



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:43 PM UTC

PDB ID : 7AU5 / pdb_00007au5
Title : Tubulin-noscapine-analogue-14e complex
Authors : Yong, C.; Devine, S.M.; Abel, A.-C.; Muthiah, D.; Gao, X.; Callaghan, R.;
Capuano, B.; Steinmetz, M.O.; Protá, A.E.; Scammels, P.J.
Deposited on : 2020-11-02
Resolution : 2.20 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

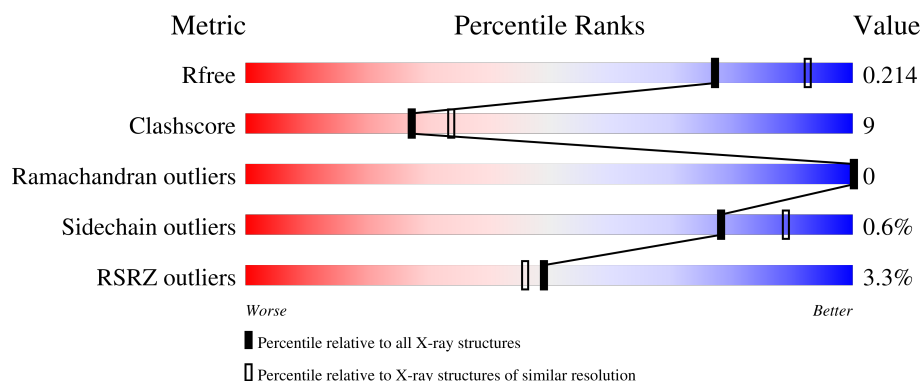
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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

Mol	Chain	Length	Quality of chain
1	A	451	0% 80% 17% .
1	C	451	0% 81% 16% .
2	B	445	2% 72% 23% 5%
2	D	445	3% 75% 21% .
3	E	143	6% 71% 15% 13%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
4	F	384	

2 Entry composition

There are 14 unique types of molecules in this entry. The entry contains 18596 atoms, of which 13 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	12	0
			3497	2214	593	665	25			
1	C	440	Total	C	N	O	S	0	8	0
			3499	2209	595	669	26			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	423	Total	C	N	O	S	0	9	0
			3401	2135	583	656	27			
2	D	426	Total	C	N	O	S	0	3	0
			3368	2112	578	650	28			

- Molecule 3 is a protein called Stathmin-4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	E	124	Total	C	N	O	S	0	4	0
			1059	652	194	207	6			

There are 2 discrepancies between the modelled and reference sequences:

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

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	F	348	Total	C	N	O	S	0	3	0
			2867	1837	492	523	15			

There are 6 discrepancies between the modelled and reference sequences:

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

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



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

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

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

Continued on next page...

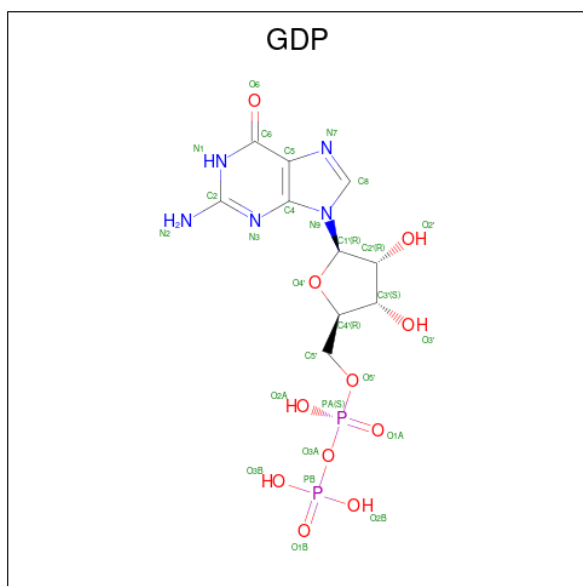
Continued from previous page...

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	1	Total	Ca	0	0
			1	1		
7	B	2	Total	Ca	0	0
			2	2		
7	C	1	Total	Ca	0	0
			1	1		
7	E	1	Total	Ca	0	0
			1	1		

- Molecule 8 is GUANOSINE-5'-DIPHOSPHATE (CCD ID: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).





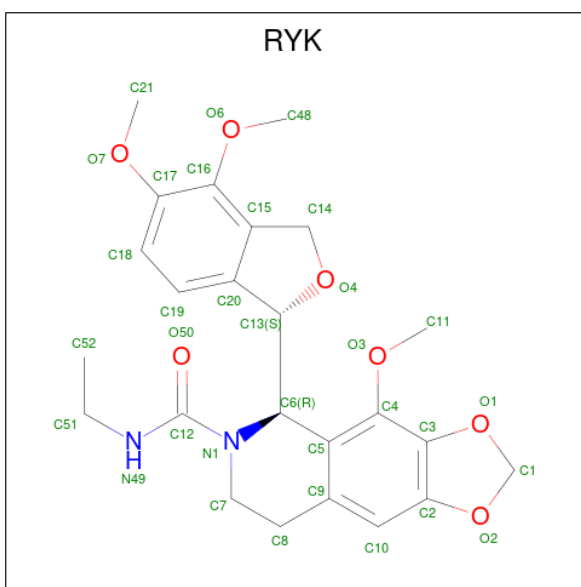
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	B	1	Total	C	N	O	S	0	0
			12	6	1	4	1		

- Molecule 10 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



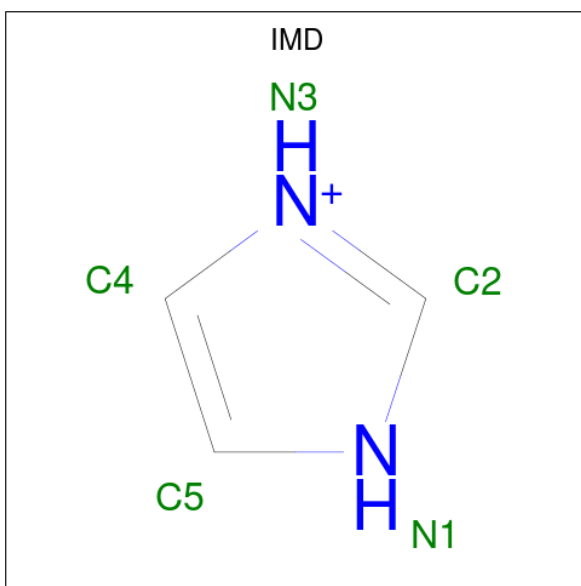
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	B	1	Total	C	H	O	0	0
			14	3	8	3		

- Molecule 11 is (5 {R})-5-[(1 {S})-4,5-dimethoxy-1,3-dihydro-2-benzofuran-1-yl]- {N}-ethyl-4-methoxy-7,8-dihydro-5 {H}-[1,3]dioxolo[4,5-g]isoquinoline-6-carboxamide (CCD ID: RYK) (formula: $C_{24}H_{28}N_2O_7$) (labeled as "Ligand of Interest" by depositor).



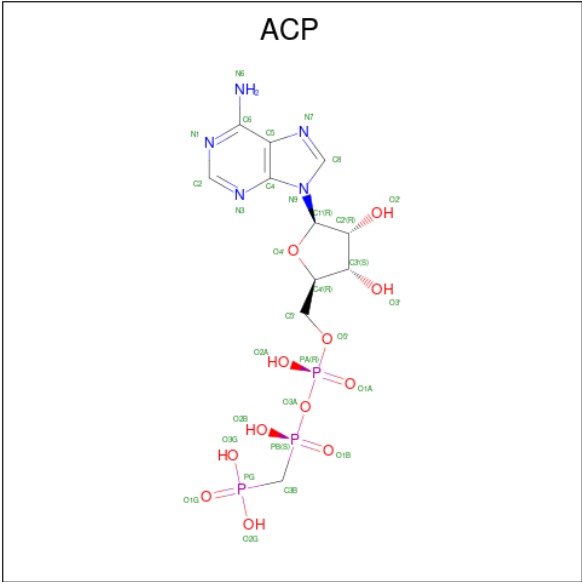
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
11	B	1	Total	C	N	O	0	0
			33	24	2	7		

- Molecule 12 is IMIDAZOLE (CCD ID: IMD) (formula: $C_3H_5N_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	C	1	Total	C	H	N	0	0
			10	3	5	2		

- Molecule 13 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (CCD ID: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).



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

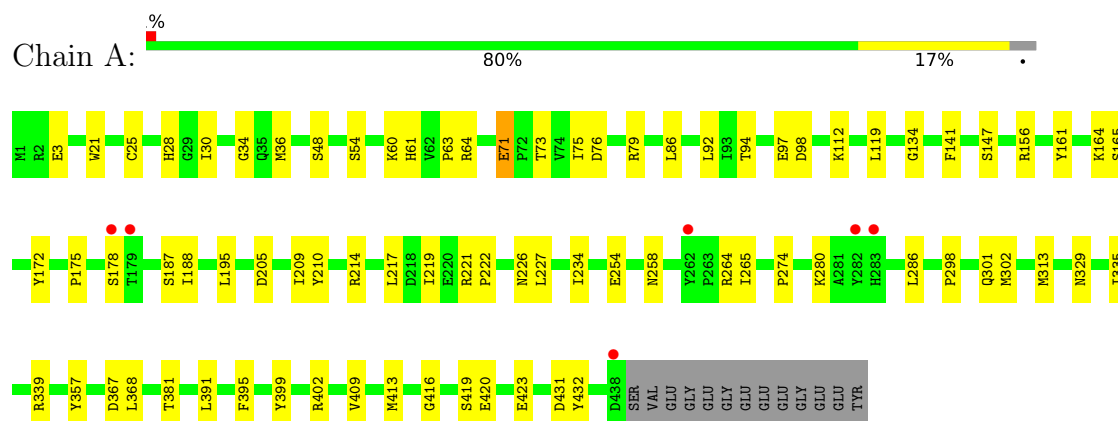
- Molecule 14 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
14	A	122	Total	O	0	0
			122	122		
14	B	150	Total	O	0	0
			150	150		
14	C	278	Total	O	0	0
			278	278		
14	D	62	Total	O	0	0
			62	62		
14	E	23	Total	O	0	0
			23	23		
14	F	40	Total	O	0	0
			40	40		

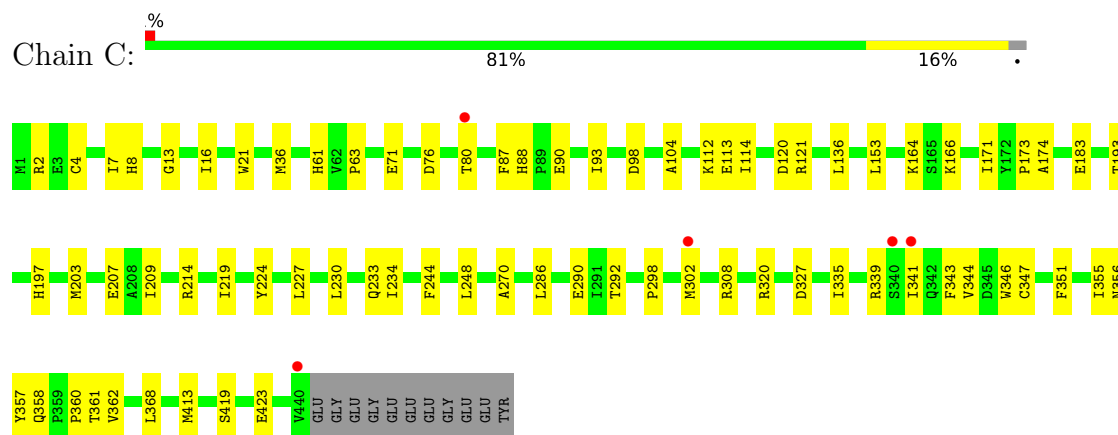
3 Residue-property plots

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.

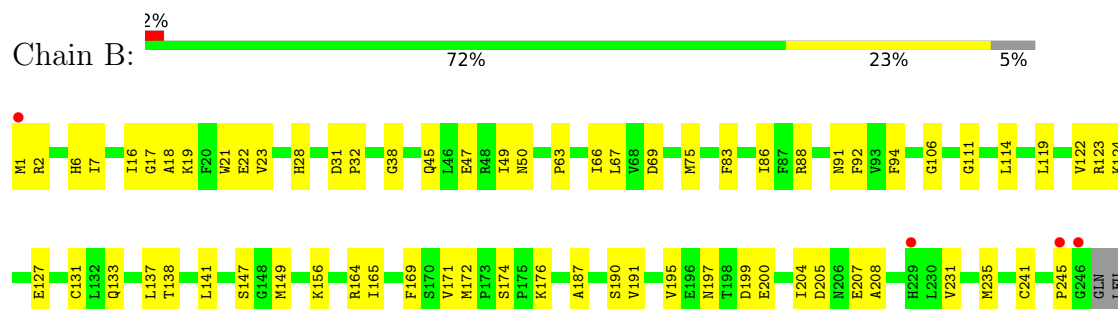
• Molecule 1: Tubulin alpha-1B chain

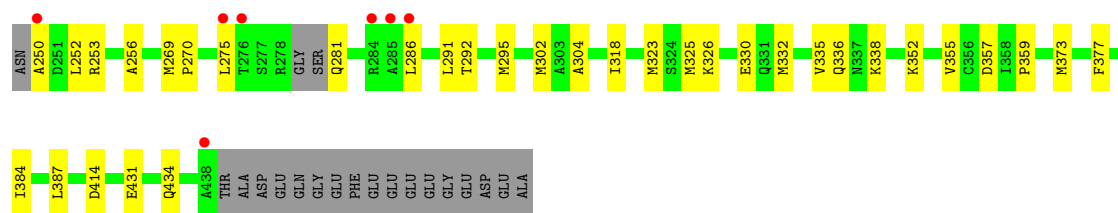


• Molecule 1: Tubulin alpha-1B chain

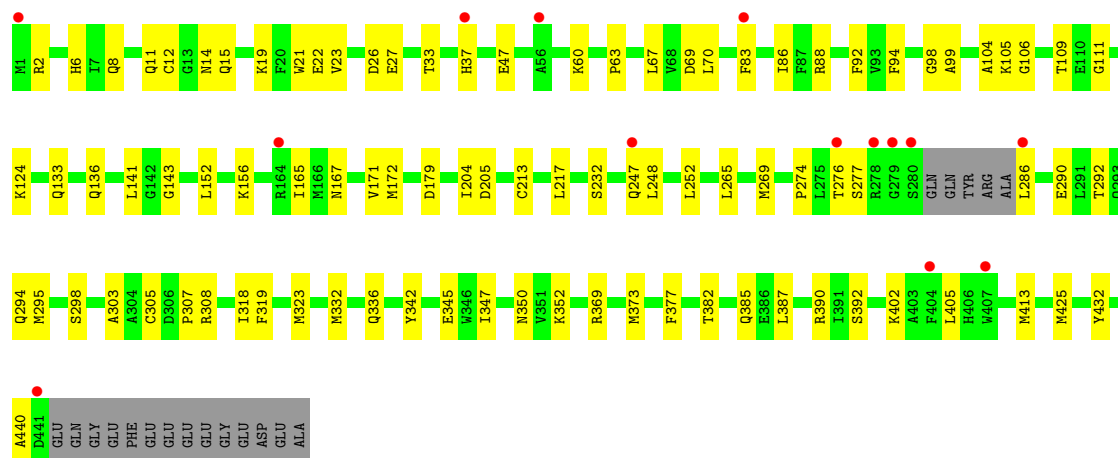
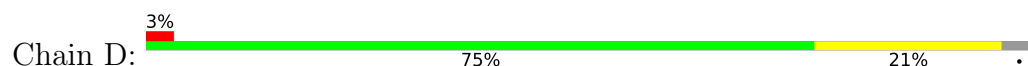


• Molecule 2: Tubulin beta-2B chain

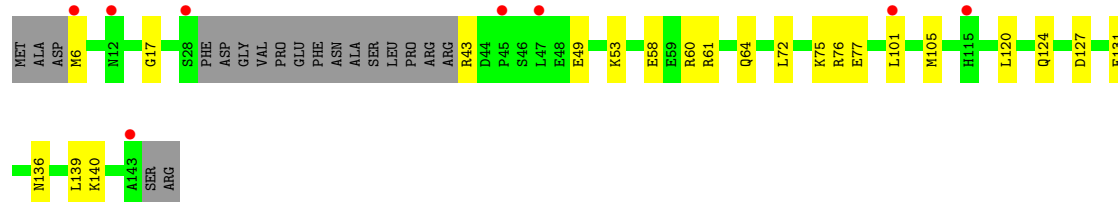
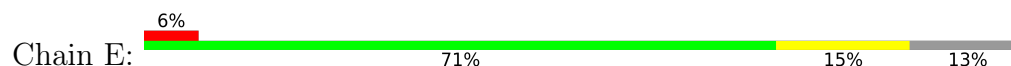




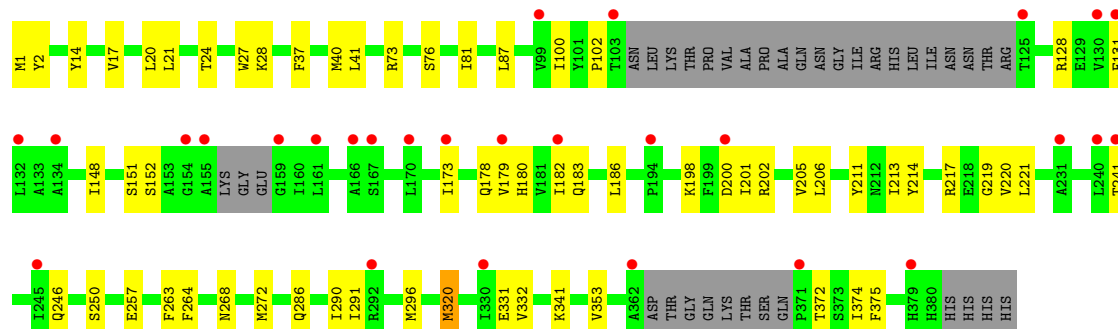
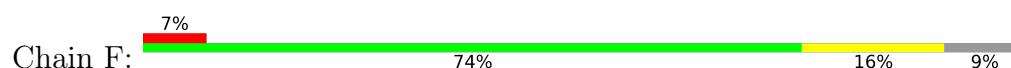
• Molecule 2: Tubulin beta-2B chain



• Molecule 3: Stathmin-4



• Molecule 4: Tubulin-Tyrosine Ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	104.64Å 157.84Å 180.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.88 – 2.20 47.88 – 2.20	Depositor EDS
% Data completeness (in resolution range)	98.6 (47.88-2.20) 98.6 (47.88-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 2.20Å)	Xtriage
Refinement program	PHENIX 1.18.2_3874, REFMAC 5.8.0258	Depositor
R, R_{free}	0.178 , 0.212 0.180 , 0.214	Depositor DCC
R_{free} test set	7481 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	51.8	Xtriage
Anisotropy	0.125	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	18596	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.44% 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: MG, RYK, GOL, GDP, CA, GTP, IMD, MES, ACP

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	0.11	0/3596	0.29	0/4880
1	C	0.13	0/3581	0.32	0/4864
2	B	0.12	0/3486	0.31	0/4717
2	D	0.12	0/3444	0.28	0/4662
3	E	0.10	0/1068	0.22	0/1417
4	F	0.09	0/2932	0.28	0/3960
All	All	0.12	0/18107	0.29	0/24500

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 [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3497	0	3421	61	0
1	C	3499	0	3396	59	0
2	B	3401	0	3282	75	0
2	D	3368	0	3251	61	0
3	E	1059	0	1071	17	0
4	F	2867	0	2836	50	0
5	A	32	0	12	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	32	0	12	1	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	1	0	0	0	0
7	B	2	0	0	0	0
7	C	1	0	0	0	0
7	E	1	0	0	0	0
8	B	28	0	12	0	0
8	D	28	0	12	3	0
9	B	12	0	12	3	0
10	B	6	8	8	0	0
11	B	33	0	0	3	0
12	C	5	5	5	0	0
13	F	31	0	14	5	0
14	A	122	0	0	1	0
14	B	150	0	0	2	0
14	C	278	0	0	7	0
14	D	62	0	0	4	0
14	E	23	0	0	3	0
14	F	40	0	0	1	0
All	All	18583	13	17344	321	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 (321) 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)
4:F:213:ILE:HD11	4:F:296[B]:MET:HE3	1.34	1.05
1:C:270:ALA:HB3	1:C:302[A]:MET:HE2	1.55	0.89
2:D:248:LEU:HD11	2:D:352:LYS:HB3	1.59	0.84
1:C:335:ILE:HG23	1:C:339:ARG:HG3	1.61	0.82
4:F:200:ASP:HB2	4:F:241:THR:HG21	1.60	0.82
4:F:1:MET:HE3	4:F:28:LYS:HB2	1.63	0.80
2:B:16[B]:ILE:HD13	2:B:231:VAL:HG11	1.63	0.79
2:B:47:GLU:HG2	2:B:245:PRO:HG3	1.65	0.77
2:B:31:ASP:HB2	2:B:32:PRO:HD2	1.65	0.77
3:E:136:ASN:OD1	3:E:140:LYS:NZ	2.17	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:352:LYS:HG3	11:B:507:RYK:C48	2.18	0.73
1:C:298:PRO:HG2	1:C:308:ARG:NH2	2.05	0.71
2:D:345:GLU:HG2	2:D:440:ALA:HB2	1.73	0.70
1:C:193[B]:THR:HG22	14:C:772:HOH:O	1.92	0.70
1:A:234:ILE:HD13	1:A:302[A]:MET:SD	2.31	0.70
2:D:295:MET:HE2	2:D:377:PHE:HB2	1.74	0.70
1:C:120[A]:ASP:OD1	14:C:601:HOH:O	2.10	0.70
1:C:76:ASP:O	1:C:80:THR:HG22	1.92	0.70
2:D:33:THR:O	2:D:60:LYS:HE3	1.93	0.69
1:C:4[B]:CYS:SG	1:C:136:LEU:HG	2.31	0.69
2:D:136:GLN:HA	2:D:167:ASN:O	1.93	0.69
1:C:361:THR:HG23	14:C:744:HOH:O	1.93	0.68
1:C:244:PHE:CD1	1:C:358:GLN:HG3	2.28	0.68
1:C:93:ILE:HD11	1:C:121:ARG:HG3	1.75	0.68
4:F:296[B]:MET:HE2	4:F:296[B]:MET:HA	1.75	0.68
3:E:77:GLU:OE1	14:E:301:HOH:O	2.12	0.67
4:F:213:ILE:CD1	4:F:296[B]:MET:HE3	2.20	0.67
4:F:100:ILE:HD12	4:F:128:ARG:HA	1.77	0.67
2:B:176:LYS:HE3	2:B:207:GLU:HB2	1.75	0.67
1:A:209:ILE:HD11	1:A:302[A]:MET:SD	2.36	0.65
1:A:175:PRO:HA	1:A:178[B]:SER:HB3	1.79	0.65
1:A:209:ILE:HG22	1:A:227:LEU:HD22	1.78	0.65
2:B:69:ASP:O	2:B:94:PHE:HA	1.97	0.65
4:F:152:SER:HB3	4:F:178:GLN:NE2	2.11	0.65
4:F:213:ILE:HD11	4:F:296[B]:MET:CE	2.19	0.64
2:D:213:CYS:HA	2:D:217:LEU:HB2	1.78	0.64
2:D:347:ILE:HG22	2:D:350:ASN:HB3	1.80	0.64
4:F:152:SER:HB3	4:F:178:GLN:HE22	1.62	0.64
1:C:270:ALA:CB	1:C:302[A]:MET:HE2	2.28	0.64
2:B:205:ASP:OD1	2:B:207:GLU:HG2	1.98	0.63
1:A:161:TYR:HB3	1:A:164:LYS:CG	2.28	0.63
4:F:151:SER:HB3	4:F:180:HIS:CD2	2.34	0.63
1:C:327:ASP:OD2	14:C:602:HOH:O	2.15	0.63
1:A:21:TRP:CZ3	1:A:63:PRO:HB3	2.34	0.63
2:D:269:MET:HG3	2:D:303:ALA:HB3	1.81	0.62
1:A:79:ARG:HG2	1:A:92:LEU:HD12	1.82	0.62
2:D:70:LEU:HD12	2:D:99:ALA:HB2	1.82	0.61
1:A:161:TYR:HB3	1:A:164:LYS:HG3	1.83	0.61
1:C:244:PHE:CG	1:C:358:GLN:HG3	2.36	0.60
2:D:172:MET:HG3	2:D:387:LEU:HD21	1.82	0.60
2:B:83:PHE:O	2:B:86:ILE:HG12	2.01	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:318:ILE:HD11	11:B:507:RYK:O2	2.01	0.60
2:D:392:SER:HB2	2:D:425:MET:HE3	1.84	0.59
2:D:143:GLY:HA3	8:D:501:GDP:O3A	2.01	0.59
2:B:88:ARG:HD2	2:B:91:ASN:OD1	2.02	0.59
1:C:248:LEU:HD12	1:C:357:TYR:OH	2.02	0.59
1:A:76:ASP:OD1	1:A:79:ARG:NH1	2.36	0.59
1:C:320:ARG:HA	1:C:356:ASN:O	2.02	0.59
2:D:83:PHE:O	2:D:86:ILE:HG22	2.02	0.59
8:D:501:GDP:O1A	14:D:601:HOH:O	2.16	0.58
2:D:23:VAL:HG21	2:D:232:SER:HB2	1.84	0.58
2:D:19:LYS:O	2:D:23:VAL:HG23	2.03	0.58
2:B:208:ALA:HB2	2:B:304:ALA:HB2	1.85	0.58
1:C:292:THR:HG22	1:C:335:ILE:CD1	2.33	0.58
2:B:22[A]:GLU:HG3	2:B:83:PHE:CE1	2.37	0.58
2:D:332:MET:O	2:D:336:GLN:HG3	2.04	0.58
4:F:186:LEU:HB2	13:F:401:ACP:H2	1.84	0.57
2:B:326:LYS:O	2:B:330:GLU:HG3	2.05	0.57
1:C:234:ILE:HD13	1:C:302[B]:MET:SD	2.45	0.57
3:E:60:ARG:O	3:E:64:GLN:HG3	2.04	0.57
2:B:88:ARG:NH2	14:B:601:HOH:O	2.37	0.57
2:D:345:GLU:CG	2:D:440:ALA:HB2	2.34	0.57
2:D:290:GLU:O	2:D:294:GLN:HG3	2.05	0.57
3:E:120:LEU:O	3:E:124:GLN:HG3	2.05	0.56
1:A:175:PRO:HA	1:A:178[A]:SER:HB2	1.85	0.56
1:C:36:MET:HB3	1:C:61:HIS:CE1	2.40	0.56
1:A:36:MET:HB3	1:A:61:HIS:CE1	2.41	0.56
1:A:217:LEU:HD21	1:A:368:LEU:HD23	1.88	0.56
2:D:432:TYR:OH	14:D:602:HOH:O	2.18	0.56
2:B:114:LEU:HD23	2:B:149:MET:HE1	1.88	0.55
2:D:323:MET:HE2	2:D:373:MET:HG2	1.88	0.55
4:F:20:LEU:O	4:F:24:THR:HG23	2.07	0.55
1:A:264[A]:ARG:NH1	1:A:431:ASP:OD2	2.40	0.55
4:F:296[B]:MET:HE2	4:F:296[B]:MET:CA	2.37	0.55
1:A:335:ILE:HG23	1:A:339:ARG:HG3	1.89	0.54
2:B:21:TRP:CZ3	2:B:63:PRO:HB3	2.43	0.54
4:F:205:VAL:HG21	4:F:291:ILE:HD13	1.89	0.54
4:F:73:ARG:HB2	4:F:76:SER:OG	2.06	0.54
1:A:416:GLY:O	1:A:420:GLU:HG3	2.08	0.54
1:A:419:SER:O	1:A:423[A]:GLU:HG3	2.08	0.54
1:A:79:ARG:HG2	1:A:92:LEU:CD1	2.38	0.54
2:B:141:LEU:HD12	2:B:172:MET:SD	2.48	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:217:ARG:HB2	4:F:374:ILE:O	2.08	0.54
2:B:67:LEU:HD22	2:B:92:PHE:CE2	2.43	0.53
1:C:98:ASP:HB2	5:C:501:GTP:O1G	2.08	0.53
2:D:171:VAL:HA	2:D:204:ILE:O	2.08	0.53
2:D:2:ARG:HB3	2:D:133:GLN:CG	2.37	0.53
4:F:37:PHE:CZ	4:F:40:MET:HE3	2.44	0.53
4:F:201:ILE:HG12	4:F:221:LEU:HG	1.90	0.53
2:B:18:ALA:O	2:B:22[B]:GLU:HG3	2.08	0.53
2:B:174:SER:OG	2:B:207:GLU:HB3	2.09	0.53
1:C:360:PRO:HB2	14:C:741:HOH:O	2.09	0.53
1:A:28:HIS:O	1:A:36:MET:HE3	2.09	0.53
2:B:16[A]:ILE:HD11	2:B:138[A]:THR:HB	1.91	0.53
1:A:63:PRO:HD3	1:A:86:LEU:HG	1.90	0.53
2:B:172:MET:HG3	2:B:387:LEU:HD11	1.90	0.53
4:F:100:ILE:CD1	4:F:128:ARG:HA	2.39	0.53
2:B:332:MET:O	2:B:336:GLN:HG2	2.09	0.52
1:C:270:ALA:O	1:C:302[B]:MET:HE2	2.08	0.52
3:E:101[A]:LEU:O	3:E:105[A]:MET:HG2	2.09	0.52
1:A:112:LYS:HE2	3:E:58:GLU:OE1	2.09	0.52
1:C:112:LYS:HE2	14:E:321:HOH:O	2.09	0.52
1:C:88[A]:HIS:HE1	1:C:90:GLU:HG3	1.74	0.52
1:A:134:GLY:HA3	1:A:165:SER:O	2.09	0.52
2:D:2:ARG:NH1	14:D:605:HOH:O	2.41	0.52
2:D:105:LYS:HA	2:D:109:THR:OG1	2.10	0.52
4:F:268:ASN:O	4:F:272:MET:HG3	2.09	0.52
2:D:269:MET:HE2	2:D:305[B]:CYS:SG	2.50	0.52
2:B:66:ILE:HD12	2:B:122:VAL:HG22	1.91	0.52
1:A:48:SER:HB2	14:A:650:HOH:O	2.08	0.51
2:B:231:VAL:O	2:B:235:MET:HG3	2.09	0.51
1:C:234:ILE:HG21	1:C:302[A]:MET:SD	2.50	0.51
1:C:248:LEU:HD13	1:C:355:ILE:HD12	1.92	0.51
1:A:210:TYR:OH	1:A:221:ARG:HD2	2.11	0.51
2:D:69:ASP:O	2:D:94:PHE:HA	2.11	0.51
1:A:254:GLU:HG2	1:A:258:ASN:ND2	2.26	0.51
1:A:409:VAL:HA	1:A:413:MET:O	2.10	0.51
2:B:270:PRO:HG2	2:B:302:MET:HB2	1.92	0.51
1:C:112:LYS:NZ	1:C:113:GLU:OE2	2.43	0.51
1:C:233:GLN:HG3	1:C:368:LEU:CD1	2.41	0.50
2:D:8:GLN:NE2	2:D:14:ASN:HA	2.26	0.50
2:B:106:GLY:O	2:B:111:GLY:HA3	2.11	0.50
2:B:241:CYS:O	2:B:250:ALA:HB1	2.12	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:209:ILE:HG22	1:C:227:LEU:HD22	1.92	0.50
1:C:104:ALA:HB2	1:C:413:MET:SD	2.52	0.50
2:D:286:LEU:HD12	2:D:290:GLU:OE1	2.12	0.50
4:F:198:LYS:HE2	4:F:320:MET:SD	2.51	0.50
1:A:141:PHE:O	1:A:147:SER:HB3	2.12	0.50
2:D:104:ALA:HB2	2:D:413:MET:SD	2.51	0.50
3:E:72:LEU:O	3:E:76:ARG:HG2	2.11	0.50
2:B:2:ARG:HA	2:B:131:CYS:O	2.12	0.50
2:B:2:ARG:HB3	2:B:133:GLN:CG	2.42	0.50
4:F:1:MET:CE	4:F:28:LYS:HB2	2.37	0.50
4:F:2:TYR:HB2	4:F:27:TRP:CD2	2.46	0.50
2:D:47:GLU:HG3	14:D:651:HOH:O	2.10	0.50
2:D:88:ARG:NH1	2:D:124:LYS:HE2	2.27	0.50
1:C:21:TRP:CZ3	1:C:63:PRO:HB3	2.48	0.49
1:C:88[A]:HIS:CE1	1:C:90:GLU:HG3	2.46	0.49
4:F:186:LEU:H	13:F:401:ACP:C2	2.24	0.49
4:F:200:ASP:O	4:F:221:LEU:HA	2.12	0.49
4:F:17:VAL:O	4:F:21:LEU:HG	2.12	0.49
1:C:419:SER:O	1:C:423:GLU:HG3	2.13	0.49
4:F:131:PHE:CE1	4:F:182:ILE:HG21	2.47	0.49
1:C:209:ILE:HG23	1:C:230:LEU:HD23	1.95	0.49
2:D:292:THR:HG22	2:D:319:PHE:HZ	1.78	0.49
4:F:151:SER:HB3	4:F:180:HIS:NE2	2.27	0.49
2:B:431:GLU:O	2:B:434:GLN:HG2	2.13	0.49
1:C:358:GLN:HB2	14:C:607:HOH:O	2.12	0.48
2:B:323:MET:SD	2:B:373:MET:HE3	2.53	0.48
1:A:97:GLU:OE2	2:B:253:ARG:NH1	2.46	0.48
1:A:357:TYR:CE2	3:E:17:GLY:HA2	2.48	0.48
2:B:292:THR:HG22	2:B:335:VAL:HG21	1.95	0.48
1:C:93:ILE:HG22	1:C:114:ILE:HD11	1.95	0.48
2:B:119:LEU:HD11	2:B:156:LYS:HB3	1.95	0.48
2:B:1:MET:CE	2:B:50[B]:ASN:HB2	2.44	0.48
2:B:357:ASP:O	2:B:359:PRO:HD3	2.14	0.48
1:A:214:ARG:HG2	1:A:219:ILE:O	2.14	0.48
1:A:265:ILE:HG23	1:A:432:TYR:CZ	2.49	0.48
2:B:123:ARG:O	2:B:127:GLU:HG3	2.13	0.48
4:F:211:TYR:CE2	4:F:296[B]:MET:HE1	2.48	0.48
2:D:298:SER:HB3	2:D:307:PRO:HD2	1.96	0.48
2:D:308:ARG:HG2	2:D:342:TYR:CZ	2.48	0.48
2:D:21:TRP:CZ3	2:D:63:PRO:HB3	2.49	0.48
2:D:141:LEU:HD12	2:D:172:MET:SD	2.53	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:F:202:ARG:HB3	4:F:220[A]:VAL:HG12	1.94	0.48
4:F:246:GLN:O	4:F:250:SER:HB3	2.14	0.48
2:D:6:HIS:CD2	2:D:21:TRP:HE1	2.32	0.48
2:D:37:HIS:O	2:D:37:HIS:ND1	2.47	0.48
2:B:2:ARG:C	2:B:133:GLN:HG3	2.39	0.47
2:B:22[B]:GLU:HG2	2:B:83:PHE:CD1	2.49	0.47
2:D:152:LEU:O	2:D:156:LYS:HG2	2.14	0.47
2:D:217:LEU:HA	2:D:277:SER:HB2	1.95	0.47
4:F:214:TYR:HB3	4:F:375:PHE:HB3	1.96	0.47
13:F:401:ACP:O1A	13:F:401:ACP:H3B2	2.14	0.47
2:B:1:MET:HE3	2:B:50[B]:ASN:HB2	1.95	0.47
2:D:205:ASP:CG	2:D:390:ARG:HH22	2.21	0.47
3:E:49:GLU:O	3:E:53:LYS:HG2	2.14	0.47
2:B:187:ALA:O	2:B:191:VAL:HG23	2.15	0.47
1:A:265:ILE:HG23	1:A:432:TYR:CE1	2.49	0.47
1:A:329:ASN:HB3	3:E:6:MET:HE3	1.96	0.47
1:C:7:ILE:HG21	1:C:153:LEU:HD21	1.97	0.47
2:D:402:LYS:HB3	2:D:405:LEU:HD12	1.96	0.47
4:F:200:ASP:HB2	4:F:241:THR:CG2	2.38	0.47
2:B:2:ARG:HB3	2:B:133:GLN:NE2	2.30	0.47
2:B:295:MET:CG	2:B:377:PHE:HB2	2.45	0.47
1:C:93:ILE:CD1	1:C:121:ARG:HG3	2.44	0.47
1:C:292:THR:HG22	1:C:335:ILE:HD12	1.97	0.47
1:A:21:TRP:CE3	1:A:63:PRO:HB3	2.50	0.47
4:F:331:GLU:HG2	4:F:332:VAL:N	2.30	0.47
2:B:199:ASP:C	2:B:200:GLU:HG3	2.39	0.46
3:E:101[A]:LEU:HD11	14:E:309:HOH:O	2.14	0.46
2:B:164[A]:ARG:HE	2:B:164[A]:ARG:HA	1.80	0.46
2:B:75:MET:HE3	2:B:92:PHE:HD2	1.80	0.46
2:B:191:VAL:O	2:B:195:VAL:HG23	2.14	0.46
1:C:344:VAL:HG21	1:C:346:TRP:CE2	2.51	0.46
4:F:372:THR:O	4:F:372:THR:HG22	2.14	0.46
2:D:2:ARG:HB3	2:D:133:GLN:HG3	1.96	0.46
2:D:12:CYS:HB2	8:D:501:GDP:C8	2.50	0.46
1:A:75:ILE:HB	1:A:94:THR:CG2	2.46	0.46
2:B:28:HIS:HB3	2:B:49:ILE:HD13	1.97	0.46
2:B:165:ILE:HG21	2:B:252:LEU:HB3	1.98	0.46
1:A:3:GLU:HG2	1:A:64:ARG:CZ	2.46	0.46
1:A:274:PRO:HB3	1:A:286:LEU:HD12	1.98	0.46
2:B:67:LEU:N	2:B:67:LEU:HD12	2.31	0.45
2:B:323:MET:HE2	2:B:373:MET:HE3	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:147:SER:OG	2:B:190:SER:OG	2.30	0.45
2:B:197:ASN:HD21	3:E:75:LYS:NZ	2.14	0.45
2:D:106:GLY:O	2:D:111:GLY:HA3	2.17	0.45
3:E:127:ASP:O	3:E:131:GLU:HG2	2.16	0.45
2:D:67:LEU:N	2:D:67:LEU:HD12	2.31	0.45
4:F:286:GLN:O	4:F:290:ILE:HG13	2.16	0.45
2:B:75:MET:HE3	2:B:92:PHE:CD2	2.52	0.45
2:B:199:ASP:OD1	9:B:504:MES:H62	2.17	0.45
2:B:323:MET:HB3	2:B:373:MET:HE3	1.97	0.45
14:B:602:HOH:O	3:E:76:ARG:HG3	2.16	0.45
2:D:67:LEU:HD22	2:D:92:PHE:CE2	2.52	0.45
4:F:263:PHE:CZ	4:F:341:LYS:HE2	2.52	0.45
1:C:214:ARG:HD2	14:C:734:HOH:O	2.15	0.45
1:C:214:ARG:HG2	1:C:219:ILE:O	2.17	0.45
2:B:1:MET:CE	2:B:50[A]:ASN:HB3	2.46	0.45
9:B:504:MES:H81	9:B:504:MES:H51	1.69	0.45
1:A:25:CYS:HB3	1:A:30:ILE:O	2.16	0.44
2:D:12:CYS:SG	2:D:171:VAL:HG21	2.57	0.44
4:F:205:VAL:CG2	4:F:291:ILE:HD13	2.47	0.44
1:A:54:SER:O	1:A:61:HIS:HA	2.17	0.44
2:D:292:THR:HG22	2:D:319:PHE:CZ	2.52	0.44
1:A:399:TYR:O	1:A:402:ARG:NH1	2.48	0.44
4:F:219:GLY:HA3	4:F:264:PHE:CZ	2.53	0.44
1:A:63:PRO:CD	1:A:86:LEU:HG	2.47	0.44
1:C:16:ILE:CD1	1:C:171:ILE:HD11	2.47	0.44
1:A:210:TYR:CE1	1:A:222:PRO:HD2	2.52	0.44
2:B:1:MET:HE3	2:B:50[A]:ASN:HB3	1.99	0.44
1:A:195:LEU:HD23	1:A:264[B]:ARG:NH2	2.32	0.43
1:C:224:TYR:HE2	2:D:247:GLN:OE1	2.00	0.43
2:D:22:GLU:HG2	2:D:83:PHE:CD1	2.53	0.43
2:B:200:GLU:OE2	2:B:256:ALA:HB2	2.18	0.43
1:C:166:LYS:HE2	1:C:197:HIS:O	2.17	0.43
1:C:174:ALA:CB	1:C:207:GLU:HB2	2.48	0.43
4:F:178:GLN:HG2	4:F:179:VAL:N	2.34	0.43
1:A:210:TYR:CZ	1:A:222:PRO:HD2	2.53	0.43
1:C:2:ARG:HA	1:C:2:ARG:NE	2.32	0.43
2:D:382:THR:O	2:D:385:GLN:HG2	2.17	0.43
2:D:274:PRO:HB3	2:D:286:LEU:HD22	2.00	0.43
1:A:71:GLU:OE1	1:A:73:THR:OG1	2.29	0.43
1:A:209:ILE:HG22	1:A:227:LEU:CD2	2.45	0.43
1:A:298:PRO:HA	1:A:301:GLN:CD	2.43	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16[A]:ILE:HG13	2:B:17:GLY:N	2.33	0.43
2:D:265:LEU:HD22	2:D:432:TYR:CZ	2.54	0.43
4:F:241:THR:HG22	13:F:401:ACP:O3'	2.19	0.42
1:A:265:ILE:HG21	1:A:313:MET:HE1	2.01	0.42
1:A:280:LYS:HB3	1:A:280:LYS:HE2	1.83	0.42
3:E:101[A]:LEU:HD12	3:E:101[A]:LEU:C	2.45	0.42
4:F:211:TYR:HE2	4:F:296[B]:MET:CE	2.32	0.42
2:B:176:LYS:CE	2:B:207:GLU:HB2	2.48	0.42
2:B:286:LEU:HD23	2:B:291:LEU:HD23	2.01	0.42
1:C:361:THR:HG22	1:C:362:VAL:N	2.34	0.42
2:D:11:GLN:O	2:D:15:GLN:HG2	2.19	0.42
1:A:175:PRO:HA	1:A:178[B]:SER:CB	2.48	0.42
2:B:7:ILE:O	2:B:137:LEU:HA	2.20	0.42
1:C:203:MET:O	1:C:302[A]:MET:HE3	2.19	0.42
4:F:102:PRO:HB3	4:F:173:ILE:HG22	2.02	0.42
1:A:188:ILE:HD12	1:A:395:PHE:HB2	2.01	0.42
2:B:286:LEU:HD23	2:B:291:LEU:CD2	2.50	0.42
1:C:21:TRP:CE3	1:C:63:PRO:HB3	2.55	0.42
2:D:165:ILE:HG21	2:D:252:LEU:HB3	2.01	0.42
1:A:21:TRP:CH2	1:A:63:PRO:HB3	2.55	0.42
4:F:2:TYR:HB3	4:F:27:TRP:CZ3	2.54	0.42
1:A:75:ILE:HD12	1:A:94:THR:HG22	2.02	0.41
1:A:119:LEU:HD11	1:A:156:ARG:HB3	2.01	0.41
1:C:164:LYS:HE2	1:C:164:LYS:HB2	1.85	0.41
2:D:70:LEU:HB3	2:D:98:GLY:HA2	2.02	0.41
1:A:226:ASN:ND2	1:A:367:ASP:OD2	2.52	0.41
2:D:318:ILE:HD12	2:D:318:ILE:N	2.35	0.41
4:F:14:TYR:HB3	4:F:41:LEU:HD13	2.00	0.41
4:F:148:ILE:HG22	4:F:183:GLN:O	2.20	0.41
1:A:187:SER:CB	1:A:391:LEU:HD21	2.50	0.41
1:A:302[B]:MET:HE3	1:A:302[B]:MET:HA	2.02	0.41
3:E:58:GLU:HG3	3:E:61:ARG:NH2	2.35	0.41
2:B:169:PHE:CD1	2:B:235:MET:HE3	2.56	0.41
4:F:186:LEU:H	13:F:401:ACP:H2	1.85	0.41
4:F:81:ILE:O	4:F:87:LEU:O	2.39	0.41
4:F:263:PHE:HB2	14:F:538:HOH:O	2.19	0.41
1:A:98:ASP:HB2	5:A:501:GTP:O2G	2.20	0.41
1:A:34:GLY:HA3	1:A:60:LYS:HG3	2.03	0.41
2:B:171:VAL:HA	2:B:204:ILE:O	2.21	0.41
1:C:63:PRO:HG2	1:C:87:PHE:CE1	2.55	0.41
1:C:270:ALA:HB3	1:C:302[A]:MET:CE	2.37	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:343:PHE:HD2	1:C:347[A]:CYS:SG	2.44	0.41
3:E:136:ASN:O	3:E:140:LYS:HG2	2.20	0.41
2:B:269:MET:HG2	2:B:384:ILE:HD13	2.02	0.41
1:C:8:HIS:HB3	1:C:13:GLY:O	2.21	0.41
1:C:71:GLU:HG2	1:C:98:ASP:HB3	2.02	0.41
1:C:286:LEU:HA	1:C:290:GLU:OE1	2.21	0.41
1:C:341:ILE:HD13	1:C:351:PHE:HZ	1.86	0.41
2:B:38:GLY:HA3	2:B:45:GLN:OE1	2.20	0.40
2:B:295:MET:HG2	2:B:377:PHE:HB2	2.03	0.40
2:D:274:PRO:HB2	2:D:276:THR:HG23	2.03	0.40
2:B:6:HIS:CD2	2:B:21:TRP:HE1	2.39	0.40
2:B:19:LYS:O	2:B:23:VAL:HG23	2.21	0.40
1:C:173:PRO:HB3	1:C:183:GLU:OE1	2.21	0.40
2:D:23:VAL:O	2:D:27:GLU:HG3	2.21	0.40
1:A:172:TYR:HB3	1:A:205:ASP:HA	2.04	0.40
1:A:187:SER:HB3	1:A:391:LEU:HD21	2.02	0.40
1:C:346:TRP:CZ3	1:C:347[C]:CYS:SG	3.14	0.40
4:F:206:LEU:HD23	4:F:353:VAL:CG2	2.52	0.40
2:B:318:ILE:HD11	11:B:507:RYK:C2	2.51	0.40
2:B:325:MET:HG2	2:B:355:VAL:HG21	2.03	0.40
2:D:26:ASP:OD2	2:D:369:ARG:HD2	2.22	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	448/451 (99%)	438 (98%)	10 (2%)	0	100	100
1	C	447/451 (99%)	436 (98%)	11 (2%)	0	100	100
2	B	426/445 (96%)	417 (98%)	9 (2%)	0	100	100
2	D	425/445 (96%)	415 (98%)	10 (2%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	124/143 (87%)	123 (99%)	1 (1%)	0	100	100
4	F	343/384 (89%)	334 (97%)	9 (3%)	0	100	100
All	All	2213/2319 (95%)	2163 (98%)	50 (2%)	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	381/379 (100%)	379 (100%)	2 (0%)	81	90
1	C	380/379 (100%)	380 (100%)	0	100	100
2	B	375/383 (98%)	371 (99%)	4 (1%)	65	79
2	D	371/383 (97%)	370 (100%)	1 (0%)	86	93
3	E	115/127 (91%)	113 (98%)	2 (2%)	53	69
4	F	314/342 (92%)	312 (99%)	2 (1%)	78	89
All	All	1936/1993 (97%)	1925 (99%)	11 (1%)	78	89

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	381	THR
2	B	124	LYS
2	B	275	LEU
2	B	281	GLN
2	B	414	ASP
2	D	179	ASP
3	E	43	ARG
3	E	139	LEU
4	F	257	GLU
4	F	320	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	GLN
1	A	309	HIS
1	A	393	HIS
2	B	59	ASN
2	B	197	ASN
2	B	281	GLN
2	B	349	ASN
2	B	385	GLN
2	B	433	GLN
2	B	434	GLN
2	B	436	GLN
1	C	133	GLN
1	C	393	HIS
2	D	331	GLN
4	F	178	GLN
4	F	260	ASN
4	F	348	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 19 ligands modelled in this entry, 10 are monoatomic - leaving 9 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
13	ACP	F	401	6	31,33,33	2.20	11 (35%)	47,52,52	1.83	12 (25%)
11	RYK	B	507	-	37,37,37	1.52	4 (10%)	48,54,54	1.69	10 (20%)
8	GDP	D	501	6	29,30,30	1.17	2 (6%)	45,47,47	1.71	5 (11%)
8	GDP	B	501	6	29,30,30	1.13	2 (6%)	45,47,47	1.72	7 (15%)
5	GTP	C	501	6	33,34,34	0.91	2 (6%)	50,54,54	1.55	10 (20%)
5	GTP	A	501	6	33,34,34	0.94	2 (6%)	50,54,54	1.52	8 (16%)
12	IMD	C	504	-	5,5,5	0.64	0	5,5,5	0.42	0
9	MES	B	504	-	12,12,12	2.24	1 (8%)	15,16,16	1.75	3 (20%)
10	GOL	B	506	-	5,5,5	0.84	0	5,5,5	0.97	0

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
13	ACP	F	401	6	-	3/19/38/38	0/3/3/3
11	RYK	B	507	-	-	4/17/45/45	0/5/5/5
8	GDP	D	501	6	-	6/16/32/32	0/3/3/3
8	GDP	B	501	6	-	5/16/32/32	0/3/3/3
5	GTP	C	501	6	-	7/22/38/38	0/3/3/3
5	GTP	A	501	6	-	9/22/38/38	0/3/3/3
12	IMD	C	504	-	-	-	0/1/1/1
9	MES	B	504	-	-	0/6/14/14	0/1/1/1
10	GOL	B	506	-	-	0/4/4/4	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	B	504	MES	C8-S	-7.48	1.67	1.77
13	F	401	ACP	PG-O1G	5.66	1.61	1.50
11	B	507	RYK	C14-C15	-5.54	1.44	1.50
13	F	401	ACP	C5-C4	4.78	1.47	1.39
13	F	401	ACP	PB-O1B	4.21	1.61	1.51
11	B	507	RYK	O4-C14	-3.97	1.36	1.43
11	B	507	RYK	C12-N1	3.96	1.48	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	F	401	ACP	PB-O3A	3.49	1.62	1.58
13	F	401	ACP	PB-O2B	-3.39	1.48	1.56
8	D	501	GDP	C5-C4	3.14	1.47	1.38
8	B	501	GDP	C5-C4	2.96	1.46	1.38
13	F	401	ACP	PG-O2G	-2.93	1.48	1.55
13	F	401	ACP	PG-O3G	2.87	1.61	1.55
13	F	401	ACP	C5-C6	2.80	1.48	1.41
13	F	401	ACP	PA-O3A	2.60	1.62	1.59
11	B	507	RYK	C6-N1	2.59	1.50	1.47
8	D	501	GDP	C6-N1	-2.37	1.34	1.38
13	F	401	ACP	C5-N7	-2.34	1.34	1.39
8	B	501	GDP	C6-N1	-2.27	1.34	1.38
5	C	501	GTP	PB-O3B	2.27	1.62	1.59
13	F	401	ACP	C8-N7	2.09	1.35	1.31
5	C	501	GTP	C2-N3	2.07	1.38	1.33
5	A	501	GTP	PA-O3A	2.06	1.61	1.59
5	A	501	GTP	C2-N3	2.06	1.38	1.33

All (55) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	501	GDP	C5-C4-N3	-5.96	118.91	128.39
13	F	401	ACP	C5-C4-N3	-5.85	118.66	126.72
8	B	501	GDP	C5-C4-N3	-5.71	119.30	128.39
8	B	501	GDP	C2-N3-C4	5.05	121.00	112.30
8	D	501	GDP	C2-N3-C4	4.95	120.83	112.30
13	F	401	ACP	N3-C4-N9	4.86	135.44	127.17
5	A	501	GTP	C5-C4-N3	-4.74	120.85	128.39
5	C	501	GTP	C5-C4-N3	-4.63	121.02	128.39
11	B	507	RYK	C13-C6-N1	4.63	118.50	110.01
5	A	501	GTP	C2-N3-C4	4.61	120.25	112.30
9	B	504	MES	C5-N4-C3	4.50	118.54	108.84
5	C	501	GTP	C2-N3-C4	4.42	119.91	112.30
8	D	501	GDP	N9-C4-N3	4.34	134.64	125.95
8	B	501	GDP	N9-C4-N3	4.27	134.48	125.95
11	B	507	RYK	C15-C20-C13	-4.09	106.46	110.25
11	B	507	RYK	C51-N49-C12	4.07	128.83	120.77
13	F	401	ACP	C2-N3-C4	3.69	120.85	111.83
13	F	401	ACP	C4-C5-N7	-3.63	106.44	110.58
8	B	501	GDP	C6-C5-N7	3.41	136.50	130.29
8	D	501	GDP	C6-C5-N7	3.39	136.46	130.29
11	B	507	RYK	C1-O2-C2	-3.16	101.08	105.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	F	401	ACP	C4-N9-C8	3.10	109.00	105.74
13	F	401	ACP	N3-C2-N1	-3.03	124.00	128.58
5	C	501	GTP	N9-C4-N3	2.86	131.66	125.95
11	B	507	RYK	O2-C2-C3	2.83	112.49	109.62
5	C	501	GTP	N9-C8-N7	-2.82	108.17	113.40
11	B	507	RYK	C5-C6-C13	-2.82	102.59	108.66
5	A	501	GTP	N9-C4-N3	2.81	131.58	125.95
5	A	501	GTP	N9-C8-N7	-2.79	108.22	113.40
13	F	401	ACP	C5-N7-C8	2.74	107.76	103.45
5	A	501	GTP	C2-N1-C6	-2.72	120.19	125.11
11	B	507	RYK	C6-N1-C12	2.65	126.01	117.24
8	D	501	GDP	C4-C5-N7	-2.64	106.48	110.67
5	A	501	GTP	C8-N7-C5	2.61	108.90	104.26
5	C	501	GTP	C8-N7-C5	2.59	108.87	104.26
5	C	501	GTP	C2-N1-C6	-2.56	120.47	125.11
11	B	507	RYK	O50-C12-N49	-2.49	116.91	123.35
8	B	501	GDP	O6-C6-C5	-2.47	120.01	126.53
5	A	501	GTP	C5-C6-N1	2.42	119.42	113.25
8	B	501	GDP	C4-C5-N7	-2.38	106.90	110.67
5	C	501	GTP	C5-C6-N1	2.38	119.31	113.25
13	F	401	ACP	PB-O3A-PA	-2.32	124.79	132.37
9	B	504	MES	O1S-S-C8	2.29	110.19	106.73
5	C	501	GTP	O2B-PB-O3A	2.25	113.37	107.27
11	B	507	RYK	C8-C9-C10	-2.17	115.62	119.91
5	A	501	GTP	O6-C6-C5	-2.16	120.84	126.53
13	F	401	ACP	C6-C5-N7	2.15	136.24	132.09
13	F	401	ACP	N9-C8-N7	-2.14	110.90	113.94
5	C	501	GTP	O6-C6-C5	-2.08	121.05	126.53
13	F	401	ACP	C2'-C1'-N9	-2.06	108.18	113.30
11	B	507	RYK	C7-C8-C9	2.06	114.89	111.34
9	B	504	MES	C6-C5-N4	-2.05	107.01	110.12
5	C	501	GTP	O2A-PA-O3A	2.04	112.79	107.27
8	B	501	GDP	C5-C6-N1	2.01	118.38	113.25
13	F	401	ACP	C3'-C2'-C1'	2.01	105.27	101.46

There are no chirality outliers.

All (34) 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

Continued on next page...

Continued from previous page...

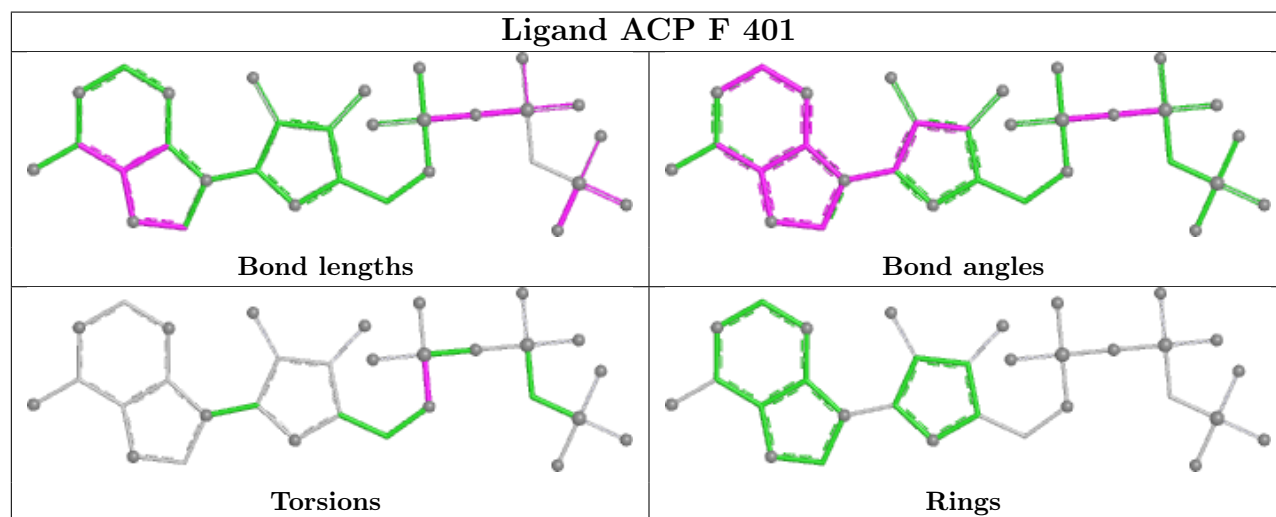
Mol	Chain	Res	Type	Atoms
5	C	501	GTP	PB-O3B-PG-O2G
5	C	501	GTP	PB-O3B-PG-O3G
5	C	501	GTP	C5'-O5'-PA-O3A
5	C	501	GTP	C5'-O5'-PA-O1A
5	C	501	GTP	C5'-O5'-PA-O2A
8	B	501	GDP	C5'-O5'-PA-O3A
8	B	501	GDP	C5'-O5'-PA-O1A
8	B	501	GDP	C5'-O5'-PA-O2A
8	D	501	GDP	C5'-O5'-PA-O3A
8	D	501	GDP	C5'-O5'-PA-O1A
8	D	501	GDP	C5'-O5'-PA-O2A
11	B	507	RYK	N1-C12-N49-C51
11	B	507	RYK	O50-C12-N49-C51
8	D	501	GDP	PA-O3A-PB-O1B
13	F	401	ACP	C5'-O5'-PA-O1A
13	F	401	ACP	C5'-O5'-PA-O2A
13	F	401	ACP	C5'-O5'-PA-O3A
5	C	501	GTP	PB-O3A-PA-O2A
11	B	507	RYK	C15-C16-O6-C48
5	A	501	GTP	PB-O3B-PG-O1G
5	A	501	GTP	PB-O3A-PA-O2A
5	C	501	GTP	C4'-C5'-O5'-PA
5	A	501	GTP	PB-O3B-PG-O2G
5	A	501	GTP	PB-O3B-PG-O3G
8	D	501	GDP	PA-O3A-PB-O2B
8	D	501	GDP	PA-O3A-PB-O3B
11	B	507	RYK	C3-C4-O3-C11
5	A	501	GTP	PB-O3A-PA-O1A
8	B	501	GDP	PB-O3A-PA-O1A
8	B	501	GDP	PB-O3A-PA-O2A
5	A	501	GTP	C4'-C5'-O5'-PA

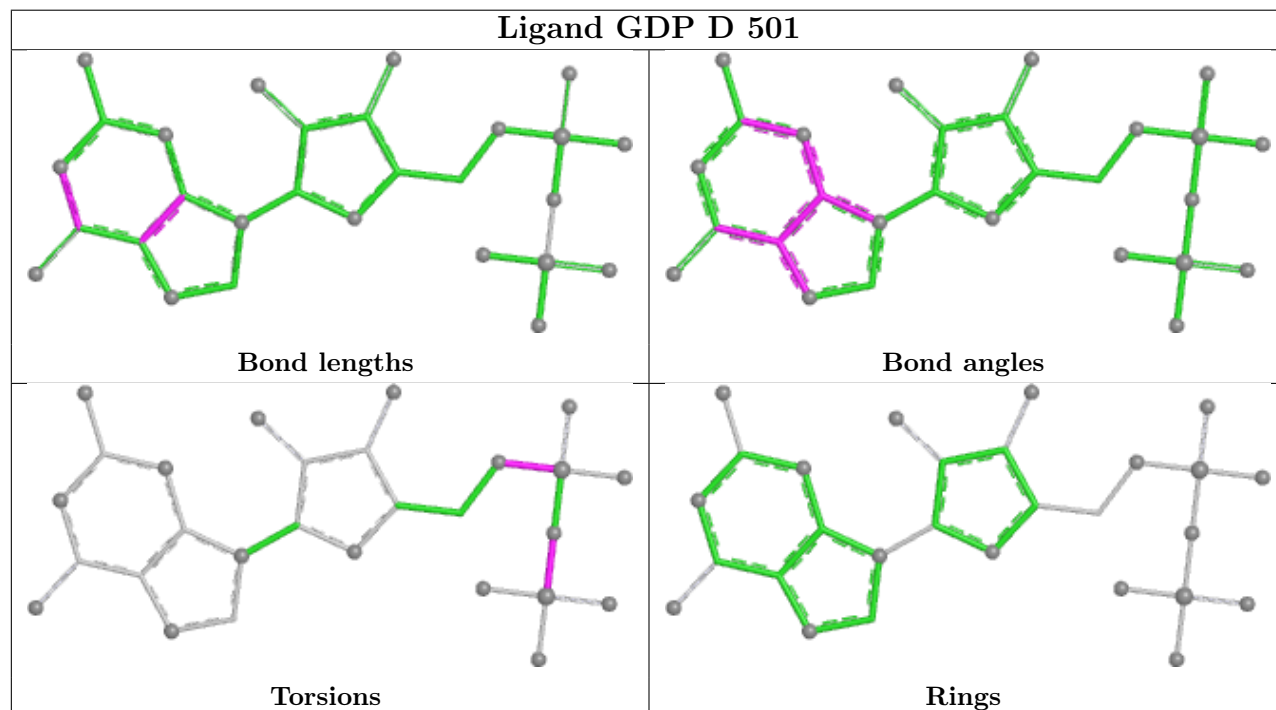
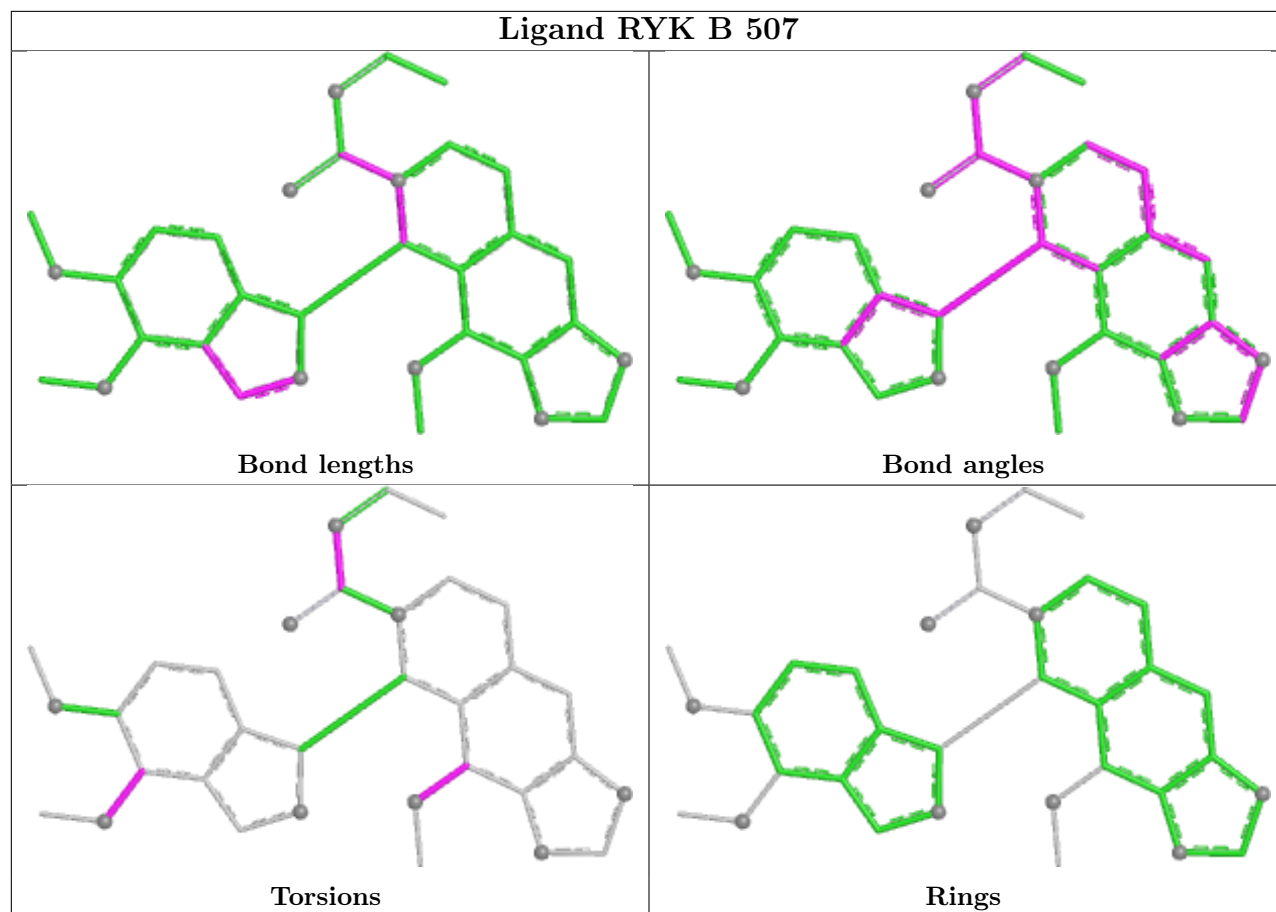
There are no ring outliers.

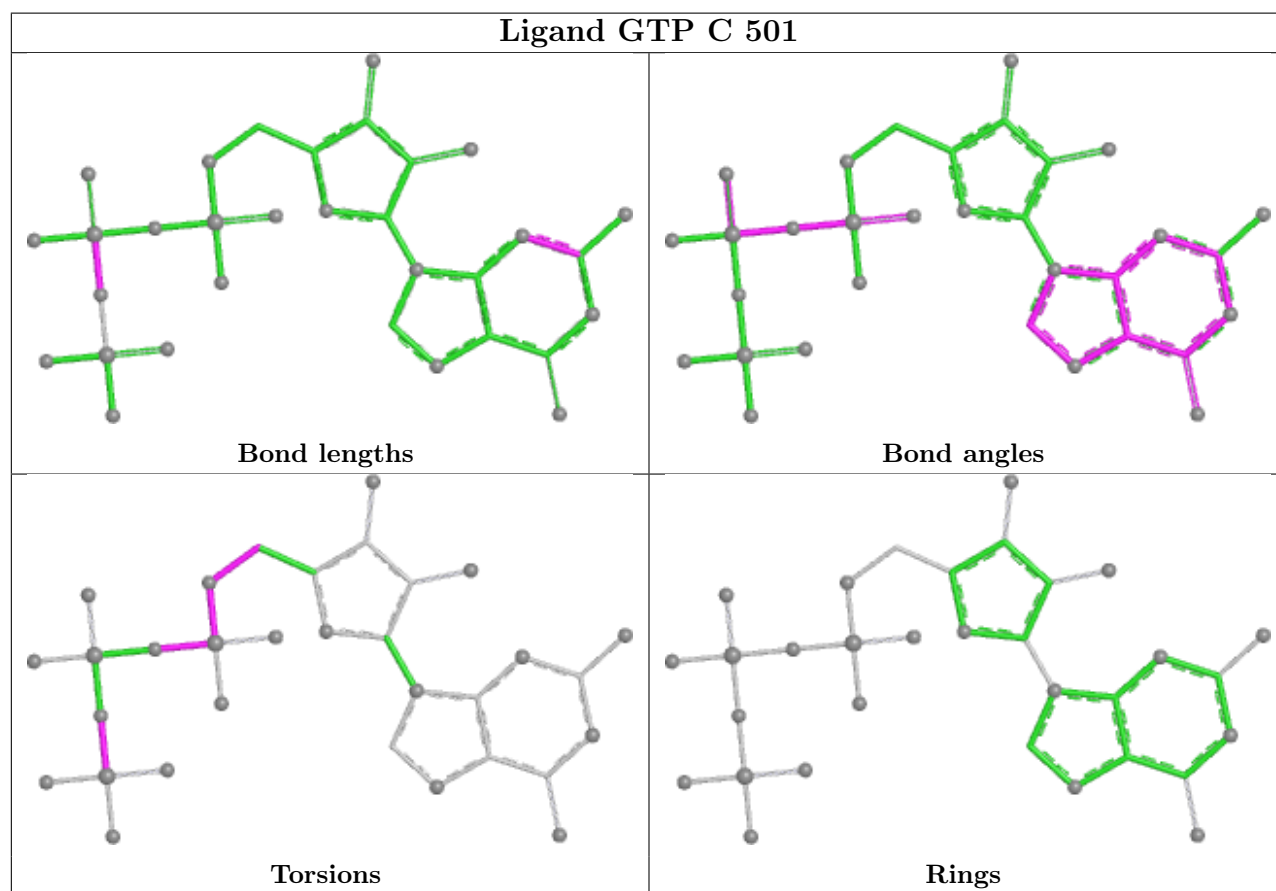
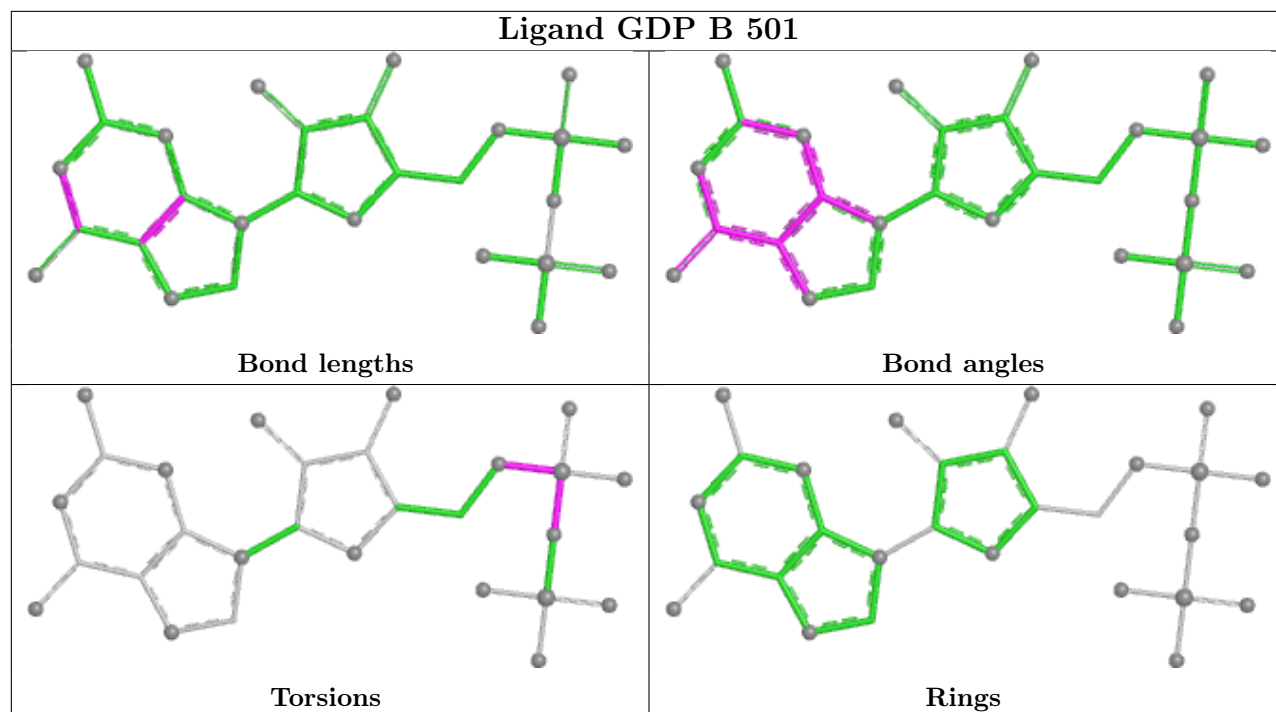
6 monomers are involved in 16 short contacts:

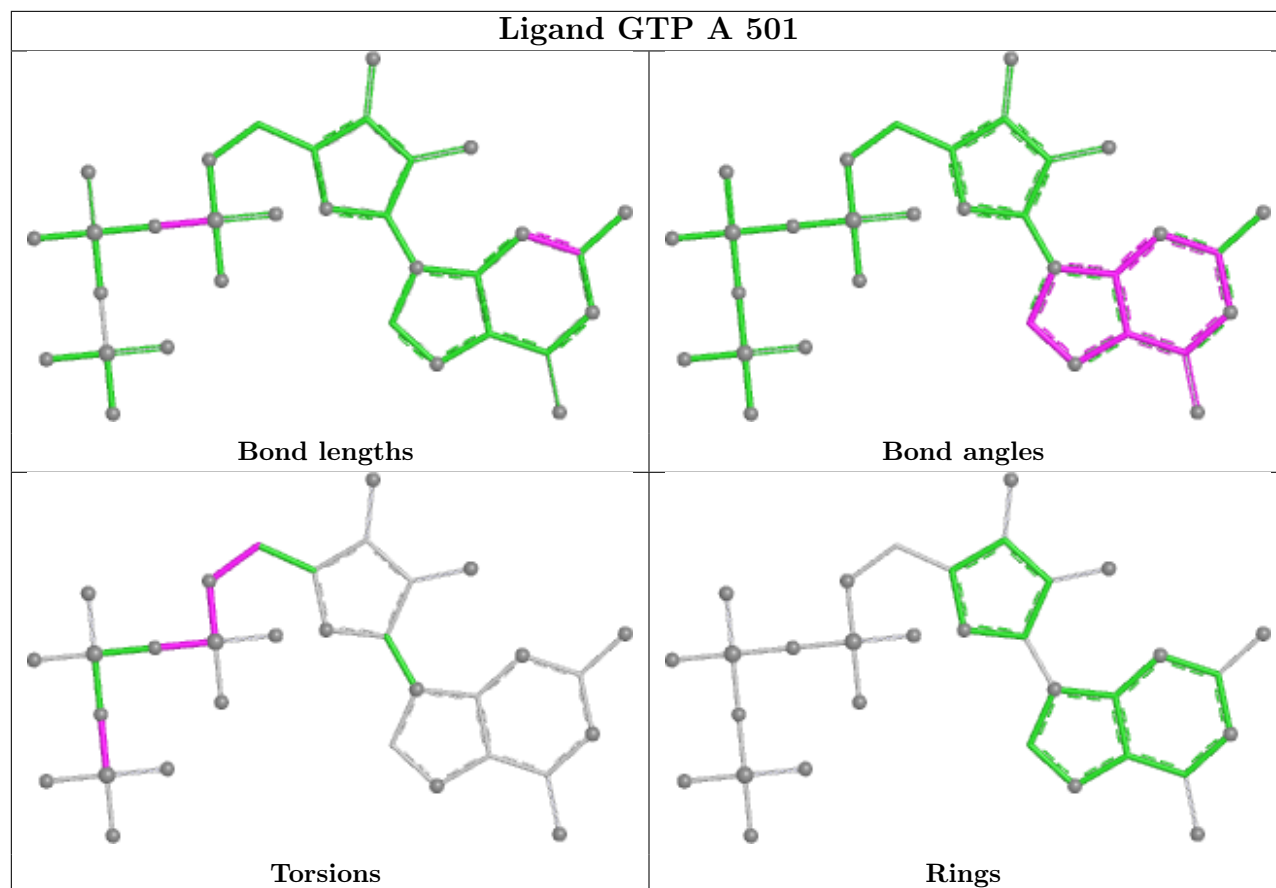
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	F	401	ACP	5	0
11	B	507	RYK	3	0
8	D	501	GDP	3	0
5	C	501	GTP	1	0
5	A	501	GTP	1	0
9	B	504	MES	3	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2		OWAB(Å ²)	Q < 0.9
1	A	438/451 (97%)	0.10	6 (1%)	73 71	28, 64, 97, 132	12 (2%)
1	C	440/451 (97%)	-0.19	5 (1%)	78 76	16, 50, 74, 124	8 (1%)
2	B	423/445 (95%)	0.07	11 (2%)	57 54	22, 59, 95, 133	11 (2%)
2	D	426/445 (95%)	0.29	14 (3%)	49 46	30, 74, 112, 131	7 (1%)
3	E	124/143 (86%)	0.60	8 (6%)	25 22	30, 78, 122, 148	4 (3%)
4	F	348/384 (90%)	0.59	28 (8%)	18 16	31, 90, 151, 188	3 (0%)
All	All	2199/2319 (94%)	0.18	72 (3%)	49 46	16, 66, 122, 188	45 (2%)

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	F	155	ALA	5.8
3	E	101[A]	LEU	5.5
2	B	246	GLY	5.5
4	F	371	PRO	3.6
4	F	240	LEU	3.5
2	D	247	GLN	3.5
4	F	179	VAL	3.5
4	F	125	THR	3.4
2	D	1	MET	3.3
3	E	143	ALA	3.2
4	F	159	GLY	3.2
1	A	179	THR	3.2
1	A	178[A]	SER	3.1
4	F	167	SER	3.1
4	F	130	VAL	3.0
1	C	440	VAL	3.0
2	D	164[A]	ARG	3.0
2	B	1	MET	3.0
1	C	340	SER	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	D	279	GLY	2.9
4	F	161	LEU	2.9
4	F	103	THR	2.9
4	F	245	ILE	2.8
2	D	37	HIS	2.8
4	F	170	LEU	2.8
2	B	438	ALA	2.8
2	D	407	TRP	2.8
4	F	362	ALA	2.8
1	C	341	ILE	2.7
4	F	132	LEU	2.7
2	D	280	SER	2.6
3	E	28	SER	2.6
2	B	250	ALA	2.6
2	B	275	LEU	2.5
2	B	276	THR	2.5
1	A	282	TYR	2.5
4	F	241	THR	2.5
3	E	12[A]	ASN	2.5
3	E	45	PRO	2.5
2	D	276	THR	2.4
2	D	278	ARG	2.4
2	B	285	ALA	2.4
4	F	194	PRO	2.4
1	A	262	TYR	2.3
4	F	134	ALA	2.3
4	F	173	ILE	2.3
2	D	286	LEU	2.3
2	B	245	PRO	2.2
4	F	154	GLY	2.2
4	F	330	ILE	2.2
1	A	438	ASP	2.2
4	F	292[A]	ARG	2.2
3	E	115[A]	HIS	2.2
4	F	182	ILE	2.2
4	F	166	ALA	2.2
2	D	404	PHE	2.1
4	F	131	PHE	2.1
2	D	56	ALA	2.1
2	D	441	ASP	2.1
3	E	47	LEU	2.1
4	F	200	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	283	HIS	2.1
4	F	231	ALA	2.1
2	B	286	LEU	2.1
2	D	83	PHE	2.1
2	B	229	HIS	2.0
4	F	99	VAL	2.0
1	C	302[A]	MET	2.0
3	E	6	MET	2.0
1	C	80	THR	2.0
4	F	379	HIS	2.0
2	B	284	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
7	CA	B	503	1/1	0.51	0.18	138,138,138,138	0
12	IMD	C	504	5/5	0.61	0.20	81,93,109,112	0
11	RYK	B	507	33/33	0.79	0.26	50,66,77,84	33
10	GOL	B	506	6/6	0.83	0.17	67,81,96,96	0
7	CA	E	201	1/1	0.88	0.13	103,103,103,103	0
13	ACP	F	401	31/31	0.88	0.10	98,109,123,125	0
6	MG	F	402	1/1	0.91	0.07	91,91,91,91	0
8	GDP	D	501	28/28	0.92	0.11	63,72,83,98	0
9	MES	B	504	12/12	0.94	0.09	53,64,75,81	0
7	CA	B	505	1/1	0.97	0.04	100,100,100,100	0
6	MG	D	502	1/1	0.97	0.05	79,79,79,79	0
5	GTP	C	501	32/32	0.98	0.06	36,42,48,50	0

Continued on next page...

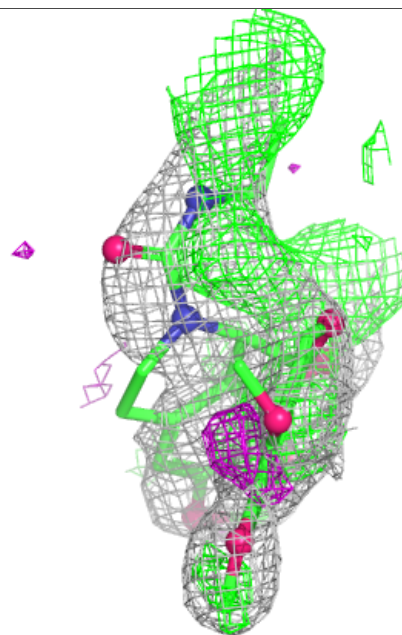
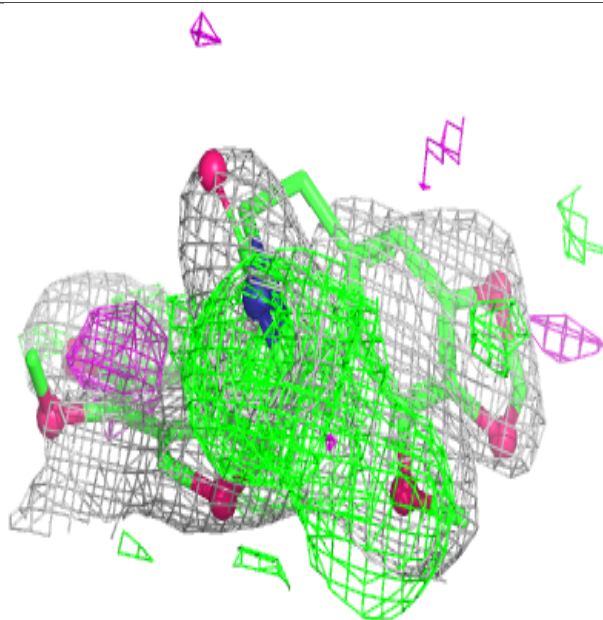
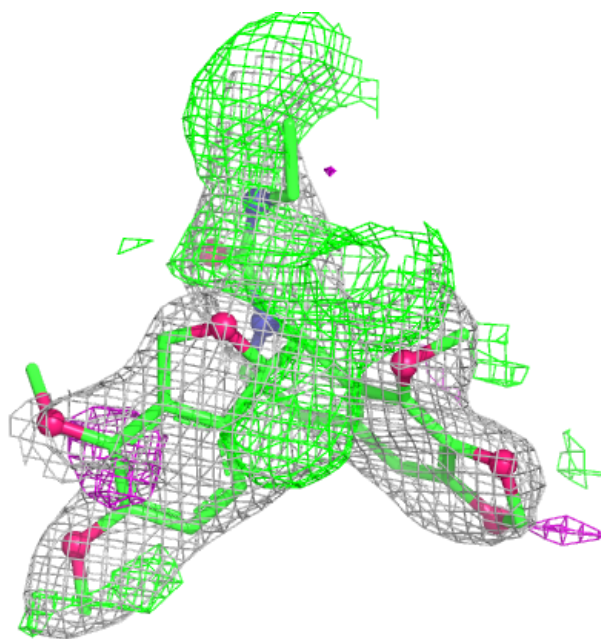
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	GTP	A	501	32/32	0.98	0.06	40,48,57,64	0
8	GDP	B	501	28/28	0.98	0.05	37,44,50,51	0
7	CA	A	503	1/1	0.99	0.03	79,79,79,79	0
6	MG	A	502	1/1	0.99	0.02	47,47,47,47	0
6	MG	C	502	1/1	0.99	0.04	42,42,42,42	0
7	CA	C	503	1/1	0.99	0.03	64,64,64,64	0
6	MG	B	502	1/1	1.00	0.08	35,35,35,35	0

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

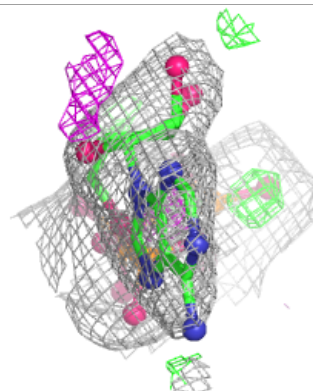
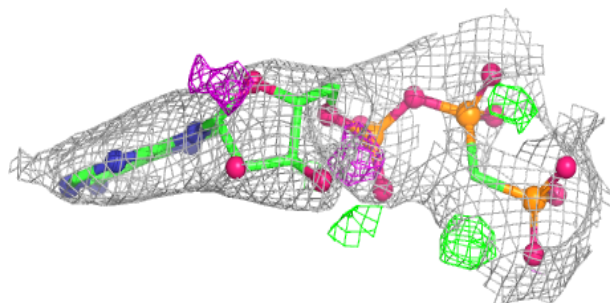
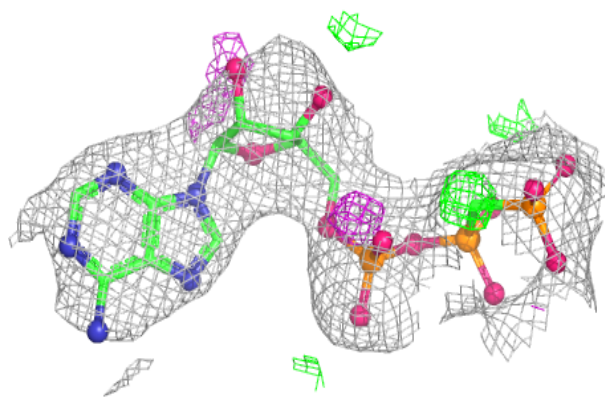
Electron density around RYK B 507:

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



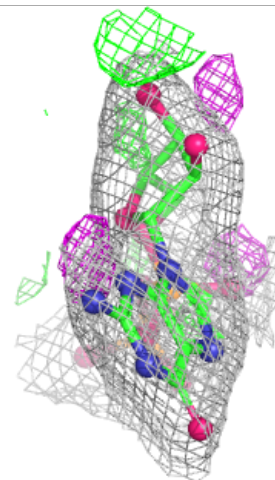
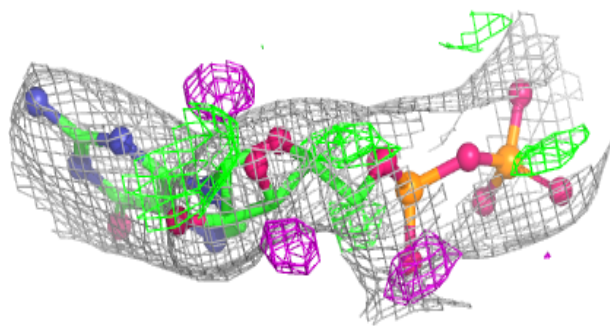
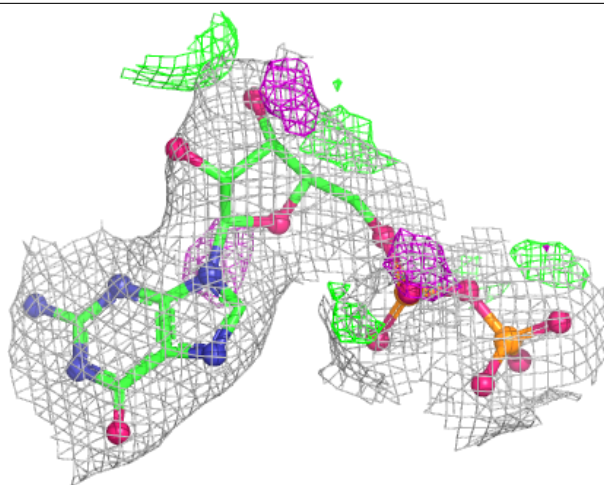
Electron density around ACP F 401:

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



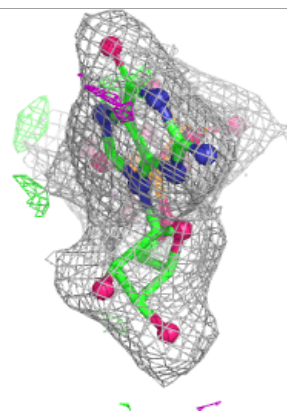
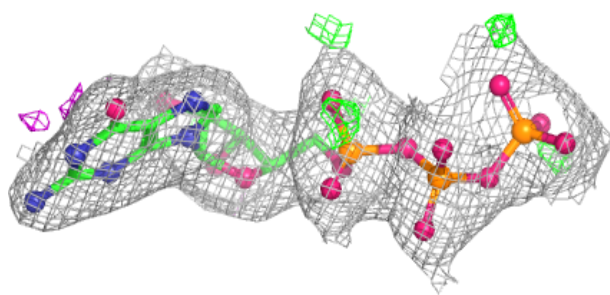
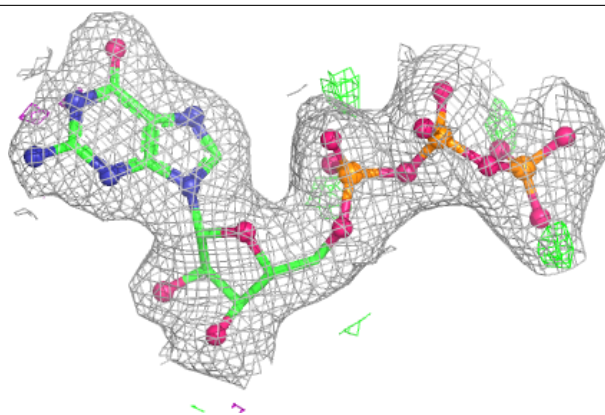
Electron density around GDP D 501:

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

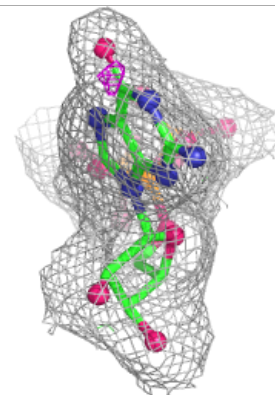
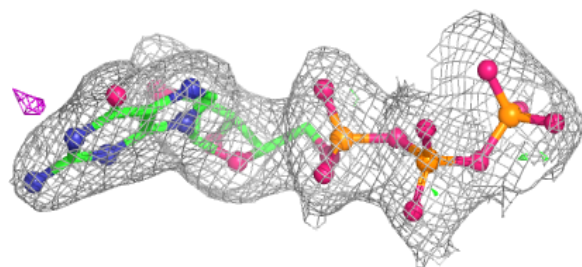
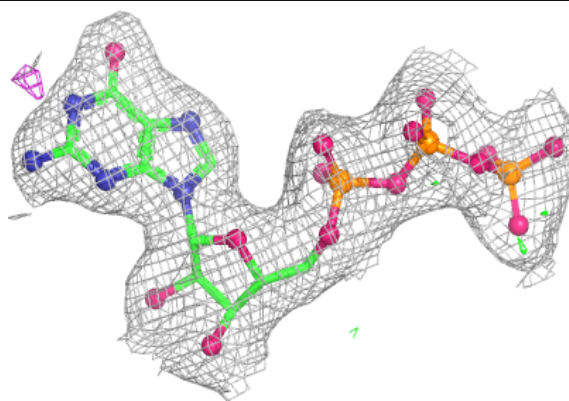


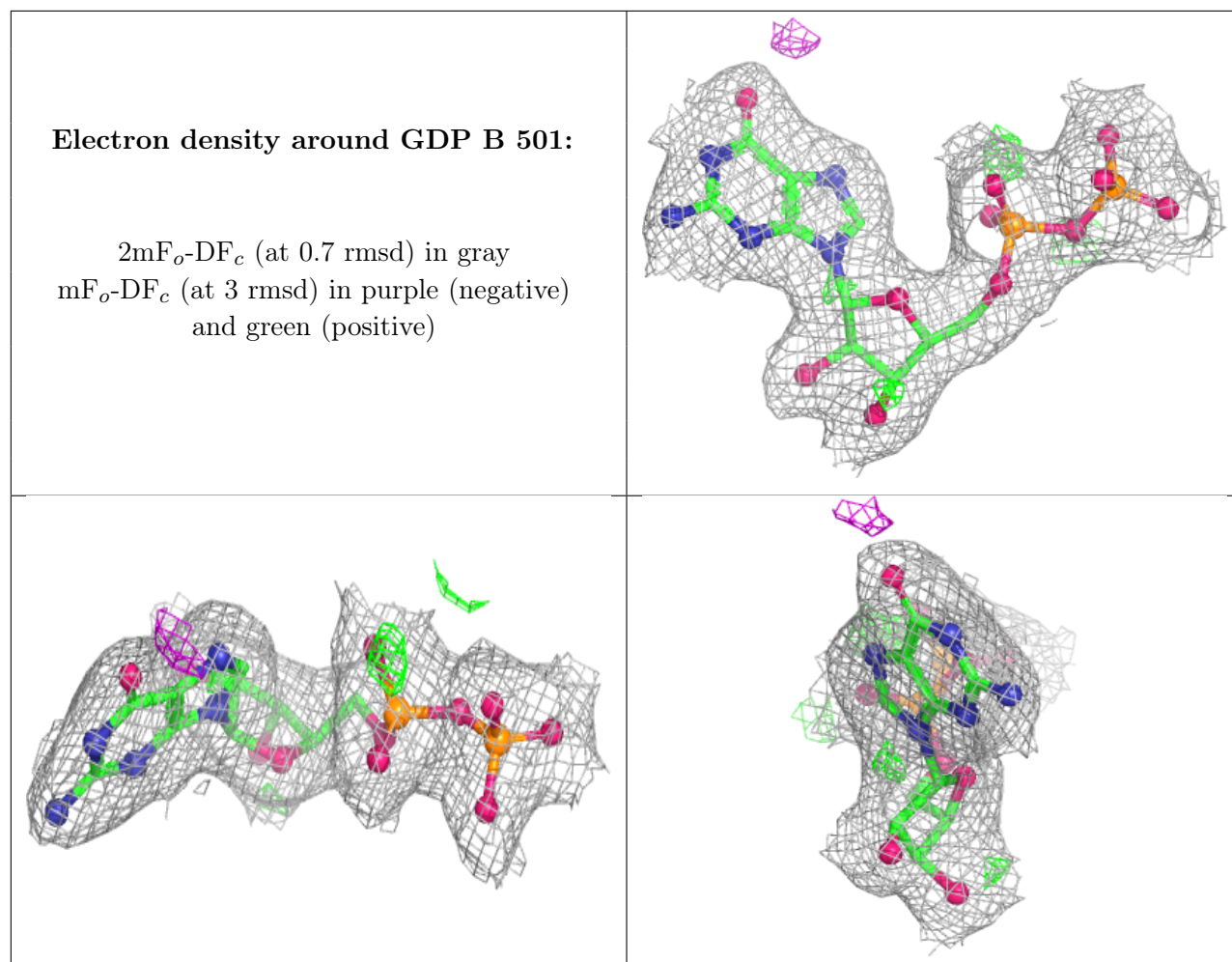
Electron density around GTP C 501:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.