



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:01 PM UTC

PDB ID : 6LSM / pdb_00006lsm
Title : Tubulin Polymerization Inhibitors
Authors : Gang, L.; Wang, Y.X.; Chen, J.J.
Deposited on : 2020-01-17
Resolution : 2.75 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

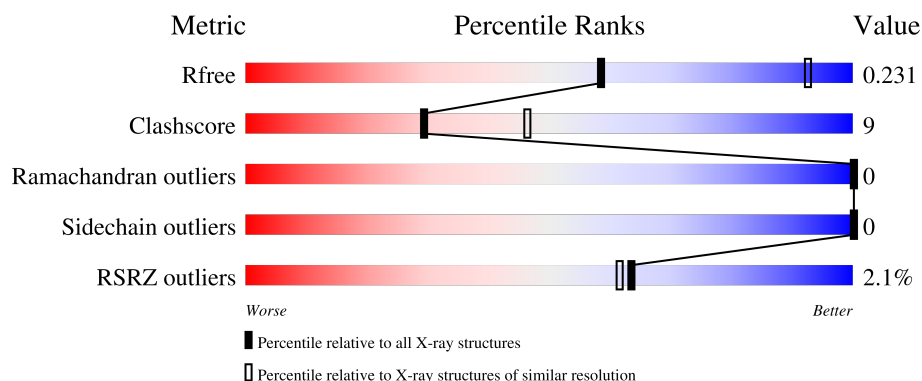
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.75 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	1009 (2.76-2.76)
Clashscore	190562	1044 (2.76-2.76)
Ramachandran outliers	187476	1024 (2.76-2.76)
Sidechain outliers	187428	1024 (2.76-2.76)
RSRZ outliers	180081	1009 (2.76-2.76)

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	% 83% 15% .
1	C	450	85% 13% .
2	B	445	% 77% 18% 5%
2	D	445	3% 73% 22% 5%
3	E	143	65% 22% 13%

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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
9	GDP	D	600	-	-	X	-

2 Entry composition

There are 13 unique types of molecules in this entry. The entry contains 17751 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	440	Total	C	N	O	S	0	1	0
			3435	2175	581	657	22			
1	C	440	Total	C	N	O	S	0	4	0
			3451	2184	585	660	22			

- Molecule 2 is a protein called Tubulin beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	424	Total	C	N	O	S	0	2	0
			3344	2104	569	645	26			
2	D	421	Total	C	N	O	S	0	2	0
			3300	2074	562	639	25			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	124	Total	C	N	O	S	0	1	0
			1021	628	184	204	5			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
E	3	MET	-	initiating methionine	UNP P63042
E	4	ALA	-	expression tag	UNP P63042

- Molecule 4 is a protein called Tubulin tyrosine ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	351	Total	C	N	O	S	0	2	0
			2891	1852	499	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		
6	D	1	Total	Mg	0	0
			1	1		

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

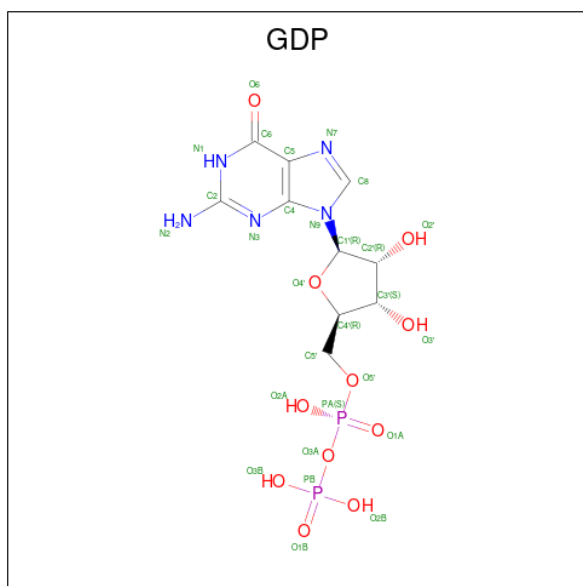
- Molecule 7 is CALCIUM ION (CCD ID: CA) (formula: Ca).

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

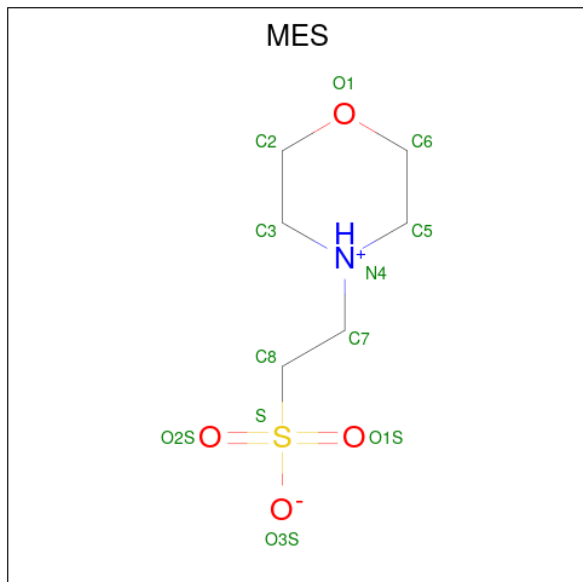
- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

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

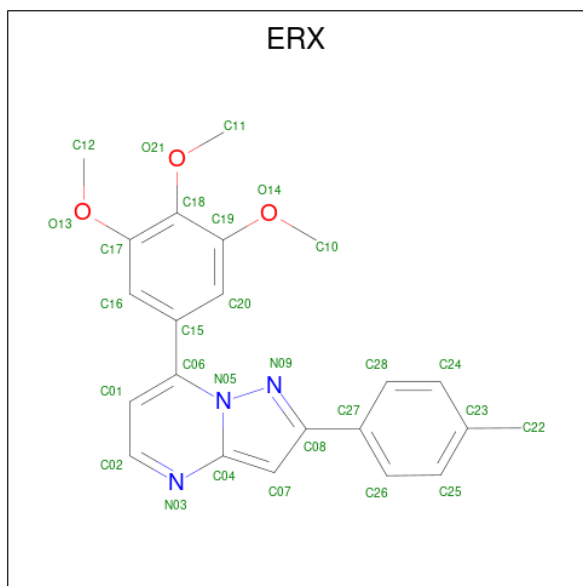


- Molecule 10 is 2-(N-MORPHOLINO)-ETHANESULFONIC ACID (CCD ID: MES) (formula: $C_6H_{13}NO_4S$).



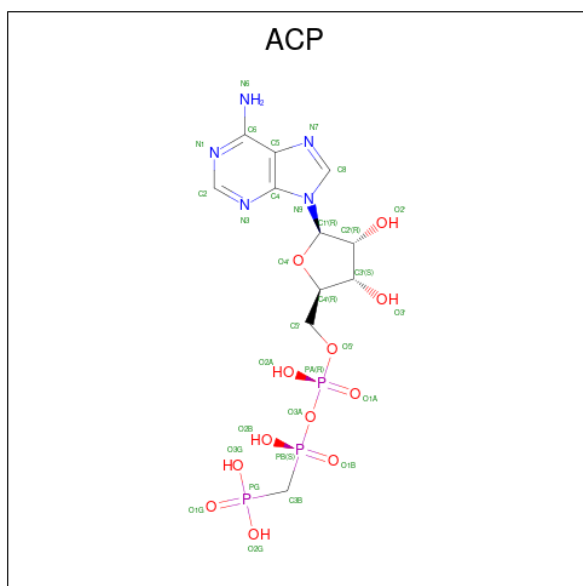
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		
10	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 11 is 2-(4-methylphenyl)-7-(3,4,5-trimethoxyphenyl)pyrazolo[1,5-a]pyrimidine (CCD ID: ERX) (formula: $C_{22}H_{21}N_3O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			28	22	3	3		

- Molecule 12 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

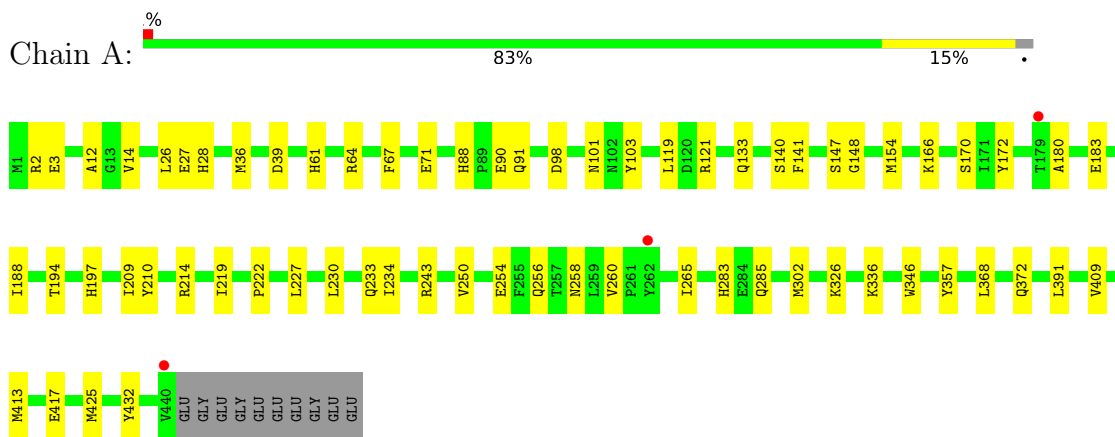
- Molecule 13 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
13	A	14	Total	O	0	0
			14	14		
13	B	27	Total	O	0	0
			27	27		
13	C	35	Total	O	0	0
			35	35		
13	D	3	Total	O	0	0
			3	3		
13	E	8	Total	O	0	0
			8	8		
13	F	8	Total	O	0	0
			8	8		

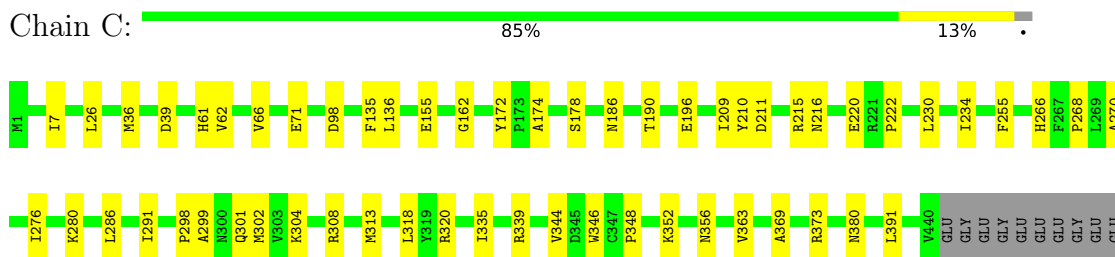
3 Residue-property plots

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

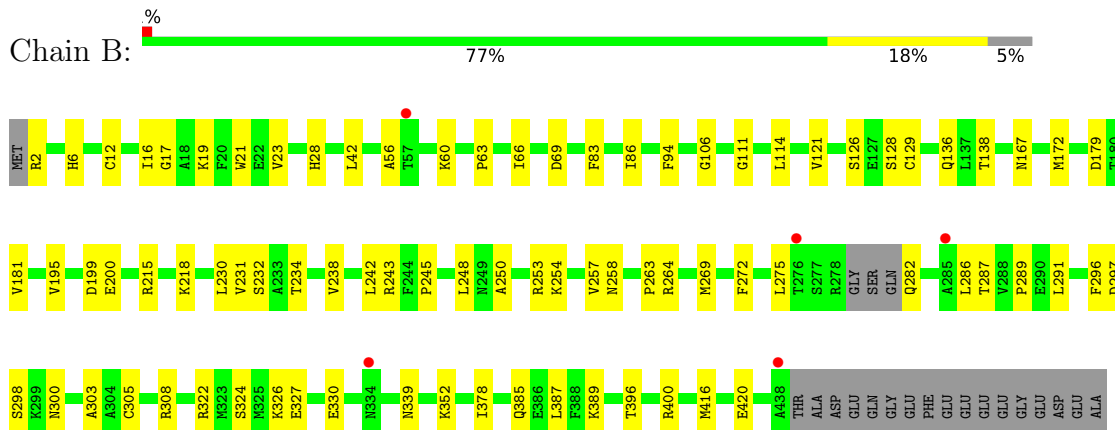
- Molecule 1: Tubulin alpha-1B chain



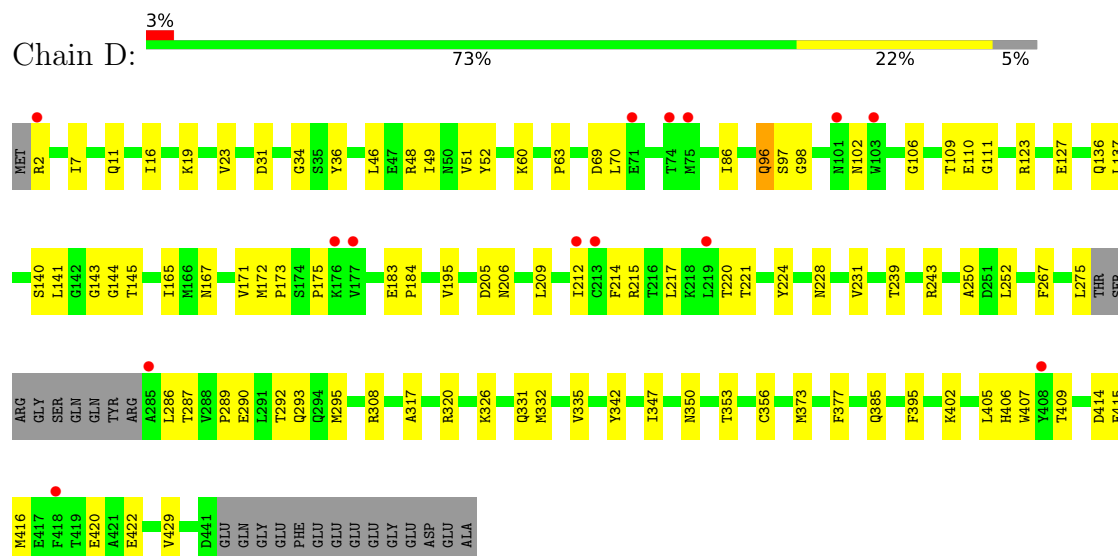
- Molecule 1: Tubulin alpha-1B chain



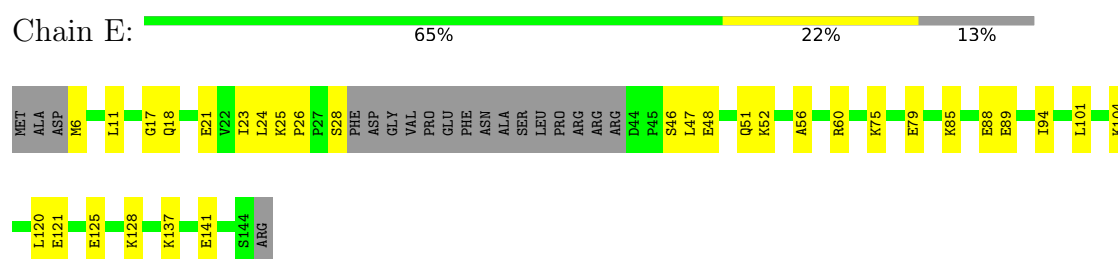
- Molecule 2: Tubulin beta chain



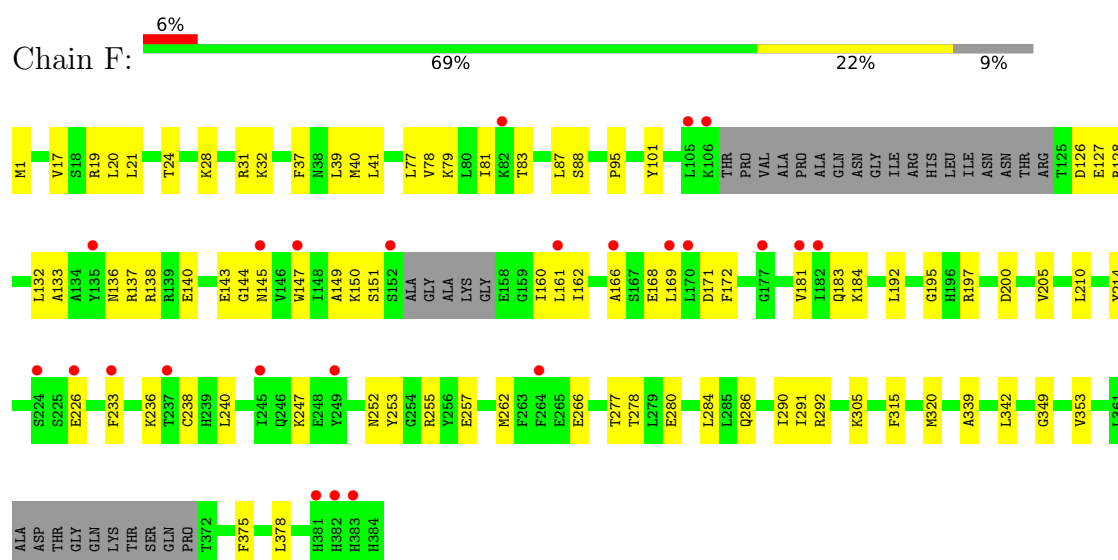
- Molecule 2: Tubulin beta chain



- Molecule 3: Stathmin-4



- Molecule 4: Tubulin tyrosine ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.55Å 158.08Å 182.23Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 2.75 29.87 – 2.75	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.87-2.75) 99.6 (29.87-2.75)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.76Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.181 , 0.227 0.188 , 0.231	Depositor DCC
R_{free} test set	2000 reflections (2.51%)	wwPDB-VP
Wilson B-factor (Å ²)	55.3	Xtriage
Anisotropy	0.145	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 47.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17751	wwPDB-VP
Average B, all atoms (Å ²)	61.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.52% 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, CA, MES, GTP, ACP, MG, ERX, CL

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	0.42	0/3516	0.65	0/4775
1	C	0.58	3/3538 (0.1%)	0.69	3/4803 (0.1%)
2	B	0.44	0/3424	0.68	0/4638
2	D	0.45	2/3376 (0.1%)	0.63	0/4576
3	E	0.43	0/1032	0.60	0/1371
4	F	0.38	0/2964	0.63	1/4003 (0.0%)
All	All	0.46	5/17850 (0.0%)	0.65	4/24166 (0.0%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	62	VAL	CA-C	-17.75	1.40	1.52
1	C	62	VAL	CA-CB	7.09	1.59	1.54
2	D	175	PRO	N-CD	-7.04	1.37	1.47
2	D	96	GLN	CA-C	6.45	1.61	1.52
1	C	62	VAL	C-N	5.43	1.40	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	62	VAL	CA-C-O	9.18	125.20	119.51
1	C	62	VAL	O-C-N	-6.59	114.45	121.11
1	C	280	LYS	CD-CE-NZ	6.58	132.97	111.90
4	F	151	SER	CB-CA-C	-5.01	101.86	112.78

There are no chirality outliers.

There are no planarity outliers.

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	3435	0	3345	50	0
1	C	3451	0	3364	35	0
2	B	3344	0	3226	59	0
2	D	3300	0	3169	76	0
3	E	1021	0	1029	26	0
4	F	2891	0	2857	60	0
5	A	32	0	12	0	0
5	C	32	0	11	0	0
6	A	1	0	0	0	0
6	B	2	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	A	1	0	0	0	0
9	B	28	0	10	2	0
9	D	28	0	12	15	0
10	B	24	0	25	5	0
11	B	28	0	0	1	0
12	F	31	0	13	3	0
13	A	14	0	0	1	0
13	B	27	0	0	5	0
13	C	35	0	0	2	0
13	D	3	0	0	0	0
13	E	8	0	0	2	0
13	F	8	0	0	0	0
All	All	17751	0	17073	300	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 (300) 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:143:GLY:HA3	9:D:600:GDP:O2A	1.45	1.14
2:D:16:ILE:HG22	2:D:228:ASN:OD1	1.74	0.88
2:D:144:GLY:N	9:D:600:GDP:O2B	2.11	0.82
2:D:206:ASN:HA	2:D:209:LEU:HD23	1.61	0.79
2:D:205:ASP:O	2:D:209:LEU:HD22	1.83	0.78
1:A:27:GLU:OE1	1:A:243:ARG:NH2	2.17	0.77
2:D:143:GLY:CA	9:D:600:GDP:O2A	2.31	0.75
1:C:255:PHE:CZ	1:C:318:LEU:HD22	2.22	0.74
1:C:36:MET:SD	1:C:39:ASP:HB2	2.31	0.70
4:F:78:VAL:HG21	4:F:181:VAL:HG21	1.75	0.68
9:D:600:GDP:H5'	9:D:600:GDP:H8	1.58	0.68
2:B:339:ASN:HA	13:B:602:HOH:O	1.95	0.67
1:C:211[A]:ASP:OD2	1:C:304:LYS:NZ	2.28	0.67
2:B:298:SER:N	10:B:505:MES:O1S	2.22	0.66
9:D:600:GDP:H8	9:D:600:GDP:C5'	2.09	0.66
3:E:11:LEU:HD11	3:E:18:GLN:HE21	1.61	0.65
4:F:128:ARG:O	4:F:132:LEU:HD12	1.96	0.65
4:F:168:GLU:O	4:F:171:ASP:HB3	1.95	0.65
4:F:192:LEU:HD22	4:F:262:MET:HE1	1.77	0.65
2:D:228:ASN:CG	9:D:600:GDP:HN1	2.05	0.65
2:B:172:MET:HG2	2:B:387:LEU:HD21	1.80	0.64
2:D:228:ASN:ND2	9:D:600:GDP:HN1	1.96	0.64
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.79	0.63
2:D:317:ALA:HB3	2:D:353:THR:HG22	1.80	0.63
4:F:197:ARG:NH2	4:F:257:GLU:OE2	2.32	0.62
4:F:277:THR:HG22	4:F:278:THR:H	1.64	0.62
2:D:16:ILE:CG2	2:D:228:ASN:OD1	2.45	0.62
1:A:209:ILE:HD11	1:A:302:MET:SD	2.41	0.61
3:E:48:GLU:O	3:E:52:LYS:HG2	2.01	0.61
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.83	0.60
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.20	0.60
2:D:145:THR:H	9:D:600:GDP:PB	2.25	0.60
2:D:136:GLN:HA	2:D:167:ASN:O	2.03	0.59
2:D:7:ILE:O	2:D:137:LEU:HD12	2.03	0.59
2:B:181:VAL:HG12	1:C:348:PRO:HG2	1.84	0.59
2:D:295:MET:HG2	2:D:377:PHE:HB2	1.84	0.59
9:D:600:GDP:C5'	9:D:600:GDP:C8	2.85	0.59
1:C:196:GLU:HB2	13:C:616:HOH:O	2.03	0.58
4:F:349:GLY:O	4:F:353:VAL:HG12	2.03	0.57
2:D:214:PHE:HD2	2:D:215:ARG:HG2	1.70	0.57
2:D:402:LYS:HG3	2:D:405:LEU:HD13	1.86	0.57
4:F:247:LYS:HD2	4:F:253:TYR:CZ	2.39	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:GLN:HA	2:B:167:ASN:O	2.04	0.57
1:C:286:LEU:HD12	13:C:610:HOH:O	2.04	0.57
2:B:12:CYS:HB2	9:B:501:GDP:C8	2.40	0.57
2:B:230:LEU:O	2:B:234:THR:HG23	2.03	0.57
2:B:167:ASN:OD1	2:B:200:GLU:HG3	2.03	0.57
2:B:263:PRO:HD2	13:B:610:HOH:O	2.04	0.57
2:D:332:MET:HG3	2:D:353:THR:HG21	1.86	0.57
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.40	0.57
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.87	0.56
2:D:70:LEU:HB3	2:D:98:GLY:HA2	1.87	0.56
4:F:210:LEU:O	4:F:305:LYS:NZ	2.38	0.56
2:D:220:THR:HG23	2:D:221:THR:HG22	1.86	0.56
2:D:239:THR:O	2:D:243:ARG:HG3	2.06	0.56
2:D:287:THR:HB	2:D:289:PRO:HD2	1.88	0.56
2:D:331:GLN:O	2:D:335:VAL:HG23	2.06	0.56
2:B:106:GLY:O	2:B:111:GLY:HA3	2.06	0.56
2:B:195:VAL:HG13	2:B:264:ARG:HB3	1.89	0.55
4:F:79:LYS:O	4:F:83:THR:OG1	2.21	0.55
4:F:280:GLU:HA	4:F:284:LEU:HB2	1.88	0.55
1:C:162:GLY:HA2	3:E:94:ILE:HD11	1.88	0.54
2:D:63:PRO:HG2	2:D:86:ILE:HG23	1.89	0.54
2:D:145:THR:N	9:D:600:GDP:O2B	2.40	0.54
1:C:174:ALA:O	1:C:178:SER:HB2	2.07	0.54
2:D:48:ARG:HH12	2:D:250:ALA:HB1	1.73	0.53
3:E:11:LEU:HD11	3:E:18:GLN:NE2	2.23	0.53
2:B:322:ARG:HG2	2:B:322:ARG:HH21	1.74	0.53
4:F:150:LYS:HD3	4:F:160:ILE:HG12	1.91	0.53
1:A:101:ASN:HD22	2:B:258:ASN:HD21	1.56	0.53
1:A:230:LEU:O	1:A:234:ILE:HD12	2.09	0.53
2:D:205:ASP:O	2:D:209:LEU:CD2	2.54	0.53
2:B:396:THR:O	2:B:400:ARG:HG2	2.08	0.53
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.91	0.52
4:F:200:ASP:OD2	12:F:402:ACP:O3'	2.27	0.52
4:F:162:ILE:HB	4:F:233:PHE:HB3	1.91	0.52
4:F:286:GLN:O	4:F:290:ILE:HG13	2.08	0.52
1:C:71:GLU:HG2	1:C:98:ASP:HB3	1.90	0.52
1:A:180:ALA:O	1:A:183:GLU:HG3	2.10	0.52
2:B:248:LEU:HD11	2:B:352:LYS:HE2	1.92	0.52
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.44	0.52
2:D:414:ASP:OD1	2:D:415:GLU:N	2.43	0.52
4:F:101:TYR:HD2	4:F:126:ASP:HB2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:TYR:CE1	1:A:148:GLY:HA2	2.45	0.52
1:A:3:GLU:HG2	1:A:64:ARG:NH2	2.25	0.51
4:F:160:ILE:HD13	4:F:240:LEU:HD21	1.92	0.51
1:C:313:MET:HE3	1:C:380:ASN:CG	2.35	0.51
2:D:69:ASP:OD1	2:D:70:LEU:N	2.44	0.51
4:F:292:ARG:HG3	4:F:378:LEU:HB3	1.93	0.51
1:C:7:ILE:HG23	1:C:66:VAL:HG13	1.93	0.51
2:D:295:MET:CG	2:D:377:PHE:HB2	2.40	0.51
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.41	0.51
2:B:308:ARG:HE	10:B:505:MES:H71	1.75	0.51
3:E:137:LYS:O	3:E:141:GLU:HG2	2.11	0.51
3:E:56:ALA:HB1	3:E:60:ARG:HH12	1.76	0.51
2:B:253:ARG:O	2:B:257:VAL:HG23	2.10	0.50
1:A:250:VAL:HG22	1:A:254:GLU:OE2	2.12	0.50
2:B:296:PHE:O	10:B:505:MES:H81	2.12	0.50
2:D:123:ARG:O	2:D:127:GLU:HG2	2.12	0.50
2:B:234:THR:O	2:B:238:VAL:HG13	2.11	0.50
4:F:136:ASN:O	4:F:140:GLU:HG3	2.10	0.50
9:D:600:GDP:C8	9:D:600:GDP:H5''	2.46	0.50
4:F:184:LYS:O	12:F:402:ACP:N6	2.44	0.50
3:E:25:LYS:HG2	3:E:26:PRO:HD2	1.93	0.49
1:A:141:PHE:O	1:A:147:SER:HB3	2.12	0.49
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.47	0.49
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.42	0.49
2:B:238:VAL:HB	2:B:378:ILE:HD11	1.92	0.49
3:E:6:MET:HE2	3:E:24:LEU:HD22	1.94	0.49
2:B:242:LEU:HA	2:B:250:ALA:HB1	1.95	0.49
2:B:286:LEU:HD23	2:B:291:LEU:HD23	1.94	0.49
1:A:326:LYS:HE2	1:A:326:LYS:H	1.78	0.49
4:F:138:ARG:NH1	4:F:144:GLY:O	2.46	0.49
3:E:125:GLU:HA	3:E:128:LYS:HG2	1.94	0.49
1:A:172:TYR:CE2	1:A:391:LEU:HD22	2.47	0.49
1:A:2:ARG:O	1:A:133:GLN:NE2	2.45	0.48
2:B:69:ASP:O	2:B:94:PHE:HA	2.14	0.48
2:B:326:LYS:HE3	2:B:330:GLU:OE2	2.13	0.48
4:F:31:ARG:HH21	4:F:32:LYS:HD3	1.78	0.48
4:F:161:LEU:HD23	4:F:172:PHE:CZ	2.49	0.48
4:F:1:MET:HE3	4:F:28:LYS:HB2	1.95	0.48
1:A:12:ALA:HB3	1:A:140:SER:HB3	1.96	0.48
2:D:416:MET:O	2:D:420:GLU:HG3	2.13	0.48
2:B:42:LEU:HD22	2:B:245:PRO:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:280:GLU:HA	4:F:284:LEU:CB	2.44	0.47
2:D:31:ASP:OD1	2:D:34:GLY:N	2.47	0.47
1:C:26:LEU:HD12	1:C:363:VAL:HG12	1.97	0.47
2:D:11:GLN:HB3	9:D:600:GDP:O1A	2.15	0.47
4:F:133:ALA:O	4:F:137:ARG:HG3	2.14	0.47
1:A:154:MET:HG3	1:A:194:THR:HG23	1.95	0.47
2:B:28:HIS:NE2	2:B:243:ARG:HB3	2.29	0.47
3:E:75:LYS:O	3:E:79:GLU:HG3	2.15	0.47
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.49	0.47
2:D:19:LYS:O	2:D:23:VAL:HG23	2.13	0.47
2:D:308:ARG:HG2	2:D:342:TYR:CZ	2.50	0.47
3:E:21:GLU:OE1	3:E:23:ILE:HD11	2.14	0.47
4:F:87:LEU:O	4:F:88:SER:OG	2.33	0.47
4:F:132:LEU:CD2	4:F:166:ALA:HB1	2.45	0.47
1:A:28:HIS:O	1:A:36:MET:HE3	2.15	0.47
2:B:16[B]:ILE:HD13	2:B:231:VAL:HG11	1.96	0.47
4:F:39:LEU:HD21	4:F:41:LEU:HD21	1.97	0.47
4:F:284:LEU:HD12	4:F:284:LEU:HA	1.63	0.47
2:D:36:TYR:CD1	2:D:46:LEU:HD21	2.49	0.47
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.51	0.46
2:D:165:ILE:HG21	2:D:252:LEU:HB3	1.96	0.46
3:E:121:GLU:O	3:E:125:GLU:HG2	2.14	0.46
1:A:336:LYS:HD3	3:E:24:LEU:CD1	2.45	0.46
2:B:234:THR:HG22	2:B:272:PHE:HB2	1.97	0.46
2:D:140:SER:HA	2:D:171:VAL:HB	1.97	0.46
2:D:228:ASN:ND2	9:D:600:GDP:N1	2.63	0.46
4:F:17:VAL:HA	4:F:20:LEU:HD12	1.96	0.46
4:F:137:ARG:HA	4:F:140:GLU:OE2	2.16	0.46
4:F:161:LEU:HD13	4:F:161:LEU:HA	1.79	0.46
2:D:51:VAL:HG13	2:D:52:TYR:CD2	2.50	0.46
1:A:88:HIS:N	1:A:91:GLN:OE1	2.38	0.46
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.51	0.46
2:B:339:ASN:ND2	13:B:602:HOH:O	2.22	0.46
1:A:101:ASN:ND2	2:B:254:LYS:HG2	2.31	0.46
1:C:186:ASN:O	1:C:190:THR:HG22	2.16	0.46
2:D:286:LEU:HD12	2:D:286:LEU:HA	1.78	0.46
1:A:166:LYS:HE2	1:A:197:HIS:O	2.16	0.46
1:A:413:MET:HE3	1:A:417:GLU:HB3	1.98	0.45
1:C:313:MET:HE3	1:C:380:ASN:ND2	2.31	0.45
2:B:282:GLN:N	13:B:608:HOH:O	2.50	0.45
2:B:303:ALA:O	2:B:305:CYS:N	2.45	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:395:PHE:CE1	2:D:422:GLU:HG3	2.51	0.45
2:D:406:HIS:CD2	2:D:407:TRP:HD1	2.34	0.45
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.52	0.45
4:F:195:GLY:HA3	4:F:197:ARG:HD3	1.99	0.45
4:F:226:GLU:HB3	4:F:238:CYS:HB3	1.98	0.45
1:A:90:GLU:O	1:A:121:ARG:HD2	2.15	0.45
1:A:141:PHE:CE1	1:A:170:SER:HB3	2.52	0.45
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.52	0.45
2:D:2:ARG:O	2:D:51:VAL:HG23	2.17	0.45
3:E:85:LYS:HE2	3:E:89:GLU:OE2	2.17	0.45
4:F:138:ARG:NH2	4:F:143:GLU:OE2	2.49	0.45
2:B:16[A]:ILE:HD11	2:B:138:THR:HB	2.00	0.44
1:C:215:ARG:HD2	1:C:216:ASN:OD1	2.18	0.44
4:F:145:ASN:OD1	4:F:147:TRP:NE1	2.49	0.44
1:A:326:LYS:HD3	1:A:326:LYS:N	2.32	0.44
1:A:336:LYS:HD3	3:E:24:LEU:HD13	1.99	0.44
2:B:16[A]:ILE:HG13	2:B:17:GLY:N	2.32	0.44
2:B:275:LEU:HD11	2:B:300:ASN:HA	1.98	0.44
3:E:28:SER:C	13:E:201:HOH:O	2.59	0.44
1:A:372:GLN:NE2	13:A:606:HOH:O	2.50	0.44
2:B:19:LYS:HG2	2:B:232:SER:OG	2.18	0.44
2:B:324:SER:OG	2:B:327:GLU:HB2	2.17	0.44
1:A:88:HIS:HB3	1:A:91:GLN:HG3	1.98	0.44
1:A:71:GLU:HG2	1:A:98:ASP:HB3	1.99	0.44
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.99	0.44
1:A:256:GLN:HG2	1:A:260:VAL:HB	1.99	0.44
1:A:233:GLN:HG3	1:A:368:LEU:HD12	2.00	0.43
1:C:210:TYR:CZ	1:C:222:PRO:HD2	2.53	0.43
4:F:339:ALA:HB3	4:F:342:LEU:HD12	2.00	0.43
2:D:48:ARG:O	2:D:51:VAL:HG12	2.19	0.43
2:D:96:GLN:NE2	2:D:97:SER:H	2.15	0.43
2:D:416:MET:HE3	2:D:416:MET:HB3	1.81	0.43
1:A:346:TRP:H	1:A:346:TRP:CD1	2.35	0.43
4:F:262:MET:SD	4:F:266:GLU:HG2	2.59	0.43
1:A:391:LEU:HD12	1:A:391:LEU:HA	1.86	0.43
2:D:70:LEU:HD23	2:D:70:LEU:HA	1.84	0.43
2:D:292:THR:HG22	2:D:335:VAL:HG21	2.00	0.43
4:F:19:ARG:HG3	4:F:20:LEU:N	2.33	0.43
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.54	0.43
4:F:95:PRO:HB2	4:F:183:GLN:CG	2.49	0.43
2:B:83:PHE:O	2:B:86:ILE:HG22	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:GLN:O	1:A:256:GLN:OE1	2.36	0.43
3:E:47:LEU:HD12	3:E:47:LEU:O	2.19	0.43
3:E:88:GLU:OE1	3:E:88:GLU:HA	2.19	0.43
4:F:150:LYS:HD3	4:F:160:ILE:CG1	2.48	0.43
4:F:169:LEU:HD23	4:F:169:LEU:HA	1.43	0.43
1:A:39:ASP:OD2	1:A:61:HIS:NE2	2.44	0.43
2:B:352:LYS:HD2	11:B:507:ERX:C08	2.49	0.43
1:C:255:PHE:CE2	1:C:318:LEU:HD22	2.54	0.43
2:B:199:ASP:OD2	10:B:504:MES:H52	2.19	0.43
2:B:287:THR:HB	2:B:289:PRO:HD2	2.00	0.43
2:D:228:ASN:OD1	9:D:600:GDP:N1	2.52	0.43
2:D:406:HIS:HA	2:D:409:THR:HG22	2.01	0.43
2:D:141:LEU:HD12	2:D:172:MET:SD	2.59	0.43
4:F:21:LEU:O	4:F:24:THR:OG1	2.24	0.43
4:F:214:TYR:HB3	4:F:375:PHE:HB3	2.01	0.43
4:F:320:MET:HE2	12:F:402:ACP:C2	2.49	0.43
2:B:56:ALA:HB3	2:B:60:LYS:HB2	2.01	0.42
1:C:215:ARG:CZ	1:C:299:ALA:HB1	2.49	0.42
3:E:46:SER:OG	3:E:48:GLU:N	2.52	0.42
2:D:106:GLY:O	2:D:111:GLY:HA3	2.19	0.42
1:C:266:HIS:O	1:C:268:PRO:HD3	2.19	0.42
4:F:161:LEU:HD23	4:F:172:PHE:CE2	2.54	0.42
2:D:172:MET:HG3	2:D:173:PRO:HD2	2.01	0.42
3:E:46:SER:OG	3:E:47:LEU:N	2.52	0.42
3:E:104:LYS:NZ	13:E:204:HOH:O	2.51	0.42
2:D:46:LEU:HA	2:D:49:ILE:HB	2.02	0.42
2:D:275:LEU:HD23	2:D:275:LEU:HA	1.85	0.42
2:D:290:GLU:O	2:D:293:GLN:HB3	2.20	0.42
1:A:12:ALA:CB	1:A:140:SER:HB3	2.50	0.42
2:B:12:CYS:HB2	9:B:501:GDP:N7	2.35	0.42
2:B:297:ASP:HA	10:B:505:MES:O1S	2.20	0.42
1:C:155:GLU:HB3	3:E:101:LEU:HD22	2.02	0.42
1:C:230:LEU:O	1:C:234:ILE:HD12	2.20	0.42
2:D:34:GLY:O	2:D:60:LYS:HA	2.20	0.42
2:D:48:ARG:NH1	2:D:250:ALA:HB1	2.34	0.42
4:F:126:ASP:OD1	4:F:127:GLU:N	2.53	0.42
4:F:205:VAL:HG22	4:F:315:PHE:HB2	2.02	0.42
2:D:228:ASN:HA	2:D:231:VAL:HG22	2.01	0.41
4:F:149:ALA:O	4:F:160:ILE:HG23	2.19	0.41
2:B:128:SER:O	2:B:128:SER:OG	2.36	0.41
3:E:120:LEU:HD23	3:E:120:LEU:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:179:ASP:O	1:C:352:LYS:NZ	2.37	0.41
2:D:212:ILE:HG22	2:D:217:LEU:HD12	2.02	0.41
2:D:228:ASN:O	2:D:231:VAL:HG22	2.20	0.41
1:C:209:ILE:HD11	1:C:302:MET:SD	2.60	0.41
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.35	0.41
2:D:385:GLN:HB2	2:D:429:VAL:HG13	2.02	0.41
4:F:205:VAL:HG11	4:F:291:ILE:HD13	2.01	0.41
2:B:28:HIS:HE1	2:B:243:ARG:O	2.03	0.41
2:B:215:ARG:O	2:B:218:LYS:NZ	2.52	0.41
1:C:135:PHE:O	1:C:136:LEU:HD23	2.20	0.41
1:C:220:GLU:OE2	2:D:326:LYS:HD3	2.20	0.41
3:E:47:LEU:HD11	3:E:51:GLN:NE2	2.35	0.41
2:D:102:ASN:ND2	2:D:407:TRP:HB3	2.35	0.41
2:D:109:THR:OG1	2:D:110:GLU:N	2.53	0.41
2:D:224:TYR:O	2:D:228:ASN:ND2	2.48	0.41
4:F:149:ALA:HB2	4:F:169:LEU:HD13	2.02	0.41
4:F:247:LYS:HD2	4:F:253:TYR:CE2	2.56	0.41
1:A:14:VAL:HG13	1:A:67:PHE:HD2	1.85	0.41
2:B:269:MET:HG3	2:B:303:ALA:HB3	2.02	0.41
9:D:600:GDP:H5'	9:D:600:GDP:C8	2.46	0.41
4:F:31:ARG:HA	4:F:31:ARG:HD2	1.73	0.41
2:B:172:MET:HE2	2:B:172:MET:HB2	1.81	0.41
2:D:195:VAL:HG22	2:D:267:PHE:CE2	2.56	0.41
1:A:26:LEU:HA	1:A:26:LEU:HD23	1.81	0.41
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.56	0.41
1:A:357:TYR:OH	3:E:18:GLN:HG3	2.20	0.41
2:B:126:SER:O	2:B:129:CYS:HB2	2.21	0.41
2:B:385:GLN:O	2:B:389:LYS:HG3	2.21	0.41
2:D:206:ASN:CA	2:D:209:LEU:HD23	2.42	0.41
2:D:373:MET:HE3	2:D:373:MET:HB3	1.75	0.41
1:A:188:ILE:HG13	1:A:425:MET:HG3	2.03	0.41
1:A:214:ARG:HG2	1:A:219:ILE:O	2.21	0.41
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.35	0.41
2:D:320:ARG:HA	2:D:356:CYS:O	2.21	0.41
1:C:270:ALA:O	1:C:302:MET:HB2	2.22	0.40
1:C:301:GLN:HE21	1:C:301:GLN:HB2	1.59	0.40
1:C:320:ARG:HA	1:C:356:ASN:O	2.22	0.40
2:D:205:ASP:C	2:D:209:LEU:CD2	2.94	0.40
2:D:290:GLU:H	2:D:290:GLU:HG2	1.71	0.40
4:F:252:ASN:O	4:F:255:ARG:HB2	2.21	0.40
2:B:66:ILE:HG12	2:B:121:VAL:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:416:MET:HE3	2:B:420:GLU:HG3	2.03	0.40
2:B:114:LEU:O	2:B:114:LEU:HG	2.21	0.40
2:D:183:GLU:HB2	2:D:184:PRO:HD3	2.02	0.40
4:F:77:LEU:O	4:F:81:ILE:HG13	2.21	0.40
4:F:168:GLU:CD	4:F:168:GLU:C	2.90	0.40
1:A:119:LEU:HD23	1:A:119:LEU:HA	1.90	0.40
1:A:409:VAL:HA	1:A:413:MET:O	2.21	0.40
1:C:276:ILE:HG23	1:C:369:ALA:HB3	2.03	0.40
1:C:291:ILE:HD13	1:C:373:ARG:HG3	2.02	0.40
2:D:402:LYS:HE2	2:D:402:LYS:HB2	1.78	0.40
1:A:283:HIS:HD2	1:A:285:GLN:NE2	2.19	0.40
2:B:2:ARG:N	13:B:613:HOH:O	2.54	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%)	422 (96%)	17 (4%)	0	100	100
1	C	441/450 (98%)	426 (97%)	15 (3%)	0	100	100
2	B	422/445 (95%)	408 (97%)	14 (3%)	0	100	100
2	D	418/445 (94%)	403 (96%)	15 (4%)	0	100	100
3	E	121/143 (85%)	119 (98%)	2 (2%)	0	100	100
4	F	345/384 (90%)	331 (96%)	14 (4%)	0	100	100
All	All	2186/2317 (94%)	2109 (96%)	77 (4%)	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%)	371 (100%)	0	100	100
1	C	374/378 (99%)	374 (100%)	0	100	100
2	B	368/383 (96%)	368 (100%)	0	100	100
2	D	361/383 (94%)	361 (100%)	0	100	100
3	E	111/127 (87%)	111 (100%)	0	100	100
4	F	319/342 (93%)	319 (100%)	0	100	100
All	All	1904/1991 (96%)	1904 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	GLN
1	A	85	GLN
1	A	101	ASN
1	A	128	GLN
1	A	285	GLN
1	A	309	HIS
1	A	393	HIS
2	B	50	ASN
2	B	59	ASN
2	B	334	ASN
2	B	339	ASN
2	B	349	ASN
2	B	385	GLN
2	B	436	GLN
1	C	15	GLN
1	C	128	GLN
1	C	256	GLN
1	C	283	HIS
1	C	285	GLN

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Mol	Chain	Res	Type
1	C	372	GLN
1	C	393	HIS
2	D	8	GLN
2	D	14	ASN
2	D	96	GLN
2	D	136	GLN
2	D	167	ASN
2	D	337	ASN
2	D	436	GLN
3	E	18	GLN
3	E	51	GLN
3	E	136	ASN
4	F	10	ASN
4	F	136	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 19 ligands modelled in this entry, 11 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
10	MES	B	505	-	12,12,12	1.63	1 (8%)	15,16,16	2.05	6 (40%)
9	GDP	D	600	-	29,30,30	1.63	8 (27%)	45,47,47	2.24	14 (31%)
9	GDP	B	501	6	29,30,30	3.68	13 (44%)	45,47,47	1.78	10 (22%)
12	ACP	F	402	6	31,33,33	3.55	11 (35%)	47,52,52	2.00	15 (31%)
10	MES	B	504	-	12,12,12	1.67	2 (16%)	15,16,16	1.90	5 (33%)
5	GTP	C	501	6	33,34,34	3.57	19 (57%)	50,54,54	1.74	13 (26%)
5	GTP	A	501	6	33,34,34	3.55	17 (51%)	50,54,54	1.59	10 (20%)
11	ERX	B	507	-	31,31,31	2.07	6 (19%)	44,44,44	3.06	16 (36%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	MES	B	505	-	-	2/6/14/14	0/1/1/1
9	GDP	D	600	-	-	5/16/32/32	0/3/3/3
9	GDP	B	501	6	-	4/16/32/32	0/3/3/3
12	ACP	F	402	6	-	6/19/38/38	0/3/3/3
10	MES	B	504	-	-	2/6/14/14	0/1/1/1
5	GTP	C	501	6	-	8/22/38/38	0/3/3/3
5	GTP	A	501	6	-	6/22/38/38	0/3/3/3
11	ERX	B	507	-	-	2/14/14/14	0/4/4/4

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	501	GDP	C3'-C4'	-8.97	1.30	1.53
12	F	402	ACP	PB-O3A	8.86	1.68	1.58
12	F	402	ACP	O4'-C1'	8.75	1.62	1.42
12	F	402	ACP	PA-O3A	8.44	1.68	1.59
9	B	501	GDP	PA-O3A	8.22	1.68	1.59
5	C	501	GTP	O4'-C1'	7.89	1.60	1.42
5	C	501	GTP	C2'-C1'	-7.85	1.28	1.53
5	A	501	GTP	C2'-C1'	-7.78	1.29	1.53
5	A	501	GTP	O4'-C1'	7.59	1.59	1.42
11	B	507	ERX	C07-C04	7.35	1.45	1.38
12	F	402	ACP	C2'-C1'	-7.09	1.31	1.53
9	B	501	GDP	O4'-C4'	7.06	1.60	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	501	GTP	PA-O3A	6.90	1.66	1.59
9	B	501	GDP	C4-N3	6.63	1.49	1.34
5	A	501	GTP	O4'-C4'	-6.52	1.30	1.45
5	C	501	GTP	O4'-C4'	-6.35	1.30	1.45
5	C	501	GTP	PB-O3B	6.20	1.66	1.59
9	B	501	GDP	C2-N2	6.14	1.48	1.34
12	F	402	ACP	O4'-C4'	-6.14	1.31	1.45
5	C	501	GTP	C4-N3	6.08	1.48	1.34
5	A	501	GTP	C4-N3	5.96	1.47	1.34
5	A	501	GTP	PB-O3B	5.75	1.65	1.59
11	B	507	ERX	C04-N05	-5.62	1.31	1.39
5	C	501	GTP	C2-N3	5.57	1.46	1.33
5	C	501	GTP	PA-O3A	5.53	1.65	1.59
5	A	501	GTP	C2-N3	5.47	1.46	1.33
9	B	501	GDP	C2-N3	4.72	1.44	1.33
12	F	402	ACP	C6-N6	4.67	1.46	1.34
5	C	501	GTP	C2-N2	4.60	1.44	1.34
5	A	501	GTP	PB-O3A	4.47	1.64	1.59
5	C	501	GTP	PB-O3A	4.06	1.63	1.59
5	A	501	GTP	C2-N2	3.95	1.43	1.34
10	B	505	MES	C8-S	3.87	1.83	1.77
9	B	501	GDP	O4'-C1'	-3.83	1.33	1.42
9	D	600	GDP	C5-N7	-3.70	1.31	1.39
10	B	504	MES	C8-S	3.50	1.82	1.77
11	B	507	ERX	C27-C08	3.47	1.52	1.47
9	D	600	GDP	C6-N1	-3.44	1.32	1.38
9	B	501	GDP	O6-C6	-3.39	1.17	1.23
5	C	501	GTP	C6-N1	3.31	1.45	1.38
9	B	501	GDP	O2'-C2'	-3.22	1.35	1.43
9	B	501	GDP	C6-N1	3.15	1.44	1.38
11	B	507	ERX	C15-C06	3.08	1.52	1.48
5	A	501	GTP	C6-N1	2.99	1.44	1.38
5	C	501	GTP	C5-C6	2.96	1.55	1.44
5	A	501	GTP	C5-C6	2.92	1.55	1.44
5	C	501	GTP	PG-O1G	2.77	1.59	1.50
12	F	402	ACP	O2'-C2'	2.76	1.49	1.43
5	A	501	GTP	C2-N1	2.72	1.44	1.37
5	C	501	GTP	C5-N7	-2.72	1.33	1.39
5	C	501	GTP	C2-N1	2.70	1.44	1.37
11	B	507	ERX	O13-C17	2.63	1.41	1.37
12	F	402	ACP	O3'-C3'	-2.61	1.36	1.43
5	A	501	GTP	O2'-C2'	2.61	1.49	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	501	GDP	C4-N9	-2.58	1.31	1.38
12	F	402	ACP	C5-C4	-2.56	1.34	1.39
10	B	504	MES	O1S-S	2.53	1.52	1.45
5	C	501	GTP	PB-O1B	2.49	1.59	1.50
5	C	501	GTP	O3'-C3'	-2.47	1.36	1.43
9	B	501	GDP	PA-O5'	2.45	1.69	1.59
9	D	600	GDP	C8-N9	-2.45	1.32	1.37
12	F	402	ACP	C5-N7	-2.39	1.34	1.39
9	D	600	GDP	C5-C4	2.39	1.45	1.38
5	A	501	GTP	O6-C6	-2.37	1.19	1.23
11	B	507	ERX	O14-C19	2.35	1.41	1.37
5	C	501	GTP	O2'-C2'	2.33	1.48	1.43
5	A	501	GTP	C5-N7	-2.30	1.34	1.39
5	C	501	GTP	O5'-C5'	-2.29	1.35	1.44
12	F	402	ACP	C8-N9	-2.18	1.33	1.37
5	C	501	GTP	C4-N9	-2.15	1.32	1.38
9	D	600	GDP	PA-O3A	-2.14	1.57	1.59
9	B	501	GDP	C5-C6	2.12	1.52	1.44
5	A	501	GTP	C4-N9	-2.09	1.32	1.38
5	A	501	GTP	O3'-C3'	-2.09	1.37	1.43
9	D	600	GDP	PA-O2A	-2.05	1.45	1.55
9	D	600	GDP	O4'-C4'	-2.05	1.40	1.45
9	D	600	GDP	C4-N9	-2.00	1.33	1.38

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	B	507	ERX	C02-N03-C04	9.83	120.28	115.82
9	D	600	GDP	C5-C4-N3	-7.56	116.36	128.39
11	B	507	ERX	C08-N09-N05	6.15	108.58	104.06
11	B	507	ERX	C01-C02-N03	-6.05	119.96	124.75
11	B	507	ERX	C08-C07-C04	-6.02	102.46	105.56
11	B	507	ERX	C07-C04-N05	5.89	109.15	105.65
9	D	600	GDP	N9-C4-N3	5.56	137.06	125.95
9	D	600	GDP	C2-N3-C4	5.31	121.45	112.30
12	F	402	ACP	N3-C2-N1	-5.29	120.58	128.58
11	B	507	ERX	O13-C17-C18	5.27	124.18	115.14
12	F	402	ACP	C5-C4-N3	-5.05	119.77	126.72
9	B	501	GDP	C1'-N9-C8	-4.69	113.40	126.73
11	B	507	ERX	O13-C17-C16	-4.66	116.06	124.08
11	B	507	ERX	C27-C08-N09	4.40	126.29	120.49
5	C	501	GTP	C5-C4-N3	-4.40	121.39	128.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	501	GTP	C5-C4-N3	-4.35	121.47	128.39
12	F	402	ACP	N6-C6-N1	-4.27	108.87	118.38
5	C	501	GTP	C2-N3-C4	4.24	119.59	112.30
10	B	505	MES	O2S-S-C8	4.23	113.12	106.73
12	F	402	ACP	N9-C8-N7	-4.03	108.21	113.94
5	A	501	GTP	C2-N3-C4	4.03	119.24	112.30
11	B	507	ERX	C07-C04-N03	-3.93	129.38	132.87
5	C	501	GTP	C2-N1-C6	-3.71	118.38	125.11
10	B	504	MES	O3S-S-O2S	-3.69	102.16	111.40
11	B	507	ERX	C02-C01-C06	-3.61	118.32	120.69
9	B	501	GDP	C1'-N9-C4	3.54	136.93	126.49
11	B	507	ERX	C27-C08-C07	-3.50	123.78	128.69
9	B	501	GDP	N9-C8-N7	-3.44	107.03	113.40
5	A	501	GTP	C2-N1-C6	-3.38	118.99	125.11
12	F	402	ACP	C5-C6-N6	3.36	131.62	123.29
11	B	507	ERX	O14-C19-C18	3.29	120.78	115.14
9	B	501	GDP	C2-N3-C4	3.28	117.95	112.30
12	F	402	ACP	C2-N3-C4	3.26	119.80	111.83
10	B	505	MES	O3S-S-O2S	-3.26	103.24	111.40
11	B	507	ERX	C12-O13-C17	3.21	122.23	117.51
9	D	600	GDP	C4'-O4'-C1'	3.14	116.40	109.47
9	B	501	GDP	C2-N1-C6	-3.12	119.46	125.11
9	B	501	GDP	C5-C4-N3	-3.11	123.44	128.39
9	D	600	GDP	O2A-PA-O1A	3.00	126.42	112.44
12	F	402	ACP	C5-N7-C8	2.98	108.14	103.45
12	F	402	ACP	N3-C4-N9	2.98	132.24	127.17
9	B	501	GDP	C5-C6-N1	2.93	120.71	113.25
9	D	600	GDP	C2-N1-C6	-2.91	119.83	125.11
5	C	501	GTP	C5-C6-N1	2.87	120.56	113.25
12	F	402	ACP	O3G-PG-C3B	2.83	113.28	106.40
9	B	501	GDP	C6-C5-N7	2.76	135.32	130.29
5	C	501	GTP	O2B-PB-O3A	2.70	114.56	107.27
10	B	505	MES	C6-C5-N4	2.69	114.21	110.12
5	A	501	GTP	N9-C8-N7	-2.68	108.44	113.40
9	D	600	GDP	O2A-PA-O5'	-2.66	95.49	107.57
5	C	501	GTP	N2-C2-N1	2.65	122.36	116.76
5	A	501	GTP	C5-C6-N1	2.61	119.91	113.25
5	C	501	GTP	O2A-PA-O3A	2.61	114.32	107.27
9	D	600	GDP	C4-C5-N7	-2.59	106.56	110.67
10	B	504	MES	O1S-S-C8	2.56	110.60	106.73
10	B	505	MES	O3S-S-C8	2.56	111.01	106.00
5	A	501	GTP	C4-C5-N7	-2.55	106.63	110.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	F	402	ACP	C4-C5-N7	-2.55	107.67	110.58
10	B	504	MES	C5-N4-C3	2.53	114.30	108.84
10	B	504	MES	C8-C7-N4	-2.51	102.86	112.36
9	D	600	GDP	O6-C6-C5	-2.48	119.98	126.53
9	B	501	GDP	O3'-C3'-C2'	-2.46	103.95	111.82
5	C	501	GTP	O5'-C5'-C4'	-2.44	100.67	108.99
9	D	600	GDP	C6-C5-N7	2.42	134.69	130.29
11	B	507	ERX	O14-C19-C20	-2.40	119.95	124.08
11	B	507	ERX	C01-C06-N05	2.39	118.06	115.22
5	A	501	GTP	C5-C4-N9	2.38	109.91	105.66
10	B	505	MES	O1-C6-C5	2.34	116.81	111.77
5	C	501	GTP	C5-C4-N9	2.34	109.84	105.66
5	A	501	GTP	C6-C5-N7	2.33	134.53	130.29
9	D	600	GDP	O4'-C4'-C5'	-2.33	101.88	109.33
5	A	501	GTP	N2-C2-N1	2.32	121.66	116.76
12	F	402	ACP	C6-C5-C4	2.30	120.32	117.18
12	F	402	ACP	PB-O3A-PA	-2.30	124.86	132.37
12	F	402	ACP	C3'-C2'-C1'	2.28	105.78	101.46
5	C	501	GTP	C4-C5-N7	-2.28	107.06	110.67
9	D	600	GDP	C5-C6-N1	2.27	119.04	113.25
10	B	504	MES	O2S-S-C8	2.27	110.16	106.73
5	C	501	GTP	C6-C5-N7	2.23	134.36	130.29
9	D	600	GDP	C3'-C2'-C1'	2.22	105.66	101.46
5	C	501	GTP	O6-C6-C5	-2.19	120.74	126.53
5	C	501	GTP	N9-C8-N7	-2.18	109.36	113.40
11	B	507	ERX	C28-C27-C08	-2.17	118.44	120.87
12	F	402	ACP	C4-N9-C8	2.14	107.98	105.74
10	B	505	MES	C6-O1-C2	2.13	116.75	109.88
9	D	600	GDP	O3B-PB-O2B	2.08	115.58	107.80
9	B	501	GDP	C4-C5-N7	-2.02	107.47	110.67
5	A	501	GTP	C8-N7-C5	2.01	107.85	104.26
12	F	402	ACP	C5-C4-N9	2.00	107.99	105.81

There are no chirality outliers.

All (35) 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

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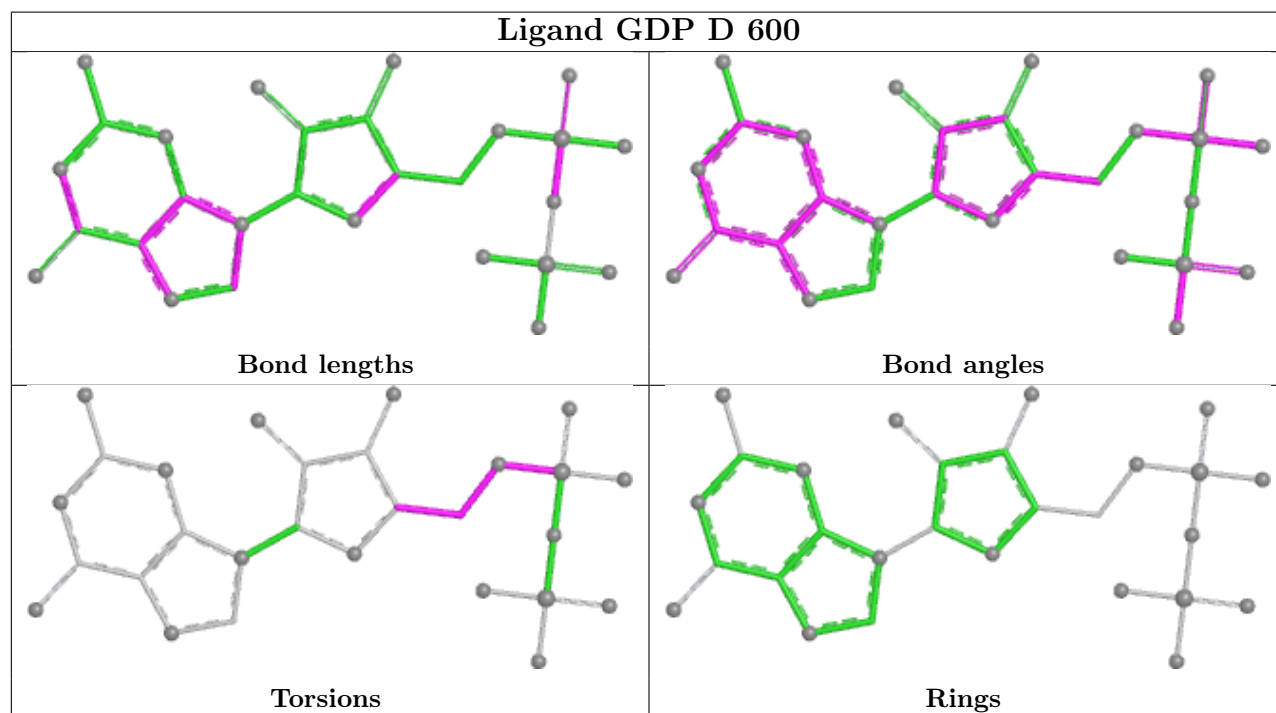
Mol	Chain	Res	Type	Atoms
5	C	501	GTP	C5'-O5'-PA-O2A
9	B	501	GDP	C5'-O5'-PA-O3A
9	B	501	GDP	C5'-O5'-PA-O1A
9	D	600	GDP	C5'-O5'-PA-O3A
9	D	600	GDP	C5'-O5'-PA-O2A
10	B	504	MES	C7-C8-S-O1S
10	B	504	MES	C7-C8-S-O2S
10	B	505	MES	C7-C8-S-O1S
12	F	402	ACP	C5'-O5'-PA-O1A
12	F	402	ACP	C5'-O5'-PA-O2A
12	F	402	ACP	C5'-O5'-PA-O3A
12	F	402	ACP	O4'-C4'-C5'-O5'
11	B	507	ERX	C16-C17-O13-C12
9	D	600	GDP	C3'-C4'-C5'-O5'
12	F	402	ACP	C3'-C4'-C5'-O5'
11	B	507	ERX	C18-C17-O13-C12
9	D	600	GDP	O4'-C4'-C5'-O5'
10	B	505	MES	C7-C8-S-O2S
5	A	501	GTP	PB-O3B-PG-O1G
5	C	501	GTP	PB-O3B-PG-O1G
9	D	600	GDP	C4'-C5'-O5'-PA
9	B	501	GDP	C5'-O5'-PA-O2A
12	F	402	ACP	PB-O3A-PA-O2A
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
9	B	501	GDP	C3'-C4'-C5'-O5'
5	C	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A

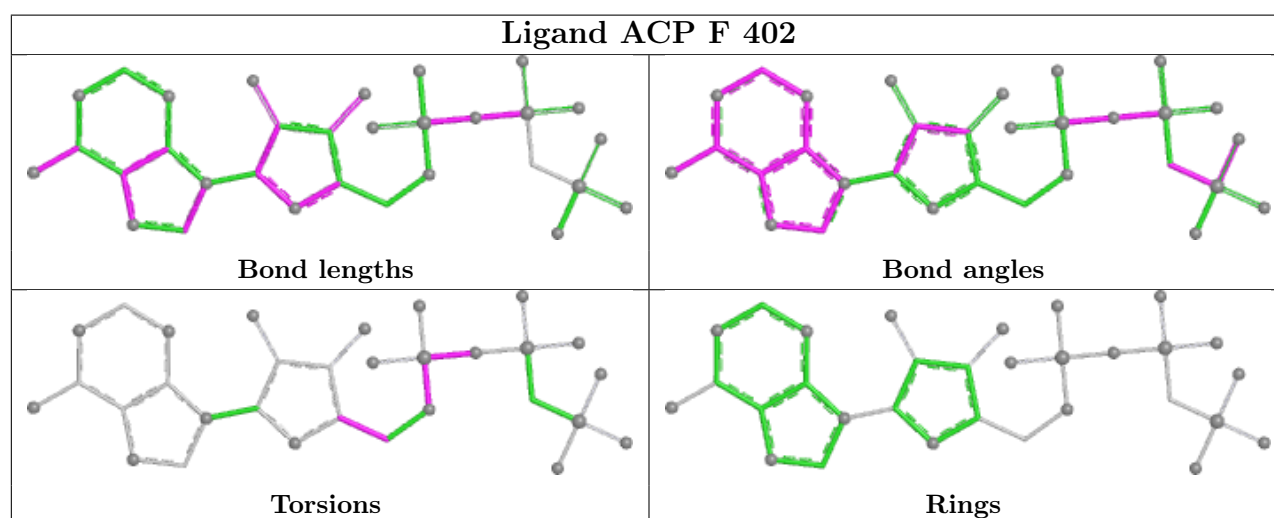
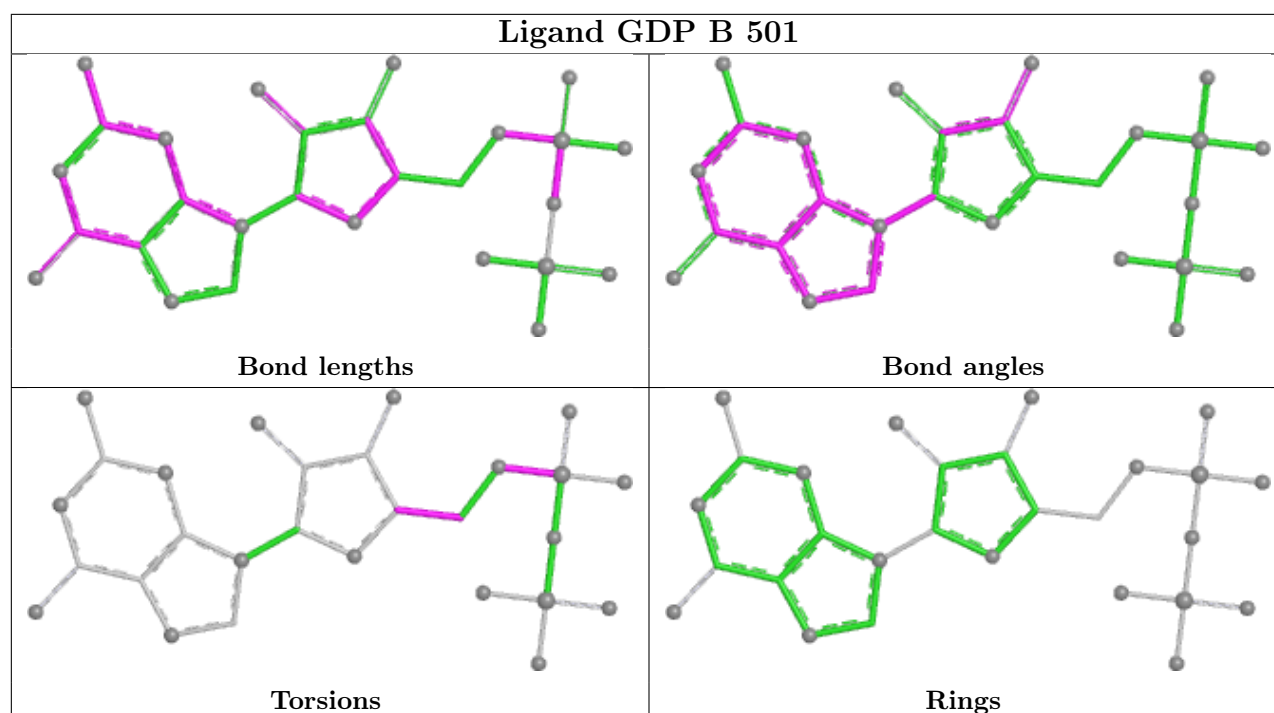
There are no ring outliers.

6 monomers are involved in 26 short contacts:

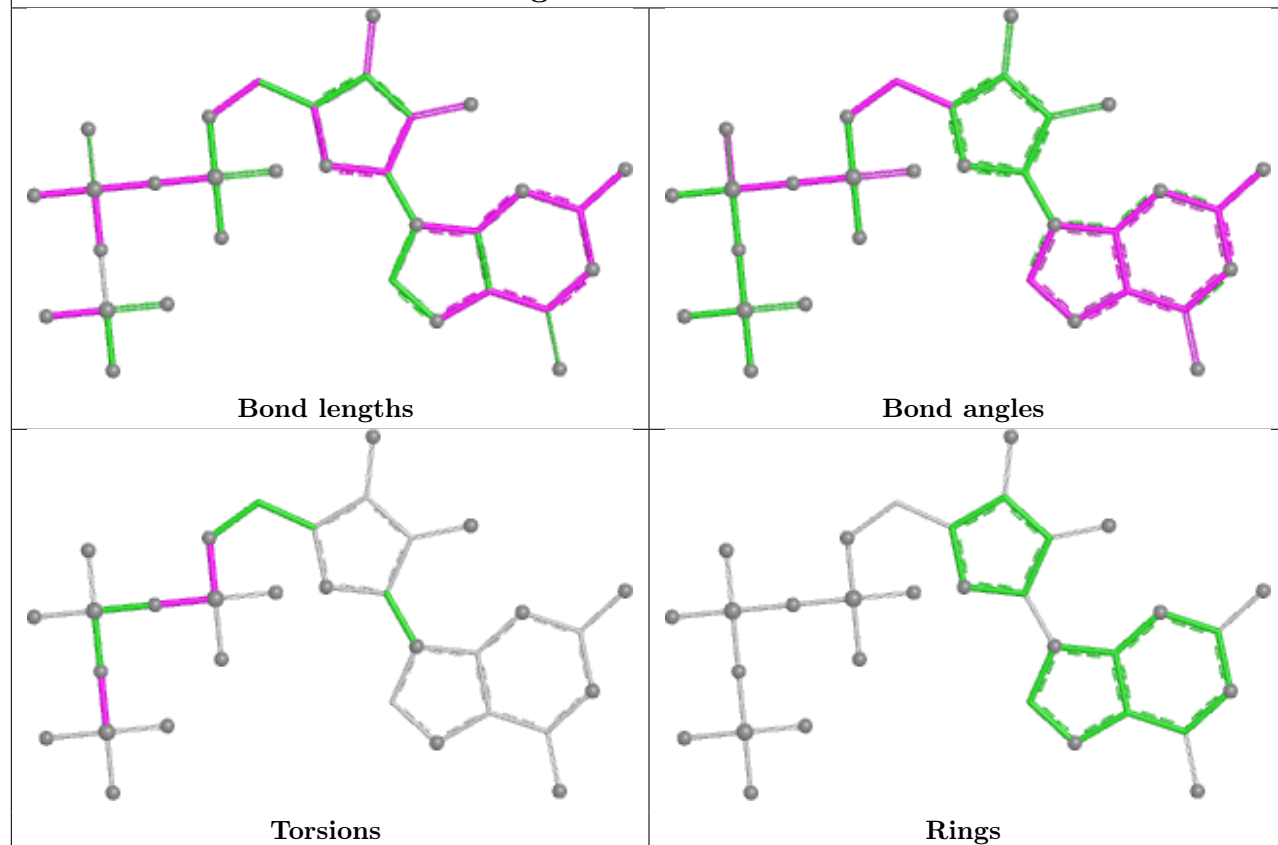
Mol	Chain	Res	Type	Clashes	Symm-Clashes
10	B	505	MES	4	0
9	D	600	GDP	15	0
9	B	501	GDP	2	0
12	F	402	ACP	3	0
10	B	504	MES	1	0
11	B	507	ERX	1	0

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.

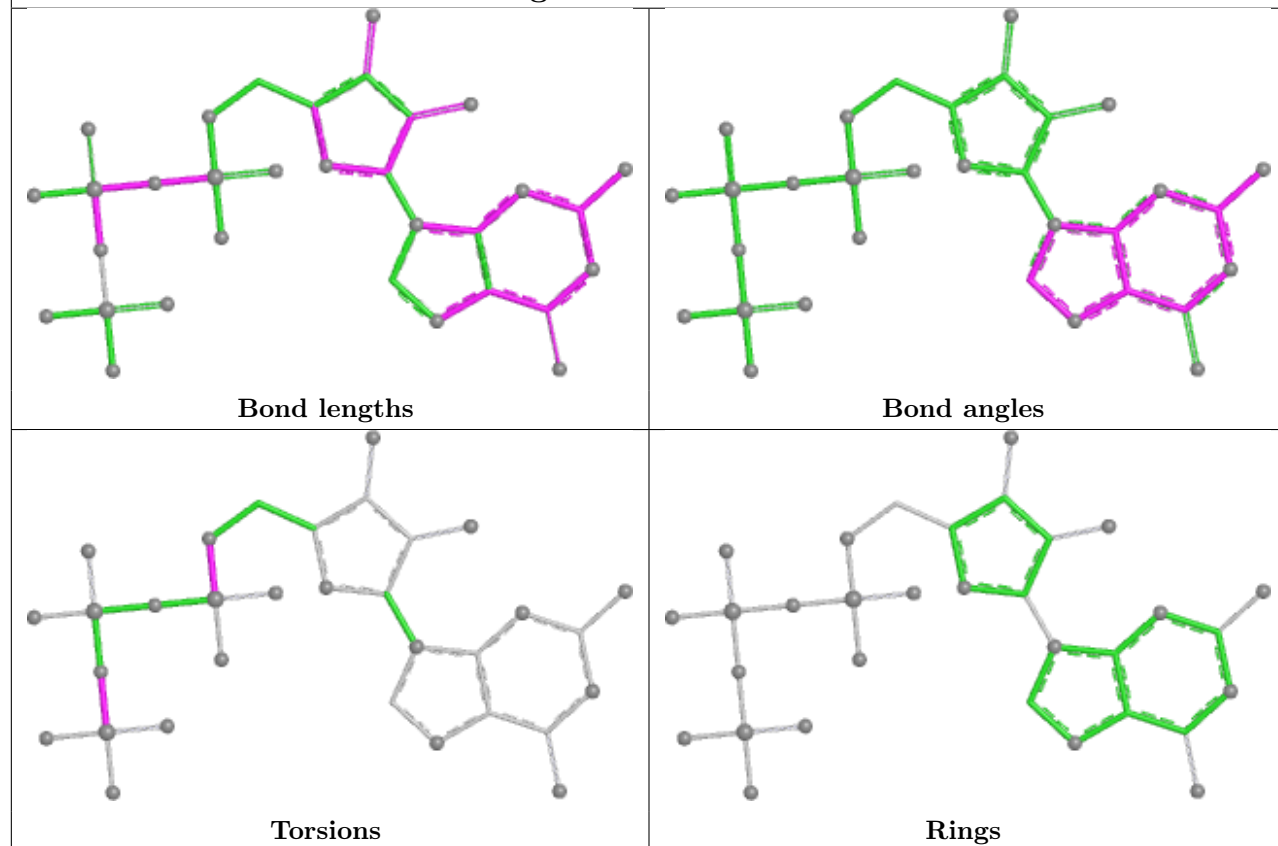


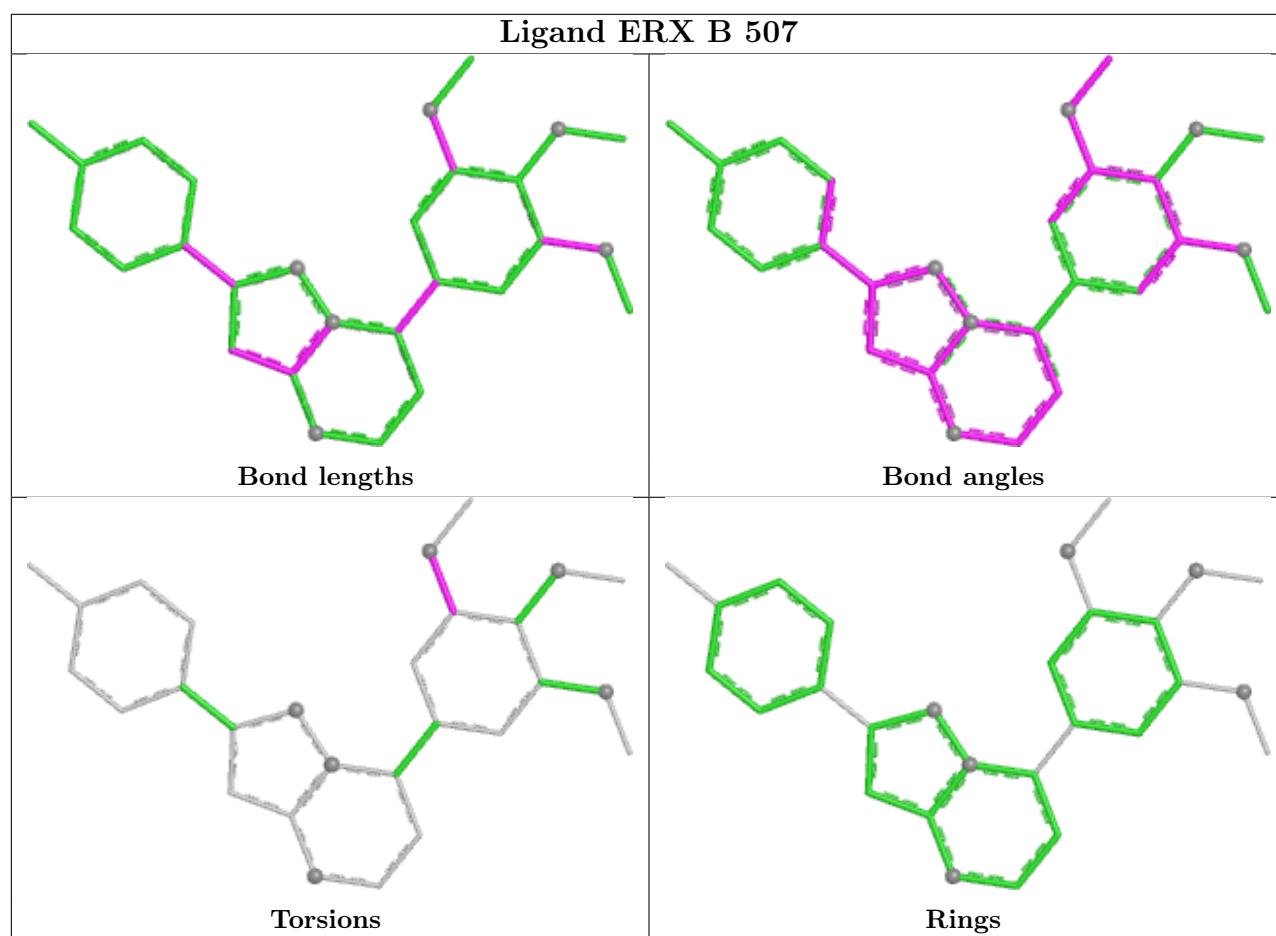


Ligand GTP C 501



Ligand GTP A 501





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	440/450 (97%)	-0.37	3 (0%) 84 84	31, 51, 80, 127	1 (0%)
1	C	440/450 (97%)	-0.75	0 100 100	22, 39, 66, 85	3 (0%)
2	B	424/445 (95%)	-0.49	5 (1%) 76 76	25, 48, 81, 130	2 (0%)
2	D	421/445 (94%)	0.22	14 (3%) 49 47	35, 69, 107, 130	1 (0%)
3	E	124/143 (86%)	0.01	0 100 100	29, 68, 109, 136	1 (0%)
4	F	351/384 (91%)	0.37	24 (6%) 23 23	33, 79, 147, 162	2 (0%)
All	All	2200/2317 (94%)	-0.22	46 (2%) 63 61	22, 57, 110, 162	10 (0%)

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	135	TYR	5.6
1	A	179	THR	4.8
4	F	166	ALA	3.9
4	F	237	THR	3.5
4	F	226	GLU	3.1
4	F	382	HIS	3.1
4	F	383	HIS	3.0
2	D	74	THR	3.0
4	F	169	LEU	3.0
2	D	212	ILE	3.0
4	F	233	PHE	2.8
2	B	57	THR	2.8
2	D	176	LYS	2.7
1	A	440	VAL	2.7
4	F	105	LEU	2.7
4	F	182	ILE	2.6
4	F	249	TYR	2.6
2	D	71	GLU	2.6
2	D	285	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
4	F	245	ILE	2.5
1	A	262	TYR	2.4
2	B	438	ALA	2.4
2	D	418	PHE	2.4
4	F	224	SER	2.4
2	D	101	ASN	2.4
4	F	177	GLY	2.3
4	F	381	HIS	2.3
2	D	213	CYS	2.3
4	F	161	LEU	2.3
4	F	264	PHE	2.3
4	F	82	LYS	2.2
4	F	145	ASN	2.2
2	D	103	TRP	2.2
2	B	285	ALA	2.2
4	F	181	VAL	2.1
4	F	147	TRP	2.1
2	D	408	TYR	2.1
4	F	106	LYS	2.1
2	B	334	ASN	2.1
2	D	75	MET	2.1
2	D	219	LEU	2.1
2	B	276	THR	2.0
4	F	170	LEU	2.0
2	D	2	ARG	2.0
4	F	152	SER	2.0
2	D	177	VAL	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

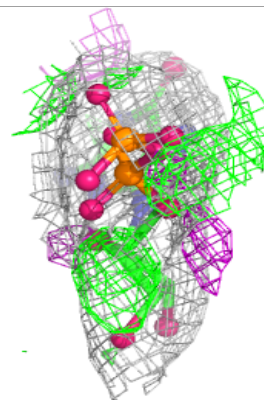
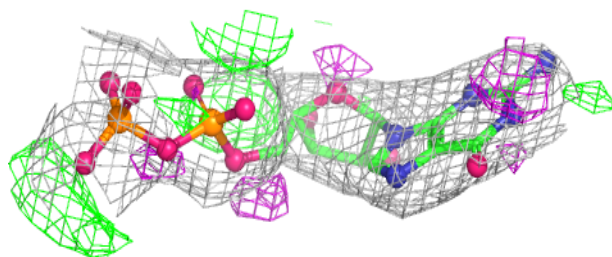
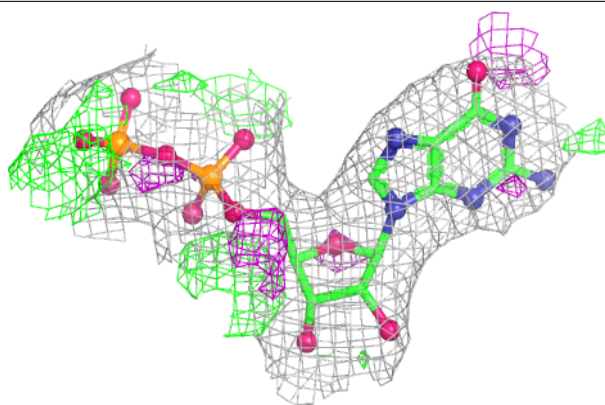
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
6	MG	F	401	1/1	0.75	0.10	94,94,94,94	0
6	MG	D	601	1/1	0.82	0.11	64,64,64,64	0
6	MG	A	502	1/1	0.82	0.13	44,44,44,44	0
6	MG	B	506	1/1	0.87	0.20	87,87,87,87	0
7	CA	A	505	1/1	0.87	0.11	113,113,113,113	0
9	GDP	D	600	28/28	0.87	0.12	52,64,92,98	0
12	ACP	F	402	31/31	0.88	0.10	77,93,124,132	0
7	CA	B	503	1/1	0.89	0.12	103,103,103,103	0
10	MES	B	505	12/12	0.90	0.12	76,84,100,107	0
8	CL	A	504	1/1	0.93	0.08	73,73,73,73	0
10	MES	B	504	12/12	0.93	0.09	40,56,79,97	0
6	MG	C	502	1/1	0.94	0.08	46,46,46,46	0
11	ERX	B	507	28/28	0.95	0.08	38,55,67,85	0
7	CA	A	503	1/1	0.98	0.10	80,80,80,80	0
5	GTP	C	501	32/32	0.98	0.05	26,34,42,43	0
5	GTP	A	501	32/32	0.98	0.06	35,41,50,54	0
9	GDP	B	501	28/28	0.99	0.04	23,34,40,41	0
7	CA	C	503	1/1	0.99	0.02	57,57,57,57	0
6	MG	B	502	1/1	0.99	0.04	36,36,36,36	0

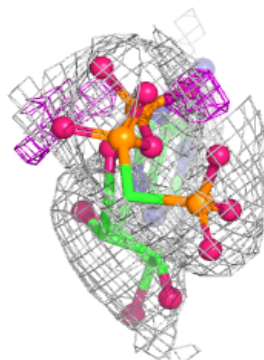
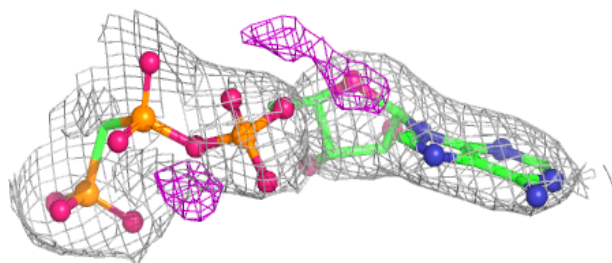
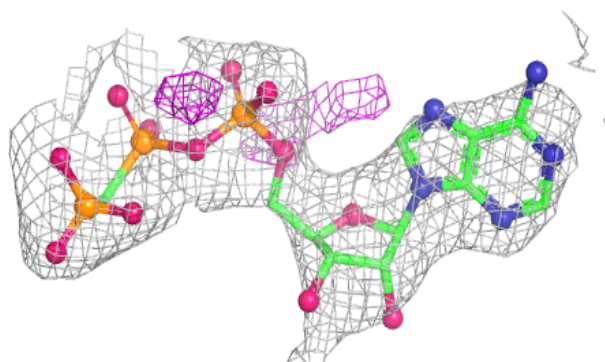
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GDP D 600:

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

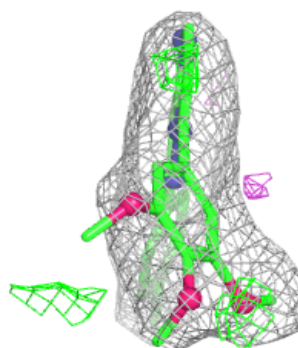
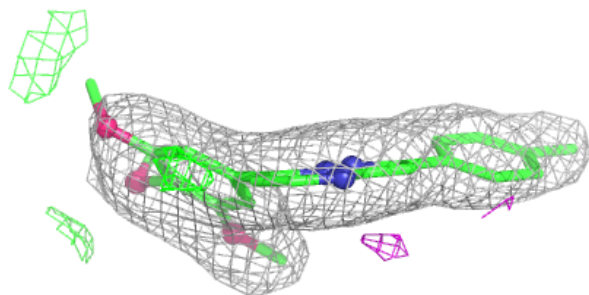
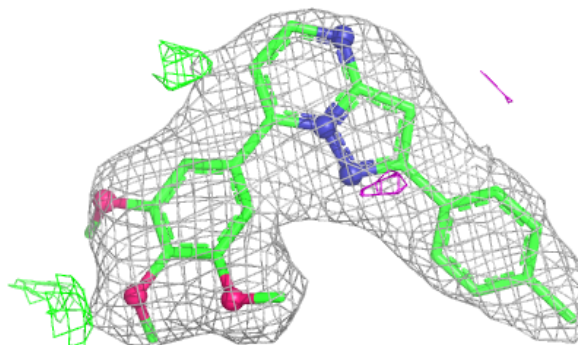
**Electron density around ACP F 402:**

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

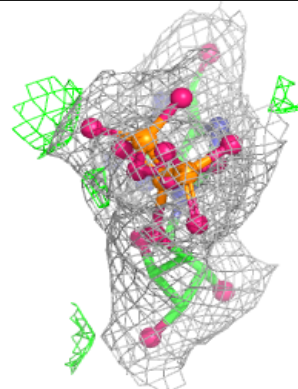
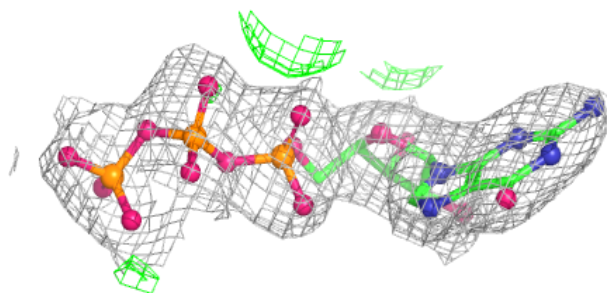
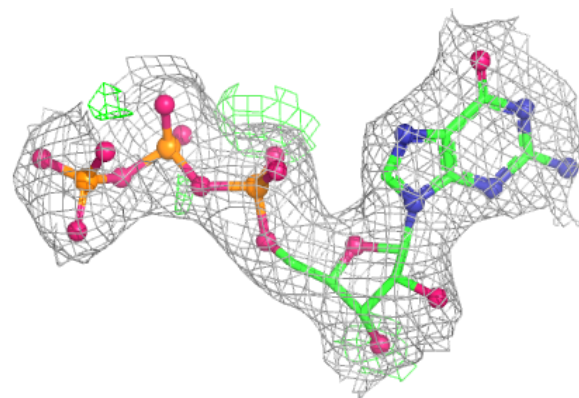


Electron density around ERX B 507:

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

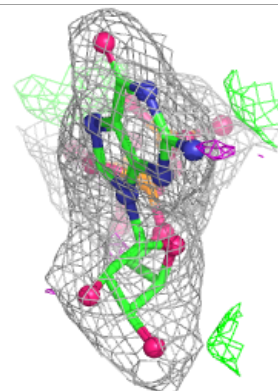
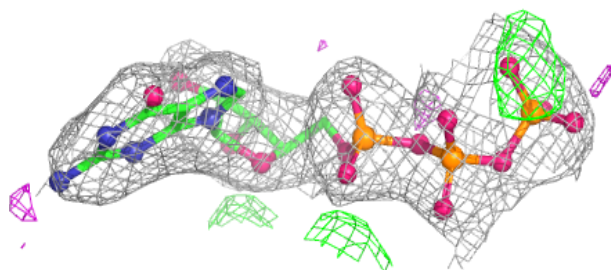
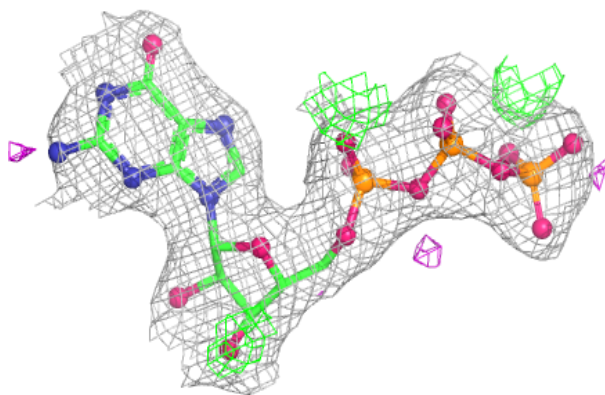
**Electron density around GTP C 501:**

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

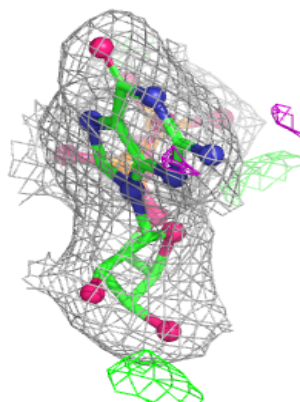
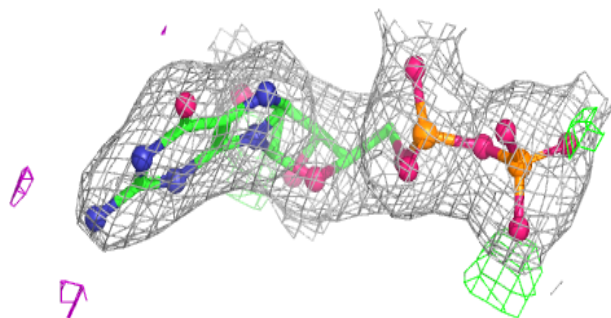
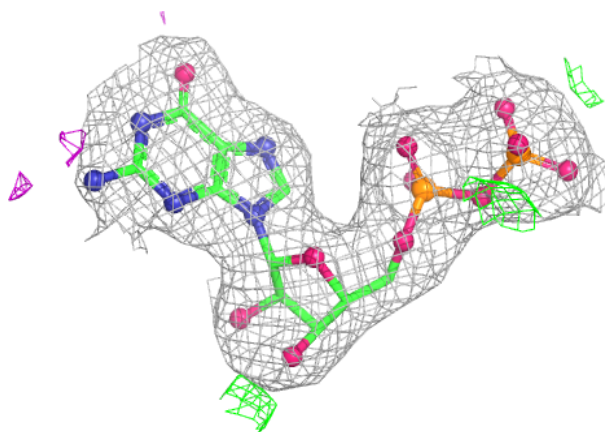


Electron density around GTP A 501:

$2mF_o-DF_c$ (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.