



# Full wwPDB X-ray Structure Validation Report ⓘ

May 27, 2026 – 04:15 PM JST

PDB ID : 9UNZ / pdb\_00009unz  
Title : Crystal structure of the V165A/S219E/A225P mutant of alanine dehydrogenase from *Geobacillus stearothermophilus* in complex with nicotinamide cytosine dinucleotide  
Authors : Hu, Y.; Guo, X.; Wang, X.; Zhao, Z.  
Deposited on : 2025-04-24  
Resolution : 2.56 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](mailto: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>.

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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	:	1.8.5 (274361), CSD as541be (2020)
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

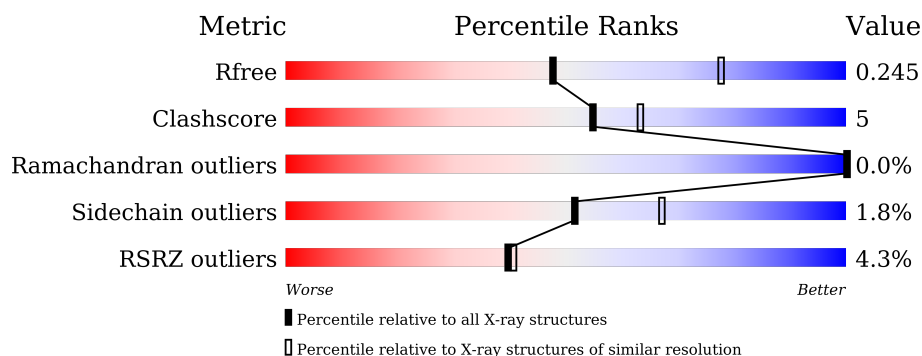
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.56 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	1853 (2.58-2.54)
Clashscore	190562	1897 (2.58-2.54)
Ramachandran outliers	187476	1875 (2.58-2.54)
Sidechain outliers	187428	1875 (2.58-2.54)
RSRZ outliers	180081	1853 (2.58-2.54)

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  $\geq 3$ , 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	372	<div> <div>18%</div> <div>81%</div> <div>18%</div> </div>
1	B	372	<div> <div>3%</div> <div>86%</div> <div>13%</div> <div>.</div> </div>
1	C	372	<div> <div>2%</div> <div>87%</div> <div>12%</div> <div>.</div> </div>
1	D	372	<div> <div>%</div> <div>85%</div> <div>15%</div> </div>
1	E	372	<div> <div>3%</div> <div>92%</div> <div>7%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
1	F	372	 3% 89% 10%
1	G	372	 4% 84% 15%
1	H	372	 5% 88% 11% •
1	I	372	 2% 87% 12% •
1	J	372	 3% 91% 8%
1	K	372	 4% 92% 8%
1	L	372	 3% 85% 14% •

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 34373 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 Alanine dehydrogenase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2765	1755	471	527	12			
1	B	371	Total	C	N	O	S	0	0	0
			2765	1755	471	527	12			
1	C	371	Total	C	N	O	S	0	0	0
			2765	1755	471	527	12			
1	D	371	Total	C	N	O	S	0	0	0
			2765	1755	471	527	12			
1	E	371	Total	C	N	O	S	0	0	0
			2765	1755	471	527	12			
1	F	371	Total	C	N	O	S	0	0	0
			2765	1755	471	527	12			
1	G	371	Total	C	N	O	S	0	0	0
			2765	1755	471	527	12			
1	H	371	Total	C	N	O	S	0	0	0
			2765	1755	471	527	12			
1	I	371	Total	C	N	O	S	0	0	0
			2765	1755	471	527	12			
1	J	371	Total	C	N	O	S	0	0	0
			2765	1755	471	527	12			
1	K	371	Total	C	N	O	S	0	0	0
			2765	1755	471	527	12			
1	L	371	Total	C	N	O	S	0	0	0
			2765	1755	471	527	12			

There are 36 discrepancies between the modelled and reference sequences:

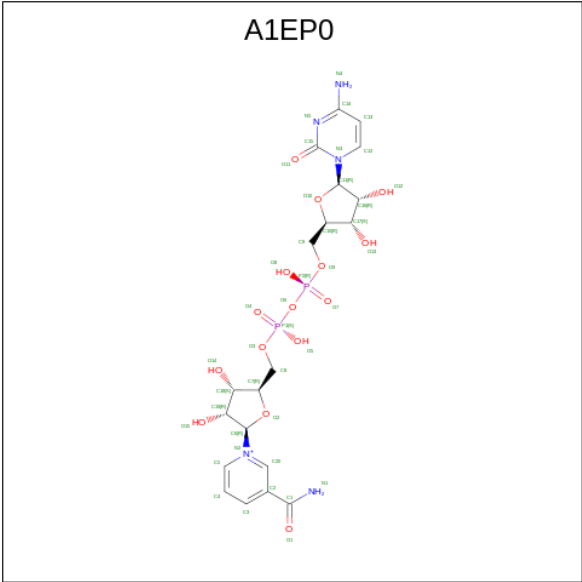
Chain	Residue	Modelled	Actual	Comment	Reference
A	165	ALA	VAL	engineered mutation	UNP A8QVZ6
A	219	GLU	SER	engineered mutation	UNP A8QVZ6
A	225	PRO	ALA	engineered mutation	UNP A8QVZ6
B	165	ALA	VAL	engineered mutation	UNP A8QVZ6
B	219	GLU	SER	engineered mutation	UNP A8QVZ6

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Chain	Residue	Modelled	Actual	Comment	Reference
B	225	PRO	ALA	engineered mutation	UNP A8QVZ6
C	165	ALA	VAL	engineered mutation	UNP A8QVZ6
C	219	GLU	SER	engineered mutation	UNP A8QVZ6
C	225	PRO	ALA	engineered mutation	UNP A8QVZ6
D	165	ALA	VAL	engineered mutation	UNP A8QVZ6
D	219	GLU	SER	engineered mutation	UNP A8QVZ6
D	225	PRO	ALA	engineered mutation	UNP A8QVZ6
E	165	ALA	VAL	engineered mutation	UNP A8QVZ6
E	219	GLU	SER	engineered mutation	UNP A8QVZ6
E	225	PRO	ALA	engineered mutation	UNP A8QVZ6
F	165	ALA	VAL	engineered mutation	UNP A8QVZ6
F	219	GLU	SER	engineered mutation	UNP A8QVZ6
F	225	PRO	ALA	engineered mutation	UNP A8QVZ6
G	165	ALA	VAL	engineered mutation	UNP A8QVZ6
G	219	GLU	SER	engineered mutation	UNP A8QVZ6
G	225	PRO	ALA	engineered mutation	UNP A8QVZ6
H	165	ALA	VAL	engineered mutation	UNP A8QVZ6
H	219	GLU	SER	engineered mutation	UNP A8QVZ6
H	225	PRO	ALA	engineered mutation	UNP A8QVZ6
I	165	ALA	VAL	engineered mutation	UNP A8QVZ6
I	219	GLU	SER	engineered mutation	UNP A8QVZ6
I	225	PRO	ALA	engineered mutation	UNP A8QVZ6
J	165	ALA	VAL	engineered mutation	UNP A8QVZ6
J	219	GLU	SER	engineered mutation	UNP A8QVZ6
J	225	PRO	ALA	engineered mutation	UNP A8QVZ6
K	165	ALA	VAL	engineered mutation	UNP A8QVZ6
K	219	GLU	SER	engineered mutation	UNP A8QVZ6
K	225	PRO	ALA	engineered mutation	UNP A8QVZ6
L	165	ALA	VAL	engineered mutation	UNP A8QVZ6
L	219	GLU	SER	engineered mutation	UNP A8QVZ6
L	225	PRO	ALA	engineered mutation	UNP A8QVZ6

- Molecule 2 is [[(2 {R},3 {S},4 {R},5 {R})-5-(3-aminocarbonylpyridin-1-ium-1-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methoxy-oxidanyl-phosphoryl] [(2 {R},3 {S},4 {R},5 {R})-5-(4-azanyl-2-oxidanylidene-pyrimidin-1-yl)-3,4-bis(oxidanyl)oxolan-2-yl]methyl hydrogen phosphate (CCD ID: A1EP0) (formula: C<sub>20</sub>H<sub>28</sub>N<sub>5</sub>O<sub>15</sub>P<sub>2</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			42	20	5	15	2		
2	B	1	Total	C	N	O	P	0	0
			42	20	5	15	2		
2	C	1	Total	C	N	O	P	0	0
			42	20	5	15	2		
2	D	1	Total	C	N	O	P	0	0
			42	20	5	15	2		
2	E	1	Total	C	N	O	P	0	0
			42	20	5	15	2		
2	F	1	Total	C	N	O	P	0	0
			42	20	5	15	2		
2	G	1	Total	C	N	O	P	0	0
			42	20	5	15	2		
2	H	1	Total	C	N	O	P	0	0
			42	20	5	15	2		
2	I	1	Total	C	N	O	P	0	0
			42	20	5	15	2		
2	J	1	Total	C	N	O	P	0	0
			42	20	5	15	2		
2	K	1	Total	C	N	O	P	0	0
			42	20	5	15	2		
2	L	1	Total	C	N	O	P	0	0
			42	20	5	15	2		

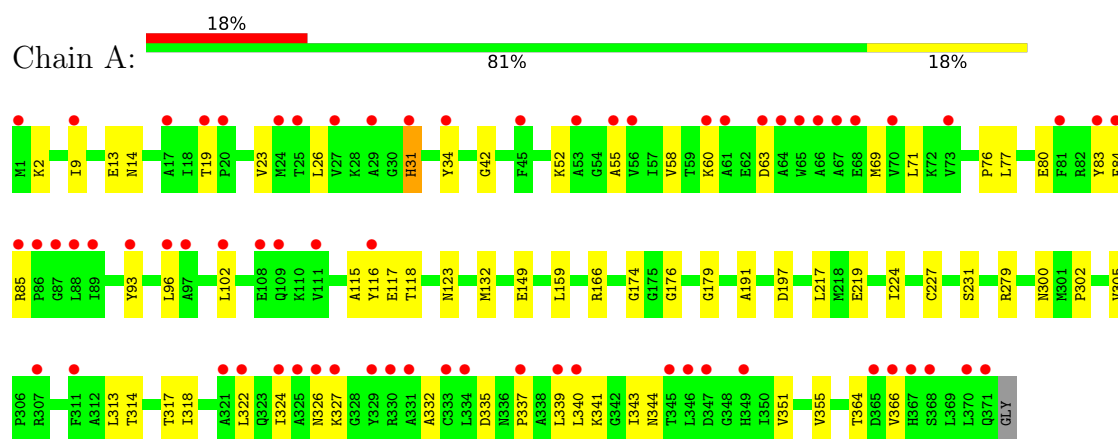
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	30	Total 30	O 30	0	0
3	B	35	Total 35	O 35	0	0
3	C	68	Total 68	O 68	0	0
3	D	65	Total 65	O 65	0	0
3	E	93	Total 93	O 93	0	0
3	F	45	Total 45	O 45	0	0
3	G	30	Total 30	O 30	0	0
3	H	50	Total 50	O 50	0	0
3	I	71	Total 71	O 71	0	0
3	J	99	Total 99	O 99	0	0
3	K	58	Total 58	O 58	0	0
3	L	45	Total 45	O 45	0	0

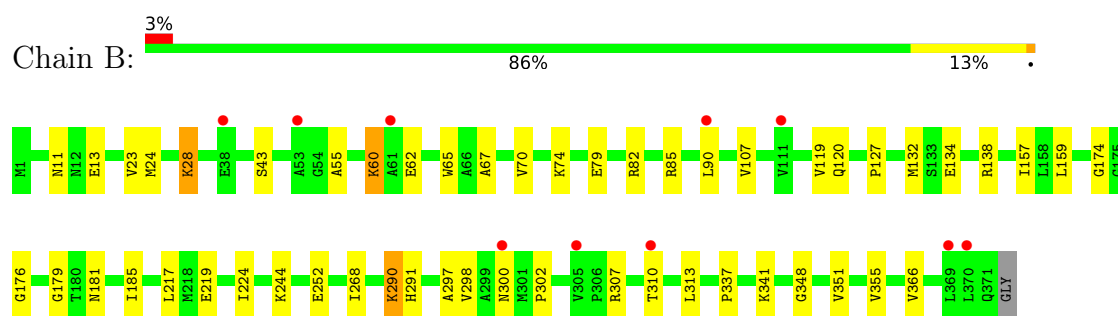
### 3 Residue-property plots [i](#)

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

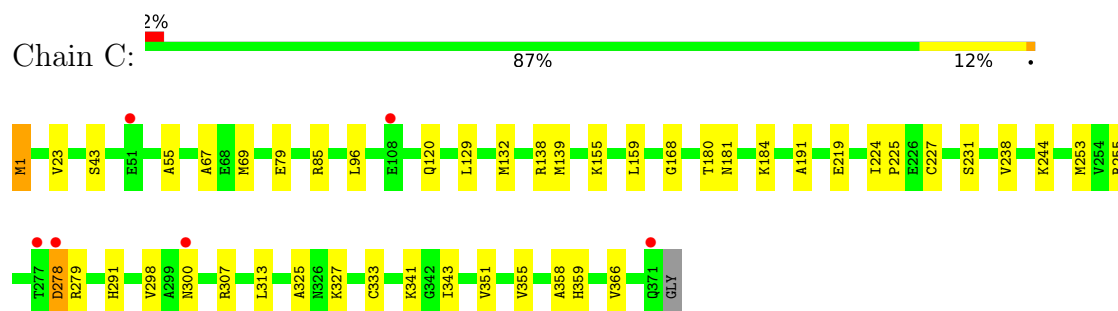
- Molecule 1: Alanine dehydrogenase



- Molecule 1: Alanine dehydrogenase

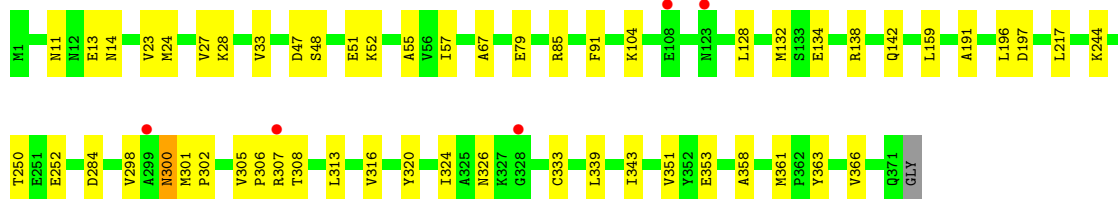
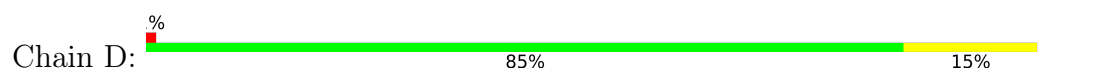


- Molecule 1: Alanine dehydrogenase

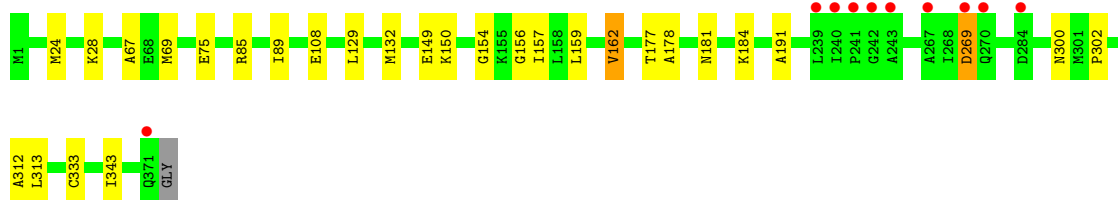
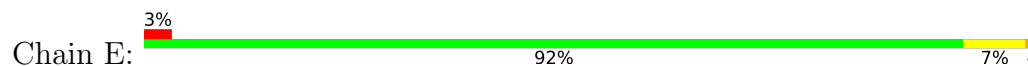


- Molecule 1: Alanine dehydrogenase

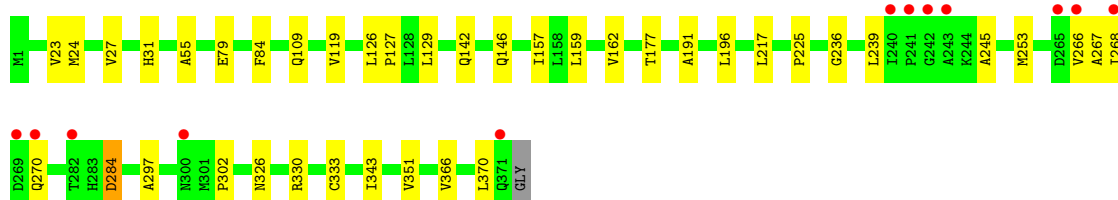
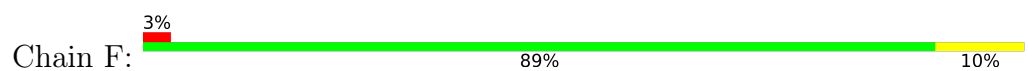




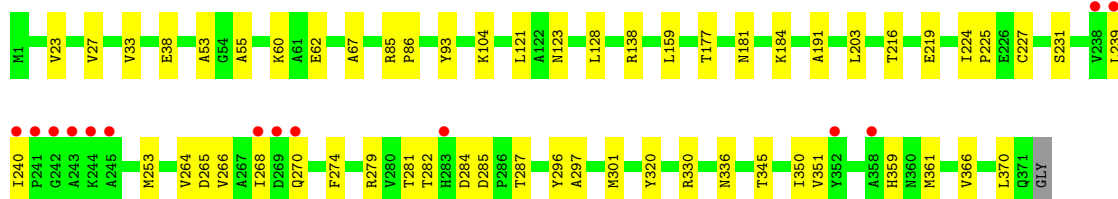
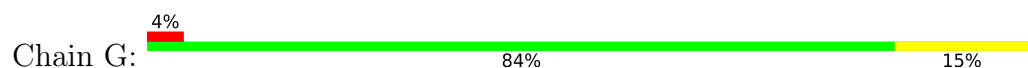
- Molecule 1: Alanine dehydrogenase



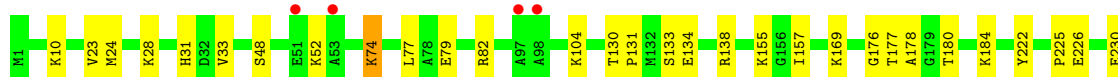
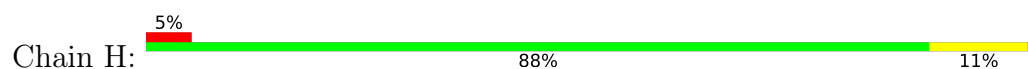
- Molecule 1: Alanine dehydrogenase



- Molecule 1: Alanine dehydrogenase

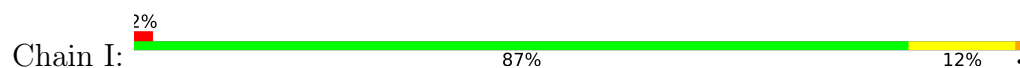


- Molecule 1: Alanine dehydrogenase

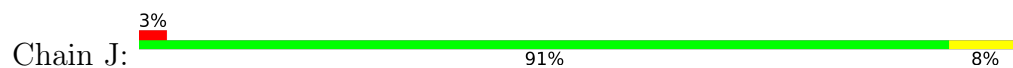




• Molecule 1: Alanine dehydrogenase



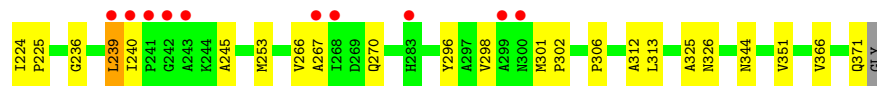
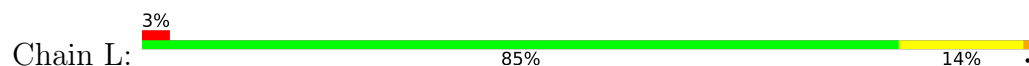
• Molecule 1: Alanine dehydrogenase



• Molecule 1: Alanine dehydrogenase



• Molecule 1: Alanine dehydrogenase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	89.44Å 155.75Å 178.09Å 90.00° 98.25° 90.00°	Depositor
Resolution (Å)	46.00 – 2.56 46.00 – 2.56	Depositor EDS
% Data completeness (in resolution range)	97.7 (46.00-2.56) 97.7 (46.00-2.56)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.80 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.15.1_3469	Depositor
R, $R_{free}$	0.193 , 0.244 0.194 , 0.245	Depositor DCC
$R_{free}$ test set	7615 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.5	Xtriage
Anisotropy	0.293	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 45.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	34373	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.46% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: A1EP0

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	0.12	0/2814	0.31	0/3829
1	B	0.13	0/2814	0.31	0/3829
1	C	0.12	0/2814	0.30	0/3829
1	D	0.13	0/2814	0.30	0/3829
1	E	0.12	0/2814	0.30	0/3829
1	F	0.12	0/2814	0.29	0/3829
1	G	0.12	0/2814	0.29	0/3829
1	H	0.12	0/2814	0.28	0/3829
1	I	0.12	0/2814	0.30	0/3829
1	J	0.12	0/2814	0.28	0/3829
1	K	0.12	0/2814	0.28	0/3829
1	L	0.12	0/2814	0.29	0/3829
All	All	0.12	0/33768	0.29	0/45948

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	2765	0	2811	46	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	2765	0	2811	31	0
1	C	2765	0	2811	24	0
1	D	2765	0	2811	32	0
1	E	2765	0	2811	17	0
1	F	2765	0	2811	21	0
1	G	2765	0	2811	34	0
1	H	2765	0	2811	29	0
1	I	2765	0	2811	29	0
1	J	2765	0	2811	19	0
1	K	2765	0	2811	16	0
1	L	2765	0	2811	35	0
2	A	42	0	0	3	0
2	B	42	0	0	2	0
2	C	42	0	0	0	0
2	D	42	0	0	2	0
2	E	42	0	0	5	0
2	F	42	0	0	4	0
2	G	42	0	0	2	0
2	H	42	0	0	7	0
2	I	42	0	0	2	0
2	J	42	0	0	2	0
2	K	42	0	0	1	0
2	L	42	0	0	2	0
3	A	30	0	0	1	0
3	B	35	0	0	0	0
3	C	68	0	0	0	0
3	D	65	0	0	0	0
3	E	93	0	0	1	0
3	F	45	0	0	0	0
3	G	30	0	0	1	0
3	H	50	0	0	0	0
3	I	71	0	0	0	0
3	J	99	0	0	2	0
3	K	58	0	0	0	0
3	L	45	0	0	0	0
All	All	34373	0	33732	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 5.

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)
1:K:10:LYS:HE3	1:K:74:LYS:HB2	1.59	0.83
1:J:24:MET:HG2	1:J:28:LYS:HE2	1.71	0.72
1:C:298:VAL:HG12	1:C:300:ASN:H	1.55	0.72
1:F:245:ALA:HB2	1:F:270:GLN:HE21	1.55	0.71
1:A:322:LEU:O	1:A:326:ASN:ND2	2.25	0.70
1:H:177:THR:HB	2:H:401:A1EP0:O5	1.91	0.69
1:I:159:LEU:HB3	1:I:191:ALA:HB2	1.74	0.68
1:H:178:ALA:H	2:H:401:A1EP0:P1	2.17	0.68
1:I:173:ILE:HG12	1:I:196:LEU:HD12	1.76	0.67
1:C:1:MET:HE3	1:C:69:MET:HB2	1.76	0.67
1:B:298:VAL:HG12	1:B:300:ASN:H	1.60	0.67
1:A:60:LYS:HE3	1:A:63:ASP:HB2	1.77	0.66
1:D:23:VAL:HG11	1:D:55:ALA:HB2	1.78	0.65
1:L:203:LEU:HG	1:L:216:THR:HB	1.78	0.64
1:A:351:VAL:HB	1:A:366:VAL:HB	1.79	0.63
1:A:31:HIS:CE1	1:A:326:ASN:HB3	2.34	0.63
1:F:302:PRO:HD2	2:F:401:A1EP0:N1	2.14	0.62
1:A:69:MET:HE2	1:A:71:LEU:HD21	1.80	0.62
1:B:219:GLU:HG3	1:B:224:ILE:HD11	1.81	0.62
1:A:58:VAL:HG11	1:A:63:ASP:HB3	1.82	0.62
1:L:177:THR:O	1:L:179:GLY:N	2.32	0.62
1:H:239:LEU:HD23	2:H:401:A1EP0:O8	2.00	0.61
1:G:359:HIS:HB3	1:G:361:MET:HE3	1.82	0.60
1:E:24:MET:HG2	1:E:28:LYS:HE2	1.84	0.60
1:G:67:ALA:O	1:G:85:ARG:NH2	2.34	0.59
1:I:312:ALA:HB2	1:J:162:VAL:HG21	1.83	0.59
1:D:67:ALA:O	1:D:85:ARG:NH2	2.34	0.59
1:C:67:ALA:O	1:C:85:ARG:NH2	2.30	0.59
1:H:79:GLU:O	1:H:82:ARG:NH1	2.36	0.59
1:E:178:ALA:N	2:E:401:A1EP0:O5	2.30	0.59
1:B:120:GLN:HB3	1:B:341:LYS:HD3	1.84	0.58
1:G:203:LEU:HD22	1:G:216:THR:HB	1.85	0.58
1:E:302:PRO:HD2	2:E:401:A1EP0:N1	2.19	0.58
1:G:23:VAL:HG22	1:G:33:VAL:HG11	1.85	0.58
1:B:13:GLU:HB2	1:B:300:ASN:HD21	1.68	0.57
1:G:159:LEU:HB3	1:G:191:ALA:HB2	1.86	0.57
1:I:123:ASN:OD1	1:I:123:ASN:N	2.35	0.57
1:F:177:THR:N	2:F:401:A1EP0:O4	2.38	0.57
1:E:132:MET:HE3	1:E:313:LEU:HB2	1.87	0.57
1:L:225:PRO:HG3	1:L:253:MET:HE2	1.87	0.57
1:L:162:VAL:HG22	1:L:163:PRO:HD2	1.85	0.57
1:E:300:ASN:HA	2:E:401:A1EP0:N1	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:219:GLU:HG3	1:L:224:ILE:HD11	1.87	0.57
1:B:23:VAL:HG11	1:B:55:ALA:HB2	1.86	0.56
1:E:269:ASP:OD1	1:E:269:ASP:N	2.39	0.56
1:A:118:THR:HG21	1:A:344:ASN:HD21	1.71	0.56
1:F:159:LEU:HB3	1:F:191:ALA:HB2	1.87	0.56
1:A:23:VAL:HG11	1:A:55:ALA:HB2	1.88	0.55
1:H:300:ASN:HA	2:H:401:A1EP0:N1	2.21	0.55
1:C:219:GLU:HG3	1:C:224:ILE:HD11	1.88	0.55
1:G:264:VAL:HG22	1:G:296:TYR:HB3	1.88	0.55
1:H:330:ARG:HG3	1:H:370:LEU:HD22	1.88	0.55
1:D:51:GLU:HG3	1:D:57:ILE:HD13	1.88	0.55
1:G:351:VAL:HB	1:G:366:VAL:HB	1.88	0.55
1:C:138:ARG:HG3	1:C:181:ASN:HB3	1.89	0.54
1:L:197:ASP:OD2	2:L:401:A1EP0:O13	2.26	0.54
1:L:1:MET:HE2	1:L:325:ALA:HA	1.89	0.54
1:C:1:MET:HE2	1:C:325:ALA:HA	1.90	0.53
1:E:156:GLY:HA3	1:L:306:PRO:HD2	1.90	0.53
1:A:84:PHE:O	1:A:85:ARG:NH1	2.42	0.53
1:H:351:VAL:HB	1:H:366:VAL:HB	1.90	0.52
1:B:82:ARG:HH12	1:H:104:LYS:HZ2	1.57	0.52
1:I:172:ILE:HG12	1:I:235:VAL:HB	1.91	0.52
1:I:177:THR:N	2:I:401:A1EP0:O4	2.42	0.52
1:C:227:CYS:O	1:C:231:SER:OG	2.19	0.52
1:F:84:PHE:O	1:F:109:GLN:NE2	2.42	0.52
1:G:104:LYS:HG3	1:G:361:MET:HE1	1.92	0.52
1:C:43:SER:O	1:C:307:ARG:NH1	2.40	0.52
1:F:268:ILE:HG12	1:F:297:ALA:HB1	1.91	0.52
1:G:268:ILE:HD13	1:G:297:ALA:HA	1.92	0.51
1:L:267:ALA:HB1	1:L:270:GLN:HB2	1.92	0.51
1:A:132:MET:HE3	1:A:313:LEU:HB2	1.91	0.51
1:B:252:GLU:OE1	1:B:252:GLU:N	2.38	0.51
1:A:26:LEU:HD23	1:A:322:LEU:HD13	1.91	0.51
1:G:239:LEU:HG	1:G:240:ILE:HG12	1.92	0.51
1:A:324:ILE:HD11	1:A:339:LEU:HD11	1.92	0.51
1:D:23:VAL:HG22	1:D:33:VAL:HG11	1.93	0.51
1:C:159:LEU:HB3	1:C:191:ALA:HB2	1.93	0.51
1:D:353:GLU:HG2	1:D:363:TYR:CZ	2.45	0.51
1:I:244:LYS:H	1:I:244:LYS:HD2	1.76	0.51
1:E:67:ALA:O	1:E:85:ARG:NH2	2.40	0.51
1:F:23:VAL:HG11	1:F:55:ALA:HB2	1.93	0.51
1:G:184:LYS:NZ	3:G:503:HOH:O	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:176:GLY:HA3	2:A:401:A1EP0:O9	2.12	0.50
1:J:67:ALA:O	1:J:85:ARG:NH2	2.42	0.50
1:K:65:TRP:O	1:K:85:ARG:NH1	2.39	0.50
1:G:60:LYS:HB3	1:G:62:GLU:HG2	1.94	0.50
1:H:24:MET:O	1:H:28:LYS:HG2	2.11	0.50
1:H:169:LYS:NZ	1:H:230:GLU:O	2.43	0.50
1:I:142:GLN:O	1:I:146:GLN:HG3	2.11	0.50
1:J:359:HIS:HB3	1:J:361:MET:HE3	1.92	0.50
1:A:14:ASN:HB3	1:A:42:GLY:HA3	1.94	0.50
1:B:302:PRO:HD3	2:B:401:A1EP0:N1	2.27	0.50
1:D:244:LYS:HE2	1:D:358:ALA:HB1	1.93	0.50
1:H:10:LYS:HG2	1:H:77:LEU:HD11	1.91	0.50
1:E:162:VAL:HG21	1:L:312:ALA:HB2	1.93	0.50
1:D:13:GLU:OE1	1:D:300:ASN:ND2	2.41	0.50
1:J:302:PRO:HD2	2:J:401:A1EP0:N1	2.27	0.49
1:B:67:ALA:O	1:B:85:ARG:NH2	2.39	0.49
1:B:268:ILE:HG12	1:B:297:ALA:HB1	1.92	0.49
1:D:24:MET:O	1:D:28:LYS:HG2	2.11	0.49
1:I:126:LEU:HD13	1:I:129:LEU:HD12	1.94	0.49
1:H:48:SER:OG	1:H:52:LYS:NZ	2.46	0.49
1:L:239:LEU:HD22	1:L:240:ILE:H	1.78	0.49
1:H:268:ILE:HD12	1:H:268:ILE:H	1.78	0.49
1:A:219:GLU:HG3	1:A:224:ILE:HD11	1.95	0.49
1:E:149:GLU:OE2	1:L:142:GLN:NE2	2.43	0.49
1:I:162:VAL:HG21	1:J:312:ALA:HB2	1.95	0.48
1:C:23:VAL:HG11	1:C:55:ALA:HB2	1.95	0.48
1:A:26:LEU:HD21	1:A:318:ILE:HD11	1.95	0.48
1:A:337:PRO:O	1:A:341:LYS:HG2	2.14	0.48
1:D:326:ASN:HB3	1:G:86:PRO:HB2	1.95	0.48
1:D:47:ASP:HB3	1:D:57:ILE:HG12	1.96	0.48
1:B:65:TRP:HA	1:B:70:VAL:HG11	1.96	0.48
1:C:278:ASP:OD1	1:C:278:ASP:N	2.39	0.48
1:G:265:ASP:HB3	1:G:268:ILE:HG13	1.96	0.48
1:H:23:VAL:HG22	1:H:33:VAL:HG11	1.95	0.48
1:H:284:ASP:OD1	1:H:284:ASP:N	2.45	0.48
1:J:333:CYS:SG	1:J:343:ILE:HD11	2.53	0.47
1:I:155:LYS:HG3	1:I:157:ILE:HG23	1.96	0.47
1:L:75:GLU:H	1:L:75:GLU:CD	2.23	0.47
1:A:2:LYS:HG3	1:A:34:TYR:CE2	2.49	0.47
1:B:43:SER:OG	1:B:310:THR:HG21	2.15	0.47
1:D:307:ARG:HA	1:D:307:ARG:HH11	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:267:ALA:HB2	2:F:401:A1EP0:O14	2.15	0.47
1:H:134:GLU:O	1:H:138:ARG:HG2	2.15	0.47
1:I:343:ILE:HG22	1:I:351:VAL:HG21	1.95	0.47
1:L:236:GLY:O	1:L:266:VAL:HG22	2.14	0.47
1:G:23:VAL:HG11	1:G:55:ALA:HB2	1.97	0.47
1:G:320:TYR:HE1	1:G:336:ASN:HD21	1.63	0.47
1:L:94:LEU:HB3	1:L:96:LEU:HG	1.96	0.47
1:A:327:LYS:HD3	1:A:332:ALA:HA	1.96	0.47
1:G:93:TYR:OH	1:G:128:LEU:O	2.24	0.47
1:K:23:VAL:HG11	1:K:55:ALA:HB2	1.96	0.47
1:C:132:MET:HE3	1:C:313:LEU:HB2	1.96	0.46
1:G:239:LEU:HB3	2:G:401:A1EP0:O8	2.15	0.46
1:J:142:GLN:O	1:J:146:GLN:HG3	2.16	0.46
1:B:337:PRO:O	1:B:341:LYS:HG3	2.16	0.46
1:D:324:ILE:HG12	1:D:339:LEU:HD21	1.98	0.46
1:K:10:LYS:HE2	1:K:10:LYS:H	1.80	0.46
1:L:197:ASP:OD1	1:L:198:ILE:N	2.49	0.46
1:D:48:SER:O	1:D:52:LYS:HG2	2.16	0.46
1:I:132:MET:HE3	1:I:313:LEU:HB2	1.98	0.46
1:I:150:LYS:HD2	1:I:154:GLY:O	2.16	0.46
1:A:76:PRO:HB2	1:A:84:PHE:HZ	1.80	0.46
1:G:345:THR:HG22	1:G:350:ILE:HD13	1.96	0.46
1:H:225:PRO:HB3	1:H:253:MET:HE2	1.98	0.46
1:D:132:MET:HE3	1:D:313:LEU:HB2	1.98	0.46
1:I:23:VAL:HG11	1:I:55:ALA:HB2	1.98	0.46
1:L:31:HIS:NE2	1:L:326:ASN:OD1	2.42	0.46
1:D:104:LYS:HE2	1:D:361:MET:HE2	1.97	0.46
1:I:23:VAL:HG22	1:I:33:VAL:HG11	1.97	0.46
1:J:132:MET:HE2	1:J:313:LEU:HB2	1.97	0.46
1:L:351:VAL:HB	1:L:366:VAL:HB	1.97	0.46
1:B:60:LYS:HG3	1:B:62:GLU:H	1.81	0.46
1:H:31:HIS:NE2	1:H:326:ASN:OD1	2.45	0.46
1:A:2:LYS:HG3	1:A:34:TYR:HE2	1.82	0.45
1:A:314:THR:HA	1:A:317:THR:HG22	1.97	0.45
1:C:333:CYS:SG	1:C:343:ILE:HD11	2.57	0.45
1:J:227:CYS:O	1:J:231:SER:OG	2.25	0.45
1:L:1:MET:HE3	1:L:1:MET:HB3	1.72	0.45
1:J:72:LYS:NZ	3:J:504:HOH:O	2.37	0.45
1:L:201:GLU:OE1	1:L:204:ARG:NH1	2.49	0.45
1:A:159:LEU:HB3	1:A:191:ALA:HB2	1.97	0.45
1:C:120:GLN:HB3	1:C:341:LYS:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:176:GLY:HA3	2:H:401:A1EP0:O7	2.16	0.45
1:H:133:SER:HB3	2:H:401:A1EP0:O5	2.15	0.45
1:A:123:ASN:N	3:A:503:HOH:O	2.49	0.45
1:F:284:ASP:OD1	1:F:284:ASP:N	2.50	0.45
1:K:268:ILE:HG13	1:K:280:VAL:HG22	1.99	0.45
1:A:227:CYS:O	1:A:231:SER:OG	2.19	0.45
1:A:327:LYS:HE2	1:A:327:LYS:HB3	1.80	0.45
1:H:330:ARG:HH11	1:H:370:LEU:HA	1.80	0.45
1:K:155:LYS:HG3	1:K:157:ILE:HG23	1.99	0.45
1:D:128:LEU:HD23	1:D:316:VAL:HG12	1.97	0.45
1:B:132:MET:HE3	1:B:313:LEU:HB2	1.99	0.45
1:D:24:MET:HA	1:D:27:VAL:HG22	1.99	0.45
1:H:333:CYS:SG	1:H:343:ILE:HD11	2.56	0.45
1:K:238:VAL:HB	1:K:273:ILE:HG21	1.98	0.45
1:L:84:PHE:O	1:L:109:GLN:NE2	2.43	0.45
1:L:140:SER:HA	1:L:301:MET:HE1	1.99	0.45
1:C:180:THR:HG22	1:C:184:LYS:HE3	1.99	0.45
1:D:159:LEU:HB3	1:D:191:ALA:HB2	1.99	0.45
1:K:23:VAL:HG22	1:K:33:VAL:HG11	1.99	0.45
1:A:9:ILE:HG23	1:A:77:LEU:HD12	2.00	0.44
1:B:176:GLY:HA3	2:B:401:A1EP0:O9	2.17	0.44
1:F:31:HIS:NE2	1:F:326:ASN:OD1	2.41	0.44
1:B:351:VAL:HB	1:B:366:VAL:HB	1.99	0.44
1:C:159:LEU:O	1:C:168:GLY:N	2.47	0.44
1:E:159:LEU:HB3	1:E:191:ALA:HB2	1.98	0.44
1:G:265:ASP:HB3	1:G:268:ILE:CG1	2.47	0.44
1:H:155:LYS:HG3	1:H:157:ILE:HG23	1.99	0.44
1:B:79:GLU:OE1	1:B:79:GLU:N	2.43	0.44
1:B:134:GLU:O	1:B:138:ARG:HD3	2.17	0.44
1:D:333:CYS:SG	1:D:343:ILE:HD11	2.57	0.44
1:G:287:THR:HG22	1:G:296:TYR:HA	1.99	0.44
1:C:351:VAL:HB	1:C:366:VAL:HB	1.98	0.44
1:K:333:CYS:SG	1:K:343:ILE:HD11	2.58	0.44
1:A:96:LEU:HD13	1:A:344:ASN:ND2	2.31	0.44
1:L:296:TYR:CE2	1:L:301:MET:HE3	2.52	0.44
1:A:58:VAL:HG12	1:A:60:LYS:H	1.82	0.44
1:G:282:THR:HG23	1:G:285:ASP:H	1.83	0.44
1:A:166:ARG:HG3	1:L:217:LEU:HD21	2.00	0.44
1:F:126:LEU:HD13	1:F:129:LEU:HD12	1.99	0.44
1:F:142:GLN:O	1:F:146:GLN:HG3	2.18	0.43
1:D:134:GLU:O	1:D:138:ARG:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:290:LYS:HD2	1:B:291:HIS:CD2	2.53	0.43
1:E:69:MET:HA	1:E:89:ILE:HB	1.98	0.43
1:I:10:LYS:HD2	1:I:77:LEU:HD11	1.99	0.43
1:I:306:PRO:HD2	1:J:156:GLY:HA3	2.00	0.43
1:J:203:LEU:HD22	1:J:216:THR:HB	2.00	0.43
1:A:115:ALA:HB1	1:A:117:GLU:CD	2.44	0.43
1:D:351:VAL:HB	1:D:366:VAL:HB	2.00	0.43
1:G:177:THR:HB	2:G:401:A1EP0:O5	2.19	0.43
1:I:351:VAL:HB	1:I:366:VAL:HB	2.00	0.43
1:K:265:ASP:HB2	1:K:274:PHE:CE2	2.53	0.43
1:A:149:GLU:OE2	1:D:142:GLN:NE2	2.48	0.43
1:A:174:GLY:O	1:A:179:GLY:HA3	2.18	0.43
1:A:197:ASP:OD2	2:A:401:A1EP0:O13	2.37	0.43
1:C:327:LYS:HG2	1:I:86:PRO:HB2	2.00	0.43
1:E:333:CYS:SG	1:E:343:ILE:HD11	2.58	0.43
1:A:302:PRO:HD3	2:A:401:A1EP0:N1	2.34	0.43
1:B:138:ARG:HG3	1:B:185:ILE:CD1	2.49	0.43
1:E:177:THR:HB	2:E:401:A1EP0:O5	2.19	0.43
1:F:333:CYS:SG	1:F:343:ILE:HD11	2.59	0.43
1:G:330:ARG:HG3	1:G:370:LEU:HD22	2.00	0.43
1:H:180:THR:HG22	1:H:184:LYS:HE2	2.00	0.43
1:I:366:VAL:HG22	1:I:370:LEU:HD13	2.01	0.43
1:K:7:LYS:HG3	1:K:39:ALA:HA	2.01	0.43
1:I:255:ARG:HE	1:I:291:HIS:CD2	2.36	0.43
1:K:202:ARG:HA	1:K:202:ARG:HD2	1.91	0.43
1:A:60:LYS:HE3	1:A:60:LYS:HB2	1.87	0.42
1:A:327:LYS:NZ	1:A:335:ASP:HB2	2.33	0.42
1:D:298:VAL:O	1:D:301:MET:HG3	2.19	0.42
1:D:197:ASP:OD2	2:D:401:A1EP0:O13	2.37	0.42
1:I:217:LEU:HD12	1:I:217:LEU:HA	1.89	0.42
1:B:11:ASN:O	1:B:300:ASN:ND2	2.52	0.42
1:C:96:LEU:O	1:C:359:HIS:NE2	2.39	0.42
1:F:236:GLY:O	1:F:266:VAL:HG22	2.18	0.42
2:J:401:A1EP0:N4	3:J:503:HOH:O	2.37	0.42
1:I:350:ILE:HD11	1:I:361:MET:HE3	2.02	0.42
1:J:14:ASN:HB3	1:J:42:GLY:HA3	2.02	0.42
1:J:23:VAL:HG11	1:J:55:ALA:HB2	2.00	0.42
1:C:155:LYS:HE3	1:C:155:LYS:HB2	1.79	0.42
1:F:24:MET:HA	1:F:27:VAL:HG22	2.02	0.42
1:G:138:ARG:HG3	1:G:181:ASN:HB3	2.02	0.42
1:G:266:VAL:HG12	1:G:301:MET:HE1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:80:GLU:HA	1:A:83:TYR:HD2	1.83	0.42
1:B:138:ARG:HD2	1:B:181:ASN:HB3	2.01	0.42
1:F:196:LEU:HG	1:F:217:LEU:HB3	2.01	0.42
1:G:265:ASP:HB2	1:G:274:PHE:CE2	2.54	0.42
1:B:217:LEU:HD12	1:B:217:LEU:HA	1.89	0.42
2:E:401:A1EP0:N4	3:E:501:HOH:O	2.37	0.42
1:G:265:ASP:HB2	1:G:274:PHE:HE2	1.84	0.42
1:J:207:ASP:OD2	1:L:184:LYS:NZ	2.53	0.42
1:L:296:TYR:CZ	1:L:298:VAL:HB	2.54	0.42
1:A:93:TYR:CE1	1:A:116:TYR:HB2	2.55	0.42
1:A:217:LEU:HD11	1:L:166:ARG:HG3	2.01	0.42
1:E:312:ALA:HB2	1:L:162:VAL:HG11	2.02	0.42
1:J:159:LEU:HD23	1:J:159:LEU:HA	1.86	0.42
1:C:225:PRO:HB3	1:C:253:MET:HE2	2.02	0.42
1:D:14:ASN:HB2	1:D:306:PRO:HG3	2.01	0.42
1:F:119:VAL:O	1:F:127:PRO:HD2	2.20	0.42
1:I:323:GLN:O	1:I:327:LYS:HD3	2.20	0.42
1:L:67:ALA:O	1:L:85:ARG:NH2	2.53	0.42
1:H:130:THR:N	1:H:131:PRO:HD2	2.34	0.42
1:L:132:MET:HE3	1:L:313:LEU:HB2	2.02	0.41
1:D:217:LEU:HD12	1:D:217:LEU:HA	1.92	0.41
1:F:225:PRO:HB3	1:F:253:MET:HG2	2.01	0.41
1:K:93:TYR:CD1	1:K:116:TYR:HB2	2.56	0.41
1:K:159:LEU:HD23	1:K:159:LEU:HA	1.88	0.41
1:L:239:LEU:HD23	1:L:245:ALA:HB2	2.01	0.41
1:A:159:LEU:HD23	1:A:159:LEU:HA	1.94	0.41
1:B:119:VAL:O	1:B:127:PRO:HD2	2.20	0.41
1:D:11:ASN:ND2	1:D:284:ASP:OD2	2.40	0.41
1:D:302:PRO:HD3	2:D:401:A1EP0:N1	2.34	0.41
1:G:219:GLU:HG3	1:G:224:ILE:HD11	2.02	0.41
1:L:302:PRO:HD2	2:L:401:A1EP0:O1	2.19	0.41
1:A:52:LYS:HE3	1:A:52:LYS:HB3	1.68	0.41
1:C:244:LYS:HE2	1:C:358:ALA:HB1	2.03	0.41
1:K:266:VAL:HG12	2:K:401:A1EP0:C20	2.50	0.41
1:G:279:ARG:HD2	1:G:281:THR:HG22	2.02	0.41
1:H:330:ARG:NH1	1:H:370:LEU:HA	2.36	0.41
1:G:227:CYS:O	1:G:231:SER:OG	2.28	0.41
1:L:89:ILE:HD13	1:L:112:VAL:HB	2.03	0.41
1:B:174:GLY:O	1:B:179:GLY:HA3	2.20	0.41
1:D:196:LEU:HA	1:D:217:LEU:O	2.20	0.41
1:I:94:LEU:HB3	1:I:96:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:10:LYS:H	1:K:10:LYS:CE	2.34	0.41
1:A:13:GLU:OE1	1:A:300:ASN:HB2	2.21	0.41
1:B:307:ARG:HD2	1:B:307:ARG:HA	1.94	0.41
1:E:150:LYS:HD2	1:E:154:GLY:O	2.20	0.41
1:G:27:VAL:HG21	1:G:53:ALA:O	2.21	0.41
1:G:225:PRO:HB3	1:G:253:MET:HE2	2.03	0.41
1:B:24:MET:O	1:B:28:LYS:HD2	2.21	0.41
1:B:159:LEU:HD23	1:B:159:LEU:HA	1.78	0.41
1:C:255:ARG:HG3	1:C:291:HIS:CD2	2.56	0.41
1:D:104:LYS:HG2	1:D:361:MET:HE1	2.02	0.41
1:F:239:LEU:HB2	2:F:401:A1EP0:C18	2.51	0.41
1:F:351:VAL:HB	1:F:366:VAL:HB	2.01	0.41
1:I:333:CYS:HB3	1:I:340:LEU:HD13	2.03	0.41
1:J:296:TYR:CZ	1:J:298:VAL:HB	2.56	0.41
1:A:217:LEU:HD12	1:A:217:LEU:HA	1.85	0.41
1:G:121:LEU:HB2	1:G:123:ASN:OD1	2.21	0.41
1:H:10:LYS:HD3	1:H:74:LYS:HD3	2.02	0.41
1:H:222:TYR:O	1:H:226:GLU:HG2	2.21	0.40
1:I:239:LEU:HB2	2:I:401:A1EP0:C18	2.52	0.40
1:L:96:LEU:HD12	1:L:344:ASN:HB3	2.03	0.40
1:D:250:THR:OG1	1:D:252:GLU:HG2	2.21	0.40
1:E:181:ASN:HA	1:E:184:LYS:HD2	2.02	0.40
1:D:320:TYR:O	1:D:324:ILE:HG13	2.22	0.40
1:H:302:PRO:HD2	2:H:401:A1EP0:N1	2.37	0.40
1:F:330:ARG:HG3	1:F:370:LEU:HD22	2.04	0.40
1:I:75:GLU:H	1:I:75:GLU:CD	2.30	0.40
1:J:351:VAL:HB	1:J:366:VAL:HB	2.03	0.40
1:A:19:THR:HG23	1:A:314:THR:HG21	2.03	0.40
1:A:31:HIS:NE2	1:A:326:ASN:HB3	2.36	0.40
1:B:70:VAL:HG23	1:B:90:LEU:HD13	2.04	0.40
1:B:107:VAL:O	1:B:348:GLY:HA2	2.22	0.40
1:C:139:MET:HE2	1:C:139:MET:HB3	1.95	0.40
1:L:142:GLN:O	1:L:146:GLN:HG3	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	369/372 (99%)	364 (99%)	5 (1%)	0	100	100
1	B	369/372 (99%)	365 (99%)	4 (1%)	0	100	100
1	C	369/372 (99%)	362 (98%)	7 (2%)	0	100	100
1	D	369/372 (99%)	366 (99%)	3 (1%)	0	100	100
1	E	369/372 (99%)	365 (99%)	4 (1%)	0	100	100
1	F	369/372 (99%)	365 (99%)	4 (1%)	0	100	100
1	G	369/372 (99%)	364 (99%)	5 (1%)	0	100	100
1	H	369/372 (99%)	367 (100%)	2 (0%)	0	100	100
1	I	369/372 (99%)	367 (100%)	2 (0%)	0	100	100
1	J	369/372 (99%)	367 (100%)	2 (0%)	0	100	100
1	K	369/372 (99%)	366 (99%)	3 (1%)	0	100	100
1	L	369/372 (99%)	364 (99%)	4 (1%)	1 (0%)	36	44
All	All	4428/4464 (99%)	4382 (99%)	45 (1%)	1 (0%)	100	100

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	L	178	ALA

### 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	290/290 (100%)	282 (97%)	8 (3%)	38	54
1	B	290/290 (100%)	283 (98%)	7 (2%)	43	59
1	C	290/290 (100%)	283 (98%)	7 (2%)	43	59
1	D	290/290 (100%)	285 (98%)	5 (2%)	53	68
1	E	290/290 (100%)	284 (98%)	6 (2%)	47	63
1	F	290/290 (100%)	286 (99%)	4 (1%)	59	73
1	G	290/290 (100%)	287 (99%)	3 (1%)	68	78
1	H	290/290 (100%)	286 (99%)	4 (1%)	59	73
1	I	290/290 (100%)	283 (98%)	7 (2%)	43	59
1	J	290/290 (100%)	290 (100%)	0	100	100
1	K	290/290 (100%)	286 (99%)	4 (1%)	59	73
1	L	290/290 (100%)	283 (98%)	7 (2%)	43	59
All	All	3480/3480 (100%)	3418 (98%)	62 (2%)	51	67

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	A	102	LEU
1	A	279	ARG
1	A	305	VAL
1	A	340	LEU
1	A	343	ILE
1	A	355	VAL
1	A	364	THR
1	B	28	LYS
1	B	60	LYS
1	B	74	LYS
1	B	157	ILE
1	B	244	LYS
1	B	290	LYS
1	B	355	VAL
1	C	1	MET
1	C	79	GLU
1	C	129	LEU
1	C	238	VAL
1	C	278	ASP
1	C	279	ARG
1	C	355	VAL

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Mol	Chain	Res	Type
1	D	79	GLU
1	D	91	PHE
1	D	300	ASN
1	D	305	VAL
1	D	308	THR
1	E	75	GLU
1	E	108	GLU
1	E	129	LEU
1	E	157	ILE
1	E	162	VAL
1	E	269	ASP
1	F	79	GLU
1	F	157	ILE
1	F	162	VAL
1	F	284	ASP
1	G	38	GLU
1	G	270	GLN
1	G	284	ASP
1	H	74	LYS
1	H	268	ILE
1	H	284	ASP
1	H	355	VAL
1	I	123	ASN
1	I	201	GLU
1	I	217	LEU
1	I	238	VAL
1	I	284	ASP
1	I	327	LYS
1	I	353	GLU
1	K	48	SER
1	K	146	GLN
1	K	252	GLU
1	K	284	ASP
1	L	1	MET
1	L	79	GLU
1	L	108	GLU
1	L	162	VAL
1	L	177	THR
1	L	239	LEU
1	L	371	GLN

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



Mol	Chain	Res	Type
1	A	12	ASN
1	A	14	ASN
1	A	31	HIS
1	A	109	GLN
1	A	146	GLN
1	A	291	HIS
1	A	315	ASN
1	A	326	ASN
1	A	344	ASN
1	B	213	GLN
1	C	109	GLN
1	C	146	GLN
1	C	152	HIS
1	D	152	HIS
1	D	336	ASN
1	E	152	HIS
1	E	283	HIS
1	F	152	HIS
1	G	12	ASN
1	G	283	HIS
1	G	336	ASN
1	G	367	HIS
1	H	109	GLN
1	H	152	HIS
1	I	291	HIS
1	I	349	HIS
1	J	367	HIS
1	K	11	ASN
1	K	14	ASN
1	K	213	GLN
1	K	336	ASN
1	L	213	GLN
1	L	283	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

12 ligands are modelled in this entry.

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
2	A1EP0	I	401	-	42,45,45	0.59	1 (2%)	58,68,68	0.69	2 (3%)
2	A1EP0	K	401	-	42,45,45	0.61	1 (2%)	58,68,68	0.64	1 (1%)
2	A1EP0	L	401	-	42,45,45	0.56	1 (2%)	58,68,68	0.80	1 (1%)
2	A1EP0	G	401	-	42,45,45	0.61	1 (2%)	58,68,68	0.65	1 (1%)
2	A1EP0	J	401	-	42,45,45	0.61	1 (2%)	58,68,68	0.61	1 (1%)
2	A1EP0	C	401	-	42,45,45	0.58	1 (2%)	58,68,68	0.72	0
2	A1EP0	B	401	-	42,45,45	0.57	1 (2%)	58,68,68	0.70	1 (1%)
2	A1EP0	D	401	-	42,45,45	0.56	1 (2%)	58,68,68	0.75	3 (5%)
2	A1EP0	A	401	-	42,45,45	0.59	1 (2%)	58,68,68	0.71	0
2	A1EP0	E	401	-	42,45,45	0.57	1 (2%)	58,68,68	0.65	1 (1%)
2	A1EP0	F	401	-	42,45,45	0.58	1 (2%)	58,68,68	0.63	0
2	A1EP0	H	401	-	42,45,45	0.58	1 (2%)	58,68,68	0.68	1 (1%)

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
2	A1EP0	I	401	-	-	10/30/62/62	0/4/4/4
2	A1EP0	K	401	-	-	16/30/62/62	0/4/4/4
2	A1EP0	L	401	-	-	8/30/62/62	0/4/4/4
2	A1EP0	G	401	-	-	10/30/62/62	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	A1EP0	J	401	-	-	15/30/62/62	0/4/4/4
2	A1EP0	C	401	-	-	6/30/62/62	0/4/4/4
2	A1EP0	B	401	-	-	8/30/62/62	0/4/4/4
2	A1EP0	D	401	-	-	8/30/62/62	0/4/4/4
2	A1EP0	A	401	-	-	8/30/62/62	0/4/4/4
2	A1EP0	E	401	-	-	13/30/62/62	0/4/4/4
2	A1EP0	F	401	-	-	17/30/62/62	0/4/4/4
2	A1EP0	H	401	-	-	11/30/62/62	0/4/4/4

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	J	401	A1EP0	C20-N2	2.62	1.38	1.35
2	G	401	A1EP0	C20-N2	2.55	1.38	1.35
2	E	401	A1EP0	C20-N2	2.55	1.38	1.35
2	I	401	A1EP0	C20-N2	2.55	1.38	1.35
2	H	401	A1EP0	C20-N2	2.54	1.38	1.35
2	K	401	A1EP0	C20-N2	2.49	1.38	1.35
2	F	401	A1EP0	C20-N2	2.42	1.37	1.35
2	C	401	A1EP0	C20-N2	2.39	1.37	1.35
2	A	401	A1EP0	C20-N2	2.38	1.37	1.35
2	D	401	A1EP0	C20-N2	2.33	1.37	1.35
2	B	401	A1EP0	C20-N2	2.29	1.37	1.35
2	L	401	A1EP0	C20-N2	2.24	1.37	1.35

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	401	A1EP0	C18-C19-C6	-3.16	96.21	100.98
2	D	401	A1EP0	O2-C6-C19	-2.35	103.49	106.93
2	D	401	A1EP0	C18-C19-C6	-2.33	97.46	100.98
2	H	401	A1EP0	O2-C6-C19	-2.22	103.68	106.93
2	I	401	A1EP0	C18-C19-C6	-2.22	97.64	100.98
2	E	401	A1EP0	O2-C6-C19	-2.20	103.71	106.93
2	K	401	A1EP0	C5-N2-C20	-2.14	120.02	121.97
2	J	401	A1EP0	C5-N2-C20	-2.12	120.04	121.97
2	G	401	A1EP0	C5-N2-C20	-2.09	120.07	121.97
2	B	401	A1EP0	C5-N2-C20	-2.07	120.08	121.97
2	D	401	A1EP0	C5-N2-C20	-2.04	120.12	121.97
2	I	401	A1EP0	O2-C6-C19	-2.02	103.98	106.93

There are no chirality outliers.

All (130) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	A1EP0	O2-C6-N2-C5
2	A	401	A1EP0	O2-C6-N2-C20
2	A	401	A1EP0	C19-C6-N2-C5
2	A	401	A1EP0	C19-C6-N2-C20
2	B	401	A1EP0	O2-C6-N2-C5
2	B	401	A1EP0	O2-C6-N2-C20
2	B	401	A1EP0	C19-C6-N2-C5
2	B	401	A1EP0	C19-C6-N2-C20
2	C	401	A1EP0	O2-C6-N2-C5
2	C	401	A1EP0	O2-C6-N2-C20
2	C	401	A1EP0	C19-C6-N2-C5
2	C	401	A1EP0	C19-C6-N2-C20
2	C	401	A1EP0	O2-C7-C8-O3
2	D	401	A1EP0	O2-C6-N2-C5
2	D	401	A1EP0	O2-C6-N2-C20
2	D	401	A1EP0	C19-C6-N2-C5
2	D	401	A1EP0	C19-C6-N2-C20
2	E	401	A1EP0	O2-C6-N2-C5
2	E	401	A1EP0	O2-C6-N2-C20
2	E	401	A1EP0	C19-C6-N2-C5
2	E	401	A1EP0	C19-C6-N2-C20
2	E	401	A1EP0	O2-C7-C8-O3
2	E	401	A1EP0	C9-O9-P2-O6
2	E	401	A1EP0	C9-O9-P2-O7
2	F	401	A1EP0	O2-C6-N2-C5
2	F	401	A1EP0	O2-C6-N2-C20
2	F	401	A1EP0	C19-C6-N2-C5
2	F	401	A1EP0	C19-C6-N2-C20
2	F	401	A1EP0	C8-O3-P1-O4
2	F	401	A1EP0	C9-O9-P2-O6
2	F	401	A1EP0	C9-O9-P2-O7
2	G	401	A1EP0	C7-C8-O3-P1
2	G	401	A1EP0	C8-O3-P1-O4
2	H	401	A1EP0	O2-C7-C8-O3
2	H	401	A1EP0	C18-C7-C8-O3
2	I	401	A1EP0	O2-C6-N2-C5
2	I	401	A1EP0	O2-C6-N2-C20
2	I	401	A1EP0	C19-C6-N2-C5
2	I	401	A1EP0	C19-C6-N2-C20
2	I	401	A1EP0	C8-O3-P1-O4

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Mol	Chain	Res	Type	Atoms
2	I	401	A1EP0	C9-O9-P2-O7
2	I	401	A1EP0	C10-C9-O9-P2
2	J	401	A1EP0	O2-C6-N2-C5
2	J	401	A1EP0	O2-C6-N2-C20
2	J	401	A1EP0	C19-C6-N2-C5
2	J	401	A1EP0	C19-C6-N2-C20
2	J	401	A1EP0	C8-O3-P1-O4
2	J	401	A1EP0	C9-O9-P2-O7
2	K	401	A1EP0	O2-C6-N2-C5
2	K	401	A1EP0	O2-C6-N2-C20
2	K	401	A1EP0	C19-C6-N2-C5
2	K	401	A1EP0	C19-C6-N2-C20
2	K	401	A1EP0	C8-O3-P1-O4
2	L	401	A1EP0	O2-C6-N2-C5
2	L	401	A1EP0	O2-C6-N2-C20
2	L	401	A1EP0	C19-C6-N2-C5
2	L	401	A1EP0	C19-C6-N2-C20
2	A	401	A1EP0	O2-C7-C8-O3
2	H	401	A1EP0	O10-C10-C9-O9
2	H	401	A1EP0	C17-C10-C9-O9
2	J	401	A1EP0	O10-C10-C9-O9
2	J	401	A1EP0	C17-C10-C9-O9
2	K	401	A1EP0	O10-C10-C9-O9
2	K	401	A1EP0	C17-C10-C9-O9
2	E	401	A1EP0	C18-C7-C8-O3
2	F	401	A1EP0	C16-C11-N3-C12
2	J	401	A1EP0	C16-C11-N3-C12
2	H	401	A1EP0	C16-C11-N3-C12
2	K	401	A1EP0	C16-C11-N3-C12
2	F	401	A1EP0	C16-C11-N3-C15
2	J	401	A1EP0	C16-C11-N3-C15
2	J	401	A1EP0	C10-C9-O9-P2
2	G	401	A1EP0	C16-C11-N3-C12
2	F	401	A1EP0	C10-C9-O9-P2
2	H	401	A1EP0	C10-C9-O9-P2
2	K	401	A1EP0	C10-C9-O9-P2
2	F	401	A1EP0	P1-O6-P2-O9
2	H	401	A1EP0	P1-O6-P2-O9
2	J	401	A1EP0	P1-O6-P2-O9
2	K	401	A1EP0	P1-O6-P2-O9
2	B	401	A1EP0	O2-C7-C8-O3
2	H	401	A1EP0	C16-C11-N3-C15

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Mol	Chain	Res	Type	Atoms
2	K	401	A1EP0	C16-C11-N3-C15
2	E	401	A1EP0	C10-C9-O9-P2
2	F	401	A1EP0	O10-C11-N3-C15
2	J	401	A1EP0	O10-C11-N3-C15
2	F	401	A1EP0	C8-O3-P1-O6
2	G	401	A1EP0	C8-O3-P1-O6
2	I	401	A1EP0	C9-O9-P2-O6
2	F	401	A1EP0	O10-C11-N3-C12
2	J	401	A1EP0	O10-C11-N3-C12
2	K	401	A1EP0	O10-C11-N3-C12
2	K	401	A1EP0	O2-C7-C8-O3
2	E	401	A1EP0	P1-O6-P2-O7
2	E	401	A1EP0	C9-O9-P2-O8
2	H	401	A1EP0	O10-C11-N3-C12
2	H	401	A1EP0	O10-C11-N3-C15
2	G	401	A1EP0	O10-C11-N3-C12
2	K	401	A1EP0	O10-C11-N3-C15
2	F	401	A1EP0	O10-C10-C9-O9
2	G	401	A1EP0	O2-C7-C8-O3
2	I	401	A1EP0	O10-C10-C9-O9
2	G	401	A1EP0	C16-C11-N3-C15
2	A	401	A1EP0	C16-C11-N3-C12
2	D	401	A1EP0	C16-C11-N3-C12
2	L	401	A1EP0	C16-C11-N3-C12
2	G	401	A1EP0	O10-C11-N3-C15
2	B	401	A1EP0	C16-C11-N3-C12
2	G	401	A1EP0	O10-C10-C9-O9
2	L	401	A1EP0	O2-C7-C8-O3
2	F	401	A1EP0	C17-C10-C9-O9
2	G	401	A1EP0	C18-C7-C8-O3
2	D	401	A1EP0	O10-C11-N3-C12
2	L	401	A1EP0	O10-C11-N3-C12
2	A	401	A1EP0	O10-C11-N3-C12
2	F	401	A1EP0	O2-C7-C8-O3
2	K	401	A1EP0	C8-O3-P1-O6
2	A	401	A1EP0	O10-C10-C9-O9
2	C	401	A1EP0	O10-C10-C9-O9
2	E	401	A1EP0	O10-C10-C9-O9
2	J	401	A1EP0	O2-C7-C8-O3
2	L	401	A1EP0	O10-C10-C9-O9
2	E	401	A1EP0	P1-O6-P2-O8
2	H	401	A1EP0	C9-O9-P2-O7

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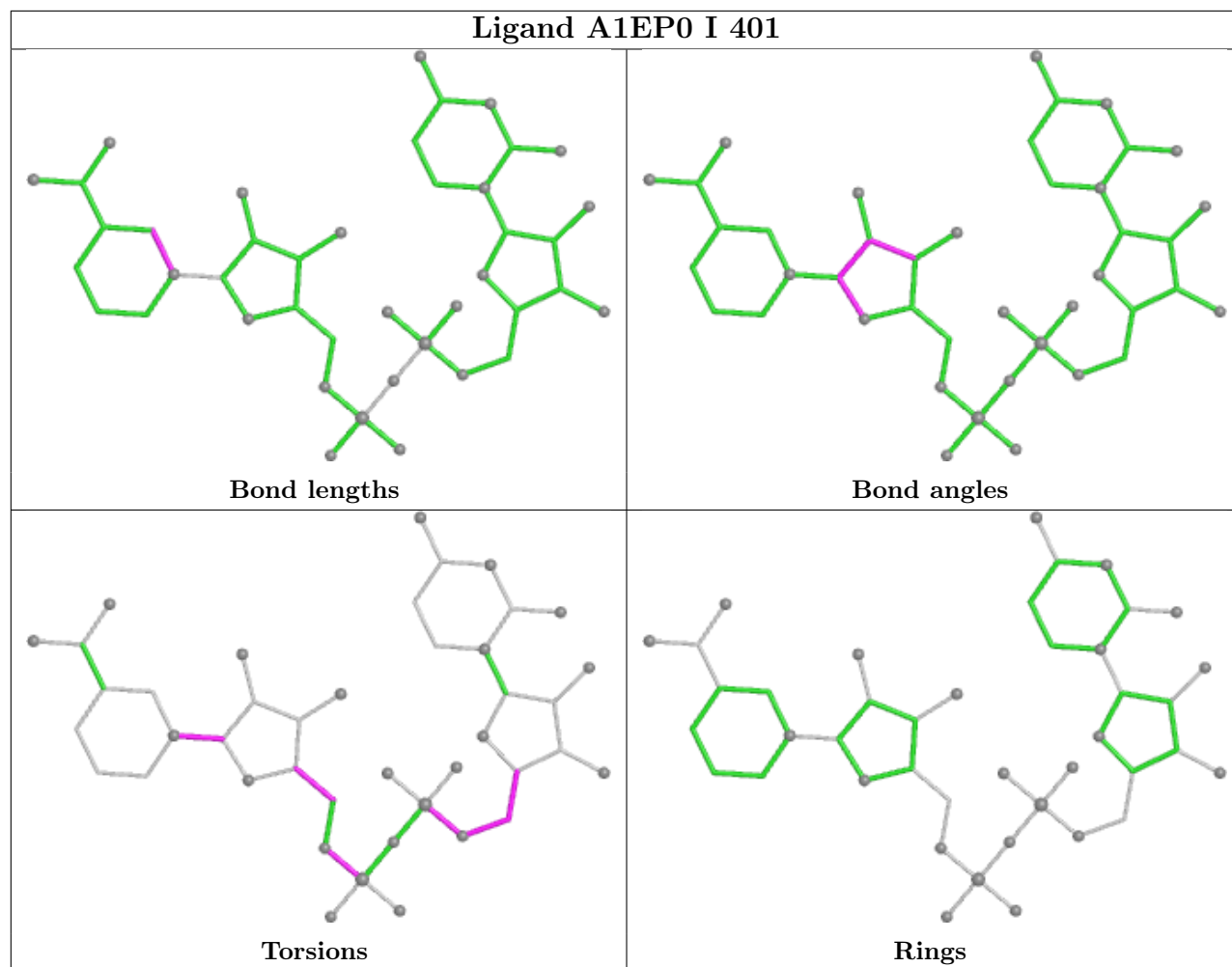
Mol	Chain	Res	Type	Atoms
2	K	401	A1EP0	C9-O9-P2-O7
2	B	401	A1EP0	O10-C10-C9-O9
2	D	401	A1EP0	O10-C10-C9-O9
2	I	401	A1EP0	O2-C7-C8-O3
2	B	401	A1EP0	O10-C11-N3-C12
2	D	401	A1EP0	C16-C11-N3-C15

There are no ring outliers.

11 monomers are involved in 32 short contacts:

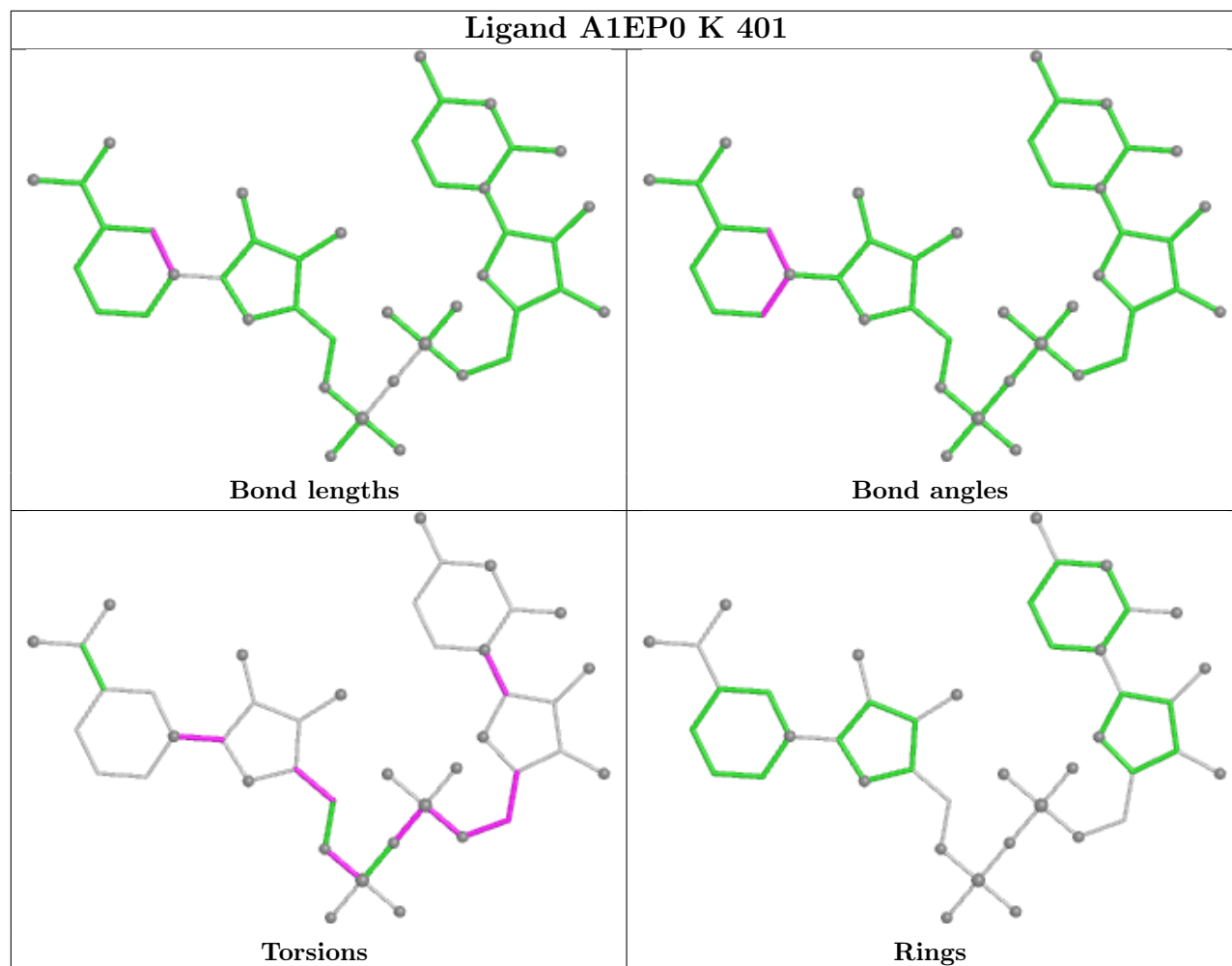
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	401	A1EP0	2	0
2	K	401	A1EP0	1	0
2	L	401	A1EP0	2	0
2	G	401	A1EP0	2	0
2	J	401	A1EP0	2	0
2	B	401	A1EP0	2	0
2	D	401	A1EP0	2	0
2	A	401	A1EP0	3	0
2	E	401	A1EP0	5	0
2	F	401	A1EP0	4	0
2	H	401	A1EP0	7	0

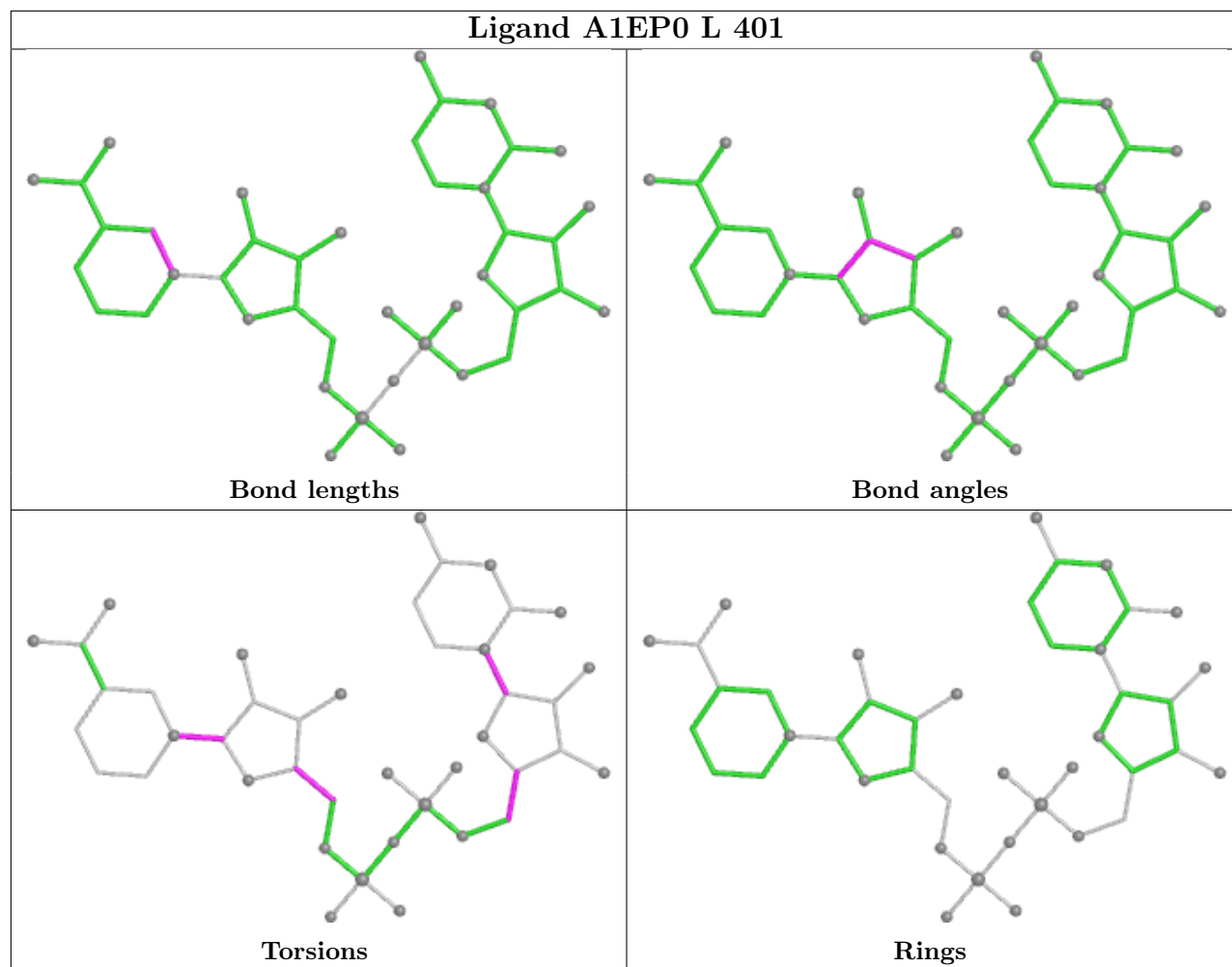
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



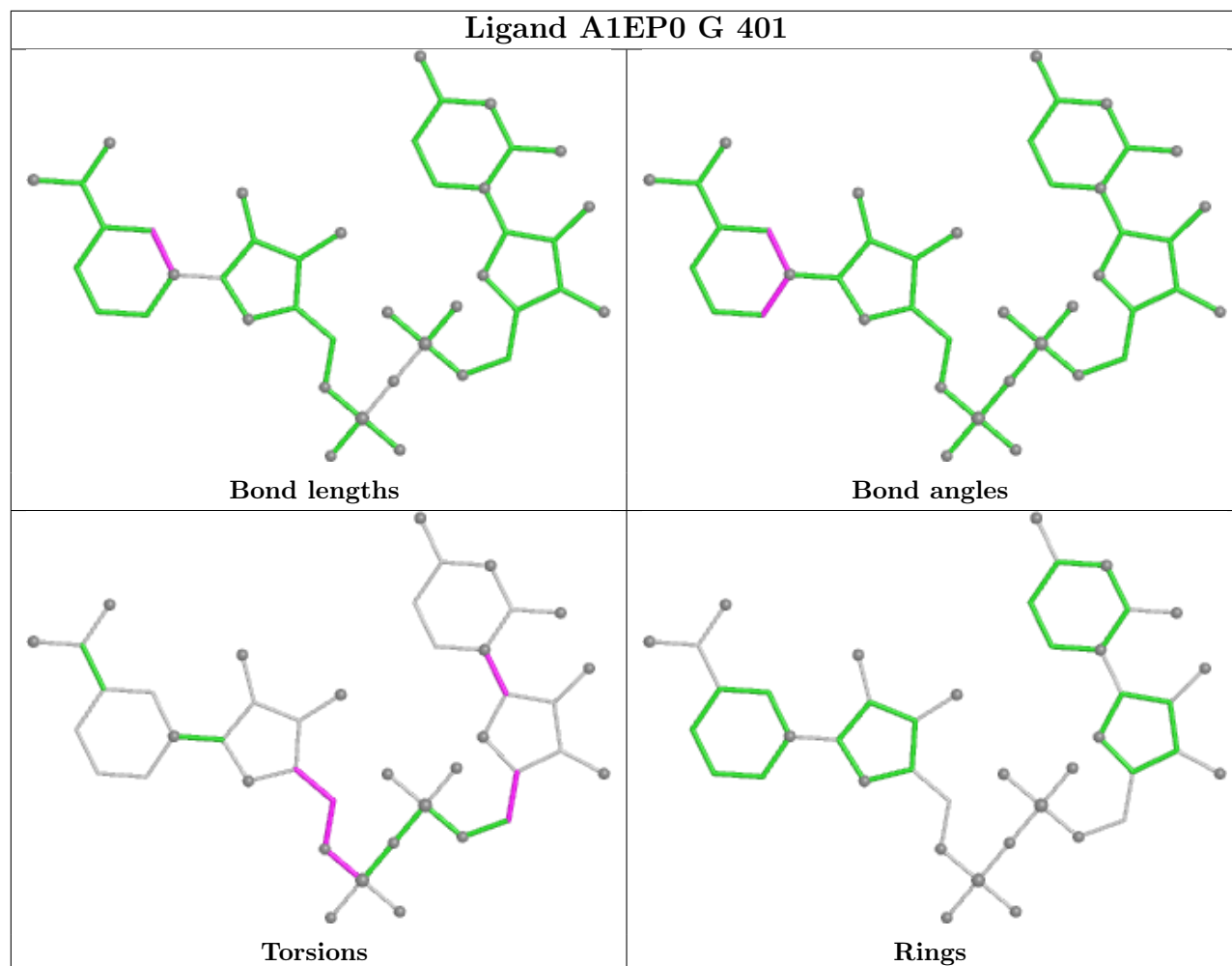


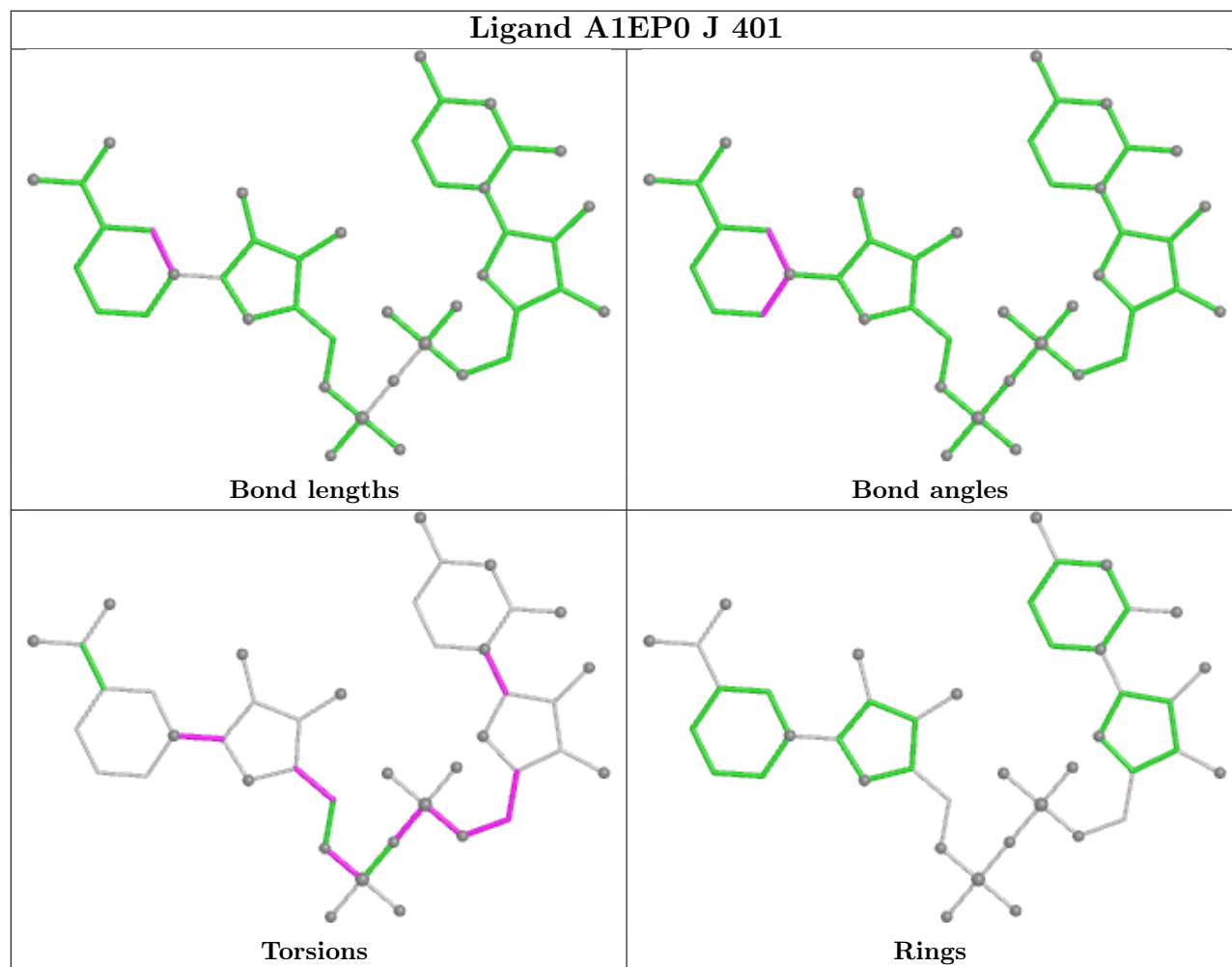
## Ligand A1EP0 K 401



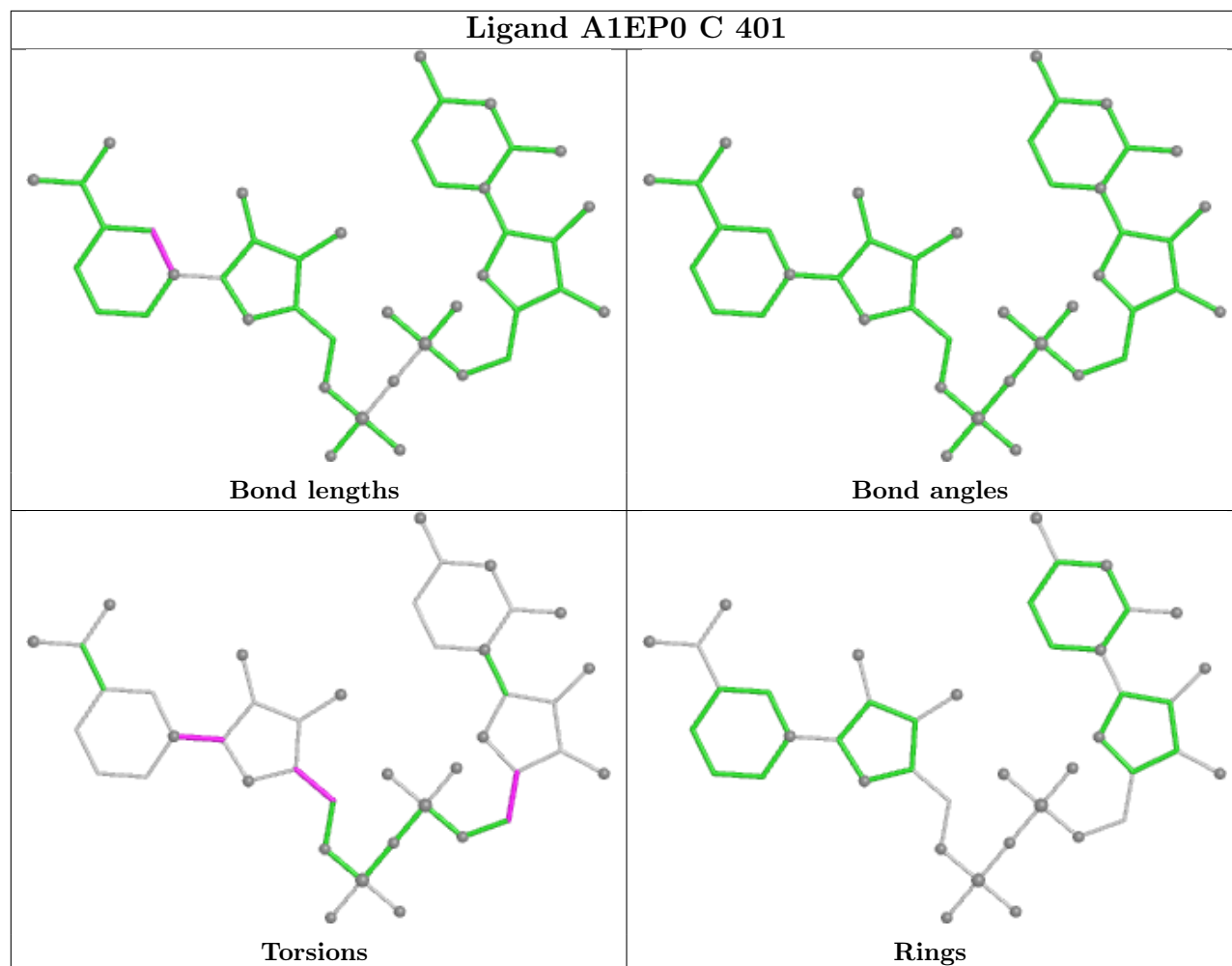


## Ligand A1EP0 G 401

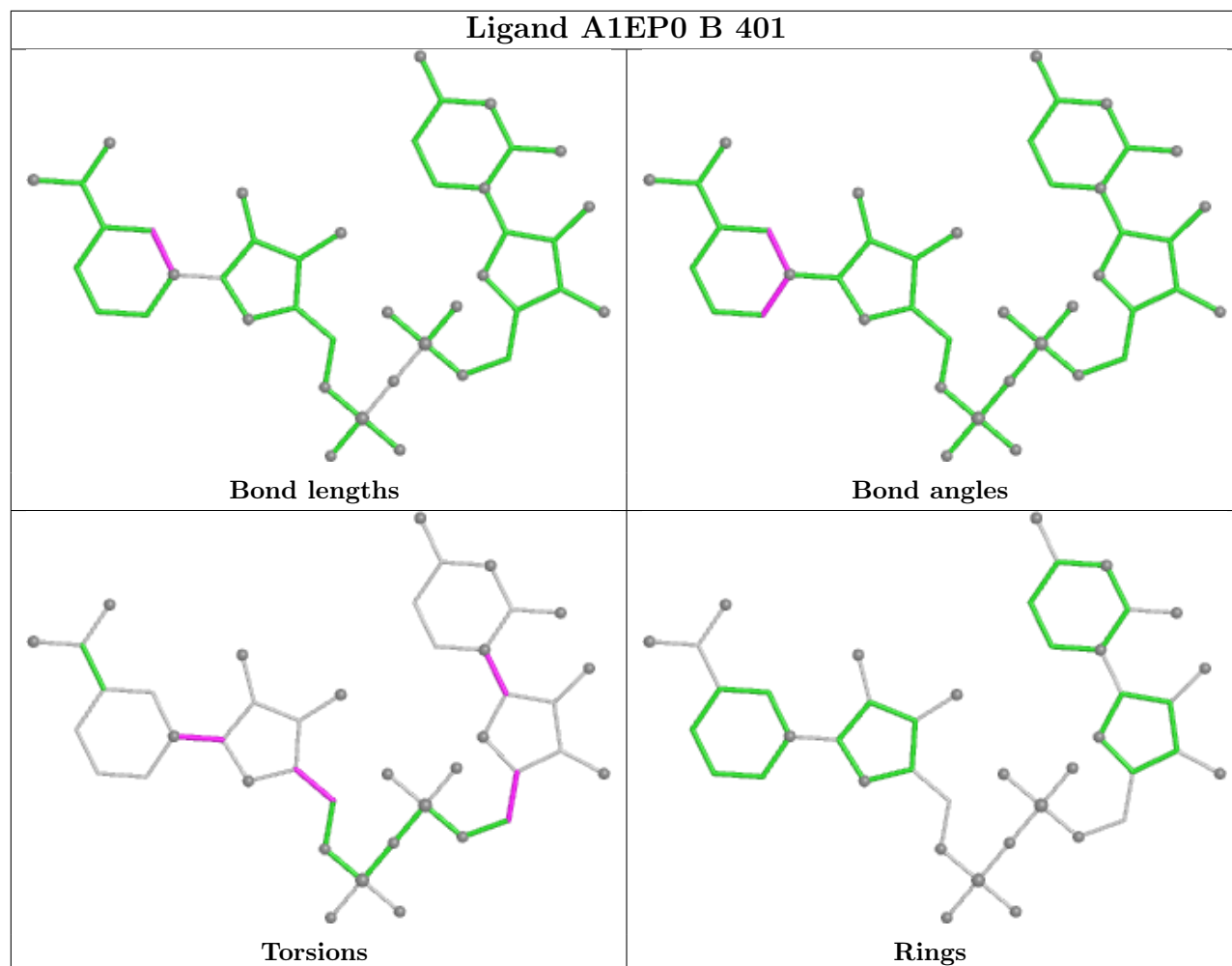




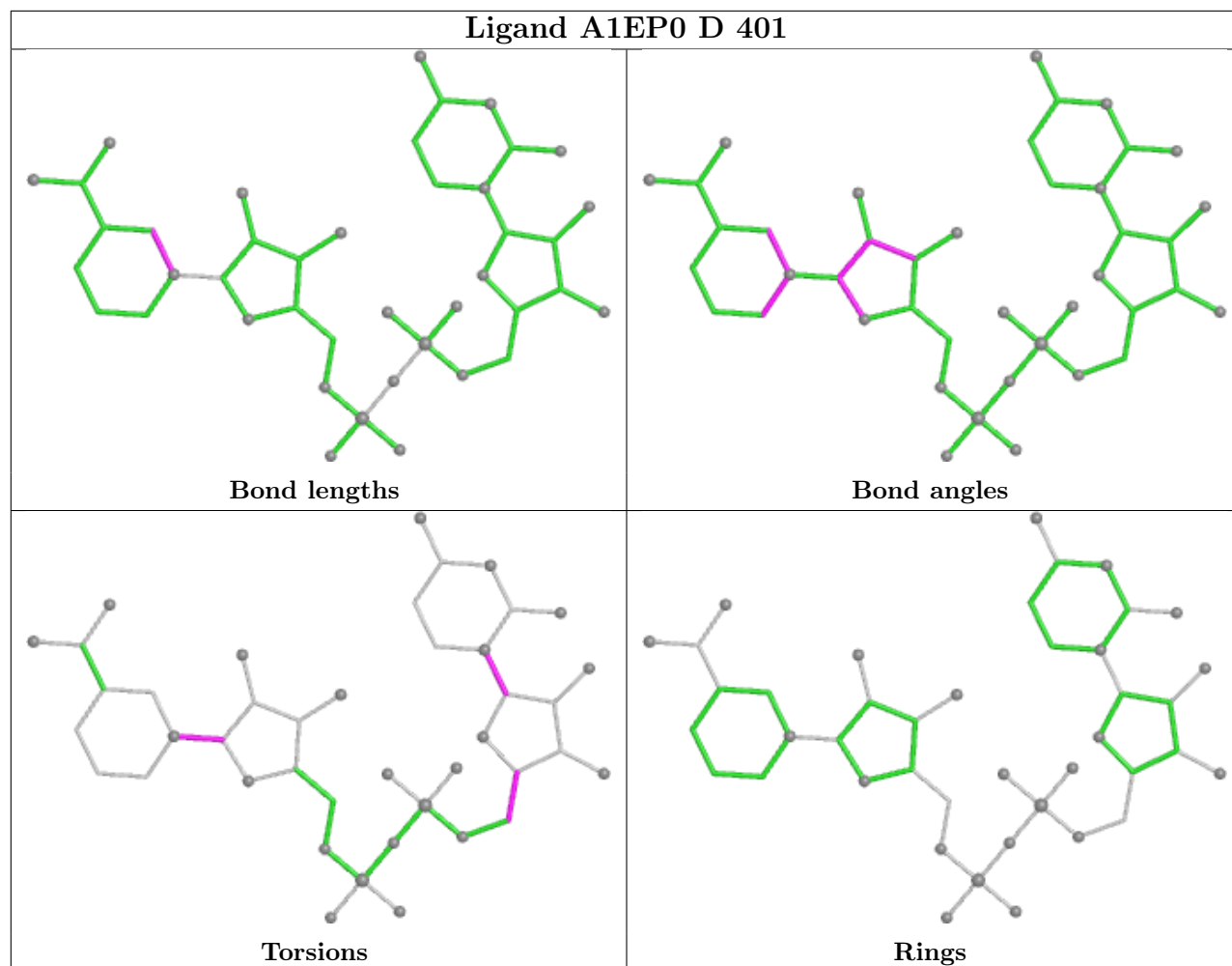
## Ligand A1EP0 C 401



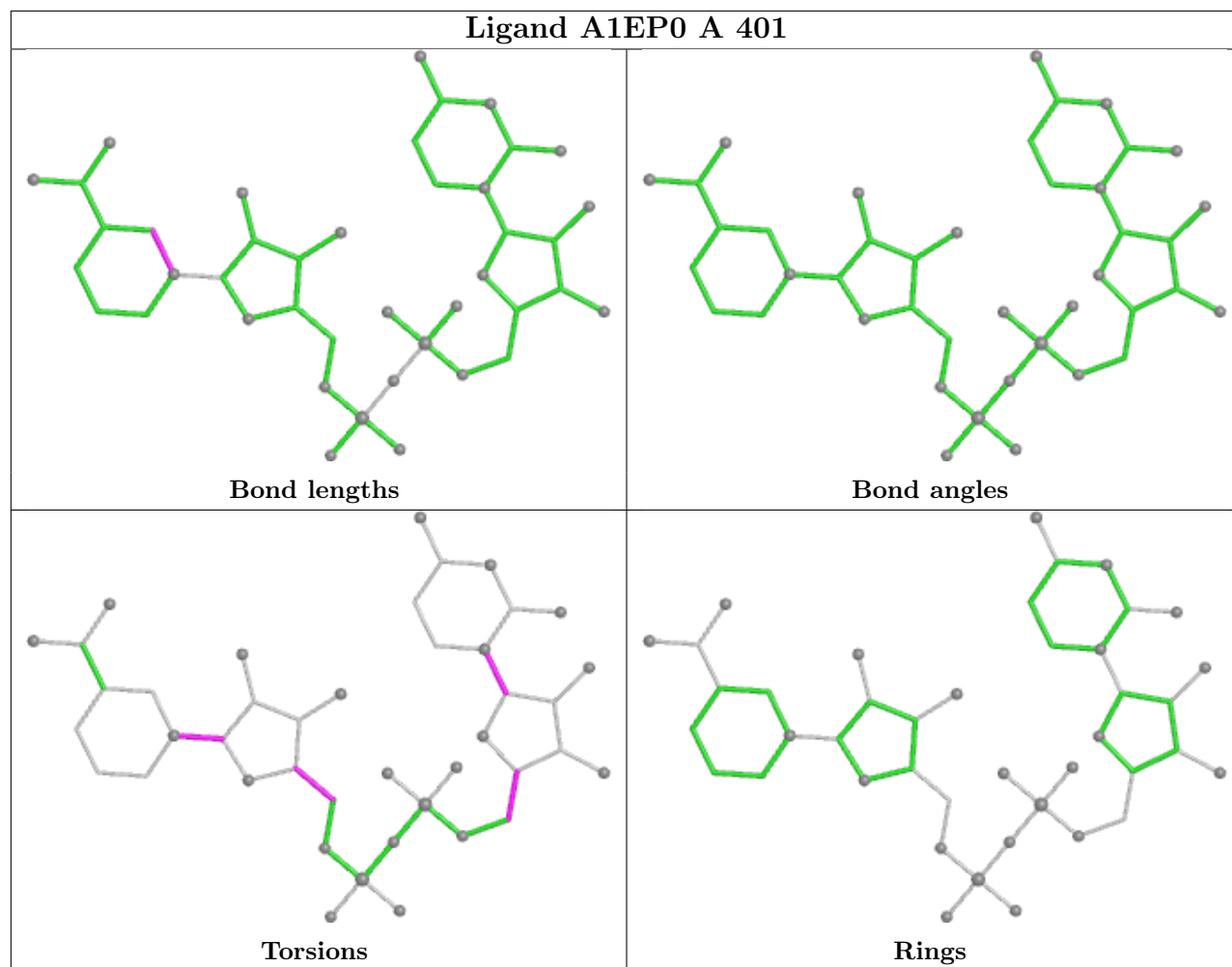
## Ligand A1EP0 B 401



## Ligand A1EP0 D 401

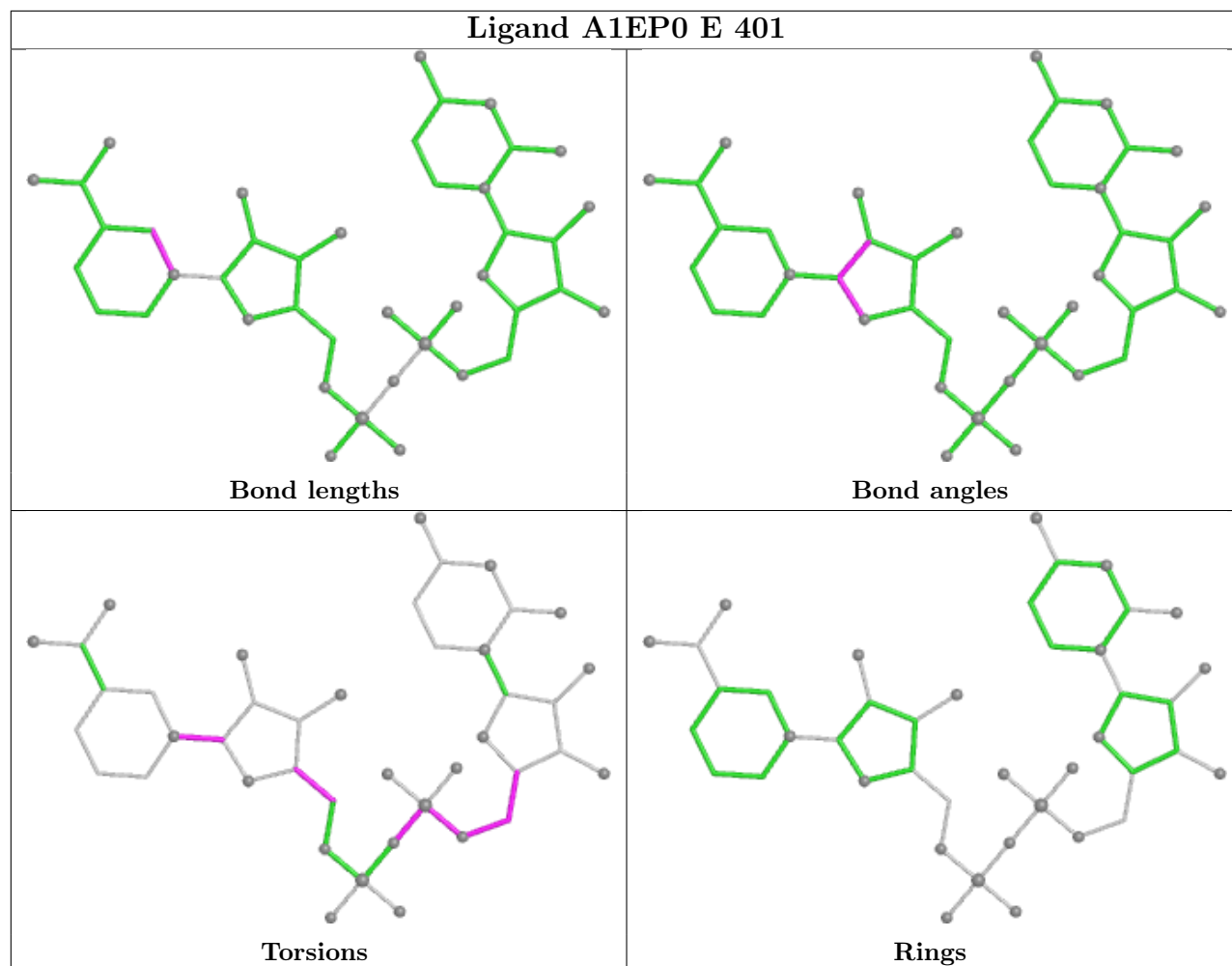


## Ligand A1EP0 A 401

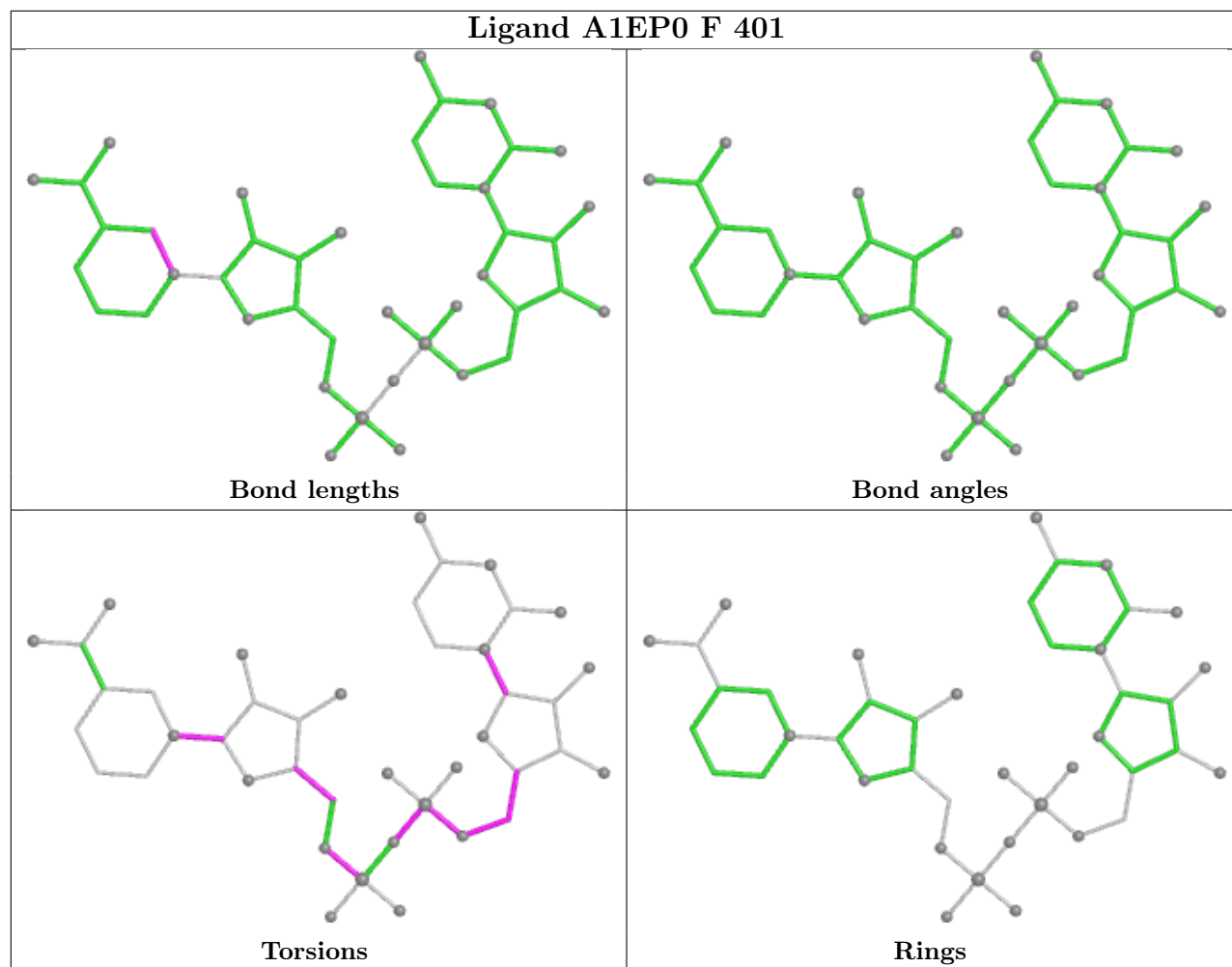


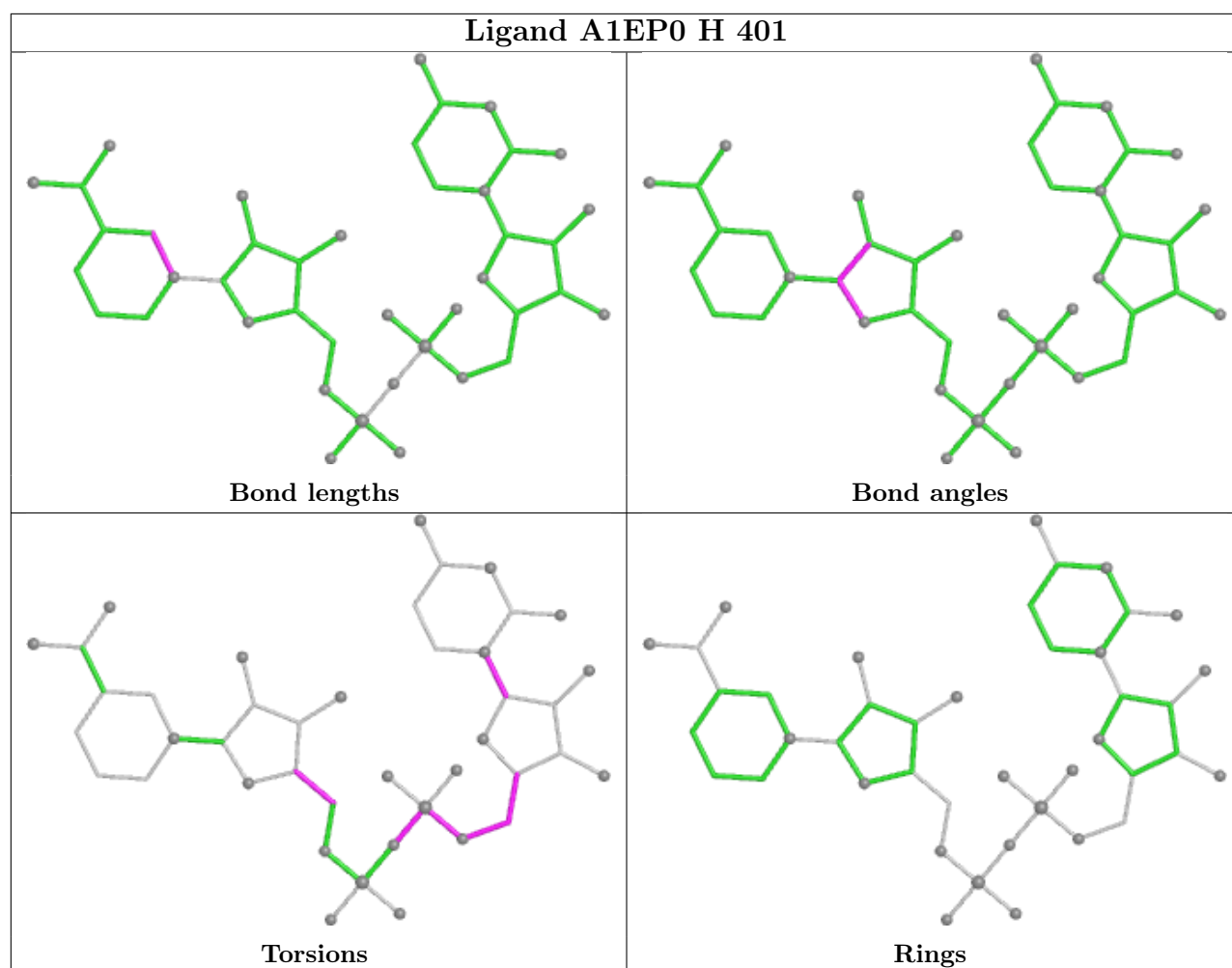


## Ligand A1EP0 E 401



## Ligand A1EP0 F 401





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	371/372 (99%)	0.89	67 (18%) 3 3	19, 52, 107, 130	0
1	B	371/372 (99%)	0.52	10 (2%) 56 58	25, 45, 72, 110	0
1	C	371/372 (99%)	0.15	6 (1%) 70 72	22, 35, 54, 84	0
1	D	371/372 (99%)	0.24	5 (1%) 75 76	22, 38, 69, 94	0
1	E	371/372 (99%)	-0.01	10 (2%) 56 58	17, 29, 54, 105	0
1	F	371/372 (99%)	0.19	12 (3%) 50 51	20, 35, 67, 105	0
1	G	371/372 (99%)	0.50	14 (3%) 44 45	23, 45, 80, 177	0
1	H	371/372 (99%)	0.45	20 (5%) 31 31	20, 41, 77, 118	0
1	I	371/372 (99%)	0.18	9 (2%) 59 61	20, 32, 62, 108	0
1	J	371/372 (99%)	0.00	10 (2%) 56 58	19, 29, 57, 100	0
1	K	371/372 (99%)	0.21	15 (4%) 42 43	20, 35, 65, 107	0
1	L	371/372 (99%)	0.31	13 (3%) 47 48	20, 38, 68, 106	0
All	All	4452/4464 (99%)	0.30	191 (4%) 40 41	17, 37, 78, 177	0

All (191) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	242	GLY	5.5
1	G	243	ALA	5.2
1	A	61	ALA	4.9
1	I	243	ALA	4.2
1	G	241	PRO	4.1
1	A	55	ALA	3.9
1	G	239	LEU	3.9
1	H	242	GLY	3.8
1	L	243	ALA	3.8
1	K	267	ALA	3.7
1	A	88	LEU	3.7

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Mol	Chain	Res	Type	RSRZ
1	F	268	ILE	3.7
1	L	239	LEU	3.7
1	A	111	VAL	3.6
1	A	334	LEU	3.6
1	C	371	GLN	3.6
1	A	68	GLU	3.5
1	A	1	MET	3.5
1	A	86	PRO	3.5
1	G	268	ILE	3.5
1	A	31	HIS	3.5
1	G	240	ILE	3.5
1	K	284	ASP	3.4
1	A	367	HIS	3.3
1	E	267	ALA	3.3
1	H	285	ASP	3.2
1	A	325	ALA	3.2
1	A	85	ARG	3.1
1	A	60	LYS	3.1
1	H	269	ASP	3.1
1	I	283	HIS	3.1
1	L	241	PRO	3.1
1	B	61	ALA	3.0
1	J	240	ILE	3.0
1	A	349	HIS	3.0
1	A	97	ALA	2.9
1	A	102	LEU	2.9
1	C	278	ASP	2.9
1	K	270	GLN	2.9
1	E	240	ILE	2.9
1	H	268	ILE	2.9
1	F	243	ALA	2.9
1	A	327	LYS	2.9
1	H	270	GLN	2.9
1	A	109	GLN	2.9
1	B	300	ASN	2.9
1	H	98	ALA	2.9
1	D	108	GLU	2.9
1	D	307	ARG	2.8
1	J	277	THR	2.8
1	H	358	ALA	2.8
1	A	93	TYR	2.8
1	A	370	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	244	LYS	2.8
1	D	123	ASN	2.8
1	B	369	LEU	2.8
1	A	368	SER	2.8
1	D	299	ALA	2.8
1	A	371	GLN	2.8
1	G	270	GLN	2.8
1	C	277	THR	2.7
1	A	311	PHE	2.7
1	L	268	ILE	2.7
1	C	300	ASN	2.7
1	F	241	PRO	2.7
1	G	245	ALA	2.7
1	I	267	ALA	2.7
1	J	267	ALA	2.7
1	H	347	ASP	2.7
1	K	10	LYS	2.7
1	J	239	LEU	2.7
1	I	222	TYR	2.7
1	L	178	ALA	2.7
1	I	284	ASP	2.6
1	K	266	VAL	2.6
1	F	269	ASP	2.6
1	G	269	ASP	2.6
1	J	269	ASP	2.6
1	A	366	VAL	2.6
1	H	243	ALA	2.6
1	A	329	TYR	2.6
1	H	240	ILE	2.6
1	A	330	ARG	2.6
1	H	284	ASP	2.6
1	I	241	PRO	2.6
1	K	241	PRO	2.6
1	K	265	ASP	2.6
1	K	108	GLU	2.6
1	A	29	ALA	2.6
1	H	97	ALA	2.6
1	A	65	TRP	2.5
1	D	328	GLY	2.5
1	K	221	SER	2.5
1	A	81	PHE	2.5
1	A	27	VAL	2.5

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Mol	Chain	Res	Type	RSRZ
1	F	300	ASN	2.5
1	L	283	HIS	2.5
1	L	267	ALA	2.5
1	A	9	ILE	2.5
1	K	240	ILE	2.5
1	A	322	LEU	2.5
1	A	307	ARG	2.5
1	J	245	ALA	2.5
1	A	347	ASP	2.5
1	A	346	LEU	2.5
1	E	371	GLN	2.5
1	A	66	ALA	2.5
1	E	284	ASP	2.4
1	A	64	ALA	2.4
1	H	241	PRO	2.4
1	F	240	ILE	2.4
1	F	266	VAL	2.4
1	A	25	THR	2.4
1	H	282	THR	2.4
1	A	87	GLY	2.4
1	K	239	LEU	2.4
1	J	283	HIS	2.4
1	A	345	THR	2.4
1	H	51	GLU	2.4
1	K	268	ILE	2.4
1	E	270	GLN	2.3
1	H	239	LEU	2.3
1	A	34	TYR	2.3
1	G	352	TYR	2.3
1	I	244	LYS	2.3
1	I	242	GLY	2.3
1	C	51	GLU	2.3
1	A	17	ALA	2.3
1	E	241	PRO	2.3
1	K	299	ALA	2.3
1	G	283	HIS	2.3
1	A	89	ILE	2.3
1	L	240	ILE	2.3
1	G	238	VAL	2.3
1	F	282	THR	2.3
1	F	371	GLN	2.3
1	B	370	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	63	ASP	2.3
1	E	243	ALA	2.2
1	L	300	ASN	2.2
1	L	242	GLY	2.2
1	E	269	ASP	2.2
1	L	299	ALA	2.2
1	A	365	ASP	2.2
1	A	326	ASN	2.2
1	H	371	GLN	2.2
1	A	340	LEU	2.2
1	A	84	PHE	2.2
1	A	73	VAL	2.2
1	A	67	ALA	2.2
1	A	19	THR	2.2
1	A	333	CYS	2.2
1	A	324	ILE	2.2
1	J	241	PRO	2.2
1	A	337	PRO	2.1
1	B	305	VAL	2.1
1	A	96	LEU	2.1
1	E	239	LEU	2.1
1	I	353	GLU	2.1
1	A	24	MET	2.1
1	A	321	ALA	2.1
1	A	331	ALA	2.1
1	G	358	ALA	2.1
1	A	108	GLU	2.1
1	J	222	TYR	2.1
1	K	269	ASP	2.1
1	L	208	ASP	2.1
1	A	339	LEU	2.1
1	E	242	GLY	2.1
1	F	242	GLY	2.1
1	K	242	GLY	2.1
1	C	108	GLU	2.1
1	A	83	TYR	2.1
1	L	212	ASP	2.1
1	A	20	PRO	2.1
1	J	270	GLN	2.0
1	A	70	VAL	2.0
1	A	53	ALA	2.0
1	H	356	ALA	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	90	LEU	2.0
1	B	38	GLU	2.0
1	F	270	GLN	2.0
1	A	45	PHE	2.0
1	A	56	VAL	2.0
1	B	111	VAL	2.0
1	B	53	ALA	2.0
1	H	53	ALA	2.0
1	B	310	THR	2.0
1	F	265	ASP	2.0
1	H	362	PRO	2.0
1	A	116	TYR	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
2	A1EP0	L	401	42/42	0.62	0.27	38,49,67,70	42
2	A1EP0	G	401	42/42	0.64	0.23	87,106,118,120	0
2	A1EP0	E	401	42/42	0.67	0.29	32,56,65,67	42
2	A1EP0	I	401	42/42	0.69	0.25	52,66,84,85	42
2	A1EP0	H	401	42/42	0.76	0.23	45,62,73,77	42
2	A1EP0	F	401	42/42	0.77	0.24	46,51,70,72	42
2	A1EP0	K	401	42/42	0.80	0.18	34,60,68,69	42
2	A1EP0	J	401	42/42	0.80	0.19	44,52,63,68	42
2	A1EP0	B	401	42/42	0.93	0.10	21,34,45,46	0
2	A1EP0	A	401	42/42	0.94	0.10	25,33,40,46	0
2	A1EP0	C	401	42/42	0.95	0.09	20,30,35,43	0

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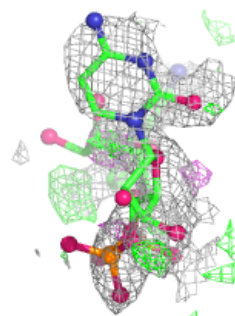
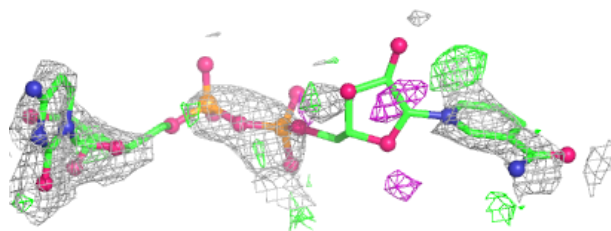
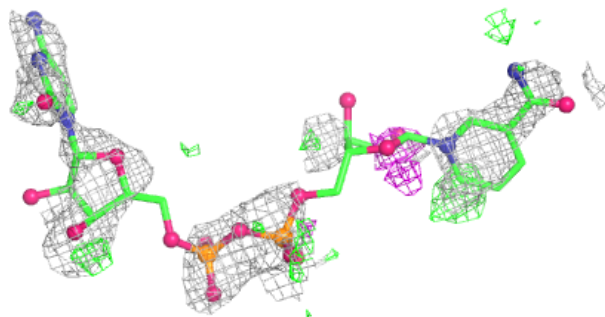
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	A1EP0	D	401	42/42	0.96	0.07	23,29,33,40	0

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.

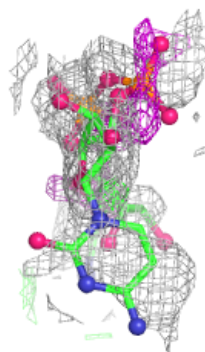
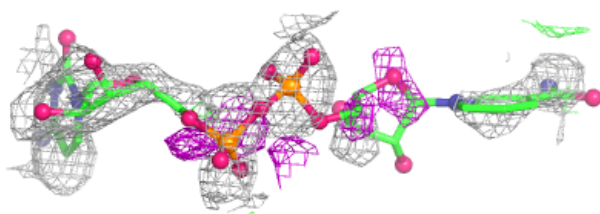
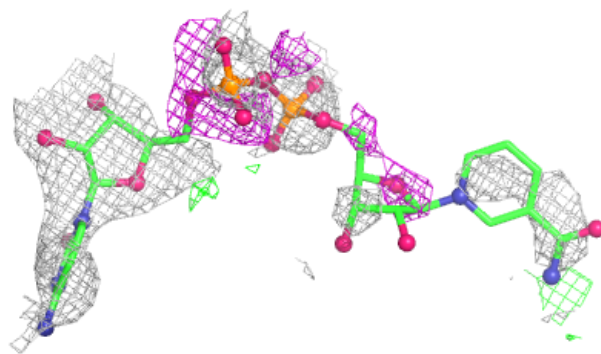
**Electron density around A1EP0 L 401:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)

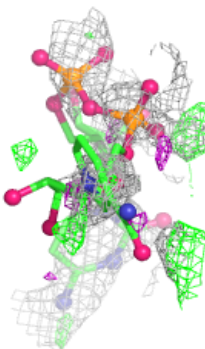
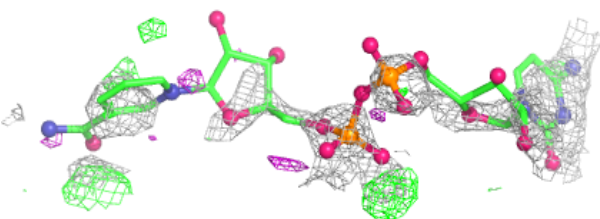
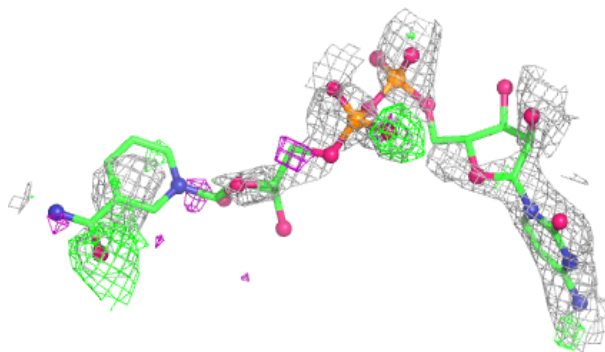


**Electron density around A1EP0 G 401:**

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

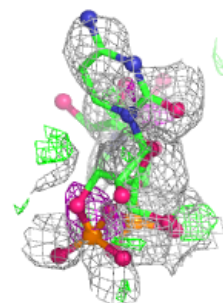
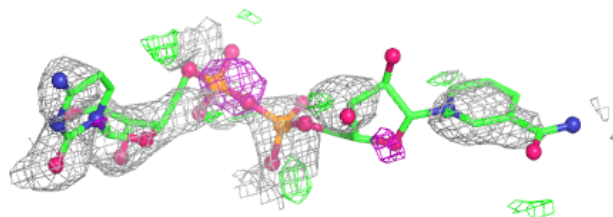
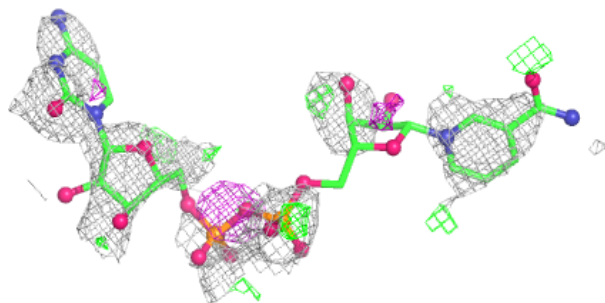
**Electron density around A1EP0 E 401:**

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

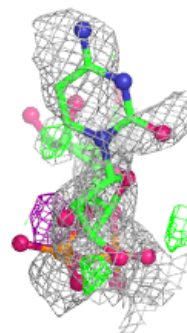
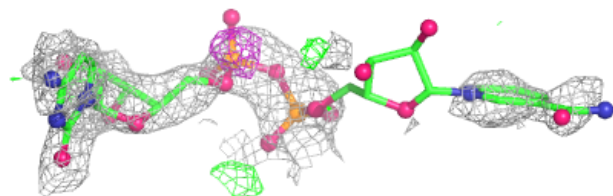
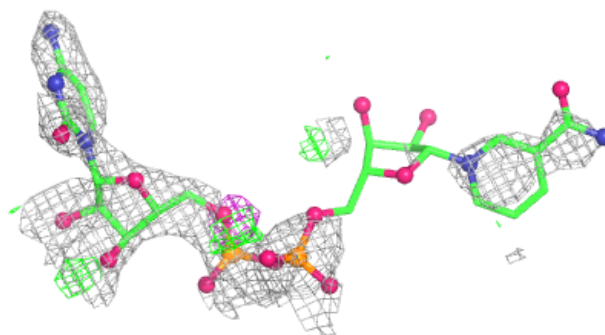


**Electron density around A1EP0 I 401:**

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

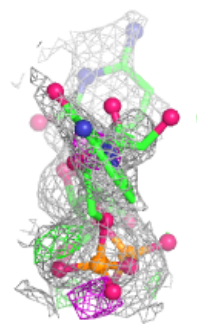
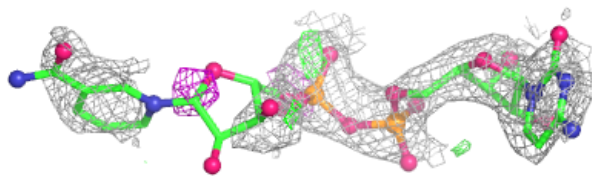
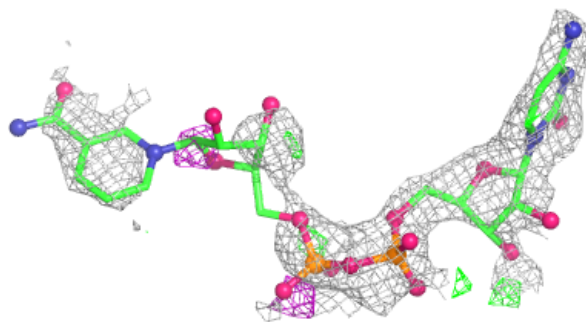
**Electron density around A1EP0 H 401:**

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

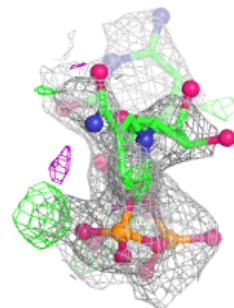
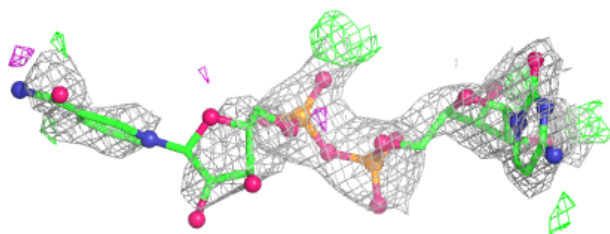
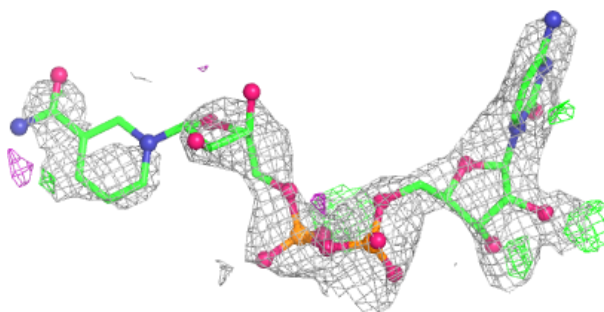


**Electron density around A1EP0 F 401:**

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

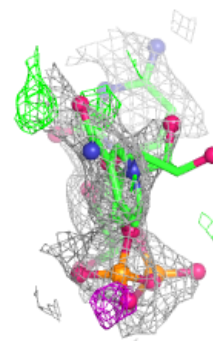
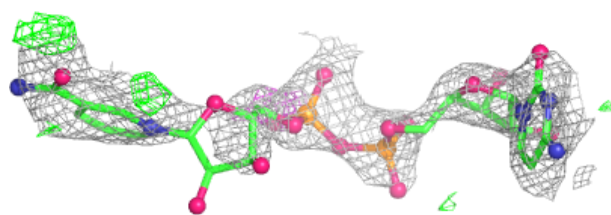
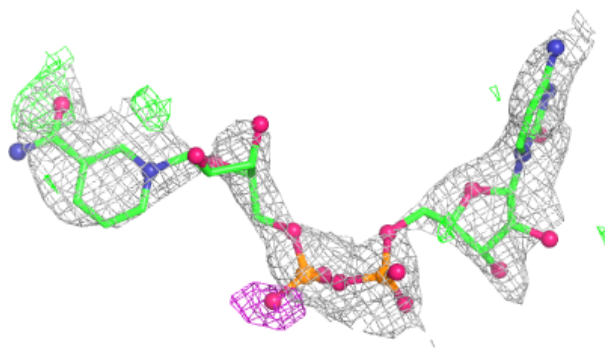
**Electron density around A1EP0 K 401:**

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

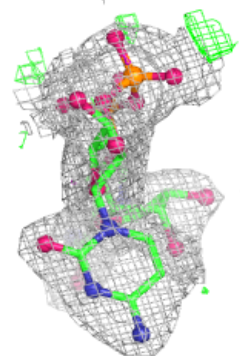
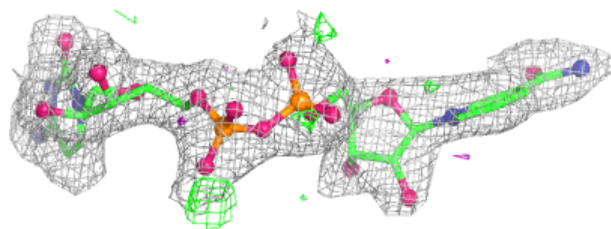
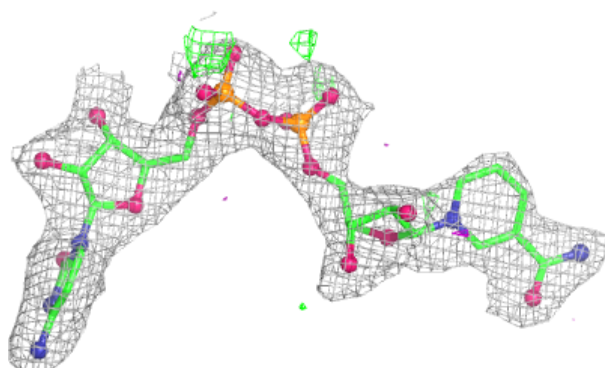


**Electron density around A1EP0 J 401:**

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

**Electron density around A1EP0 B 401:**

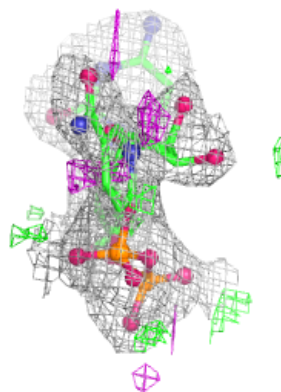
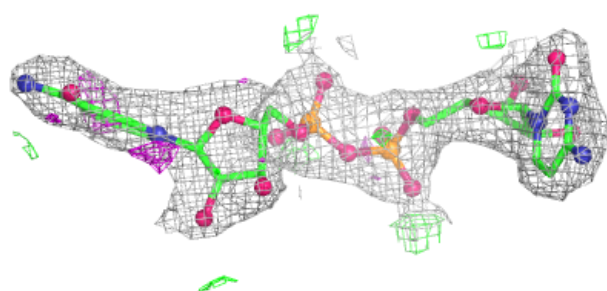
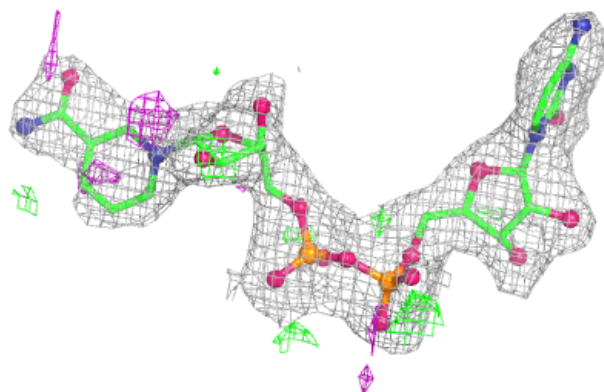
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



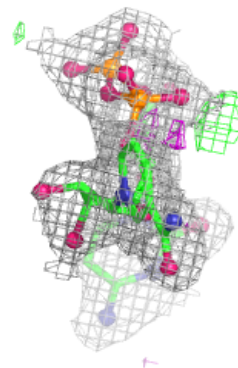
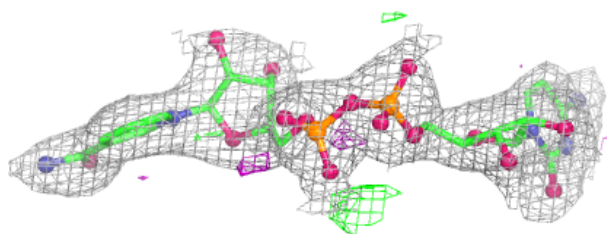
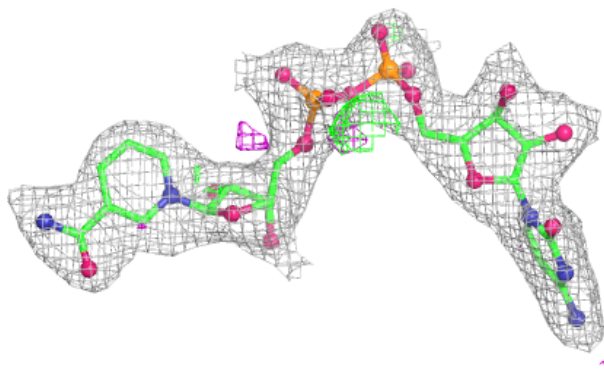


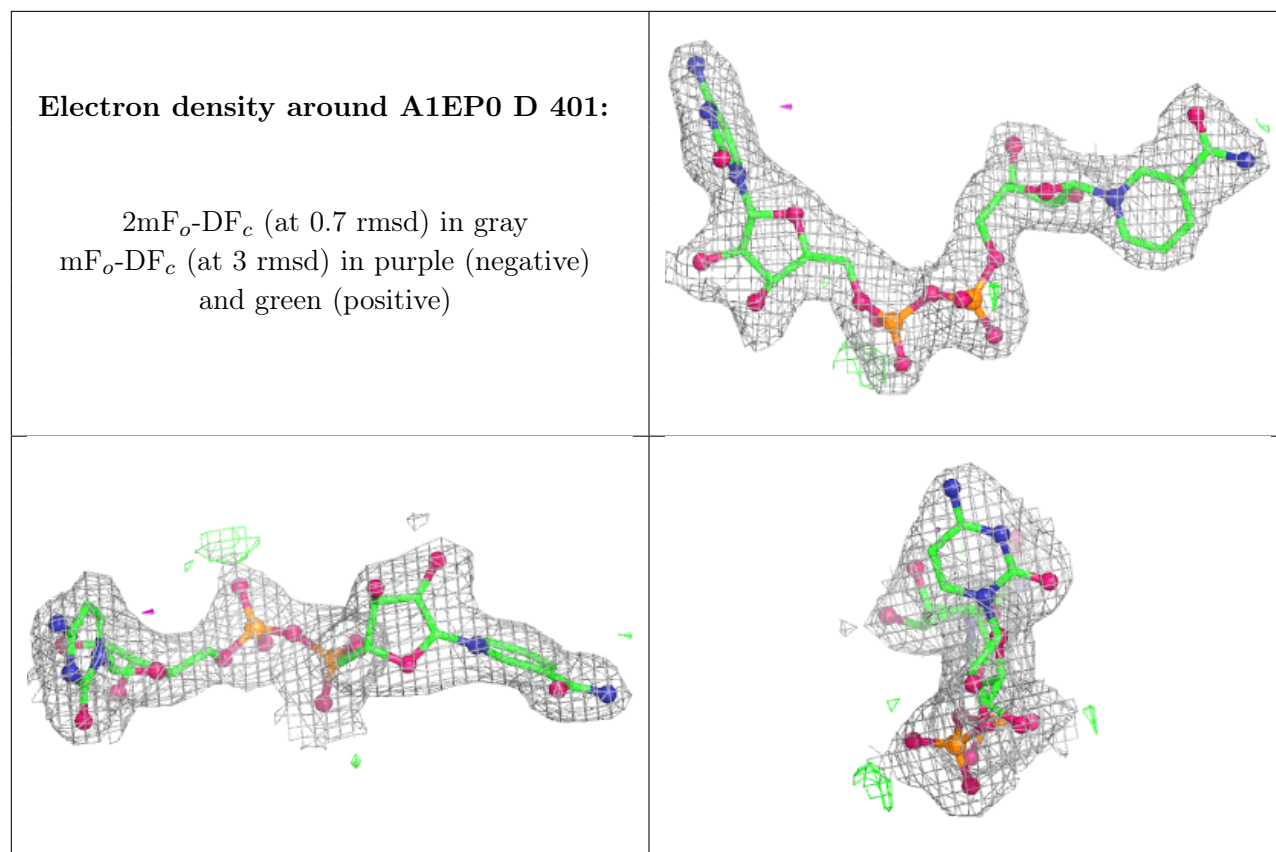
**Electron density around A1EP0 A 401:**

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

**Electron density around A1EP0 C 401:**

$2mF_o-DF_c$  (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.