wwPDB X-ray Structure Validation Summary Report (i)

Oct 25, 2023 – 03:44 AM EDT

PDB ID	:	3EX7
Title	:	The crystal structure of EJC in its transition state
Authors	:	Andersen, G.R.; Nielsen, K.H.
Deposited on	:	2008-10-16
Resolution	:	2.30 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:

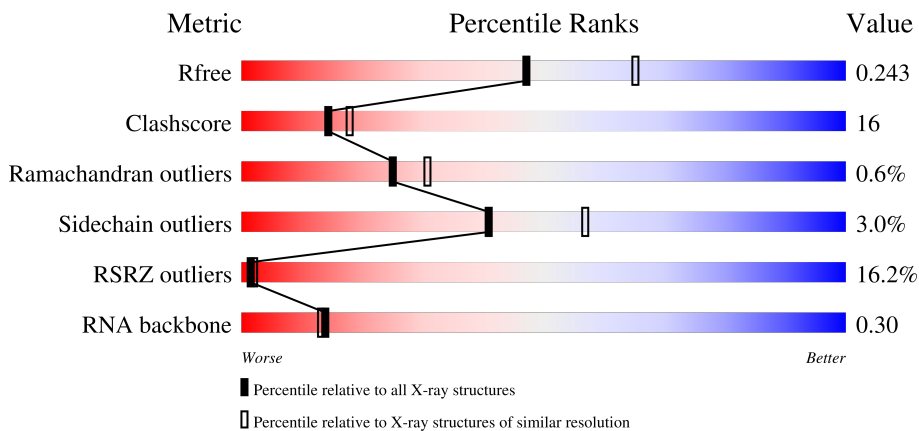|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & 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	Percentile Ranks	Value
Rfree		0.243
Clashscore		16
Ramachandran outliers		0.6%
Sidechain outliers		3.0%
RSRZ outliers		16.2%
RNA backbone		0.30

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	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)
RNA backbone	3102	1090 (2.70-1.90)

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	146	2% / 79% / 18% / ..
1	E	146	38% / 51% / 45% / . .
2	B	126	10% / 51% / 22% / . / 25%
2	G	126	44% / 39% / 33% / 28%

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Mol	Chain	Length	Quality of chain
3	C	413	4% / 76% / 17% / 5%
3	H	413	14% / 65% / 27% / 5%
4	D	146	6% / 23% / 14% / 61%
4	I	146	9% / 24% / 18% / 58%
5	F	6	50% / 17% / 17% / 17%
5	J	6	33% / 17% / 33% / 17%

2 Entry composition ⓘ

There are 9 unique types of molecules in this entry. The entry contains 11856 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 Protein mago nashi homolog.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	144	Total 1196	C 772	N 200	O 221	S 3	0	0	0
1	E	142	Total 1182	C 765	N 198	O 216	S 3	0	0	0

- Molecule 2 is a protein called RNA-binding protein 8A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	94	Total 750	C 476	N 126	O 145	S 3	0	0	0
2	G	91	Total 730	C 463	N 122	O 142	S 3	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	175	LEU	-	expression tag	UNP Q9Y5S9
B	176	GLU	-	expression tag	UNP Q9Y5S9
G	175	LEU	-	expression tag	UNP Q9Y5S9
G	176	GLU	-	expression tag	UNP Q9Y5S9

- Molecule 3 is a protein called Eukaryotic initiation factor 4A-III.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	392	Total 3148	C 1987	N 548	O 594	S 19	0	0	0
3	H	392	Total 3148	C 1987	N 548	O 594	S 19	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	412	LEU	-	expression tag	UNP P38919
C	413	GLU	-	expression tag	UNP P38919
H	412	LEU	-	expression tag	UNP P38919
H	413	GLU	-	expression tag	UNP P38919

- Molecule 4 is a protein called Protein CASC3.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	D	57	Total 491	C 306	N 93	O 92	0	0	0
4	I	62	Total 533	C 333	N 101	O 99	0	0	0

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	6	Total 117	C 54	N 12	O 46	P 5	0	0	0
5	J	6	Total 117	C 54	N 12	O 46	P 5	0	0	0

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total 27	C 10	N 5	O 10	P 2	0	0

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W O R L D W I D E
wwPDB
PROTEIN DATA BANK

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	H	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 7 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF$_3$).
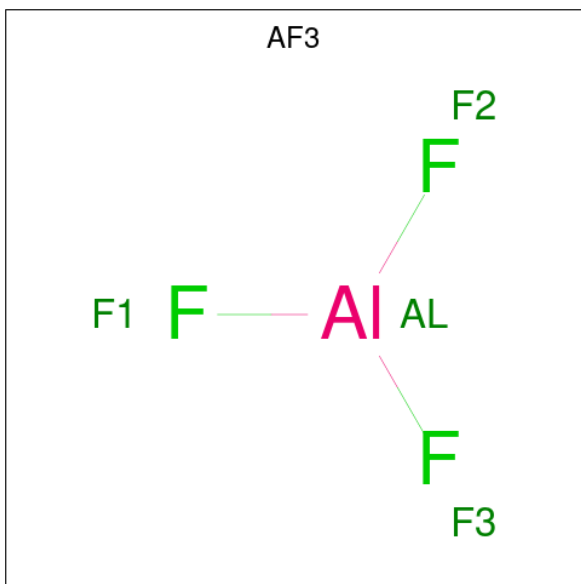
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	Al	F	0	0
			4	1	3		
7	H	1	Total	Al	F	0	0
			4	1	3		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Mg	0	0
			1	1		
8	H	1	Total	Mg	0	0
			1	1		

- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	72	Total	O	0	0
			72	72		
9	B	15	Total	O	0	0
			15	15		

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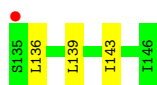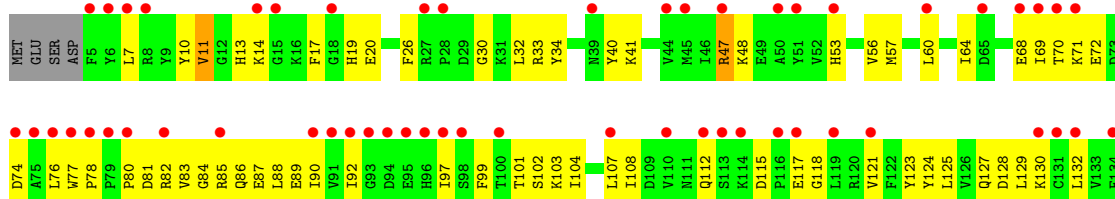| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	C	158	Total 158	O 158	0	0
9	D	25	Total 25	O 25	0	0
9	E	3	Total 3	O 3	0	0
9	G	2	Total 2	O 2	0	0
9	H	76	Total 76	O 76	0	0
9	I	18	Total 18	O 18	0	0
9	F	6	Total 6	O 6	0	0
9	J	5	Total 5	O 5	0	0

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 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.
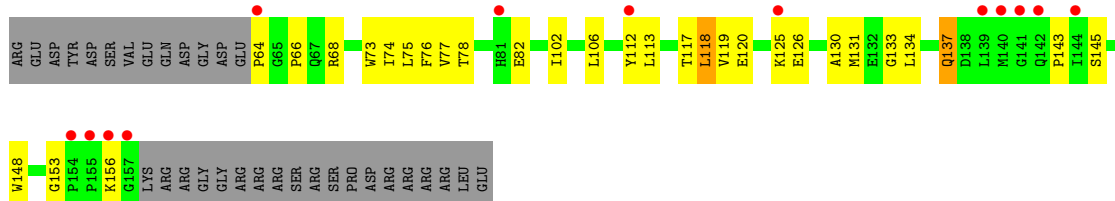
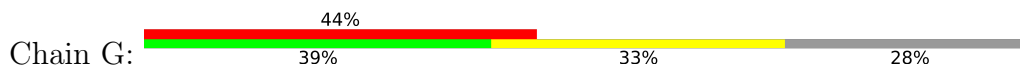• Molecule 1: Protein mago nashi homolog
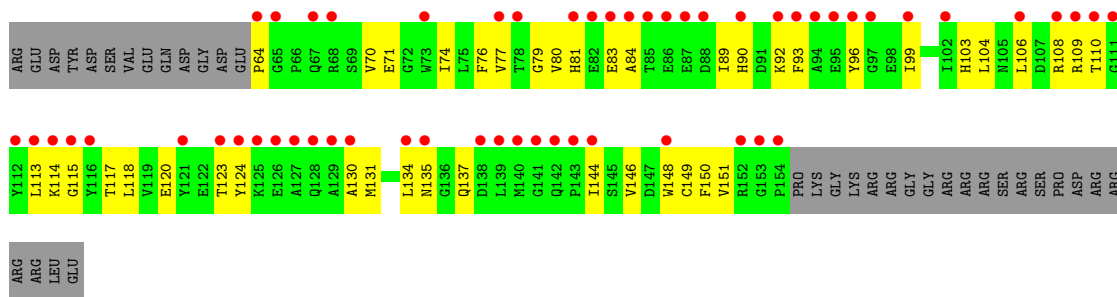

• Molecule 1: Protein mago nashi homolog
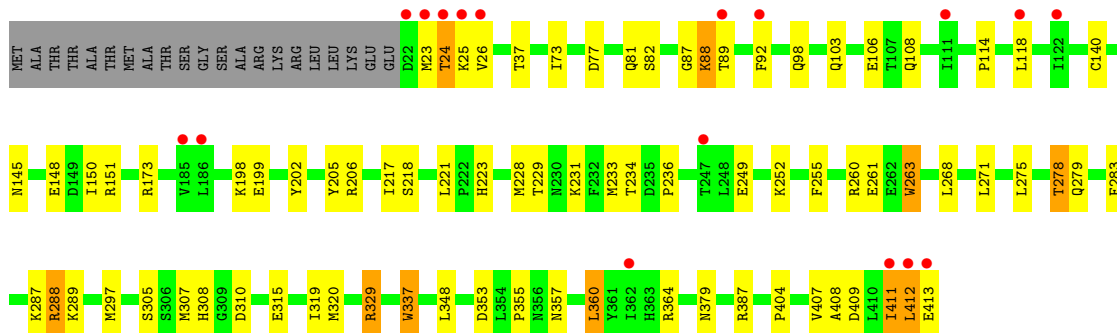

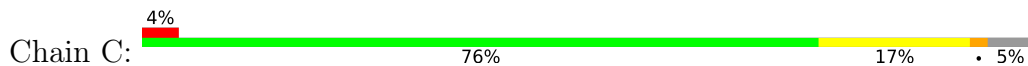• Molecule 2: RNA-binding protein 8A
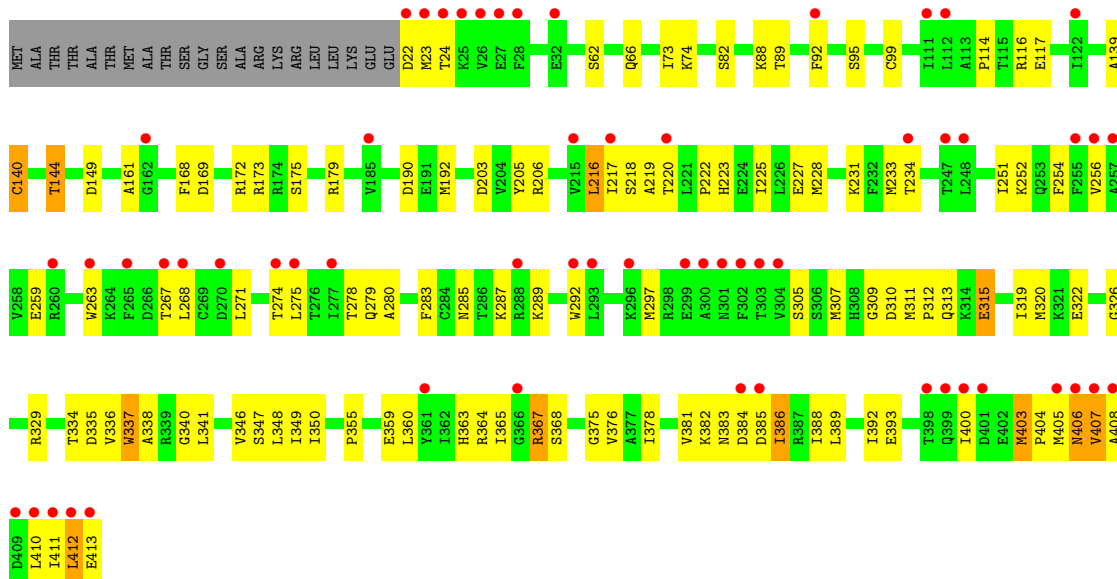

• Molecule 2: RNA-binding protein 8A

ARG GLU ASP TYR ASP SER VAL GLU GLN ASP GLY ASP GLU P64 G65 P66 Q67 R68 S69 V70 E71 G72 W73 I74 L75 F76 V77 T78 G79 V80 H81 E82 E83 A84 T85 E86 E87 D88 I89 H90 D91 K92 F93 A94 E95 Y96 G97 E98 I99 I102 H103 L104 N105 L106 D107 R108 R109 T110 G111

Y112 L113 K114 G115 Y116 T117 L118 V119 E120 Y121 E122 T123 Y124 K125 E126 A127 Q128 A129 A130 M131 L134 N135 G136 Q137 D138 L139 M140 G141 Q142 P143 I144 S145 V146 D147 W148 C149 F150 V151 R152 G153 P154 PRO LYS LYS ARG ARG GLY ARG ARG SER ARG SER PRO ASP ARG ARG

ARG ARG LEU GLU

• **Molecule 3: Eukaryotic initiation factor 4A-III**

Chain C:

4%

76%   17%   • 5%

MET ALA THR THR ALA THR MET ALA THR SER GLY SER ALA ARG LYS LEU LEU GLU LYS GLU D22 M23 T24 K25 V26 T37 I73 D77 Q81 S82 G87 K88 T89 F92 Q98 Q103 E106 T107 Q108 I111 P114 L118 I122 C140

N145 E148 D149 I150 R151 R173 V185 L186 K198 E199 Y202 Y205 R206 I217 S218 L221 P222 H223 M228 T229 N230 K231 F232 M233 T234 D235 P236 T247 L248 E249 K252 F255 R260 E261 E262 W263 L268 L271 L275 T278 Q279 F283

K287 R288 K289 M297 S305 S306 M307 H308 G309 D310 E315 I319 M320 R329 W337 L348 D353 L354 P355 N356 N357 L360 Y361 I362 H363 R364 N379 R387 P404 V407 A408 D409 L410 I411 L412 E413

• **Molecule 3: Eukaryotic initiation factor 4A-III**

Chain H:

14%

65%   27%   • 5%

MET ALA THR THR ALA THR MET ALA THR SER GLY SER ALA ARG LYS LEU LEU GLU LYS GLU D22 M23 T24 K25 V26 E27 F28 E32 S62 Q66 I73 K74 S82 K88 T89 F92 S95 C99 I111 L112 A113 P114 T115 R116 E117 I122 A139

C140 T144 D149 A161 G162 F168 D169 R172 R173 R174 S175 R179 V185 D190 E191 M192 D203 V204 Y205 R206 V215 I216 I217 S218 A219 T220 L221 P222 H223 E224 I225 L226 E227 M228 K231 F232 M233 T234 T247 L248 I251 K252 Q253 F254 F255 V256 A257

V258 E259 R260 W263 K264 F265 D266 T267 L268 C269 D270 L271 T274 L275 T276 I277 T278 Q279 A280 F283 C284 N285 T286 K287 R288 K289 W292 L293 K296 M297 R298 E299 A300 N301 F302 T303 V304 S305 S306 M307 H308 G309 D310 M311 P312 Q313 K314 E315 I319 M320 K321 E322 G326

R329 T334 D335 V336 W337 A338 R339 G340 L341 V346 S347 L348 I349 I350 P355 E359 L360 Y361 I362 H363 R364 I365 G366 R367 S368 G375 V376 A377 I378 V381 K382 N383 D384 I386 R387 I388 L389 I392 E393 T398 Q399 I400 E402 M403 P404 M405 N406 V407 A408

D409 L410 I411 L412 E413

• **Molecule 4: Protein CASC3**

Chain D:

6%

23%   14%   •   61%

THR LYS SER THR VAL THR GLY GLU ARG GLN SER GLY ASP GLY GLN GLU SER THR GLU PRO VAL GLU ASN LYS VAL GLY LYS LYS GLY PRO LYS HIS LEU ASP D172 D173 E174 D175 R176 K177 N178 P179 I182 P183 L193 R194 GLY GLN THR GLN GLU GLU GLU VAL ARG PRO LYS GLY

ARG GLN ARG LYS LEU TRP LYS ASP GLU G216 H220 D221 K222 F223 R224 E225 D226 E227 S232 R233 Q234 E235 L236 Y240 R245 S246 A247 H248 N249 PRO ASP ASP ILE LYS PRO ARG ARG ILE ARG LYS PRO ARG TYR GLY SER PRO PRO GLN ARG ASP PRO ASN TRP ASN GLY GLU

ARG LEU ASN LYS SER HIS ARG

- Molecule 4: Protein CASC3

Chain I:

THR LYS SER THR VAL THR GLY GLU ARG GLN SER GLY ASP GLY GLN GLU SER THR GLU PRO VAL GLU ASN LYS VAL GLY LYS LYS GLY P167 K168 H169 L170 D175 R176 K177 N178 P179 A180 Y181 I182 P183 R184 K185 G186 L187 F188 F189 D192 L193 R194 GLY GLN THR GLN GLU GLU GLU

VAL ARG PRO LYS GLY ARG GLN ARG LYS LEU TRP LYS ASP GLU G216 R217 H220 D221 Q228 L236 I237 G241 Y242 D243 I244 R245 S246 A247 H248 N249 PRO ASP ASP ILE LYS PRO ARG ARG ILE ARG LYS PRO ARG TYR GLY SER PRO PRO GLN ARG ASP PRO ASN TRP ASN GLY

GLU ARG LEU ASN LYS SER HIS ARG

- Molecule 5: RNA (5'-R(*UP*UP*UP*UP*UP*U)-3')

Chain F:

- Molecule 5: RNA (5'-R(*UP*UP*UP*UP*UP*U)-3')

Chain J:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	182.04Å 100.75Å 145.88Å 90.00° 112.08° 90.00°	Depositor
Resolution (Å)	39.06 – 2.30 39.06 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.3 (39.06-2.30) 99.3 (39.06-2.30)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	1.53 (at 2.29Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.206 , 0.251 0.200 , 0.243	Depositor DCC
R_{free} test set	2144 reflections (1.99%)	wwPDB-VP
Wilson B-factor (Å^2)	34.6	Xtriage
Anisotropy	0.788	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 59.7	EDS
L-test for twinning[2]	$< |L| > = 0.48, < L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.015 for 1/2*h-3/2*k,-1/2*h-1/2*k,-1/2*h+1/2*k-l 0.017 for 1/2*h+3/2*k,1/2*h-1/2*k,-1/2*h-1/2*k-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	11856	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.12% 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, AF3

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	0.54	1/1225 (0.1%)	0.65	0/1648
1	E	0.27	0/1211	0.44	0/1629
2	B	0.36	0/769	0.53	0/1040
2	G	0.26	0/748	0.42	0/1012
3	C	0.50	1/3197 (0.0%)	0.66	0/4314
3	H	0.40	1/3197 (0.0%)	0.57	0/4314
4	D	0.42	0/503	0.55	0/673
4	I	0.33	0/547	0.50	0/732
5	F	0.88	0/128	2.89	7/196 (3.6%)
5	J	0.84	0/128	1.49	2/196 (1.0%)
All	All	0.44	3/11653 (0.0%)	0.68	9/15754 (0.1%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	140	CYS	CB-SG	-5.69	1.72	1.81
1	A	131	CYS	CB-SG	-5.13	1.73	1.81
3	C	140	CYS	CB-SG	-5.05	1.73	1.81

The worst 5 of 9 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	F	6	U	C1'-O4'-C4'	-30.07	85.84	109.90
5	J	1	U	P-O3'-C3'	9.53	131.14	119.70
5	F	6	U	N1-C1'-C2'	9.41	126.23	114.00
5	F	6	U	C5'-C4'-C3'	7.93	128.70	116.00
5	J	1	U	C1'-O4'-C4'	-7.46	103.93	109.90

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	1196	0	1182	17	0
1	E	1182	0	1173	63	0
2	B	750	0	713	18	0
2	G	730	0	690	36	0
3	C	3148	0	3189	76	0
3	H	3148	0	3189	115	0
4	D	491	0	455	24	0
4	I	533	0	498	34	0
5	F	117	0	62	7	0
5	J	117	0	62	7	0
6	C	27	0	12	1	0
6	H	27	0	12	0	0
7	C	4	0	0	0	0
7	H	4	0	0	1	0
8	C	1	0	0	0	0
8	H	1	0	0	0	0
9	A	72	0	0	1	0
9	B	15	0	0	2	0
9	C	158	0	0	6	0
9	D	25	0	0	2	0
9	E	3	0	0	1	0
9	F	6	0	0	0	0
9	G	2	0	0	0	0
9	H	76	0	0	3	0
9	I	18	0	0	1	0
9	J	5	0	0	0	0
All	All	11856	0	11237	352	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 16.

The worst 5 of 352 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)
3:C:268:LEU:HD23	3:C:297:MET:HE3	1.36	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:I:169:HIS:HD2	5:F:5:U:H3	1.02	0.99
4:I:183:PRO:HG2	5:J:1:U:H5"	1.44	0.97
1:E:69:ILE:HG13	1:E:125:LEU:HD22	1.51	0.92
3:H:88:LYS:HG2	3:H:217:ILE:HG23	1.52	0.89

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	142/146 (97%)	137 (96%)	5 (4%)	0	100	100
1	E	140/146 (96%)	127 (91%)	12 (9%)	1 (1%)	22	26
2	B	92/126 (73%)	90 (98%)	1 (1%)	1 (1%)	14	15
2	G	89/126 (71%)	81 (91%)	8 (9%)	0	100	100
3	C	390/413 (94%)	380 (97%)	9 (2%)	1 (0%)	41	50
3	H	390/413 (94%)	371 (95%)	15 (4%)	4 (1%)	15	17
4	D	53/146 (36%)	51 (96%)	2 (4%)	0	100	100
4	I	58/146 (40%)	54 (93%)	3 (5%)	1 (2%)	9	8
All	All	1354/1662 (82%)	1291 (95%)	55 (4%)	8 (1%)	25	31

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	I	245	ARG
3	H	335	ASP
3	H	406	ASN
2	B	137	GLN
3	C	412	LEU

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	132/134 (98%)	128 (97%)	4 (3%)	41	57
1	E	130/134 (97%)	129 (99%)	1 (1%)	81	91
2	B	78/107 (73%)	77 (99%)	1 (1%)	69	82
2	G	76/107 (71%)	76 (100%)	0	100	100
3	C	347/363 (96%)	334 (96%)	13 (4%)	34	48
3	H	347/363 (96%)	333 (96%)	14 (4%)	31	44
4	D	50/130 (38%)	48 (96%)	2 (4%)	31	44
4	I	55/130 (42%)	53 (96%)	2 (4%)	35	49
All	All	1215/1468 (83%)	1178 (97%)	37 (3%)	41	57

5 of 37 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
3	H	337	TRP
4	I	245	ARG
3	H	360	LEU
3	H	403	MET
3	C	288	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
2	G	90	HIS
4	I	220	HIS
2	G	128	GLN
4	I	248	HIS
3	H	399	GLN

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
5	F	5/6 (83%)	1 (20%)	0
5	J	6/6 (100%)	2 (33%)	1 (16%)
All	All	11/12 (91%)	3 (27%)	1 (9%)

All (3) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
5	F	6	U
5	J	2	U
5	J	3	U

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
5	J	1	U

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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\#|Z| > 2$
7	AF3	H	415	-	0,3,3	-	-	-		
7	AF3	C	415	-	0,3,3	-	-	-		
6	ADP	H	414	-	24,29,29	1.11	2 (8%)	29,45,45	1.52	7 (24%)
6	ADP	C	414	-	24,29,29	1.05	2 (8%)	29,45,45	1.40	6 (20%)

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
6	ADP	H	414	-	-	1/12/32/32	0/3/3/3
6	ADP	C	414	-	-	1/12/32/32	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	414	ADP	C5-C4	2.77	1.48	1.40
6	C	414	ADP	C5-C4	2.35	1.47	1.40
6	C	414	ADP	C2-N3	2.05	1.35	1.32
6	H	414	ADP	O4'-C1'	2.03	1.43	1.41

The worst 5 of 13 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	414	ADP	N3-C2-N1	-3.52	123.18	128.68
6	H	414	ADP	N3-C2-N1	-3.10	123.83	128.68
6	C	414	ADP	C4-C5-N7	-2.61	106.68	109.40
6	H	414	ADP	PA-O3A-PB	-2.60	123.89	132.83
6	H	414	ADP	C4-C5-N7	-2.54	106.75	109.40

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	414	ADP	PA-O3A-PB-O2B
6	C	414	ADP	PA-O3A-PB-O2B

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	415	AF3	1	0
6	C	414	ADP	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 H 414

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP C 414

Bond lengths

Bond angles

Torsions

Rings
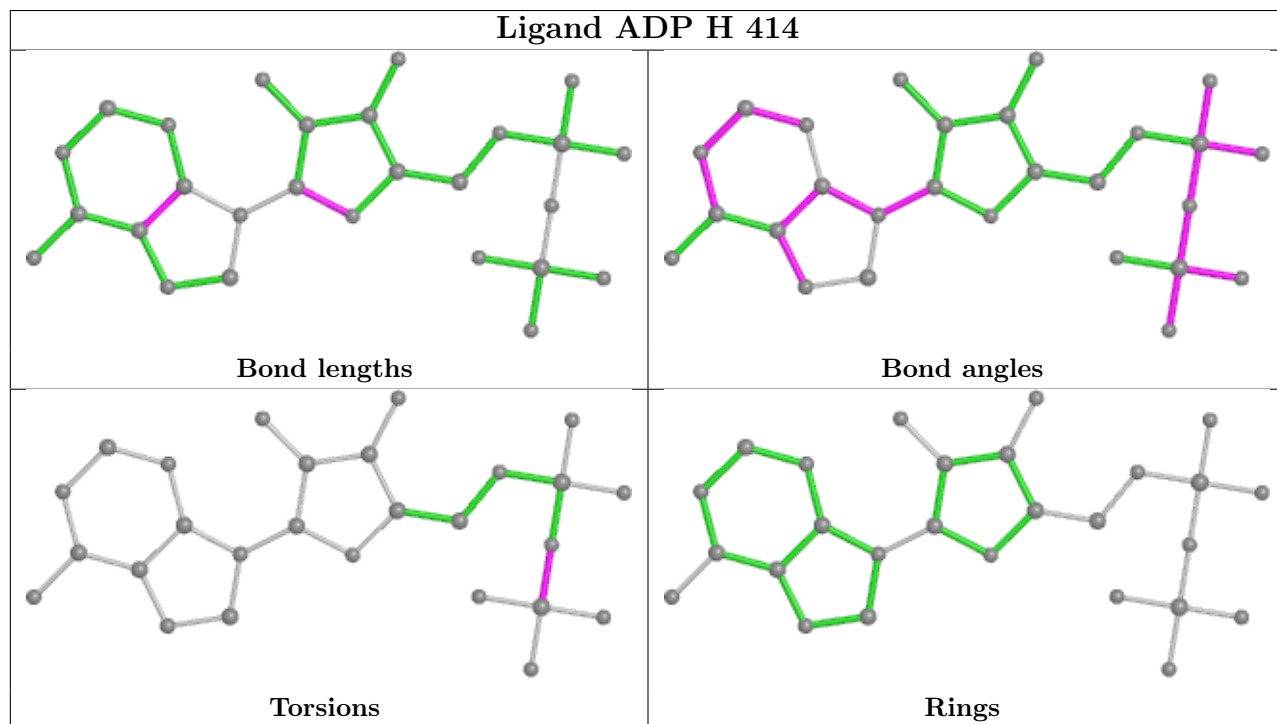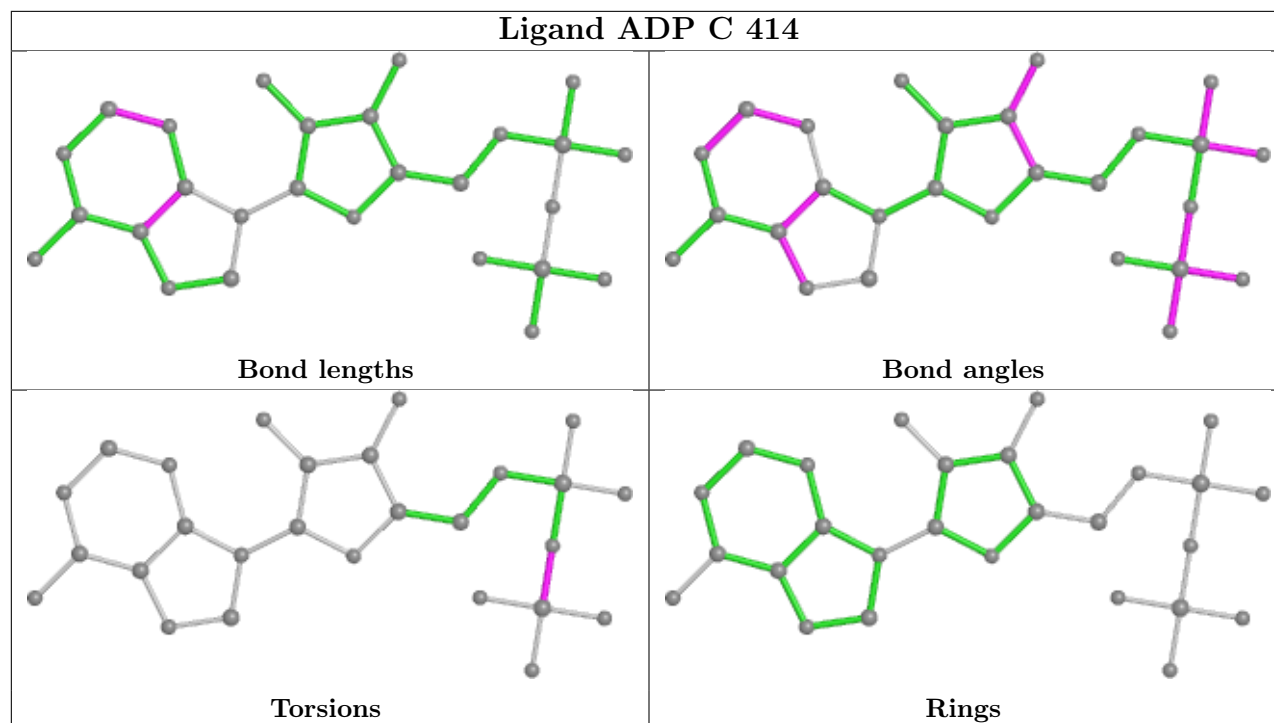
5.7 Other polymers ⓘ

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 ⓘ

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(Å²)	Q<0.9
1	A	144/146 (98%)	-0.10	3 (2%)	63	70	24, 34, 65, 120	0
1	E	142/146 (97%)	1.92	55 (38%)	0	0	81, 119, 190, 266	0
2	B	94/126 (74%)	0.52	13 (13%)	2	4	35, 61, 98, 160	0
2	G	91/126 (72%)	3.01	56 (61%)	0	0	92, 128, 176, 192	0
3	C	392/413 (94%)	0.10	17 (4%)	35	42	23, 35, 63, 142	0
3	H	392/413 (94%)	0.66	59 (15%)	2	3	33, 61, 144, 267	0
4	D	57/146 (39%)	0.74	9 (15%)	2	2	29, 52, 148, 167	0
4	I	62/146 (42%)	0.97	13 (20%)	1	1	37, 73, 140, 185	0
5	F	6/6 (100%)	0.23	0	100	100	35, 39, 45, 74	0
5	J	6/6 (100%)	0.02	0	100	100	55, 63, 75, 104	0
All	All	1386/1674 (82%)	0.71	225 (16%)	1	2	23, 52, 155, 267	0

The worst 5 of 225 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	H	405	MET	11.4
2	G	139	LEU	11.0
4	D	172	ASP	10.2
4	D	174	GLU	10.0
2	G	84	ALA	9.4

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

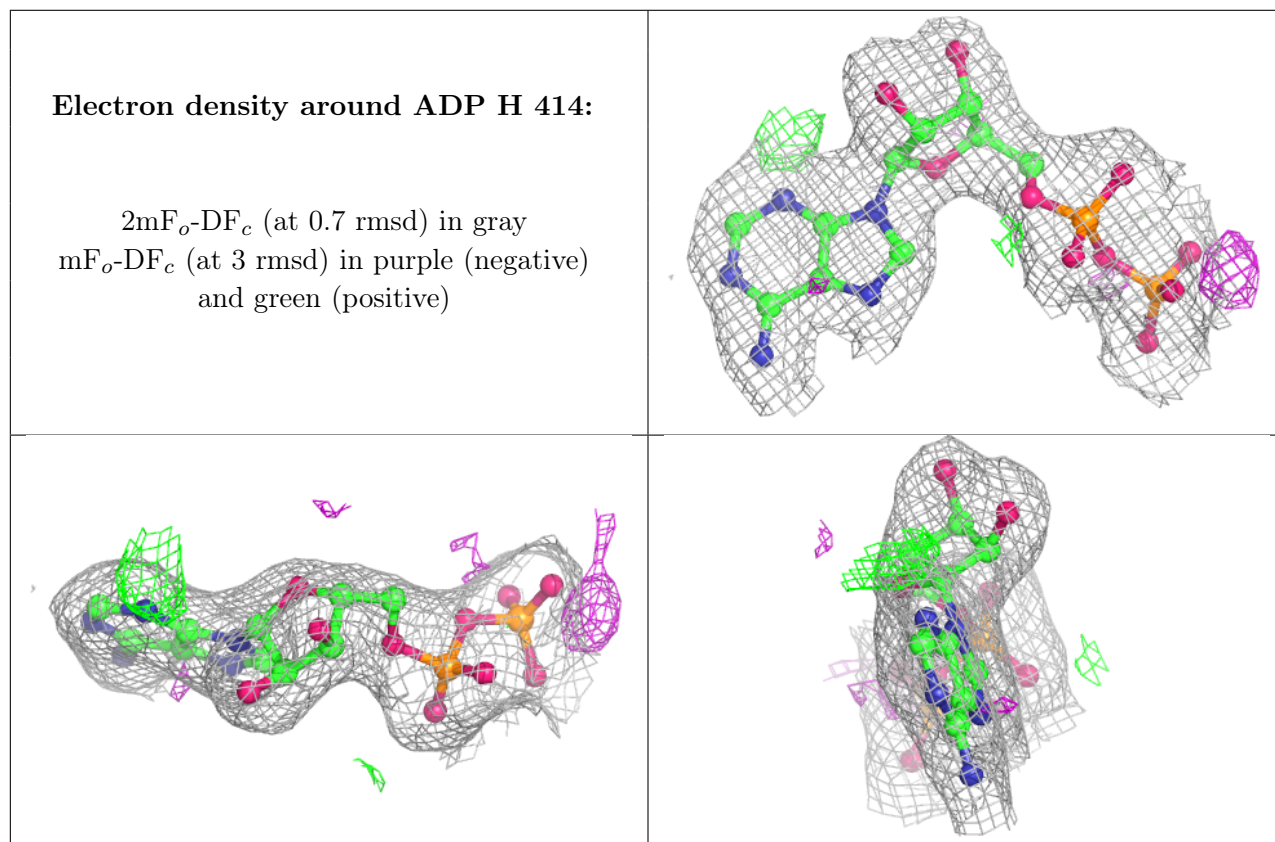There are no non-standard protein/DNA/RNA residues in this entry.

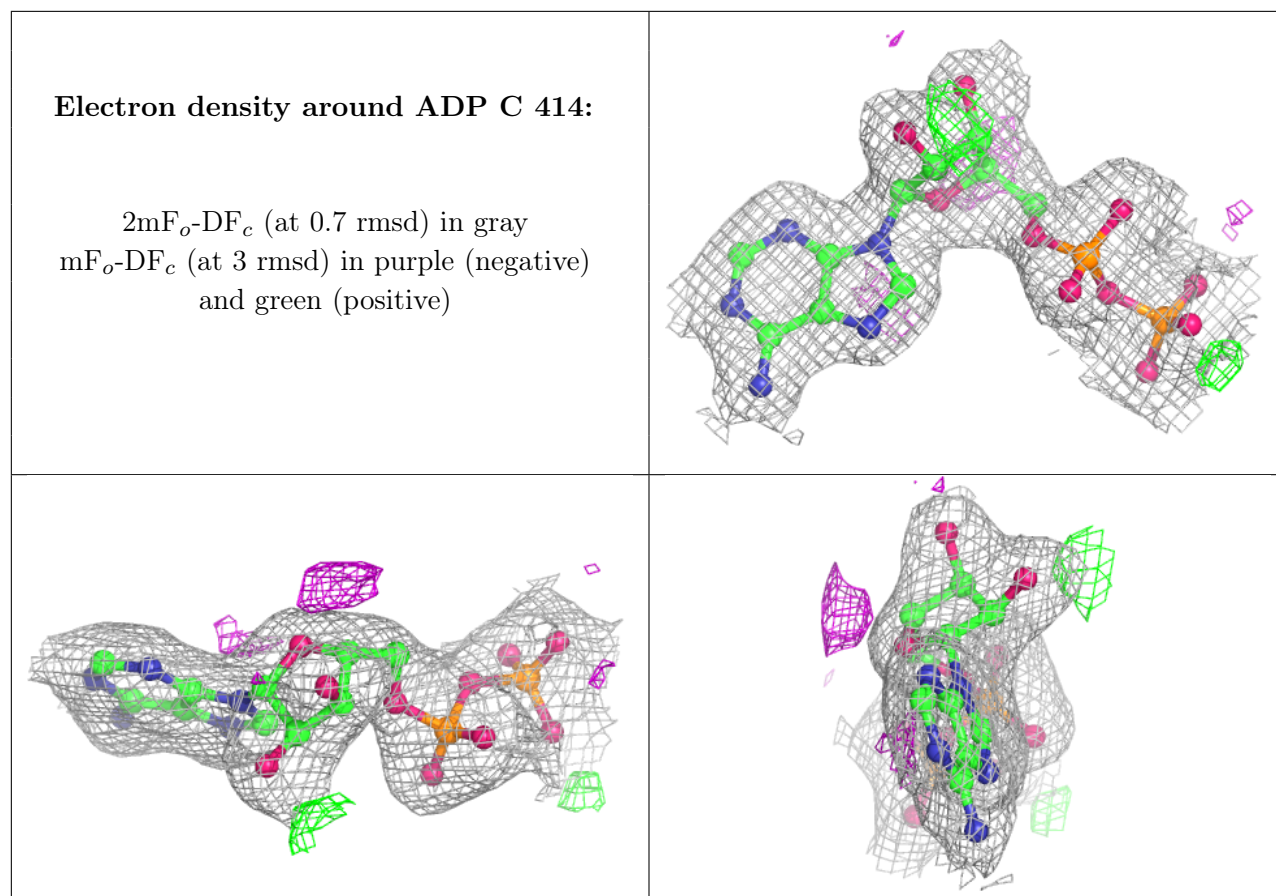## 6.3　Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4　Ligands ⓘ

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	AF3	H	415	4/4	0.80	0.34	52,66,72,214	0
7	AF3	C	415	4/4	0.91	0.27	37,42,60,145	0
8	MG	H	416	1/1	0.92	0.18	40,40,40,40	0
6	ADP	H	414	27/27	0.94	0.13	35,44,54,61	0
8	MG	C	416	1/1	0.97	0.28	32,32,32,32	0
6	ADP	C	414	27/27	0.98	0.15	19,28,36,40	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 ADP H 414:

$2mF_o\text{-}DF_c$ (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 414:

$2mF_o$-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.