Full wwPDB X-ray Structure Validation Report ⓘ

Feb 28, 2024 – 08:32 PM EST

PDB ID	:	5S4Y
Title	:	Tubulin-Z2856434857-complex
Authors	:	Muehlethaler, T.; Gioia, D.; Prota, A.E.; Sharpe, M.E.; Cavalli, A.; Steinmetz, M.O.
Deposited on	:	2020-11-08
Resolution	:	2.30 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

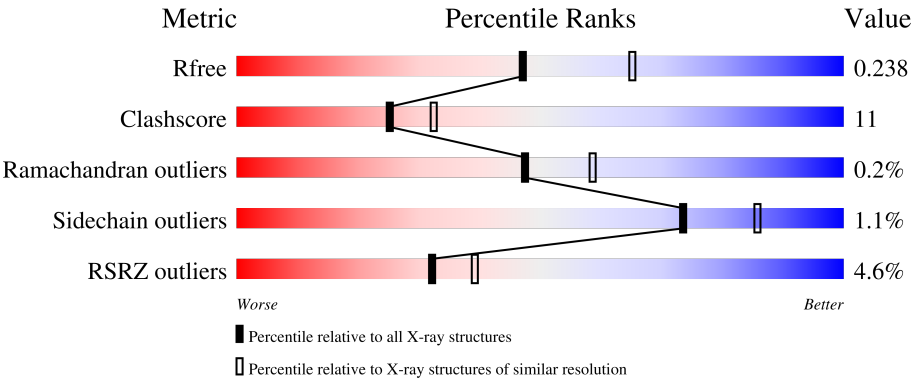
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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

Mol	Chain	Length	Quality of chain
1	A	451	3% 73% 23%
1	C	451	3% 75% 22%
2	B	445	4% 74% 21%
2	D	445	4% 70% 25% 5%
3	E	143	6% 68% 18% 14%

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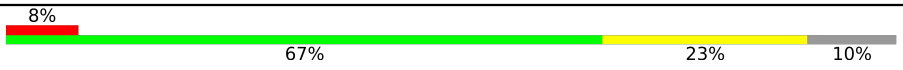
Mol	Chain	Length	Quality of chain
4	F	384	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 17863 atoms, of which 30 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	438	Total	C	N	O	S	0	0	0
			3424	2167	582	653	22			
1	C	440	Total	C	N	O	S	0	1	0
			3443	2178	585	657	23			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	426	Total	C	N	O	S	2	1	0
			3356	2108	574	647	27			
2	D	424	Total	C	N	O	S	5	0	0
			3333	2093	568	645	27			

- Molecule 3 is a protein called Stathmin-4.

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

There are 2 discrepancies between the modelled and reference sequences:

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

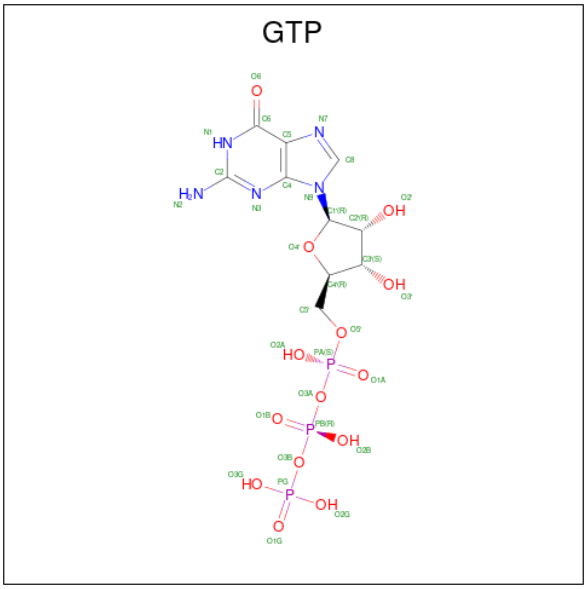
- Molecule 4 is a protein called Tubulin-Tyrosine Ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	346	Total	C	N	O	S	0	0	0
			2843	1823	489	517	14			

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 (three-letter code: 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 (three-letter code: MG) (formula: Mg).

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

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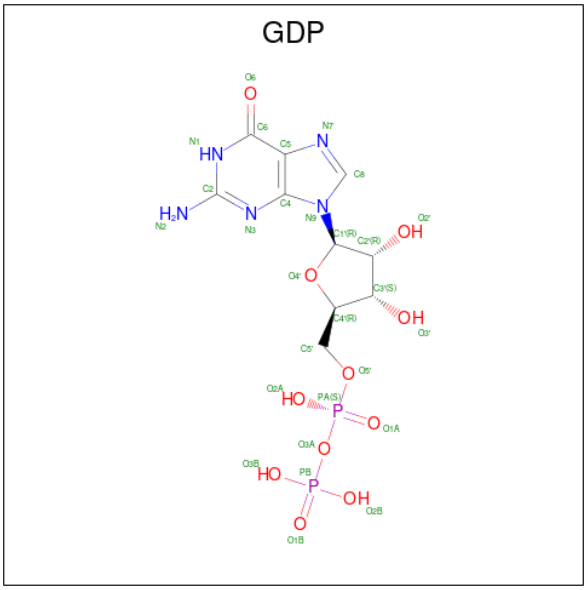
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	F	1	Total Mg 1 1	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

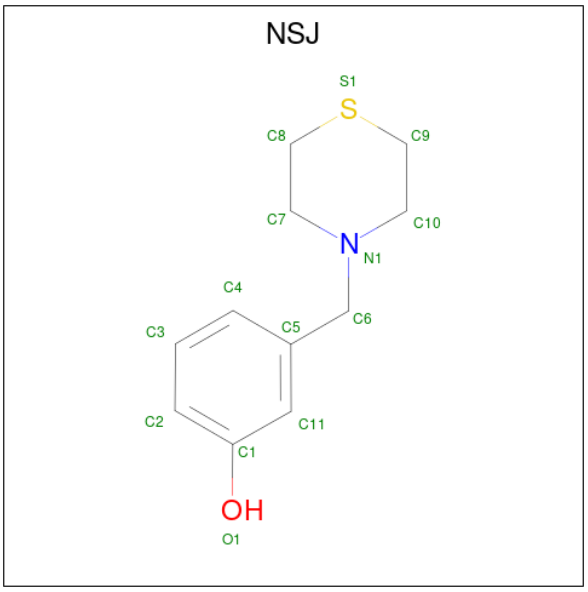
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	2	Total Ca 2 2	0	0
7	B	1	Total Ca 1 1	0	0
7	C	1	Total Ca 1 1	0	0

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



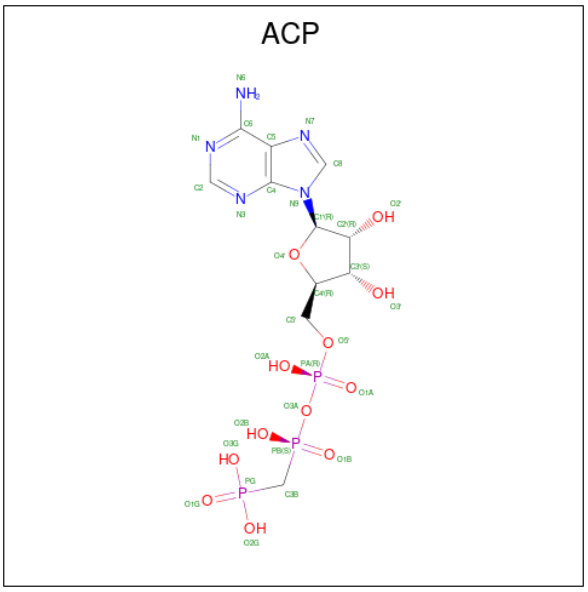
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total C N O P 28 10 5 11 2	0	0
8	D	1	Total C N O P 28 10 5 11 2	0	0

- Molecule 9 is 3-[(thiomorpholin-4-yl)methyl]phenol (three-letter code: NSJ) (formula: $C_{11}H_{15}NOS$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
9	B	1	Total	C	H	N	O	S	0	0
			29	11	15	1	1	1		
9	B	1	Total	C	H	N	O	S	0	0
			29	11	15	1	1	1		

- Molecule 10 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

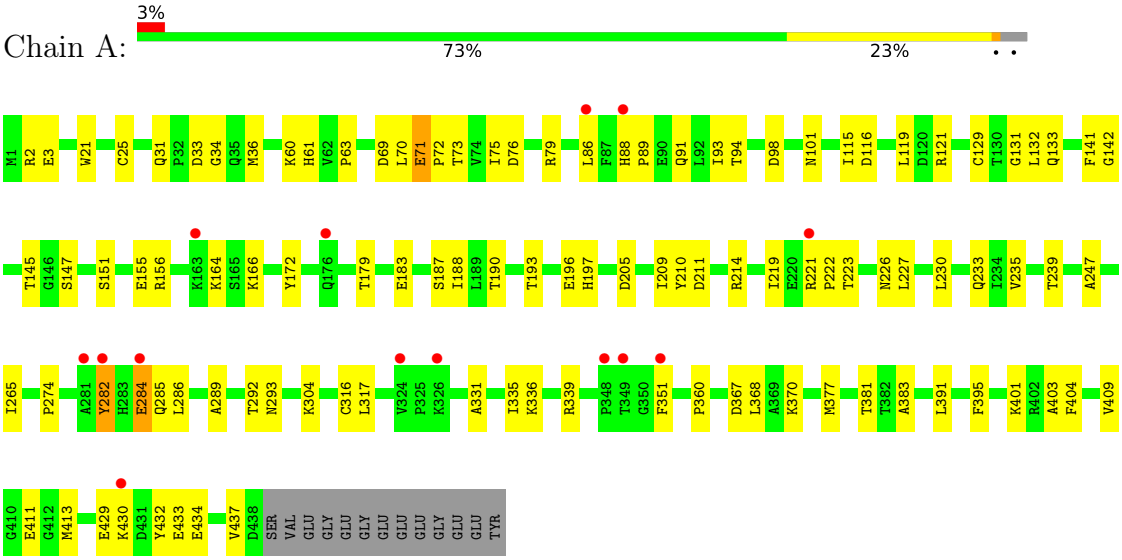
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	51	Total O 51 51	0	0
11	B	35	Total O 35 35	0	0
11	C	116	Total O 116 116	0	0
11	D	16	Total O 16 16	0	0
11	E	5	Total O 5 5	0	0
11	F	9	Total O 9 9	0	0

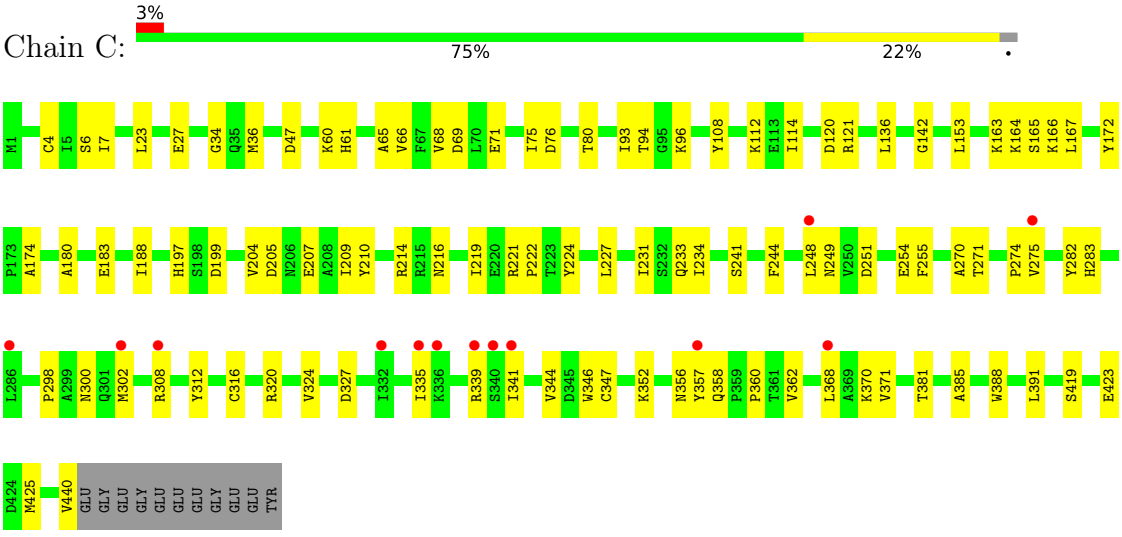
3 Residue-property plots (i)

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.

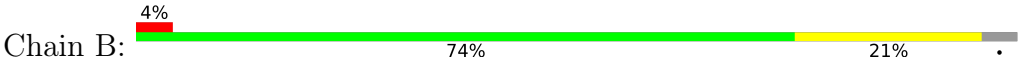
• Molecule 1: Tubulin alpha-1B chain

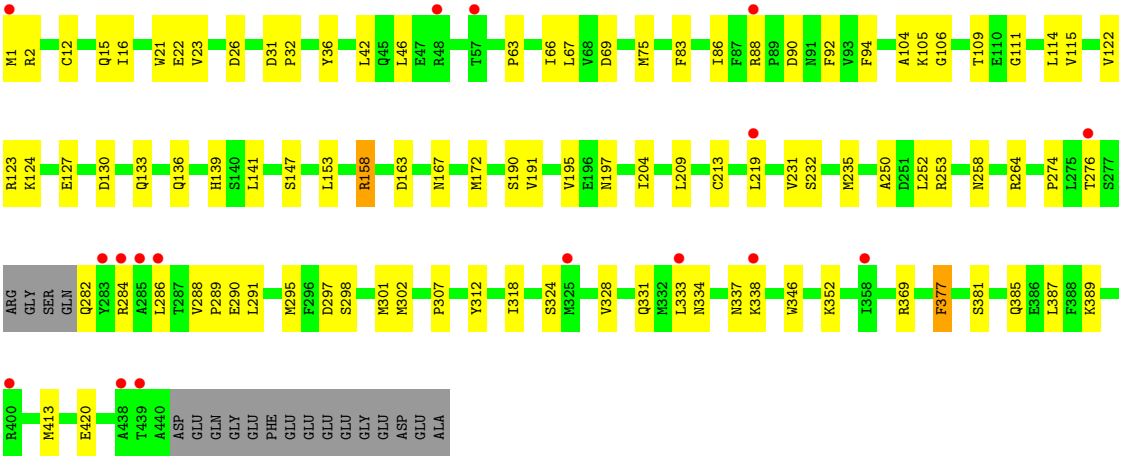


• Molecule 1: Tubulin alpha-1B chain

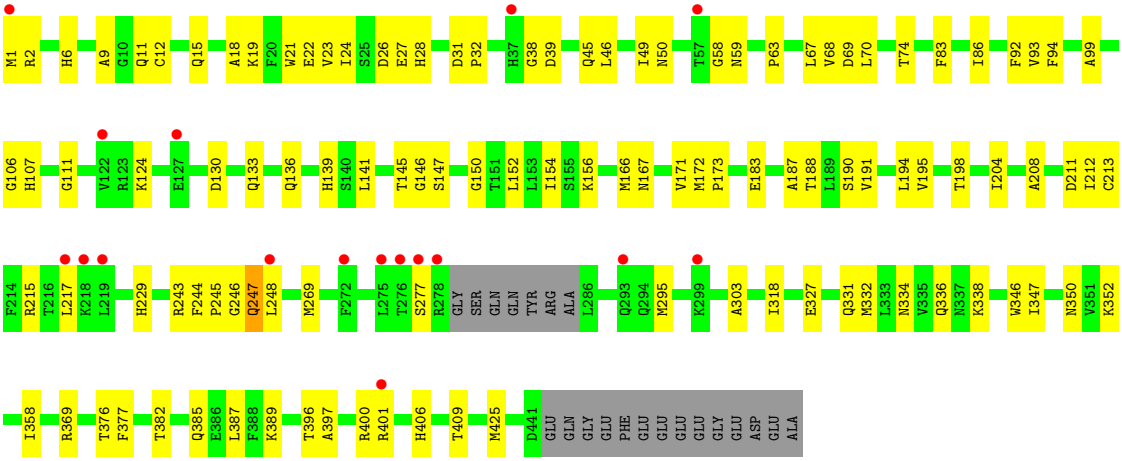


• Molecule 2: Tubulin beta-2B chain

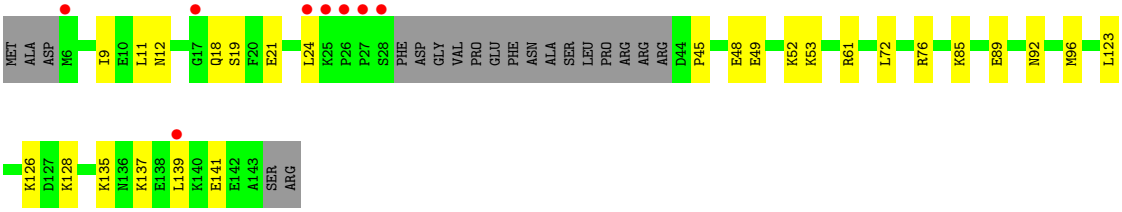




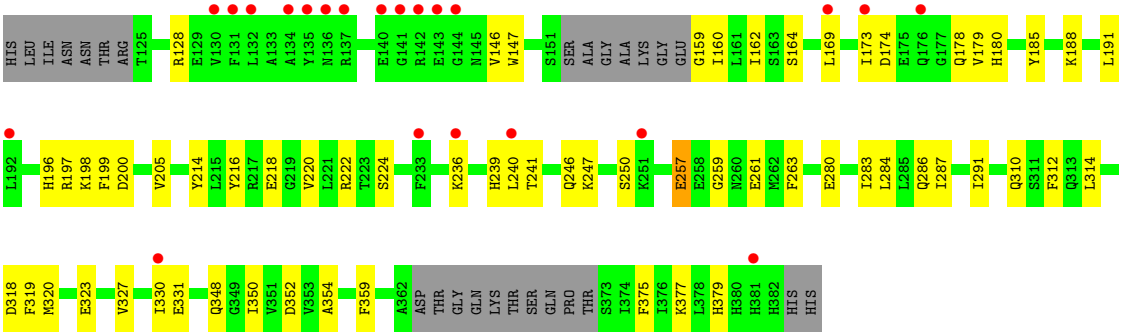
• Molecule 2: Tubulin beta-2B chain



• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-Tyrosine Ligase


HIS LEU ILE ASN ASN THR ARG T125 R128 E129 V130 F131 L132 A133 A134 Y135 N136 R137 E140 G141 R142 E143 G144 N145 V146 W147 S151 SER ALA GLY ALA LYS GLY GLU G159 I160 L161 I162 S163 S164 L169 I173 D174 E175 Q176 G177 Q178 V179 H180 Y185 K188 L191
L192 H196 R197 K198 F199 D200 V205 Y214 L215 Y216 R217 E218 G219 V220 L221 R222 T223 S224 F233 K236 H239 L240 T241 Q246 K247 S250 K251 E257 E258 G259 N260 E261 M262 F263 E280 I283 L284 L285 Q286 I287 I291 Q310 S311 F312 Q313 L314
D318 F319 M320 E323 V327 I330 E331 Q348 G349 I350 V351 D352 V353 A354 F359 A362 ASP THR GLY GLN LYS THR SER GLN PRO THR S373 I374 F375 I376 K377 L378 H379 H380 H381 H382 HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	104.14Å 157.78Å 178.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	78.89 – 2.30 118.28 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (78.89-2.30) 99.9 (118.28-2.30)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.12 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874	Depositor
R, R_{free}	0.200 , 0.238 0.201 , 0.238	Depositor DCC
R_{free} test set	6495 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å^2)	69.6	Xtriage
Anisotropy	0.141	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 57.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	17863	wwPDB-VP
Average B, all atoms (Å^2)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.54% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NSJ, ACP, GDP, CA, MG, GTP

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	0.25	0/3502	0.41	0/4754
1	C	0.26	0/3521	0.42	0/4780
2	B	0.25	0/3430	0.42	0/4645
2	D	0.25	0/3406	0.41	0/4613
3	E	0.23	0/1022	0.35	0/1356
4	F	0.24	0/2909	0.40	0/3930
All	All	0.25	0/17790	0.41	0/24078

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	3424	0	3335	71	0
1	C	3443	0	3352	70	0
2	B	3356	0	3231	77	0
2	D	3333	0	3214	78	0
3	E	1014	0	1029	19	0
4	F	2843	0	2806	67	0
5	A	32	0	12	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	2	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
8	B	28	0	12	2	0
8	D	28	0	12	3	0
9	B	28	30	0	0	0
10	F	31	0	14	4	0
11	A	51	0	0	2	0
11	B	35	0	0	2	0
11	C	116	0	0	1	0
11	D	16	0	0	1	0
11	E	5	0	0	0	0
11	F	9	0	0	1	0
All	All	17833	30	17029	371	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 11.

All (371) 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)
1:A:381:THR:HG22	1:A:383:ALA:H	1.24	1.01
4:F:102:PRO:HG2	4:F:105:LEU:HD13	1.52	0.92
4:F:236:LYS:HB3	4:F:240:LEU:HD13	1.58	0.86
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.59	0.84
2:B:2:ARG:HB2	2:B:133:GLN:HG3	1.58	0.83
1:C:209:ILE:HD11	1:C:302:MET:CE	2.10	0.82
4:F:241:THR:OG1	10:F:401:ACP:O3'	1.98	0.80
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.65	0.79
1:C:234:ILE:HD13	1:C:302:MET:CE	2.12	0.78
2:D:397:ALA:O	2:D:401:ARG:NH1	2.17	0.78
2:B:163:ASP:O	2:B:253[A]:ARG:NH2	2.18	0.77
1:A:71:GLU:OE2	1:A:73:THR:OG1	2.01	0.76
1:C:76:ASP:O	1:C:80:THR:HG22	1.85	0.76
1:C:209:ILE:HD11	1:C:302:MET:HE3	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:ILE:HD13	1:C:302:MET:HE1	1.66	0.75
2:D:172:MET:HG3	2:D:387:LEU:HD11	1.68	0.74
4:F:241:THR:HG1	10:F:401:ACP:HO3'	1.30	0.74
4:F:331:GLU:OE2	10:F:401:ACP:O3G	2.05	0.74
2:D:334:ASN:HD21	2:D:338:LYS:HE3	1.53	0.74
4:F:128:ARG:NH2	4:F:174:ASP:OD1	2.22	0.73
2:B:420:GLU:OE1	11:B:601:HOH:O	2.07	0.73
2:B:15:GLN:NE2	8:B:501:GDP:O6	2.21	0.72
2:B:284:ARG:NH2	2:B:290:GLU:OE2	2.22	0.72
2:D:83:PHE:O	2:D:86:ILE:HG22	1.90	0.72
4:F:102:PRO:HG2	4:F:105:LEU:CD1	2.21	0.70
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.28	0.69
1:A:293:ASN:OD1	1:A:339:ARG:NH2	2.24	0.69
2:B:2:ARG:HB2	2:B:133:GLN:CG	2.22	0.69
2:D:136:GLN:HA	2:D:167:ASN:O	1.93	0.68
2:B:274:PRO:HB3	2:B:286:LEU:HD22	1.75	0.67
1:C:320:ARG:HA	1:C:356:ASN:O	1.93	0.67
2:B:133:GLN:OE1	2:B:252:LEU:HG	1.94	0.67
4:F:348:GLN:NE2	4:F:352:ASP:OD1	2.28	0.67
1:C:47:ASP:OD2	11:C:601:HOH:O	2.12	0.66
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.76	0.66
2:B:69:ASP:O	2:B:94:PHE:HA	1.95	0.66
4:F:286:GLN:HG3	11:F:506:HOH:O	1.96	0.66
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.29	0.65
2:D:188:THR:HG23	2:D:425:MET:HE2	1.79	0.65
1:A:71:GLU:HG2	1:A:72:PRO:HD2	1.79	0.64
2:B:191:VAL:O	2:B:195:VAL:HG23	1.97	0.64
2:D:141:LEU:HD22	2:D:190:SER:HB3	1.78	0.64
2:D:397:ALA:HA	2:D:400:ARG:NH1	2.11	0.64
1:A:429:GLU:OE2	11:A:601:HOH:O	2.14	0.64
1:C:254:GLU:HG2	1:C:352:LYS:HE2	1.78	0.64
4:F:200:ASP:OD1	4:F:222:ARG:HB2	1.98	0.64
2:B:23:VAL:HG21	2:B:232:SER:HB3	1.80	0.63
8:D:501:GDP:O1A	11:D:601:HOH:O	2.15	0.63
4:F:147:TRP:HB2	4:F:169:LEU:HD11	1.79	0.63
2:D:46:LEU:HA	2:D:49:ILE:HB	1.79	0.63
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.80	0.63
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.34	0.62
1:C:233:GLN:HG3	1:C:368:LEU:HD12	1.80	0.62
2:D:248:LEU:HD21	2:D:352:LYS:HB3	1.80	0.62
1:C:312:TYR:CD1	1:C:341:ILE:HG23	2.34	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LEU:O	1:A:164:LYS:NZ	2.32	0.62
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.80	0.62
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.35	0.62
2:D:1:MET:CE	2:D:50:ASN:HB2	2.29	0.61
2:D:334:ASN:ND2	2:D:338:LYS:HE3	2.15	0.61
1:A:88:HIS:CD2	1:A:91:GLN:HG3	2.34	0.61
11:B:615:HOH:O	1:C:163:LYS:HD2	2.00	0.61
4:F:147:TRP:HB2	4:F:169:LEU:CD1	2.31	0.61
4:F:314:LEU:HD22	4:F:350:ILE:HD11	1.82	0.60
3:E:48:GLU:OE2	3:E:52:LYS:NZ	2.27	0.60
2:B:83:PHE:O	2:B:86:ILE:HG22	2.01	0.60
2:D:11:GLN:O	2:D:15:GLN:HG2	2.02	0.60
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.84	0.60
2:D:69:ASP:O	2:D:94:PHE:HA	2.01	0.60
1:C:180:ALA:O	1:C:183:GLU:HG3	2.02	0.60
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.16	0.59
2:D:244:PHE:O	2:D:246:GLY:N	2.34	0.59
2:B:286:LEU:HD23	2:B:291:LEU:HD23	1.85	0.59
3:E:128:LYS:O	3:E:128:LYS:HD3	2.02	0.59
4:F:16:GLU:OE2	4:F:19:ARG:NH2	2.36	0.58
4:F:216:TYR:CZ	4:F:218:GLU:HB2	2.38	0.58
2:D:187:ALA:O	2:D:191:VAL:HG23	2.04	0.58
1:C:4[A]:CYS:SG	1:C:136:LEU:HG	2.44	0.58
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.39	0.58
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.85	0.58
4:F:96:GLU:OE2	4:F:98:TYR:OH	2.14	0.57
2:B:301:MET:HE1	2:B:377:PHE:HZ	1.68	0.57
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.86	0.57
2:D:26:ASP:OD2	2:D:369:ARG:HD2	2.04	0.57
2:D:217:LEU:HA	2:D:277:SER:HB3	1.86	0.57
2:B:123:ARG:O	2:B:127:GLU:HG3	2.05	0.57
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.34	0.57
2:D:152:LEU:O	2:D:156:LYS:HG2	2.04	0.57
2:B:136:GLN:HA	2:B:167:ASN:O	2.05	0.56
2:D:106:GLY:O	2:D:111:GLY:HA3	2.05	0.56
2:B:2:ARG:HB2	2:B:133:GLN:HE21	1.68	0.56
2:B:147:SER:OG	2:B:190:SER:OG	2.22	0.56
2:B:26:ASP:OD1	2:B:369:ARG:NH2	2.37	0.56
2:D:1:MET:HE2	2:D:50:ASN:HB2	1.85	0.56
4:F:14:TYR:HB3	4:F:41:LEU:HD13	1.86	0.56
4:F:38:ASN:HB3	4:F:359:PHE:CE1	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:282:TYR:O	1:C:283:HIS:HB2	2.04	0.56
1:C:270:ALA:O	1:C:302:MET:HG2	2.05	0.56
2:B:1:MET:HB2	2:B:130:ASP:OD2	2.05	0.56
1:C:270:ALA:HB3	1:C:302:MET:HG3	1.88	0.56
1:C:249:ASN:OD1	1:C:356:ASN:ND2	2.35	0.55
4:F:47:LEU:HD23	4:F:48:PRO:HD2	1.88	0.55
1:C:234:ILE:HD13	1:C:302:MET:SD	2.46	0.55
1:A:34:GLY:HA3	1:A:60:LYS:HG3	1.87	0.55
2:B:286:LEU:HD23	2:B:291:LEU:CD2	2.37	0.55
2:D:332:MET:O	2:D:336:GLN:HG3	2.06	0.55
4:F:198:LYS:HG2	4:F:199:PHE:H	1.71	0.55
1:A:336:LYS:HG3	3:E:24:LEU:HD13	1.89	0.54
2:B:147:SER:HG	2:B:190:SER:HG	1.52	0.54
1:C:34:GLY:HA3	1:C:60:LYS:HG3	1.88	0.54
4:F:100:ILE:HD12	4:F:128:ARG:HA	1.88	0.54
2:B:337:ASN:OD1	4:F:36:ARG:HD3	2.08	0.54
2:D:141:LEU:HD22	2:D:190:SER:CB	2.37	0.54
4:F:216:TYR:CE2	4:F:218:GLU:HB2	2.42	0.54
1:A:93:ILE:HD11	1:A:121:ARG:HG3	1.90	0.54
4:F:159:GLY:C	4:F:160:ILE:HD12	2.28	0.54
1:A:166:LYS:HE2	1:A:197:HIS:O	2.07	0.54
2:D:141:LEU:HD12	2:D:172:MET:SD	2.47	0.54
1:C:214:ARG:HG2	1:C:219:ILE:O	2.08	0.54
4:F:61:LEU:HD11	4:F:312:PHE:HD1	1.73	0.54
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.43	0.54
2:B:324:SER:O	2:B:328:VAL:HG23	2.08	0.54
1:A:430:LYS:O	1:A:434:GLU:HG3	2.08	0.53
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.89	0.53
2:D:2:ARG:HB3	2:D:133:GLN:HG2	1.89	0.53
3:E:123:LEU:HD23	3:E:126:LYS:HD3	1.91	0.53
1:C:75:ILE:HD12	1:C:94:THR:HG22	1.91	0.53
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.43	0.53
1:A:247:ALA:N	11:A:602:HOH:O	2.41	0.53
1:A:360:PRO:O	1:A:370:LYS:NZ	2.35	0.53
1:C:165:SER:HA	1:C:199:ASP:OD2	2.09	0.53
4:F:178:GLN:N	4:F:178:GLN:OE1	2.41	0.53
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.09	0.53
1:C:241:SER:HA	1:C:249:ASN:OD1	2.08	0.53
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.43	0.53
2:B:16:ILE:HD13	2:B:231:VAL:HG11	1.91	0.53
1:C:227:LEU:O	1:C:231:ILE:HG13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:124:LYS:C	2:D:124:LYS:HD3	2.29	0.52
2:D:23:VAL:O	2:D:27:GLU:HG3	2.08	0.52
4:F:236:LYS:HB3	4:F:240:LEU:CD1	2.36	0.52
2:D:145:THR:HB	8:D:501:GDP:O2B	2.10	0.52
1:A:433:GLU:HG3	1:A:437:VAL:HG21	1.91	0.52
4:F:100:ILE:CD1	4:F:128:ARG:HA	2.39	0.52
1:A:71:GLU:HG2	1:A:72:PRO:CD	2.38	0.52
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.91	0.52
3:E:137:LYS:HE2	3:E:141:GLU:OE2	2.09	0.52
3:E:12:ASN:O	3:E:18:GLN:HB2	2.09	0.52
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.10	0.52
1:C:108:TYR:O	1:C:112:LYS:HG2	2.09	0.52
2:D:38:GLY:HA3	2:D:45:GLN:OE1	2.09	0.52
2:D:21:TRP:CE3	2:D:24:ILE:HD11	2.45	0.52
4:F:17:VAL:O	4:F:21:LEU:HG	2.10	0.52
4:F:19:ARG:HD2	4:F:19:ARG:O	2.10	0.52
2:D:147:SER:HB2	2:D:190:SER:OG	2.09	0.51
1:C:204:VAL:HG13	1:C:302:MET:HE3	1.93	0.51
1:A:69:ASP:O	1:A:94:THR:HA	2.11	0.51
2:B:141:LEU:HD12	2:B:172:MET:SD	2.51	0.51
1:A:88:HIS:HB2	1:A:89:PRO:HD2	1.92	0.51
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.93	0.51
1:C:419:SER:O	1:C:423:GLU:HG3	2.11	0.51
1:C:23:LEU:O	1:C:27:GLU:HG3	2.10	0.50
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.40	0.50
2:D:154:ILE:HG23	2:D:166:MET:HG2	1.93	0.50
2:B:301:MET:HE1	2:B:377:PHE:CZ	2.45	0.50
2:D:327:GLU:O	2:D:331:GLN:HG2	2.12	0.50
4:F:198:LYS:O	4:F:199:PHE:HB3	2.11	0.50
1:C:142:GLY:HA3	1:C:183:GLU:OE1	2.10	0.50
2:D:208:ALA:O	2:D:212:ILE:HG13	2.11	0.50
2:D:171:VAL:HA	2:D:204:ILE:O	2.12	0.50
4:F:280:GLU:HA	4:F:284:LEU:HB3	1.94	0.50
1:A:188:ILE:HD12	1:A:395:PHE:CD2	2.46	0.50
1:A:142:GLY:HA3	1:A:183:GLU:HG2	1.92	0.50
2:B:36:TYR:CD1	2:B:46:LEU:HD21	2.46	0.50
4:F:162:ILE:HD13	4:F:185:TYR:CE1	2.46	0.50
2:B:286:LEU:HD12	2:B:290:GLU:OE1	2.11	0.50
2:D:19:LYS:O	2:D:23:VAL:HG23	2.12	0.49
3:E:48:GLU:CG	3:E:52:LYS:HE3	2.42	0.49
2:B:88:ARG:NH1	2:B:90:ASP:HB2	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:67:LEU:HD22	2:D:92:PHE:CE2	2.47	0.49
2:B:2:ARG:CG	2:B:133:GLN:HE21	2.26	0.49
1:A:233:GLN:HG3	1:A:368:LEU:CD1	2.43	0.49
1:A:403:ALA:O	1:A:404:PHE:HB2	2.12	0.49
1:A:179:THR:HA	2:B:352:LYS:HD2	1.95	0.48
1:A:247:ALA:HB3	3:E:19:SER:OG	2.13	0.48
1:C:172:TYR:CE2	1:C:391:LEU:HD22	2.48	0.48
1:A:187:SER:HB3	1:A:391:LEU:HD21	1.95	0.48
1:A:289:ALA:HA	1:A:331:ALA:HB1	1.96	0.48
2:B:295:MET:SD	2:B:377:PHE:HB3	2.53	0.48
2:B:385:GLN:OE1	2:B:389:LYS:HE3	2.13	0.48
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.48	0.48
2:D:346:TRP:CE3	2:D:347:ILE:HG13	2.48	0.48
3:E:9:ILE:HD11	3:E:21:GLU:OE1	2.13	0.48
2:B:114:LEU:O	2:B:114:LEU:HG	2.13	0.48
2:D:67:LEU:N	2:D:67:LEU:HD12	2.28	0.48
2:D:146:GLY:O	2:D:150:GLY:HA3	2.14	0.48
1:A:119:LEU:HD12	1:A:156:ARG:NH2	2.29	0.48
2:B:31:ASP:HB2	2:B:32:PRO:CD	2.43	0.48
2:B:124:LYS:HD3	2:B:124:LYS:C	2.33	0.48
2:D:11:GLN:HA	2:D:74:THR:HG21	1.94	0.48
4:F:146:VAL:HG22	4:F:164:SER:HB3	1.94	0.48
2:B:334:ASN:HD21	2:B:338:LYS:HD2	1.78	0.48
1:C:93:ILE:CG2	1:C:114:ILE:HD11	2.43	0.48
1:C:188:ILE:HG13	1:C:425:MET:HG3	1.96	0.48
2:B:195:VAL:CG1	2:B:264:ARG:HE	2.26	0.48
1:C:224:TYR:HE2	2:D:247:GLN:HE21	1.61	0.48
3:E:11:LEU:HD11	3:E:18:GLN:OE1	2.14	0.48
4:F:283:ILE:HG23	4:F:327:VAL:CG2	2.43	0.48
1:A:289:ALA:HA	1:A:331:ALA:CB	2.44	0.47
1:C:440:VAL:HG12	1:C:440:VAL:O	2.14	0.47
1:A:3:GLU:OE1	1:A:129:CYS:HB3	2.13	0.47
2:D:107:HIS:O	2:D:152:LEU:HD22	2.14	0.47
2:D:318:ILE:N	2:D:318:ILE:HD12	2.29	0.47
1:A:401:LYS:HG3	2:B:346:TRP:CE3	2.49	0.47
3:E:85:LYS:O	3:E:89:GLU:HG3	2.14	0.47
3:E:92:ASN:O	3:E:96:MET:HG2	2.14	0.47
4:F:24:THR:O	4:F:26:GLN:HG3	2.14	0.47
4:F:38:ASN:HB3	4:F:359:PHE:CZ	2.49	0.47
1:A:101:ASN:HD22	2:B:258:ASN:HD21	1.62	0.47
2:B:276:THR:HG21	2:B:282:GLN:HA	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:69:ASP:O	1:C:94:THR:HA	2.15	0.47
1:C:174:ALA:HB1	1:C:207:GLU:HB2	1.96	0.47
4:F:287:ILE:HG23	4:F:319:PHE:CZ	2.50	0.47
2:B:209:LEU:CD2	2:B:302:MET:HG3	2.45	0.47
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.49	0.47
1:C:271:THR:HG23	1:C:300:ASN:O	2.15	0.47
1:A:142:GLY:CA	1:A:183:GLU:HG2	2.45	0.47
1:A:211:ASP:OD2	1:A:304:LYS:NZ	2.24	0.47
1:A:331:ALA:O	1:A:335:ILE:HG13	2.15	0.47
1:A:2:ARG:HB3	1:A:131:GLY:O	2.14	0.47
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.33	0.47
4:F:318:ASP:OD2	10:F:401:ACP:O2G	2.33	0.47
2:D:406:HIS:HA	2:D:409:THR:OG1	2.15	0.46
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.45	0.46
1:A:209:ILE:HG23	1:A:230:LEU:HD23	1.97	0.46
1:A:292:THR:HG22	1:A:335:ILE:CD1	2.46	0.46
2:B:12:CYS:HB2	8:B:501:GDP:C8	2.51	0.46
2:B:42:LEU:N	2:B:42:LEU:HD12	2.31	0.46
1:C:209:ILE:HD11	1:C:302:MET:HE1	1.91	0.46
1:C:362:VAL:HG22	1:C:370:LYS:HD3	1.97	0.46
3:E:135:LYS:NZ	3:E:139:LEU:HD11	2.30	0.46
1:C:324:VAL:HG22	1:C:327:ASP:OD2	2.15	0.46
4:F:173:ILE:HD13	4:F:180:HIS:HB2	1.97	0.46
2:B:297:ASP:OD1	2:B:298:SER:N	2.48	0.46
2:D:9:ALA:HA	2:D:68:VAL:O	2.16	0.46
3:E:135:LYS:O	3:E:139:LEU:HG	2.15	0.46
2:B:2:ARG:CB	2:B:133:GLN:HE21	2.28	0.46
2:B:115:VAL:HG23	2:B:153:LEU:HD23	1.97	0.46
2:D:1:MET:HG3	2:D:50:ASN:HB2	1.98	0.46
4:F:246:GLN:O	4:F:250:SER:HB3	2.16	0.46
4:F:101:TYR:CD2	4:F:179:VAL:HG22	2.51	0.46
4:F:350:ILE:O	4:F:354:ALA:HB3	2.16	0.46
4:F:377:LYS:HD3	4:F:379:HIS:CE1	2.50	0.45
4:F:280:GLU:OE1	4:F:284:LEU:HD23	2.16	0.45
4:F:283:ILE:HG23	4:F:327:VAL:HG21	1.99	0.45
2:B:301:MET:HE3	2:B:307:PRO:HG2	1.99	0.45
4:F:224:SER:HB2	4:F:241:THR:HG22	1.98	0.45
1:A:433:GLU:HG3	1:A:437:VAL:CG2	2.46	0.45
2:D:1:MET:HG3	2:D:50:ASN:CB	2.47	0.45
2:B:231:VAL:O	2:B:235:MET:HG3	2.17	0.45
1:C:244:PHE:CE1	1:C:358:GLN:HG2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:191:LEU:HD12	4:F:196:HIS:CE1	2.52	0.45
4:F:259:GLY:O	4:F:261:GLU:HG3	2.17	0.45
1:A:223:THR:O	1:A:227:LEU:HG	2.16	0.45
2:B:209:LEU:HD23	2:B:302:MET:HG3	1.99	0.45
2:D:382:THR:O	2:D:385:GLN:HG2	2.17	0.45
2:B:104:ALA:HB2	2:B:413:MET:SD	2.56	0.45
1:C:75:ILE:HB	1:C:94:THR:HG21	1.99	0.45
1:C:136:LEU:HD23	1:C:167:LEU:HB2	1.98	0.45
1:C:210:TYR:CE1	1:C:222:PRO:HD2	2.52	0.45
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.99	0.45
2:B:158:ARG:NH1	2:B:197:ASN:O	2.50	0.44
1:C:385:ALA:HA	1:C:388:TRP:CD1	2.52	0.44
1:A:285:GLN:HA	1:A:285:GLN:NE2	2.31	0.44
1:C:172:TYR:HB3	1:C:205:ASP:HA	1.99	0.44
2:B:289:PRO:HG3	2:B:331:GLN:NE2	2.33	0.44
1:A:75:ILE:HD12	1:A:94:THR:HG22	1.98	0.44
2:B:21:TRP:CE3	2:B:63:PRO:HB3	2.53	0.44
2:B:105:LYS:HA	2:B:109:THR:OG1	2.18	0.44
2:D:68:VAL:HA	2:D:93:VAL:O	2.18	0.44
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.47	0.44
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.53	0.44
2:B:67:LEU:N	2:B:67:LEU:HD12	2.33	0.44
2:B:334:ASN:OD1	2:B:338:LYS:HD3	2.18	0.44
1:C:335:ILE:HG23	1:C:339:ARG:HD2	2.01	0.43
2:D:173:PRO:HB3	2:D:183:GLU:OE1	2.18	0.43
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.53	0.43
2:B:334:ASN:ND2	2:B:338:LYS:HD2	2.32	0.43
2:D:295:MET:HE1	2:D:376:THR:C	2.38	0.43
1:A:2:ARG:HB2	1:A:133:GLN:HE21	1.82	0.43
1:A:235:VAL:O	1:A:239:THR:HG23	2.18	0.43
1:C:216:ASN:HB3	1:C:275:VAL:O	2.19	0.43
2:B:312:TYR:CD1	2:B:381:SER:HB2	2.53	0.43
2:D:211:ASP:O	2:D:215:ARG:HB2	2.19	0.43
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.00	0.43
1:A:284:GLU:CD	1:A:284:GLU:H	2.21	0.43
1:A:351:PHE:HE1	3:E:24:LEU:HD11	1.82	0.43
2:B:42:LEU:HD12	2:B:42:LEU:H	1.83	0.43
2:D:31:ASP:HB2	2:D:32:PRO:CD	2.49	0.43
4:F:58:LEU:HD23	4:F:58:LEU:HA	1.91	0.43
2:D:387:LEU:HD23	2:D:387:LEU:C	2.40	0.43
4:F:3:THR:HA	4:F:28:LYS:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:SER:HB2	1:A:193:THR:OG1	2.18	0.43
2:B:2:ARG:HB2	2:B:133:GLN:NE2	2.33	0.43
2:B:106:GLY:O	2:B:111:GLY:HA3	2.19	0.43
2:B:115:VAL:HG23	2:B:153:LEU:CD2	2.49	0.43
1:C:6:SER:O	1:C:65:ALA:HA	2.19	0.43
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.49	0.42
3:E:72:LEU:O	3:E:76:ARG:HG2	2.19	0.42
4:F:188:LYS:HB3	4:F:323:GLU:CD	2.39	0.42
1:A:187:SER:CB	1:A:391:LEU:HD21	2.49	0.42
3:E:45:PRO:HA	3:E:49:GLU:OE1	2.19	0.42
1:A:71:GLU:HG2	1:A:72:PRO:N	2.33	0.42
4:F:220:VAL:HG12	4:F:263:PHE:CE1	2.54	0.42
2:D:191:VAL:O	2:D:195:VAL:HG23	2.19	0.42
2:D:244:PHE:CE1	2:D:358:ILE:HD12	2.55	0.42
4:F:247:LYS:HG2	4:F:247:LYS:O	2.19	0.42
1:A:31:GLN:HB2	1:A:33:ASP:OD1	2.19	0.42
1:A:155:GLU:OE1	3:E:53:LYS:NZ	2.48	0.42
1:C:425:MET:HB3	1:C:425:MET:HE3	1.85	0.42
4:F:61:LEU:HD12	4:F:310:GLN:O	2.20	0.42
4:F:214:TYR:HB3	4:F:375:PHE:HB3	2.02	0.42
1:C:66:VAL:HG12	1:C:68:VAL:HG23	2.01	0.42
1:C:96:LYS:NZ	2:D:130:ASP:OD1	2.49	0.42
2:D:18:ALA:O	2:D:22:GLU:HG3	2.20	0.42
2:D:69:ASP:HA	2:D:145:THR:HG21	2.02	0.42
4:F:185:TYR:OH	4:F:239:HIS:HB3	2.20	0.42
1:A:196:GLU:OE1	1:A:196:GLU:HA	2.19	0.42
2:B:36:TYR:CE2	2:B:46:LEU:HD11	2.55	0.42
2:B:387:LEU:C	2:B:387:LEU:HD23	2.39	0.42
1:A:25:CYS:SG	1:A:86:LEU:HD11	2.60	0.41
1:C:274:PRO:HG2	1:C:371:VAL:HG11	2.01	0.41
2:D:70:LEU:HD12	2:D:99:ALA:HB2	2.02	0.41
2:B:204:ILE:HD13	2:B:231:VAL:HG13	2.02	0.41
2:B:288:VAL:HB	2:B:289:PRO:HD3	2.02	0.41
1:C:368:LEU:HD23	1:C:368:LEU:HA	1.89	0.41
2:D:334:ASN:HD21	2:D:338:LYS:CE	2.29	0.41
2:D:385:GLN:O	2:D:389:LYS:HG3	2.21	0.41
4:F:197:ARG:NH1	4:F:257:GLU:OE2	2.51	0.41
4:F:240:LEU:HD12	4:F:240:LEU:N	2.35	0.41
1:A:141:PHE:O	1:A:147:SER:HB3	2.21	0.41
2:B:195:VAL:HG11	2:B:264:ARG:HE	1.84	0.41
1:A:274:PRO:HB3	1:A:286:LEU:HD12	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:LEU:HD13	4:F:57:GLY:HA3	2.03	0.41
2:D:28:HIS:NE2	2:D:243:ARG:HB3	2.36	0.41
1:A:317:LEU:HD23	1:A:377:MET:HG3	2.03	0.41
2:D:396:THR:O	2:D:400:ARG:HG2	2.21	0.41
1:A:214:ARG:HG2	1:A:219:ILE:O	2.21	0.41
2:B:213:CYS:HB3	2:B:219:LEU:HD12	2.03	0.41
1:A:409:VAL:HA	1:A:413:MET:O	2.21	0.41
2:B:22:GLU:HG3	2:B:83:PHE:CE1	2.55	0.41
2:D:2:ARG:O	2:D:133:GLN:NE2	2.44	0.41
1:C:255:PHE:CD1	1:C:316:CYS:HB3	2.56	0.41
4:F:47:LEU:HD23	4:F:48:PRO:CD	2.50	0.41
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.56	0.40
1:C:360:PRO:HG2	1:C:371:VAL:HG23	2.03	0.40
2:D:58:GLY:O	2:D:59:ASN:HB2	2.22	0.40
2:D:295:MET:HE2	2:D:377:PHE:CB	2.40	0.40
4:F:3:THR:OG1	4:F:37:PHE:HA	2.20	0.40
4:F:320:MET:HE3	4:F:320:MET:HB3	1.98	0.40
1:A:70:LEU:HD12	1:A:145:THR:OG1	2.21	0.40
1:C:75:ILE:HB	1:C:94:THR:CG2	2.51	0.40
1:C:166:LYS:HE2	1:C:197:HIS:O	2.21	0.40
1:A:411:GLU:O	3:E:61:ARG:HD3	2.20	0.40
1:C:341:ILE:HD12	1:C:341:ILE:N	2.36	0.40
2:D:31:ASP:HB2	2:D:32:PRO:HD2	2.03	0.40
2:D:194:LEU:HD22	2:D:198:THR:HG21	2.03	0.40
1:A:147:SER:HB2	1:A:190:THR:HB	2.03	0.40
1:C:164:LYS:HE3	1:C:164:LYS:HB2	1.97	0.40
4:F:320:MET:HG3	4:F:330:ILE:HD11	2.02	0.40
1:A:115:ILE:HG23	1:A:116:ASP:N	2.36	0.40
4:F:377:LYS:HD3	4:F:379:HIS:NE2	2.37	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	436/451 (97%)	426 (98%)	9 (2%)	1 (0%)	47	58
1	C	439/451 (97%)	430 (98%)	9 (2%)	0	100	100
2	B	423/445 (95%)	410 (97%)	12 (3%)	1 (0%)	47	58
2	D	420/445 (94%)	408 (97%)	11 (3%)	1 (0%)	47	58
3	E	119/143 (83%)	118 (99%)	1 (1%)	0	100	100
4	F	338/384 (88%)	324 (96%)	13 (4%)	1 (0%)	41	50
All	All	2175/2319 (94%)	2116 (97%)	55 (2%)	4 (0%)	47	58

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	245	PRO
1	A	282	TYR
2	B	250	ALA
4	F	88	SER

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	369/379 (97%)	364 (99%)	5 (1%)	67	81
1	C	372/379 (98%)	366 (98%)	6 (2%)	62	78
2	B	367/383 (96%)	363 (99%)	4 (1%)	73	86
2	D	367/383 (96%)	363 (99%)	4 (1%)	73	86
3	E	110/127 (87%)	110 (100%)	0	100	100
4	F	312/342 (91%)	310 (99%)	2 (1%)	86	94
All	All	1897/1993 (95%)	1876 (99%)	21 (1%)	73	86

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU

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Mol	Chain	Res	Type
1	A	221	ARG
1	A	282	TYR
1	A	284	GLU
1	A	316	CYS
2	B	139	HIS
2	B	158	ARG
2	B	318	ILE
2	B	377	PHE
1	C	71	GLU
1	C	120	ASP
1	C	221	ARG
1	C	251	ASP
1	C	347	CYS
1	C	381	THR
2	D	39	ASP
2	D	139	HIS
2	D	229	HIS
2	D	247	GLN
4	F	91	CYS
4	F	257	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	101	ASN
1	A	300	ASN
2	B	15	GLN
2	B	247	GLN
2	B	282	GLN
2	B	294	GLN
1	C	11	GLN
2	D	294	GLN
4	F	180	HIS
4	F	229	ASN
4	F	269	GLN
4	F	333	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 16 ligands modelled in this entry, 9 are monoatomic - leaving 7 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	NSJ	B	505	-	15,15,15	0.66	0	19,19,19	1.22	3 (15%)
8	GDP	D	501	6	24,30,30	0.93	1 (4%)	30,47,47	1.17	4 (13%)
9	NSJ	B	504	-	15,15,15	0.66	0	19,19,19	1.13	2 (10%)
8	GDP	B	501	6	24,30,30	0.96	1 (4%)	30,47,47	1.09	3 (10%)
5	GTP	C	501	6	26,34,34	1.12	2 (7%)	32,54,54	1.39	6 (18%)
10	ACP	F	401	6	27,33,33	1.44	5 (18%)	32,52,52	1.50	4 (12%)
5	GTP	A	501	6	26,34,34	1.14	1 (3%)	32,54,54	1.38	6 (18%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	NSJ	B	505	-	-	0/4/12/12	0/2/2/2
8	GDP	D	501	6	-	2/12/32/32	0/3/3/3
9	NSJ	B	504	-	-	0/4/12/12	0/2/2/2
8	GDP	B	501	6	-	3/12/32/32	0/3/3/3
5	GTP	C	501	6	-	9/18/38/38	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
10	ACP	F	401	6	-	9/15/38/38	0/3/3/3
5	GTP	A	501	6	-	7/18/38/38	0/3/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	501	GTP	C5-C6	-4.09	1.39	1.47
5	C	501	GTP	C5-C6	-4.02	1.39	1.47
10	F	401	ACP	PG-O3G	3.07	1.61	1.54
10	F	401	ACP	PB-O3A	3.07	1.61	1.58
10	F	401	ACP	PG-O2G	3.04	1.61	1.54
10	F	401	ACP	C5-C4	2.56	1.47	1.40
8	B	501	GDP	C6-N1	-2.36	1.34	1.37
8	D	501	GDP	C6-N1	-2.34	1.34	1.37
10	F	401	ACP	PB-O2B	2.30	1.61	1.56
5	C	501	GTP	C2-N3	2.05	1.38	1.33

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	F	401	ACP	PB-O3A-PA	-4.05	119.71	132.56
10	F	401	ACP	C3'-C2'-C1'	3.58	106.37	100.98
10	F	401	ACP	N3-C2-N1	-3.12	123.80	128.68
5	C	501	GTP	C5-C6-N1	3.08	119.39	113.95
5	C	501	GTP	C8-N7-C5	3.07	108.84	102.99
5	A	501	GTP	C5-C6-N1	3.06	119.36	113.95
5	A	501	GTP	C8-N7-C5	3.00	108.71	102.99
8	D	501	GDP	PA-O3A-PB	-3.00	122.54	132.83
5	A	501	GTP	PA-O3A-PB	-2.89	122.90	132.83
5	C	501	GTP	PB-O3B-PG	-2.84	123.06	132.83
5	C	501	GTP	PA-O3A-PB	-2.81	123.17	132.83
5	C	501	GTP	C2-N1-C6	-2.76	120.02	125.10
5	A	501	GTP	PB-O3B-PG	-2.73	123.46	132.83
9	B	505	NSJ	C10-C9-S1	-2.62	109.20	112.51
8	B	501	GDP	PA-O3A-PB	-2.60	123.91	132.83
5	A	501	GTP	C2-N1-C6	-2.58	120.34	125.10
9	B	504	NSJ	C8-C7-N1	-2.57	110.08	111.85
9	B	505	NSJ	C9-C10-N1	-2.55	110.09	111.85
10	F	401	ACP	C4-C5-N7	-2.53	106.76	109.40
8	B	501	GDP	C5-C6-N1	2.52	118.40	113.95
9	B	504	NSJ	C9-C10-N1	-2.39	110.20	111.85
8	B	501	GDP	C8-N7-C5	2.33	107.43	102.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	D	501	GDP	C8-N7-C5	2.29	107.36	102.99
8	D	501	GDP	C5-C6-N1	2.28	117.98	113.95
9	B	505	NSJ	C7-C8-S1	-2.19	109.75	112.51
5	A	501	GTP	O6-C6-C5	-2.11	120.26	124.37
8	D	501	GDP	C3'-C2'-C1'	2.10	104.15	100.98
5	C	501	GTP	O6-C6-C5	-2.00	120.46	124.37

There are no chirality outliers.

All (30) 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-O1A
5	A	501	GTP	C5'-O5'-PA-O2A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O2A
10	F	401	ACP	PB-C3B-PG-O1G
10	F	401	ACP	PB-C3B-PG-O2G
10	F	401	ACP	PB-C3B-PG-O3G
10	F	401	ACP	PG-C3B-PB-O1B
10	F	401	ACP	PG-C3B-PB-O2B
10	F	401	ACP	PG-C3B-PB-O3A
10	F	401	ACP	C5'-O5'-PA-O2A
10	F	401	ACP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3B-PG-O1G
10	F	401	ACP	C5'-O5'-PA-O1A
5	C	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	C4'-C5'-O5'-PA
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	A	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O3A
5	A	501	GTP	PB-O3A-PA-O1A
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	PB-O3A-PA-O1A

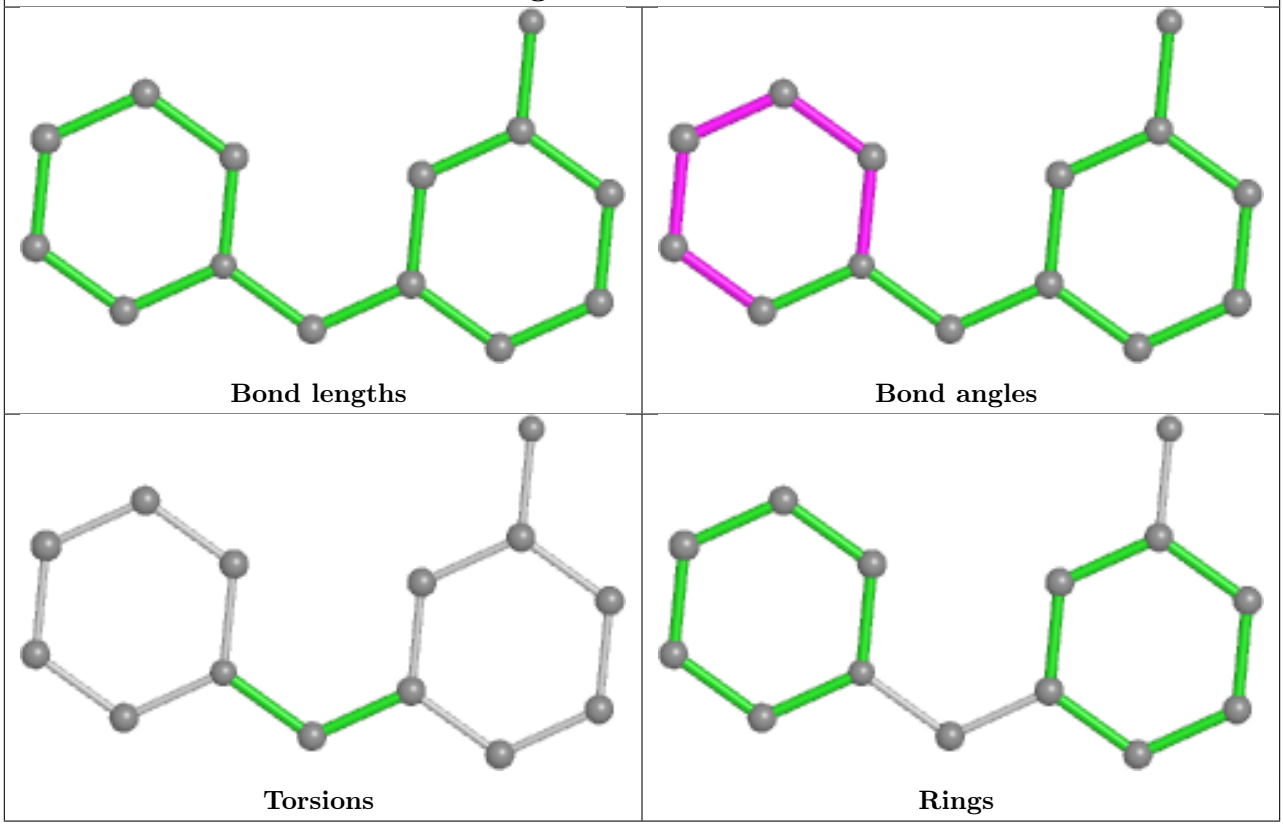
There are no ring outliers.

4 monomers are involved in 10 short contacts:

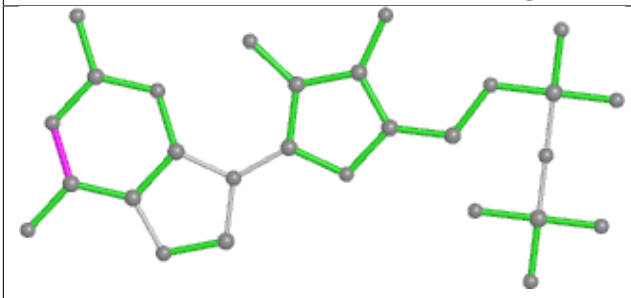
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	501	GDP	3	0
8	B	501	GDP	2	0
10	F	401	ACP	4	0
5	A	501	GTP	1	0

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 then 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.

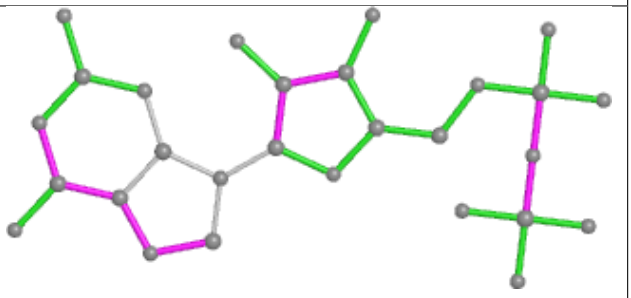
Ligand NSJ B 505



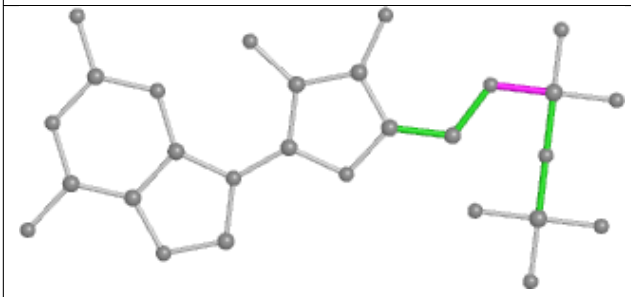
Ligand GDP D 501



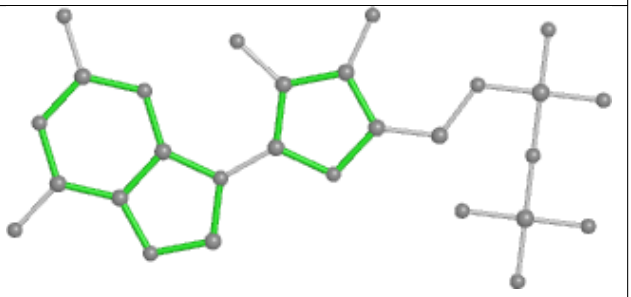
Bond lengths



Bond angles

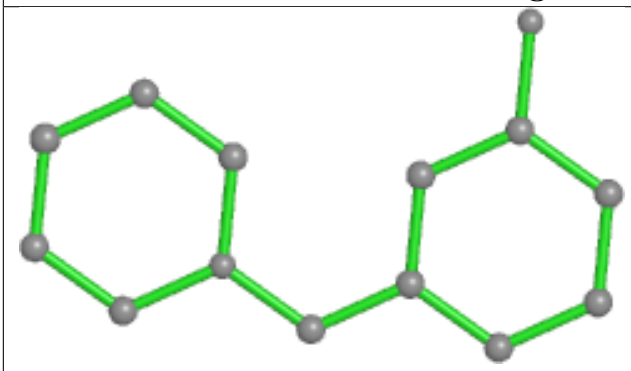


Torsions

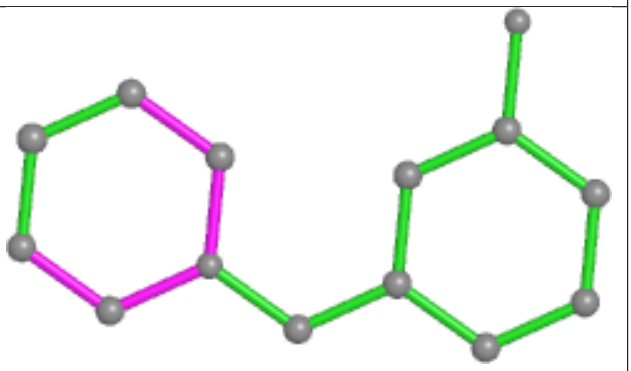


Rings

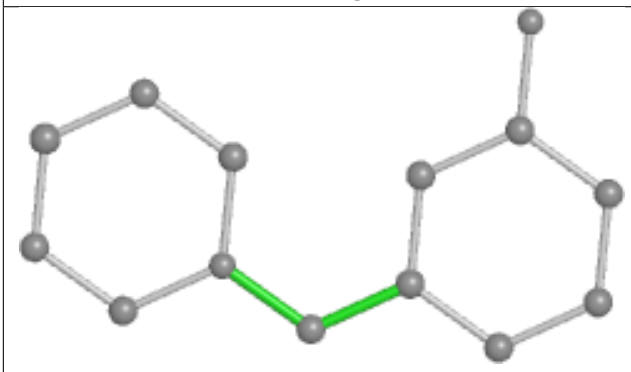
Ligand NSJ B 504



Bond lengths



Bond angles



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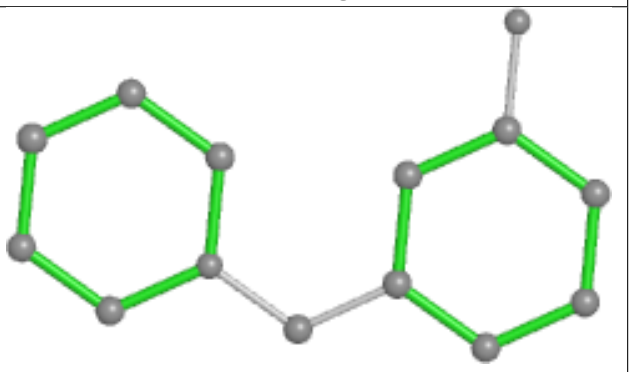
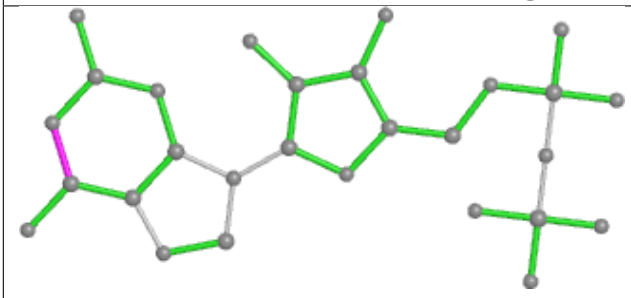
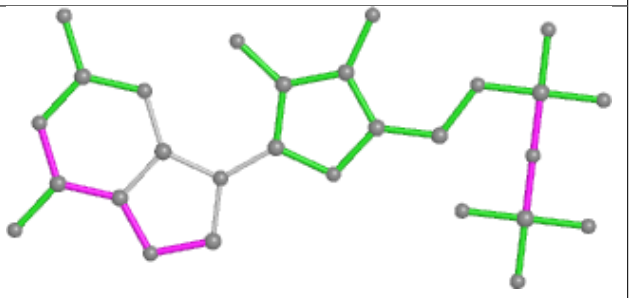


Rings

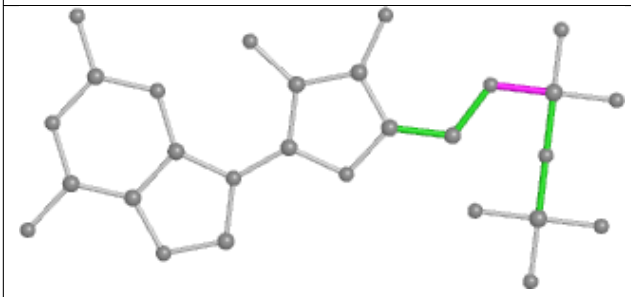
Ligand GDP B 501



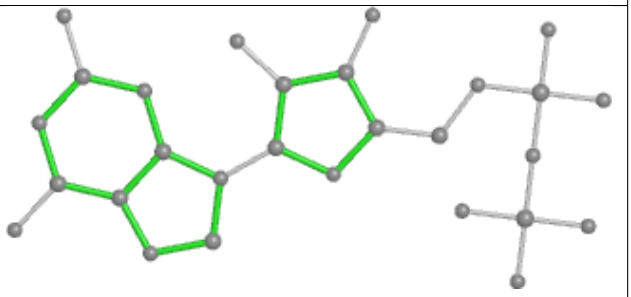
Bond lengths



Bond angles

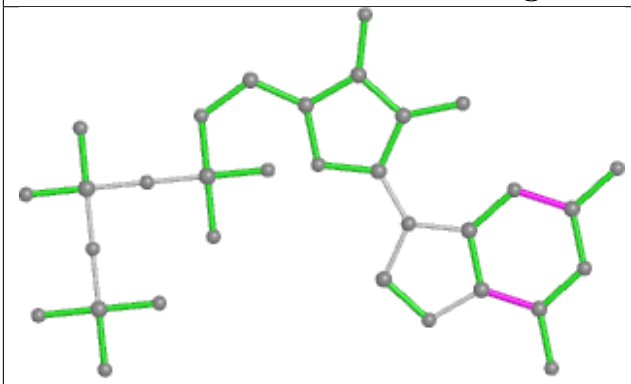


Torsions

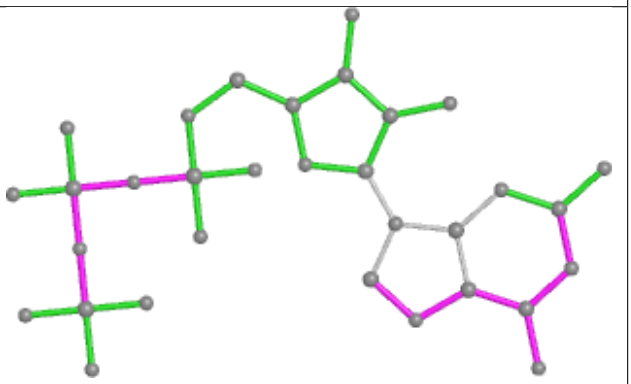


Rings

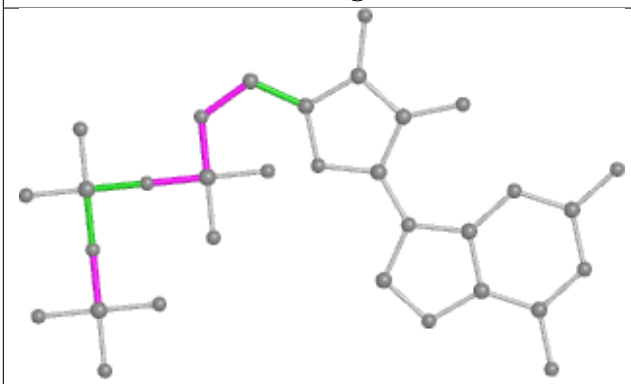
Ligand GTP C 501



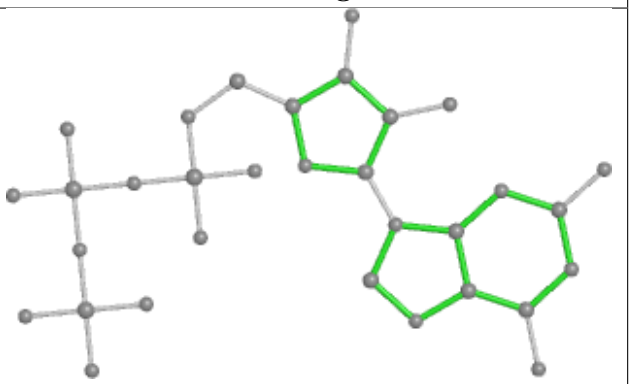
Bond lengths



Bond angles

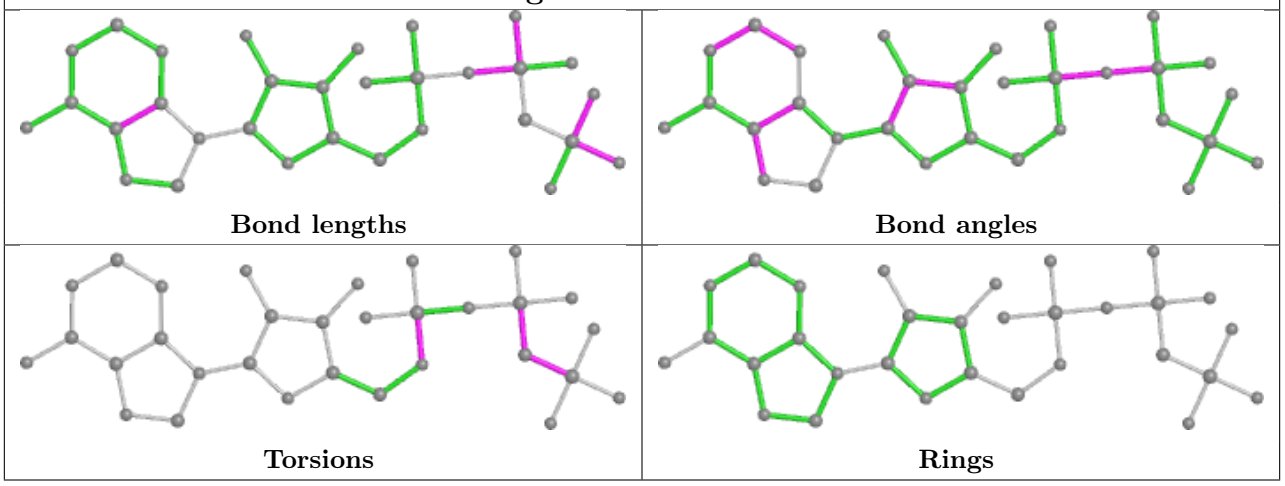


Torsions

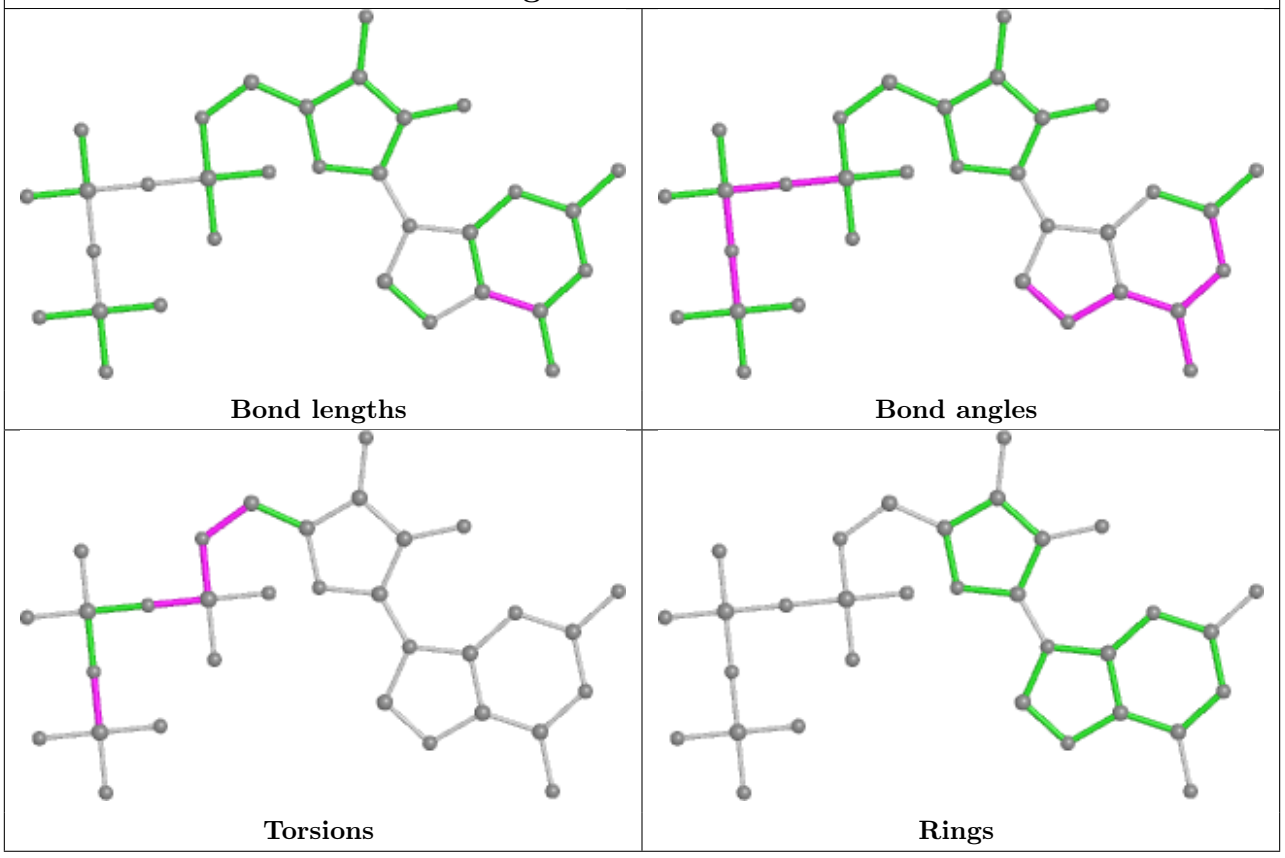


Rings

Ligand ACP F 401



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, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	438/451 (97%)	0.44	14 (3%)	47	54	56, 77, 117, 190	0
1	C	440/451 (97%)	0.48	13 (2%)	50	57	54, 68, 100, 139	0
2	B	426/445 (95%)	0.58	17 (3%)	38	45	54, 76, 118, 173	2 (0%)
2	D	424/445 (95%)	0.52	17 (4%)	38	45	62, 87, 122, 155	4 (0%)
3	E	123/143 (86%)	0.72	8 (6%)	18	24	63, 91, 132, 166	0
4	F	346/384 (90%)	0.64	32 (9%)	9	12	66, 100, 163, 210	0
All	All	2197/2319 (94%)	0.54	101 (4%)	32	39	54, 81, 132, 210	6 (0%)

All (101) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	90	SER	8.4
2	B	284	ARG	8.2
2	D	276	THR	7.5
3	E	24	LEU	6.5
2	B	283	TYR	6.1
4	F	173	ILE	5.7
3	E	26	PRO	5.1
2	D	1	MET	4.9
4	F	105	LEU	4.9
4	F	143	GLU	4.9
4	F	169	LEU	4.7
3	E	25	LYS	4.7
2	D	219	LEU	4.7
2	B	276	THR	4.6
2	D	277	SER	4.4
3	E	27	PRO	4.4
1	A	282	TYR	4.2
4	F	131	PHE	4.1
2	B	1	MET	3.9

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Mol	Chain	Res	Type	RSRZ
4	F	136	ASN	3.8
2	B	285	ALA	3.8
4	F	89	GLU	3.8
4	F	135	TYR	3.7
2	D	275	LEU	3.7
2	D	248	LEU	3.6
1	C	341	ILE	3.6
4	F	144	GLY	3.5
1	A	349	THR	3.5
1	C	286	LEU	3.5
1	C	248	LEU	3.5
2	D	57	THR	3.4
4	F	137	ARG	3.4
1	A	88	HIS	3.3
1	C	335	ILE	3.3
2	D	37	HIS	3.2
4	F	233	PHE	3.2
2	B	57	THR	3.2
1	C	357	TYR	3.2
1	C	368	LEU	3.2
1	C	340	SER	3.1
4	F	251	LYS	3.1
4	F	240	LEU	3.1
4	F	132	LEU	3.0
4	F	99	VAL	3.0
2	B	439	THR	2.9
2	D	217	LEU	2.9
2	D	293	GLN	2.9
2	D	278	ARG	2.9
3	E	139	LEU	2.9
1	A	221	ARG	2.9
4	F	130	VAL	2.9
2	B	400	ARG	2.9
3	E	6	MET	2.8
4	F	140	GLU	2.8
1	A	281	ALA	2.8
1	A	86	LEU	2.8
2	D	122	VAL	2.7
4	F	142	ARG	2.7
1	A	348	PRO	2.7
1	C	308	ARG	2.7
4	F	103	THR	2.7

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Mol	Chain	Res	Type	RSRZ
4	F	381	HIS	2.7
2	B	286	LEU	2.6
1	C	339	ARG	2.6
2	B	219	LEU	2.6
2	B	325	MET	2.5
4	F	134	ALA	2.5
3	E	28	SER	2.5
2	D	299	LYS	2.5
3	E	17	GLY	2.5
1	C	336	LYS	2.4
1	A	351	PHE	2.4
2	D	127	GLU	2.4
1	A	430	LYS	2.3
1	A	324	VAL	2.3
1	A	284	GLU	2.3
4	F	17	VAL	2.3
4	F	236	LYS	2.3
4	F	192	LEU	2.2
4	F	36	ARG	2.2
4	F	176	GLN	2.2
4	F	141	GLY	2.2
1	C	302	MET	2.2
2	B	88	ARG	2.2
1	A	163	LYS	2.2
2	D	218	LYS	2.2
4	F	104	ASN	2.2
2	B	358	ILE	2.2
1	A	326	LYS	2.2
2	B	338	LYS	2.1
2	D	272	PHE	2.1
4	F	98	TYR	2.1
1	C	275	VAL	2.1
2	B	438	ALA	2.1
4	F	330	ILE	2.1
1	A	176	GLN	2.1
1	C	332	ILE	2.0
2	D	401	ARG	2.0
2	B	333	LEU	2.0
4	F	100	ILE	2.0
2	B	48	ARG	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 monosaccharides in this entry.

6.4 Ligands (i)

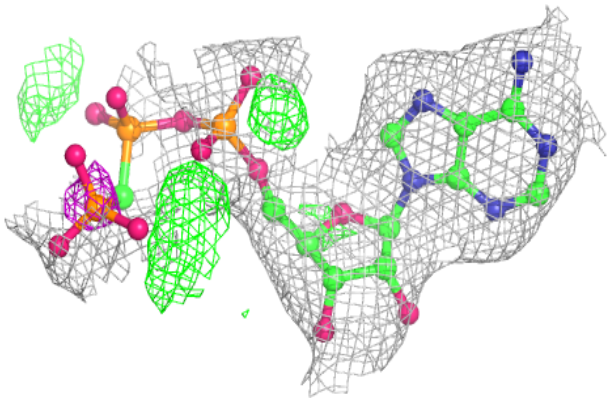
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

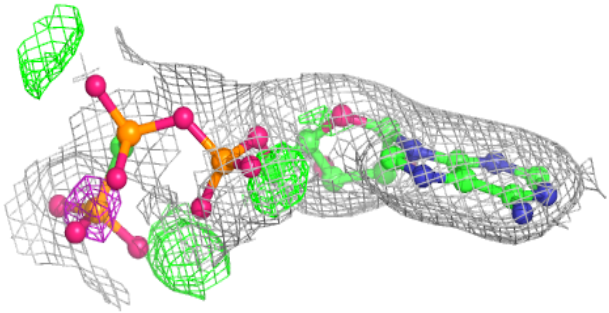
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
7	CA	A	503	1/1	0.83	0.11	108,108,108,108	0
10	ACP	F	401	31/31	0.86	0.14	95,106,120,131	0
6	MG	A	502	1/1	0.88	0.15	59,59,59,59	0
9	NSJ	B	504	14/14	0.89	0.20	69,77,90,92	29
7	CA	A	504	1/1	0.91	0.11	104,104,104,104	0
6	MG	B	502	1/1	0.93	0.19	57,57,57,57	0
9	NSJ	B	505	14/14	0.94	0.17	65,75,89,90	29
7	CA	B	503	1/1	0.95	0.07	114,114,114,114	0
8	GDP	D	501	28/28	0.96	0.17	74,80,91,103	0
6	MG	F	402	1/1	0.96	0.19	92,92,92,92	0
6	MG	D	502	1/1	0.96	0.20	77,77,77,77	0
7	CA	C	503	1/1	0.96	0.12	90,90,90,90	0
6	MG	C	502	1/1	0.97	0.15	61,61,61,61	0
5	GTP	C	501	32/32	0.98	0.17	49,58,61,66	0
5	GTP	A	501	32/32	0.98	0.16	50,60,66,67	0
8	GDP	B	501	28/28	0.99	0.17	53,61,65,66	0

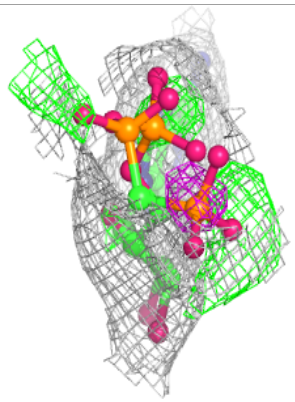
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

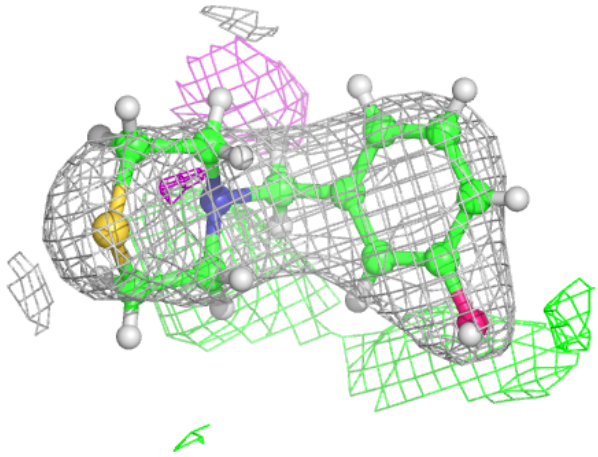


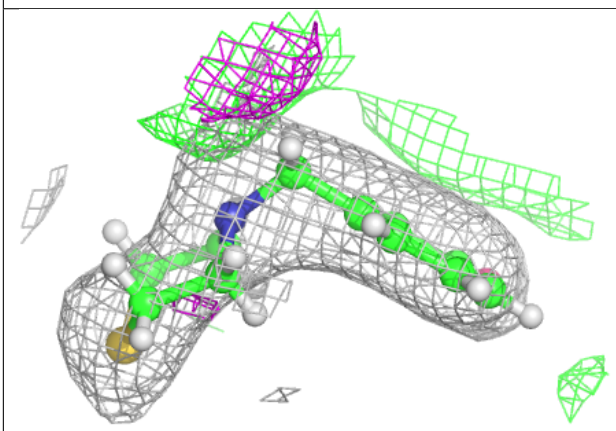


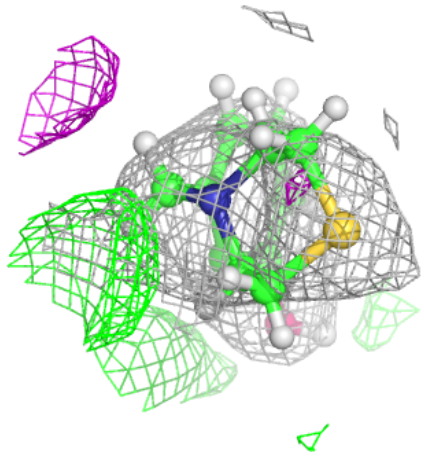


Electron density around NSJ B 504:

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

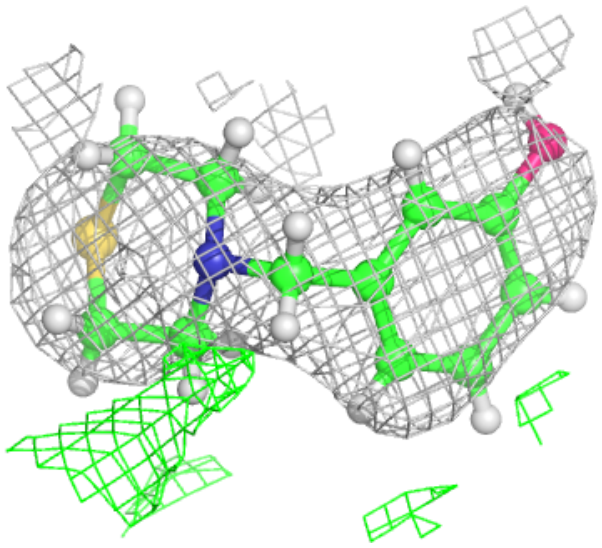


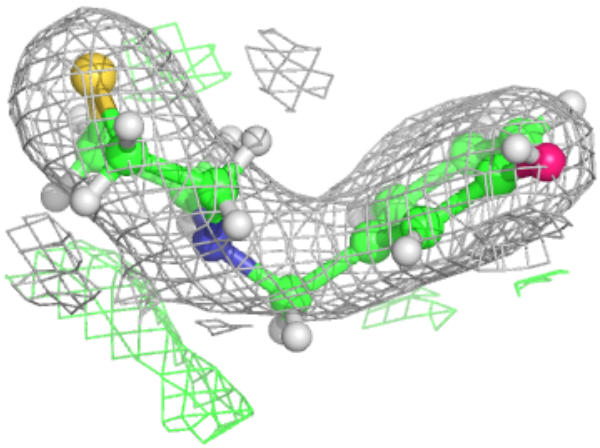


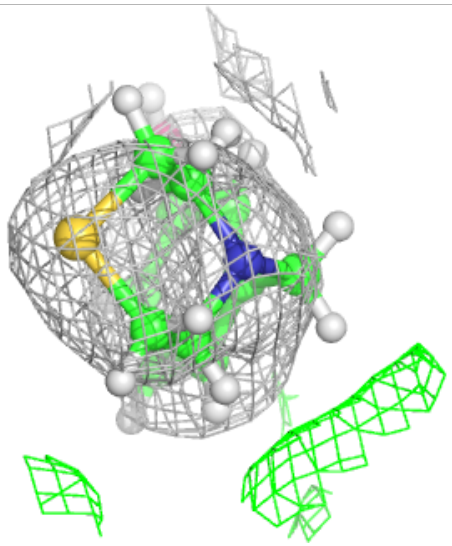


Electron density around NSJ B 505:

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

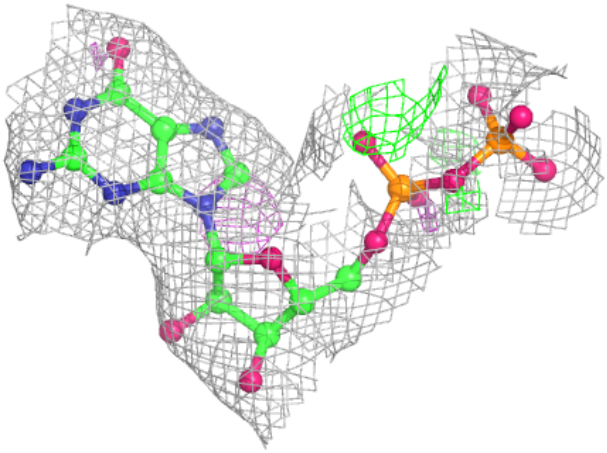


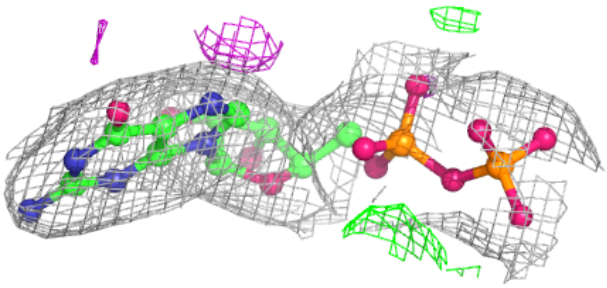


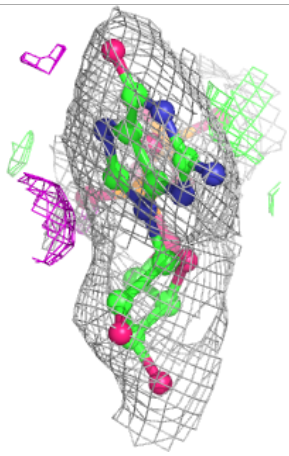


Electron density around GDP D 501:

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

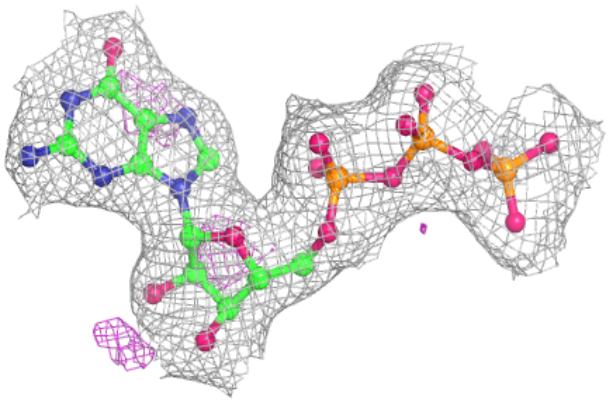


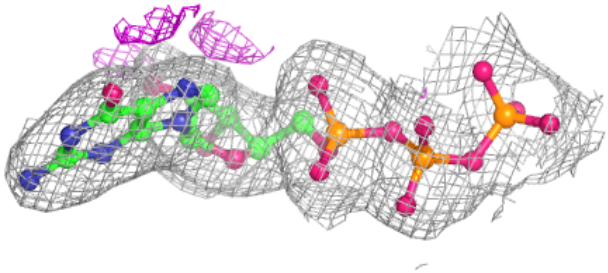


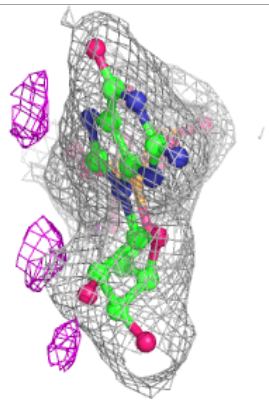


Electron density around GTP C 501:

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

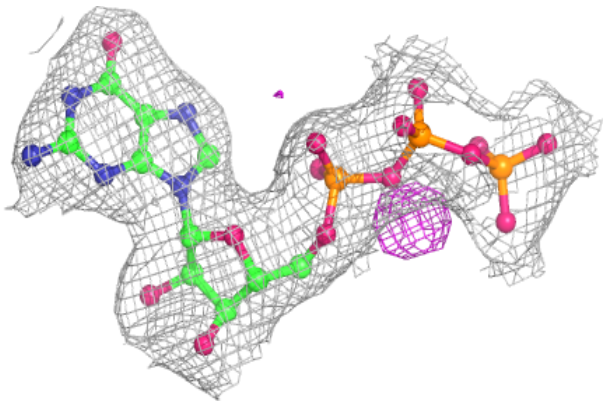


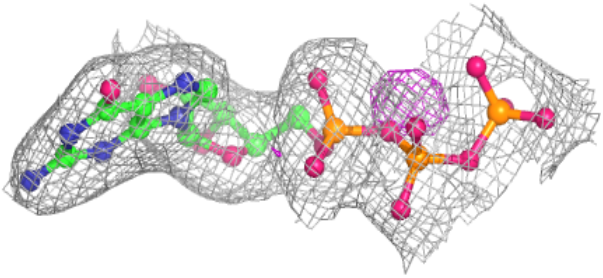


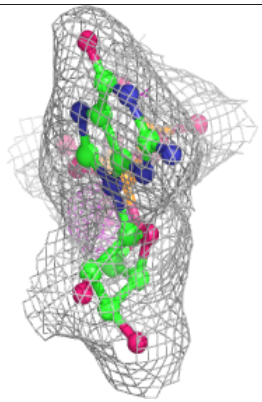


Electron density around GTP A 501:

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

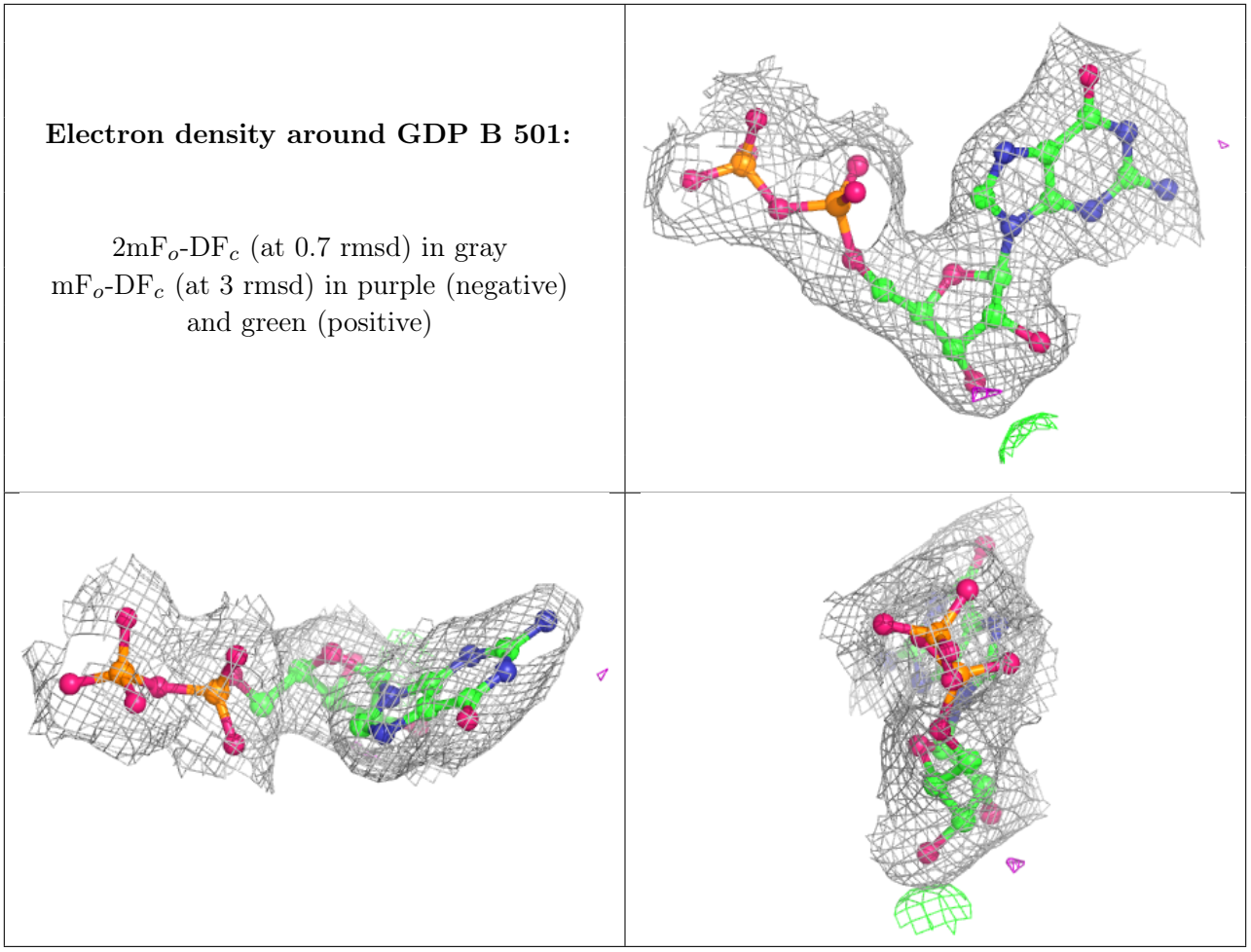






Electron density around GDP B 501:

$2mF_o$-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

There are no such residues in this entry.