



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:26 AM UTC

PDB ID : 7VMG / pdb_00007vmg
Title : Crystal structure of tubulin with 17j
Authors : Jifa, Z.; Lun, T.
Deposited on : 2021-10-08
Resolution : 2.39 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:

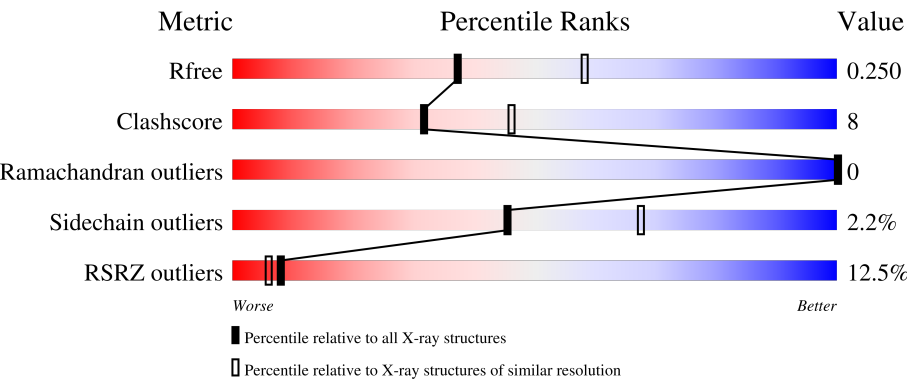
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 i

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.39 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	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	450	3% 86% 12% .
1	C	450	3% 82% 14% ..
2	B	445	4% 82% 13% 5%
2	D	445	25% 66% 27% . 6%
3	E	143	15% 66% 20% . 14%

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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
8	CL	D	503	-	-	-	X

2 Entry composition

There are 12 unique types of molecules in this entry. The entry contains 17851 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Tubulin alpha-1B chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	437	Total	C	N	O	S	0	4	0
			3427	2170	580	653	24			
1	C	440	Total	C	N	O	S	0	9	0
			3468	2195	585	663	25			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	4	0
			3364	2116	575	647	26			
2	D	420	Total	C	N	O	S	0	1	0
			3291	2069	557	639	26			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	123	Total	C	N	O	S	0	2	0
			1026	633	186	202	5			

There are 2 discrepancies between the modelled and reference sequences:

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

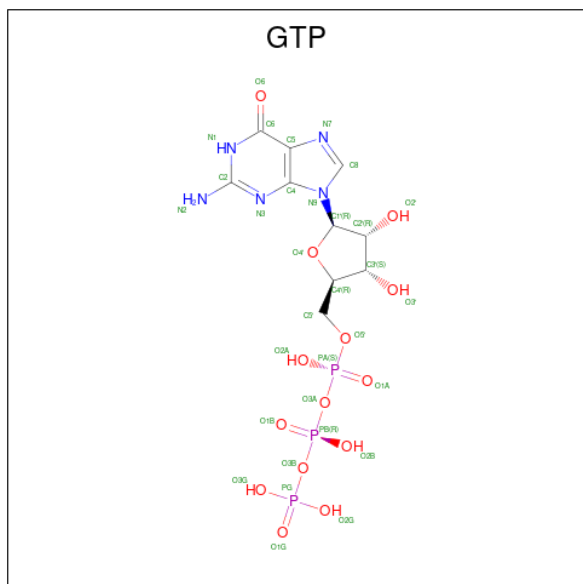
- Molecule 4 is a protein called TTL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	346	Total	C	N	O	S	0	5	0
			2856	1835	487	519	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
F	379	HIS	-	expression tag	UNP E1BQ43
F	380	HIS	-	expression tag	UNP E1BQ43
F	381	HIS	-	expression tag	UNP E1BQ43
F	382	HIS	-	expression tag	UNP E1BQ43
F	383	HIS	-	expression tag	UNP E1BQ43
F	384	HIS	-	expression tag	UNP E1BQ43

- Molecule 5 is GUANOSINE-5'-TRIPHOSPHATE (CCD ID: GTP) (formula: $C_{10}H_{16}N_5O_{14}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			32	10	5	14	3		
5	C	1	Total	C	N	O	P	0	0
			32	10	5	14	3		

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

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

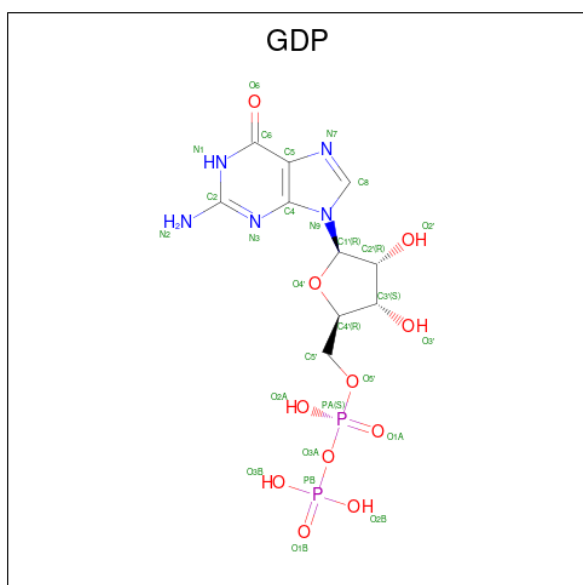
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

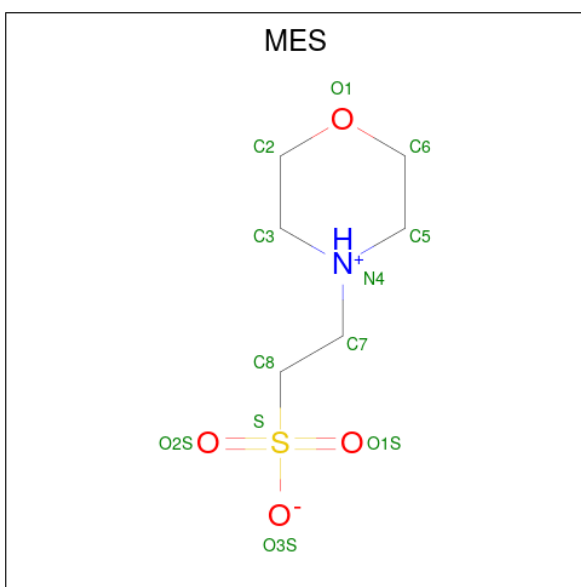
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	1	Total	Ca	1	0
			1	1		
7	C	1	Total	Ca	0	0
			1	1		

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

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

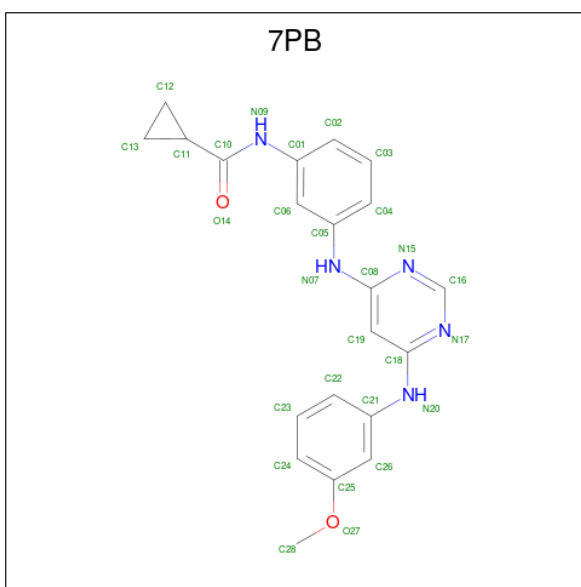
- Molecule 9 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).





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

- Molecule 11 is N-[3-[[6-[(3-methoxyphenyl)amino]pyrimidin-4-yl]amino]phenyl]cyclopropa necarboxamide (CCD ID: 7PB) (formula: C₂₁H₂₁N₅O₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			28	21	5	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	D	1	Total	C	N	O	0	0
			28	21	5	2		

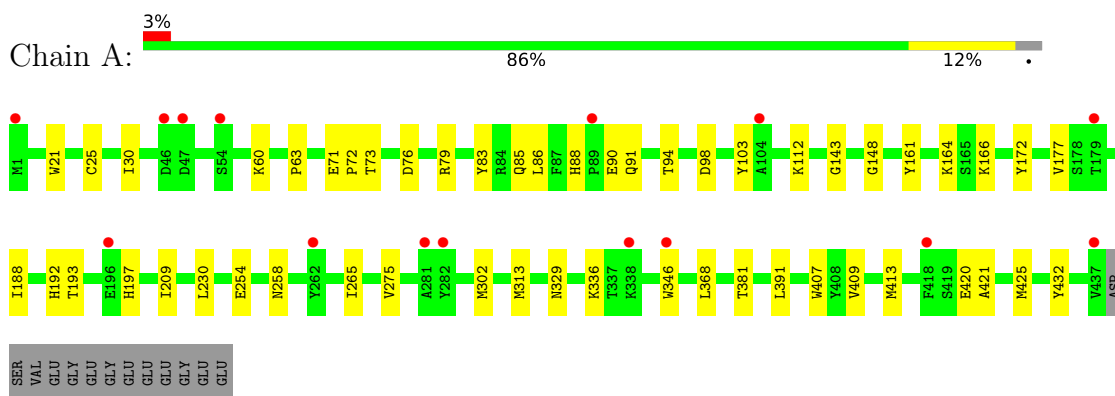
- Molecule 12 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
12	A	55	Total	O	0	0
			55	55		
12	B	51	Total	O	0	0
			51	51		
12	C	82	Total	O	0	0
			82	82		
12	D	4	Total	O	0	0
			4	4		
12	E	5	Total	O	0	0
			5	5		
12	F	15	Total	O	0	0
			15	15		

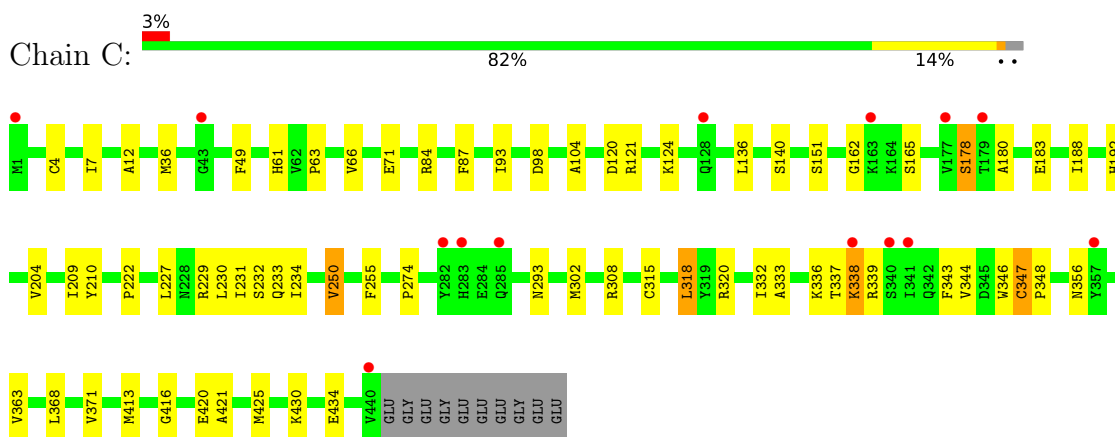
3 Residue-property plots [i](#)

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

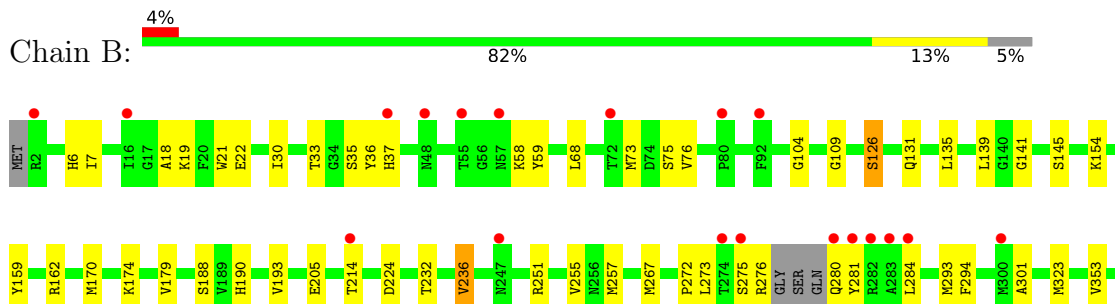
• Molecule 1: Tubulin alpha-1B chain

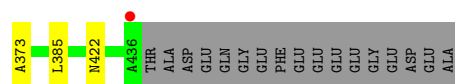


• Molecule 1: Tubulin alpha-1B chain

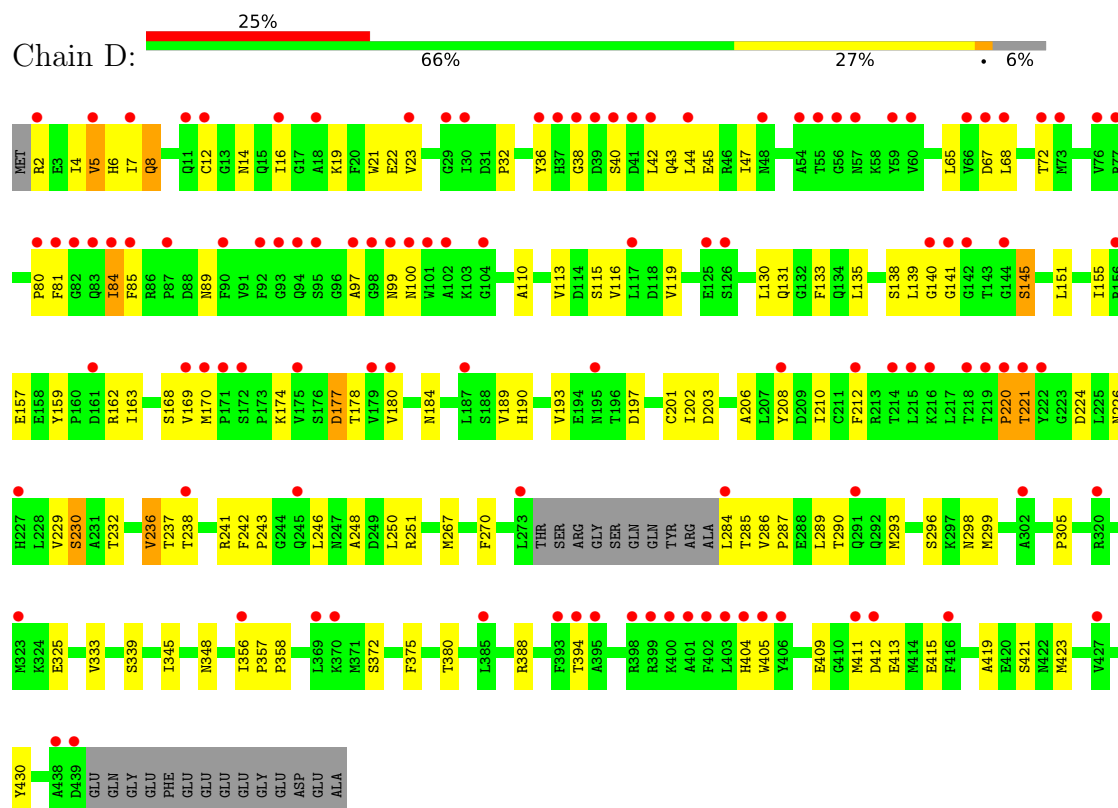


• Molecule 2: Tubulin beta-2B chain

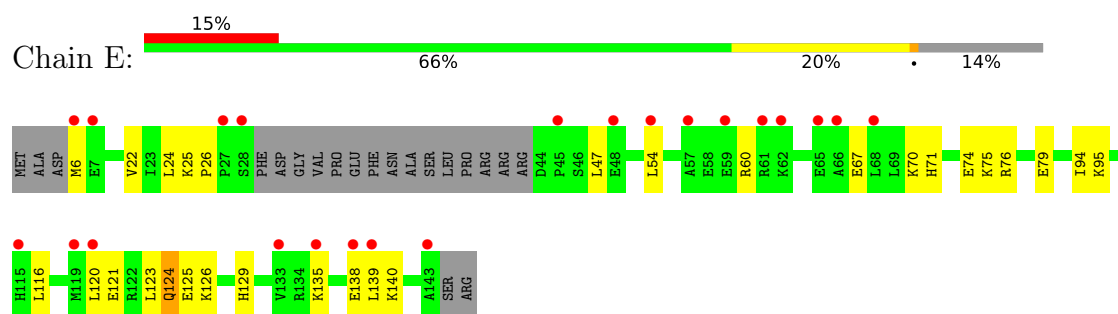




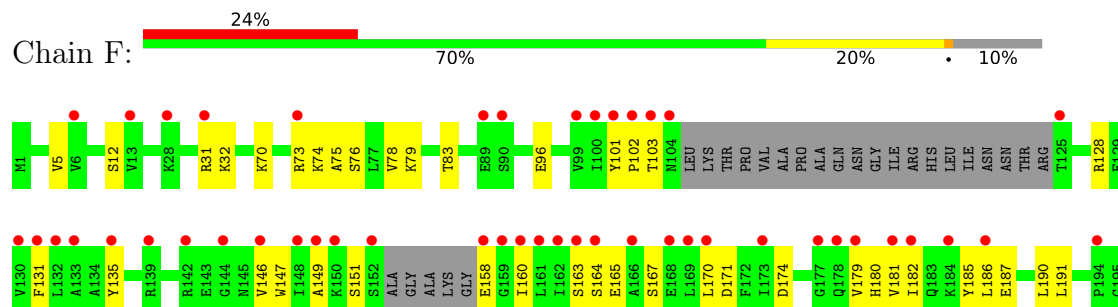
• Molecule 2: Tubulin beta-2B chain

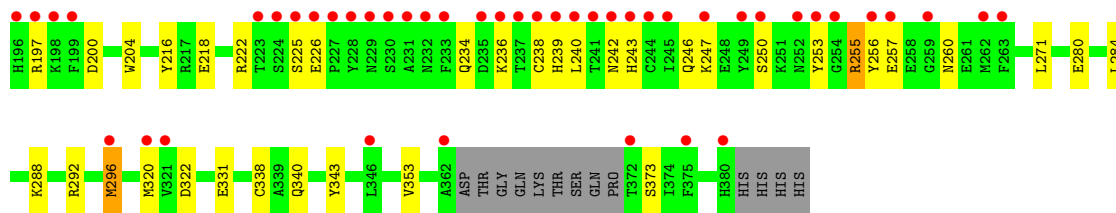


• Molecule 3: Stathmin-4



• Molecule 4: TTL





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.33Å 158.21Å 182.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	91.24 – 2.39 91.24 – 2.39	Depositor EDS
% Data completeness (in resolution range)	99.7 (91.24-2.39) 95.6 (91.24-2.39)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.15 (at 2.40Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.210 , 0.250 0.212 , 0.250	Depositor DCC
R_{free} test set	2000 reflections (1.65%)	wwPDB-VP
Wilson B-factor (Å ²)	52.2	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	17851	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.25% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MES, CL, GTP, 7PB, GDP, MG, 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	0.40	0/3517	0.59	0/4776
1	C	0.46	0/3570	0.65	1/4847 (0.0%)
2	B	0.45	0/3447	0.65	0/4667
2	D	0.45	0/3364	0.69	4/4560 (0.1%)
3	E	0.47	0/1041	0.66	0/1382
4	F	0.32	0/2935	0.56	0/3966
All	All	0.42	0/17874	0.63	5/24198 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
4	F	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	220	PRO	N-CA-C	7.55	128.03	112.47
1	C	338	LYS	CA-CB-CG	6.32	126.74	114.10
2	D	251	ARG	N-CA-C	5.99	117.89	111.36
2	D	242	PHE	CA-C-N	-5.33	114.43	119.76
2	D	242	PHE	C-N-CA	-5.33	114.43	119.76

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	F	234	GLN	Peptide

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3427	0	3340	36	0
1	C	3468	0	3388	42	0
2	B	3364	0	3249	43	0
2	D	3291	0	3155	88	0
3	E	1026	0	1042	31	0
4	F	2856	0	2837	52	0
5	A	32	0	12	2	0
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
7	A	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
8	D	1	0	0	0	0
9	B	28	0	12	1	0
9	D	28	0	12	1	0
10	B	24	0	26	4	0
11	B	28	0	0	1	0
11	D	28	0	0	2	0
12	A	55	0	0	1	0
12	B	51	0	0	0	0
12	C	82	0	0	2	0
12	D	4	0	0	1	0
12	E	5	0	0	0	0
12	F	15	0	0	0	0
All	All	17851	0	17085	282	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 (282) 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)
2:B:251:ARG:NH2	10:B:503:MES:O1S	2.02	0.92
2:D:99:ASN:HD22	2:D:178:THR:HG21	1.39	0.87
1:A:112:LYS:HD2	3:E:54:LEU:HB3	1.56	0.87
2:D:131:GLN:HB2	2:D:250:LEU:HD12	1.57	0.86
1:A:88:HIS:NE2	1:A:90:GLU:HG3	1.98	0.79
2:B:36:TYR:O	2:B:37:HIS:ND1	2.15	0.79
1:C:229:ARG:HD2	1:C:363:VAL:HG11	1.64	0.78
4:F:128:ARG:HE	4:F:170:LEU:HD22	1.50	0.76
2:D:221:THR:HG23	2:D:224:ASP:H	1.51	0.76
4:F:128:ARG:HH21	4:F:170:LEU:HB3	1.52	0.73
2:D:206:ALA:O	2:D:210:ILE:HG13	1.87	0.73
4:F:186:LEU:HD12	4:F:320:MET:HE2	1.70	0.72
3:E:6:MET:HE2	3:E:24:LEU:CD2	2.20	0.71
1:A:60:LYS:NZ	1:A:85:GLN:O	2.23	0.71
1:C:36:MET:HE3	1:C:61:HIS:CD2	2.26	0.70
1:A:88:HIS:CD2	1:A:90:GLU:HG3	2.27	0.69
2:D:221:THR:HG22	2:D:224:ASP:HB2	1.75	0.68
4:F:31:ARG:HE	4:F:32:LYS:H	1.40	0.68
2:B:251:ARG:CZ	10:B:503:MES:O1S	2.08	0.68
1:A:161:TYR:HB3	1:A:164:LYS:HD3	1.75	0.67
4:F:135:TYR:OH	4:F:165:GLU:HA	1.93	0.67
2:D:67:ASP:OD2	2:D:72:THR:HG21	1.95	0.67
2:B:280:GLN:HG3	2:B:281:TYR:H	1.59	0.67
2:D:220:PRO:O	2:D:221:THR:HG22	1.96	0.66
2:B:73:MET:HA	2:B:76:VAL:HG12	1.78	0.66
3:E:6:MET:HE2	3:E:24:LEU:HD21	1.77	0.66
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.78	0.66
2:B:267:MET:HG3	2:B:301:ALA:HB3	1.80	0.64
2:D:99:ASN:ND2	2:D:178:THR:HG21	2.12	0.64
4:F:226:GLU:OE1	4:F:238:CYS:HB3	1.98	0.63
2:B:154:LYS:NZ	3:E:76:ARG:HD2	2.13	0.63
3:E:121:GLU:HA	3:E:124:GLN:HG2	1.81	0.62
2:D:65:LEU:HD11	2:D:85:PHE:HD2	1.64	0.61
4:F:246:GLN:O	4:F:250:SER:HB3	1.99	0.61
2:D:202:ILE:HD13	2:D:229:VAL:HG13	1.82	0.61
2:D:2:ARG:N	2:D:131:GLN:HG2	2.16	0.61
2:D:40:SER:H	2:D:43:GLN:HE22	1.49	0.61
2:D:236:VAL:O	11:D:502:7PB:N09	2.34	0.61
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.83	0.60
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.29	0.60
1:C:178:SER:HB2	1:C:183:GLU:OE2	2.00	0.60
2:D:141:GLY:HA3	9:D:501:GDP:O3A	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:139:LEU:HD21	2:D:168:SER:HB3	1.82	0.60
2:D:139:LEU:HA	2:D:145[A]:SER:HB3	1.82	0.60
2:B:170:MET:HG3	2:B:385:LEU:HD21	1.83	0.59
2:B:323:MET:SD	2:B:353:VAL:HG21	2.42	0.59
1:A:79:ARG:NH2	1:A:94:THR:OG1	2.35	0.58
4:F:128:ARG:HA	4:F:131:PHE:HB3	1.85	0.58
2:D:32:PRO:HB3	2:D:81:PHE:HA	1.86	0.58
2:D:221:THR:CG2	2:D:224:ASP:H	2.16	0.58
3:E:67:GLU:O	3:E:70:LYS:HE3	2.04	0.57
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.84	0.57
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.44	0.57
2:D:45:GLU:OE1	2:D:243:PRO:HG2	2.03	0.57
2:D:412:ASP:OD1	2:D:413:GLU:N	2.38	0.57
1:A:265:ILE:HG21	1:A:313:MET:HE1	1.86	0.57
4:F:103:THR:HG22	4:F:174:ASP:HB3	1.88	0.56
1:C:234:ILE:HD13	1:C:302:MET:SD	2.45	0.56
4:F:78:VAL:HG21	4:F:181:VAL:HG21	1.88	0.56
2:D:130:LEU:O	2:D:162:ARG:NH1	2.35	0.55
4:F:103:THR:N	4:F:174:ASP:OD1	2.39	0.55
2:D:44:LEU:HA	2:D:47:ILE:HB	1.87	0.55
4:F:236:LYS:HB2	4:F:240:LEU:HD22	1.87	0.55
2:D:285:THR:HB	2:D:287:PRO:HD2	1.87	0.55
4:F:340:GLN:HA	4:F:343:TYR:HD2	1.72	0.55
2:B:145:SER:HB2	2:B:188:SER:OG	2.07	0.55
2:B:104:GLY:O	2:B:109:GLY:HA3	2.06	0.55
2:D:140:GLY:O	2:D:184:ASN:ND2	2.31	0.54
2:B:190:HIS:O	2:B:193:VAL:HG12	2.06	0.54
2:D:19:LYS:O	2:D:23:VAL:HG23	2.08	0.54
4:F:5:VAL:HG13	4:F:32:LYS:HA	1.89	0.54
2:B:174:LYS:HD2	2:B:205:GLU:OE1	2.08	0.54
2:D:16:ILE:HD11	2:D:169:VAL:HG21	1.89	0.53
2:B:236:VAL:O	11:B:505:7PB:N09	2.42	0.52
1:A:209:ILE:HD11	1:A:302:MET:SD	2.49	0.52
2:B:154:LYS:HZ3	3:E:76:ARG:HD2	1.74	0.52
2:B:224:ASP:OD1	2:B:276:ARG:NH2	2.41	0.52
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.92	0.52
2:D:293:MET:HE2	2:D:375:PHE:HB2	1.92	0.52
2:B:18:ALA:O	2:B:22:GLU:HG3	2.10	0.52
2:D:189:VAL:HG11	2:D:423:MET:HG3	1.91	0.52
2:D:44:LEU:HD23	2:D:47:ILE:HD13	1.91	0.52
2:D:248:ALA:HB1	11:D:502:7PB:N07	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:126:SER:O	2:B:126:SER:OG	2.23	0.52
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.45	0.51
2:D:36:TYR:CD2	2:D:44:LEU:HD11	2.46	0.51
3:E:139:LEU:C	3:E:140:LYS:HD3	2.34	0.51
4:F:190:LEU:HB2	4:F:322:ASP:O	2.10	0.51
2:D:155:ILE:O	2:D:159:TYR:N	2.40	0.51
2:D:270:PHE:O	2:D:298:ASN:HB3	2.11	0.51
2:B:275:SER:OG	2:B:276:ARG:N	2.44	0.51
3:E:60:ARG:HG3	3:E:60:ARG:HH11	1.76	0.51
2:D:65:LEU:HD11	2:D:85:PHE:CD2	2.46	0.51
3:E:47:LEU:HD12	3:E:47:LEU:O	2.11	0.51
4:F:79:LYS:O	4:F:83:THR:OG1	2.20	0.51
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.46	0.50
1:A:83:TYR:HD2	1:A:86:LEU:HD22	1.77	0.50
2:D:67:ASP:OD1	2:D:68:LEU:N	2.45	0.49
2:D:232:THR:O	2:D:236:VAL:HG13	2.12	0.49
2:D:174:LYS:HD2	2:D:208:TYR:CD2	2.47	0.49
4:F:31:ARG:NE	4:F:32:LYS:H	2.09	0.49
1:C:84:ARG:HG2	1:C:84:ARG:HH11	1.77	0.49
4:F:151:SER:HB3	4:F:180:HIS:CE1	2.47	0.49
4:F:31:ARG:HE	4:F:31:ARG:HA	1.78	0.49
1:A:275:VAL:HG13	1:A:368:LEU:HD21	1.94	0.49
2:D:19:LYS:NZ	2:D:22:GLU:OE1	2.36	0.49
2:D:22:GLU:OE2	2:D:80:PRO:HG2	2.13	0.49
2:D:409:GLU:OE1	2:D:409:GLU:HA	2.12	0.49
1:A:346:TRP:H	1:A:346:TRP:CD1	2.30	0.49
1:A:177:VAL:O	1:A:177:VAL:HG22	2.12	0.48
1:C:227:LEU:O	1:C:231:ILE:HG13	2.13	0.48
3:E:116:LEU:O	3:E:120:LEU:HD12	2.13	0.48
2:B:281:TYR:O	2:B:281:TYR:CD1	2.66	0.48
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.49	0.48
3:E:70:LYS:HD2	3:E:71:HIS:N	2.28	0.48
3:E:124:GLN:HG3	3:E:125:GLU:N	2.28	0.48
4:F:74:LYS:NZ	4:F:331:GLU:OE1	2.46	0.48
3:E:25:LYS:C	3:E:25:LYS:HD3	2.38	0.48
3:E:60:ARG:HG3	3:E:60:ARG:NH1	2.29	0.48
4:F:247:LYS:NZ	4:F:253:TYR:OH	2.46	0.48
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.96	0.48
1:C:430:LYS:O	1:C:434:GLU:HG3	2.13	0.48
4:F:102:PRO:HA	4:F:174:ASP:OD1	2.14	0.48
1:A:83:TYR:CD2	1:A:86:LEU:HD22	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:31:ARG:HE	4:F:32:LYS:N	2.11	0.48
1:A:420:GLU:OE1	12:A:601:HOH:O	2.20	0.47
1:A:25:CYS:HB3	1:A:30:ILE:O	2.15	0.47
2:D:89:ASN:HA	2:D:119:VAL:HG11	1.95	0.47
3:E:70:LYS:O	3:E:74:GLU:HG3	2.13	0.47
3:E:75:LYS:O	3:E:79:GLU:HG3	2.14	0.47
1:A:188:ILE:HG23	1:A:425:MET:HG3	1.96	0.47
2:B:35:SER:OG	2:B:58:LYS:HE2	2.14	0.47
2:B:139:LEU:HA	2:B:145:SER:HB3	1.95	0.47
4:F:73:ARG:O	4:F:76:SER:HB2	2.14	0.47
1:C:250:VAL:HG22	1:C:255:PHE:CZ	2.48	0.47
1:C:255:PHE:CZ	1:C:318:LEU:HD22	2.50	0.47
1:A:166:LYS:HE2	1:A:197:HIS:O	2.14	0.47
4:F:292:ARG:NH1	4:F:296[B]:MET:SD	2.88	0.47
1:A:143:GLY:HA3	5:A:501:GTP:O3A	2.14	0.47
1:C:416:GLY:O	1:C:420[B]:GLU:HB2	2.15	0.47
2:D:4:ILE:HG12	2:D:250:LEU:HD11	1.97	0.47
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.50	0.46
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.97	0.46
2:D:246:LEU:HD23	2:D:246:LEU:HA	1.67	0.46
2:D:290:THR:HG22	2:D:333:VAL:HG21	1.96	0.46
4:F:103:THR:CG2	4:F:174:ASP:HB3	2.44	0.46
3:E:25:LYS:HD3	3:E:26:PRO:O	2.15	0.46
4:F:167:SER:O	4:F:171:ASP:HB2	2.15	0.46
1:C:204:VAL:HG13	1:C:302:MET:HG3	1.98	0.46
2:D:110:ALA:O	2:D:113:VAL:HG12	2.16	0.46
2:D:2:ARG:C	2:D:131:GLN:HE21	2.24	0.46
2:D:170:MET:HE1	2:D:201:CYS:C	2.41	0.46
2:D:170:MET:HE1	2:D:202:ILE:N	2.30	0.46
2:D:356:ILE:HD12	2:D:357:PRO:HD2	1.96	0.46
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.33	0.46
2:B:7:ILE:O	2:B:135:LEU:HA	2.15	0.46
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.98	0.46
3:E:25:LYS:NZ	3:E:26:PRO:O	2.41	0.46
1:C:36:MET:HE1	1:C:49:PHE:CE1	2.52	0.45
2:D:12:CYS:CB	2:D:138:SER:HB3	2.46	0.45
2:D:170:MET:HB2	2:D:170:MET:HE2	1.55	0.45
2:D:36:TYR:CZ	2:D:38:GLY:HA3	2.51	0.45
2:D:100:ASN:ND2	2:D:405:TRP:HB3	2.32	0.45
4:F:75:ALA:O	4:F:79:LYS:HG3	2.16	0.45
4:F:260:ASN:N	4:F:260:ASN:HD22	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:332:ILE:O	1:C:336:LYS:HG2	2.16	0.45
4:F:151:SER:HB3	4:F:180:HIS:NE2	2.32	0.45
2:D:68:LEU:HD12	2:D:97:ALA:HB2	1.98	0.45
2:D:81:PHE:O	2:D:84:ILE:HG22	2.16	0.45
1:C:274:PRO:HG2	1:C:371:VAL:HG11	1.99	0.45
4:F:200:ASP:OD1	4:F:222:ARG:HB2	2.17	0.45
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.89	0.44
4:F:255[B]:ARG:HD3	4:F:256:TYR:CE1	2.52	0.44
1:C:104:ALA:HB2	1:C:413:MET:SD	2.57	0.44
1:C:320:ARG:HA	1:C:356:ASN:O	2.18	0.44
2:D:237:THR:O	2:D:241:ARG:HG3	2.17	0.44
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.17	0.44
1:A:192:HIS:CG	1:A:421:ALA:HA	2.53	0.44
2:D:203:ASP:OD2	2:D:388:ARG:NH1	2.44	0.44
4:F:31:ARG:NE	4:F:31:ARG:HA	2.32	0.44
4:F:243:HIS:ND1	4:F:243:HIS:O	2.50	0.44
1:A:72:PRO:HB2	1:A:76:ASP:OD2	2.17	0.44
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.52	0.44
2:B:154:LYS:HZ1	3:E:76:ARG:HD2	1.81	0.44
2:B:294:PHE:HB3	10:B:504:MES:H31	1.98	0.44
1:C:229:ARG:O	1:C:232:SER:OG	2.34	0.44
2:D:6:HIS:CE1	2:D:21:TRP:HE1	2.35	0.44
3:E:70:LYS:HD2	3:E:70:LYS:C	2.42	0.44
4:F:284:LEU:O	4:F:288:LYS:HG3	2.17	0.44
2:D:7:ILE:O	2:D:135:LEU:HD12	2.17	0.44
2:D:163:ILE:HA	2:D:197:ASP:OD2	2.17	0.44
2:D:212:PHE:CD1	2:D:212:PHE:C	2.95	0.44
1:C:229:ARG:HD2	1:C:363:VAL:CG1	2.40	0.44
4:F:158:GLU:N	4:F:160:ILE:HD11	2.33	0.44
1:A:71:GLU:OE1	1:A:73:THR:OG1	2.29	0.44
1:C:233:GLN:HG3	1:C:368:LEU:HD12	2.00	0.43
2:D:221:THR:HG22	2:D:224:ASP:CB	2.45	0.43
1:A:409:VAL:HA	1:A:413:MET:O	2.18	0.43
2:B:293:MET:HE3	2:B:373:ALA:HB1	1.99	0.43
3:E:135:LYS:O	3:E:138:GLU:HG3	2.18	0.43
4:F:200:ASP:OD1	4:F:222:ARG:NE	2.49	0.43
1:C:12:ALA:HB3	1:C:140:SER:HB3	2.00	0.43
1:A:88:HIS:HB3	1:A:91:GLN:OE1	2.18	0.43
2:B:159:TYR:HB3	2:B:162[B]:ARG:HG2	2.00	0.43
2:B:68:LEU:HA	2:B:68:LEU:HD23	1.74	0.43
2:D:404:HIS:CD2	2:D:405:TRP:HD1	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:146:VAL:HG23	4:F:187:GLU:OE2	2.18	0.43
1:C:293[A]:ASN:CG	1:C:339:ARG:HH21	2.26	0.43
2:B:30:ILE:HD13	2:B:59:TYR:HB2	2.01	0.43
2:D:8:GLN:NE2	2:D:14:ASN:HA	2.33	0.43
4:F:101:TYR:CD2	4:F:179:VAL:HG22	2.54	0.43
2:B:139:LEU:HD12	2:B:170:MET:SD	2.59	0.43
2:D:411:MET:HE2	2:D:411:MET:HB3	1.71	0.43
4:F:191:LEU:HD23	4:F:197:ARG:C	2.44	0.43
2:D:22:GLU:HG3	2:D:81:PHE:CD1	2.53	0.43
4:F:163:SER:OG	4:F:164:SER:N	2.51	0.43
1:C:93:ILE:HD11	1:C:121:ARG:HG3	2.00	0.42
1:C:308:ARG:HD2	12:C:664:HOH:O	2.19	0.42
2:D:296:SER:HB3	2:D:305:PRO:HD2	2.01	0.42
2:D:190:HIS:ND1	2:D:419:ALA:HA	2.34	0.42
4:F:340:GLN:HA	4:F:343:TYR:CD2	2.53	0.42
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.34	0.42
1:A:329:ASN:OD1	3:E:22:VAL:HG21	2.19	0.42
4:F:96:GLU:HG2	4:F:147:TRP:HH2	1.83	0.42
1:C:333:ALA:O	1:C:337:THR:HG23	2.20	0.42
2:D:5:VAL:HG13	2:D:133:PHE:CD2	2.55	0.42
2:D:5:VAL:HG12	2:D:130:LEU:HD11	2.02	0.42
2:D:267:MET:HE3	2:D:267:MET:HB2	1.88	0.42
2:D:286:VAL:HB	2:D:325:GLU:HG2	2.01	0.42
2:D:157:GLU:HA	3:E:123:LEU:HD13	2.01	0.42
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.55	0.42
1:C:120[B]:ASP:CG	1:C:124:LYS:HZ1	2.27	0.42
2:D:68:LEU:HD23	2:D:68:LEU:HA	1.90	0.42
2:D:345:ILE:HG22	2:D:348:ASN:HB3	2.01	0.42
2:B:190:HIS:CD2	2:B:422:ASN:OD1	2.73	0.42
2:B:272:PRO:HB3	2:B:284:LEU:HD22	2.02	0.42
1:C:192:HIS:CG	1:C:421:ALA:HA	2.55	0.42
2:D:380:THR:HA	2:D:430:TYR:CD1	2.55	0.42
3:E:6:MET:HE2	3:E:24:LEU:HD22	2.01	0.42
2:D:65:LEU:HD21	2:D:85:PHE:CE2	2.55	0.42
4:F:242:ASN:OD1	4:F:242:ASN:N	2.52	0.41
2:D:415:GLU:OE1	3:E:129:HIS:NE2	2.48	0.41
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.55	0.41
2:D:358:PRO:HB2	12:D:602:HOH:O	2.20	0.41
2:B:33:THR:O	2:B:58:LYS:NZ	2.42	0.41
2:B:141:GLY:HA3	9:B:501:GDP:O3A	2.21	0.41
4:F:246:GLN:NE2	4:F:260:ASN:OD1	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ALA:HB3	1:C:183:GLU:HG3	2.02	0.41
4:F:149:ALA:HB2	4:F:182:ILE:HG22	2.03	0.41
1:C:302:MET:N	1:C:302:MET:HE2	2.35	0.41
2:D:40:SER:N	2:D:43:GLN:HE22	2.16	0.41
1:A:72:PRO:HA	1:A:94:THR:HG21	2.02	0.41
2:B:267:MET:HE3	2:B:267:MET:HB2	1.68	0.41
1:C:356:ASN:ND2	12:C:607:HOH:O	2.53	0.41
2:D:40:SER:HB3	2:D:42:LEU:H	1.85	0.41
1:A:88:HIS:CD2	1:A:90:GLU:H	2.38	0.41
2:B:257:MET:HE3	2:B:257:MET:HB3	1.79	0.41
2:B:280:GLN:HG3	2:B:281:TYR:N	2.30	0.41
2:D:65:LEU:HD21	2:D:85:PHE:CD2	2.56	0.41
3:E:139:LEU:HB3	3:E:140:LYS:HE3	2.01	0.41
4:F:70:LYS:HB2	4:F:70:LYS:HE3	1.78	0.41
4:F:185:TYR:OH	4:F:239:HIS:HB3	2.21	0.41
1:A:209:ILE:HG23	1:A:230:LEU:HD23	2.03	0.41
2:D:296:SER:HA	2:D:299:MET:HG2	2.03	0.41
3:E:67:GLU:O	3:E:70:LYS:HG3	2.20	0.41
1:C:7:ILE:HG23	1:C:66:VAL:HG13	2.02	0.40
2:D:12:CYS:SG	2:D:138:SER:HB3	2.61	0.40
1:A:407:TRP:CE2	2:B:255:VAL:HA	2.56	0.40
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.56	0.40
1:C:343:PHE:HD2	1:C:347[A]:CYS:SG	2.43	0.40
2:D:36:TYR:CE1	2:D:38:GLY:HA3	2.56	0.40
2:D:151:LEU:O	2:D:155:ILE:HG13	2.21	0.40
2:D:177:ASP:OD1	2:D:177:ASP:N	2.48	0.40
2:D:226:ASN:O	2:D:230:SER:HB2	2.22	0.40
4:F:204:TRP:CZ2	4:F:338:CYS:HA	2.56	0.40
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.56	0.40
2:B:19:LYS:HE3	2:B:19:LYS:HB3	1.66	0.40
2:B:273:LEU:HD23	2:B:273:LEU:HA	1.57	0.40
2:B:232:THR:O	2:B:236:VAL:HG13	2.22	0.40
1:C:338:LYS:HG2	1:C:338:LYS:O	2.22	0.40
3:E:95:LYS:HA	3:E:95:LYS:HD2	1.92	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	439/450 (98%)	427 (97%)	12 (3%)	0	100	100
1	C	446/450 (99%)	437 (98%)	9 (2%)	0	100	100
2	B	424/445 (95%)	412 (97%)	12 (3%)	0	100	100
2	D	416/445 (94%)	397 (95%)	19 (5%)	0	100	100
3	E	121/143 (85%)	119 (98%)	2 (2%)	0	100	100
4	F	343/384 (89%)	322 (94%)	21 (6%)	0	100	100
All	All	2189/2317 (94%)	2114 (97%)	75 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	371/378 (98%)	368 (99%)	3 (1%)	73	86
1	C	379/378 (100%)	368 (97%)	11 (3%)	37	60
2	B	370/383 (97%)	365 (99%)	5 (1%)	59	79
2	D	361/383 (94%)	342 (95%)	19 (5%)	20	36
3	E	112/127 (88%)	110 (98%)	2 (2%)	51	73
4	F	315/342 (92%)	305 (97%)	10 (3%)	34	56
All	All	1908/1991 (96%)	1858 (97%)	50 (3%)	45	63

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	193[A]	THR
1	A	193[B]	THR
1	A	381	THR
2	B	75	SER
2	B	126	SER
2	B	131	GLN
2	B	214	THR
2	B	236	VAL
1	C	151[A]	SER
1	C	151[B]	SER
1	C	165[A]	SER
1	C	165[B]	SER
1	C	178	SER
1	C	250	VAL
1	C	315[A]	CYS
1	C	315[B]	CYS
1	C	318	LEU
1	C	347[A]	CYS
1	C	347[B]	CYS
2	D	5	VAL
2	D	8	GLN
2	D	84	ILE
2	D	115	SER
2	D	116	VAL
2	D	145[A]	SER
2	D	177	ASP
2	D	180	VAL
2	D	193	VAL
2	D	221	THR
2	D	230	SER
2	D	236	VAL
2	D	238	THR
2	D	284	LEU
2	D	289	LEU
2	D	339	SER
2	D	372	SER
2	D	394	THR
2	D	421	SER
3	E	124	GLN
3	E	126	LYS
4	F	12	SER
4	F	225	SER

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Mol	Chain	Res	Type
4	F	255[A]	ARG
4	F	255[B]	ARG
4	F	271[A]	LEU
4	F	271[B]	LEU
4	F	296[A]	MET
4	F	296[B]	MET
4	F	353	VAL
4	F	373	SER

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	11	GLN
1	A	356	ASN
2	B	48	ASN
2	B	165	ASN
2	B	191	GLN
2	B	332	ASN
2	B	347	ASN
2	B	383	GLN
2	B	434	GLN
1	C	15	GLN
1	C	283	HIS
2	D	6	HIS
2	D	8	GLN
2	D	99	ASN
2	D	100	ASN
2	D	195	ASN
2	D	292	GLN
2	D	329	GLN
3	E	71	HIS
3	E	92	ASN
3	E	103	GLN
4	F	310	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 15 ligands modelled in this entry, 7 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
9	GDP	D	501	-	29,30,30	1.20	4 (13%)	45,47,47	1.81	6 (13%)
11	7PB	D	502	-	31,31,31	3.33	17 (54%)	42,42,42	4.65	21 (50%)
10	MES	B	503	-	12,12,12	1.05	1 (8%)	15,16,16	2.80	4 (26%)
5	GTP	A	501	6	33,34,34	1.24	2 (6%)	50,54,54	1.61	10 (20%)
9	GDP	B	501	6	29,30,30	1.06	1 (3%)	45,47,47	1.94	12 (26%)
11	7PB	B	505	-	31,31,31	2.55	12 (38%)	42,42,42	3.27	13 (30%)
5	GTP	C	501	6	33,34,34	0.91	2 (6%)	50,54,54	1.64	9 (18%)
10	MES	B	504	-	12,12,12	1.51	1 (8%)	15,16,16	2.64	8 (53%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GDP	D	501	-	-	4/16/32/32	0/3/3/3
11	7PB	D	502	-	-	0/18/20/20	0/4/4/4
10	MES	B	503	-	-	3/6/14/14	0/1/1/1
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GDP	B	501	6	-	3/16/32/32	0/3/3/3
11	7PB	B	505	-	-	1/18/20/20	0/4/4/4
5	GTP	C	501	6	-	7/22/38/38	0/3/3/3
10	MES	B	504	-	-	0/6/14/14	0/1/1/1

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	D	502	7PB	C08-N07	8.03	1.52	1.38
11	D	502	7PB	O27-C25	7.25	1.52	1.37
11	B	505	7PB	C08-N07	6.51	1.50	1.38
11	B	505	7PB	O27-C25	6.12	1.49	1.37
11	D	502	7PB	C21-N20	5.60	1.53	1.40
11	D	502	7PB	C18-N20	5.49	1.48	1.38
11	D	502	7PB	C10-N09	5.46	1.48	1.35
11	B	505	7PB	C21-N20	5.44	1.52	1.40
5	A	501	GTP	PB-O3B	5.06	1.65	1.59
11	D	502	7PB	C01-N09	4.70	1.51	1.41
10	B	504	MES	C8-S	4.30	1.83	1.77
11	D	502	7PB	C23-C22	4.27	1.46	1.38
11	B	505	7PB	C18-N20	3.87	1.45	1.38
11	B	505	7PB	C10-N09	3.75	1.44	1.35
11	D	502	7PB	C05-N07	3.64	1.48	1.40
11	B	505	7PB	C23-C24	3.50	1.44	1.38
11	D	502	7PB	O27-C28	3.48	1.52	1.42
11	D	502	7PB	C23-C24	3.29	1.44	1.38
9	D	501	GDP	C5-C4	3.21	1.47	1.38
11	D	502	7PB	C03-C04	3.17	1.44	1.38
11	D	502	7PB	C16-N15	3.04	1.39	1.33
11	B	505	7PB	C05-N07	2.89	1.47	1.40
11	D	502	7PB	C13-C12	2.78	1.58	1.48
9	B	501	GDP	C5-C4	2.78	1.46	1.38
11	D	502	7PB	C06-C05	2.66	1.43	1.39
11	B	505	7PB	C23-C22	2.61	1.43	1.38
11	D	502	7PB	C16-N17	2.50	1.38	1.33
9	D	501	GDP	PA-O3A	2.46	1.62	1.59
11	D	502	7PB	C02-C01	2.41	1.43	1.39
11	B	505	7PB	O27-C28	2.38	1.49	1.42
10	B	503	MES	C8-S	2.33	1.80	1.77
11	B	505	7PB	C16-N15	2.27	1.38	1.33
11	D	502	7PB	O14-C10	2.24	1.27	1.23
9	D	501	GDP	C6-N1	-2.22	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	B	505	7PB	C01-N09	2.19	1.46	1.41
5	A	501	GTP	C2-N3	2.18	1.38	1.33
5	C	501	GTP	C2-N3	2.18	1.38	1.33
9	D	501	GDP	C5-N7	-2.17	1.34	1.39
11	B	505	7PB	C03-C04	2.10	1.42	1.38
5	C	501	GTP	PB-O3B	2.06	1.61	1.59

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	D	502	7PB	C13-C11-C10	-23.03	94.73	117.24
11	B	505	7PB	C12-C11-C10	-12.66	104.86	117.24
11	B	505	7PB	C13-C11-C10	-10.56	106.92	117.24
11	D	502	7PB	C12-C11-C10	-9.24	108.21	117.24
11	B	505	7PB	N17-C16-N15	-8.19	116.18	128.58
10	B	503	MES	O3S-S-O1S	-7.63	92.31	111.40
11	D	502	7PB	N17-C16-N15	-7.40	117.38	128.58
9	D	501	GDP	C5-C4-N3	-6.08	118.72	128.39
11	D	502	7PB	C04-C05-C06	6.06	126.98	119.66
9	B	501	GDP	C5-C4-N3	-5.43	119.75	128.39
9	B	501	GDP	C2-N3-C4	5.34	121.49	112.30
10	B	504	MES	C5-N4-C3	5.33	120.33	108.84
11	D	502	7PB	C23-C22-C21	-5.10	113.85	119.73
9	D	501	GDP	C2-N3-C4	4.94	120.81	112.30
5	C	501	GTP	C5-C4-N3	-4.64	121.00	128.39
5	C	501	GTP	C2-N3-C4	4.60	120.22	112.30
5	A	501	GTP	C5-C4-N3	-4.49	121.25	128.39
11	D	502	7PB	C05-C06-C01	-4.46	112.86	119.67
10	B	503	MES	O3S-S-C8	4.46	114.73	106.00
11	D	502	7PB	C28-O27-C25	-4.35	108.17	117.50
9	B	501	GDP	N9-C4-N3	4.35	134.65	125.95
9	D	501	GDP	N9-C4-N3	4.34	134.62	125.95
11	B	505	7PB	O14-C10-C11	-4.33	115.50	122.19
11	D	502	7PB	C01-N09-C10	-4.26	117.64	127.37
5	A	501	GTP	C2-N3-C4	4.13	119.41	112.30
10	B	504	MES	O3S-S-O2S	-4.12	101.09	111.40
10	B	503	MES	O1S-S-C8	4.03	112.82	106.73
10	B	504	MES	C6-C5-N4	3.88	116.02	110.12
9	B	501	GDP	C6-C5-N7	3.67	136.98	130.29
11	D	502	7PB	C02-C01-N09	-3.53	108.56	120.41
11	B	505	7PB	C04-C05-C06	3.37	123.73	119.66
11	D	502	7PB	C02-C01-C06	3.33	123.68	119.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	D	501	GDP	C6-C5-N7	3.32	136.33	130.29
5	A	501	GTP	C8-N7-C5	3.17	109.91	104.26
5	C	501	GTP	O2A-PA-O3A	3.16	115.81	107.27
10	B	504	MES	O2S-S-C8	3.10	111.41	106.73
11	D	502	7PB	C03-C04-C05	-3.06	116.20	119.73
11	D	502	7PB	C04-C05-N07	-3.03	110.34	120.61
11	D	502	7PB	C22-C23-C24	3.03	124.14	120.24
10	B	503	MES	C5-N4-C3	3.02	115.35	108.84
5	C	501	GTP	N9-C8-N7	-3.01	107.82	113.40
9	B	501	GDP	O6-C6-C5	-2.99	118.64	126.53
5	A	501	GTP	N9-C8-N7	-2.97	107.89	113.40
5	C	501	GTP	C8-N7-C5	2.92	109.46	104.26
11	B	505	7PB	C11-C10-N09	2.91	120.78	115.16
10	B	504	MES	C2-C3-N4	2.83	114.42	110.12
9	D	501	GDP	C4-C5-N7	-2.82	106.20	110.67
11	B	505	7PB	C21-N20-C18	-2.81	121.52	128.75
5	A	501	GTP	O2A-PA-O3A	2.81	114.86	107.27
11	B	505	7PB	C05-C06-C01	-2.76	115.45	119.67
10	B	504	MES	C7-N4-C5	-2.75	103.91	111.24
5	C	501	GTP	C2-N1-C6	-2.75	120.12	125.11
11	B	505	7PB	C02-C01-C06	2.70	122.92	119.66
10	B	504	MES	C7-N4-C3	-2.66	104.16	111.24
5	A	501	GTP	C4-C5-N7	-2.65	106.47	110.67
11	B	505	7PB	C19-C08-N15	-2.65	119.45	122.92
9	B	501	GDP	C4-C5-N7	-2.60	106.55	110.67
5	A	501	GTP	C5'-C4'-C3'	-2.60	105.87	115.21
11	D	502	7PB	C21-N20-C18	-2.51	122.30	128.75
11	B	505	7PB	C16-N15-C08	2.48	123.37	115.25
11	B	505	7PB	C01-N09-C10	-2.43	121.83	127.37
5	A	501	GTP	N9-C4-N3	2.42	130.79	125.95
11	D	502	7PB	C21-C26-C25	2.42	122.74	119.18
11	B	505	7PB	C05-N07-C08	-2.39	122.61	128.75
11	D	502	7PB	C11-C10-N09	2.38	119.75	115.16
11	D	502	7PB	C19-C08-N15	-2.37	119.80	122.92
5	C	501	GTP	C5-C6-N1	2.36	119.26	113.25
9	B	501	GDP	C8-N7-C5	2.35	108.45	104.26
11	D	502	7PB	C06-C01-N09	2.35	127.76	120.13
11	D	502	7PB	C16-N15-C08	2.34	122.92	115.25
5	C	501	GTP	C4-C5-N7	-2.34	106.96	110.67
9	D	501	GDP	O2A-PA-O3A	2.28	113.44	107.27
5	C	501	GTP	N9-C4-N3	2.25	130.44	125.95
10	B	504	MES	O3S-S-C8	2.21	110.33	106.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	501	GDP	N9-C8-N7	-2.20	109.31	113.40
5	A	501	GTP	O2B-PB-O3A	2.17	113.13	107.27
9	B	501	GDP	C8-N9-C4	2.16	110.08	106.03
9	B	501	GDP	O2B-PB-O3A	2.14	111.81	104.64
11	D	502	7PB	O14-C10-C11	-2.12	118.92	122.19
5	A	501	GTP	C2-N1-C6	-2.11	121.29	125.11
11	D	502	7PB	C13-C11-C12	2.10	62.04	58.80
9	B	501	GDP	O4'-C1'-N9	-2.05	103.70	108.36
9	B	501	GDP	C5-C6-N1	2.03	118.42	113.25

There are no chirality outliers.

All (24) torsion outliers are listed below:

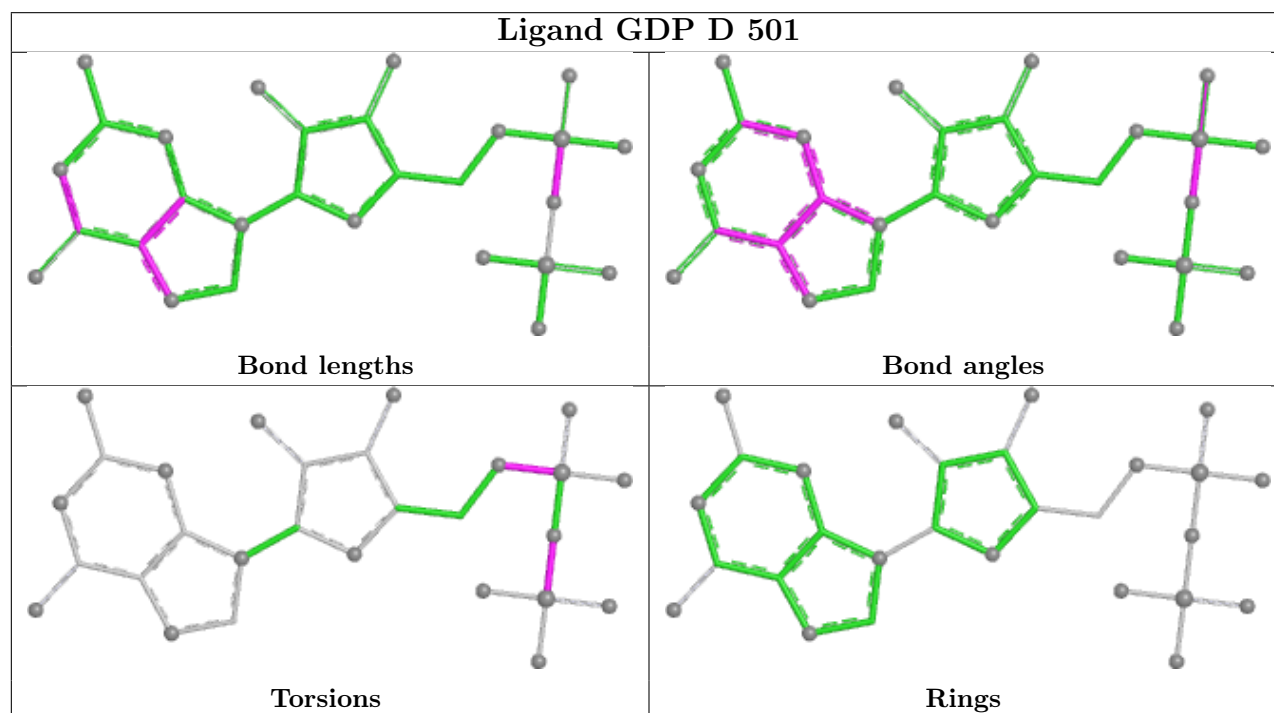
Mol	Chain	Res	Type	Atoms
5	A	501	GTP	C5'-O5'-PA-O3A
5	A	501	GTP	C5'-O5'-PA-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O1A
9	B	501	GDP	C5'-O5'-PA-O2A
9	D	501	GDP	C5'-O5'-PA-O3A
9	D	501	GDP	C5'-O5'-PA-O1A
9	D	501	GDP	C5'-O5'-PA-O2A
10	B	503	MES	C7-C8-S-O3S
10	B	503	MES	C7-C8-S-O1S
10	B	503	MES	C7-C8-S-O2S
5	A	501	GTP	PB-O3B-PG-O1G
9	D	501	GDP	PA-O3A-PB-O3B
5	C	501	GTP	C4'-C5'-O5'-PA
11	B	505	7PB	C19-C08-N07-C05
5	A	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3A-PA-O2A

There are no ring outliers.

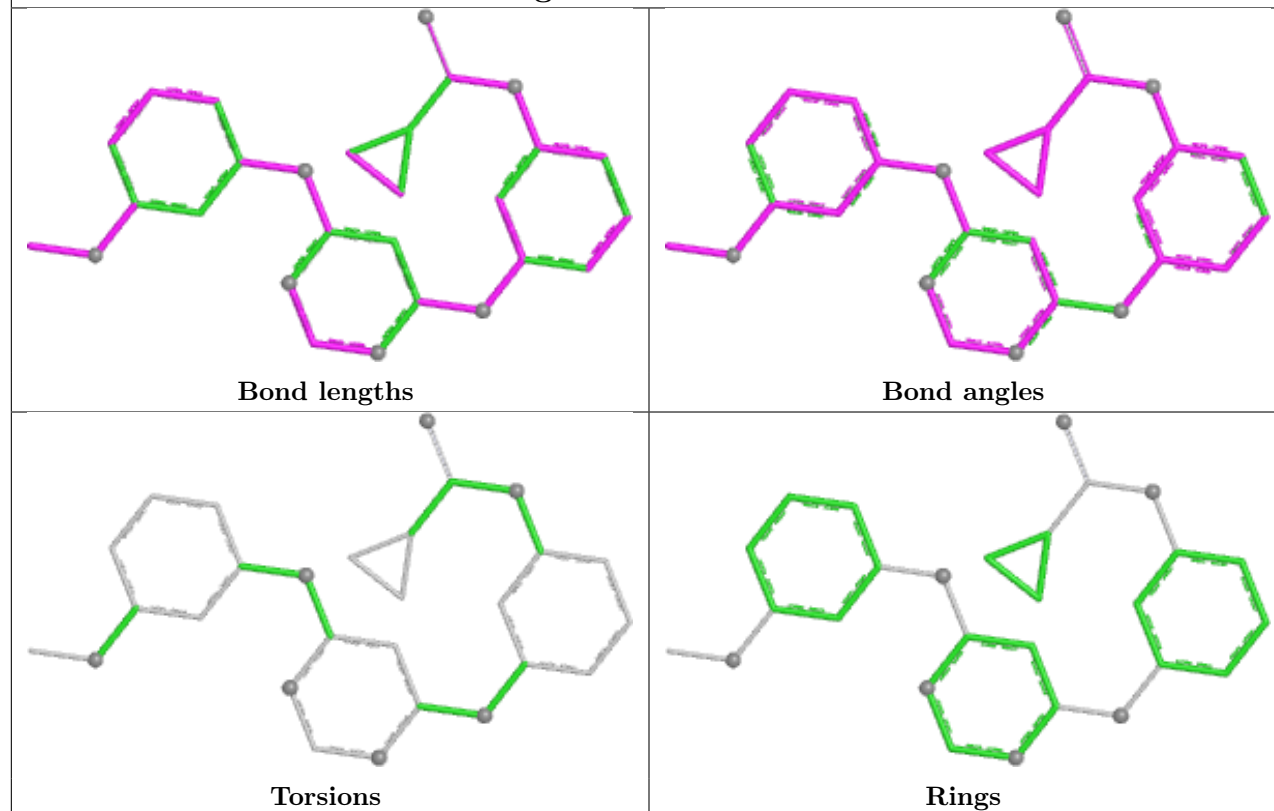
7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	D	501	GDP	1	0
11	D	502	7PB	2	0
10	B	503	MES	3	0
5	A	501	GTP	2	0
9	B	501	GDP	1	0
11	B	505	7PB	1	0
10	B	504	MES	1	0

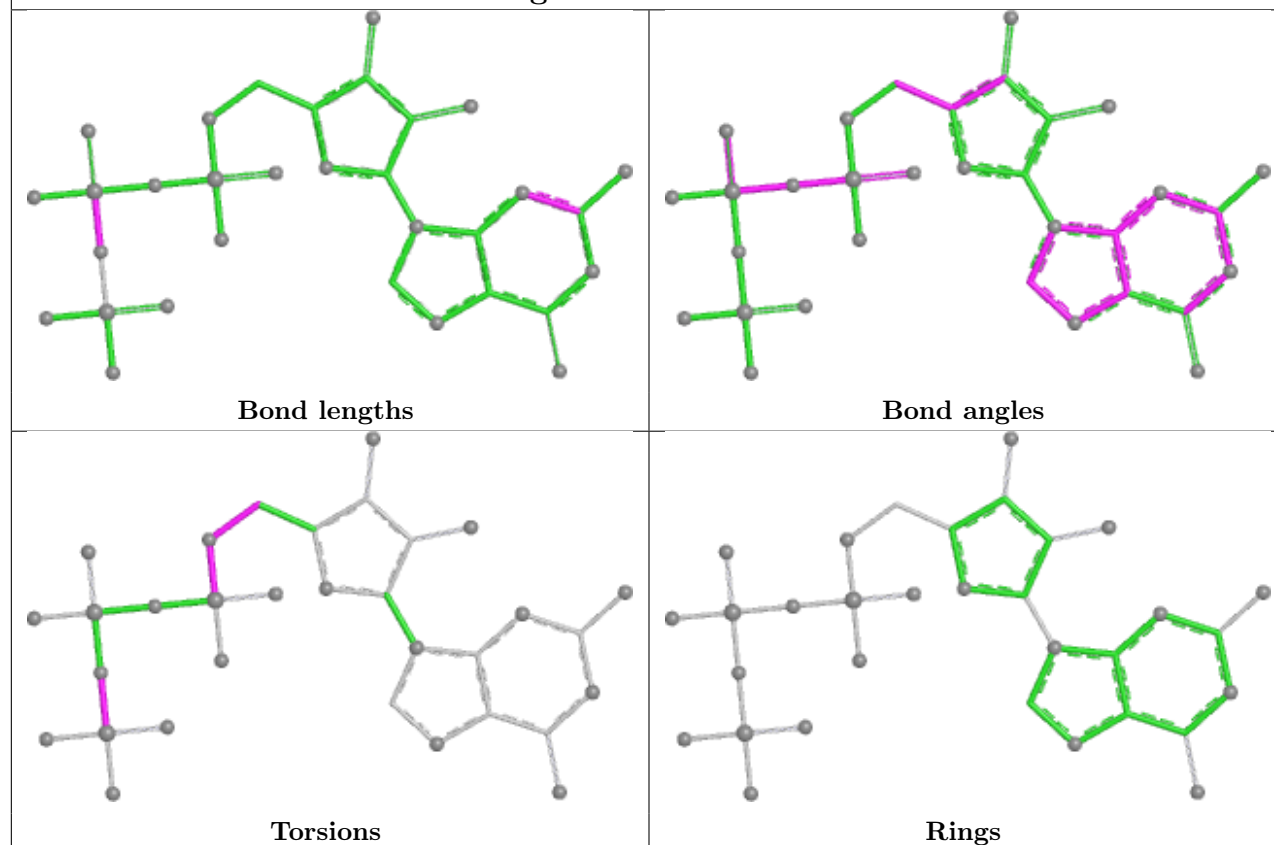
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

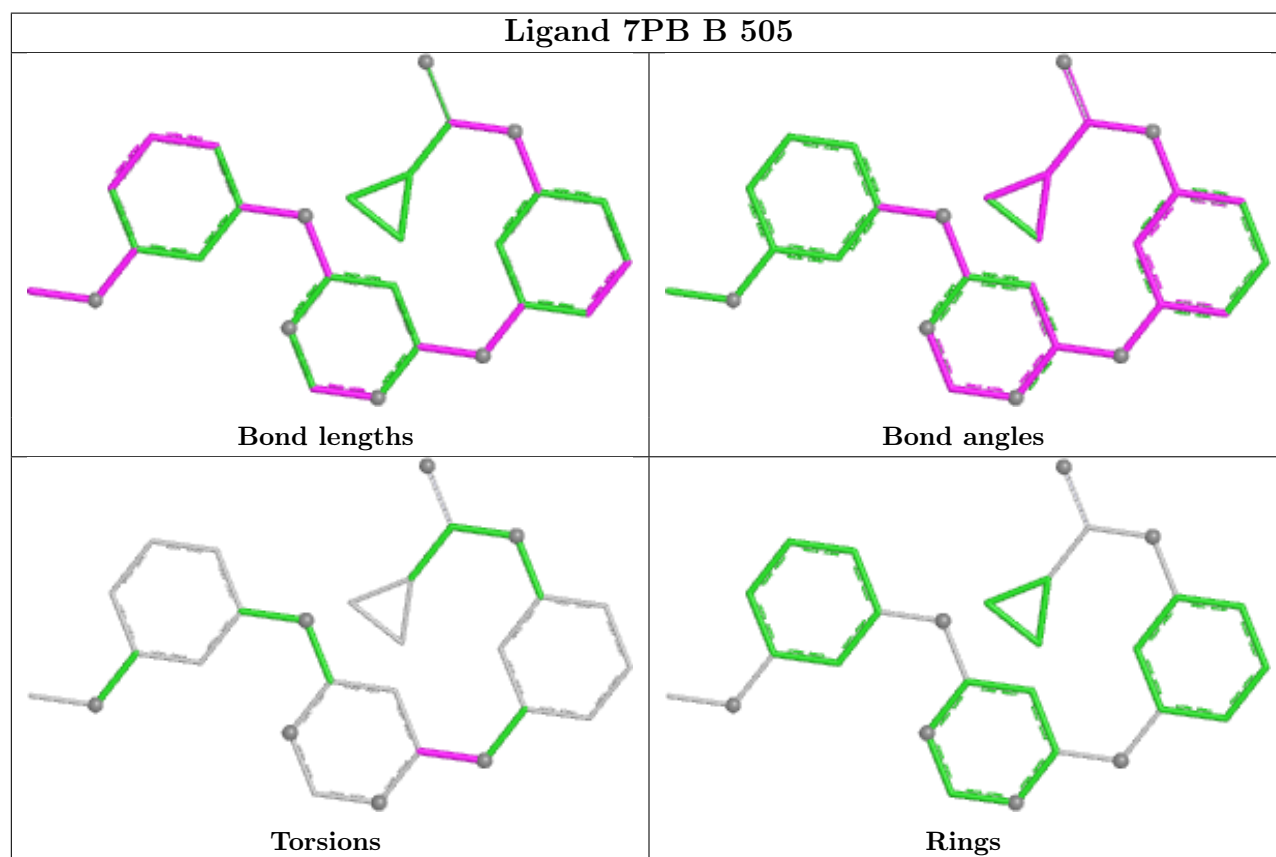
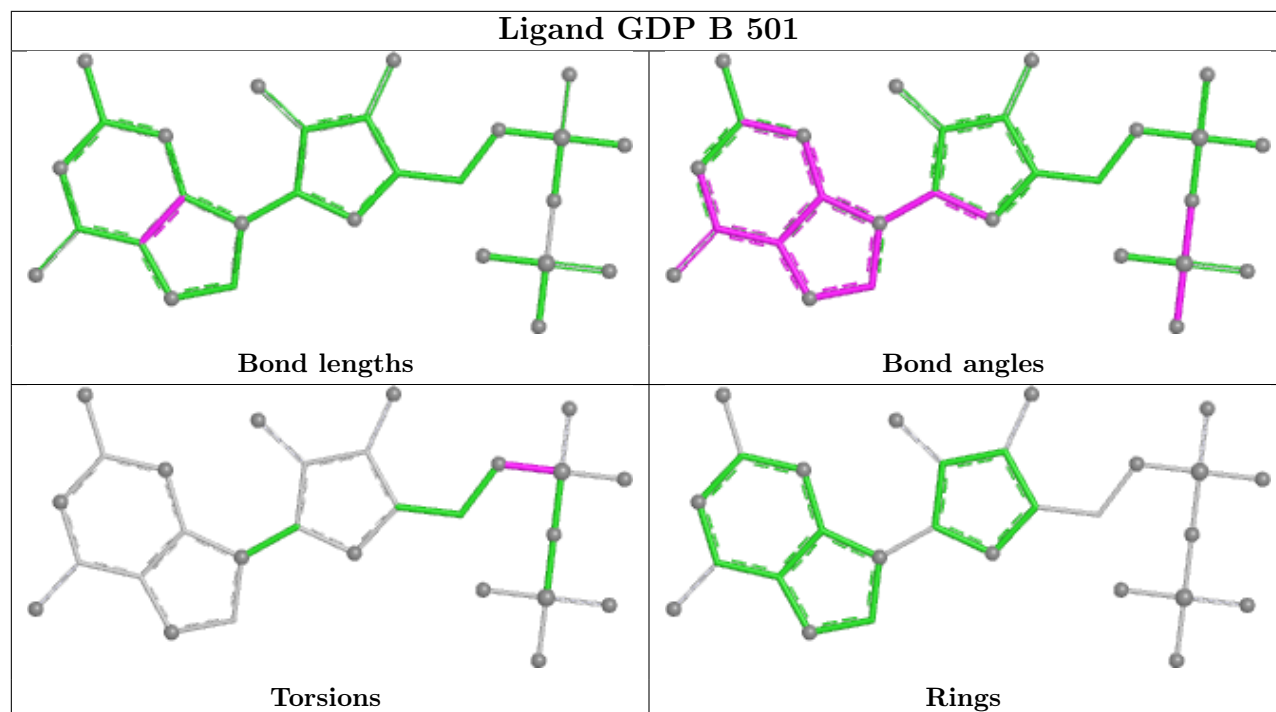


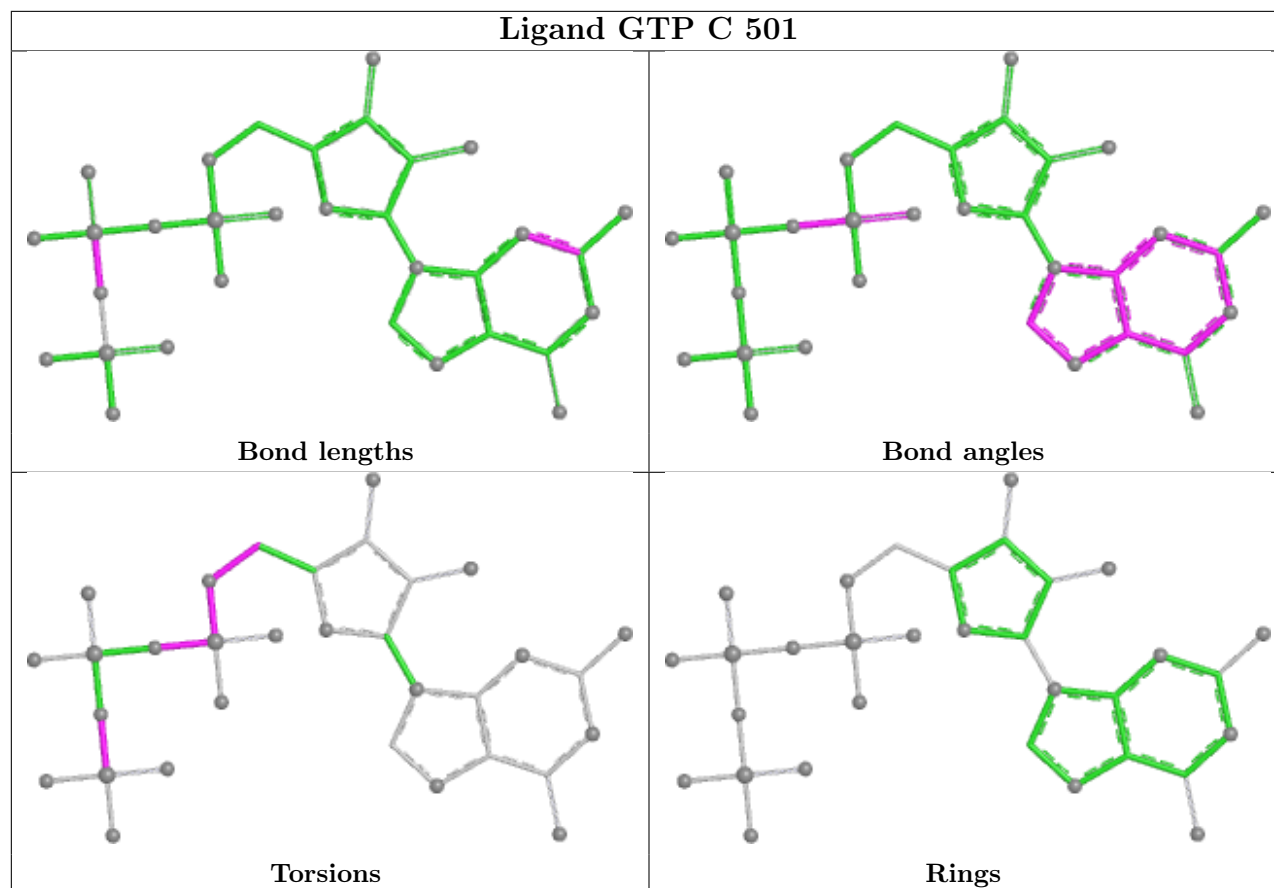
Ligand 7PB D 502



Ligand GTP A 501







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	437/450 (97%)	0.45	15 (3%)	48 44	31, 53, 74, 89	4 (0%)
1	C	440/450 (97%)	0.21	14 (3%)	50 46	27, 46, 68, 88	8 (1%)
2	B	424/445 (95%)	0.41	20 (4%)	36 32	26, 51, 78, 116	7 (1%)
2	D	420/445 (94%)	1.42	110 (26%)	1 1	44, 75, 99, 126	2 (0%)
3	E	123/143 (86%)	1.29	22 (17%)	3 3	35, 74, 104, 130	2 (1%)
4	F	346/384 (90%)	1.27	92 (26%)	1 1	36, 77, 142, 163	5 (1%)
All	All	2190/2317 (94%)	0.76	273 (12%)	8 6	26, 59, 104, 163	28 (1%)

All (273) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	169	LEU	7.8
2	D	402	PHE	5.4
2	B	57	ASN	5.3
4	F	225	SER	5.2
3	E	143	ALA	4.7
2	D	140	GLY	4.7
4	F	240	LEU	4.7
2	B	281	TYR	4.7
2	D	73	MET	4.6
4	F	245	ILE	4.4
1	A	262	TYR	4.3
2	D	54	ALA	4.3
2	D	39	ASP	4.2
1	C	338	LYS	4.2
4	F	166	ALA	4.1
2	D	72	THR	4.1
3	E	28	SER	4.0
4	F	161	LEU	4.0
4	F	125	THR	4.0

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Mol	Chain	Res	Type	RSRZ
1	C	340	SER	4.0
2	D	401	ALA	4.0
4	F	173	ILE	4.0
1	C	282	TYR	3.9
2	D	37	HIS	3.9
4	F	239	HIS	3.9
4	F	170	LEU	3.8
2	D	284	LEU	3.8
2	D	99	ASN	3.8
2	D	55	THR	3.7
4	F	372	THR	3.7
3	E	6	MET	3.7
2	D	92	PHE	3.7
4	F	146	VAL	3.7
2	D	219	THR	3.7
4	F	132	LEU	3.6
2	B	247	ASN	3.6
2	D	411	MET	3.5
2	D	84	ILE	3.5
1	C	283	HIS	3.5
4	F	380	HIS	3.5
2	B	283	ALA	3.4
2	D	36	TYR	3.4
4	F	362	ALA	3.4
2	D	141	GLY	3.4
4	F	249	TYR	3.4
2	D	175	VAL	3.4
2	D	212	PHE	3.3
4	F	233	PHE	3.3
4	F	158	GLU	3.2
4	F	244	CYS	3.2
4	F	237	THR	3.2
3	E	61	ARG	3.2
2	D	16	ILE	3.2
2	D	394	THR	3.2
2	B	436	ALA	3.1
1	C	440	VAL	3.1
4	F	179	VAL	3.1
1	A	196	GLU	3.1
2	D	416	PHE	3.1
4	F	100	ILE	3.1
2	D	101	TRP	3.1

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Mol	Chain	Res	Type	RSRZ
2	D	97	ALA	3.1
3	E	62	LYS	3.1
2	D	215	LEU	3.1
4	F	242	ASN	3.0
4	F	102	PRO	3.0
2	D	117	LEU	3.0
4	F	228	TYR	3.0
4	F	144	GLY	3.0
4	F	90	SER	3.0
2	D	44	LEU	2.9
2	D	93	GLY	2.9
4	F	252	ASN	2.9
4	F	346	LEU	2.9
2	D	220	PRO	2.9
4	F	28	LYS	2.9
2	D	405	TRP	2.9
2	D	395	ALA	2.8
4	F	231	ALA	2.8
2	B	72	THR	2.8
4	F	101	TYR	2.8
4	F	186	LEU	2.8
2	D	302	ALA	2.8
4	F	168	GLU	2.8
2	D	404	HIS	2.8
2	B	274	THR	2.8
4	F	99	VAL	2.8
2	D	57	ASN	2.7
2	D	439	ASP	2.7
4	F	160	ILE	2.7
4	F	229	ASN	2.7
1	A	104	ALA	2.7
1	C	43	GLY	2.7
2	D	82	GLY	2.7
1	A	346	TRP	2.7
2	D	81	PHE	2.7
2	D	29	GLY	2.7
2	B	275	SER	2.7
1	A	1	MET	2.7
3	E	119	MET	2.7
1	A	282	TYR	2.7
2	D	245	GLN	2.7
2	D	85	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
4	F	375	PHE	2.7
2	D	180	VAL	2.7
4	F	130	VAL	2.7
2	D	80	PRO	2.7
2	B	282	ARG	2.7
2	D	369	LEU	2.7
4	F	133	ALA	2.6
4	F	253	TYR	2.6
4	F	263	PHE	2.6
2	D	66	VAL	2.6
2	D	76	VAL	2.6
2	D	427	VAL	2.6
1	C	341	ILE	2.6
2	D	227	HIS	2.6
2	D	273	LEU	2.6
3	E	68	LEU	2.6
2	D	98	GLY	2.6
4	F	103	THR	2.6
4	F	162	ILE	2.6
2	B	2	ARG	2.6
2	D	412	ASP	2.6
2	D	144	GLY	2.6
2	D	126	SER	2.6
1	C	163	LYS	2.6
2	D	48	ASN	2.6
4	F	235	ASP	2.6
2	B	55	THR	2.6
3	E	139	LEU	2.5
2	D	100	ASN	2.5
4	F	131	PHE	2.5
4	F	199	PHE	2.5
2	D	30	ILE	2.5
2	B	280	GLN	2.5
2	D	102	ALA	2.5
4	F	259	GLY	2.5
4	F	241	THR	2.5
2	D	320	ARG	2.5
4	F	256	TYR	2.5
3	E	57	ALA	2.5
4	F	149	ALA	2.5
2	D	38	GLY	2.5
2	D	214	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	418	PHE	2.5
2	D	399	ARG	2.5
4	F	182	ILE	2.5
2	D	208	TYR	2.5
2	D	56	GLY	2.5
2	D	104	GLY	2.5
1	A	179	THR	2.4
2	B	214	THR	2.4
2	D	156	ARG	2.4
1	C	177	VAL	2.4
1	A	46	ASP	2.4
2	D	195	ASN	2.4
2	D	2	ARG	2.4
4	F	177	GLY	2.4
4	F	194	PRO	2.4
2	D	221	THR	2.4
2	D	90	PHE	2.4
4	F	150	LYS	2.4
4	F	247	LYS	2.4
1	C	128	GLN	2.4
4	F	226	GLU	2.4
4	F	159	GLY	2.4
4	F	164	SER	2.4
4	F	250	SER	2.4
2	D	23	VAL	2.4
4	F	296[A]	MET	2.4
2	D	11	GLN	2.4
3	E	48	GLU	2.4
3	E	135	LYS	2.3
2	D	169	VAL	2.3
4	F	13	VAL	2.3
3	E	120	LEU	2.3
4	F	232	ASN	2.3
4	F	135	TYR	2.3
2	D	218	THR	2.3
2	D	323	MET	2.3
4	F	224	SER	2.3
2	D	356	ILE	2.3
2	D	179	VAL	2.3
4	F	104	ASN	2.3
3	E	27	PRO	2.3
4	F	227	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
2	D	406	TYR	2.3
2	D	172	SER	2.3
2	D	94	GLN	2.3
2	D	42	LEU	2.3
2	D	12	CYS	2.3
4	F	230	SER	2.3
4	F	89	GLU	2.3
2	B	16[A]	ILE	2.3
2	B	284	LEU	2.2
2	D	393	PHE	2.2
1	A	281	ALA	2.2
2	D	238	THR	2.2
3	E	138	GLU	2.2
1	A	54	SER	2.2
4	F	178	GLN	2.2
4	F	181	VAL	2.2
1	A	89	PRO	2.2
1	C	1	MET	2.2
2	D	87	PRO	2.2
4	F	254	GLY	2.2
2	D	7	ILE	2.2
2	D	68	LEU	2.2
2	D	187	LEU	2.2
1	A	437	VAL	2.2
2	D	67	ASP	2.2
4	F	197	ARG	2.2
2	D	83	GLN	2.2
4	F	243	HIS	2.2
1	C	357	TYR	2.2
2	D	59	TYR	2.2
3	E	45	PRO	2.2
1	C	285	GLN	2.2
4	F	196	HIS	2.2
1	C	179	THR	2.2
2	D	95	SER	2.2
4	F	152	SER	2.2
3	E	133	VAL	2.1
4	F	6	VAL	2.1
2	D	125	GLU	2.1
2	D	370	LYS	2.1
3	E	59	GLU	2.1
4	F	257	GLU	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	291	GLN	2.1
2	D	18	ALA	2.1
2	B	300	MET	2.1
3	E	54	LEU	2.1
4	F	198	LYS	2.1
3	E	7	GLU	2.1
2	D	40	SER	2.1
4	F	223	THR	2.1
4	F	236	LYS	2.1
2	B	48	ASN	2.1
2	B	37	HIS	2.1
3	E	115[A]	HIS	2.1
4	F	321	VAL	2.1
4	F	73	ARG	2.1
4	F	238	CYS	2.1
2	D	438	ALA	2.1
4	F	184	LYS	2.1
2	D	170	MET	2.1
4	F	320	MET	2.1
2	D	385	LEU	2.1
2	D	403	LEU	2.1
2	D	41	ASP	2.1
2	D	161	ASP	2.1
4	F	148	ILE	2.1
2	B	80	PRO	2.1
2	D	222	TYR	2.1
2	D	400	LYS	2.0
3	E	65	GLU	2.0
3	E	66	ALA	2.0
2	D	5	VAL	2.0
2	D	60	VAL	2.0
2	D	398	ARG	2.0
4	F	139	ARG	2.0
2	D	142	GLY	2.0
2	B	92	PHE	2.0
2	D	216	LYS	2.0
4	F	262	MET	2.0
4	F	163	SER	2.0
1	A	47	ASP	2.0
2	D	77	ARG	2.0
2	D	171	PRO	2.0
4	F	31	ARG	2.0

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Mol	Chain	Res	Type	RSRZ
4	F	142	ARG	2.0
1	A	338	LYS	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](#)

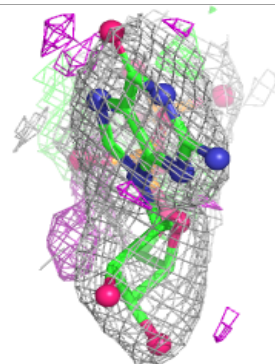
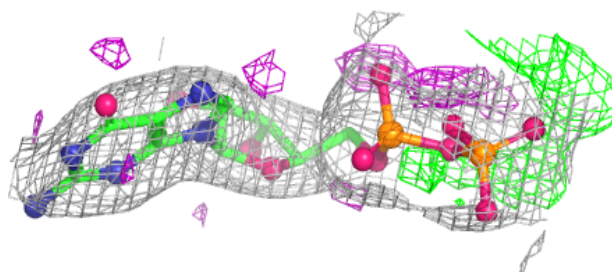
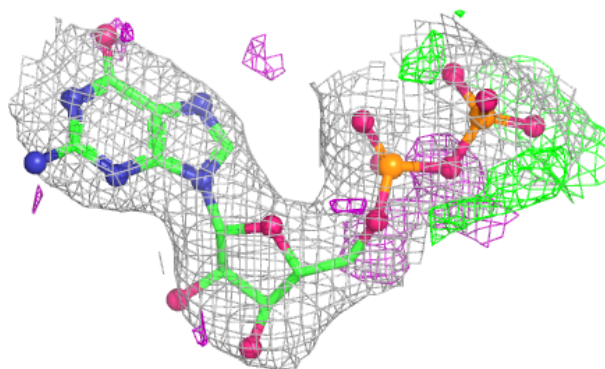
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	CL	D	503	1/1	0.72	0.47	120,120,120,120	0
9	GDP	D	501	28/28	0.86	0.14	67,74,85,88	0
10	MES	B	503	12/12	0.90	0.12	45,59,77,81	0
11	7PB	D	502	28/28	0.93	0.12	51,63,68,70	0
11	7PB	B	505	28/28	0.95	0.11	38,49,57,58	0
7	CA	A	503	1/1	-	-	73,73,73,73	1
10	MES	B	504	12/12	0.96	0.10	57,65,71,80	0
8	CL	A	504	1/1	-	-	74,74,74,74	1
7	CA	C	503	1/1	0.96	0.04	59,59,59,59	0
6	MG	B	502	1/1	0.96	0.05	36,36,36,36	0
5	GTP	A	501	32/32	0.97	0.06	35,43,47,51	0
9	GDP	B	501	28/28	0.98	0.06	34,42,47,51	0
5	GTP	C	501	32/32	0.98	0.05	33,40,43,49	0
6	MG	A	502	1/1	0.99	0.04	47,47,47,47	0
6	MG	C	502	1/1	0.99	0.02	41,41,41,41	0

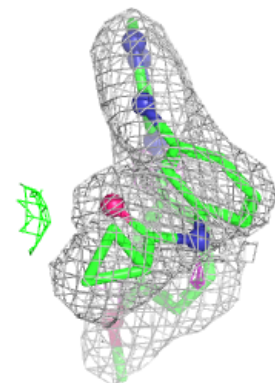
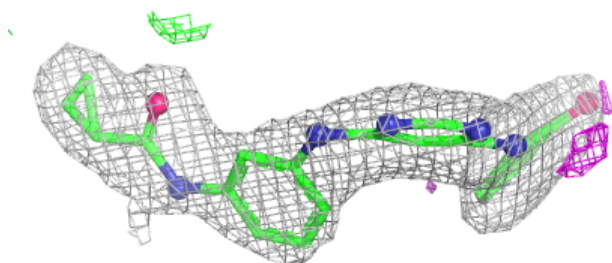
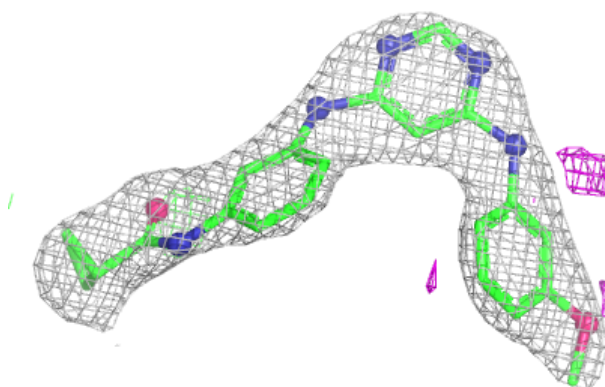
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP D 501:

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

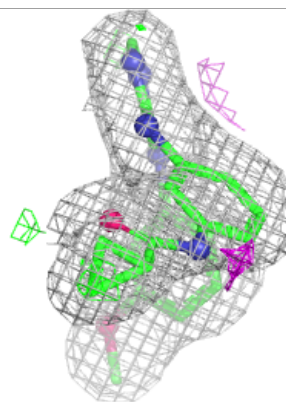
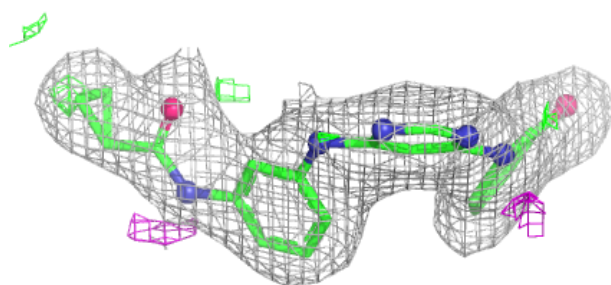
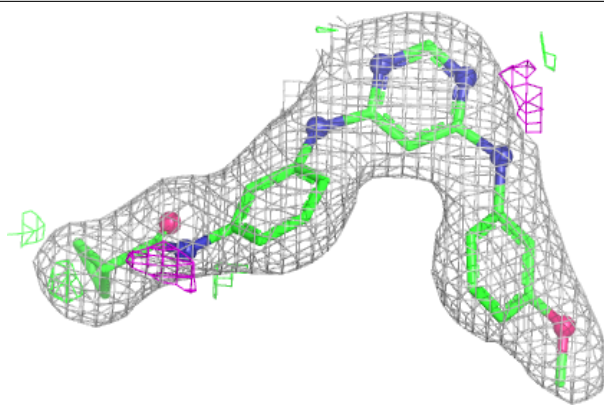
**Electron density around 7PB D 502:**

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

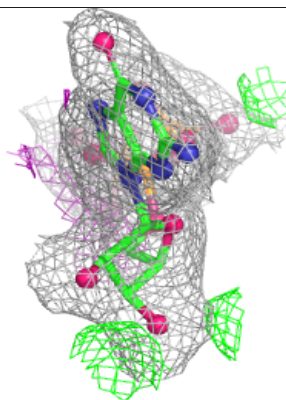
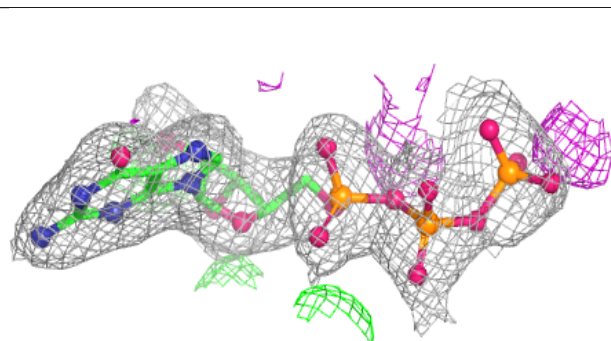
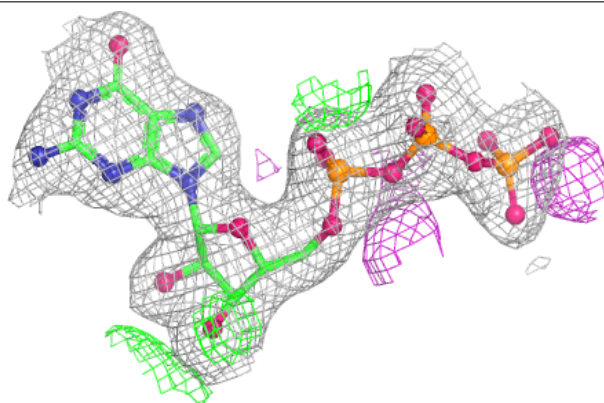


Electron density around 7PB B 505:

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

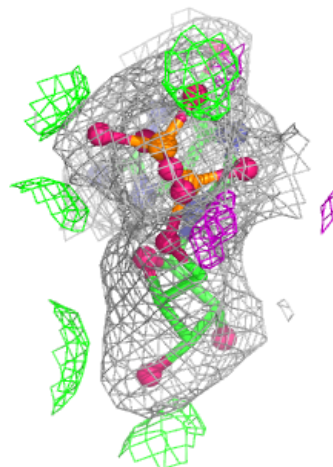
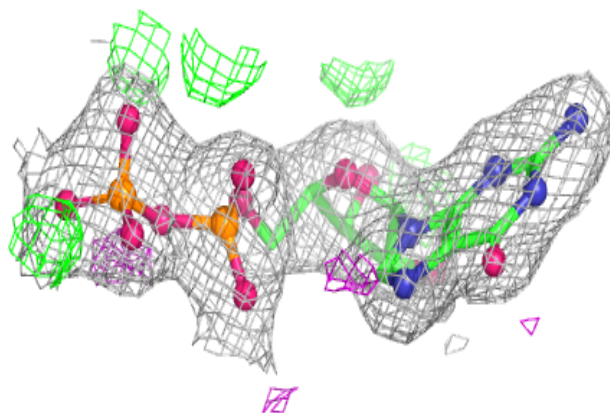
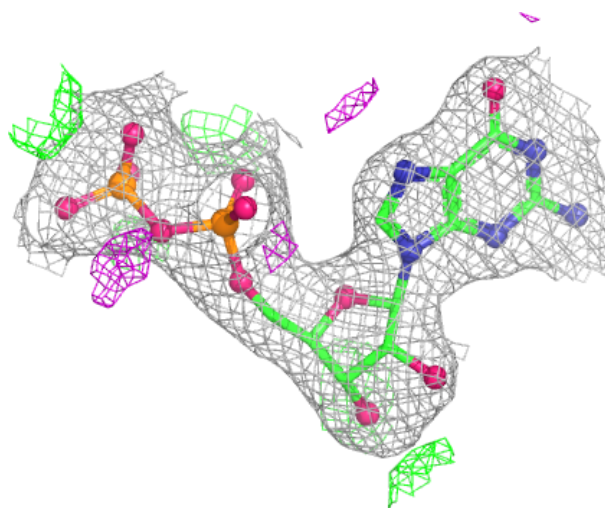
**Electron density around GTP A 501:**

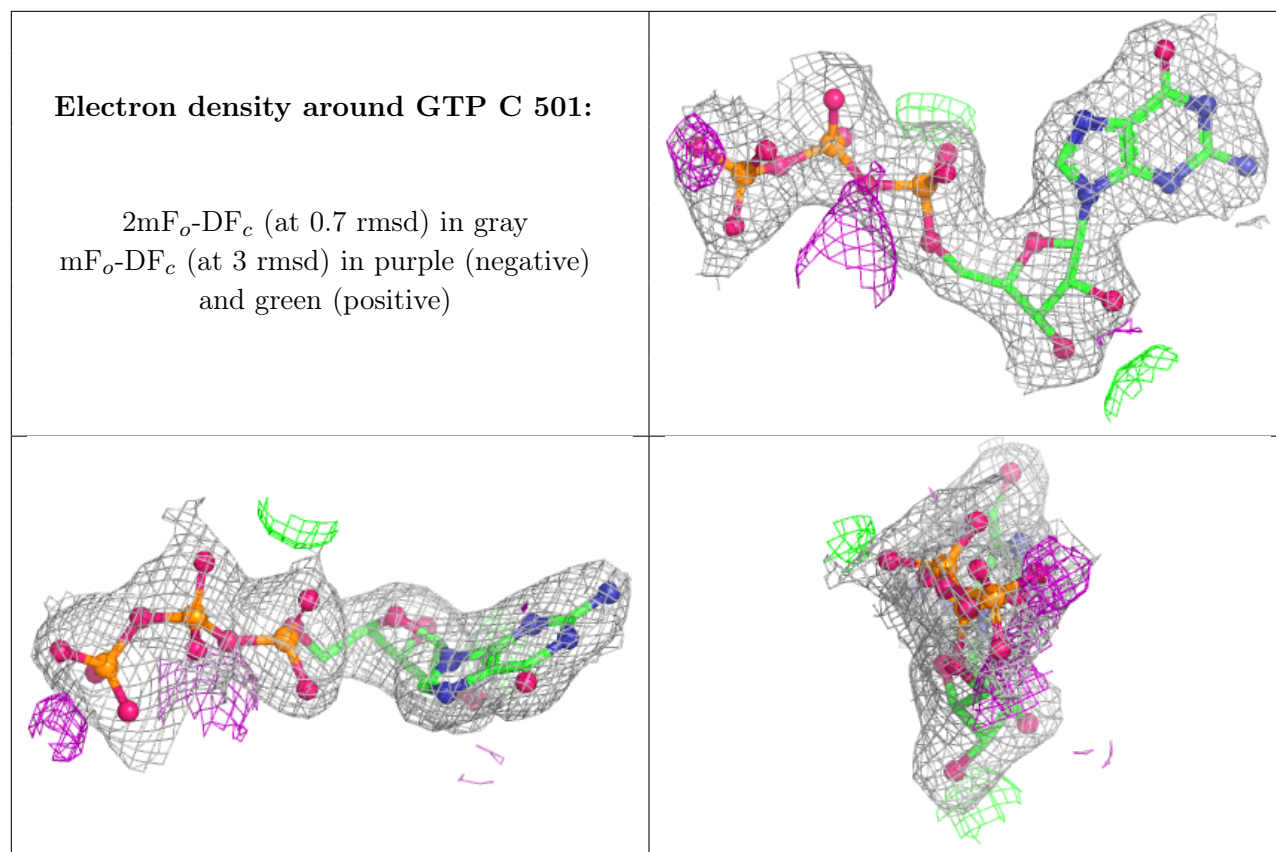
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 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.