	4:F:73:ARG:HH11	1.85	0.42
2:B:2:ARG:HB2	2:B:2:ARG:NH1	2.35	0.41
2:B:248:LEU:HD23	2:B:354:ALA:HB2	2.01	0.41
2:D:75:MET:HG3	2:D:94:PHE:CB	2.49	0.41
4:F:99:VAL:O	4:F:100:ILE:HD13	2.20	0.41
1:A:12:ALA:HB3	1:A:140:SER:HB3	2.02	0.41
1:A:390[A]:ARG:HD2	4:F:54:HIS:CD2	2.55	0.41
2:D:182:VAL:O	2:D:185:TYR:HB2	2.20	0.41
1:A:88:HIS:N	1:A:91:GLN:OE1	2.27	0.41
1:A:123:ARG:HA	1:A:123:ARG:HD3	1.85	0.41
1:C:402:ARG:HE	1:C:415:GLU:CD	2.28	0.41
4:F:169:LEU:O	4:F:170:LEU:C	2.63	0.41
4:F:246:GLN:O	4:F:250:SER:HB2	2.21	0.41
4:F:279:LEU:HG	4:F:284:LEU:HG	2.01	0.41
2:B:312:TYR:CD1	2:B:381:SER:HB2	2.55	0.41
11:B:507:GDF:C10	11:B:507:GDF:C04	2.64	0.41
1:A:180:ALA:O	1:A:183:GLU:HG3	2.21	0.41
2:B:209:LEU:HB3	2:B:227:LEU:HG	2.03	0.41
1:A:320:ARG:HG3	12:A:618:HOH:O	2.20	0.41
2:B:31:ASP:HB2	2:B:32:PRO:HD2	2.02	0.41
1:C:72:PRO:HA	1:C:94:THR:HG21	2.03	0.41
1:C:351:PHE:CD1	1:C:351:PHE:N	2.88	0.41
2:D:295:MET:CE	2:D:375:ALA:HB1	2.42	0.41
3:E:135:LYS:HD2	3:E:135:LYS:HA	1.81	0.41
4:F:86:GLU:H	4:F:86:GLU:CD	2.26	0.41
4:F:236:LYS:O	4:F:240:LEU:HB2	2.20	0.41
1:A:209:ILE:HG23	1:A:209:ILE:HD12	1.68	0.41
1:A:409:VAL:HA	1:A:413:MET:O	2.21	0.41
2:D:138:THR:HG22	2:D:169:PHE:HB2	2.03	0.41
2:D:165:ILE:HG21	2:D:252:LEU:HB3	2.02	0.41
2:D:400:ARG:HA	2:D:400:ARG:HD3	1.69	0.41
3:E:80:ARG:HH11	3:E:80:ARG:HD2	1.73	0.41
4:F:217:ARG:HG2	4:F:374:ILE:O	2.21	0.41
1:A:363:VAL:HA	1:A:364:PRO:HD3	1.96	0.41
2:B:158:ARG:CZ	10:B:504:MES:H21	2.51	0.41
2:D:204:ILE:CG2	2:D:209:LEU:HD11	2.50	0.41
4:F:21:LEU:O	4:F:24:THR:OG1	2.32	0.41
4:F:101:TYR:HD2	4:F:126:ASP:CB	2.34	0.40
1:C:162:GLY:HA2	3:E:94:ILE:HD11	2.03	0.40
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.04	0.40
4:F:2:TYR:HB2	4:F:27:TRP:CD2	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:184:LYS:HD2	4:F:184:LYS:HA	1.85	0.40
2:D:160:GLU:OE2	12:D:702:HOH:O	2.22	0.40
2:B:164[B]:ARG:HA	2:B:164[B]:ARG:HD2	1.91	0.40
2:D:274:PRO:HB3	2:D:286:LEU:HD22	2.04	0.40
2:D:347:ILE:HG22	2:D:350:ASN:HB3	2.03	0.40
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.56	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	442/451 (98%)	430 (97%)	12 (3%)	0	100	100
1	C	445/451 (99%)	437 (98%)	8 (2%)	0	100	100
2	B	432/445 (97%)	417 (96%)	15 (4%)	0	100	100
2	D	419/445 (94%)	404 (96%)	14 (3%)	1 (0%)	43	63
3	E	122/143 (85%)	118 (97%)	4 (3%)	0	100	100
4	F	346/384 (90%)	323 (93%)	22 (6%)	1 (0%)	36	55
All	All	2206/2319 (95%)	2129 (96%)	75 (3%)	2 (0%)	48	68

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	F	32	LYS
2	D	340	SER

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	236/379 (62%)	235 (100%)	1 (0%)	84	93
1	C	378/379 (100%)	376 (100%)	2 (0%)	81	92
2	B	374/383 (98%)	372 (100%)	2 (0%)	81	92
2	D	366/383 (96%)	366 (100%)	0	100	100
3	E	114/127 (90%)	114 (100%)	0	100	100
4	F	319/342 (93%)	317 (99%)	2 (1%)	78	91
All	All	1787/1993 (90%)	1780 (100%)	7 (0%)	87	93

All (7) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	402	ARG
2	B	39[A]	ASP
2	B	39[B]	ASP
1	C	165[A]	SER
1	C	165[B]	SER
4	F	271[A]	LEU
4	F	271[B]	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	301	GLN
1	A	358	GLN
2	B	8	GLN
2	B	11	GLN
2	B	15	GLN
2	B	136	GLN
2	B	229	HIS
2	B	300	ASN
2	B	349	ASN
1	C	285	GLN

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Mol	Chain	Res	Type
1	C	293	ASN
2	D	8	GLN
2	D	14	ASN
2	D	91	ASN
2	D	167	ASN
2	D	197	ASN
2	D	337	ASN
2	D	426	ASN
2	D	436	GLN
3	E	92	ASN
3	E	103	GLN
4	F	340	GLN

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 17 ligands modelled in this entry, 10 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	$\# Z > 2$
5	GTP	C	501	6	33,34,34	1.04	1 (3%)	50,54,54	1.60	9 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GTP	D	602	6	33,34,34	0.91	1 (3%)	50,54,54	1.70	10 (20%)
9	GDP	B	501	6	29,30,30	1.18	2 (6%)	45,47,47	1.87	11 (24%)
10	MES	B	504	-	12,12,12	2.31	4 (33%)	15,16,16	2.90	10 (66%)
5	GTP	A	501	6	33,34,34	1.35	5 (15%)	50,54,54	1.56	9 (18%)
10	MES	B	505	-	12,12,12	2.48	1 (8%)	15,16,16	2.34	6 (40%)
11	GDF	B	507	-	61,65,65	4.67	29 (47%)	77,104,104	3.42	39 (50%)

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	-	6/22/38/38	0/3/3/3
5	GTP	D	602	6	-	5/22/38/38	0/3/3/3
9	GDP	B	501	6	-	5/16/32/32	0/3/3/3
10	MES	B	504	-	-	4/6/14/14	0/1/1/1
5	GTP	A	501	6	-	5/22/38/38	0/3/3/3
10	MES	B	505	-	-	2/6/14/14	0/1/1/1
11	GDF	B	507	-	-	4/30/127/127	0/7/9/9

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	507	GDF	C43-C12	13.31	1.54	1.39
11	B	507	GDF	C43-N44	12.24	1.60	1.39
11	B	507	GDF	C03-C10	11.60	1.80	1.53
11	B	507	GDF	C03-C04	-9.92	1.33	1.51
11	B	507	GDF	C47-C46	-9.40	1.21	1.56
11	B	507	GDF	C04-C05	8.88	1.48	1.32
11	B	507	GDF	O52-C47	8.86	1.58	1.42
10	B	505	MES	C8-S	-7.75	1.66	1.77
11	B	507	GDF	C31-C28	7.75	1.64	1.50
11	B	507	GDF	C25-C26	6.40	1.59	1.54
11	B	507	GDF	C39-C14	6.20	1.51	1.39
11	B	507	GDF	C16-C17	5.78	1.46	1.37
11	B	507	GDF	C09-C11	-5.62	1.43	1.55
11	B	507	GDF	O36-C35	5.55	1.43	1.33
11	B	507	GDF	C31-N33	5.53	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	507	GDF	C13-C14	5.50	1.47	1.39
11	B	507	GDF	C11-C12	-5.38	1.43	1.51
10	B	504	MES	C8-S	-5.22	1.70	1.77
11	B	507	GDF	O54-C53	-4.41	1.35	1.44
11	B	507	GDF	C15-C16	4.38	1.61	1.52
11	B	507	GDF	O49-C48	4.24	1.41	1.33
11	B	507	GDF	C42-C39	4.08	1.45	1.38
11	B	507	GDF	O40-C39	4.05	1.43	1.37
10	B	504	MES	O1S-S	3.94	1.56	1.45
5	A	501	GTP	PA-O3A	3.79	1.63	1.59
10	B	504	MES	O2S-S	3.67	1.55	1.45
5	A	501	GTP	PB-O3A	3.53	1.63	1.59
11	B	507	GDF	O54-C55	3.42	1.42	1.35
11	B	507	GDF	C46-N44	3.37	1.54	1.47
11	B	507	GDF	C32-N33	-3.35	1.41	1.46
9	B	501	GDP	C5-C4	3.21	1.47	1.38
11	B	507	GDF	C16-N24	-2.93	1.33	1.38
11	B	507	GDF	C11-C10	-2.88	1.45	1.55
11	B	507	GDF	C15-C35	2.76	1.57	1.53
5	A	501	GTP	PB-O3B	2.63	1.62	1.59
10	B	504	MES	O3S-S	2.29	1.55	1.47
5	A	501	GTP	O4'-C4'	-2.26	1.40	1.45
5	D	602	GTP	C2-N3	2.25	1.38	1.33
11	B	507	GDF	C56-C55	2.14	1.56	1.49
11	B	507	GDF	C22-C23	2.11	1.43	1.39
9	B	501	GDP	C5-N7	-2.07	1.34	1.39
5	C	501	GTP	C5-N7	-2.06	1.34	1.39
5	A	501	GTP	C5-N7	-2.01	1.35	1.39

All (94) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	507	GDF	C47-C46-N44	12.19	129.59	112.81
11	B	507	GDF	C43-N44-C46	-11.61	93.01	108.99
11	B	507	GDF	C11-C10-C03	-8.14	112.16	118.20
11	B	507	GDF	C45-N44-C46	8.02	138.55	119.14
10	B	504	MES	C5-N4-C3	7.19	124.33	108.84
11	B	507	GDF	O40-C39-C14	7.11	123.63	116.59
11	B	507	GDF	C53-O54-C55	-6.55	107.72	117.65
11	B	507	GDF	C10-C03-C04	5.80	114.06	108.27
9	B	501	GDP	C5-C4-N3	-5.49	119.66	128.39
11	B	507	GDF	C26-C32-N33	5.38	118.25	110.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	602	GTP	C5-C4-N3	-5.11	120.26	128.39
11	B	507	GDF	O49-C48-C47	4.94	120.34	112.21
5	D	602	GTP	C2-N3-C4	4.94	120.81	112.30
9	B	501	GDP	C2-N3-C4	4.93	120.78	112.30
10	B	504	MES	O2S-S-C8	4.91	114.14	106.73
5	A	501	GTP	C5-C4-N3	-4.80	120.75	128.39
10	B	505	MES	C5-N4-C3	4.77	119.12	108.84
5	C	501	GTP	C2-N3-C4	4.59	120.20	112.30
11	B	507	GDF	O36-C35-C15	4.58	118.60	111.21
10	B	505	MES	O1S-S-C8	4.57	113.63	106.73
9	B	501	GDP	N9-C4-N3	4.49	134.94	125.95
11	B	507	GDF	O40-C39-C42	-4.35	116.58	124.08
11	B	507	GDF	O54-C55-C56	4.31	118.77	111.09
5	C	501	GTP	C5-C4-N3	-4.28	121.58	128.39
11	B	507	GDF	O54-C53-C47	4.26	112.95	106.29
5	A	501	GTP	C2-N3-C4	4.25	119.62	112.30
11	B	507	GDF	C09-C11-C12	-4.00	105.09	112.36
9	B	501	GDP	C6-C5-N7	3.77	137.15	130.29
11	B	507	GDF	O52-C47-C46	3.51	120.07	108.08
5	D	602	GTP	N9-C4-N3	3.49	132.93	125.95
11	B	507	GDF	C53-C47-C46	-3.32	102.39	109.23
11	B	507	GDF	C17-C16-N24	-3.31	106.44	109.95
10	B	504	MES	O1-C6-C5	-3.30	104.66	111.77
11	B	507	GDF	C06-N07-C10	3.22	120.63	112.48
5	A	501	GTP	C2-N1-C6	-3.19	119.32	125.11
11	B	507	GDF	C13-C14-C39	3.12	121.23	116.80
5	C	501	GTP	N9-C8-N7	-3.08	107.69	113.40
5	D	602	GTP	C2-N1-C6	-3.05	119.57	125.11
11	B	507	GDF	C06-N07-C08	2.96	126.60	116.36
5	D	602	GTP	N9-C8-N7	-2.93	107.97	113.40
10	B	505	MES	C7-N4-C3	2.87	118.90	111.24
11	B	507	GDF	C03-C10-N07	2.87	117.76	111.72
9	B	501	GDP	O6-C6-C5	-2.85	119.00	126.53
5	A	501	GTP	N9-C8-N7	-2.85	108.12	113.40
5	A	501	GTP	N9-C4-N3	2.84	131.63	125.95
5	D	602	GTP	C5-C6-N1	2.83	120.46	113.25
5	C	501	GTP	O2B-PB-O3A	2.82	114.89	107.27
9	B	501	GDP	O2A-PA-O3A	2.81	114.88	107.27
11	B	507	GDF	C12-C11-C46	-2.78	97.78	102.11
11	B	507	GDF	C22-C23-C18	-2.67	119.60	122.19
5	C	501	GTP	N9-C4-N3	2.66	131.28	125.95
10	B	504	MES	C7-N4-C5	2.66	118.33	111.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C8-N7-C5	2.66	109.00	104.26
5	C	501	GTP	C2-N1-C6	-2.64	120.31	125.11
5	D	602	GTP	C8-N7-C5	2.61	108.92	104.26
11	B	507	GDF	O49-C48-O51	-2.61	119.46	123.95
11	B	507	GDF	C47-C46-C11	2.61	119.57	114.18
11	B	507	GDF	C03-C04-C05	-2.58	118.38	123.88
11	B	507	GDF	C12-C43-N44	-2.57	108.12	110.93
5	C	501	GTP	C8-N7-C5	2.54	108.79	104.26
11	B	507	GDF	O51-C48-C47	-2.50	120.08	123.92
10	B	504	MES	C6-O1-C2	2.50	117.96	109.88
10	B	505	MES	C2-C3-N4	-2.49	106.34	110.12
11	B	507	GDF	C46-C11-C10	2.48	118.26	114.07
11	B	507	GDF	C15-C16-N24	2.48	126.09	119.98
11	B	507	GDF	C09-C11-C10	2.45	107.07	101.85
5	C	501	GTP	O6-C6-C5	-2.45	120.06	126.53
9	B	501	GDP	C4-C5-N7	-2.44	106.80	110.67
5	A	501	GTP	C5-C6-N1	2.43	119.44	113.25
9	B	501	GDP	C5-C6-N1	2.37	119.30	113.25
11	B	507	GDF	C06-C05-C04	2.36	126.80	123.13
5	D	602	GTP	O6-C6-C5	-2.36	120.31	126.53
10	B	505	MES	O3S-S-C8	2.34	110.59	106.00
5	A	501	GTP	O2A-PA-O3A	2.34	113.59	107.27
5	C	501	GTP	C5-C6-N1	2.29	119.09	113.25
11	B	507	GDF	C45-N44-C43	2.29	128.03	120.94
10	B	505	MES	O1-C2-C3	2.28	116.68	111.77
10	B	504	MES	C7-N4-C3	2.27	117.29	111.24
11	B	507	GDF	C42-C39-C14	-2.26	119.79	122.11
5	A	501	GTP	O6-C6-C5	-2.25	120.59	126.53
9	B	501	GDP	C8-N9-C4	2.23	110.20	106.03
11	B	507	GDF	C41-O40-C39	-2.22	114.26	117.51
5	D	602	GTP	O2G-PG-O3B	2.21	112.05	104.64
5	D	602	GTP	O3G-PG-O3B	2.21	112.03	104.64
11	B	507	GDF	C34-C17-C16	-2.12	124.62	128.45
10	B	504	MES	O2S-S-O1S	-2.11	106.96	113.82
11	B	507	GDF	O36-C35-O38	-2.10	120.34	123.95
11	B	507	GDF	C23-N24-C16	2.09	111.95	109.06
10	B	504	MES	C6-C5-N4	-2.08	106.96	110.12
9	B	501	GDP	C8-N7-C5	2.06	107.93	104.26
10	B	504	MES	C2-C3-N4	2.06	113.25	110.12
10	B	504	MES	O1S-S-C8	2.02	109.77	106.73
11	B	507	GDF	C05-C06-N07	2.01	115.76	110.94
9	B	501	GDP	N9-C8-N7	-2.01	109.67	113.40

There are no chirality outliers.

All (31) 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	D	602	GTP	C5'-O5'-PA-O3A
5	D	602	GTP	C5'-O5'-PA-O1A
5	D	602	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
10	B	504	MES	C8-C7-N4-C5
10	B	504	MES	C7-C8-S-O1S
10	B	504	MES	C7-C8-S-O3S
10	B	505	MES	C8-C7-N4-C3
11	B	507	GDF	O51-C48-O49-C50
11	B	507	GDF	C47-C48-O49-C50
5	D	602	GTP	PB-O3B-PG-O1G
10	B	505	MES	C8-C7-N4-C5
10	B	504	MES	C7-C8-S-O2S
5	A	501	GTP	PB-O3B-PG-O1G
5	D	602	GTP	PB-O3B-PG-O2G
11	B	507	GDF	C42-C39-O40-C41
5	C	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	PB-O3B-PG-O1G
11	B	507	GDF	C14-C39-O40-C41
9	B	501	GDP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
9	B	501	GDP	PB-O3A-PA-O1A

There are no ring outliers.

5 monomers are involved in 13 short contacts:

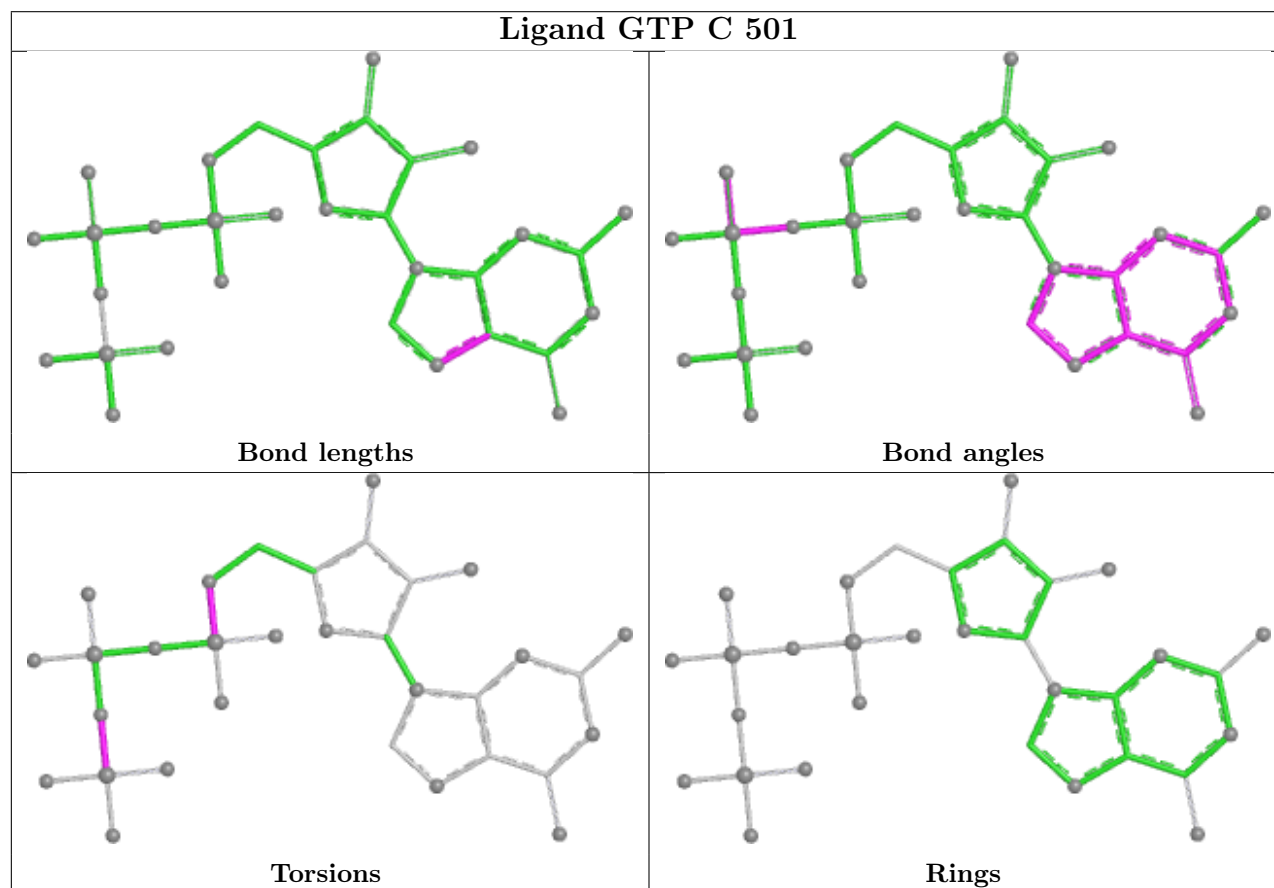
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	501	GTP	1	0
9	B	501	GDP	1	0
10	B	504	MES	4	0
10	B	505	MES	2	0

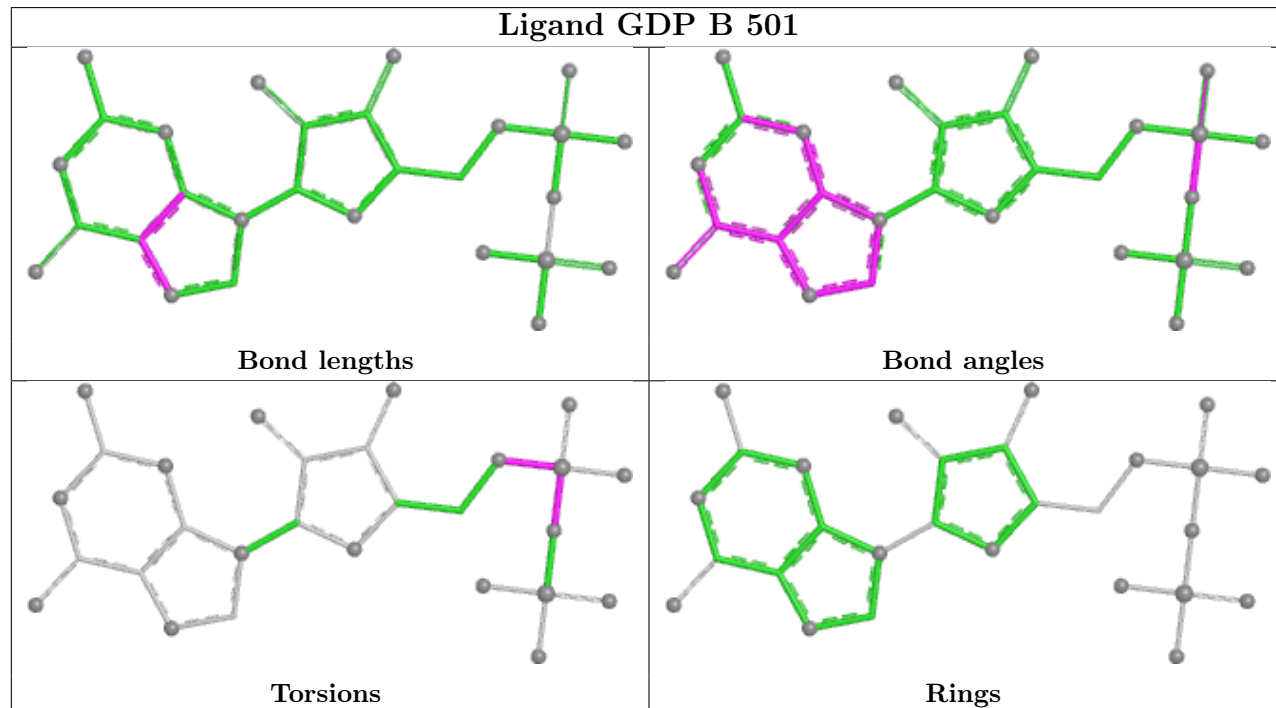
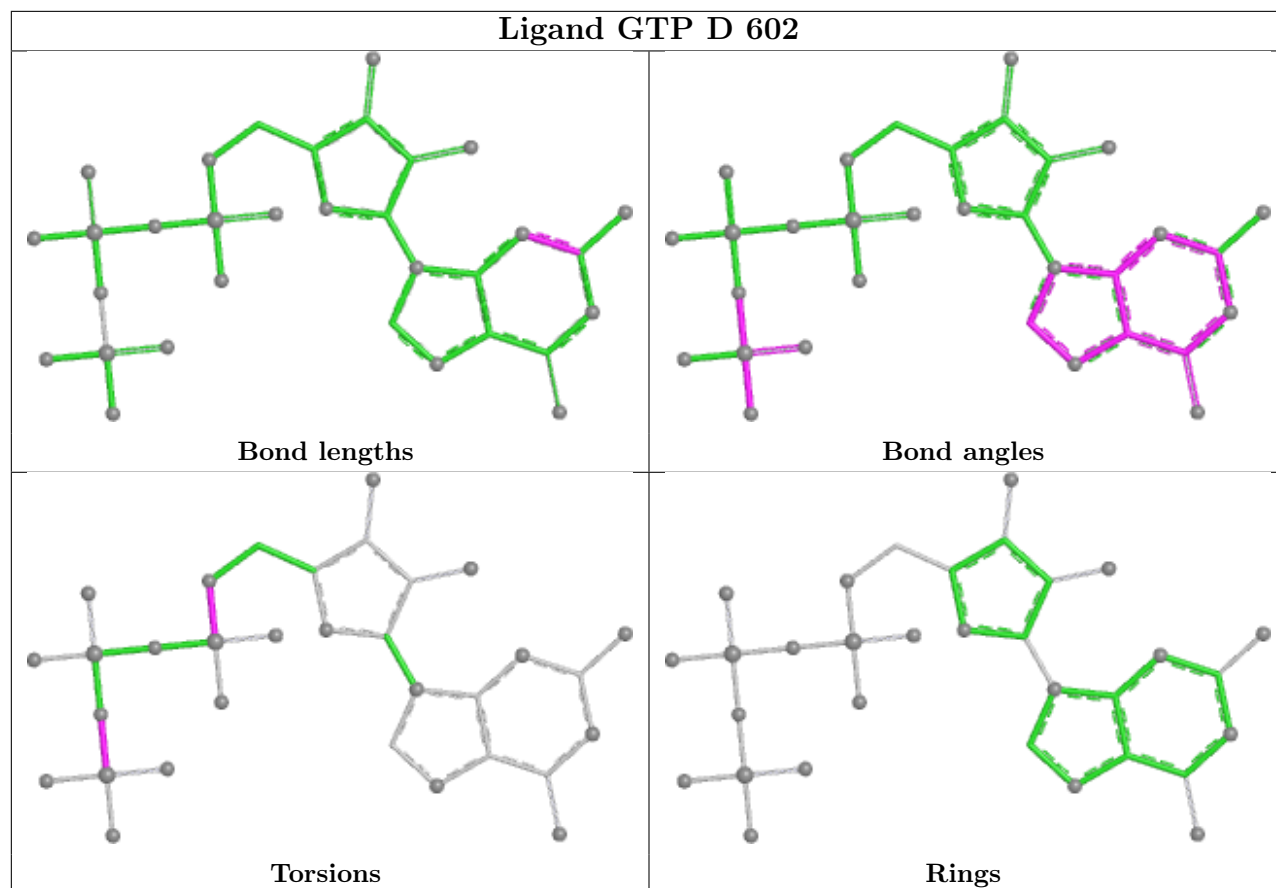
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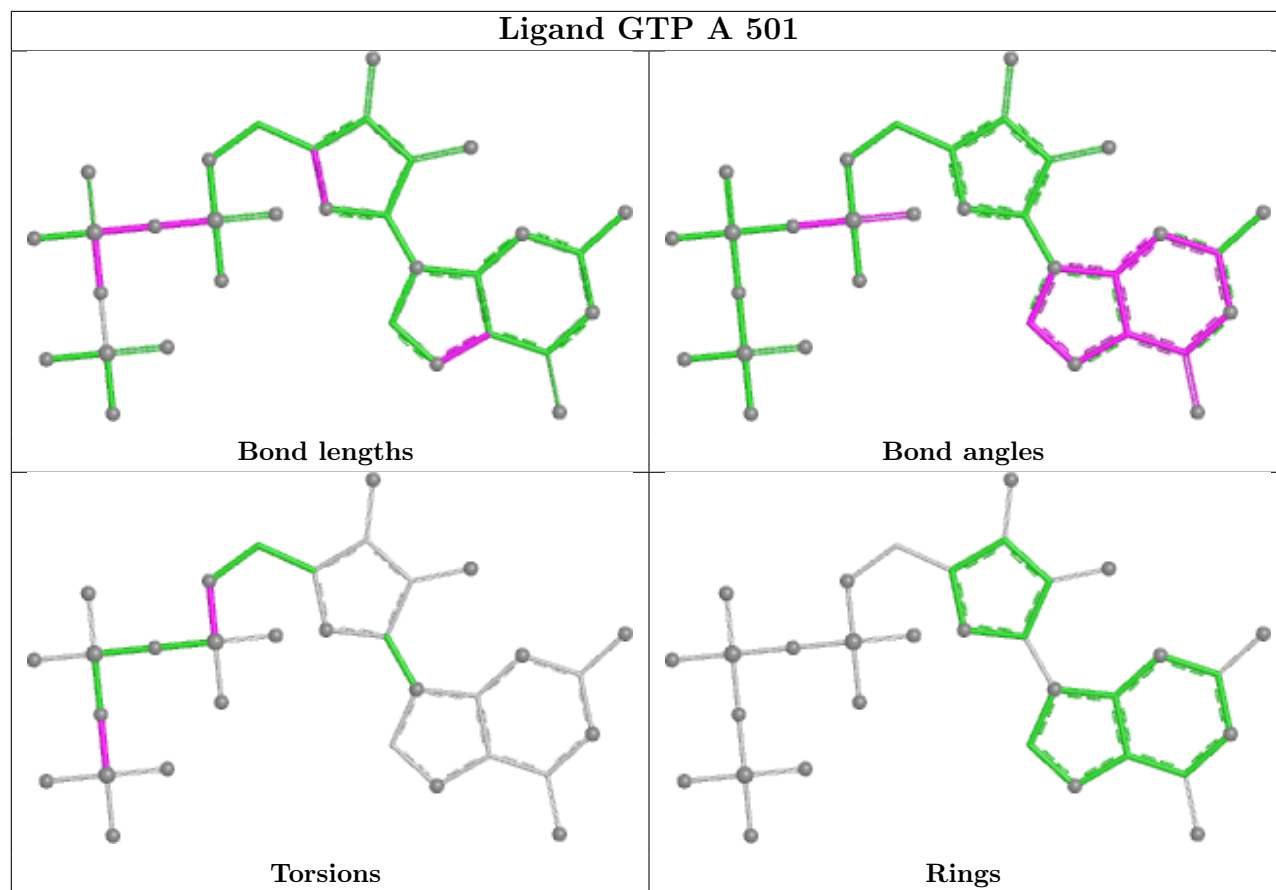
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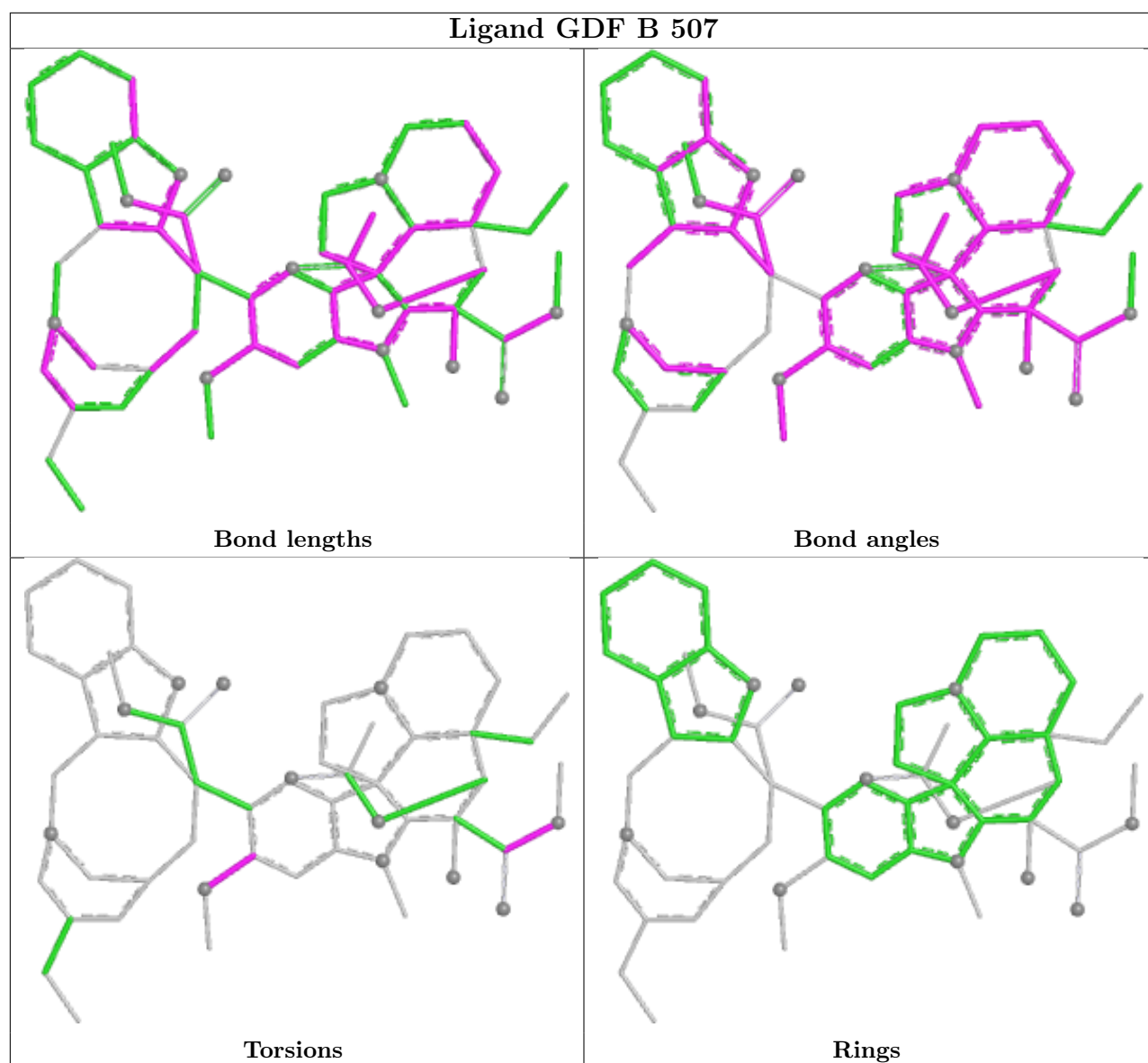
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	507	GDF	5	0

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 [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	438/451 (97%)	-0.02	7 (1%) 70 67	18, 41, 63, 80	6 (1%)
1	C	440/451 (97%)	-0.07	7 (1%) 70 67	17, 35, 47, 56	8 (1%)
2	B	430/445 (96%)	-0.10	12 (2%) 55 50	22, 36, 62, 78	5 (1%)
2	D	420/445 (94%)	0.48	20 (4%) 35 31	26, 56, 77, 88	5 (1%)
3	E	122/143 (85%)	0.86	12 (9%) 13 11	24, 55, 78, 91	4 (3%)
4	F	350/384 (91%)	1.05	61 (17%) 4 3	29, 67, 117, 136	4 (1%)
All	All	2200/2319 (94%)	0.27	119 (5%) 31 27	17, 44, 83, 136	32 (1%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	57	THR	5.1
4	F	105	LEU	5.1
4	F	152	SER	5.0
4	F	177	GLY	4.8
4	F	231	ALA	4.7
4	F	130	VAL	4.6
4	F	167	SER	4.1
4	F	133	ALA	3.9
4	F	90	SER	3.9
4	F	243	HIS	3.7
4	F	249	TYR	3.7
1	C	285	GLN	3.6
4	F	176	GLN	3.6
4	F	132	LEU	3.5
4	F	169	LEU	3.5
4	F	134	ALA	3.4
4	F	253	TYR	3.4
2	B	57	THR	3.3
4	F	233	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
4	F	383	HIS	3.2
4	F	235	ASP	3.1
2	D	400	ARG	3.1
4	F	381	HIS	3.1
4	F	161	LEU	3.1
4	F	170	LEU	3.0
4	F	89	GLU	3.0
3	E	139	LEU	3.0
4	F	254	GLY	3.0
4	F	141	GLY	3.0
4	F	131	PHE	3.0
4	F	137	ARG	2.9
4	F	140	GLU	2.9
2	D	50	ASN	2.9
4	F	136	ASN	2.9
4	F	166	ALA	2.9
4	F	159	GLY	2.8
4	F	234	GLN	2.8
4	F	70	LYS	2.8
3	E	28	SER	2.8
2	D	37	HIS	2.8
1	C	340	SER	2.8
2	D	220	THR	2.8
3	E	140	LYS	2.8
2	B	281	GLN	2.8
3	E	115[A]	HIS	2.8
1	C	163	LYS	2.7
4	F	251	LYS	2.7
1	A	438	ASP	2.7
2	D	441	ASP	2.7
4	F	144	GLY	2.7
4	F	146	VAL	2.7
2	D	96	GLN	2.7
4	F	380	HIS	2.7
4	F	384	HIS	2.7
4	F	232	ASN	2.6
2	D	58	GLY	2.6
3	E	142	GLU	2.6
3	E	114	ALA	2.6
1	A	262	TYR	2.6
2	D	98	GLY	2.6
4	F	139	ARG	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	282	TYR	2.5
2	B	75	MET	2.5
3	E	10	GLU	2.5
4	F	340	GLN	2.5
4	F	148	ILE	2.5
4	F	236	LYS	2.5
2	B	74	THR	2.5
3	E	45	PRO	2.4
4	F	103	THR	2.4
2	D	179	ASP	2.4
2	D	15	GLN	2.4
4	F	172	PHE	2.4
2	B	282	GLN	2.4
4	F	91	CYS	2.4
2	D	94	PHE	2.4
3	E	121	GLU	2.4
2	D	308	ARG	2.3
2	D	369	ARG	2.3
2	B	322	ARG	2.3
4	F	227	PRO	2.3
2	D	286	LEU	2.3
2	D	416	MET	2.3
4	F	75	ALA	2.2
4	F	104	ASN	2.2
4	F	142	ARG	2.3
2	D	397	ALA	2.2
4	F	245	ILE	2.2
1	A	163	LYS	2.2
2	B	283	TYR	2.2
2	B	166	MET	2.2
4	F	182	ILE	2.2
4	F	207	VAL	2.2
4	F	178	GLN	2.2
1	C	284	GLU	2.2
1	A	346	TRP	2.2
4	F	382	HIS	2.1
4	F	175	GLU	2.1
3	E	27	PRO	2.1
2	D	404	PHE	2.1
1	A	437	VAL	2.1
3	E	133	VAL	2.1
1	A	77	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	B	85	GLN	2.1
4	F	158	GLU	2.1
1	C	357	TYR	2.1
2	D	75	MET	2.1
2	B	247	GLN	2.1
1	C	337	THR	2.1
4	F	135	TYR	2.1
2	D	38	GLY	2.0
4	F	125	THR	2.0
1	C	1	MET	2.0
2	B	1	MET	2.0
3	E	105[A]	MET	2.0
4	F	362	ALA	2.0
4	F	168	GLU	2.0
4	F	173	ILE	2.0
2	B	37	HIS	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.

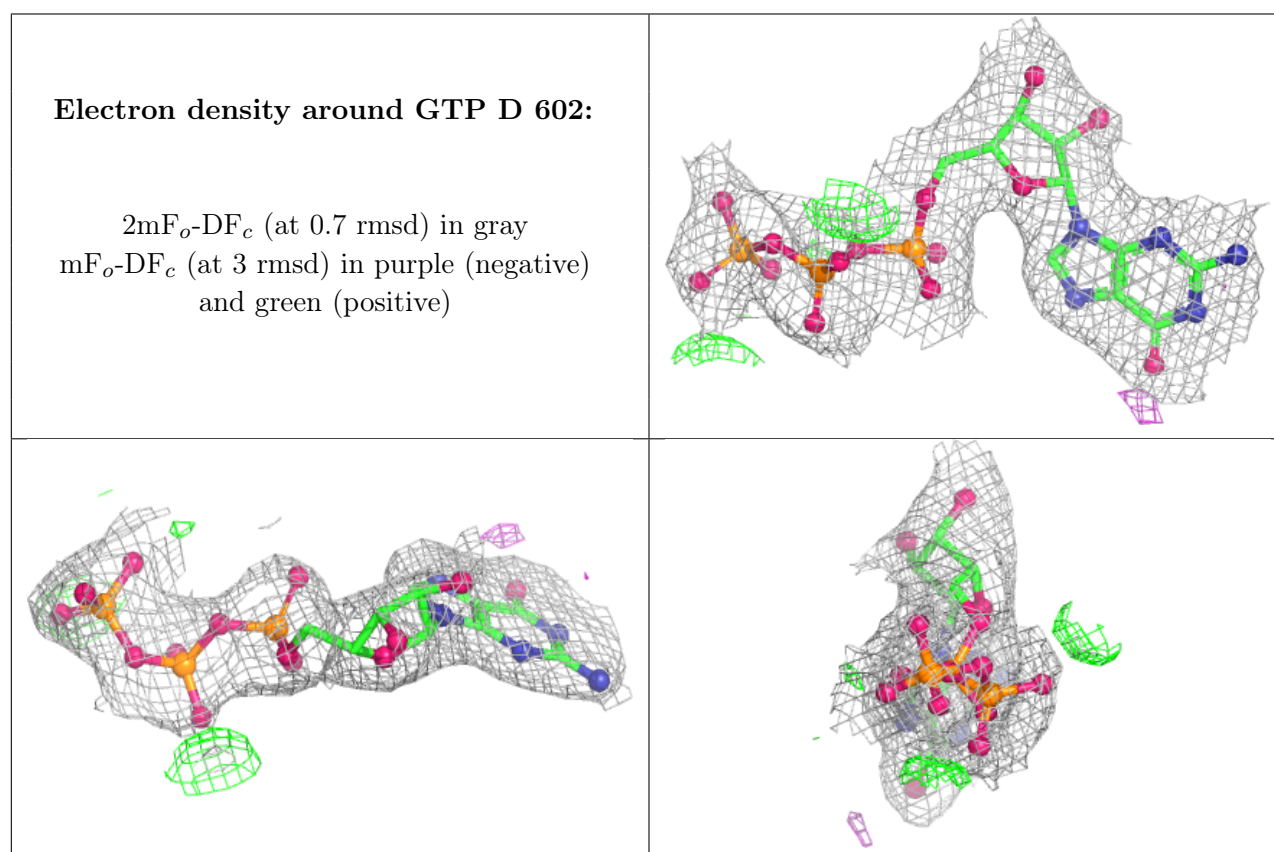
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	CA	B	503	1/1	-0.01	0.51	187,187,187,187	0
6	MG	B	506	1/1	0.65	0.46	89,89,89,89	0
7	CA	E	201	1/1	0.88	0.22	91,91,91,91	0
6	MG	D	601	1/1	0.90	0.15	63,63,63,63	0
6	MG	A	502	1/1	0.91	0.27	44,44,44,44	0
6	MG	C	502	1/1	0.92	0.13	37,37,37,37	0
8	CL	A	504	1/1	0.93	0.09	51,51,51,51	0

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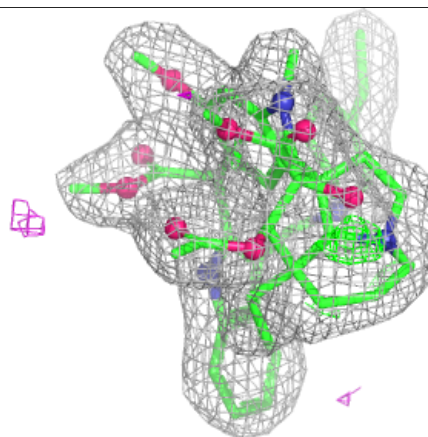
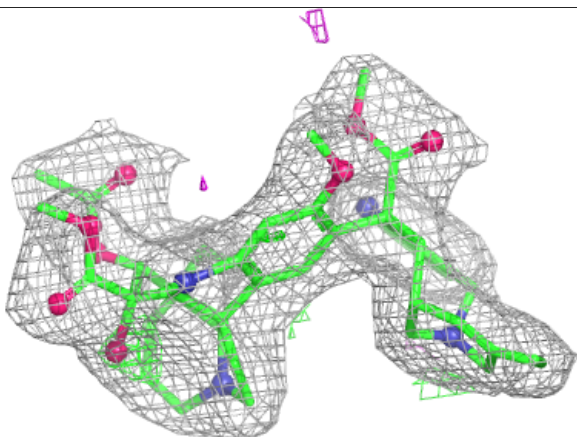
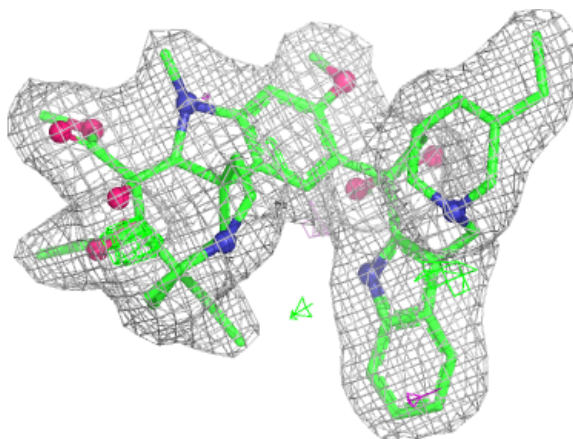
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
10	MES	B	504	12/12	0.93	0.10	41,46,68,74	0
5	GTP	D	602	32/32	0.94	0.11	51,63,81,84	0
6	MG	B	502	1/1	0.95	0.09	58,58,58,58	0
10	MES	B	505	12/12	0.95	0.09	32,41,63,67	0
11	GDF	B	507	57/57	0.95	0.11	35,41,50,56	0
7	CA	A	503	1/1	0.96	0.04	55,55,55,55	0
5	GTP	A	501	32/32	0.97	0.09	28,39,58,59	0
5	GTP	C	501	32/32	0.98	0.07	28,34,38,40	0
7	CA	C	503	1/1	0.98	0.07	50,50,50,50	0
9	GDP	B	501	28/28	0.98	0.05	18,22,29,30	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.

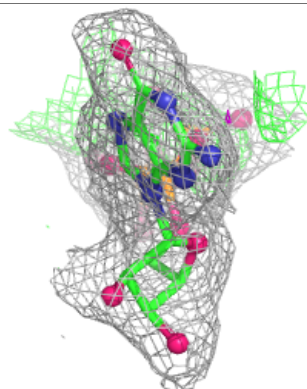
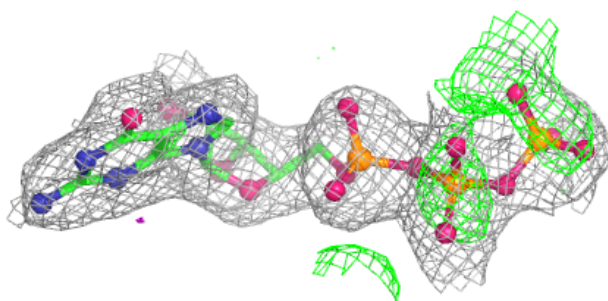
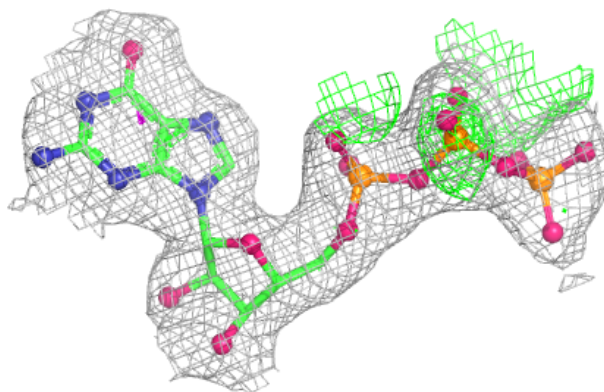


Electron density around GDF B 507:

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

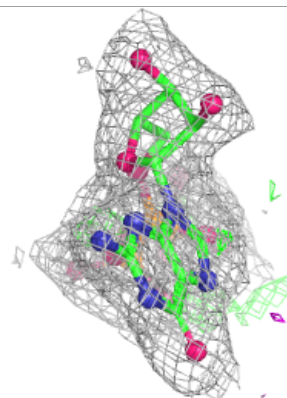
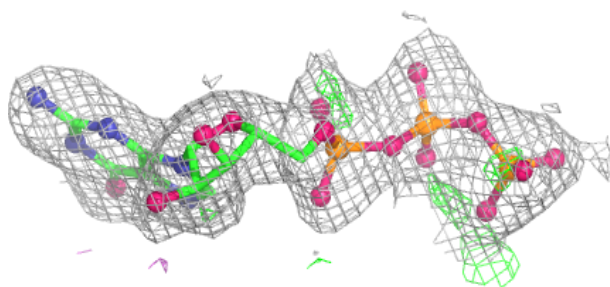
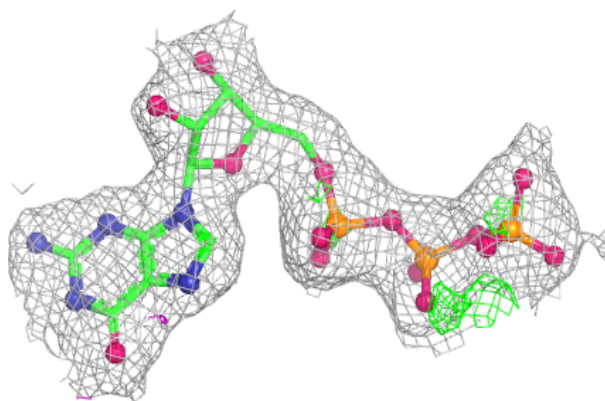
**Electron density around GTP A 501:**

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

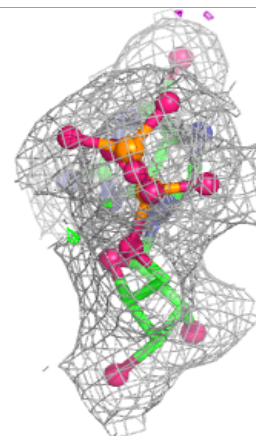
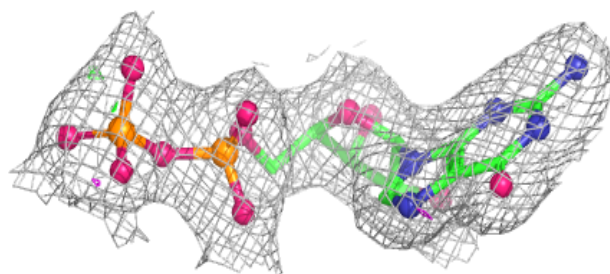
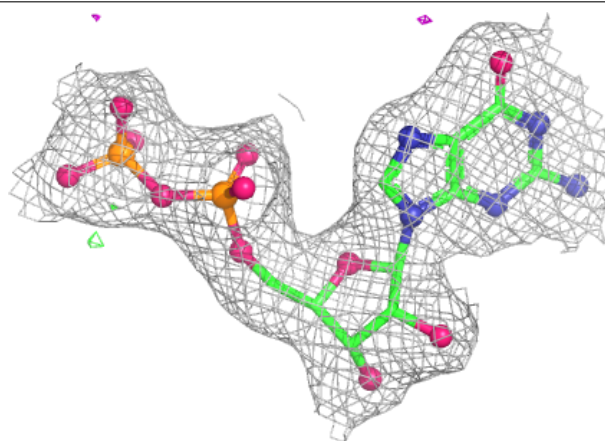


Electron density around GTP C 501:

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

**Electron density around GDP B 501:**

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



6.5 Other polymers [i](#)

There are no such residues in this entry.