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wwPDB X-ray Structure Validation Summary Report (i)

Aug 27, 2023 – 03:41 PM EDT

PDB ID	:	3ICE
Title	:	Rho transcription termination factor bound to RNA and ADP-BeF3
Authors	:	Thomsen, N.D.; Berger, J.M.
Deposited on	:	2009-07-17
Resolution	:	2.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

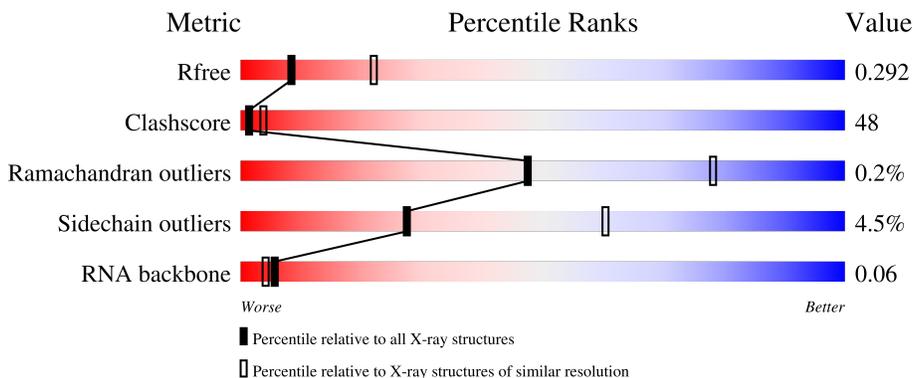|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 2.80 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	Percentile Ranks	Value
Rfree		0.292
Clashscore		48
Ramachandran outliers		0.2%
Sidechain outliers		4.5%
RNA backbone		0.06

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	422	35% 56% • 6%
1	B	422	44% 50% • •
1	C	422	39% 58% • •
1	D	422	41% 55% • •
1	E	422	37% 55% • •
1	F	422	29% 62% • 6%

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Mol	Chain	Length	Quality of chain
2	G	12	17%　　33%　　50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	SPD	E	504	-	-	X	-

2   Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 19558 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Transcription termination factor rho.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	398	Total	C	N	O	S	Se	0	0	0
			3133	1974	556	589	1	13			
1	B	408	Total	C	N	O	S	Se	0	1	0
			3214	2024	568	606	1	15			
1	C	413	Total	C	N	O	S	Se	0	0	0
			3251	2047	576	613	1	14			
1	D	410	Total	C	N	O	S	Se	0	1	0
			3230	2035	570	608	1	16			
1	E	407	Total	C	N	O	S	Se	0	0	0
			3202	2017	566	604	1	14			
1	F	396	Total	C	N	O	S	Se	0	1	0
			3111	1959	553	584	1	14			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MSE	-	expression tag	UNP P0AG30
A	-1	GLY	-	expression tag	UNP P0AG30
A	0	HIS	-	expression tag	UNP P0AG30
B	-2	MSE	-	expression tag	UNP P0AG30
B	-1	GLY	-	expression tag	UNP P0AG30
B	0	HIS	-	expression tag	UNP P0AG30
C	-2	MSE	-	expression tag	UNP P0AG30
C	-1	GLY	-	expression tag	UNP P0AG30
C	0	HIS	-	expression tag	UNP P0AG30
D	-2	MSE	-	expression tag	UNP P0AG30
D	-1	GLY	-	expression tag	UNP P0AG30
D	0	HIS	-	expression tag	UNP P0AG30
E	-2	MSE	-	expression tag	UNP P0AG30
E	-1	GLY	-	expression tag	UNP P0AG30
E	0	HIS	-	expression tag	UNP P0AG30
F	-2	MSE	-	expression tag	UNP P0AG30
F	-1	GLY	-	expression tag	UNP P0AG30

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Chain	Residue	Modelled	Actual	Comment	Reference
F	0	HIS	-	expression tag	UNP P0AG30

- Molecule 2 is a RNA chain called 5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP* U)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	P			
2	G	6	121	54	12	49	6	0	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
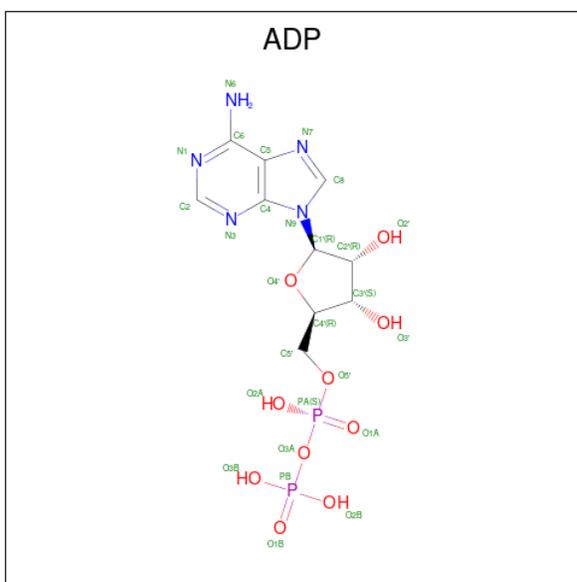
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	27	10	5	10	2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	F	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total 1	Mg 1	0	0
4	B	1	Total 1	Mg 1	0	0
4	C	1	Total 1	Mg 1	0	0
4	D	1	Total 1	Mg 1	0	0
4	E	1	Total 1	Mg 1	0	0
4	F	1	Total 1	Mg 1	0	0

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3).
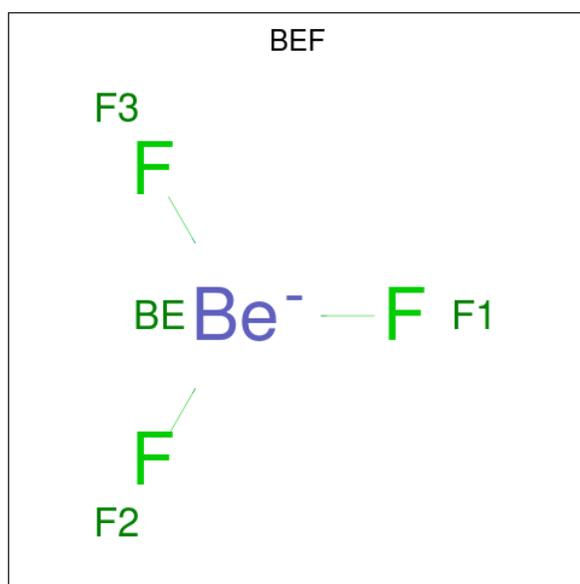
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 4	Be 1	F 3	0	0
5	B	1	Total 4	Be 1	F 3	0	0
5	C	1	Total 4	Be 1	F 3	0	0
5	D	1	Total 4	Be 1	F 3	0	0
5	E	1	Total 4	Be 1	F 3	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	F	1	Total 4	Be 1	F 3	0	0

- Molecule 6 is SPERMIDINE (three-letter code: SPD) (formula: $C_7H_{19}N_3$).

SPD
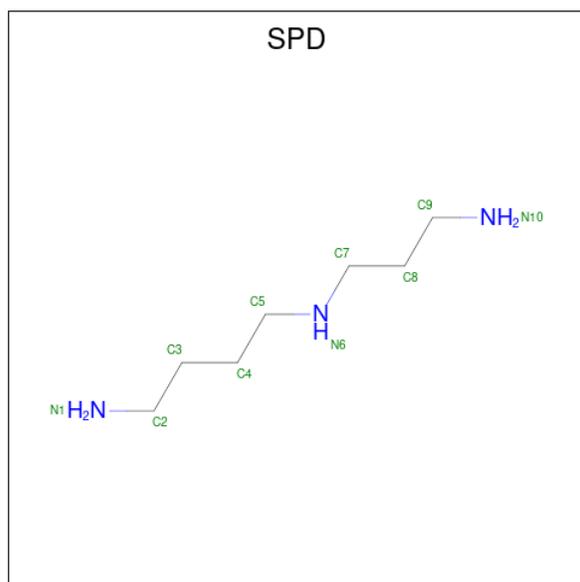
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	E	1	Total 10	C 7	N 3	0	0
6	G	1	Total 10	C 7	N 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	18	Total 18	O 18	0	0
7	B	19	Total 19	O 19	0	0
7	C	19	Total 19	O 19	0	0
7	D	13	Total 13	O 13	0	0
7	E	9	Total 9	O 9	0	0
7	F	4	Total 4	O 4	0	0

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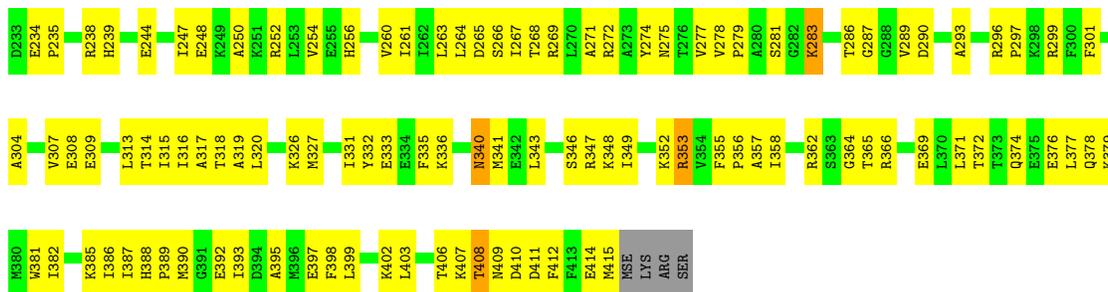| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	G	2	Total 2	O 2	0	0

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. 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. 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.

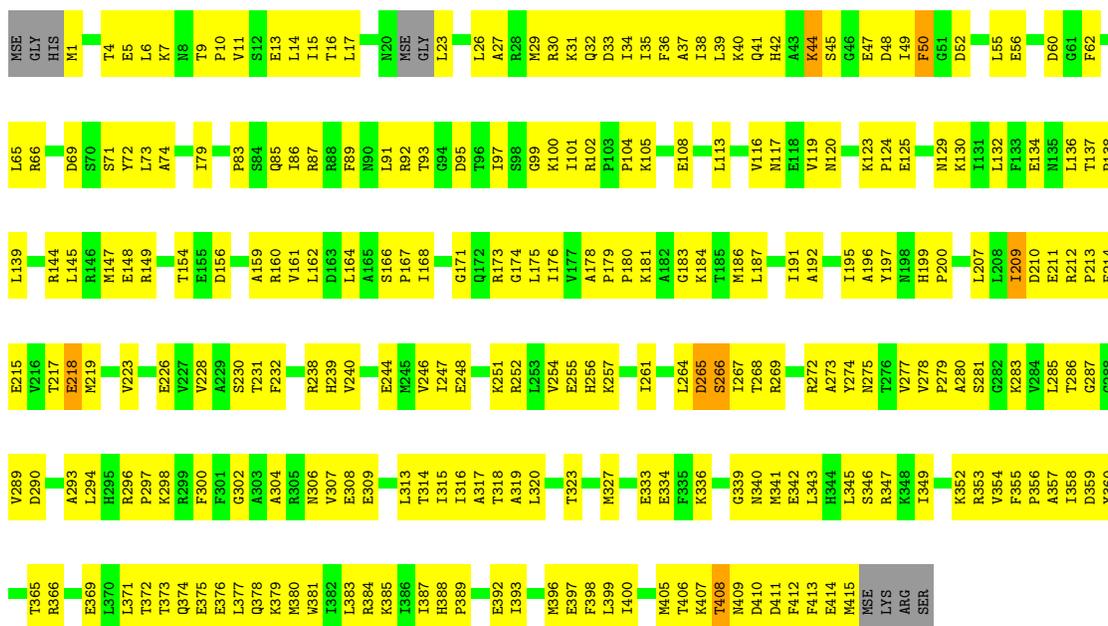- Molecule 1: Transcription termination factor rho

Chain A:

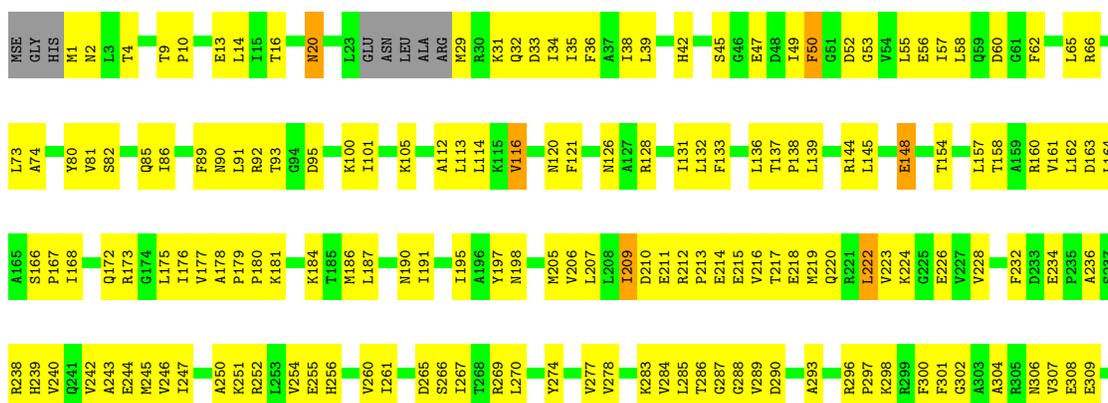
- Molecule 1: Transcription termination factor rho

Chain B:

• Molecule 1: Transcription termination factor rho

Chain C:

• Molecule 1: Transcription termination factor rho

Chain D:

L313 T314 I315 I316 A317 T318 A319 L320 I321 D322 G324 S325 K326 M327 D328 E329 V330 I331 Y332 E333 F335 T338 G339 N340 M341 E342 L343 H344 L345 S346 I349 K352 R353 V354 F355 P356 A357 I358 S363 G364 T365 R366 E369 L370 L371 T372 T373 Q374 E375 L377 Q378 K379

M380 W381 I382 I386 I387 H388 P389 M390 G391 E392 I393 D394 A395 M396 E397 F398 L399 I400 N401 K402 L403 A404 M405 T406 K407 T408 N409 D410 D411 F412 F413 E414 M415 MSE LYS ARG SER

• Molecule 1: Transcription termination factor rho

Chain E:

MSE GLY HIS M1 N2 L3 T4 E5 L6 V11 E19 N20 M21 GLY LEU GLU ASN LEU ALA ARG MSE R30 K31 Q32 D33 I34 I35 F36 A37 I38 L39 K40 Q41 H42 A43 K44 S45 G46 E47 D48 I49 F50 G53 V54 L55 E56 I57 L58 Q59 D60 G61 F62 G63 F64 L65 R66

S70 S71 Y72 L73 A74 G75 P76 I79 Y80 F89 N90 L91 R92 T93 T96 I97 S98 G99 K100 I101 R102 P103 P104 K105 E106 G107 E108 F111 A112 L113 L114 K115 V116 N117 E118 V119 N120 F121 D122 R128 L132 F133 E134 T137 P138 L139 H140 A141 N142 S143 R144 L145 R146

M147 T154 E155 D156 L157 T158 A159 R160 V161 L162 D163 L164 A165 S166 P167 I168 G169 R170 G171 Q172 R173 G174 L175 I176 V177 A178 P179 P180 K181 A182 G183 K184 T185 M186 L187 L188 Q189 N190 I191 A192 Q193 S194 I195 D201 M205 I209 D210 E211 R212 P213 E214 E215 V216 T217 E218 M219

Q220 R221 L222 V223 V227 S230 T231 F232 D233 E234 P235 A236 S237 R238 H239 V240 Q241 M245 V246 I247 E248 K249 A250 K251 R252 L253 V254 E255 H256 D259 V260 I261 I262 L263 L264 D265 S266 I267 T268 R269 L270 A271 R272 A273 Y274 N275 T276 V277 V278 K283 V284 L285 T286 G287 G288

V289 D290 A291 N292 A293 L294 H295 R296 P297 K298 R299 F300 F301 G302 A303 A304 R305 N306 V307 E308 L313 T314 I315 I316 A317 T318 A319 L320 I321 D322 T323 G324 S325 K326 M327 D328 E329 V330 I331 Y332 E333 E334 G339 N340 M341 E342 L343 H344 L345 S346 R347 K348 I349 A350 E351 K352 R353 V354

F355 P356 A357 I358 T365 R366 K367 L370 L371 E375 E376 K379 M380 W381 I382 L383 R384 K385 I386 I387 H388 P389 M390 G391 E392 I393 D394 A395 M396 E397 F398 L399 I400 N401 K402 L403 T406 K407 T408 N409 D410 D411 F412 M415 MSE LYS ARG SER

• Molecule 1: Transcription termination factor rho

Chain F:

MSE GLY HIS M1 N2 E5 L6 T9 P10 VAL SER GLU LEU ILE THR LEU GLY GLU ASN MSE GLY LEU GLU ASN LEU ALA ARG MSE R30 K31 Q32 D33 I34 I35 F36 A37 I38 L39 K40 Q41 H42 A43 K44 E47 D48 I49 F50 G53 V54 L55 E56 I57 L58 Q59 D60 G61

F62 G63 F64 L65 R66 D69 S70 S71 Y72 L73 A74 I79 Y80 V81 S82 P83 S84 Q85 I86 R87 R88 F89 N90 L91 R92 T93 G94 D95 T96 I97 S98 I101 R102 P103 P104 K105 E106 G107 E108 R109 Y110 F111 A112 L113 L114 E118 V119 N120 F121 D122 K123 P124 E125 R128

I131 L132 F133 L136 T137 P138 L139 H140 A141 N142 S143 R144 L145 R146 M147 E148 R149 G150 N151 G152 S153 T154 E155 D156 L157 T158 A159 R160 V161 L162 D163 S166 P167 I168 G169 R170 G171 Q172 R173 G174 L175 I176 V177 A178 P179 P180 K181 A182 G183 K184 T185 M186 L187 L188 Q189 N190 I191 A192

I195 A196 Y197 L204 M205 V206 L207 I208 I209 D210 E211 R212 P213 E214 E215 V216 M219 L222 V223 K224 G225 E226 V227 V228 A229 S230 T231 F232 D233 E234 P235 A236 S237 R238 H239 V242 A243 E244 M245 V246 I247 E248 K249 A250 K251 R252 L253 V254 E255 H256 K257 K258 I261 I262

L263 L264 D265 S266 I267 T268 R269 L270 A271 R272 A273 Y274 N275 T276 V277 V278 P279 A280 S281 G282 K283 G287 G288 V289 D290 A291 N292 A293 L294 H295 R296 P297 K298 R299 F300 F301 A304 V307 E308 E309 T314 I315 I316 A317 T318 A319 L320 T323 G324 S325 K326 M327 D328 E329 V330

I331 Y332 E333 E334 F335 K336 G337 N340 M341 H344 L345 S346 R347 K348 I349 K352 R353 V354 F355 P356 A357 I358 D359 Y360 T365 R366 K367 E368 E369 L370 L371 Q374 E375 L377 Q378 K379 M380 W381 I382 L383 R384 K385 I386 I387 H388 P389 M390 I393 F398 L399 I400 N401

K402 L403 A404 M405 T406 K407 T408 N409 D410 D411 F412 F413 E414 M415 MSE LYS ARG SER

• Molecule 2: 5'-R(P*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*UP*U)-3'

Chain G: 17%   33%   50%

U1 U2 U3 U4 U5 U6 U U U U U U

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	69.23Å 127.03Å 127.17Å 60.48° 90.26° 89.77°	Depositor
Resolution (Å)	41.88 – 2.80 41.88 – 2.80	Depositor EDS
% Data completeness (in resolution range)	94.7 (41.88-2.80) 91.6 (41.88-2.80)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.86 (at 2.81Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.270 , 0.295 0.264 , 0.292	Depositor DCC
R_{free} test set	4440 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å^2)	49.8	Xtriage
Anisotropy	0.628	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 5.3	EDS
L-test for twinning[2]	$< |L| > = 0.30$, $< L^2 > = 0.13$	Xtriage
Estimated twinning fraction	0.389 for h,k-l,k 0.389 for h,l,-k+l 0.336 for h,-l,k-l 0.336 for h,-k+l,-k 0.317 for h,-k,-l 0.210 for -h,k,k-l 0.208 for -h,-k+l,l 0.208 for -h,-l,-k 0.216 for -h,l,k 0.208 for -h,-k,-k+l 0.208 for -h,k-l,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	19558	wwPDB-VP
Average B, all atoms (Å^2)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.14% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: MG, ADP, SPD, BEF

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	0.66	0/3169	0.54	0/4249
1	B	0.66	0/3248	0.52	0/4351
1	C	0.67	0/3286	0.52	0/4405
1	D	0.66	0/3264	0.52	0/4372
1	E	0.63	0/3237	0.53	0/4339
1	F	0.60	0/3149	0.55	0/4220
2	G	0.66	0/132	0.83	0/200
All	All	0.65	0/19485	0.53	0/26136

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	3133	0	3201	331	0
1	B	3214	0	3283	251	0
1	C	3251	0	3323	257	0
1	D	3230	0	3303	291	0
1	E	3202	0	3271	356	0
1	F	3111	0	3154	427	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	G	121	0	61	43	0
3	A	27	0	12	3	0
3	B	27	0	12	2	0
3	C	27	0	12	4	0
3	D	27	0	12	4	0
3	E	27	0	12	5	0
3	F	27	0	12	8	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
5	C	4	0	0	0	0
5	D	4	0	0	0	0
5	E	4	0	0	1	0
5	F	4	0	0	1	0
6	E	10	0	19	32	0
6	G	10	0	19	5	0
7	A	18	0	0	1	0
7	B	19	0	0	3	0
7	C	19	0	0	1	0
7	D	13	0	0	1	0
7	E	9	0	0	2	0
7	F	4	0	0	0	0
7	G	2	0	0	0	0
All	All	19558	0	19706	1871	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 48.

The worst 5 of 1871 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:1:U:C2'	2:G:2:U:H5'	1.52	1.36
1:D:178:ALA:HB3	1:D:184:LYS:CD	1.57	1.33
1:E:241:GLN:NE2	6:E:504:SPD:H71	1.42	1.33
1:D:407:LYS:NZ	1:D:409:ASN:HB3	1.53	1.23
1:A:120:ASN:HB2	1:A:256:HIS:CE1	1.76	1.19

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	394/422 (93%)	351 (89%)	42 (11%)	1 (0%)	41	72
1	B	404/422 (96%)	388 (96%)	15 (4%)	1 (0%)	47	78
1	C	409/422 (97%)	385 (94%)	23 (6%)	1 (0%)	47	78
1	D	406/422 (96%)	366 (90%)	39 (10%)	1 (0%)	47	78
1	E	403/422 (96%)	384 (95%)	19 (5%)	0	100	100
1	F	392/422 (93%)	375 (96%)	17 (4%)	0	100	100
All	All	2408/2532 (95%)	2249 (93%)	155 (6%)	4 (0%)	47	78

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	414	GLU
1	A	322	ASP
1	B	218	GLU
1	C	231	THR

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	341/344 (99%)	326 (96%)	15 (4%)	28	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	350/344 (102%)	338 (97%)	12 (3%)	37	71
1	C	354/344 (103%)	341 (96%)	13 (4%)	34	68
1	D	352/344 (102%)	336 (96%)	16 (4%)	27	60
1	E	349/344 (102%)	329 (94%)	20 (6%)	20	50
1	F	334/344 (97%)	317 (95%)	17 (5%)	24	55
All	All	2080/2064 (101%)	1987 (96%)	93 (4%)	27	60

5 of 93 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	32	GLN
1	E	323	THR
1	E	38	ILE
1	E	106	GLU
1	E	398	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	59	GLN
1	C	388	HIS
1	F	189	GLN
1	E	239	HIS
1	F	90	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	G	5/12 (41%)	4 (80%)	0

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	G	2	U
2	G	3	U
2	G	5	U
2	G	6	U

There are no RNA pucker outliers to report.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 20 ligands modelled in this entry, 6 are monoatomic - leaving 14 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	$\#|Z| > 2$
5	BEF	A	1002	3	0,3,3	-	-	-		
5	BEF	E	503	3	0,3,3	-	-	-		
5	BEF	D	1002	3	0,3,3	-	-	-		
3	ADP	B	1000	4,5	24,29,29	1.01	2 (8%)	29,45,45	1.44	6 (20%)
3	ADP	F	1000	4,5	24,29,29	1.03	2 (8%)	29,45,45	1.66	9 (31%)
5	BEF	C	1002	3	0,3,3	-	-	-		
3	ADP	D	1000	4,5	24,29,29	0.99	1 (4%)	29,45,45	1.44	4 (13%)
6	SPD	E	504	-	9,9,9	0.61	0	8,8,8	0.77	0
3	ADP	A	1000	4,5	24,29,29	0.99	1 (4%)	29,45,45	1.43	5 (17%)
5	BEF	B	1002	3	0,3,3	-	-	-		
3	ADP	E	501	4,5	24,29,29	1.01	2 (8%)	29,45,45	1.47	5 (17%)
3	ADP	C	1000	4,5	24,29,29	1.12	3 (12%)	29,45,45	1.34	4 (13%)
6	SPD	G	101	-	9,9,9	0.61	0	8,8,8	0.52	0
5	BEF	F	1002	3	0,3,3	-	-	-		

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
3	ADP	B	1000	4,5	-	3/12/32/32	0/3/3/3
3	ADP	F	1000	4,5	-	6/12/32/32	0/3/3/3
3	ADP	D	1000	4,5	-	0/12/32/32	0/3/3/3
6	SPD	E	504	-	-	5/7/7/7	-
3	ADP	A	1000	4,5	-	2/12/32/32	0/3/3/3
3	ADP	E	501	4,5	-	0/12/32/32	0/3/3/3
3	ADP	C	1000	4,5	-	4/12/32/32	0/3/3/3
6	SPD	G	101	-	-	3/7/7/7	-

The worst 5 of 11 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	1000	ADP	C5-C4	2.52	1.47	1.40
3	E	501	ADP	C5-C4	2.48	1.47	1.40
3	F	1000	ADP	O4'-C1'	2.44	1.44	1.41
3	F	1000	ADP	C5-C4	2.42	1.47	1.40
3	B	1000	ADP	C5-C4	2.35	1.47	1.40

The worst 5 of 33 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1000	ADP	N3-C2-N1	-3.71	122.89	128.68
3	D	1000	ADP	N3-C2-N1	-3.68	122.93	128.68
3	E	501	ADP	N3-C2-N1	-3.67	122.94	128.68
3	F	1000	ADP	N3-C2-N1	-3.66	122.96	128.68
3	A	1000	ADP	N3-C2-N1	-3.66	122.96	128.68

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1000	ADP	PA-O3A-PB-O3B
3	C	1000	ADP	O4'-C4'-C5'-O5'
3	F	1000	ADP	C5'-O5'-PA-O1A
3	F	1000	ADP	C5'-O5'-PA-O2A
6	G	101	SPD	C3-C4-C5-N6

There are no ring outliers.

10 monomers are involved in 64 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	503	BEF	1	0
3	B	1000	ADP	2	0
3	F	1000	ADP	8	0
3	D	1000	ADP	4	0
6	E	504	SPD	32	0
3	A	1000	ADP	3	0
3	E	501	ADP	5	0
3	C	1000	ADP	4	0
6	G	101	SPD	5	0
5	F	1002	BEF	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 ADP B 1000

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP F 1000

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP D 1000

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP A 1000

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP E 501

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP C 1000

Bond lengths

Bond angles

Torsions

Rings
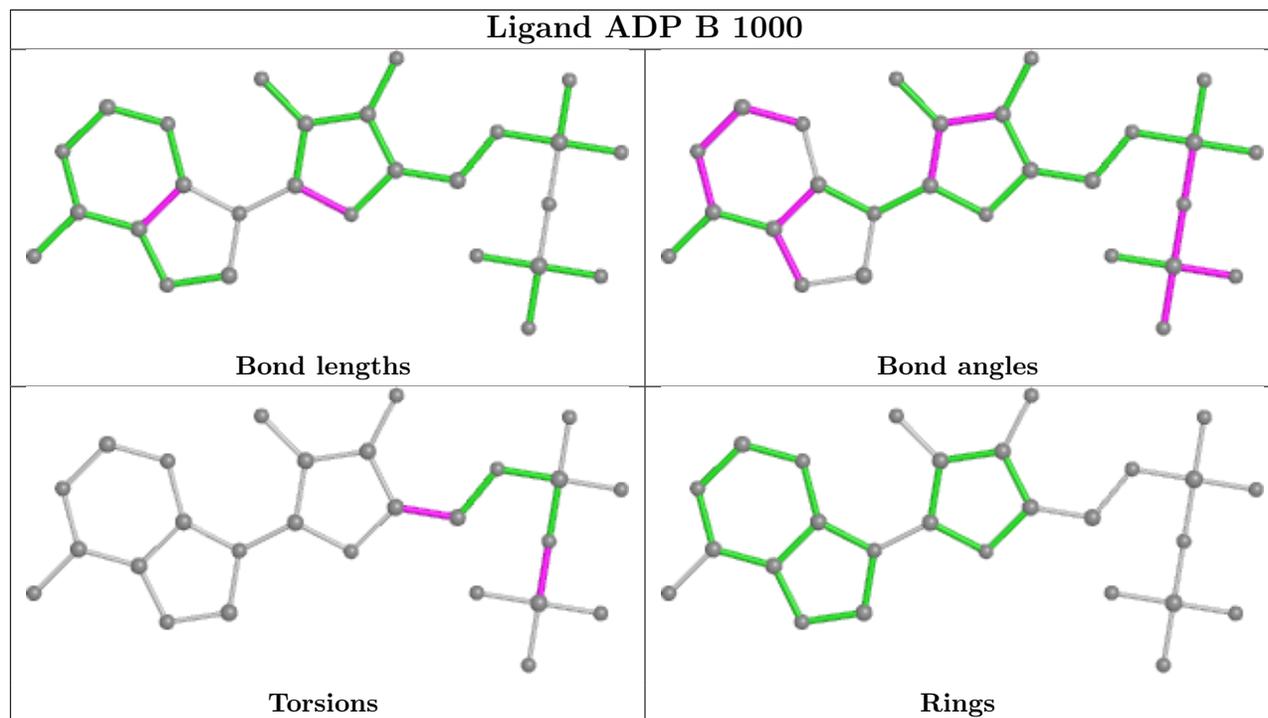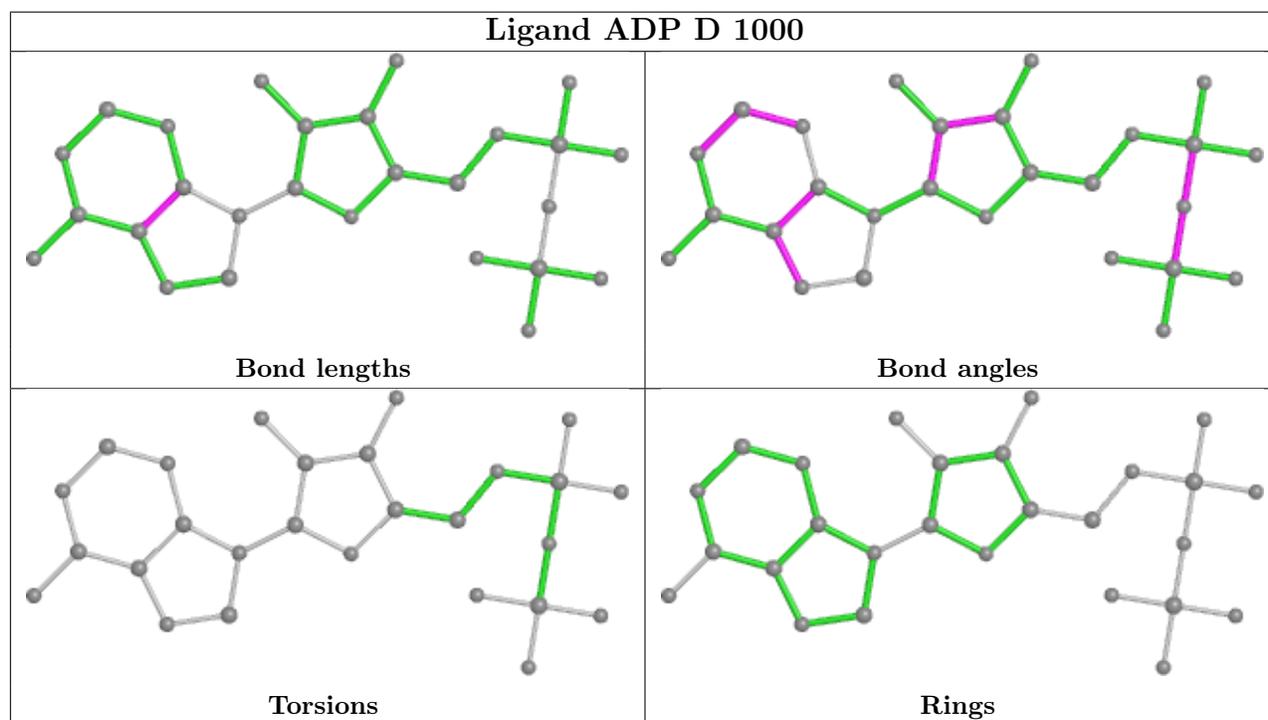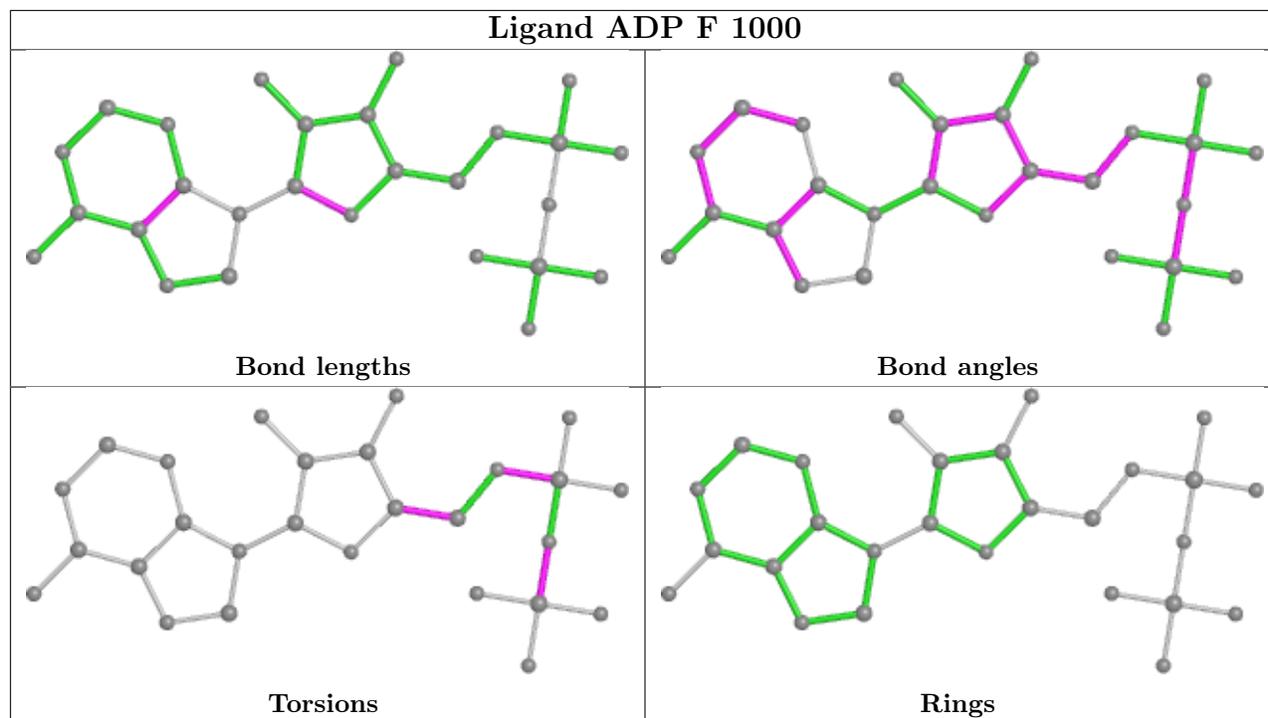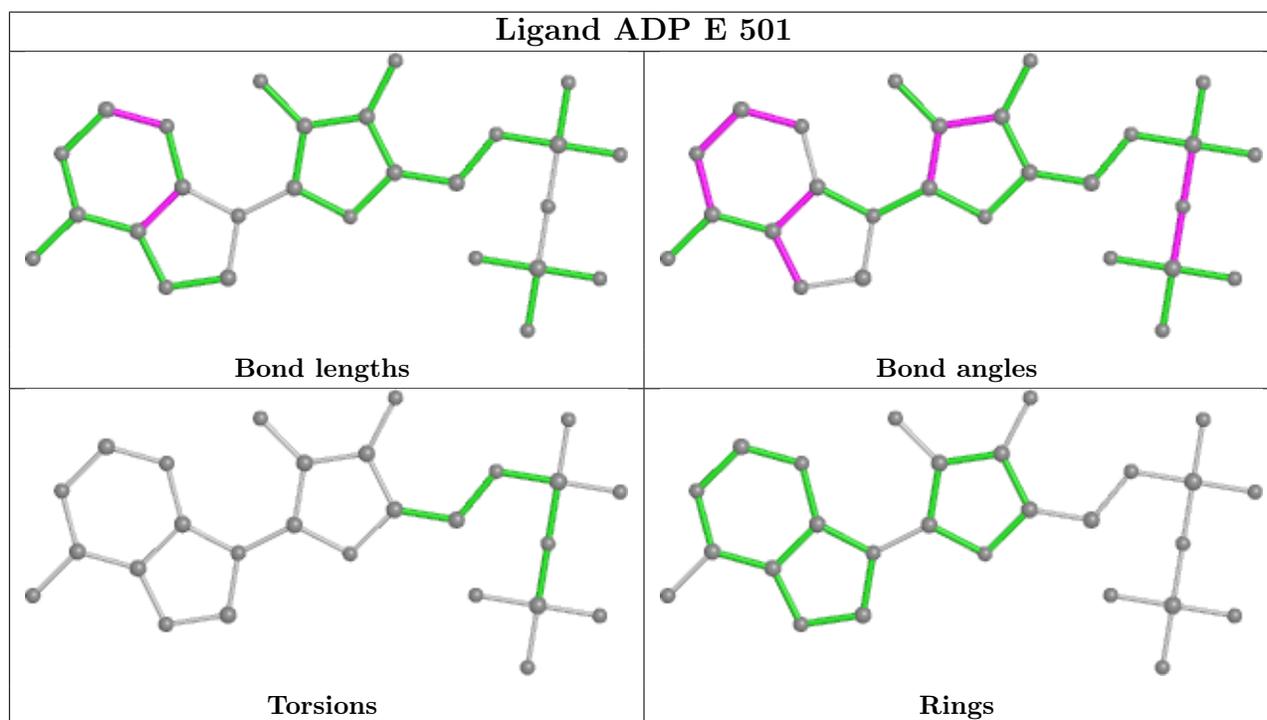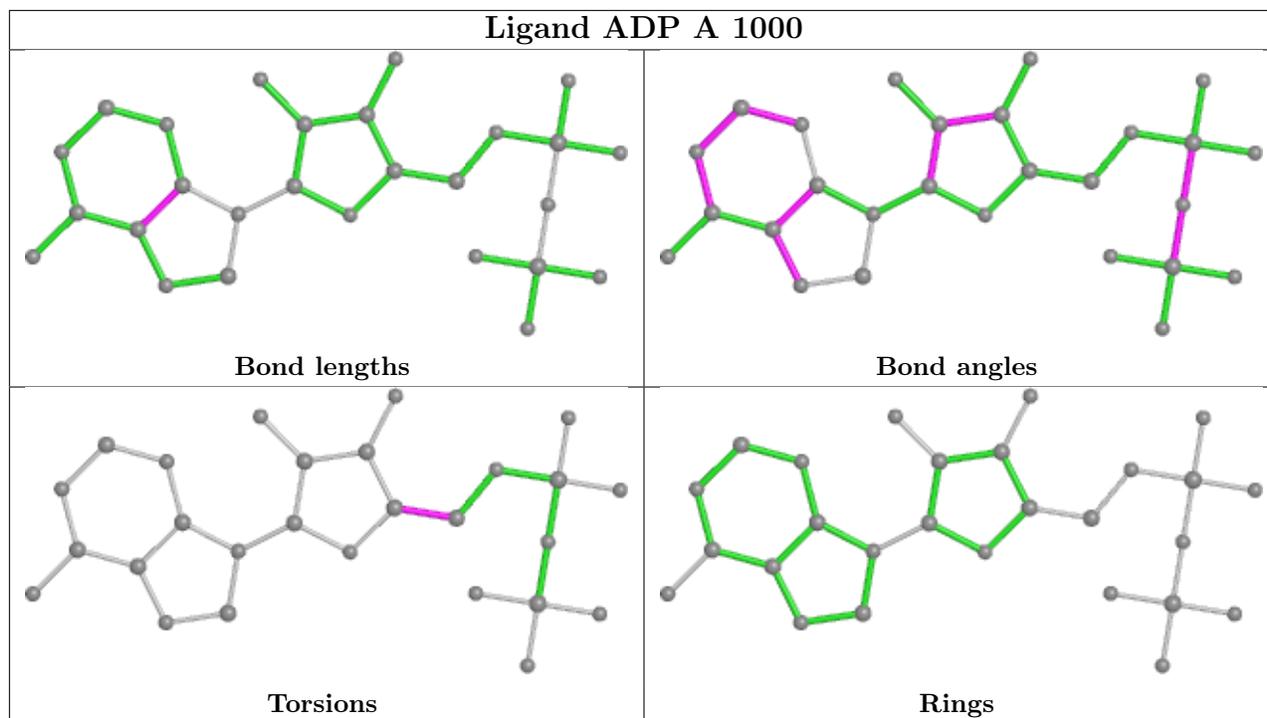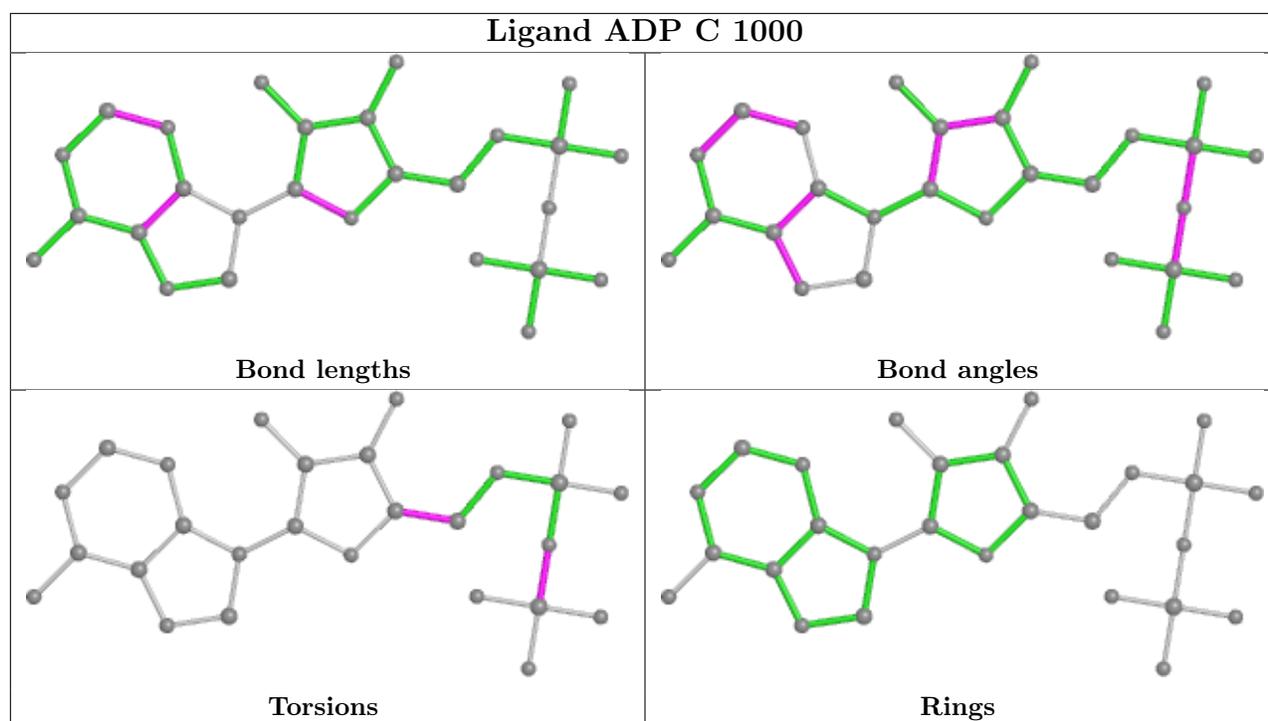
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6   Fit of model and data ⓘ

6.1   Protein, DNA and RNA chains ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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

Unable to reproduce the depositors R factor - this section is therefore empty.

6.3   Carbohydrates ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

6.4   Ligands ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.

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.
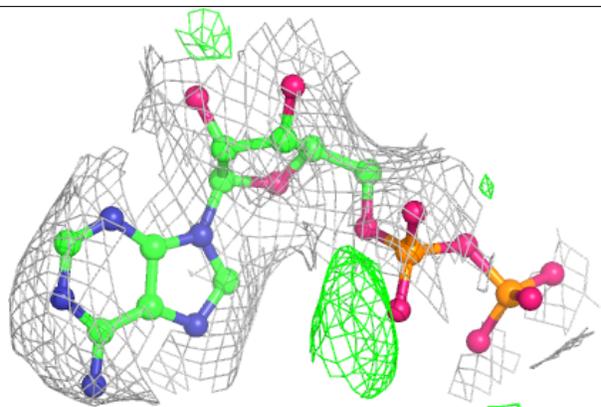
Electron density around ADP A 1000:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
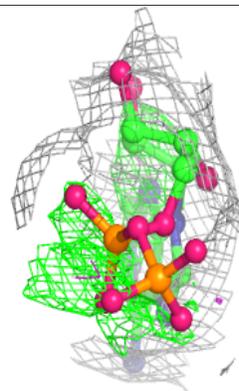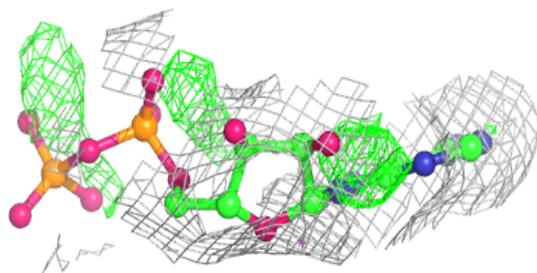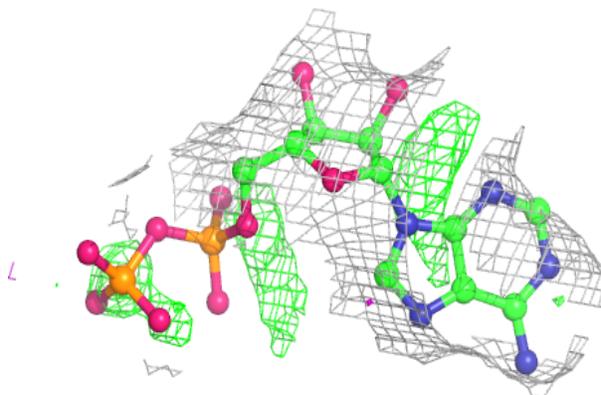mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
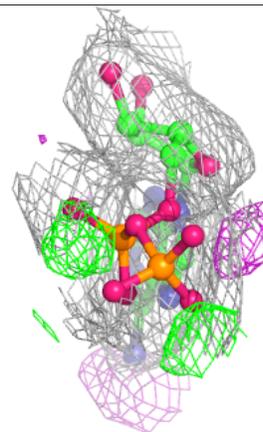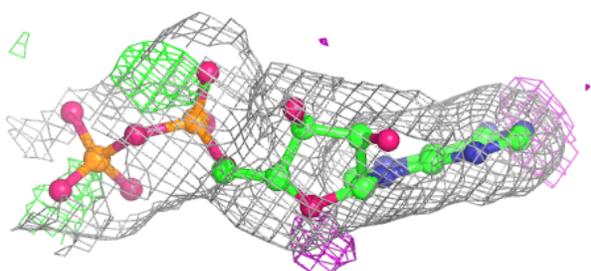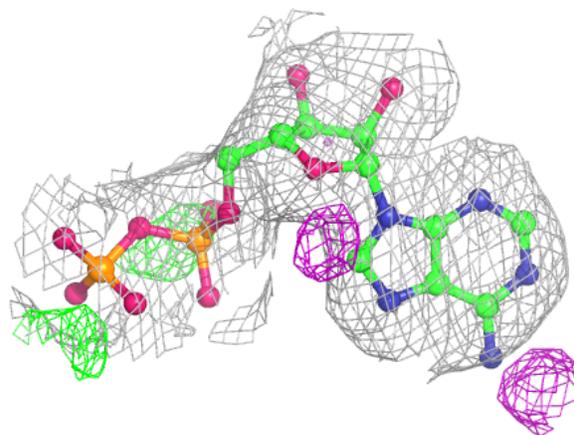
Electron density around ADP B 1000:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
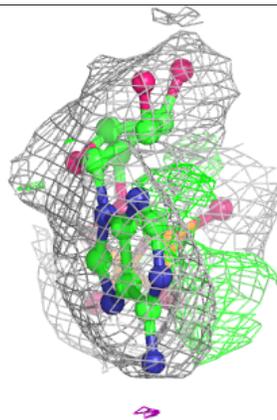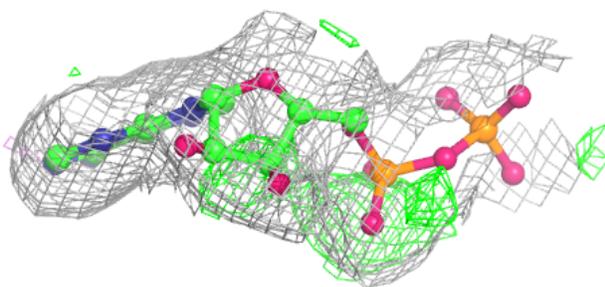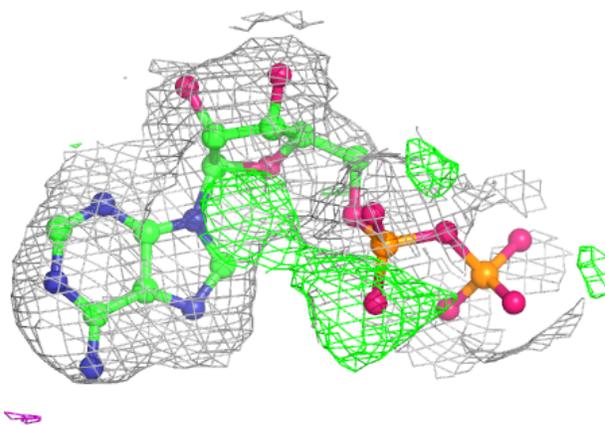
Electron density around ADP C 1000:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
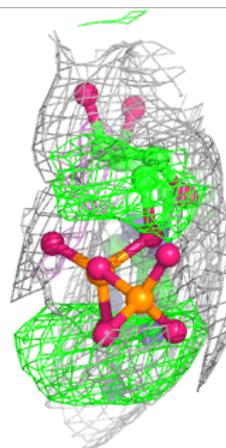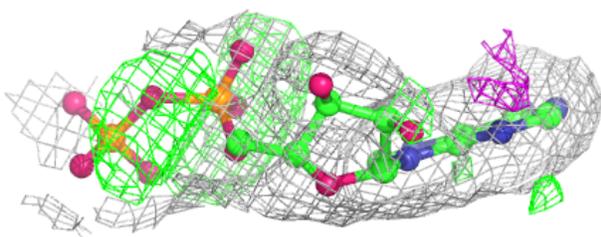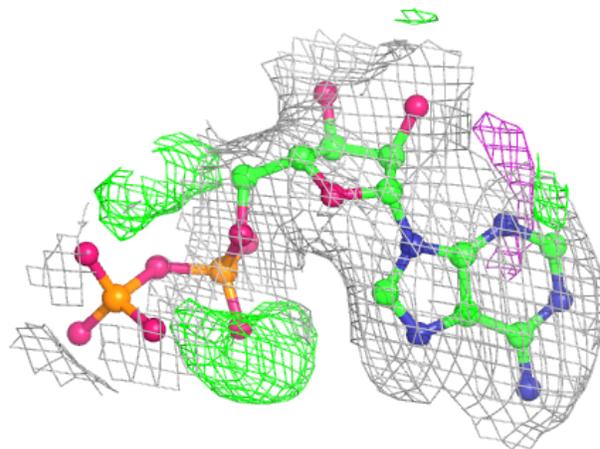
Electron density around ADP D 1000:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
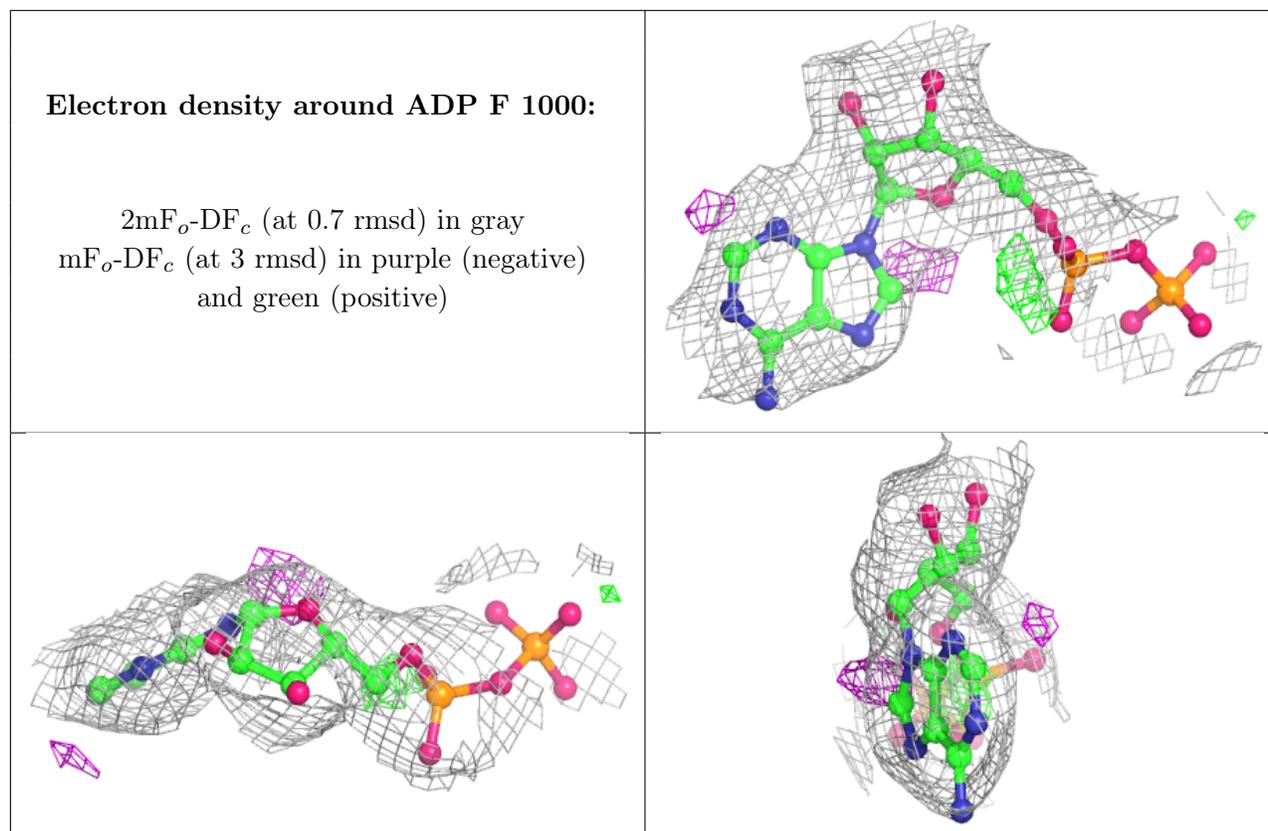and green (positive)
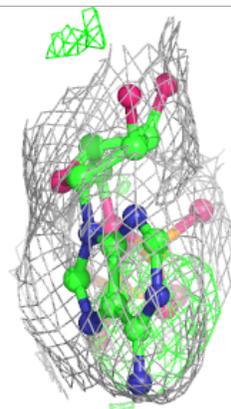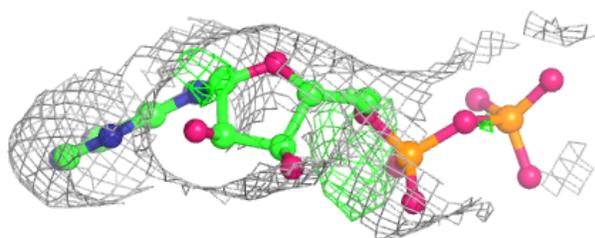
Electron density around ADP E 501:

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

Electron density around ADP F 1000:

$2mF_o$-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 ⓘ

Unable to reproduce the depositors R factor - this section is therefore empty.