



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 26, 2026 – 09:05 AM EDT

PDB ID : 7VMK / pdb_00007vmk
Title : Crystal structure of tubulin with 3
Authors : Jifa, Z.; Lun, T.
Deposited on : 2021-10-08
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:

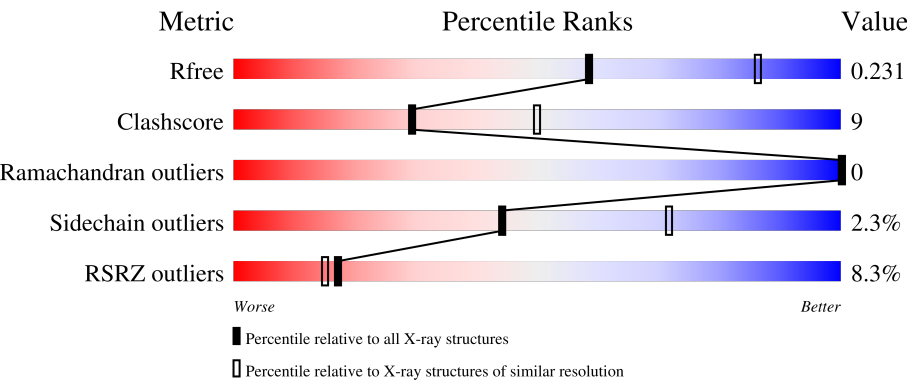
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal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

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	450	2% 80% 18%
1	C	450	% 83% 14%
2	B	445	4% 79% 16%
2	D	445	11% 67% 27% 5%
3	E	143	9% 72% 14% 14%

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Mol	Chain	Length	Quality of chain
4	F	384	24% 68% 23% 9%

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17937 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	439	Total	C	N	O	S	0	6	0
			3458	2188	587	659	24			
1	C	440	Total	C	N	O	S	0	8	0
			3467	2195	585	661	26			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	425	Total	C	N	O	S	0	4	0
			3378	2122	580	649	27			
2	D	421	Total	C	N	O	S	0	2	0
			3309	2080	562	641	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	3	0
			1031	636	187	203	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 Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	351	Total	C	N	O	S	0	4	0
			2909	1867	502	525	15			

There are 6 discrepancies between the modelled and reference sequences:

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

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



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

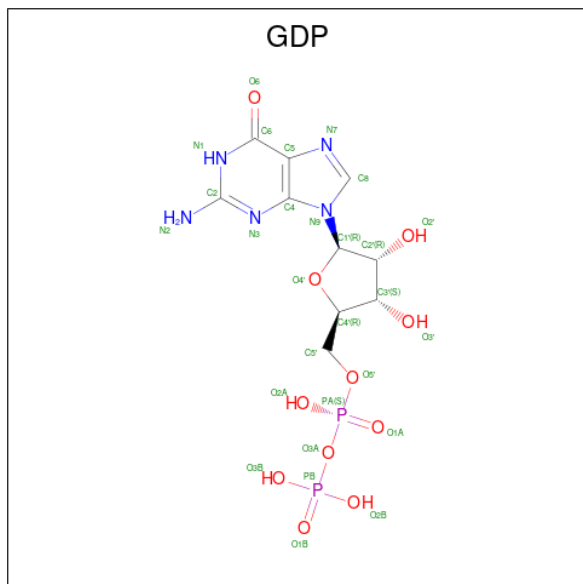
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: $C_{10}H_{15}N_5O_{11}P_2$).



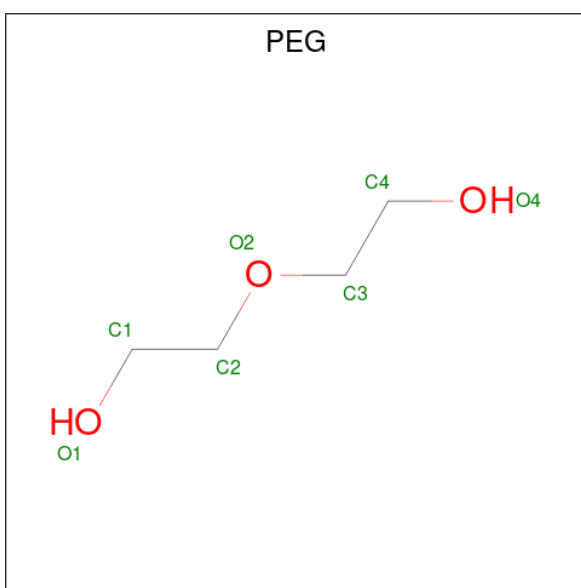
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N O P 28 10 5 11 2	0	0
8	D	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 9 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



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

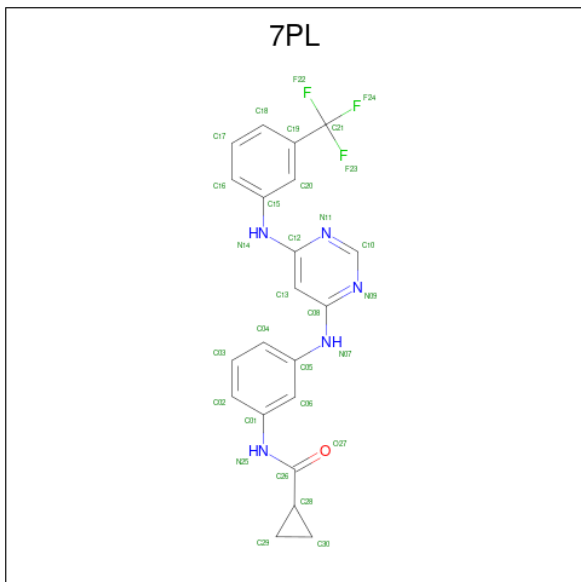
- Molecule 10 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	B	1	Total	C	O	0	0
			7	4	3		

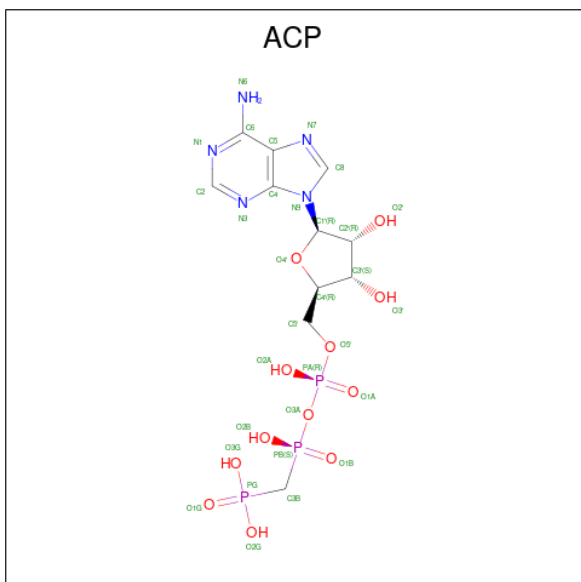
- Molecule 11 is N-[3-[[[6-[[3-(trifluoromethyl)phenyl]amino]pyrimidin-4-yl]amino]phenyl]c

cyclopropanecarboxamide (CCD ID: 7PL) (formula: $\text{C}_{21}\text{H}_{18}\text{F}_3\text{N}_5\text{O}$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	F	N	O	0	0
			30	21	3	5	1		

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $\text{C}_{11}\text{H}_{18}\text{N}_5\text{O}_{12}\text{P}_3$).



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

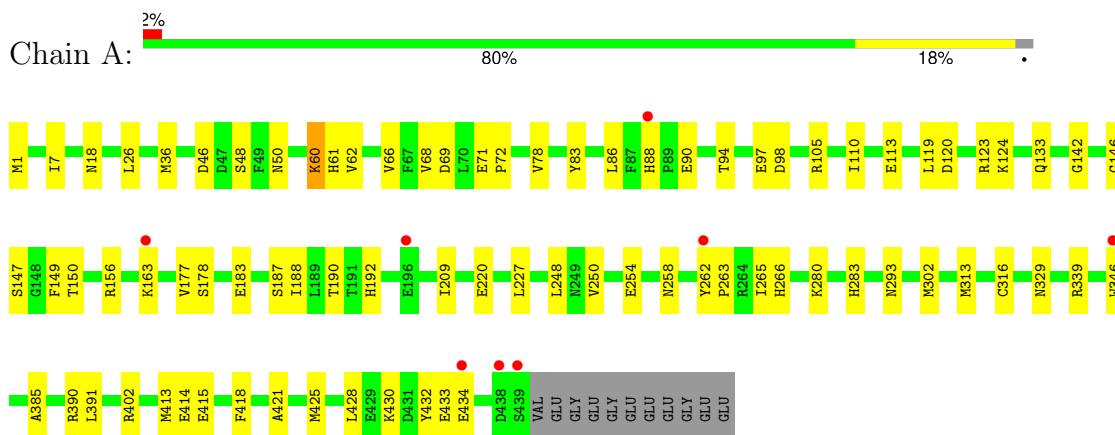
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	30	Total 30	O 30	0	0
13	B	38	Total 38	O 38	0	0
13	C	81	Total 81	O 81	0	0
13	D	10	Total 10	O 10	0	0
13	E	3	Total 3	O 3	0	0
13	F	3	Total 3	O 3	0	0

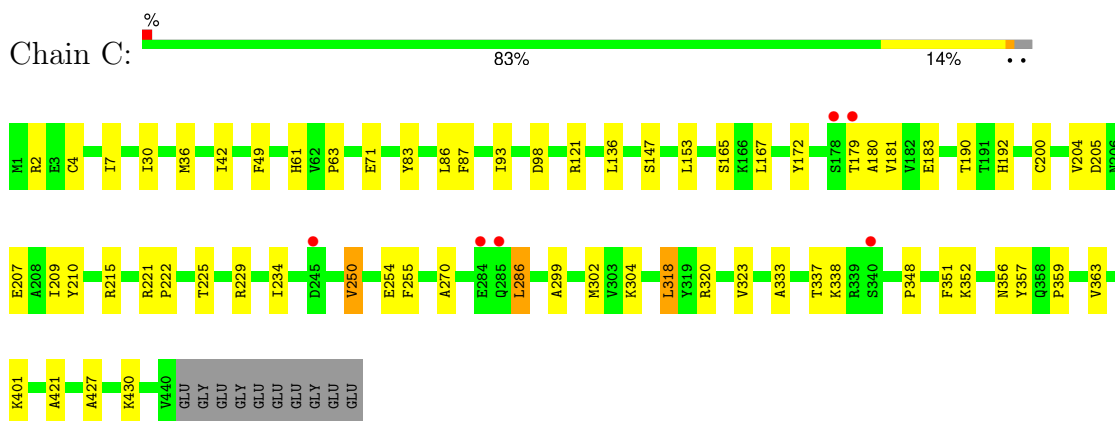
3 Residue-property plots [i](#)

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

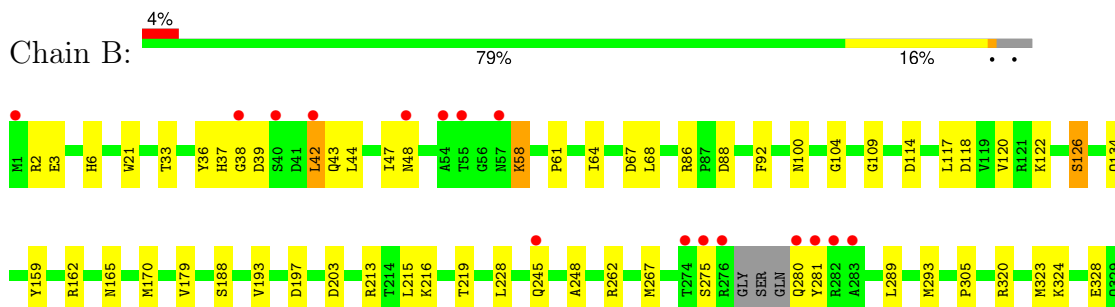
- Molecule 1: Tubulin alpha-1B chain



- Molecule 1: Tubulin alpha-1B chain

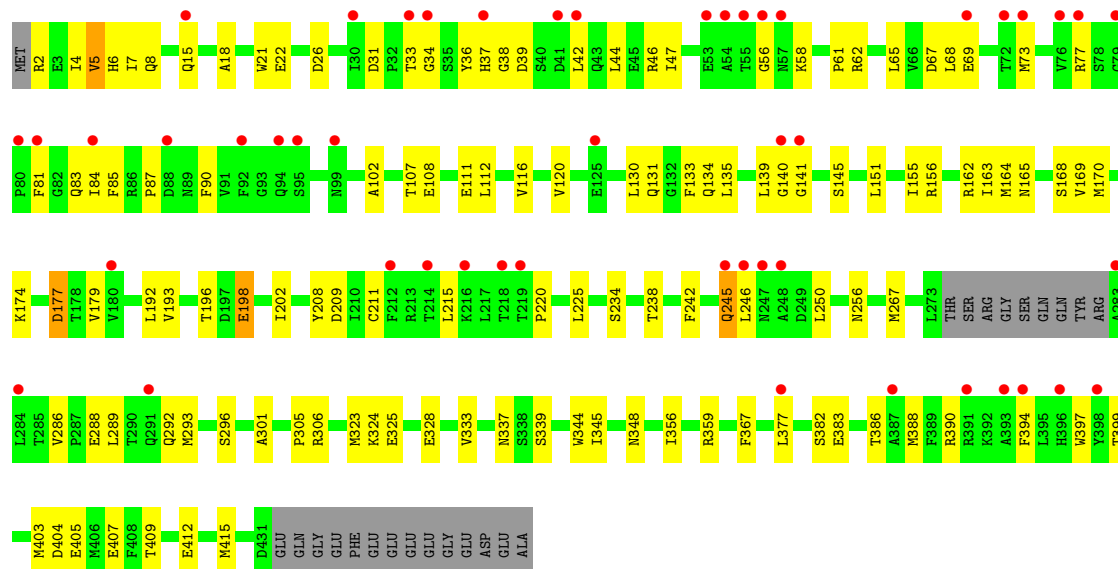


- Molecule 2: Tubulin beta-2B chain

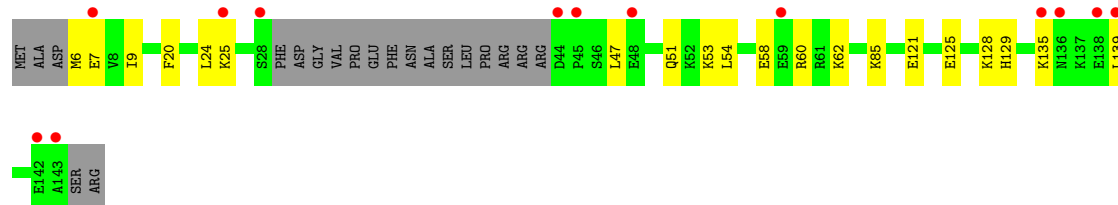




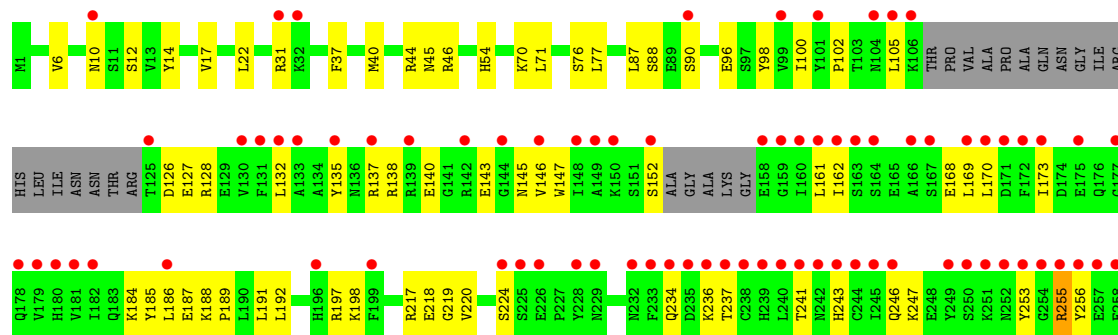
• Molecule 2: Tubulin beta-2B chain

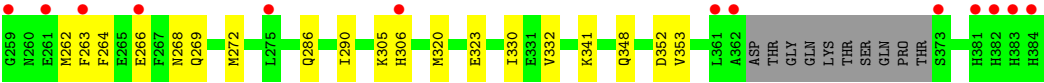


• Molecule 3: Stathmin-4



• Molecule 4: Tubulin tyrosine ligase





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.83Å 157.51Å 182.19Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.73 – 2.50 49.73 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.3 (49.73-2.50) 98.2 (49.73-2.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.19_4092	Depositor
R, R_{free}	0.194 , 0.232 0.194 , 0.231	Depositor DCC
R_{free} test set	2000 reflections (1.91%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.6	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	17937	wwPDB-VP
Average B, all atoms (Å ²)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.58% 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: GDP, ACP, CA, MG, GTP, PEG, MES, 7PL

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	0.47	0/3554	0.65	0/4824
1	C	0.52	0/3566	0.69	0/4841
2	B	0.47	0/3461	0.65	0/4685
2	D	0.45	1/3385 (0.0%)	0.65	3/4586 (0.1%)
3	E	0.46	0/1049	0.62	1/1393 (0.1%)
4	F	0.35	0/2989	0.55	0/4036
All	All	0.46	1/18004 (0.0%)	0.64	4/24365 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	69	GLU	CA-C	-6.81	1.47	1.52

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	140	GLY	N-CA-C	6.60	120.47	112.49
2	D	69	GLU	CA-C-N	-5.59	114.24	120.45
2	D	69	GLU	C-N-CA	-5.59	114.24	120.45
3	E	25	LYS	CB-CA-C	5.42	120.85	110.17

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	3458	0	3379	56	0
1	C	3467	0	3387	46	0
2	B	3378	0	3269	55	0
2	D	3309	0	3187	91	0
3	E	1031	0	1048	11	0
4	F	2909	0	2886	54	0
5	A	32	0	12	0	0
5	C	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
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	0	0
9	B	24	0	26	4	0
10	B	7	0	10	3	0
11	B	30	0	0	1	0
12	F	31	0	13	1	0
13	A	30	0	0	0	0
13	B	38	0	0	1	0
13	C	81	0	0	1	0
13	D	10	0	0	3	0
13	E	3	0	0	1	0
13	F	3	0	0	0	0
All	All	17937	0	17253	302	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 (302) 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:D:179:VAL:HG12	2:D:388:MET:HE3	1.44	0.98
4:F:128:ARG:HD2	4:F:170:LEU:HD22	1.58	0.86
1:A:220:GLU:HG2	2:B:324:LYS:HD2	1.58	0.84
2:B:170:MET:HG2	2:B:377:LEU:HD21	1.62	0.82
4:F:186:LEU:HD23	4:F:320[B]:MET:HE1	1.61	0.81
2:D:73:MET:HE3	2:D:90:PHE:HD2	1.46	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:GLY:HA3	1:A:183:GLU:HG2	1.67	0.76
2:D:18:ALA:O	2:D:22:GLU:HG3	1.88	0.74
1:A:430:LYS:NZ	1:A:433:GLU:OE1	2.22	0.73
2:B:324:LYS:O	2:B:328:GLU:HG3	1.89	0.72
1:C:234:ILE:HG21	1:C:302[B]:MET:SD	2.30	0.72
2:D:386:THR:O	2:D:390:ARG:HG2	1.90	0.71
1:C:427:ALA:HA	1:C:430:LYS:HE3	1.73	0.70
2:D:179:VAL:HG12	2:D:388:MET:CE	2.19	0.70
4:F:192:LEU:HD22	4:F:262:MET:HE1	1.72	0.70
2:D:81:PHE:O	2:D:84:ILE:HG22	1.92	0.70
1:C:36:MET:HE3	1:C:61:HIS:CD2	2.28	0.69
2:D:293:MET:HE2	2:D:367:PHE:HB2	1.75	0.69
1:A:414:GLU:OE2	3:E:60:ARG:NH1	2.27	0.68
2:D:44:LEU:HA	2:D:47:ILE:HB	1.76	0.68
2:B:323:MET:SD	2:B:353:VAL:HG21	2.34	0.68
2:B:38:GLY:HA3	2:B:43:GLN:OE1	1.93	0.67
4:F:320[B]:MET:HE2	4:F:330:ILE:HD11	1.77	0.66
2:D:170:MET:HG2	2:D:377:LEU:HD11	1.78	0.66
4:F:126:ASP:OD1	4:F:127:GLU:N	2.29	0.65
2:D:4:ILE:HG12	2:D:250:LEU:HD11	1.79	0.65
2:D:56:GLY:HA3	2:D:58:LYS:NZ	2.12	0.65
2:B:332:ASN:O	2:B:336:LYS:HG2	1.98	0.64
2:D:36:TYR:CD2	2:D:44:LEU:HD11	2.33	0.63
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.80	0.63
4:F:102:PRO:HD2	4:F:105:LEU:HD12	1.81	0.63
4:F:188:LYS:HG2	4:F:323:GLU:CD	2.24	0.62
2:D:5:VAL:HG22	2:D:133:PHE:CD2	2.34	0.62
2:D:286:VAL:HB	2:D:325:GLU:HG2	1.82	0.62
2:B:126:SER:O	2:B:126:SER:OG	2.19	0.61
1:A:293:ASN:OD1	1:A:339:ARG:NH1	2.34	0.61
2:D:324:LYS:O	2:D:328:GLU:HG3	2.00	0.61
2:D:288:GLU:O	2:D:292:GLN:HG3	2.01	0.61
2:B:293:MET:HG2	2:B:367:PHE:HB2	1.83	0.61
1:C:204:VAL:HG22	1:C:302[B]:MET:CE	2.30	0.61
2:D:409:THR:O	2:D:412:GLU:HB3	2.02	0.60
1:A:60:LYS:HD3	1:A:62:VAL:HG22	1.83	0.60
4:F:189:PRO:HG2	4:F:191:LEU:HD21	1.84	0.60
4:F:237:THR:O	4:F:246:GLN:NE2	2.35	0.60
2:D:37:HIS:CG	2:D:37:HIS:O	2.56	0.59
2:D:238:THR:HG22	13:D:707:HOH:O	2.02	0.59
1:A:414:GLU:OE2	3:E:60:ARG:CZ	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:VAL:HG12	1:C:348:PRO:HG2	1.84	0.59
4:F:266:GLU:N	4:F:266:GLU:OE1	2.37	0.58
2:B:203:ASP:OD2	2:B:380:ARG:NH2	2.36	0.58
2:B:213:ARG:O	2:B:216:LYS:HE2	2.03	0.58
4:F:31:ARG:H	4:F:31:ARG:HD3	1.68	0.58
2:D:36:TYR:CE1	2:D:38:GLY:HA3	2.38	0.58
1:A:220:GLU:CG	2:B:324:LYS:HD2	2.31	0.58
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.85	0.58
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.86	0.57
1:C:225:THR:O	1:C:229:ARG:HG3	2.03	0.57
2:B:100:ASN:HB2	10:B:507:PEG:H11	1.87	0.57
2:B:330:MET:HG3	2:B:351:THR:HG21	1.86	0.57
1:A:147:SER:HB2	1:A:190:THR:HB	1.86	0.57
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.39	0.57
2:D:165:ASN:OD1	2:D:198:GLU:HG3	2.05	0.57
4:F:138:ARG:HB3	4:F:145:ASN:CG	2.30	0.57
2:D:139:LEU:HA	2:D:145[A]:SER:HB3	1.86	0.56
1:A:413:MET:HE2	1:A:418:PHE:CE1	2.41	0.56
2:D:296:SER:HB3	2:D:305:PRO:HD2	1.88	0.56
1:C:221:ARG:HG3	2:D:323:MET:HB3	1.87	0.56
2:D:179:VAL:CG1	2:D:388:MET:HE3	2.29	0.56
4:F:128:ARG:CD	4:F:170:LEU:HD22	2.34	0.55
1:C:323:VAL:O	1:C:357:TYR:HE1	1.89	0.55
1:C:255:PHE:CZ	1:C:318:LEU:HD22	2.41	0.55
2:B:280:GLN:HG3	2:B:281:TYR:H	1.72	0.55
2:B:118:ASP:O	2:B:122:LYS:HE2	2.07	0.54
1:C:250:VAL:HG22	1:C:255:PHE:CE2	2.42	0.54
4:F:263:PHE:CE2	4:F:341:LYS:HE2	2.42	0.54
2:D:102:ALA:HB2	2:D:403:MET:SD	2.48	0.54
1:A:88:HIS:CE1	1:A:90:GLU:HB2	2.43	0.54
4:F:247:LYS:HD2	4:F:253:TYR:CE2	2.43	0.54
1:C:270:ALA:HB3	1:C:302[B]:MET:SD	2.48	0.53
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.47	0.53
4:F:220[A]:VAL:HG12	4:F:263:PHE:CE1	2.44	0.53
13:B:622:HOH:O	1:C:2:ARG:HD2	2.07	0.53
1:C:333:ALA:O	1:C:337:THR:HG23	2.08	0.53
2:B:2:ARG:HD3	2:B:3:GLU:CD	2.34	0.53
1:C:36:MET:HE1	1:C:49:PHE:CE1	2.43	0.53
2:D:139:LEU:HD21	2:D:168:SER:HB3	1.91	0.53
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.27	0.53
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:ARG:NH1	1:C:299:ALA:HB1	2.24	0.52
4:F:161:LEU:HD21	4:F:168:GLU:HG3	1.90	0.52
1:A:97:GLU:OE2	1:A:105:ARG:NH2	2.43	0.52
2:B:100:ASN:HD22	10:B:507:PEG:H12	1.75	0.52
2:D:141:GLY:O	2:D:145[A]:SER:OG	2.24	0.52
3:E:125:GLU:OE1	3:E:128:LYS:HD2	2.10	0.52
2:B:215:LEU:HD11	2:B:228:LEU:HD21	1.92	0.51
4:F:132:LEU:HD21	4:F:170:LEU:HD11	1.91	0.51
1:C:204:VAL:HG22	1:C:302[B]:MET:HE3	1.91	0.51
1:C:204:VAL:HG13	1:C:302[B]:MET:HE3	1.92	0.51
2:B:42:LEU:CD1	2:B:42:LEU:N	2.72	0.51
2:B:48:ASN:H	2:B:48:ASN:ND2	2.08	0.51
2:D:2:ARG:O	2:D:131:GLN:NE2	2.41	0.51
2:D:56:GLY:HA3	2:D:58:LYS:HZ1	1.74	0.51
1:A:402:ARG:NH1	1:A:415:GLU:OE2	2.42	0.50
1:C:180:ALA:HB3	1:C:183:GLU:HG3	1.93	0.50
3:E:53:LYS:HG3	3:E:54:LEU:N	2.24	0.50
4:F:263:PHE:CD2	4:F:341:LYS:HE2	2.46	0.50
2:B:21:TRP:CZ3	2:B:61:PRO:HB3	2.46	0.50
4:F:96:GLU:OE2	4:F:98:TYR:OH	2.26	0.50
4:F:138:ARG:HG3	4:F:143:GLU:HB2	1.92	0.50
4:F:234:GLN:O	4:F:236:LYS:NZ	2.45	0.50
2:D:211:CYS:HA	2:D:215:LEU:HB2	1.94	0.50
2:B:197:ASP:OD2	9:B:504:MES:H52	2.12	0.50
1:A:209:ILE:HD11	1:A:302:MET:SD	2.51	0.50
4:F:217:ARG:HG3	4:F:218:GLU:HG2	1.94	0.50
1:C:401:LYS:HG3	2:D:344:TRP:CE3	2.47	0.50
3:E:7:GLU:HG2	3:E:9:ILE:HG22	1.93	0.49
1:A:71:GLU:HB2	1:A:98:ASP:HB3	1.94	0.49
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.27	0.49
2:D:5:VAL:HG22	2:D:133:PHE:HD2	1.77	0.49
4:F:247:LYS:HA	4:F:253:TYR:CD2	2.47	0.49
2:B:215:LEU:HD13	2:B:275:SER:HB3	1.94	0.49
2:D:267:MET:HG3	2:D:301:ALA:HB3	1.95	0.49
4:F:31:ARG:HD3	4:F:31:ARG:N	2.27	0.49
2:B:197:ASP:OD1	9:B:504:MES:H32	2.13	0.49
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.46	0.49
2:D:134:GLN:HA	2:D:165:ASN:O	2.13	0.49
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.30	0.49
1:A:329:ASN:HD21	3:E:20:PHE:HE2	1.61	0.49
1:C:179:THR:HG21	2:D:246:LEU:HD13	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.95	0.48
3:E:47:LEU:O	3:E:51:GLN:HG2	2.13	0.48
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.95	0.48
2:D:164:MET:HG3	2:D:196:THR:HG22	1.95	0.48
4:F:70:LYS:HA	4:F:76:SER:HB3	1.93	0.48
1:A:83:TYR:CD1	1:A:86:LEU:HD22	2.49	0.48
4:F:45:ASN:ND2	4:F:46:ARG:HG3	2.29	0.48
4:F:269:GLN:HA	4:F:272:MET:HE3	1.96	0.48
2:B:33:THR:O	2:B:58:LYS:NZ	2.41	0.48
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.49	0.48
2:B:39:ASP:N	2:B:39:ASP:OD1	2.47	0.48
2:D:165:ASN:CG	2:D:198:GLU:HG3	2.39	0.48
2:D:242:PHE:CE1	2:D:356:ILE:HD12	2.49	0.47
4:F:100:ILE:HG22	4:F:173:ILE:HG21	1.96	0.47
2:D:26:ASP:OD2	2:D:359:ARG:HD3	2.15	0.47
4:F:255[B]:ARG:HD2	4:F:256:TYR:CD1	2.50	0.47
1:A:248:LEU:HD21	1:A:316[B]:CYS:SG	2.55	0.47
2:B:262:ARG:HH12	2:B:414:ASN:HD21	1.61	0.47
2:B:392:LYS:HE3	2:B:405:GLU:CD	2.40	0.47
1:C:83:TYR:HD2	1:C:86:LEU:HD22	1.79	0.47
2:D:169:VAL:HA	2:D:202:ILE:O	2.15	0.47
2:B:392:LYS:HE3	2:B:405:GLU:OE2	2.15	0.47
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.97	0.47
2:D:56:GLY:HA3	2:D:58:LYS:HZ2	1.79	0.47
2:B:44:LEU:HA	2:B:47:ILE:HB	1.96	0.47
2:B:406:MET:HE3	2:B:410:GLU:HG3	1.97	0.47
3:E:58:GLU:HG2	3:E:62:LYS:HD2	1.95	0.47
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.50	0.47
2:B:67:ASP:O	2:B:92:PHE:HA	2.15	0.47
2:B:104:GLY:O	2:B:109:GLY:HA3	2.15	0.47
1:C:42:ILE:HD12	1:C:42:ILE:N	2.30	0.47
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.96	0.46
2:D:234:SER:O	2:D:238:THR:HG23	2.15	0.46
1:A:280:LYS:HD3	1:A:283:HIS:HB2	1.97	0.46
1:C:167:LEU:HG	1:C:200:CYS:HB3	1.97	0.46
2:D:394:PHE:O	2:D:397:TRP:HB2	2.16	0.46
1:A:123:ARG:HG3	1:A:123:ARG:HH11	1.81	0.46
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.50	0.46
4:F:330:ILE:HD13	4:F:330:ILE:HA	1.78	0.46
1:A:1:MET:HE2	1:A:50:ASN:HB2	1.98	0.46
1:C:204:VAL:HG22	1:C:302[B]:MET:HE1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:68:LEU:HD23	2:D:112:LEU:HD22	1.97	0.46
1:A:263:PRO:O	1:A:266:HIS:HD2	1.99	0.46
2:B:320:ARG:HB3	2:B:320:ARG:NH1	2.31	0.46
3:E:85:LYS:NZ	13:E:201:HOH:O	2.37	0.46
1:A:60:LYS:HD3	1:A:62:VAL:CG2	2.44	0.46
2:B:86[A]:ARG:HH11	2:B:88:ASP:HB2	1.80	0.46
12:F:401:ACP:H8	12:F:401:ACP:H5'2	1.96	0.46
2:D:73:MET:HE3	2:D:90:PHE:CD2	2.37	0.46
2:D:107:THR:OG1	2:D:108:GLU:N	2.48	0.45
2:D:245:GLN:H	2:D:245:GLN:HG3	1.46	0.45
2:D:404:ASP:OD1	2:D:405:GLU:N	2.48	0.45
4:F:146:VAL:HB	4:F:187:GLU:OE2	2.16	0.45
2:D:131:GLN:HB3	2:D:250:LEU:HD12	1.97	0.45
9:B:504:MES:H31	9:B:504:MES:H81	1.79	0.45
1:C:209:ILE:HD11	1:C:302[A]:MET:HG3	1.97	0.45
1:C:215:ARG:CZ	1:C:299:ALA:HB1	2.47	0.45
2:D:107:THR:O	2:D:111:GLU:HG2	2.17	0.45
2:D:2:ARG:C	2:D:131:GLN:HE21	2.24	0.45
2:D:31:ASP:OD1	2:D:31:ASP:C	2.60	0.45
1:C:286:LEU:H	1:C:286:LEU:HD12	1.81	0.45
1:C:36:MET:HE1	1:C:49:PHE:CD1	2.52	0.45
2:D:151:LEU:O	2:D:155:ILE:HG13	2.17	0.45
2:D:267:MET:HB2	2:D:267:MET:HE3	1.86	0.45
1:A:98:ASP:C	1:A:98:ASP:OD1	2.60	0.45
1:A:123:ARG:HG3	1:A:123:ARG:NH1	2.32	0.45
4:F:44:ARG:HE	4:F:44:ARG:HB3	1.57	0.45
4:F:132:LEU:HA	4:F:135:TYR:HB3	1.98	0.45
1:A:192:HIS:CG	1:A:421:ALA:HA	2.52	0.45
1:A:265:ILE:HG21	1:A:313:MET:HE1	1.98	0.45
2:B:289:LEU:HD23	2:B:289:LEU:HA	1.69	0.45
1:C:320:ARG:HA	1:C:356:ASN:O	2.17	0.45
2:D:67:ASP:OD1	2:D:68:LEU:N	2.49	0.44
1:A:430:LYS:HD2	1:A:430:LYS:HA	1.51	0.44
1:C:147:SER:HB2	1:C:190:THR:HB	1.98	0.44
4:F:286:GLN:O	4:F:290:ILE:HG13	2.17	0.44
2:B:21:TRP:CE3	2:B:61:PRO:HB3	2.52	0.44
1:C:30:ILE:HD11	1:C:36:MET:HE2	2.00	0.44
2:D:289:LEU:HD12	2:D:289:LEU:HA	1.85	0.44
2:D:156:ARG:HG2	13:D:701:HOH:O	2.18	0.44
2:B:134:GLN:HA	2:B:165:ASN:O	2.18	0.44
1:A:1:MET:HE2	1:A:50:ASN:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.53	0.44
2:D:85:PHE:O	2:D:87:PRO:HD3	2.18	0.44
2:D:165:ASN:ND2	2:D:250:LEU:HD22	2.33	0.44
2:B:332:ASN:HD21	2:B:336:LYS:HE3	1.82	0.43
2:D:407:GLU:OE1	3:E:129:HIS:NE2	2.50	0.43
1:A:346:TRP:H	1:A:346:TRP:CD1	2.36	0.43
2:D:209:ASP:OD1	2:D:209:ASP:N	2.50	0.43
4:F:14:TYR:HA	4:F:17:VAL:HB	2.00	0.43
2:B:197:ASP:OD2	9:B:504:MES:H71	2.19	0.43
3:E:6:MET:HE2	3:E:24:LEU:HG	2.01	0.43
2:B:248:ALA:HA	11:B:508:7PL:N09	2.33	0.43
1:A:18:ASN:OD1	1:A:78:VAL:HG22	2.19	0.43
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.54	0.43
2:D:220:PRO:HD3	13:D:704:HOH:O	2.19	0.43
2:D:65:LEU:HD12	2:D:65:LEU:H	1.83	0.43
2:D:383:GLU:O	2:D:386:THR:HG22	2.18	0.43
1:A:142:GLY:CA	1:A:183:GLU:HG2	2.44	0.43
2:B:64:ILE:HD13	2:B:120:VAL:HG22	2.00	0.43
2:D:5:VAL:HG12	2:D:62:ARG:CD	2.49	0.43
2:B:245:GLN:H	2:B:245:GLN:CD	2.27	0.43
2:D:7:ILE:O	2:D:135:LEU:HD12	2.18	0.43
4:F:184:LYS:HD3	4:F:185:TYR:N	2.33	0.43
1:C:359:PRO:HB2	13:C:609:HOH:O	2.18	0.42
2:D:33:THR:HG22	2:D:33:THR:O	2.19	0.42
4:F:77:LEU:HD12	4:F:77:LEU:HA	1.84	0.42
4:F:161:LEU:HD22	4:F:168:GLU:OE2	2.18	0.42
1:A:69:ASP:O	1:A:94:THR:HA	2.19	0.42
2:B:2:ARG:HD3	2:B:3:GLU:OE2	2.19	0.42
2:D:77:ARG:HG3	2:D:90:PHE:CZ	2.55	0.42
2:B:159:TYR:HB3	2:B:162[B]:ARG:HG2	2.00	0.42
1:C:207:GLU:OE2	1:C:304:LYS:NZ	2.47	0.42
2:D:163:ILE:HD13	2:D:163:ILE:HA	1.86	0.42
2:B:68:LEU:HD23	2:B:68:LEU:HA	1.92	0.42
4:F:305:LYS:HD3	4:F:306:HIS:NE2	2.35	0.42
1:A:120[B]:ASP:OD1	1:A:124:LYS:NZ	2.50	0.42
2:B:170:MET:CG	2:B:377:LEU:HD21	2.39	0.42
1:C:192:HIS:CG	1:C:421:ALA:HA	2.54	0.42
1:A:7:ILE:HG12	1:A:66:VAL:CG1	2.49	0.42
1:A:68:VAL:HG11	1:A:149:PHE:CE2	2.54	0.42
1:A:83:TYR:HD1	1:A:86:LEU:HD22	1.83	0.42
2:D:386:THR:OG1	2:D:390:ARG:NE	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:GLU:OE1	1:A:434:GLU:HA	2.17	0.42
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.55	0.42
2:D:46:ARG:HA	2:D:46:ARG:HD2	1.78	0.42
4:F:71:LEU:HD23	4:F:332:VAL:HG11	2.02	0.42
1:A:1:MET:SD	1:A:1:MET:C	3.03	0.42
1:A:119:LEU:HD11	1:A:156:ARG:HB3	2.01	0.42
1:A:146:GLY:O	1:A:150:THR:HB	2.19	0.42
1:C:93:ILE:HD11	1:C:121:ARG:HG3	2.02	0.42
2:D:333:VAL:O	2:D:337:ASN:HB2	2.19	0.42
4:F:31:ARG:H	4:F:31:ARG:CD	2.32	0.42
1:A:390[B]:ARG:HD2	4:F:54:HIS:CD2	2.54	0.41
2:D:116:VAL:O	2:D:120:VAL:HG23	2.20	0.41
2:B:267:MET:HE1	2:B:305:PRO:HG3	2.01	0.41
2:D:399:THR:HG22	2:D:403:MET:O	2.19	0.41
4:F:198:LYS:HB3	4:F:241:THR:CG2	2.50	0.41
1:A:428:LEU:HA	1:A:428:LEU:HD12	1.73	0.41
2:B:36:TYR:O	2:B:37:HIS:CD2	2.73	0.41
2:B:332:ASN:ND2	2:B:336:LYS:HE3	2.34	0.41
2:D:68:LEU:HD23	2:D:68:LEU:HA	1.89	0.41
4:F:137:ARG:HA	4:F:140:GLU:OE1	2.20	0.41
2:B:397:TRP:CZ3	10:B:507:PEG:H32	2.56	0.41
1:A:262:TYR:CD1	1:A:262:TYR:C	2.99	0.41
1:C:351:PHE:N	1:C:351:PHE:CD1	2.88	0.41
1:A:188:ILE:HD12	1:A:425:MET:HG3	2.02	0.41
2:D:36:TYR:CZ	2:D:38:GLY:HA3	2.55	0.41
1:C:221:ARG:NE	2:D:323:MET:HE3	2.35	0.41
2:D:293:MET:HE3	2:D:293:MET:HB2	1.96	0.41
2:D:174:LYS:HD3	2:D:208:TYR:HD2	1.85	0.41
4:F:138:ARG:NH1	4:F:184:LYS:HZ2	2.18	0.41
4:F:243:HIS:O	4:F:243:HIS:ND1	2.54	0.41
2:D:34:GLY:O	2:D:58:LYS:HA	2.21	0.41
2:D:61:PRO:HD3	2:D:84:ILE:HG12	2.03	0.41
2:D:177:ASP:OD1	2:D:177:ASP:N	2.35	0.41
2:D:245:GLN:HE21	2:D:245:GLN:HB2	1.73	0.41
4:F:87:LEU:O	4:F:88:SER:OG	2.32	0.40
2:B:114:ASP:HA	2:B:117:LEU:HD12	2.04	0.40
1:A:26:LEU:HD23	1:A:26:LEU:HA	1.87	0.40
1:A:110:ILE:O	1:A:113:GLU:HG3	2.22	0.40
1:C:181:VAL:H	2:D:256:ASN:ND2	2.19	0.40
2:D:65:LEU:HD12	2:D:65:LEU:N	2.37	0.40
2:D:130:LEU:HB3	2:D:162:ARG:HH11	1.85	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:TYR:C	1:A:262:TYR:HD1	2.29	0.40
1:A:385:ALA:HB2	1:A:432:TYR:CG	2.56	0.40
2:D:192:LEU:HD23	2:D:192:LEU:HA	1.90	0.40
2:D:345:ILE:HG22	2:D:348:ASN:HB3	2.03	0.40
4:F:197:ARG:HD2	4:F:224:SER:O	2.20	0.40
1:A:1:MET:HB3	1:A:46:ASP:HB2	2.03	0.40
2:B:363:MET:HE3	2:B:363:MET:HB3	1.81	0.40
2:D:382:SER:HB2	2:D:415:MET:HE3	2.02	0.40
4:F:268:ASN:ND2	4:F:272:MET:HE2	2.36	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	443/450 (98%)	426 (96%)	17 (4%)	0	100	100
1	C	445/450 (99%)	430 (97%)	15 (3%)	0	100	100
2	B	425/445 (96%)	409 (96%)	16 (4%)	0	100	100
2	D	418/445 (94%)	399 (96%)	19 (4%)	0	100	100
3	E	122/143 (85%)	120 (98%)	2 (2%)	0	100	100
4	F	347/384 (90%)	326 (94%)	21 (6%)	0	100	100
All	All	2200/2317 (95%)	2110 (96%)	90 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	376/378 (100%)	369 (98%)	7 (2%)	50	76
1	C	378/378 (100%)	372 (98%)	6 (2%)	55	79
2	B	372/383 (97%)	366 (98%)	6 (2%)	55	79
2	D	364/383 (95%)	351 (96%)	13 (4%)	31	58
3	E	113/127 (89%)	110 (97%)	3 (3%)	39	67
4	F	321/342 (94%)	311 (97%)	10 (3%)	35	62
All	All	1924/1991 (97%)	1879 (98%)	45 (2%)	44	72

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	SER
1	A	60	LYS
1	A	133	GLN
1	A	163	LYS
1	A	177	VAL
1	A	178	SER
1	A	250	VAL
2	B	42	LEU
2	B	58	LYS
2	B	126	SER
2	B	188	SER
2	B	193	VAL
2	B	219	THR
1	C	165	SER
1	C	250	VAL
1	C	286	LEU
1	C	318	LEU
1	C	338	LYS
1	C	363	VAL
2	D	5	VAL
2	D	8	GLN
2	D	15	GLN
2	D	39	ASP
2	D	42	LEU
2	D	83	GLN
2	D	177	ASP
2	D	193	VAL

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Mol	Chain	Res	Type
2	D	198	GLU
2	D	225	LEU
2	D	245	GLN
2	D	306	ARG
2	D	339	SER
3	E	121	GLU
3	E	135	LYS
3	E	139	LEU
4	F	6	VAL
4	F	10	ASN
4	F	12	SER
4	F	22	LEU
4	F	90	SER
4	F	152	SER
4	F	162	ILE
4	F	255[A]	ARG
4	F	255[B]	ARG
4	F	353	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	101	ASN
1	A	329	ASN
1	A	393	HIS
2	B	15	GLN
2	B	37	HIS
2	B	190	HIS
2	B	247	ASN
2	B	256	ASN
2	B	337	ASN
2	B	347	ASN
2	B	414	ASN
1	C	61	HIS
1	C	101	ASN
1	C	356	ASN
1	C	393	HIS
2	D	11	GLN
2	D	15	GLN
2	D	256	ASN
2	D	329	GLN

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Mol	Chain	Res	Type
3	E	18	GLN
3	E	103	GLN
4	F	45	ASN
4	F	310	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, 8 are monoatomic - leaving 9 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
11	7PL	B	508	-	33,33,33	1.78	8 (24%)	47,47,47	1.48	6 (12%)
5	GTP	A	501	6	33,34,34	1.28	4 (12%)	50,54,54	1.59	9 (18%)
5	GTP	C	501	6	33,34,34	1.19	2 (6%)	50,54,54	1.54	7 (14%)
9	MES	B	504	-	12,12,12	1.84	3 (25%)	15,16,16	2.00	5 (33%)
8	GDP	B	501	6	29,30,30	1.28	4 (13%)	45,47,47	1.73	6 (13%)
8	GDP	D	600	-	29,30,30	1.23	2 (6%)	45,47,47	1.86	10 (22%)
10	PEG	B	507	-	6,6,6	0.66	0	5,5,5	0.50	0
9	MES	B	505	-	12,12,12	1.45	3 (25%)	15,16,16	1.60	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
12	ACP	F	401	-	31,33,33	3.51	10 (32%)	47,52,52	2.35	15 (31%)

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
11	7PL	B	508	-	-	2/22/24/24	0/4/4/4
5	GTP	A	501	6	-	4/22/38/38	0/3/3/3
5	GTP	C	501	6	-	9/22/38/38	0/3/3/3
9	MES	B	504	-	-	5/6/14/14	0/1/1/1
8	GDP	B	501	6	-	5/16/32/32	0/3/3/3
8	GDP	D	600	-	-	4/16/32/32	0/3/3/3
10	PEG	B	507	-	-	4/4/4/4	-
9	MES	B	505	-	-	0/6/14/14	0/1/1/1
12	ACP	F	401	-	-	2/19/38/38	0/3/3/3

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	F	401	ACP	PB-O3A	9.12	1.68	1.58
12	F	401	ACP	O4'-C1'	8.60	1.61	1.42
12	F	401	ACP	PA-O3A	7.87	1.68	1.59
12	F	401	ACP	C2'-C1'	-7.21	1.30	1.53
12	F	401	ACP	O4'-C4'	-6.25	1.31	1.45
11	B	508	7PL	C26-N25	4.88	1.46	1.35
9	B	504	MES	C8-S	4.51	1.83	1.77
12	F	401	ACP	C6-N6	4.38	1.45	1.34
11	B	508	7PL	C08-N07	4.31	1.46	1.38
11	B	508	7PL	C12-N14	3.93	1.45	1.38
5	C	501	GTP	PB-O3B	3.82	1.63	1.59
8	D	600	GDP	C5-C4	3.56	1.48	1.38
5	A	501	GTP	PA-O3A	3.38	1.63	1.59
5	C	501	GTP	PA-O3A	3.23	1.63	1.59
5	A	501	GTP	PB-O3B	3.17	1.62	1.59
8	B	501	GDP	C5-C4	3.17	1.47	1.38
8	B	501	GDP	PA-O3A	2.96	1.62	1.59
9	B	504	MES	O2S-S	2.94	1.53	1.45
12	F	401	ACP	O3'-C3'	-2.93	1.35	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	501	GTP	PB-O3A	2.81	1.62	1.59
9	B	505	MES	C8-S	2.77	1.81	1.77
12	F	401	ACP	C5-C4	-2.74	1.34	1.39
9	B	505	MES	O2S-S	2.74	1.52	1.45
11	B	508	7PL	C15-N14	2.71	1.46	1.40
9	B	504	MES	O1S-S	2.69	1.52	1.45
5	A	501	GTP	C2-N3	2.67	1.39	1.33
12	F	401	ACP	O2'-C2'	2.55	1.49	1.43
8	D	600	GDP	C6-N1	-2.54	1.34	1.38
11	B	508	7PL	C01-N25	2.45	1.46	1.41
12	F	401	ACP	C5-N7	-2.43	1.34	1.39
8	B	501	GDP	C6-N1	-2.36	1.34	1.38
11	B	508	7PL	C05-N07	2.34	1.45	1.40
11	B	508	7PL	C21-C19	2.22	1.54	1.49
11	B	508	7PL	C28-C26	2.20	1.55	1.51
9	B	505	MES	O1S-S	2.19	1.51	1.45
8	B	501	GDP	C2-N3	2.00	1.38	1.33

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	401	ACP	N3-C2-N1	-5.98	119.53	128.58
12	F	401	ACP	N6-C6-N1	-5.95	105.13	118.38
11	B	508	7PL	N11-C10-N09	-5.76	119.86	128.58
8	B	501	GDP	C5-C4-N3	-5.62	119.45	128.39
8	D	600	GDP	C5-C4-N3	-5.56	119.55	128.39
5	A	501	GTP	C5-C4-N3	-5.17	120.16	128.39
12	F	401	ACP	C5-C4-N3	-4.90	119.97	126.72
12	F	401	ACP	C5-C6-N6	4.77	135.10	123.29
8	B	501	GDP	C2-N3-C4	4.56	120.15	112.30
8	B	501	GDP	N9-C4-N3	4.46	134.87	125.95
12	F	401	ACP	N9-C8-N7	-4.31	107.81	113.94
5	A	501	GTP	C2-N3-C4	4.24	119.61	112.30
8	D	600	GDP	C2-N3-C4	4.18	119.50	112.30
5	C	501	GTP	C2-N3-C4	4.17	119.49	112.30
5	C	501	GTP	C5-C4-N3	-4.09	121.88	128.39
9	B	504	MES	O2S-S-C8	4.07	112.88	106.73
9	B	504	MES	C2-C3-N4	4.03	116.25	110.12
8	D	600	GDP	N9-C4-N3	3.92	133.80	125.95
8	D	600	GDP	C6-C5-N7	3.89	137.36	130.29
12	F	401	ACP	O3G-PG-C3B	3.65	115.25	106.40
5	C	501	GTP	N9-C8-N7	-3.52	106.87	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	401	ACP	C2-N3-C4	3.50	120.39	111.83
11	B	508	7PL	C29-C28-C26	-3.44	113.87	117.24
12	F	401	ACP	C3'-C2'-C1'	3.42	107.92	101.46
8	D	600	GDP	O2B-PB-O3A	3.35	115.88	104.64
8	B	501	GDP	C6-C5-N7	3.23	136.17	130.29
8	D	600	GDP	C4-C5-N7	-3.18	105.64	110.67
5	A	501	GTP	N9-C4-N3	3.18	132.30	125.95
5	A	501	GTP	C8-N7-C5	3.10	109.78	104.26
12	F	401	ACP	C5-N7-C8	3.07	108.27	103.45
11	B	508	7PL	C15-N14-C12	-3.02	120.98	128.75
9	B	504	MES	C5-N4-C3	2.98	115.26	108.84
5	C	501	GTP	C8-N7-C5	2.97	109.55	104.26
9	B	505	MES	O2S-S-C8	2.91	111.13	106.73
5	A	501	GTP	N9-C8-N7	-2.91	108.01	113.40
9	B	505	MES	C5-N4-C3	2.89	115.07	108.84
12	F	401	ACP	N3-C4-N9	2.82	131.97	127.17
5	A	501	GTP	C2-N1-C6	-2.79	120.04	125.11
9	B	505	MES	C8-C7-N4	-2.73	102.04	112.36
9	B	504	MES	O2S-S-O1S	-2.71	105.01	113.82
12	F	401	ACP	C5'-C4'-C3'	-2.65	105.67	115.21
11	B	508	7PL	C13-C08-N09	-2.52	119.61	122.92
5	C	501	GTP	N9-C4-N3	2.52	130.99	125.95
12	F	401	ACP	C4-C5-N7	-2.51	107.71	110.58
12	F	401	ACP	O3G-PG-O1G	-2.48	105.97	112.39
8	B	501	GDP	C4-C5-N7	-2.47	106.76	110.67
5	A	501	GTP	C4-C5-N7	-2.46	106.78	110.67
12	F	401	ACP	C4-N9-C8	2.29	108.14	105.74
9	B	505	MES	O3S-S-O2S	-2.29	105.68	111.40
8	B	501	GDP	O6-C6-C5	-2.26	120.56	126.53
8	D	600	GDP	O3B-PB-O1B	2.19	119.35	110.83
5	A	501	GTP	O5'-PA-O1A	2.18	117.56	108.94
8	D	600	GDP	O2A-PA-O3A	2.15	113.09	107.27
8	D	600	GDP	C8-N7-C5	2.14	108.07	104.26
5	C	501	GTP	O2B-PB-O3A	2.11	112.98	107.27
8	D	600	GDP	O2B-PB-O1B	-2.10	102.65	110.83
5	A	501	GTP	C5-C6-N1	2.09	118.56	113.25
5	C	501	GTP	C4-C5-N7	-2.07	107.39	110.67
12	F	401	ACP	C5-C4-N9	2.07	108.07	105.81
9	B	504	MES	O1-C2-C3	2.06	116.20	111.77
11	B	508	7PL	C30-C28-C26	2.04	119.23	117.24
11	B	508	7PL	C10-N09-C08	2.03	121.89	115.25

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	501	GTP	PB-O3B-PG-O2G
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
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	D	600	GDP	C5'-O5'-PA-O3A
8	D	600	GDP	C5'-O5'-PA-O1A
8	D	600	GDP	C5'-O5'-PA-O2A
9	B	504	MES	C8-C7-N4-C3
9	B	504	MES	C7-C8-S-O2S
9	B	504	MES	C7-C8-S-O3S
9	B	504	MES	C7-C8-S-O1S
10	B	507	PEG	O1-C1-C2-O2
9	B	504	MES	N4-C7-C8-S
10	B	507	PEG	C1-C2-O2-C3
8	B	501	GDP	C5'-O5'-PA-O2A
10	B	507	PEG	C4-C3-O2-C2
5	C	501	GTP	C4'-C5'-O5'-PA
8	D	600	GDP	C4'-C5'-O5'-PA
12	F	401	ACP	PB-O3A-PA-O1A
12	F	401	ACP	PB-O3A-PA-O2A
8	B	501	GDP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3A-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A
11	B	508	7PL	N09-C08-N07-C05
10	B	507	PEG	O2-C3-C4-O4
11	B	508	7PL	C13-C08-N07-C05
8	B	501	GDP	PB-O3A-PA-O1A

There are no ring outliers.

4 monomers are involved in 9 short contacts:

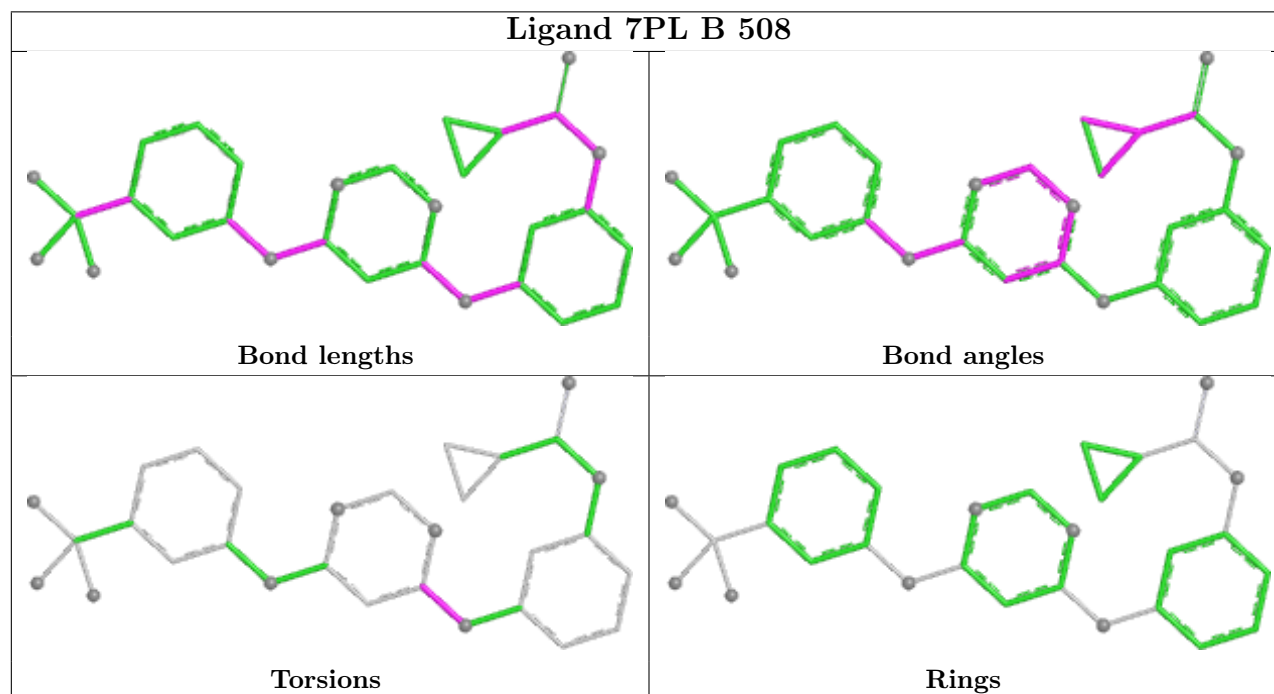
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	B	508	7PL	1	0

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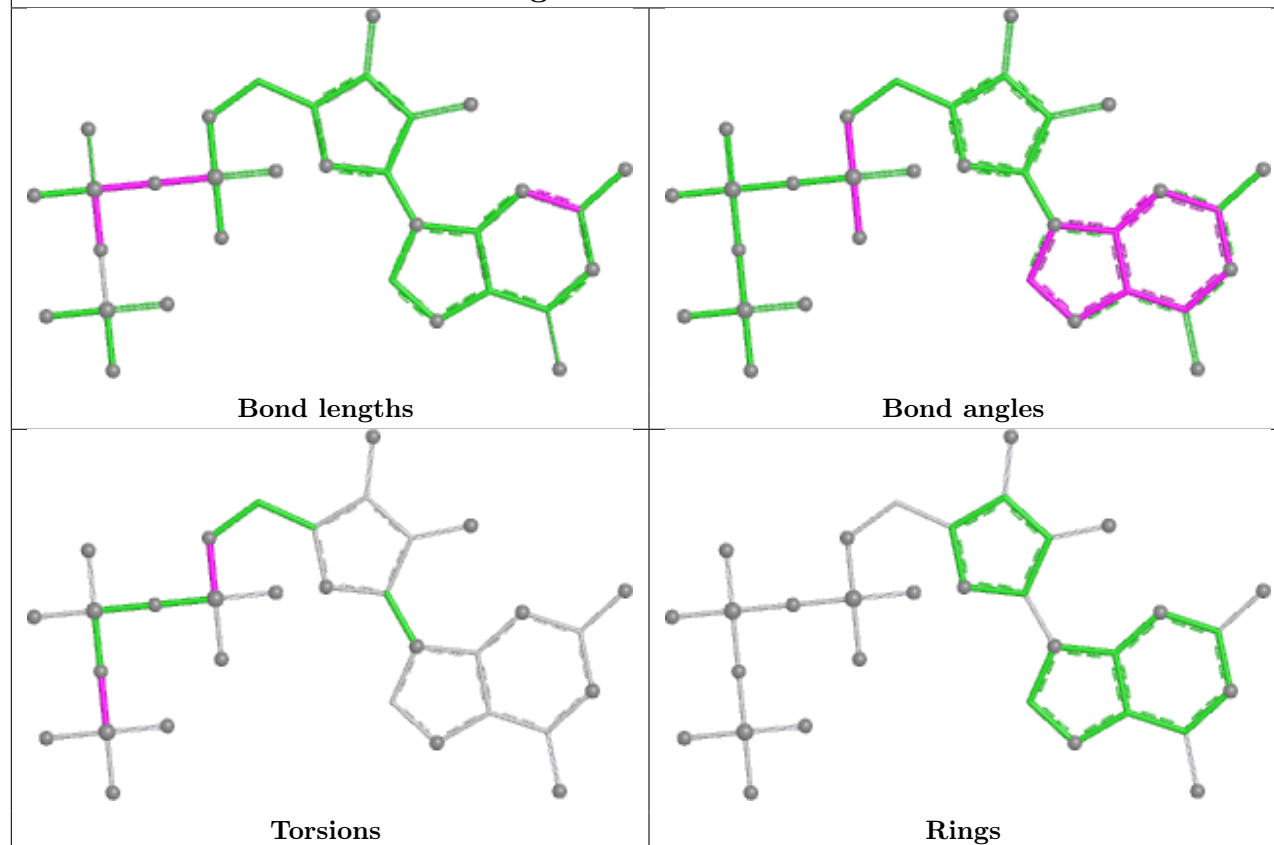
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	504	MES	4	0
10	B	507	PEG	3	0
12	F	401	ACP	1	0

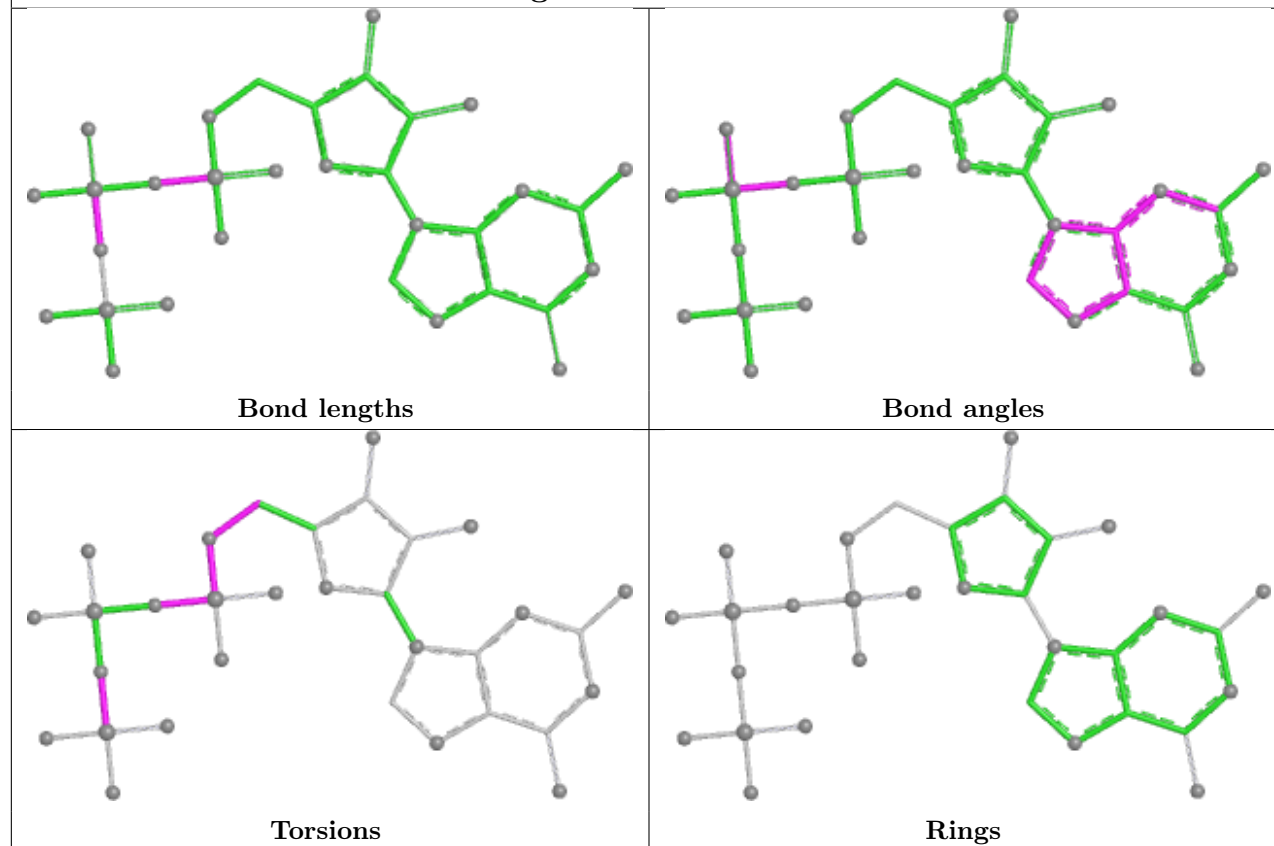
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

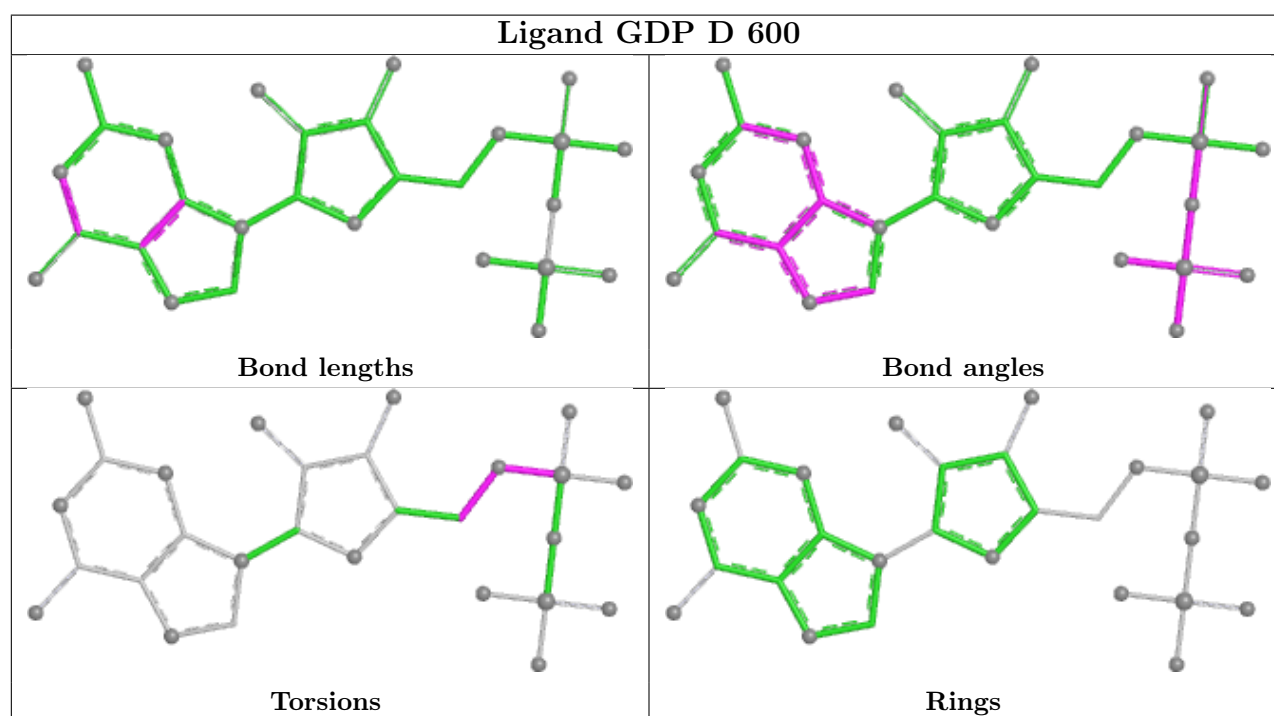
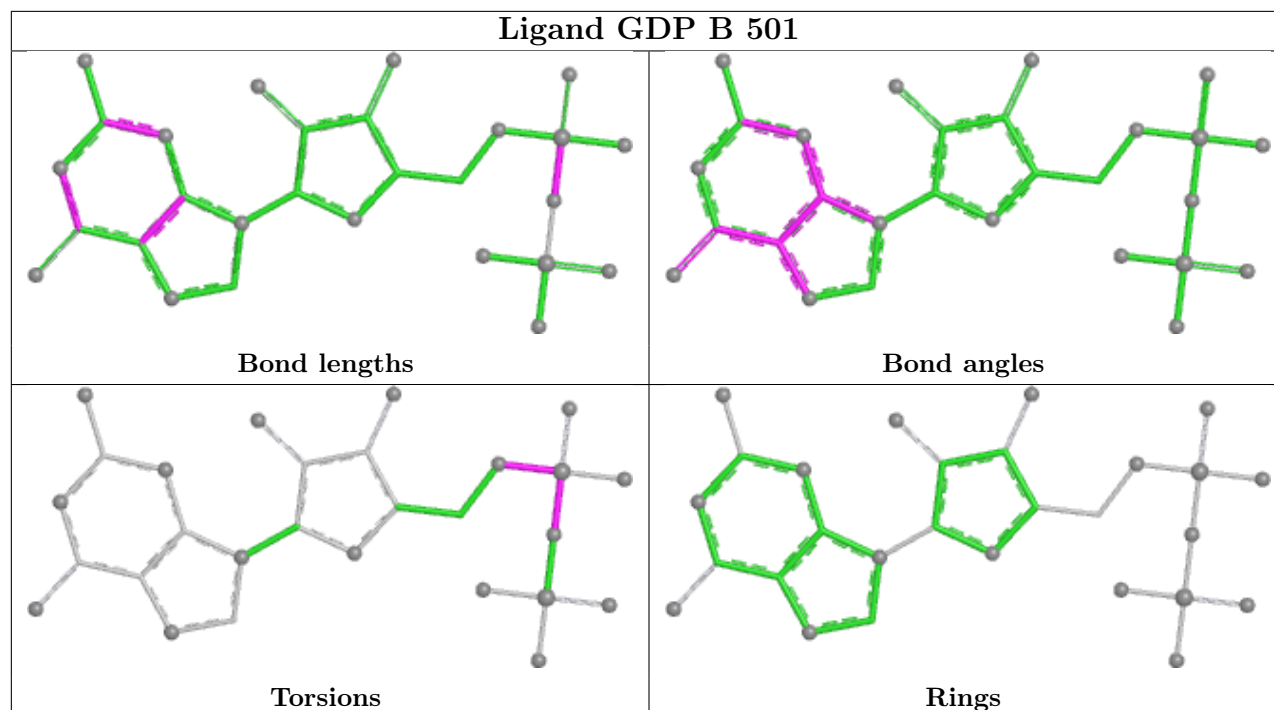


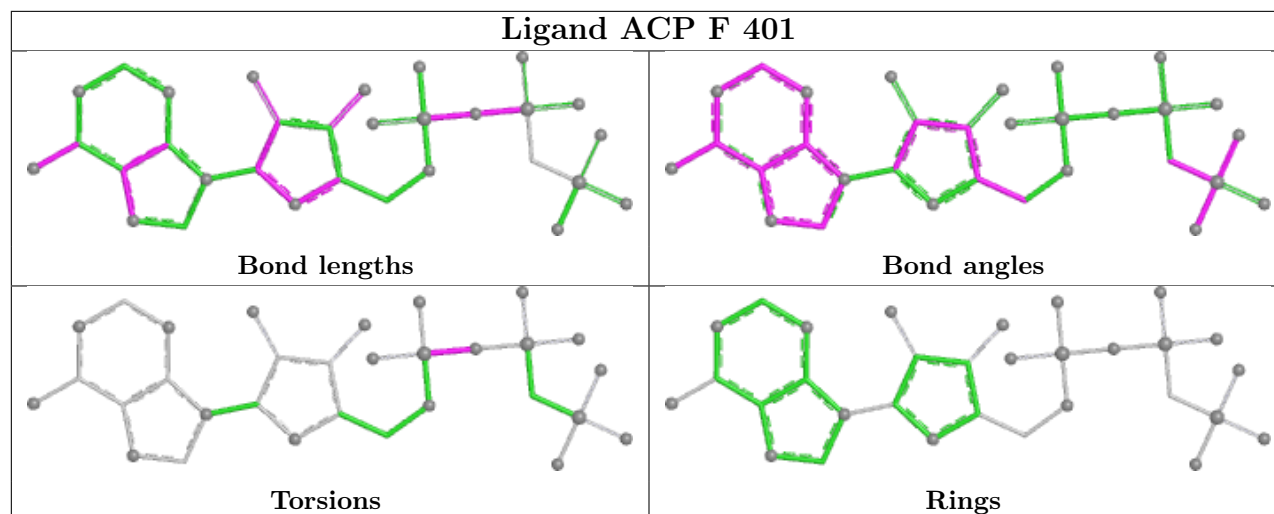
Ligand GTP A 501



Ligand GTP C 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	439/450 (97%)	-0.06	8 (1%) 67 64	17, 37, 59, 114	6 (1%)
1	C	440/450 (97%)	-0.35	6 (1%) 73 70	16, 29, 50, 73	7 (1%)
2	B	425/445 (95%)	0.01	16 (3%) 44 39	18, 36, 67, 103	5 (1%)
2	D	421/445 (94%)	0.90	49 (11%) 9 8	28, 58, 89, 119	2 (0%)
3	E	123/143 (86%)	0.89	13 (10%) 11 9	24, 51, 86, 116	3 (2%)
4	F	351/384 (91%)	1.16	91 (25%) 1 1	28, 64, 128, 150	4 (1%)
All	All	2199/2317 (94%)	0.33	183 (8%) 17 15	16, 43, 92, 150	27 (1%)

All (183) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	105	LEU	5.6
4	F	159	GLY	5.3
3	E	143	ALA	5.3
1	A	262	TYR	4.9
2	D	284	LEU	4.8
4	F	233	PHE	4.8
2	B	1	MET	4.7
2	D	283	ALA	4.5
2	B	275	SER	4.5
4	F	125	THR	4.5
2	D	92	PHE	4.1
4	F	169	LEU	4.1
2	D	248	ALA	4.0
4	F	106	LYS	4.0
2	D	37	HIS	4.0
4	F	152	SER	4.0
2	D	55	THR	3.9
4	F	225	SER	3.9
2	D	245	GLN	3.9

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Mol	Chain	Res	Type	RSRZ
2	D	393	ALA	3.9
4	F	249	TYR	3.8
4	F	362	ALA	3.8
4	F	259	GLY	3.8
1	C	179	THR	3.7
4	F	244	CYS	3.6
4	F	158	GLU	3.6
1	C	340	SER	3.5
2	B	281	TYR	3.5
2	D	33	THR	3.5
2	D	80	PRO	3.5
4	F	253	TYR	3.4
2	B	276	ARG	3.4
2	B	57	ASN	3.4
4	F	144	GLY	3.4
2	D	99	ASN	3.4
4	F	381	HIS	3.4
1	A	439	SER	3.4
2	B	55	THR	3.3
4	F	245	ILE	3.3
2	B	282	ARG	3.3
4	F	164	SER	3.3
2	D	141	GLY	3.3
2	D	219	THR	3.3
1	C	284	GLU	3.2
4	F	130	VAL	3.2
4	F	242	ASN	3.2
4	F	255[A]	ARG	3.2
2	B	38	GLY	3.2
2	D	57	ASN	3.2
2	D	84	ILE	3.1
4	F	160	ILE	3.1
4	F	133	ALA	3.1
2	D	73	MET	3.1
4	F	177	GLY	3.1
4	F	132	LEU	3.0
4	F	275[A]	LEU	3.0
3	E	139	LEU	3.0
4	F	104	ASN	3.0
4	F	251	LYS	3.0
4	F	162	ILE	3.0
4	F	170	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
2	D	247	ASN	3.0
4	F	250	SER	2.9
2	D	30	ILE	2.9
3	E	138	GLU	2.9
4	F	146	VAL	2.9
4	F	166	ALA	2.9
4	F	226	GLU	2.9
4	F	182	ILE	2.9
4	F	232	ASN	2.8
4	F	101	TYR	2.8
4	F	167	SER	2.8
2	D	42	LEU	2.8
2	D	125	GLU	2.8
2	D	79	GLY	2.8
4	F	181	VAL	2.8
2	D	72	THR	2.8
2	B	280	GLN	2.8
4	F	257	GLU	2.8
2	D	81	PHE	2.8
4	F	161	LEU	2.7
3	E	48	GLU	2.7
2	D	54	ALA	2.7
4	F	235	ASP	2.7
4	F	199	PHE	2.7
4	F	252	ASN	2.7
1	A	163	LYS	2.7
3	E	28	SER	2.7
4	F	224	SER	2.7
4	F	236	LYS	2.7
4	F	256	TYR	2.7
2	D	94	GLN	2.7
4	F	254	GLY	2.6
2	D	394	PHE	2.6
4	F	90	SER	2.6
4	F	149	ALA	2.6
2	D	88	ASP	2.6
3	E	135	LYS	2.6
4	F	142	ARG	2.6
4	F	148	ILE	2.6
4	F	263	PHE	2.6
2	B	274	THR	2.6
4	F	171	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
4	F	186	LEU	2.5
2	D	95	SER	2.5
4	F	135	TYR	2.5
1	A	438	ASP	2.5
2	D	41	ASP	2.5
2	D	396	HIS	2.5
4	F	32	LYS	2.5
4	F	172	PHE	2.5
4	F	241	THR	2.5
3	E	44	ASP	2.5
1	C	285	GLN	2.5
4	F	243	HIS	2.5
4	F	163	SER	2.5
4	F	237	THR	2.5
1	C	245	ASP	2.4
2	B	42	LEU	2.4
4	F	196	HIS	2.4
4	F	179	VAL	2.4
2	D	214	THR	2.4
4	F	266	GLU	2.4
4	F	373	SER	2.4
4	F	234	GLN	2.4
2	D	387	ALA	2.4
2	D	291	GLN	2.4
3	E	25	LYS	2.4
4	F	246	GLN	2.3
4	F	228	TYR	2.3
4	F	229	ASN	2.3
3	E	7	GLU	2.3
2	D	218	THR	2.3
2	D	34	GLY	2.3
2	D	377	LEU	2.3
1	A	346	TRP	2.3
2	B	40	SER	2.3
2	D	56	GLY	2.3
2	D	76	VAL	2.3
4	F	178	GLN	2.3
4	F	239	HIS	2.3
4	F	383	HIS	2.3
2	D	69	GLU	2.3
4	F	382	HIS	2.2
2	D	216	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
4	F	361	LEU	2.2
1	A	196	GLU	2.2
4	F	131	PHE	2.2
2	D	391	ARG	2.2
1	C	178	SER	2.2
1	A	434	GLU	2.2
4	F	258	GLU	2.2
4	F	31	ARG	2.2
2	D	212	PHE	2.2
3	E	45	PRO	2.2
2	B	283	ALA	2.2
4	F	10	ASN	2.2
2	D	15	GLN	2.2
4	F	306	HIS	2.2
4	F	173	ILE	2.2
2	D	53	GLU	2.2
4	F	180	HIS	2.1
2	D	246	LEU	2.1
2	D	180	VAL	2.1
2	B	245	GLN	2.1
2	B	48	ASN	2.1
4	F	137	ARG	2.1
4	F	175	GLU	2.1
4	F	150	LYS	2.1
2	B	54	ALA	2.1
2	D	77	ARG	2.1
4	F	139	ARG	2.1
4	F	384	HIS	2.1
2	D	140	GLY	2.1
4	F	99	VAL	2.0
3	E	136	ASN	2.0
4	F	240	LEU	2.0
3	E	59	GLU	2.0
4	F	261	GLU	2.0
1	A	88	HIS	2.0
4	F	238	CYS	2.0
3	E	142	GLU	2.0
2	D	398	TYR	2.0

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

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](#)

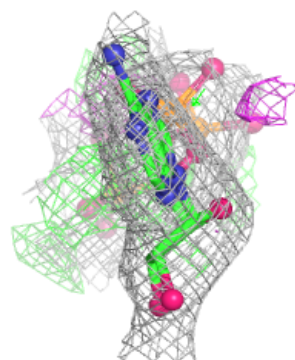
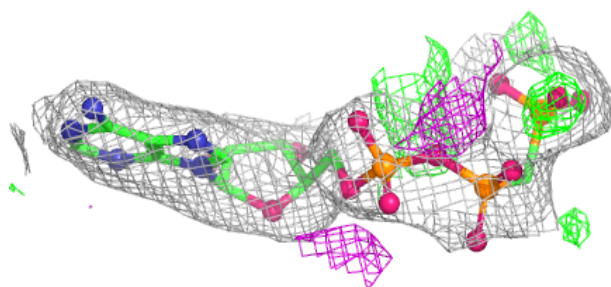
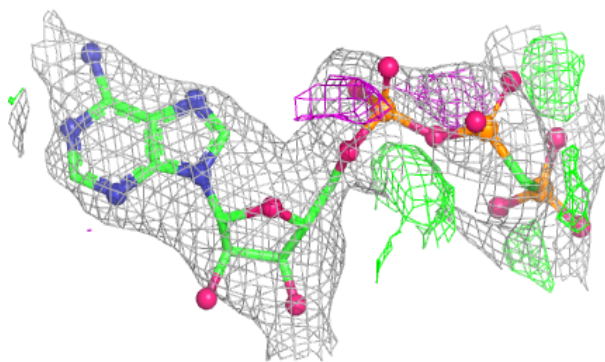
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
12	ACP	F	401	31/31	0.72	0.17	75,85,103,111	0
10	PEG	B	507	7/7	0.80	0.27	34,48,55,56	0
7	CA	B	503	1/1	0.80	0.20	91,91,91,91	0
7	CA	C	503	1/1	0.84	0.16	43,43,43,43	0
6	MG	B	506	1/1	0.87	0.34	66,66,66,66	0
6	MG	C	502	1/1	0.87	0.24	33,33,33,33	0
8	GDP	D	600	28/28	0.88	0.14	53,58,68,73	0
7	CA	A	504	1/1	0.92	0.26	110,110,110,110	0
9	MES	B	505	12/12	0.92	0.11	50,52,60,67	0
9	MES	B	504	12/12	0.95	0.08	29,35,54,57	0
7	CA	A	503	1/1	0.95	0.06	54,54,54,54	0
11	7PL	B	508	30/30	0.96	0.07	25,35,41,45	0
5	GTP	A	501	32/32	0.98	0.06	21,28,33,45	0
5	GTP	C	501	32/32	0.98	0.05	18,25,30,33	0
6	MG	A	502	1/1	0.99	0.03	30,30,30,30	0
6	MG	B	502	1/1	0.99	0.02	27,27,27,27	0
8	GDP	B	501	28/28	0.99	0.05	20,26,33,35	0

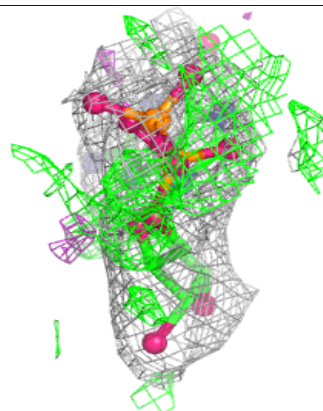
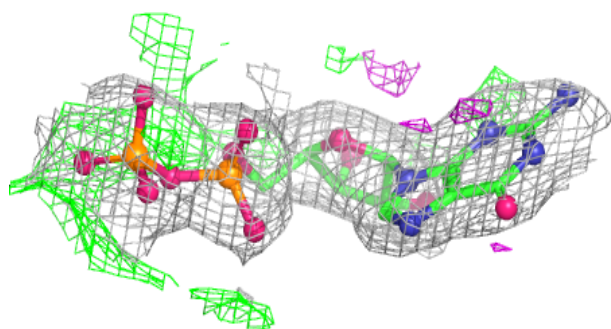
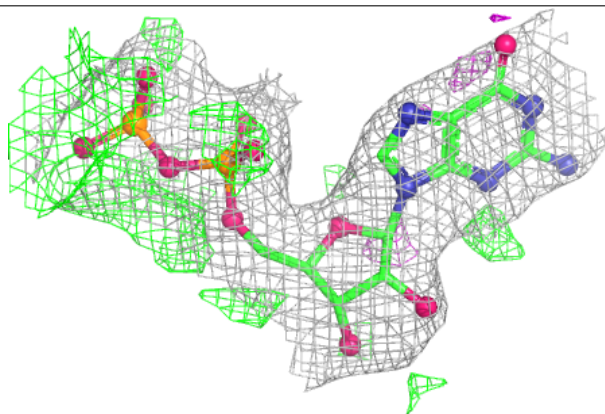
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACP F 401:

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

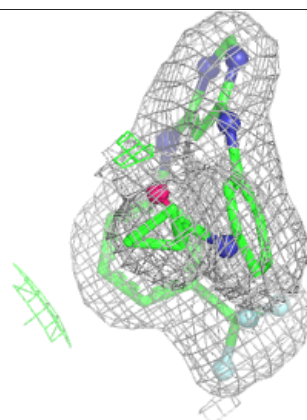
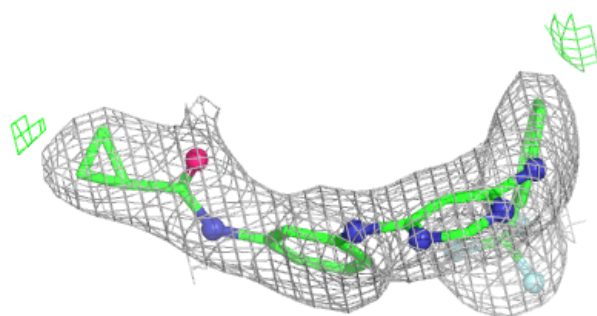
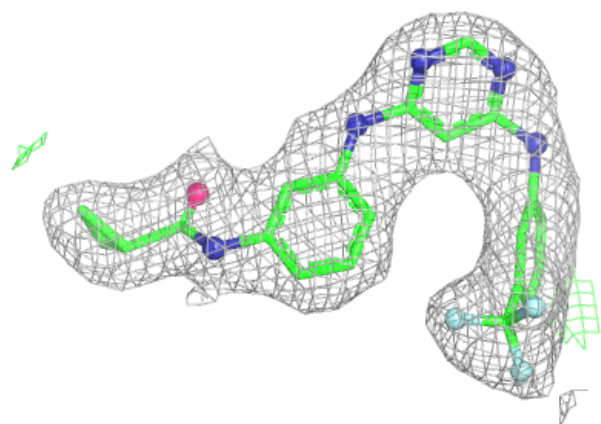
**Electron density around GDP D 600:**

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

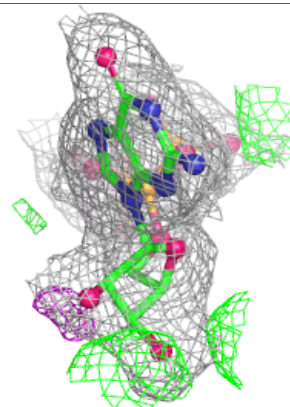
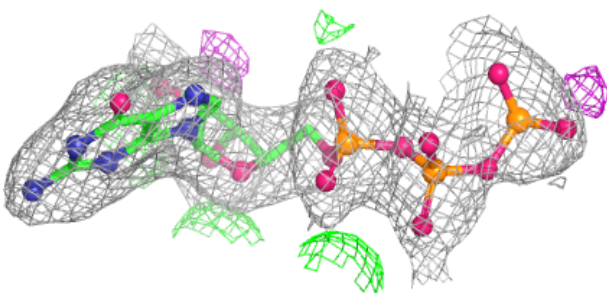
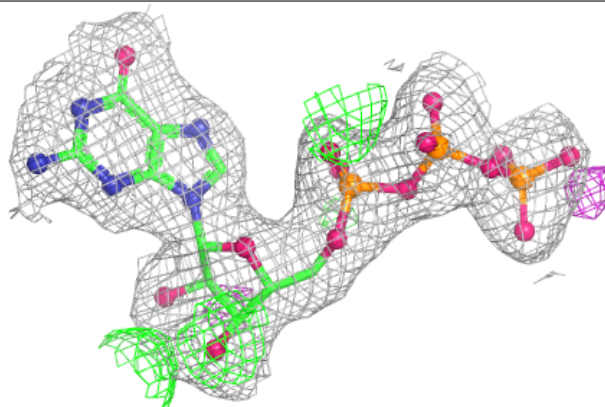


Electron density around 7PL B 508:

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

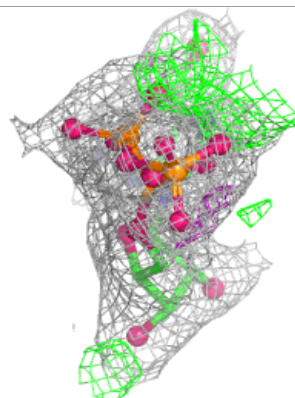
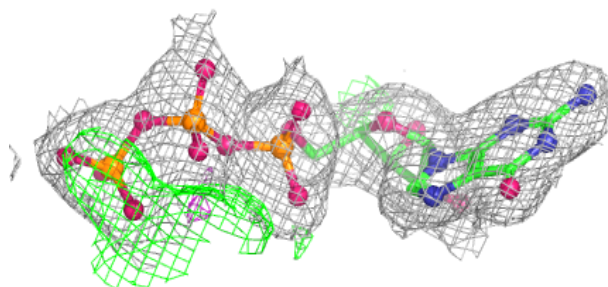
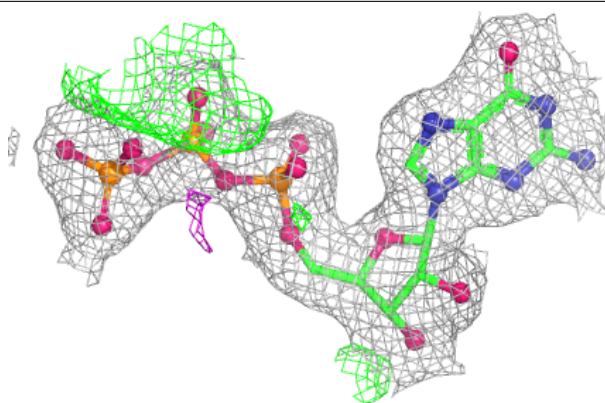
**Electron density around GTP A 501:**

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



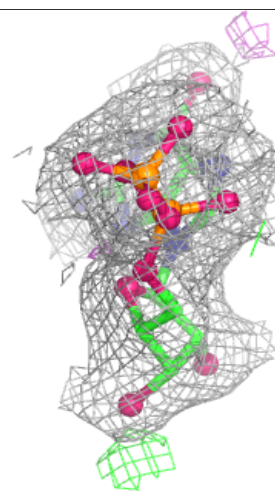
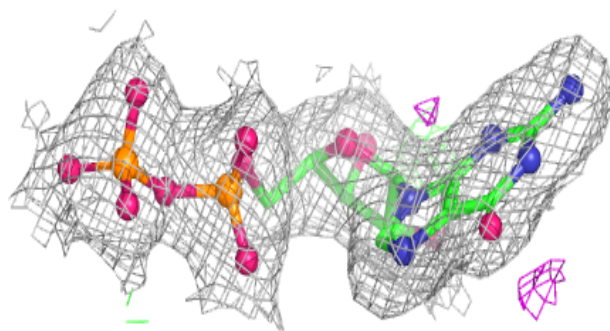
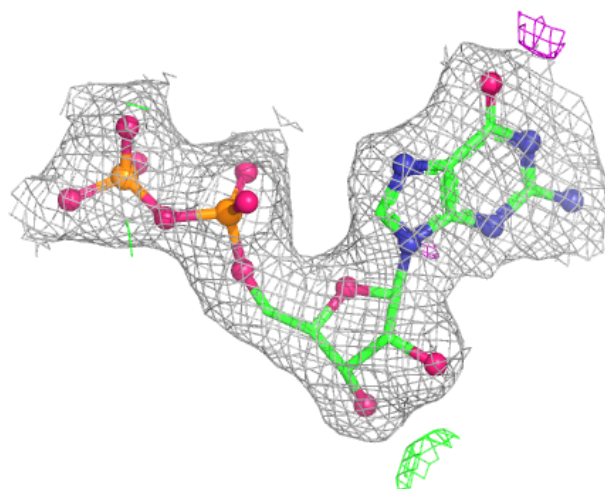
Electron density around GTP C 501:

$2mF_o-DF_c$ (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.