



# Full wwPDB X-ray Structure Validation Report i

Sep 26, 2022 – 05:27 pm BST

PDB ID : 7QYS  
Title : Crystal structure of RimK from *Pseudomonas syringae* DC3000  
Authors : Thompson, C.M.A.; Little, R.H.; Stevenson, C.E.M.; Lawson, D.M.; Malone, J.G.  
Deposited on : 2022-01-29  
Resolution : 2.90 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 i 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](#) i) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.4, CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.31.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0267  
CCP4 : 7.1.010 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

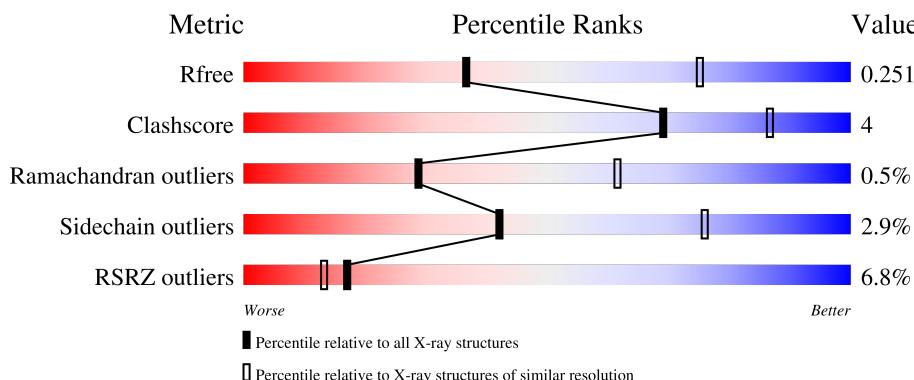
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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  $\geq 3$ , 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.



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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
2	ADP	A	401	-	-	-	X
2	ADP	C	401	-	-	-	X
2	ADP	D	401	-	-	-	X
2	ADP	K	401	-	-	-	X
2	ADP	M	401	-	-	-	X
2	ADP	O	401	-	-	-	X

## 2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 34293 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 Probable alpha-L-glutamate ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	290	Total 2166	C 1365	N 383	O 402	S 16	0	0	0
1	B	281	Total 2073	C 1309	N 360	O 388	S 16	0	0	0
1	C	282	Total 2108	C 1332	N 369	O 391	S 16	0	0	0
1	D	291	Total 2165	C 1362	N 385	O 402	S 16	0	0	0
1	E	292	Total 2153	C 1359	N 375	O 403	S 16	0	0	0
1	F	284	Total 2121	C 1338	N 371	O 396	S 16	0	0	0
1	G	282	Total 2106	C 1331	N 366	O 393	S 16	0	0	0
1	H	284	Total 2115	C 1338	N 368	O 393	S 16	0	0	0
1	I	282	Total 2080	C 1315	N 359	O 390	S 16	0	0	0
1	J	286	Total 2101	C 1327	N 361	O 397	S 16	0	0	0
1	K	283	Total 2106	C 1329	N 366	O 395	S 16	0	0	0
1	L	294	Total 2178	C 1374	N 381	O 406	S 17	0	0	0
1	M	290	Total 2155	C 1359	N 380	O 400	S 16	0	0	0
1	N	290	Total 2105	C 1330	N 365	O 394	S 16	0	0	0
1	O	290	Total 2147	C 1355	N 375	O 401	S 16	0	0	0
1	P	286	Total 2117	C 1338	N 368	O 395	S 16	0	0	0

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	302	LEU	-	expression tag	UNP Q88AZ9
A	303	GLU	-	expression tag	UNP Q88AZ9
A	304	HIS	-	expression tag	UNP Q88AZ9
A	305	HIS	-	expression tag	UNP Q88AZ9
A	306	HIS	-	expression tag	UNP Q88AZ9
A	307	HIS	-	expression tag	UNP Q88AZ9
A	308	HIS	-	expression tag	UNP Q88AZ9
A	309	HIS	-	expression tag	UNP Q88AZ9
B	302	LEU	-	expression tag	UNP Q88AZ9
B	303	GLU	-	expression tag	UNP Q88AZ9
B	304	HIS	-	expression tag	UNP Q88AZ9
B	305	HIS	-	expression tag	UNP Q88AZ9
B	306	HIS	-	expression tag	UNP Q88AZ9
B	307	HIS	-	expression tag	UNP Q88AZ9
B	308	HIS	-	expression tag	UNP Q88AZ9
B	309	HIS	-	expression tag	UNP Q88AZ9
C	302	LEU	-	expression tag	UNP Q88AZ9
C	303	GLU	-	expression tag	UNP Q88AZ9
C	304	HIS	-	expression tag	UNP Q88AZ9
C	305	HIS	-	expression tag	UNP Q88AZ9
C	306	HIS	-	expression tag	UNP Q88AZ9
C	307	HIS	-	expression tag	UNP Q88AZ9
C	308	HIS	-	expression tag	UNP Q88AZ9
C	309	HIS	-	expression tag	UNP Q88AZ9
D	302	LEU	-	expression tag	UNP Q88AZ9
D	303	GLU	-	expression tag	UNP Q88AZ9
D	304	HIS	-	expression tag	UNP Q88AZ9
D	305	HIS	-	expression tag	UNP Q88AZ9
D	306	HIS	-	expression tag	UNP Q88AZ9
D	307	HIS	-	expression tag	UNP Q88AZ9
D	308	HIS	-	expression tag	UNP Q88AZ9
D	309	HIS	-	expression tag	UNP Q88AZ9
E	302	LEU	-	expression tag	UNP Q88AZ9
E	303	GLU	-	expression tag	UNP Q88AZ9
E	304	HIS	-	expression tag	UNP Q88AZ9
E	305	HIS	-	expression tag	UNP Q88AZ9
E	306	HIS	-	expression tag	UNP Q88AZ9
E	307	HIS	-	expression tag	UNP Q88AZ9
E	308	HIS	-	expression tag	UNP Q88AZ9
E	309	HIS	-	expression tag	UNP Q88AZ9
F	302	LEU	-	expression tag	UNP Q88AZ9
F	303	GLU	-	expression tag	UNP Q88AZ9

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Chain	Residue	Modelled	Actual	Comment	Reference
F	304	HIS	-	expression tag	UNP Q88AZ9
F	305	HIS	-	expression tag	UNP Q88AZ9
F	306	HIS	-	expression tag	UNP Q88AZ9
F	307	HIS	-	expression tag	UNP Q88AZ9
F	308	HIS	-	expression tag	UNP Q88AZ9
F	309	HIS	-	expression tag	UNP Q88AZ9
G	302	LEU	-	expression tag	UNP Q88AZ9
G	303	GLU	-	expression tag	UNP Q88AZ9
G	304	HIS	-	expression tag	UNP Q88AZ9
G	305	HIS	-	expression tag	UNP Q88AZ9
G	306	HIS	-	expression tag	UNP Q88AZ9
G	307	HIS	-	expression tag	UNP Q88AZ9
G	308	HIS	-	expression tag	UNP Q88AZ9
G	309	HIS	-	expression tag	UNP Q88AZ9
H	302	LEU	-	expression tag	UNP Q88AZ9
H	303	GLU	-	expression tag	UNP Q88AZ9
H	304	HIS	-	expression tag	UNP Q88AZ9
H	305	HIS	-	expression tag	UNP Q88AZ9
H	306	HIS	-	expression tag	UNP Q88AZ9
H	307	HIS	-	expression tag	UNP Q88AZ9
H	308	HIS	-	expression tag	UNP Q88AZ9
H	309	HIS	-	expression tag	UNP Q88AZ9
I	302	LEU	-	expression tag	UNP Q88AZ9
I	303	GLU	-	expression tag	UNP Q88AZ9
I	304	HIS	-	expression tag	UNP Q88AZ9
I	305	HIS	-	expression tag	UNP Q88AZ9
I	306	HIS	-	expression tag	UNP Q88AZ9
I	307	HIS	-	expression tag	UNP Q88AZ9
I	308	HIS	-	expression tag	UNP Q88AZ9
I	309	HIS	-	expression tag	UNP Q88AZ9
J	302	LEU	-	expression tag	UNP Q88AZ9
J	303	GLU	-	expression tag	UNP Q88AZ9
J	304	HIS	-	expression tag	UNP Q88AZ9
J	305	HIS	-	expression tag	UNP Q88AZ9
J	306	HIS	-	expression tag	UNP Q88AZ9
J	307	HIS	-	expression tag	UNP Q88AZ9
J	308	HIS	-	expression tag	UNP Q88AZ9
J	309	HIS	-	expression tag	UNP Q88AZ9
K	302	LEU	-	expression tag	UNP Q88AZ9
K	303	GLU	-	expression tag	UNP Q88AZ9
K	304	HIS	-	expression tag	UNP Q88AZ9
K	305	HIS	-	expression tag	UNP Q88AZ9

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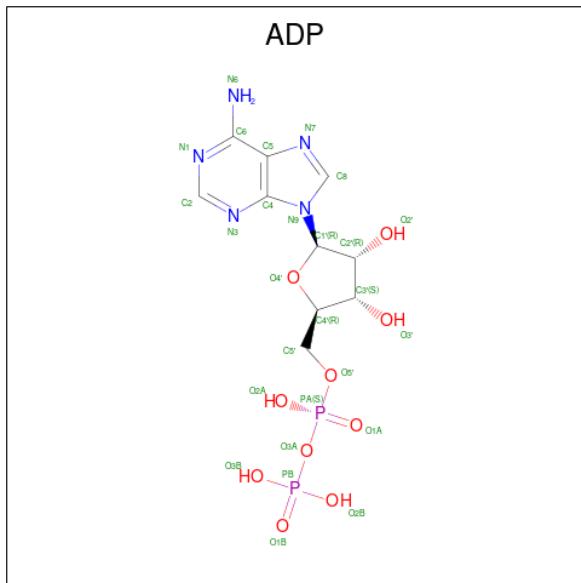
Chain	Residue	Modelled	Actual	Comment	Reference
K	306	HIS	-	expression tag	UNP Q88AZ9
K	307	HIS	-	expression tag	UNP Q88AZ9
K	308	HIS	-	expression tag	UNP Q88AZ9
K	309	HIS	-	expression tag	UNP Q88AZ9
L	302	LEU	-	expression tag	UNP Q88AZ9
L	303	GLU	-	expression tag	UNP Q88AZ9
L	304	HIS	-	expression tag	UNP Q88AZ9
L	305	HIS	-	expression tag	UNP Q88AZ9
L	306	HIS	-	expression tag	UNP Q88AZ9
L	307	HIS	-	expression tag	UNP Q88AZ9
L	308	HIS	-	expression tag	UNP Q88AZ9
L	309	HIS	-	expression tag	UNP Q88AZ9
M	302	LEU	-	expression tag	UNP Q88AZ9
M	303	GLU	-	expression tag	UNP Q88AZ9
M	304	HIS	-	expression tag	UNP Q88AZ9
M	305	HIS	-	expression tag	UNP Q88AZ9
M	306	HIS	-	expression tag	UNP Q88AZ9
M	307	HIS	-	expression tag	UNP Q88AZ9
M	308	HIS	-	expression tag	UNP Q88AZ9
M	309	HIS	-	expression tag	UNP Q88AZ9
N	302	LEU	-	expression tag	UNP Q88AZ9
N	303	GLU	-	expression tag	UNP Q88AZ9
N	304	HIS	-	expression tag	UNP Q88AZ9
N	305	HIS	-	expression tag	UNP Q88AZ9
N	306	HIS	-	expression tag	UNP Q88AZ9
N	307	HIS	-	expression tag	UNP Q88AZ9
N	308	HIS	-	expression tag	UNP Q88AZ9
N	309	HIS	-	expression tag	UNP Q88AZ9
O	302	LEU	-	expression tag	UNP Q88AZ9
O	303	GLU	-	expression tag	UNP Q88AZ9
O	304	HIS	-	expression tag	UNP Q88AZ9
O	305	HIS	-	expression tag	UNP Q88AZ9
O	306	HIS	-	expression tag	UNP Q88AZ9
O	307	HIS	-	expression tag	UNP Q88AZ9
O	308	HIS	-	expression tag	UNP Q88AZ9
O	309	HIS	-	expression tag	UNP Q88AZ9
P	302	LEU	-	expression tag	UNP Q88AZ9
P	303	GLU	-	expression tag	UNP Q88AZ9
P	304	HIS	-	expression tag	UNP Q88AZ9
P	305	HIS	-	expression tag	UNP Q88AZ9
P	306	HIS	-	expression tag	UNP Q88AZ9
P	307	HIS	-	expression tag	UNP Q88AZ9

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Chain	Residue	Modelled	Actual	Comment	Reference
P	308	HIS	-	expression tag	UNP Q88AZ9
P	309	HIS	-	expression tag	UNP Q88AZ9

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</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
			27	10	5	10	2		
2	B	1	Total C N O P					0	0
			27	10	5	10	2		
2	C	1	Total C N O P					0	0
			27	10	5	10	2		
2	D	1	Total C N O P					0	0
			27	10	5	10	2		
2	E	1	Total C N O P					0	0
			27	10	5	10	2		
2	G	1	Total C N O P					0	0
			27	10	5	10	2		
2	H	1	Total C N O P					0	0
			27	10	5	10	2		
2	J	1	Total C N O P					0	0
			27	10	5	10	2		
2	K	1	Total C N O P					0	0
			27	10	5	10	2		
2	M	1	Total C N O P					0	0
			27	10	5	10	2		

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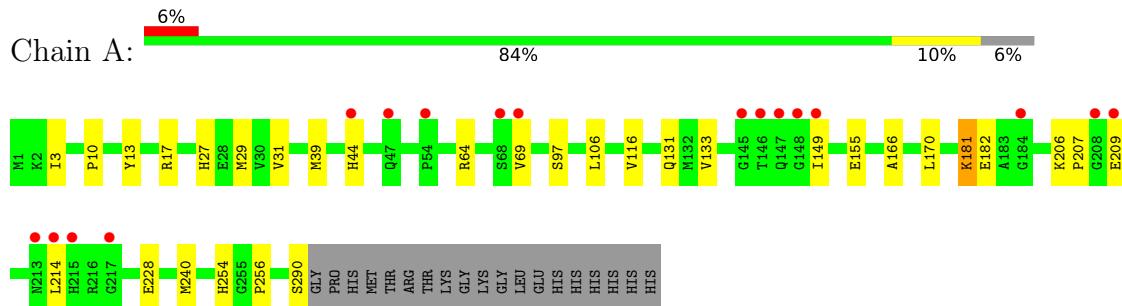
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	O	1	27	10	5	10	2	0	0

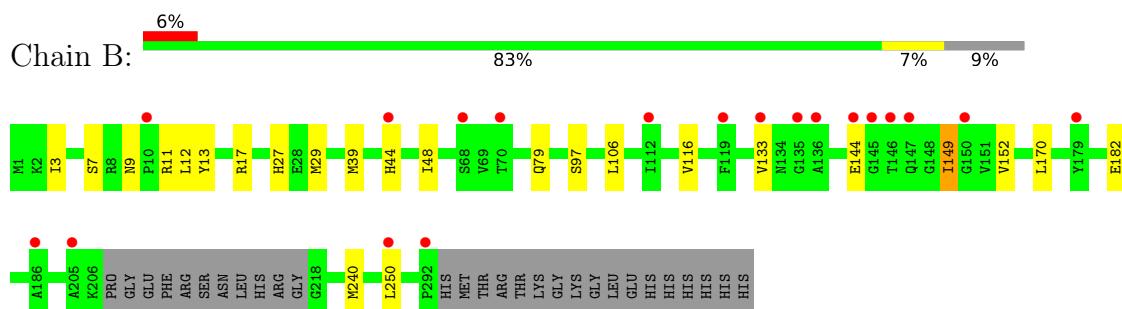
### 3 Residue-property plots [\(i\)](#)

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.

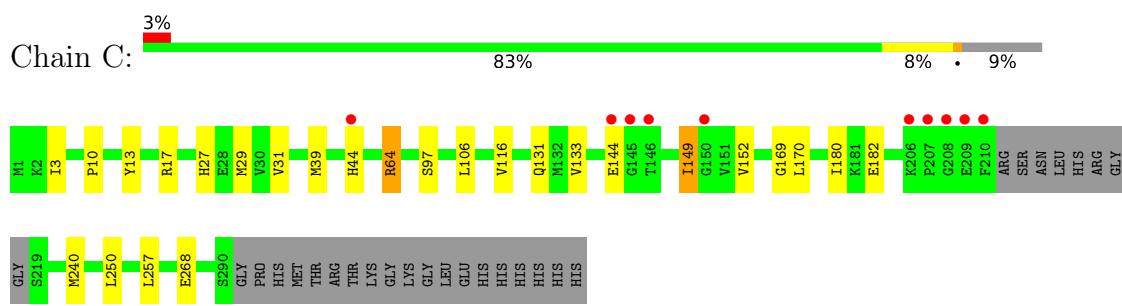
- Molecule 1: Probable alpha-L-glutamate ligase



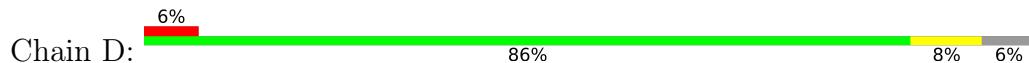
- Molecule 1: Probable alpha-L-glutamate ligase



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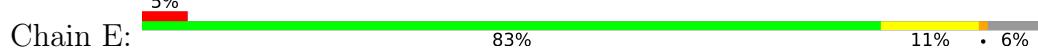
- Molecule 1: Probable alpha-L-glutamate ligase





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#### • Molecule 1: Probable alpha L glutamate ligase

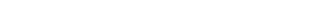


- Molecule 1: Probable alpha-L-glutamate ligase

Chain F: 4% 80%



- Molecule 1: Probable alpha-L-glutamate ligase

Chain G:  3% 80%

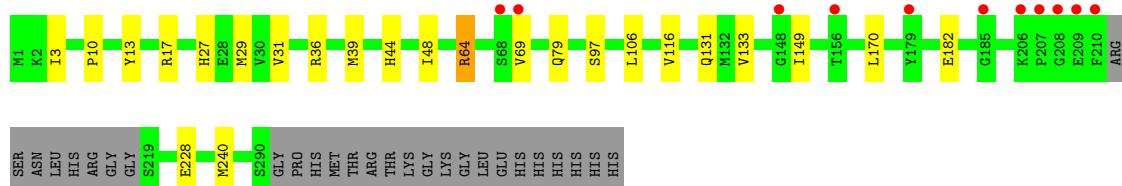


- Molecule 1: Probable alpha-L-glutamate ligase

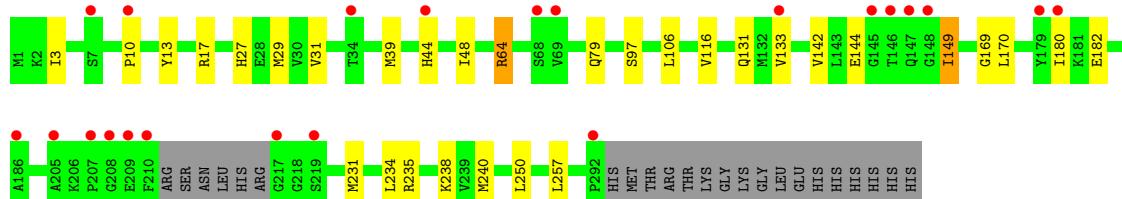
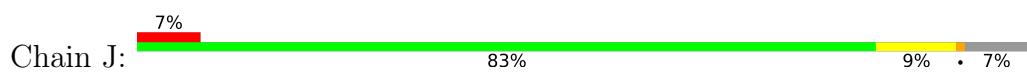
Chain H:  6% 83%



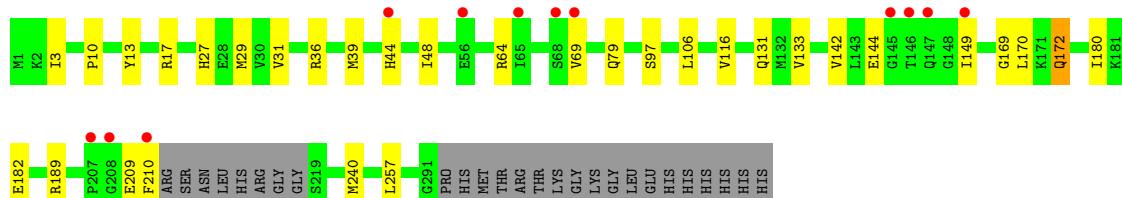
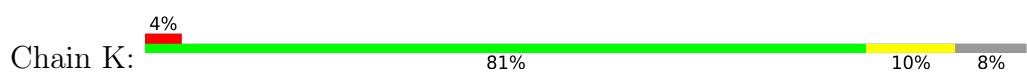
- Molecule 1: Probable alpha-L-glutamate ligase



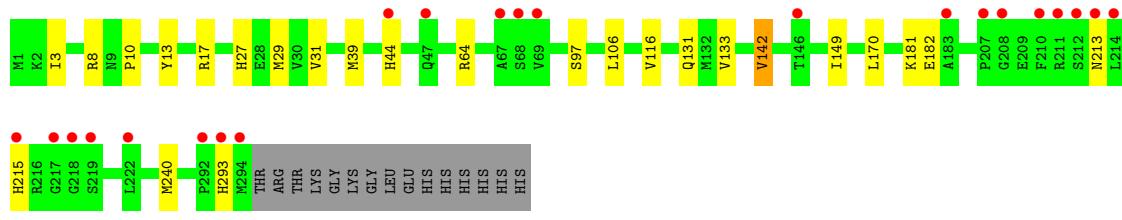
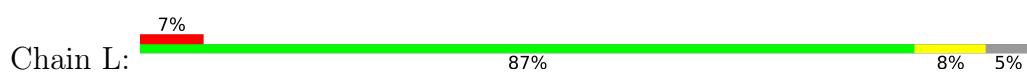
- Molecule 1: Probable alpha-L-glutamate ligase



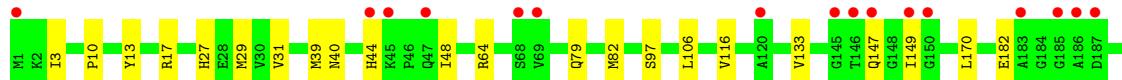
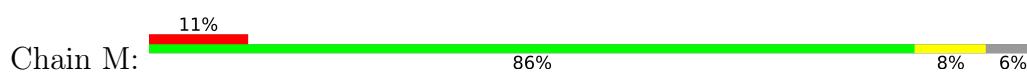
- Molecule 1: Probable alpha-L-glutamate ligase



- Molecule 1: Probable alpha-L-glutamate ligase

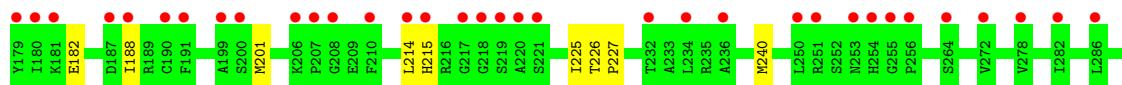


- Molecule 1: Probable alpha-L-glutamate ligase

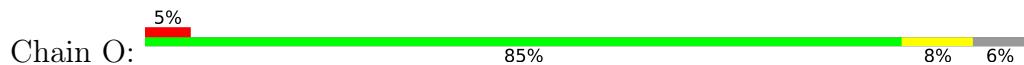




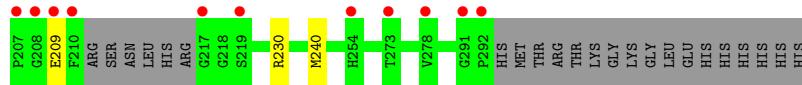
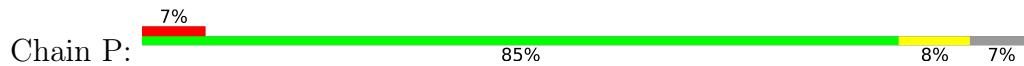
- Molecule 1: Probable alpha-L-glutamate ligase



- Molecule 1: Probable alpha-L-glutamate ligase



- Molecule 1: Probable alpha-L-glutamate ligase



## 4 Data and refinement statistics i

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	95.91Å 96.09Å 156.99Å 88.94° 84.37° 89.97°	Depositor
Resolution (Å)	49.80 – 2.90 49.80 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.9 (49.80-2.90) 98.9 (49.80-2.90)	Depositor EDS
$R_{merge}$	0.16	Depositor
$R_{sym}$	(Not available)	Depositor
$< I/\sigma(I) >$ <sup>1</sup>	1.50 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
$R$ , $R_{free}$	0.237 , 0.248 0.240 , 0.251	Depositor DCC
$R_{free}$ test set	5890 reflections (4.82%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	56.3	Xtriage
Anisotropy	0.559	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	(Not available) , (Not available)	EDS
L-test for twinning <sup>2</sup>	$<  L  > = 0.43$ , $< L^2 > = 0.26$	Xtriage
Estimated twinning fraction	0.104 for -h,k,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	34293	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.94% 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  $< |L| >$ ,  $< L^2 >$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section:  
ADP

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	0.67	0/2197	0.79	2/2968 (0.1%)
1	B	0.70	1/2102 (0.0%)	0.78	0/2848
1	C	0.67	0/2138	0.84	3/2891 (0.1%)
1	D	0.67	0/2196	0.79	3/2969 (0.1%)
1	E	0.69	0/2185	0.84	6/2959 (0.2%)
1	F	0.67	0/2151	0.84	3/2907 (0.1%)
1	G	0.67	0/2136	0.78	2/2889 (0.1%)
1	H	0.67	0/2146	0.79	3/2903 (0.1%)
1	I	0.67	0/2110	0.84	4/2857 (0.1%)
1	J	0.68	0/2131	0.84	3/2887 (0.1%)
1	K	0.66	0/2136	0.81	3/2889 (0.1%)
1	L	0.67	0/2211	0.79	2/2991 (0.1%)
1	M	0.66	0/2186	0.78	2/2955 (0.1%)
1	N	0.68	0/2136	0.79	2/2897 (0.1%)
1	O	0.67	0/2178	0.77	2/2946 (0.1%)
1	P	0.67	0/2148	0.79	2/2906 (0.1%)
All	All	0.67	1/34487 (0.0%)	0.81	42/46662 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	7	SER	CA-CB	-5.58	1.44	1.52

All (42) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	64	ARG	NE-CZ-NH1	-12.41	114.10	120.30
1	I	64	ARG	NE-CZ-NH2	12.40	126.50	120.30
1	J	64	ARG	NE-CZ-NH1	-12.13	114.24	120.30
1	C	64	ARG	NE-CZ-NH2	12.06	126.33	120.30
1	J	64	ARG	NE-CZ-NH2	11.84	126.22	120.30
1	F	64	ARG	NE-CZ-NH1	-11.62	114.49	120.30
1	F	64	ARG	NE-CZ-NH2	11.56	126.08	120.30
1	I	64	ARG	NE-CZ-NH1	-11.45	114.57	120.30
1	K	189	ARG	NE-CZ-NH1	-9.73	115.43	120.30
1	C	64	ARG	CG-CD-NE	-7.70	95.62	111.80
1	E	64	ARG	NE-CZ-NH2	-7.42	116.59	120.30
1	D	64	ARG	CG-CD-NE	-7.41	96.23	111.80
1	L	64	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	A	64	ARG	NE-CZ-NH1	-7.34	116.63	120.30
1	I	64	ARG	CG-CD-NE	-7.30	96.47	111.80
1	A	64	ARG	NE-CZ-NH2	7.29	123.94	120.30
1	J	64	ARG	CG-CD-NE	-7.11	96.87	111.80
1	F	64	ARG	CG-CD-NE	-7.10	96.89	111.80
1	G	64	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	P	64	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	H	64	ARG	NE-CZ-NH2	-6.87	116.87	120.30
1	K	64	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	N	64	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	O	64	ARG	NE-CZ-NH2	-6.65	116.97	120.30
1	M	64	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	E	70	THR	CA-CB-CG2	6.48	121.48	112.40
1	P	64	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	L	64	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	H	235	ARG	NE-CZ-NH2	5.69	123.14	120.30
1	H	64	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	E	64	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	G	64	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	E	39	MET	CA-CB-CG	5.41	122.49	113.30
1	E	45	LYS	CB-CA-C	5.33	121.07	110.40
1	O	64	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	N	64	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	D	64	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	K	36	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	D	64	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	M	64	ARG	NE-CZ-NH1	5.11	122.86	120.30
1	E	39	MET	CG-SD-CE	5.04	108.27	100.20
1	I	36	ARG	CG-CD-NE	5.01	122.31	111.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	44	HIS	Mainchain

## 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	2166	0	2212	27	0
1	B	2073	0	2084	17	0
1	C	2108	0	2148	18	1
1	D	2165	0	2197	19	0
1	E	2153	0	2176	19	1
1	F	2121	0	2161	34	0
1	G	2106	0	2141	20	0
1	H	2115	0	2151	24	0
1	I	2080	0	2085	16	0
1	J	2101	0	2113	23	0
1	K	2106	0	2131	18	0
1	L	2178	0	2200	13	0
1	M	2155	0	2195	16	0
1	N	2105	0	2095	21	0
1	O	2147	0	2179	18	0
1	P	2117	0	2145	15	0
2	A	27	0	12	0	0
2	B	27	0	12	1	0
2	C	27	0	12	1	0
2	D	27	0	12	0	0
2	E	27	0	12	0	0
2	G	27	0	12	0	0
2	H	27	0	12	0	0
2	J	27	0	12	1	0
2	K	27	0	12	0	0
2	M	27	0	12	0	0
2	O	27	0	12	0	0
All	All	34293	0	34545	252	1

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 4.

All (252) 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:I:228:GLU:HG2	1:O:272:VAL:HG21	1.47	0.92
1:N:226:THR:HG22	1:N:227:PRO:HD2	1.55	0.89
1:A:181:LYS:HB2	1:F:11:ARG:CB	2.02	0.88
1:N:170:LEU:HD13	1:P:170:LEU:HD13	1.60	0.84
1:E:40:ASN:ND2	1:F:132:MET:O	2.12	0.81
1:B:9:ASN:HB3	1:B:12:LEU:HD22	1.61	0.81
1:J:144:GLU:HB2	1:J:149:ILE:HD11	1.62	0.81
1:A:181:LYS:CG	1:F:11:ARG:CB	2.60	0.80
1:A:170:LEU:HD23	1:C:149:ILE:HG21	1.62	0.80
1:I:228:GLU:CG	1:O:272:VAL:HG21	2.14	0.78
1:A:155:GLU:OE1	1:F:16:ARG:NH2	2.19	0.76
1:P:149:ILE:HD12	1:P:150:GLY:N	2.01	0.76
1:H:149:ILE:HD12	1:H:150:GLY:N	2.01	0.76
1:D:149:ILE:HD12	1:D:150:GLY:N	2.01	0.75
1:A:181:LYS:CB	1:F:11:ARG:CB	2.64	0.75
1:F:152:VAL:HG22	1:H:166:ALA:HB2	1.69	0.72
1:F:67:ALA:HB1	1:F:146:THR:OG1	1.91	0.71
1:F:10:PRO:HB3	1:F:31:VAL:HG11	1.73	0.71
1:I:10:PRO:HB3	1:I:31:VAL:HG11	1.74	0.70
1:H:10:PRO:HB3	1:H:31:VAL:HG11	1.74	0.70
1:M:10:PRO:HB3	1:M:31:VAL:HG11	1.72	0.70
1:J:10:PRO:HB3	1:J:31:VAL:HG11	1.73	0.69
1:G:111:GLY:O	1:J:231:MET:HG3	1.92	0.69
1:O:10:PRO:HB3	1:O:31:VAL:HG11	1.75	0.69
1:L:10:PRO:HB3	1:L:31:VAL:HG11	1.73	0.69
1:D:10:PRO:HB3	1:D:31:VAL:HG11	1.73	0.68
1:K:10:PRO:HB3	1:K:31:VAL:HG11	1.76	0.68
1:A:10:PRO:HB3	1:A:31:VAL:HG11	1.74	0.68
1:E:10:PRO:HB3	1:E:31:VAL:HG11	1.74	0.68
1:G:10:PRO:HB3	1:G:31:VAL:HG11	1.75	0.68
1:N:10:PRO:HB3	1:N:31:VAL:HG11	1.74	0.68
1:C:10:PRO:HB3	1:C:31:VAL:HG11	1.76	0.68
1:N:188:ILE:HG21	1:N:225:ILE:HD12	1.76	0.68
1:P:10:PRO:HB3	1:P:31:VAL:HG11	1.74	0.68
1:O:206:LYS:HG2	1:O:217:GLY:O	1.94	0.67
1:M:170:LEU:HD13	1:O:170:LEU:HD13	1.76	0.67
1:H:142:VAL:HB	1:H:149:ILE:HD11	1.77	0.67
1:M:149:ILE:CG2	1:O:169:GLY:C	2.63	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:181:LYS:HG3	1:F:11:ARG:CB	2.25	0.66
1:B:149:ILE:HG21	1:D:170:LEU:HD23	1.77	0.66
1:K:142:VAL:CG1	1:K:172:GLN:HG2	2.26	0.66
1:P:142:VAL:HB	1:P:149:ILE:HD11	1.76	0.66
1:A:290:SER:C	1:O:195:ASP:OD2	2.34	0.65
1:D:142:VAL:HB	1:D:149:ILE:HD11	1.76	0.65
1:B:152:VAL:HG22	1:D:166:ALA:HB2	1.78	0.65
1:A:155:GLU:OE1	1:F:16:ARG:CZ	2.45	0.64
1:H:189:ARG:HD3	1:H:248:ASP:OD1	2.00	0.61
1:E:149:ILE:CG2	1:G:169:GLY:C	2.70	0.61
1:D:189:ARG:HD3	1:D:248:ASP:OD1	2.02	0.60
1:G:228:GLU:HB2	1:J:238:LYS:HB3	1.84	0.60
1:F:152:VAL:HG22	1:H:166:ALA:CB	2.32	0.60
1:N:226:THR:HG22	1:N:227:PRO:CD	2.30	0.60
1:N:188:ILE:HG21	1:N:225:ILE:CD1	2.32	0.59
1:G:189:ARG:HD3	1:G:248:ASP:OD1	2.02	0.59
1:J:170:LEU:HD13	1:L:170:LEU:HD13	1.84	0.58
1:J:144:GLU:HB2	1:J:149:ILE:CD1	2.32	0.58
1:E:166:ALA:HB2	1:G:152:VAL:HG22	1.85	0.58
1:N:170:LEU:CD1	1:P:170:LEU:HD13	2.31	0.57
1:D:142:VAL:C	1:D:143:LEU:HD12	2.25	0.57
1:E:3:ILE:HD12	1:E:29:MET:HE1	1.87	0.56
1:M:3:ILE:HD12	1:M:29:MET:HE1	1.86	0.56
1:A:166:ALA:HB2	1:C:152:VAL:HG22	1.86	0.56
1:M:40:ASN:ND2	1:N:132:MET:O	2.37	0.56
1:A:170:LEU:HD13	1:C:170:LEU:HD13	1.87	0.55
1:K:3:ILE:HD12	1:K:29:MET:HE1	1.87	0.55
1:A:181:LYS:HD2	1:F:11:ARG:CB	2.36	0.55
1:O:3:ILE:HD12	1:O:29:MET:HE1	1.88	0.55
1:G:231:MET:SD	1:J:234:LEU:HB3	2.47	0.55
1:G:3:ILE:HD12	1:G:29:MET:HE1	1.89	0.55
1:H:44:HIS:CG	1:H:45:LYS:H	2.25	0.55
1:G:144:GLU:HB2	1:G:149:ILE:HG13	1.89	0.55
1:M:216:ARG:O	1:M:216:ARG:HG3	2.08	0.54
1:O:206:LYS:HA	1:O:206:LYS:HE2	1.89	0.54
1:D:3:ILE:HD12	1:D:29:MET:HE1	1.90	0.54
1:K:144:GLU:HB2	1:K:149:ILE:HG13	1.88	0.54
1:I:170:LEU:HD13	1:K:170:LEU:HD13	1.89	0.54
1:A:181:LYS:CD	1:F:11:ARG:CB	2.85	0.53
1:P:3:ILE:HD12	1:P:29:MET:HE1	1.91	0.53
1:H:149:ILE:HD12	1:H:150:GLY:H	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:144:GLU:HB2	1:F:149:ILE:HG13	1.90	0.53
1:M:149:ILE:HG22	1:O:169:GLY:HA3	1.91	0.53
1:L:27:HIS:HB2	1:L:29:MET:HE3	1.92	0.52
1:D:149:ILE:HD12	1:D:150:GLY:H	1.74	0.52
1:P:149:ILE:HD12	1:P:150:GLY:H	1.72	0.52
1:A:149:ILE:CG2	1:C:169:GLY:C	2.77	0.52
1:A:254:HIS:CE1	1:G:11:ARG:NH2	2.78	0.52
1:F:27:HIS:HB2	1:F:29:MET:HE3	1.91	0.52
1:J:3:ILE:HD12	1:J:29:MET:HE1	1.91	0.52
1:B:3:ILE:HD12	1:B:29:MET:HE1	1.92	0.51
1:H:27:HIS:HB2	1:H:29:MET:HE3	1.92	0.51
1:G:228:GLU:OE2	1:J:235:ARG:HG2	2.10	0.51
1:C:27:HIS:HB2	1:C:29:MET:HE3	1.92	0.51
1:C:144:GLU:HB2	1:C:149:ILE:HD13	1.92	0.51
1:J:142:VAL:HG12	1:J:149:ILE:HD12	1.92	0.51
1:B:27:HIS:HB2	1:B:29:MET:HE3	1.93	0.50
1:A:3:ILE:HD12	1:A:29:MET:HE1	1.94	0.50
1:A:27:HIS:HB2	1:A:29:MET:HE3	1.93	0.50
1:I:3:ILE:HD12	1:I:29:MET:HE1	1.92	0.50
1:J:27:HIS:HB2	1:J:29:MET:HE3	1.93	0.50
1:C:144:GLU:CB	1:C:149:ILE:HD13	2.42	0.50
1:E:42:ALA:HB2	1:F:108:SER:OG	2.12	0.50
1:N:27:HIS:HB2	1:N:29:MET:HE3	1.93	0.50
1:P:27:HIS:HB2	1:P:29:MET:HE3	1.94	0.50
1:B:144:GLU:CB	1:B:149:ILE:HD13	2.41	0.50
1:E:149:ILE:HG23	1:G:169:GLY:C	2.33	0.49
1:D:27:HIS:HB2	1:D:29:MET:HE3	1.94	0.49
1:P:142:VAL:HB	1:P:149:ILE:CD1	2.43	0.49
1:B:144:GLU:HB2	1:B:149:ILE:HD13	1.94	0.49
1:H:3:ILE:HD12	1:H:29:MET:HE1	1.94	0.49
1:I:27:HIS:HB2	1:I:29:MET:HE3	1.94	0.49
1:D:142:VAL:HB	1:D:149:ILE:CD1	2.43	0.48
1:I:97:SER:HA	1:I:240:MET:HE2	1.96	0.48
1:O:27:HIS:HB2	1:O:29:MET:HE3	1.95	0.48
1:K:27:HIS:HB2	1:K:29:MET:HE3	1.95	0.48
1:L:3:ILE:HD12	1:L:29:MET:HE1	1.95	0.48
1:B:250:LEU:HD21	2:B:401:ADP:C2	2.48	0.48
1:F:144:GLU:HB3	1:F:149:ILE:HD11	1.96	0.48
1:F:170:LEU:HD21	1:H:172:GLN:HE21	1.77	0.48
1:G:27:HIS:HB2	1:G:29:MET:HE3	1.95	0.48
1:J:97:SER:HA	1:J:240:MET:HE2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3:ILE:HD12	1:C:29:MET:HE1	1.95	0.48
1:M:97:SER:HA	1:M:240:MET:HE2	1.96	0.48
1:B:97:SER:HA	1:B:240:MET:HE2	1.96	0.48
1:E:41:ILE:CG1	1:F:117:THR:HB	2.44	0.47
1:M:82:MET:HG2	1:N:109:ARG:HD3	1.95	0.47
1:F:3:ILE:HD12	1:F:29:MET:HE1	1.97	0.47
1:J:250:LEU:HD21	2:J:401:ADP:C2	2.49	0.47
1:H:142:VAL:HB	1:H:149:ILE:CD1	2.43	0.47
1:N:170:LEU:HG	1:P:149:ILE:HD13	1.95	0.47
1:E:27:HIS:HB2	1:E:29:MET:HE3	1.96	0.47
1:H:97:SER:HA	1:H:240:MET:HE2	1.96	0.47
1:N:97:SER:HA	1:N:240:MET:HE2	1.96	0.47
1:B:170:LEU:HD13	1:D:170:LEU:HD13	1.95	0.47
1:A:97:SER:HA	1:A:240:MET:HE2	1.97	0.47
1:C:13:TYR:CE2	1:C:17:ARG:HG3	2.50	0.47
1:F:170:LEU:CD2	1:H:172:GLN:HE21	2.28	0.47
1:N:3:ILE:HD12	1:N:29:MET:HE1	1.95	0.47
1:E:142:VAL:HG23	1:E:149:ILE:HB	1.96	0.47
1:H:13:TYR:CE2	1:H:17:ARG:HG3	2.50	0.47
1:L:13:TYR:CE2	1:L:17:ARG:HG3	2.50	0.47
1:P:13:TYR:CE2	1:P:17:ARG:HG3	2.50	0.47
1:F:152:VAL:CG2	1:H:166:ALA:CB	2.93	0.47
1:G:97:SER:HA	1:G:240:MET:HE2	1.96	0.47
1:H:142:VAL:CB	1:H:149:ILE:HD11	2.45	0.47
1:E:109:ARG:HD3	1:F:82:MET:HG2	1.97	0.47
1:E:142:VAL:HG22	1:E:150:GLY:H	1.80	0.47
1:M:27:HIS:HB2	1:M:29:MET:HE3	1.96	0.47
1:N:13:TYR:CE2	1:N:17:ARG:HG3	2.50	0.46
1:J:13:TYR:CE2	1:J:17:ARG:HG3	2.51	0.46
1:K:13:TYR:CE2	1:K:17:ARG:HG3	2.50	0.46
1:O:13:TYR:CE2	1:O:17:ARG:HG3	2.50	0.46
1:M:13:TYR:CE2	1:M:17:ARG:HG3	2.50	0.46
1:B:13:TYR:CE2	1:B:17:ARG:HG3	2.50	0.46
1:F:97:SER:HA	1:F:240:MET:HE2	1.96	0.46
1:G:144:GLU:HB3	1:G:149:ILE:HD11	1.97	0.46
1:I:13:TYR:CE2	1:I:17:ARG:HG3	2.51	0.46
1:A:13:TYR:CE2	1:A:17:ARG:HG3	2.51	0.46
1:E:13:TYR:CE2	1:E:17:ARG:HG3	2.51	0.46
1:I:170:LEU:HD23	1:K:149:ILE:HG21	1.97	0.46
1:N:226:THR:CG2	1:N:227:PRO:HD2	2.35	0.46
1:D:13:TYR:CE2	1:D:17:ARG:HG3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:SER:HA	1:E:240:MET:HE2	1.98	0.46
1:I:149:ILE:CG2	1:K:169:GLY:C	2.84	0.46
1:J:170:LEU:HD21	1:L:142:VAL:HG21	1.96	0.46
1:C:97:SER:HA	1:C:240:MET:HE2	1.97	0.46
1:G:13:TYR:CE2	1:G:17:ARG:HG3	2.50	0.46
1:J:149:ILE:HD13	1:L:170:LEU:HD23	1.97	0.46
1:M:149:ILE:HG23	1:O:169:GLY:O	2.16	0.46
1:D:97:SER:HA	1:D:240:MET:HE2	1.96	0.45
1:E:41:ILE:HG12	1:F:117:THR:HB	1.97	0.45
1:P:97:SER:HA	1:P:240:MET:HE2	1.96	0.45
1:P:142:VAL:CB	1:P:149:ILE:HD11	2.45	0.45
1:K:97:SER:HA	1:K:240:MET:HE2	1.98	0.45
1:O:97:SER:HA	1:O:240:MET:HE2	1.97	0.45
1:F:13:TYR:CE2	1:F:17:ARG:HG3	2.50	0.45
1:J:169:GLY:O	1:L:149:ILE:CG2	2.65	0.45
1:J:149:ILE:HD13	1:L:170:LEU:CD2	2.47	0.45
1:N:188:ILE:CG2	1:N:225:ILE:CD1	2.95	0.45
1:G:44:HIS:ND1	1:G:45:LYS:N	2.54	0.44
1:P:116:VAL:HG12	1:P:133:VAL:HG13	1.99	0.44
1:A:116:VAL:HG12	1:A:133:VAL:HG13	2.00	0.44
1:K:116:VAL:HG12	1:K:133:VAL:HG13	2.00	0.44
1:L:116:VAL:HG12	1:L:133:VAL:HG13	1.99	0.44
1:A:170:LEU:HD13	1:C:170:LEU:CD1	2.48	0.44
1:J:169:GLY:C	1:L:149:ILE:CG2	2.86	0.44
1:L:97:SER:HA	1:L:240:MET:HE2	1.98	0.44
1:A:206:LYS:HB2	1:A:207:PRO:HD2	2.00	0.44
1:B:116:VAL:HG12	1:B:133:VAL:HG13	2.00	0.44
1:I:116:VAL:HG12	1:I:133:VAL:HG13	1.99	0.44
1:I:149:ILE:CG2	1:K:169:GLY:O	2.66	0.44
1:D:116:VAL:HG12	1:D:133:VAL:HG13	1.99	0.43
1:E:116:VAL:HG12	1:E:133:VAL:HG13	2.00	0.43
1:K:142:VAL:HG13	1:K:172:GLN:HB3	2.00	0.43
1:O:116:VAL:HG12	1:O:133:VAL:HG13	2.00	0.43
1:H:116:VAL:HG12	1:H:133:VAL:HG13	1.99	0.43
1:N:116:VAL:HG12	1:N:133:VAL:HG13	1.99	0.43
1:A:228:GLU:HG3	1:A:256:PRO:HG3	2.01	0.43
1:E:48:ILE:HD11	1:E:79:GLN:HB3	2.01	0.43
1:I:149:ILE:HG23	1:K:169:GLY:O	2.18	0.43
1:F:48:ILE:HD11	1:F:79:GLN:HB3	2.01	0.43
1:K:144:GLU:HB3	1:K:149:ILE:HD11	1.99	0.43
1:M:116:VAL:HG12	1:M:133:VAL:HG13	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ILE:HG22	1:C:169:GLY:HA3	2.01	0.43
1:A:155:GLU:OE1	1:F:16:ARG:NE	2.52	0.43
1:B:48:ILE:HD11	1:B:79:GLN:HB3	2.00	0.43
1:B:9:ASN:HB3	1:B:12:LEU:CD2	2.42	0.43
1:B:170:LEU:HG	1:D:149:ILE:HD13	2.01	0.43
1:D:142:VAL:CB	1:D:149:ILE:HD11	2.45	0.42
1:F:166:ALA:HA	1:H:150:GLY:CA	2.49	0.42
1:A:170:LEU:HD23	1:C:149:ILE:CG2	2.42	0.42
1:J:116:VAL:HG12	1:J:133:VAL:HG13	2.00	0.42
1:N:48:ILE:HD11	1:N:79:GLN:HB3	2.01	0.42
1:F:166:ALA:HA	1:H:150:GLY:HA3	2.01	0.42
1:G:116:VAL:HG12	1:G:133:VAL:HG13	2.01	0.42
1:J:48:ILE:HD11	1:J:79:GLN:HB3	2.01	0.42
1:D:143:LEU:HD12	1:D:143:LEU:N	2.35	0.42
1:F:116:VAL:HG12	1:F:133:VAL:HG13	2.00	0.42
1:L:3:ILE:HD12	1:L:29:MET:CE	2.50	0.42
1:C:116:VAL:HG12	1:C:133:VAL:HG13	2.01	0.42
1:J:3:ILE:HD12	1:J:29:MET:CE	2.50	0.42
1:K:180:ILE:HD13	1:K:257:LEU:HD12	2.01	0.42
1:B:3:ILE:HD12	1:B:29:MET:CE	2.49	0.42
1:P:3:ILE:HD12	1:P:29:MET:CE	2.50	0.42
1:D:3:ILE:HD12	1:D:29:MET:CE	2.50	0.41
1:F:180:ILE:HD13	1:F:257:LEU:HD12	2.02	0.41
1:C:180:ILE:HD13	1:C:257:LEU:HD12	2.02	0.41
1:F:3:ILE:HD12	1:F:29:MET:CE	2.50	0.41
1:A:3:ILE:HD12	1:A:29:MET:CE	2.50	0.41
1:H:3:ILE:HD12	1:H:29:MET:CE	2.50	0.41
1:N:3:ILE:HD12	1:N:29:MET:CE	2.50	0.41
1:C:3:ILE:HD12	1:C:29:MET:CE	2.50	0.41
1:I:149:ILE:HG21	1:K:170:LEU:HD23	2.02	0.41
1:G:3:ILE:HD12	1:G:29:MET:CE	2.50	0.41
1:F:162:SER:OG	1:H:152:VAL:HA	2.21	0.41
1:G:180:ILE:HD13	1:G:257:LEU:HD12	2.02	0.41
1:H:142:VAL:CG1	1:H:149:ILE:HD11	2.51	0.41
1:M:3:ILE:HD12	1:M:29:MET:CE	2.50	0.41
1:E:180:ILE:HD13	1:E:257:LEU:HD12	2.03	0.41
1:N:188:ILE:CG2	1:N:225:ILE:HD11	2.51	0.41
1:C:250:LEU:HD21	2:C:401:ADP:C2	2.56	0.40
1:B:9:ASN:CG	1:B:12:LEU:HD13	2.41	0.40
1:E:3:ILE:HD12	1:E:29:MET:CE	2.51	0.40
1:H:48:ILE:HD11	1:H:79:GLN:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:3:ILE:HD12	1:I:29:MET:CE	2.50	0.40
1:O:3:ILE:HD12	1:O:29:MET:CE	2.50	0.40
1:K:48:ILE:HD11	1:K:79:GLN:HB3	2.03	0.40
1:M:48:ILE:HD11	1:M:79:GLN:HB3	2.03	0.40
1:O:48:ILE:HD11	1:O:79:GLN:HB3	2.03	0.40
1:I:48:ILE:HD11	1:I:79:GLN:HB3	2.04	0.40
1:J:180:ILE:HD13	1:J:257:LEU:HD12	2.03	0.40
1:M:149:ILE:CG2	1:O:169:GLY:O	2.69	0.40
1:N:201:MET:CE	1:N:214:LEU:HD11	2.51	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:268:GLU:OE2	1:E:228:GLU:OE1[1_545]	1.75	0.45

## 5.3 Torsion angles [\(i\)](#)

### 5.3.1 Protein backbone [\(i\)](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	288/309 (93%)	274 (95%)	12 (4%)	2 (1%)	22 54
1	B	277/309 (90%)	266 (96%)	10 (4%)	1 (0%)	34 66
1	C	278/309 (90%)	266 (96%)	11 (4%)	1 (0%)	34 66
1	D	289/309 (94%)	274 (95%)	14 (5%)	1 (0%)	41 71
1	E	290/309 (94%)	276 (95%)	13 (4%)	1 (0%)	41 71
1	F	280/309 (91%)	267 (95%)	12 (4%)	1 (0%)	34 66
1	G	278/309 (90%)	266 (96%)	10 (4%)	2 (1%)	22 54
1	H	280/309 (91%)	268 (96%)	11 (4%)	1 (0%)	34 66
1	I	278/309 (90%)	266 (96%)	10 (4%)	2 (1%)	22 54

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	J	282/309 (91%)	271 (96%)	10 (4%)	1 (0%)	34 66
1	K	279/309 (90%)	267 (96%)	10 (4%)	2 (1%)	22 54
1	L	292/309 (94%)	276 (94%)	14 (5%)	2 (1%)	22 54
1	M	288/309 (93%)	275 (96%)	12 (4%)	1 (0%)	41 71
1	N	288/309 (93%)	273 (95%)	14 (5%)	1 (0%)	41 71
1	O	288/309 (93%)	274 (95%)	12 (4%)	2 (1%)	22 54
1	P	282/309 (91%)	268 (95%)	13 (5%)	1 (0%)	34 66
All	All	4537/4944 (92%)	4327 (95%)	188 (4%)	22 (0%)	29 61

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	HIS
1	B	44	HIS
1	C	44	HIS
1	D	44	HIS
1	F	44	HIS
1	G	44	HIS
1	H	44	HIS
1	I	44	HIS
1	J	44	HIS
1	K	44	HIS
1	L	44	HIS
1	M	44	HIS
1	N	44	HIS
1	O	44	HIS
1	P	44	HIS
1	L	293	HIS
1	E	44	HIS
1	A	69	VAL
1	G	69	VAL
1	I	69	VAL
1	O	69	VAL
1	K	69	VAL

### 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	229/254 (90%)	222 (97%)	7 (3%)	40 74
1	B	215/254 (85%)	210 (98%)	5 (2%)	50 80
1	C	223/254 (88%)	217 (97%)	6 (3%)	44 77
1	D	227/254 (89%)	221 (97%)	6 (3%)	46 77
1	E	226/254 (89%)	218 (96%)	8 (4%)	36 70
1	F	225/254 (89%)	217 (96%)	8 (4%)	35 69
1	G	223/254 (88%)	216 (97%)	7 (3%)	40 74
1	H	223/254 (88%)	216 (97%)	7 (3%)	40 74
1	I	216/254 (85%)	211 (98%)	5 (2%)	50 80
1	J	220/254 (87%)	214 (97%)	6 (3%)	44 77
1	K	222/254 (87%)	215 (97%)	7 (3%)	39 73
1	L	228/254 (90%)	219 (96%)	9 (4%)	32 66
1	M	227/254 (89%)	221 (97%)	6 (3%)	46 77
1	N	215/254 (85%)	210 (98%)	5 (2%)	50 80
1	O	226/254 (89%)	220 (97%)	6 (3%)	44 77
1	P	222/254 (87%)	215 (97%)	7 (3%)	39 73
All	All	3567/4064 (88%)	3462 (97%)	105 (3%)	42 76

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	39	MET
1	A	106	LEU
1	A	131	GLN
1	A	181	LYS
1	A	182	GLU
1	A	209	GLU
1	A	214	LEU
1	B	11	ARG
1	B	39	MET
1	B	106	LEU
1	B	149	ILE
1	B	182	GLU

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Mol	Chain	Res	Type
1	C	39	MET
1	C	64	ARG
1	C	106	LEU
1	C	131	GLN
1	C	149	ILE
1	C	182	GLU
1	D	39	MET
1	D	64	ARG
1	D	106	LEU
1	D	131	GLN
1	D	171	LYS
1	D	182	GLU
1	E	39	MET
1	E	106	LEU
1	E	131	GLN
1	E	147	GLN
1	E	182	GLU
1	E	209	GLU
1	E	214	LEU
1	E	238	LYS
1	F	8	ARG
1	F	39	MET
1	F	64	ARG
1	F	106	LEU
1	F	131	GLN
1	F	182	GLU
1	F	209	GLU
1	F	210	PHE
1	G	39	MET
1	G	51	ARG
1	G	106	LEU
1	G	131	GLN
1	G	182	GLU
1	G	209	GLU
1	G	238	LYS
1	H	39	MET
1	H	44	HIS
1	H	51	ARG
1	H	106	LEU
1	H	182	GLU
1	H	189	ARG
1	H	235	ARG

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Mol	Chain	Res	Type
1	I	39	MET
1	I	64	ARG
1	I	106	LEU
1	I	131	GLN
1	I	182	GLU
1	J	39	MET
1	J	64	ARG
1	J	106	LEU
1	J	131	GLN
1	J	149	ILE
1	J	182	GLU
1	K	39	MET
1	K	106	LEU
1	K	131	GLN
1	K	172	GLN
1	K	182	GLU
1	K	209	GLU
1	K	210	PHE
1	L	8	ARG
1	L	39	MET
1	L	106	LEU
1	L	131	GLN
1	L	142	VAL
1	L	181	LYS
1	L	182	GLU
1	L	213	ASN
1	L	215	HIS
1	M	39	MET
1	M	106	LEU
1	M	147	GLN
1	M	182	GLU
1	M	216	ARG
1	M	228	GLU
1	N	39	MET
1	N	106	LEU
1	N	131	GLN
1	N	182	GLU
1	N	215	HIS
1	O	39	MET
1	O	106	LEU
1	O	131	GLN
1	O	182	GLU

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Mol	Chain	Res	Type
1	O	206	LYS
1	O	209	GLU
1	P	39	MET
1	P	51	ARG
1	P	106	LEU
1	P	131	GLN
1	P	182	GLU
1	P	209	GLU
1	P	230	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	GLN
1	A	254	HIS
1	B	172	GLN
1	C	131	GLN
1	C	172	GLN
1	D	131	GLN
1	E	131	GLN
1	F	131	GLN
1	F	172	GLN
1	G	131	GLN
1	G	172	GLN
1	H	172	GLN
1	I	131	GLN
1	J	131	GLN
1	J	172	GLN
1	K	131	GLN
1	L	131	GLN
1	N	131	GLN
1	O	131	GLN
1	P	131	GLN

### 5.3.3 RNA [\(i\)](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [\(i\)](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [\(i\)](#)

11 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	ADP	O	401	-	24,29,29	0.64	0	29,45,45	0.71	1 (3%)
2	ADP	K	401	-	24,29,29	0.67	0	29,45,45	0.70	1 (3%)
2	ADP	A	401	-	24,29,29	0.63	0	29,45,45	0.77	1 (3%)
2	ADP	M	401	-	24,29,29	0.63	0	29,45,45	0.76	1 (3%)
2	ADP	C	401	-	24,29,29	0.65	0	29,45,45	0.78	1 (3%)
2	ADP	G	401	-	24,29,29	0.66	0	29,45,45	0.75	1 (3%)
2	ADP	J	401	-	24,29,29	0.64	0	29,45,45	0.71	1 (3%)
2	ADP	E	401	-	24,29,29	0.64	0	29,45,45	0.74	1 (3%)
2	ADP	H	401	-	24,29,29	0.66	0	29,45,45	0.71	1 (3%)
2	ADP	B	401	-	24,29,29	0.65	0	29,45,45	0.68	1 (3%)
2	ADP	D	401	-	24,29,29	0.65	0	29,45,45	0.71	1 (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
2	ADP	O	401	-	-	2/12/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	ADP	K	401	-	-	5/12/32/32	0/3/3/3
2	ADP	A	401	-	-	5/12/32/32	0/3/3/3
2	ADP	M	401	-	-	4/12/32/32	0/3/3/3
2	ADP	C	401	-	-	4/12/32/32	0/3/3/3
2	ADP	G	401	-	-	2/12/32/32	0/3/3/3
2	ADP	J	401	-	-	1/12/32/32	0/3/3/3
2	ADP	E	401	-	-	3/12/32/32	0/3/3/3
2	ADP	H	401	-	-	8/12/32/32	0/3/3/3
2	ADP	B	401	-	-	0/12/32/32	0/3/3/3
2	ADP	D	401	-	-	2/12/32/32	0/3/3/3

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
2	A	401	ADP	C5-C6-N6	2.33	123.89	120.35
2	G	401	ADP	C5-C6-N6	2.32	123.88	120.35
2	H	401	ADP	C5-C6-N6	2.29	123.83	120.35
2	K	401	ADP	C5-C6-N6	2.28	123.82	120.35
2	M	401	ADP	C5-C6-N6	2.23	123.74	120.35
2	E	401	ADP	C5-C6-N6	2.22	123.73	120.35
2	B	401	ADP	C5-C6-N6	2.22	123.73	120.35
2	D	401	ADP	C5-C6-N6	2.22	123.73	120.35
2	O	401	ADP	C5-C6-N6	2.22	123.72	120.35
2	J	401	ADP	C5-C6-N6	2.19	123.68	120.35
2	C	401	ADP	C5-C6-N6	2.11	123.56	120.35

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	ADP	C5'-O5'-PA-O1A
2	A	401	ADP	C5'-O5'-PA-O2A
2	C	401	ADP	O4'-C4'-C5'-O5'
2	D	401	ADP	C5'-O5'-PA-O1A
2	D	401	ADP	C5'-O5'-PA-O3A
2	H	401	ADP	C5'-O5'-PA-O2A
2	H	401	ADP	C5'-O5'-PA-O3A
2	H	401	ADP	O4'-C4'-C5'-O5'

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Mol	Chain	Res	Type	Atoms
2	K	401	ADP	PA-O3A-PB-O2B
2	M	401	ADP	PA-O3A-PB-O2B
2	C	401	ADP	C3'-C4'-C5'-O5'
2	E	401	ADP	O4'-C4'-C5'-O5'
2	G	401	ADP	O4'-C4'-C5'-O5'
2	H	401	ADP	C3'-C4'-C5'-O5'
2	K	401	ADP	O4'-C4'-C5'-O5'
2	K	401	ADP	C3'-C4'-C5'-O5'
2	A	401	ADP	O4'-C4'-C5'-O5'
2	A	401	ADP	C3'-C4'-C5'-O5'
2	E	401	ADP	C3'-C4'-C5'-O5'
2	G	401	ADP	C3'-C4'-C5'-O5'
2	C	401	ADP	PB-O3A-PA-O5'
2	O	401	ADP	O4'-C4'-C5'-O5'
2	A	401	ADP	C5'-O5'-PA-O3A
2	H	401	ADP	C5'-O5'-PA-O1A
2	O	401	ADP	C3'-C4'-C5'-O5'
2	H	401	ADP	PA-O3A-PB-O1B
2	J	401	ADP	O4'-C4'-C5'-O5'
2	M	401	ADP	O4'-C4'-C5'-O5'
2	H	401	ADP	PA-O3A-PB-O2B
2	H	401	ADP	PA-O3A-PB-O3B
2	K	401	ADP	PA-O3A-PB-O3B
2	M	401	ADP	PA-O3A-PB-O3B
2	C	401	ADP	C5'-O5'-PA-O1A
2	E	401	ADP	C5'-O5'-PA-O1A
2	K	401	ADP	C5'-O5'-PA-O1A
2	M	401	ADP	PA-O3A-PB-O1B

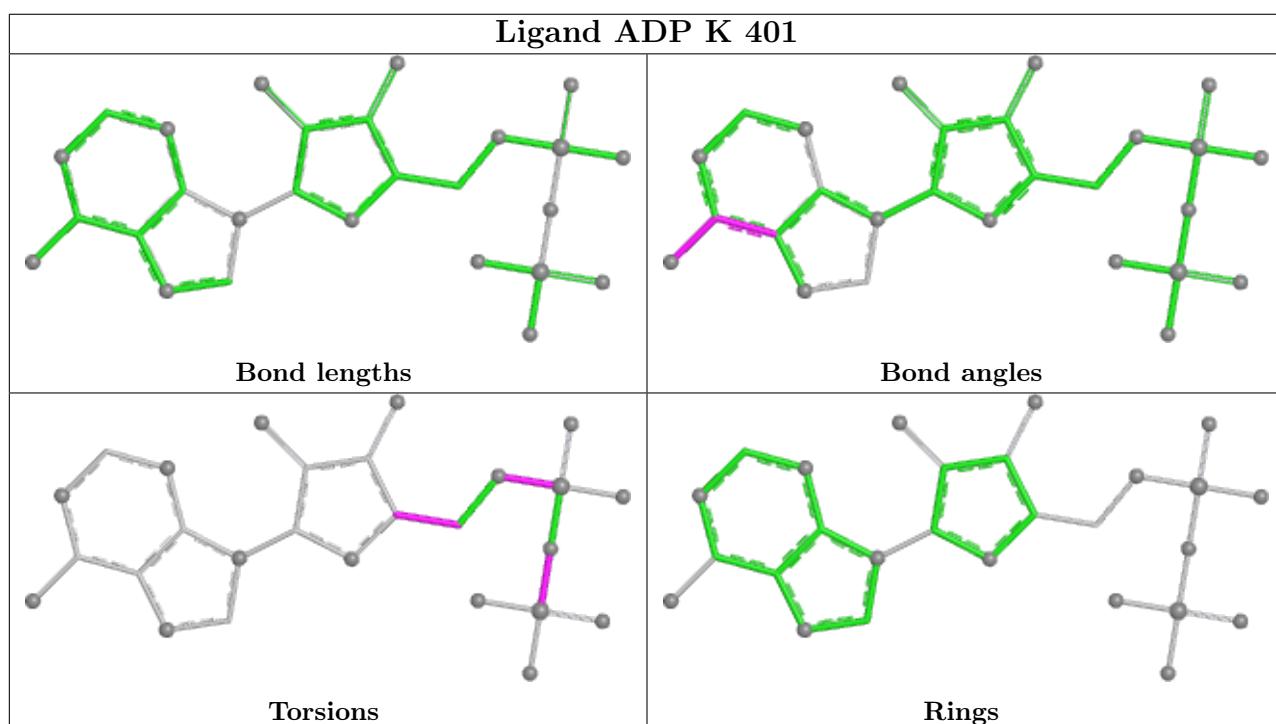
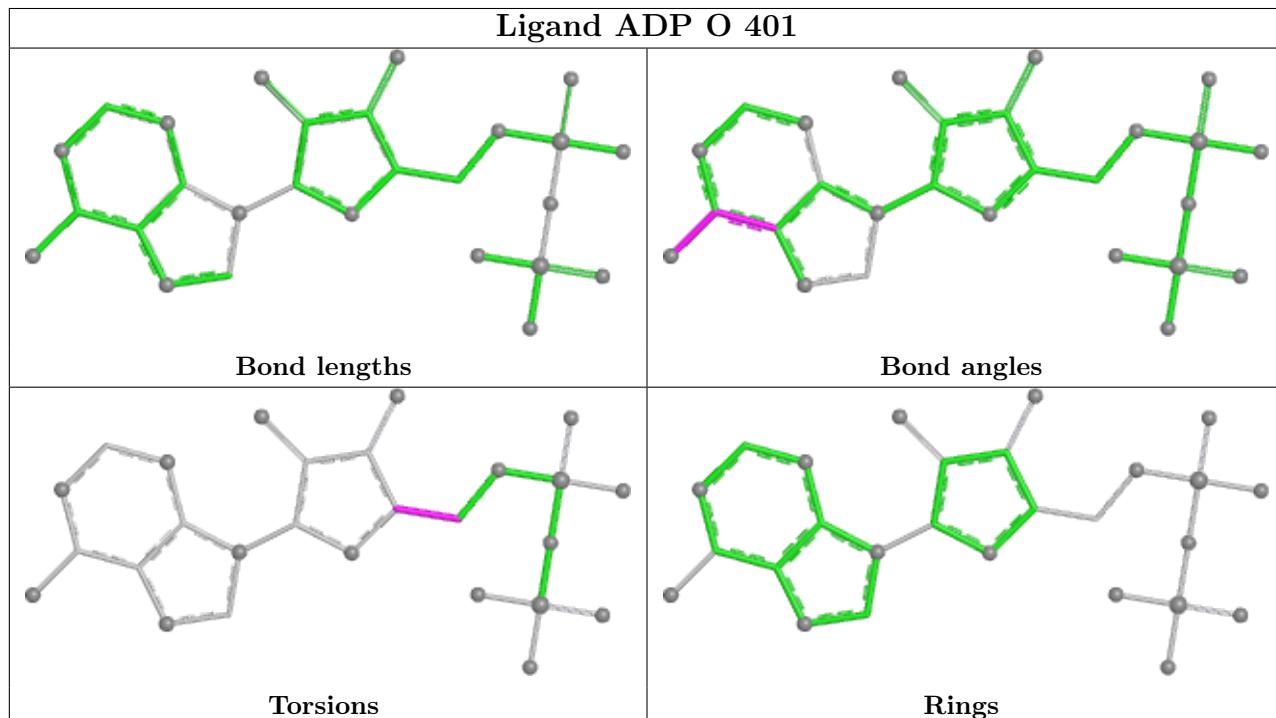
There are no ring outliers.

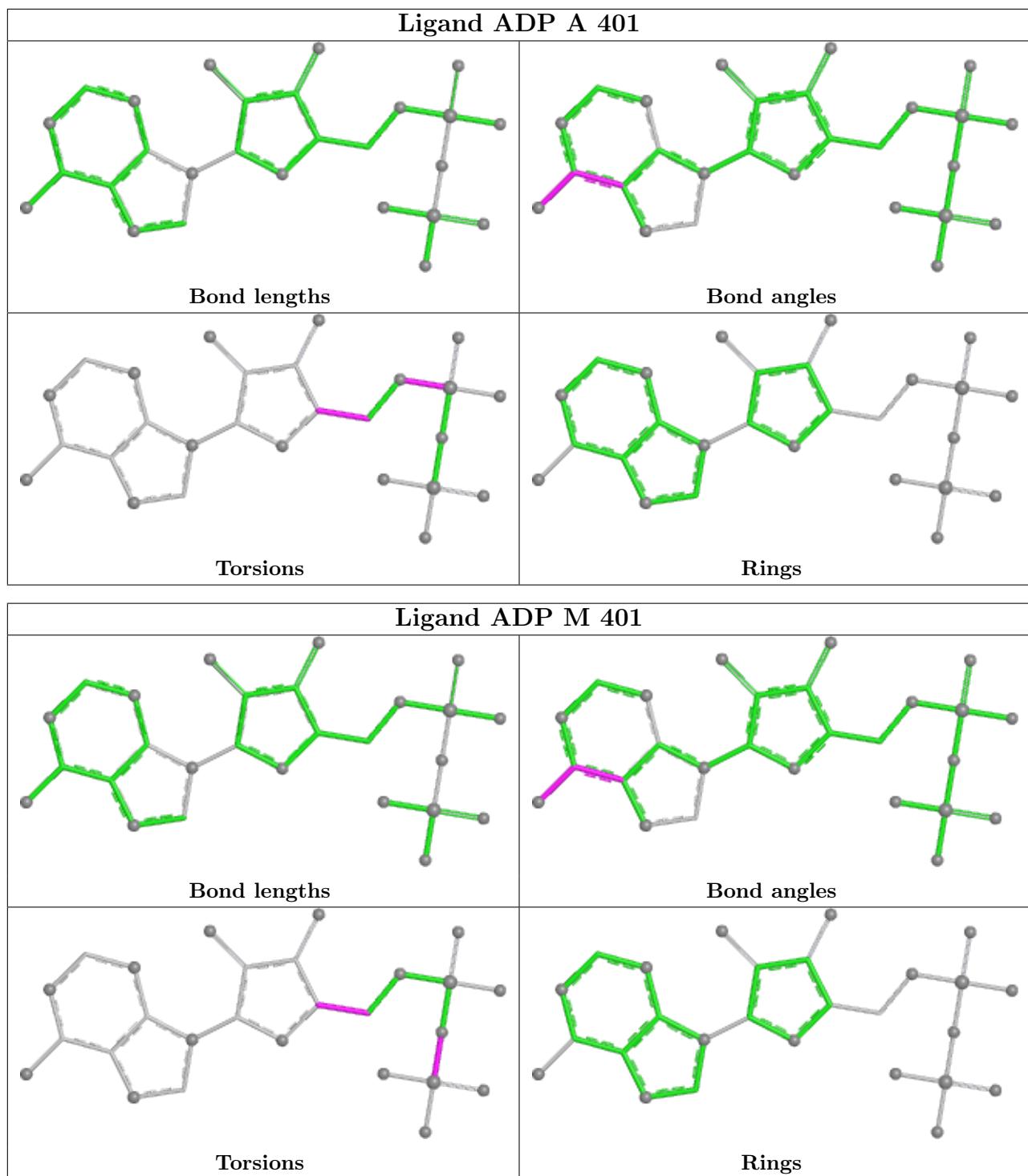
3 monomers are involved in 3 short contacts:

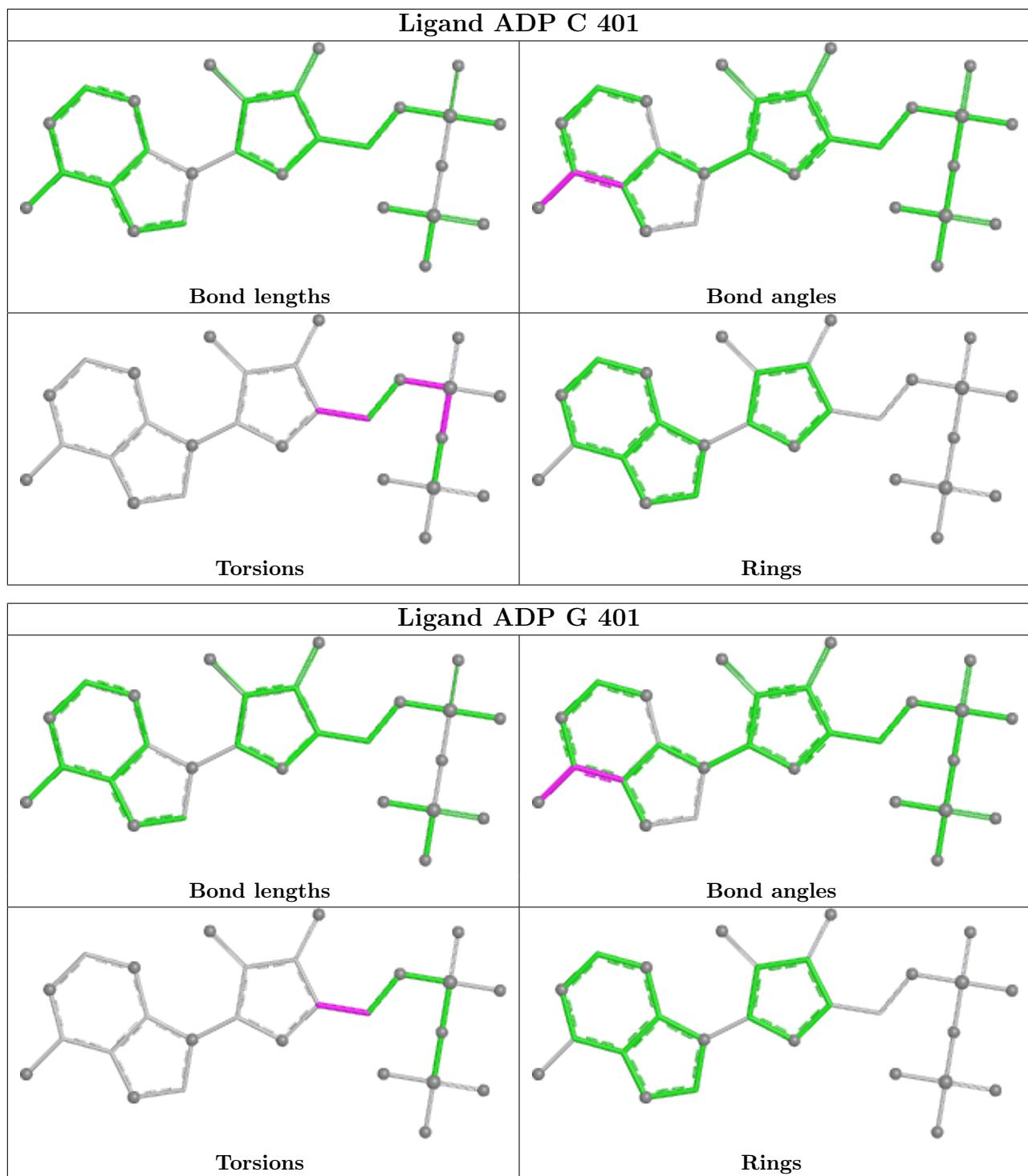
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	401	ADP	1	0
2	J	401	ADP	1	0
2	B	401	ADP	1	0

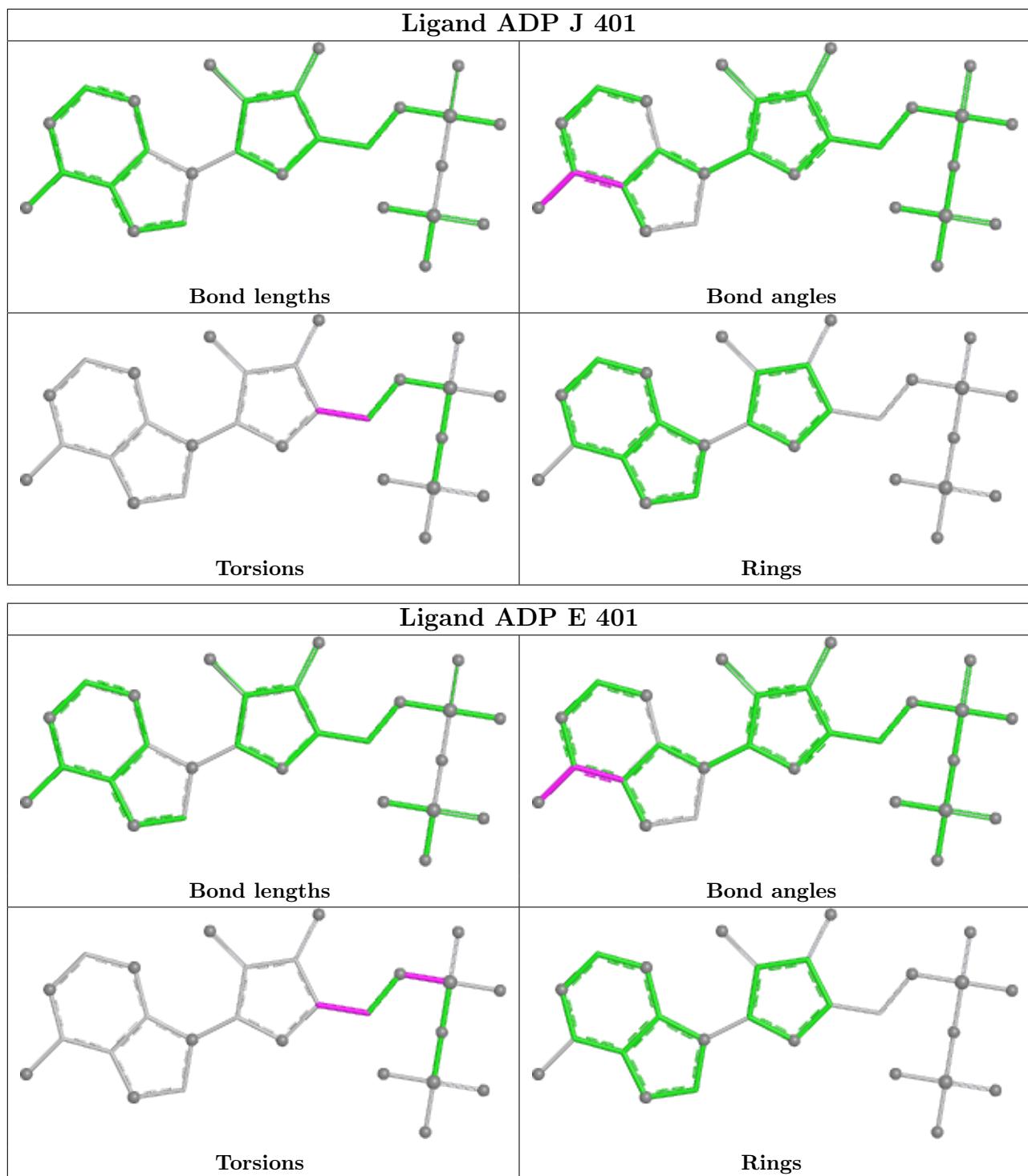
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

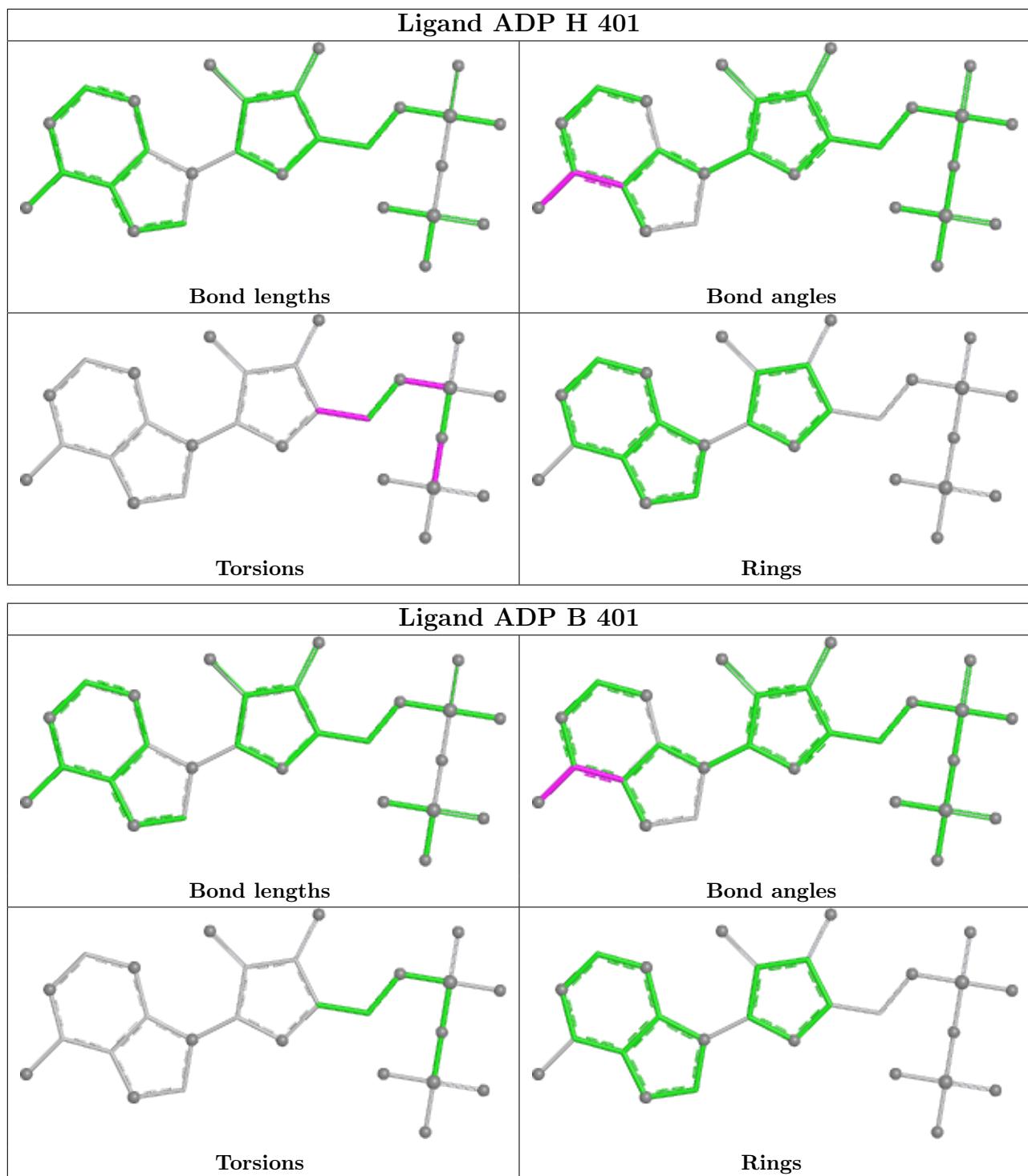
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

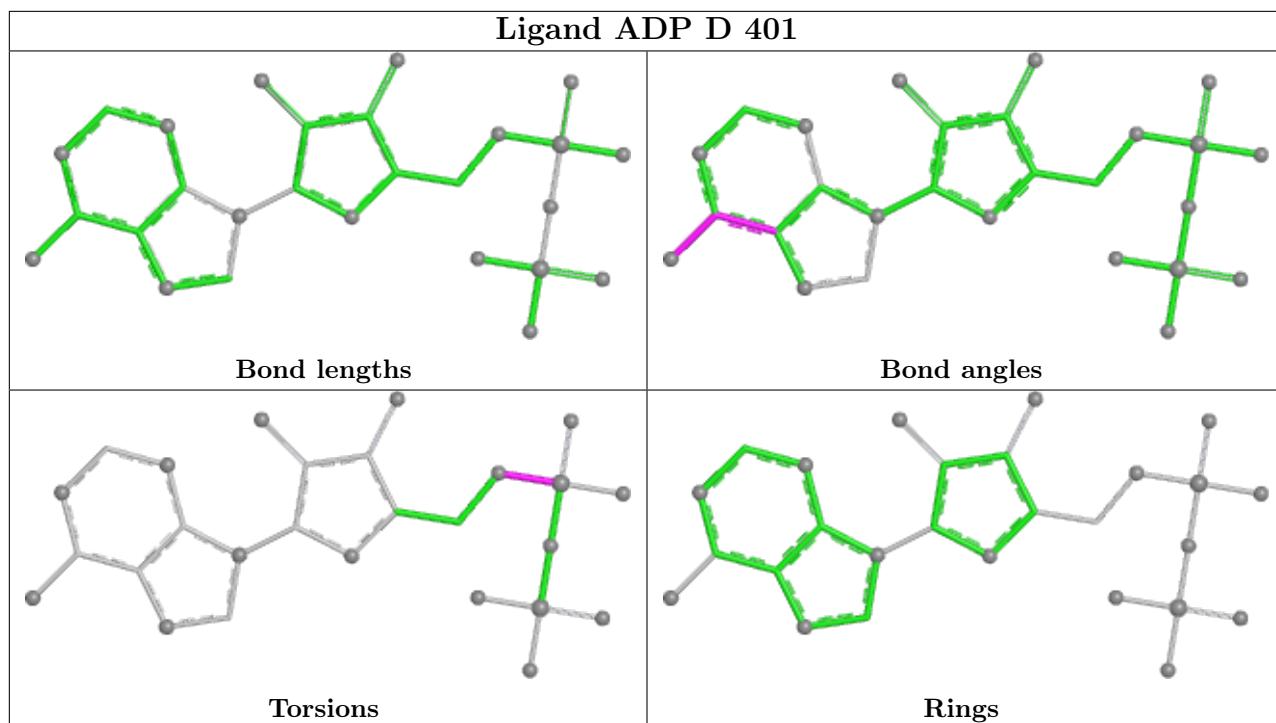












## 5.7 Other polymers [\(i\)](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data [\(i\)](#)

### 6.1 Protein, DNA and RNA chains [\(i\)](#)

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	290/309 (93%)	0.51	17 (5%) 22 18	36, 60, 117, 149	0
1	B	281/309 (90%)	0.65	19 (6%) 17 13	40, 58, 93, 134	0
1	C	282/309 (91%)	0.45	10 (3%) 44 38	38, 53, 96, 145	0
1	D	291/309 (94%)	0.56	20 (6%) 16 13	40, 54, 118, 156	0
1	E	292/309 (94%)	0.46	14 (4%) 30 27	32, 54, 113, 137	0
1	F	284/309 (91%)	0.48	11 (3%) 39 35	38, 58, 102, 170	0
1	G	282/309 (91%)	0.39	8 (2%) 53 49	33, 51, 93, 146	0
1	H	284/309 (91%)	0.57	17 (5%) 21 18	36, 53, 103, 159	0
1	I	282/309 (91%)	0.55	11 (3%) 39 35	42, 63, 108, 165	0
1	J	286/309 (92%)	0.58	22 (7%) 13 10	42, 61, 110, 182	0
1	K	283/309 (91%)	0.46	12 (4%) 36 32	37, 58, 108, 162	0
1	L	294/309 (95%)	0.62	22 (7%) 14 11	46, 66, 124, 165	0
1	M	290/309 (93%)	0.83	33 (11%) 5 3	45, 75, 131, 168	0
1	N	290/309 (93%)	1.13	56 (19%) 1 0	60, 95, 147, 199	0
1	O	290/309 (93%)	0.63	15 (5%) 27 23	46, 66, 122, 157	0
1	P	286/309 (92%)	0.58	23 (8%) 12 9	44, 64, 115, 158	0
All	All	4587/4944 (92%)	0.59	310 (6%) 17 13	32, 61, 119, 199	0

All (310) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	207	PRO	12.9
1	O	213	ASN	10.2
1	J	207	PRO	9.5
1	I	210	PHE	9.1
1	M	215	HIS	8.2

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Mol	Chain	Res	Type	RSRZ
1	B	145	GLY	7.8
1	J	208	GLY	7.8
1	E	146	THR	7.7
1	P	208	GLY	7.3
1	O	210	PHE	7.2
1	H	208	GLY	6.9
1	M	208	GLY	6.7
1	N	217	GLY	6.6
1	P	207	PRO	6.5
1	C	207	PRO	6.3
1	M	210	PHE	6.3
1	J	210	PHE	6.2
1	D	146	THR	6.1
1	K	210	PHE	6.1
1	M	209	GLU	6.1
1	H	207	PRO	6.0
1	O	214	LEU	6.0
1	I	208	GLY	5.9
1	N	207	PRO	5.8
1	G	207	PRO	5.7
1	N	208	GLY	5.7
1	M	213	ASN	5.7
1	I	209	GLU	5.6
1	H	69	VAL	5.5
1	L	212	SER	5.5
1	O	217	GLY	5.4
1	L	215	HIS	5.3
1	H	146	THR	5.3
1	M	214	LEU	5.2
1	O	207	PRO	5.2
1	L	207	PRO	5.2
1	L	294	MET	5.1
1	C	208	GLY	5.1
1	I	207	PRO	5.1
1	D	211	ARG	5.0
1	A	214	LEU	5.0
1	I	68	SER	4.9
1	J	146	THR	4.8
1	H	67	ALA	4.7
1	K	207	PRO	4.6
1	A	215	HIS	4.6
1	B	146	THR	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	147	GLN	4.6
1	E	215	HIS	4.5
1	D	44	HIS	4.5
1	P	44	HIS	4.5
1	F	147	GLN	4.5
1	E	69	VAL	4.4
1	N	219	SER	4.4
1	L	213	ASN	4.4
1	N	180	ILE	4.4
1	A	208	GLY	4.4
1	O	211	ARG	4.3
1	P	146	THR	4.3
1	N	67	ALA	4.2
1	N	146	THR	4.2
1	I	206	LYS	4.2
1	E	147	GLN	4.2
1	O	44	HIS	4.1
1	N	10	PRO	4.1
1	L	214	LEU	4.1
1	H	210	PHE	4.1
1	A	146	THR	4.0
1	O	69	VAL	4.0
1	M	45	LYS	4.0
1	C	209	GLU	4.0
1	J	292	PRO	4.0
1	N	250	LEU	4.0
1	D	213	ASN	3.9
1	L	68	SER	3.9
1	D	210	PHE	3.9
1	N	210	PHE	3.9
1	H	205	ALA	3.9
1	J	217	GLY	3.9
1	H	185	GLY	3.9
1	K	145	GLY	3.9
1	J	69	VAL	3.8
1	N	1	MET	3.8
1	G	210	PHE	3.8
1	L	218	GLY	3.8
1	M	212	SER	3.8
1	M	183	ALA	3.8
1	F	10	PRO	3.8
1	D	214	LEU	3.8

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Mol	Chain	Res	Type	RSRZ
1	I	185	GLY	3.8
1	A	217	GLY	3.8
1	B	292	PRO	3.7
1	D	69	VAL	3.7
1	E	145	GLY	3.7
1	I	148	GLY	3.7
1	L	208	GLY	3.7
1	L	217	GLY	3.7
1	C	210	PHE	3.7
1	N	253	ASN	3.7
1	A	145	GLY	3.6
1	N	190	CYS	3.6
1	P	43	SER	3.6
1	E	217	GLY	3.6
1	N	218	GLY	3.6
1	K	69	VAL	3.6
1	E	213	ASN	3.6
1	G	69	VAL	3.6
1	N	22	GLY	3.6
1	B	44	HIS	3.6
1	E	207	PRO	3.6
1	N	290	SER	3.5
1	K	146	THR	3.5
1	F	145	GLY	3.5
1	L	293	HIS	3.5
1	L	183	ALA	3.5
1	B	68	SER	3.4
1	J	180	ILE	3.4
1	N	289	ASN	3.4
1	N	13	TYR	3.3
1	F	210	PHE	3.3
1	N	187	ASP	3.3
1	D	217	GLY	3.3
1	A	149	ILE	3.3
1	N	232	THR	3.3
1	N	278	VAL	3.3
1	M	68	SER	3.3
1	B	179	TYR	3.3
1	N	109	ARG	3.2
1	L	219	SER	3.2
1	H	149	ILE	3.2
1	P	292	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	M	147	GLN	3.2
1	M	146	THR	3.2
1	N	234	LEU	3.2
1	F	67	ALA	3.2
1	J	205	ALA	3.2
1	N	11	ARG	3.2
1	A	148	GLY	3.2
1	N	191	PHE	3.2
1	P	210	PHE	3.2
1	G	206	LYS	3.1
1	A	213	ASN	3.1
1	K	147	GLN	3.1
1	K	208	GLY	3.1
1	M	145	GLY	3.1
1	N	69	VAL	3.0
1	N	214	LEU	3.0
1	A	184	GLY	3.0
1	H	209	GLU	3.0
1	G	208	GLY	3.0
1	J	145	GLY	3.0
1	N	160	ALA	3.0
1	L	44	HIS	3.0
1	H	183	ALA	3.0
1	J	219	SER	3.0
1	O	147	GLN	3.0
1	D	207	PRO	2.9
1	O	146	THR	2.9
1	D	215	HIS	2.9
1	E	148	GLY	2.9
1	M	47	GLN	2.9
1	C	206	LYS	2.9
1	F	146	THR	2.9
1	L	146	THR	2.9
1	C	44	HIS	2.9
1	K	44	HIS	2.9
1	D	208	GLY	2.9
1	F	208	GLY	2.9
1	N	200	SER	2.8
1	P	219	SER	2.8
1	J	186	ALA	2.8
1	M	216	ARG	2.8
1	N	181	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	P	145	GLY	2.8
1	F	207	PRO	2.8
1	G	150	GLY	2.8
1	F	184	GLY	2.7
1	P	291	GLY	2.7
1	H	187	ASP	2.7
1	K	68	SER	2.7
1	P	68	SER	2.7
1	B	147	GLN	2.7
1	I	179	TYR	2.7
1	H	145	GLY	2.7
1	N	179	TYR	2.7
1	O	149	ILE	2.7
1	O	212	SER	2.7
1	M	206	LYS	2.7
1	M	217	GLY	2.7
1	A	69	VAL	2.7
1	L	69	VAL	2.7
1	B	119	PHE	2.7
1	J	209	GLU	2.6
1	E	214	LEU	2.6
1	D	147	GLN	2.6
1	L	222	LEU	2.6
1	B	10	PRO	2.6
1	J	148	GLY	2.6
1	B	135	GLY	2.6
1	E	68	SER	2.6
1	O	148	GLY	2.6
1	J	147	GLN	2.5
1	N	117	THR	2.5
1	N	272	VAL	2.5
1	J	7	SER	2.5
1	E	185	GLY	2.5
1	N	44	HIS	2.5
1	H	150	GLY	2.5
1	P	188	ILE	2.5
1	C	146	THR	2.5
1	P	209	GLU	2.5
1	D	68	SER	2.5
1	P	156	THR	2.5
1	J	10	PRO	2.5
1	N	59	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	44	HIS	2.5
1	N	221	SER	2.5
1	P	254	HIS	2.5
1	M	185	GLY	2.5
1	E	188	ILE	2.5
1	O	43	SER	2.5
1	N	206	LYS	2.5
1	M	211	ARG	2.4
1	B	205	ALA	2.4
1	C	150	GLY	2.4
1	L	67	ALA	2.4
1	N	236	ALA	2.4
1	N	254	HIS	2.4
1	B	250	LEU	2.4
1	D	205	ALA	2.4
1	F	179	TYR	2.4
1	N	47	GLN	2.4
1	A	209	GLU	2.4
1	N	215	HIS	2.4
1	A	68	SER	2.4
1	N	255	GLY	2.4
1	N	116	VAL	2.4
1	D	185	GLY	2.4
1	C	144	GLU	2.4
1	H	148	GLY	2.4
1	B	70	THR	2.4
1	N	264	SER	2.4
1	M	149	ILE	2.4
1	M	219	SER	2.4
1	N	251	ARG	2.4
1	L	210	PHE	2.3
1	M	191	PHE	2.3
1	L	292	PRO	2.3
1	P	273	THR	2.3
1	B	136	ALA	2.3
1	N	86	PHE	2.3
1	M	1	MET	2.3
1	P	67	ALA	2.3
1	B	133	VAL	2.3
1	A	54	PRO	2.3
1	L	211	ARG	2.3
1	M	186	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	I	69	VAL	2.3
1	D	218	GLY	2.3
1	J	179	TYR	2.3
1	N	188	ILE	2.3
1	P	69	VAL	2.2
1	F	150	GLY	2.2
1	D	273	THR	2.2
1	J	44	HIS	2.2
1	H	147	GLN	2.2
1	M	69	VAL	2.2
1	N	133	VAL	2.2
1	C	145	GLY	2.2
1	N	68	SER	2.2
1	P	190	CYS	2.2
1	J	34	THR	2.2
1	L	47	GLN	2.2
1	M	218	GLY	2.2
1	B	112	ILE	2.2
1	D	191	PHE	2.2
1	N	286	LEU	2.2
1	B	186	ALA	2.2
1	J	68	SER	2.2
1	N	147	GLN	2.2
1	K	149	ILE	2.2
1	N	199	ALA	2.1
1	N	282	ILE	2.1
1	B	144	GLU	2.1
1	E	216	ARG	2.1
1	J	133	VAL	2.1
1	M	277	ASP	2.1
1	M	150	GLY	2.1
1	N	256	PRO	2.1
1	P	278	VAL	2.1
1	P	183	ALA	2.1
1	A	47	GLN	2.1
1	M	187	ASP	2.1
1	M	205	ALA	2.1
1	B	150	GLY	2.1
1	O	184	GLY	2.1
1	I	156	THR	2.1
1	N	164	ILE	2.1
1	G	143	LEU	2.0

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Mol	Chain	Res	Type	RSRZ
1	H	68	SER	2.0
1	D	222	LEU	2.0
1	K	65	ILE	2.0
1	G	146	THR	2.0
1	K	56	GLU	2.0
1	P	185	GLY	2.0
1	D	172	GLN	2.0
1	M	44	HIS	2.0
1	M	120	ALA	2.0
1	N	220	ALA	2.0
1	P	217	GLY	2.0

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

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

## 6.3 Carbohydrates [\(i\)](#)

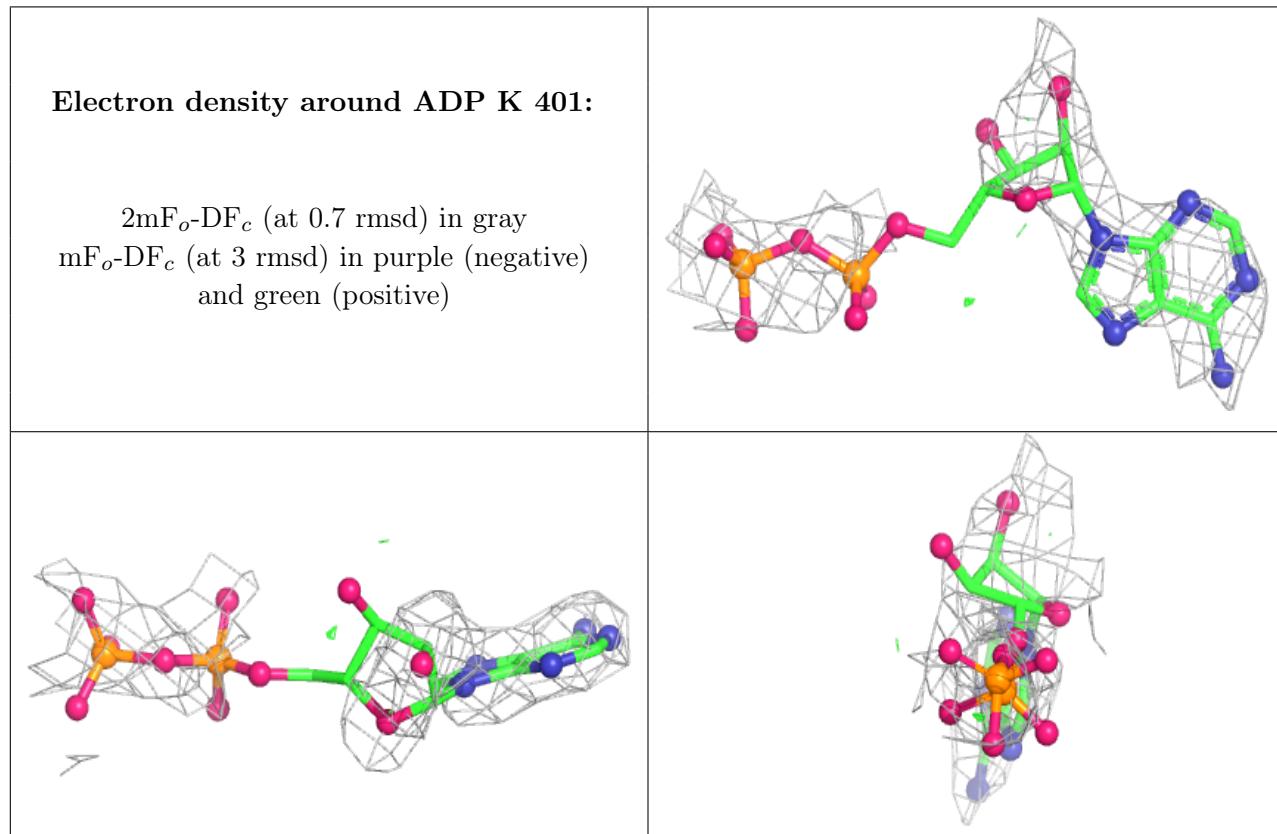
There are no monosaccharides in this entry.

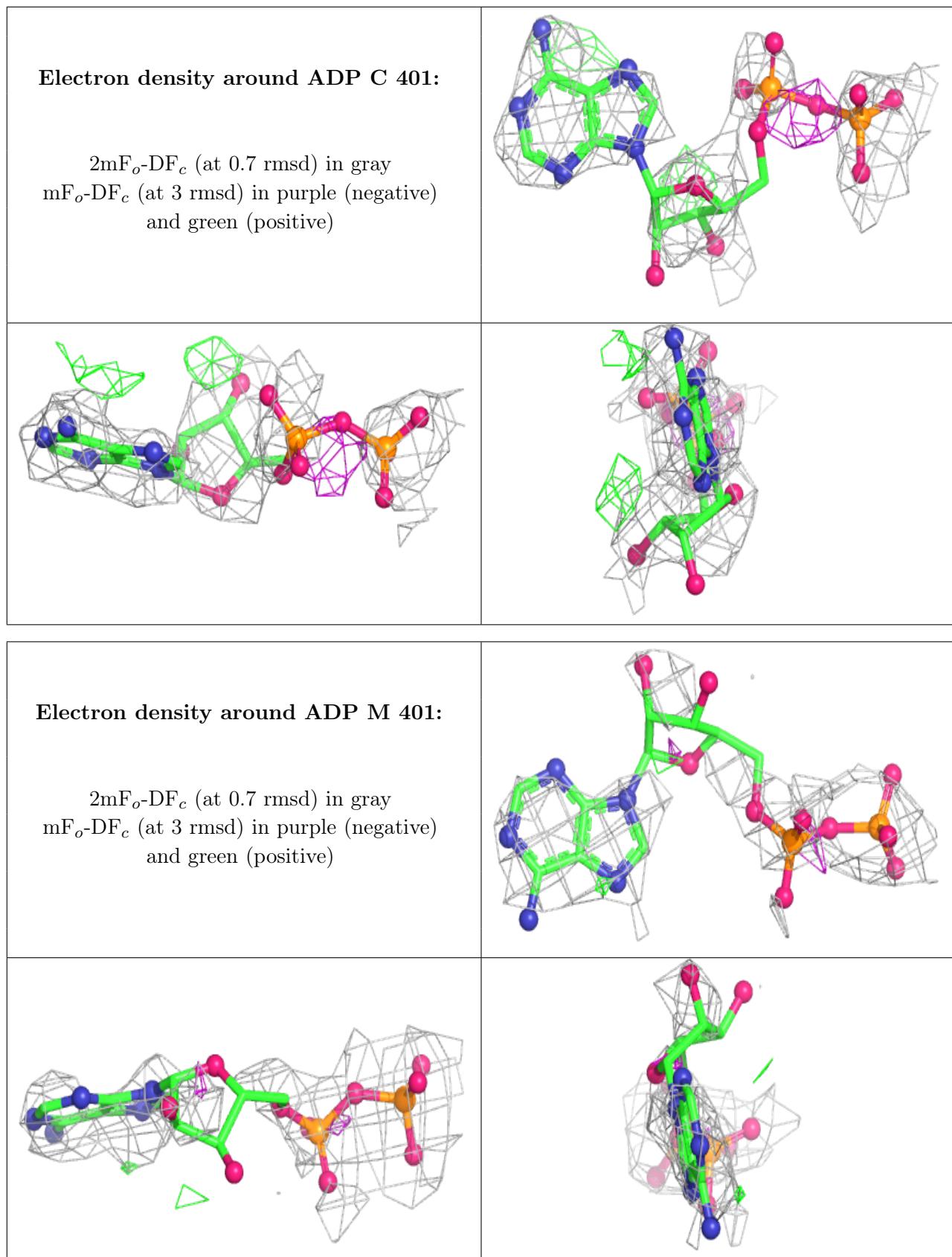
## 6.4 Ligands [\(i\)](#)

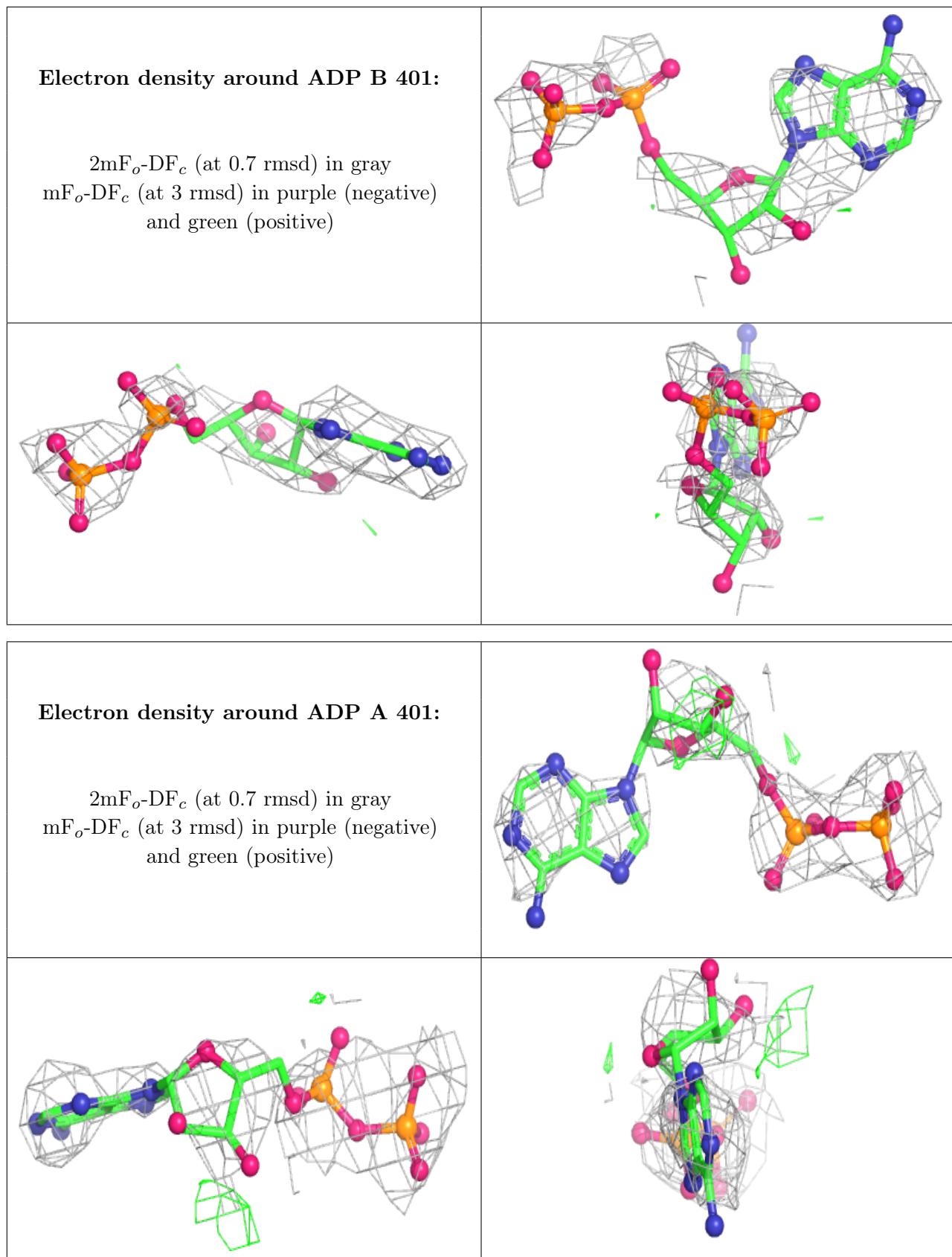
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q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

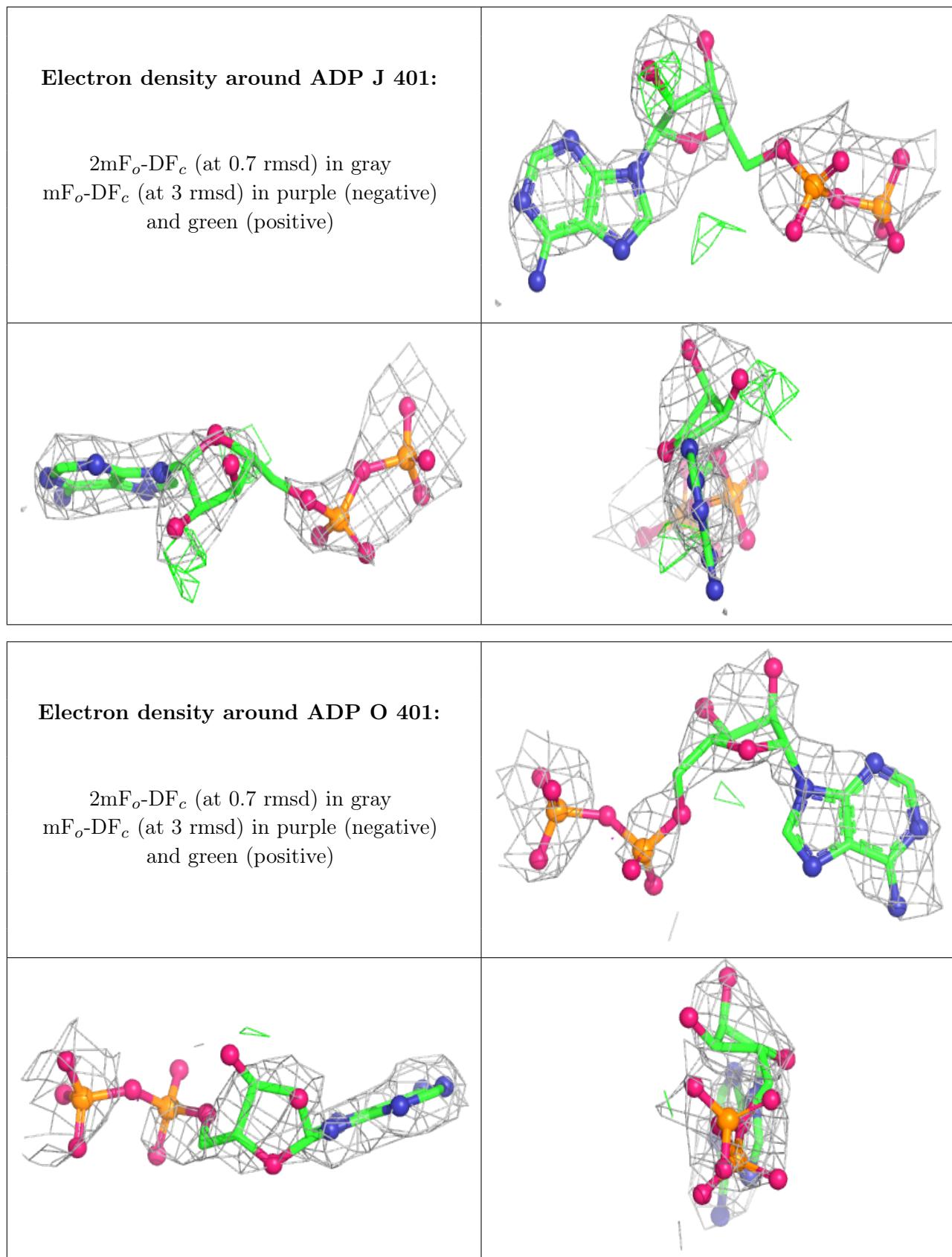
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	ADP	K	401	27/27	0.62	0.45	84,101,123,126	27
2	ADP	C	401	27/27	0.64	0.42	66,78,97,97	27
2	ADP	M	401	27/27	0.66	0.44	69,83,92,94	27
2	ADP	B	401	27/27	0.68	0.39	87,105,118,121	27
2	ADP	A	401	27/27	0.69	0.48	71,81,85,87	27
2	ADP	J	401	27/27	0.70	0.37	66,75,92,93	27
2	ADP	O	401	27/27	0.70	0.44	72,88,111,113	27
2	ADP	G	401	27/27	0.73	0.36	62,74,91,92	27
2	ADP	D	401	27/27	0.74	0.44	72,84,104,105	27
2	ADP	H	401	27/27	0.74	0.35	72,82,94,96	27
2	ADP	E	401	27/27	0.74	0.38	64,78,85,86	27

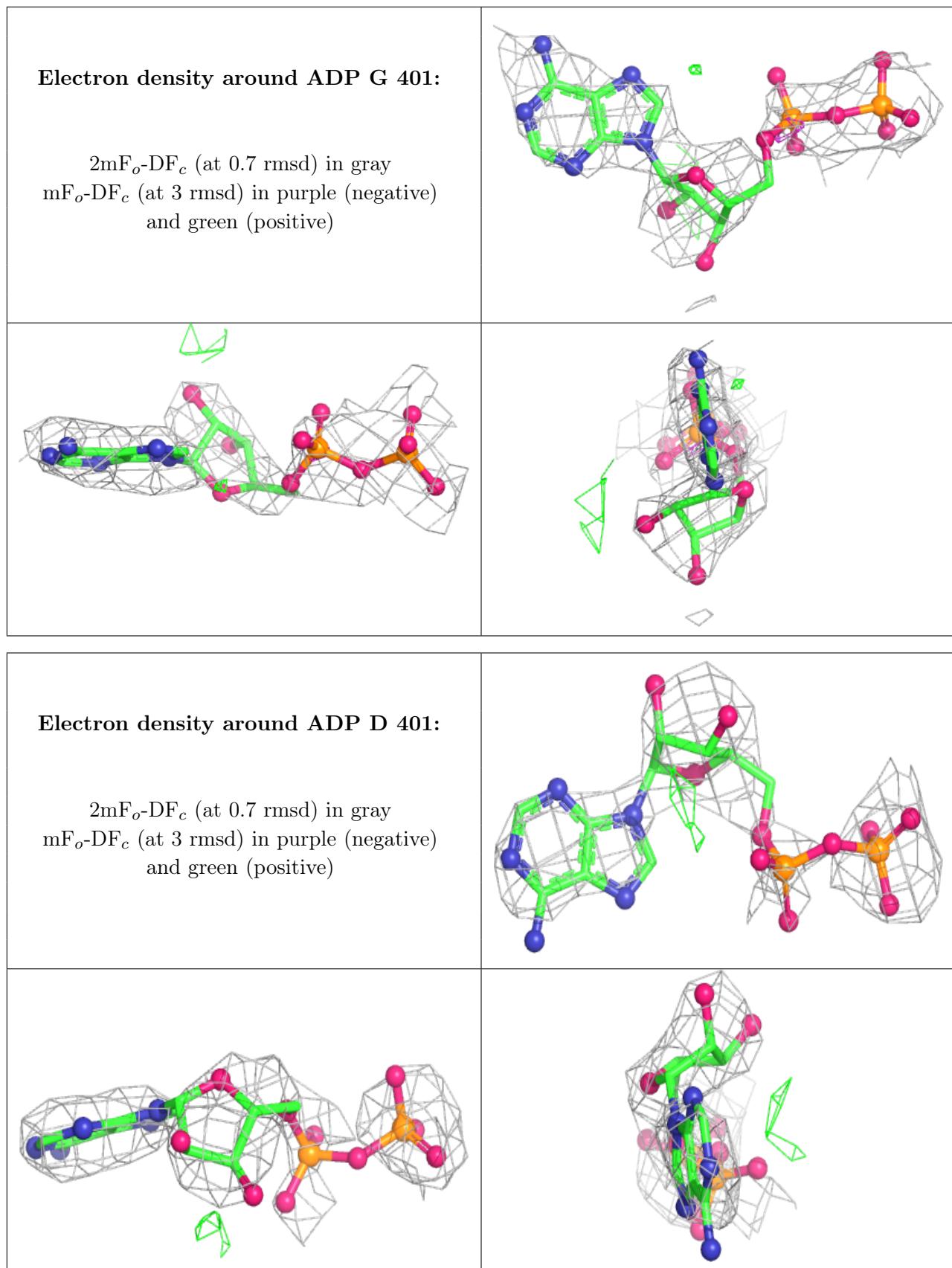
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

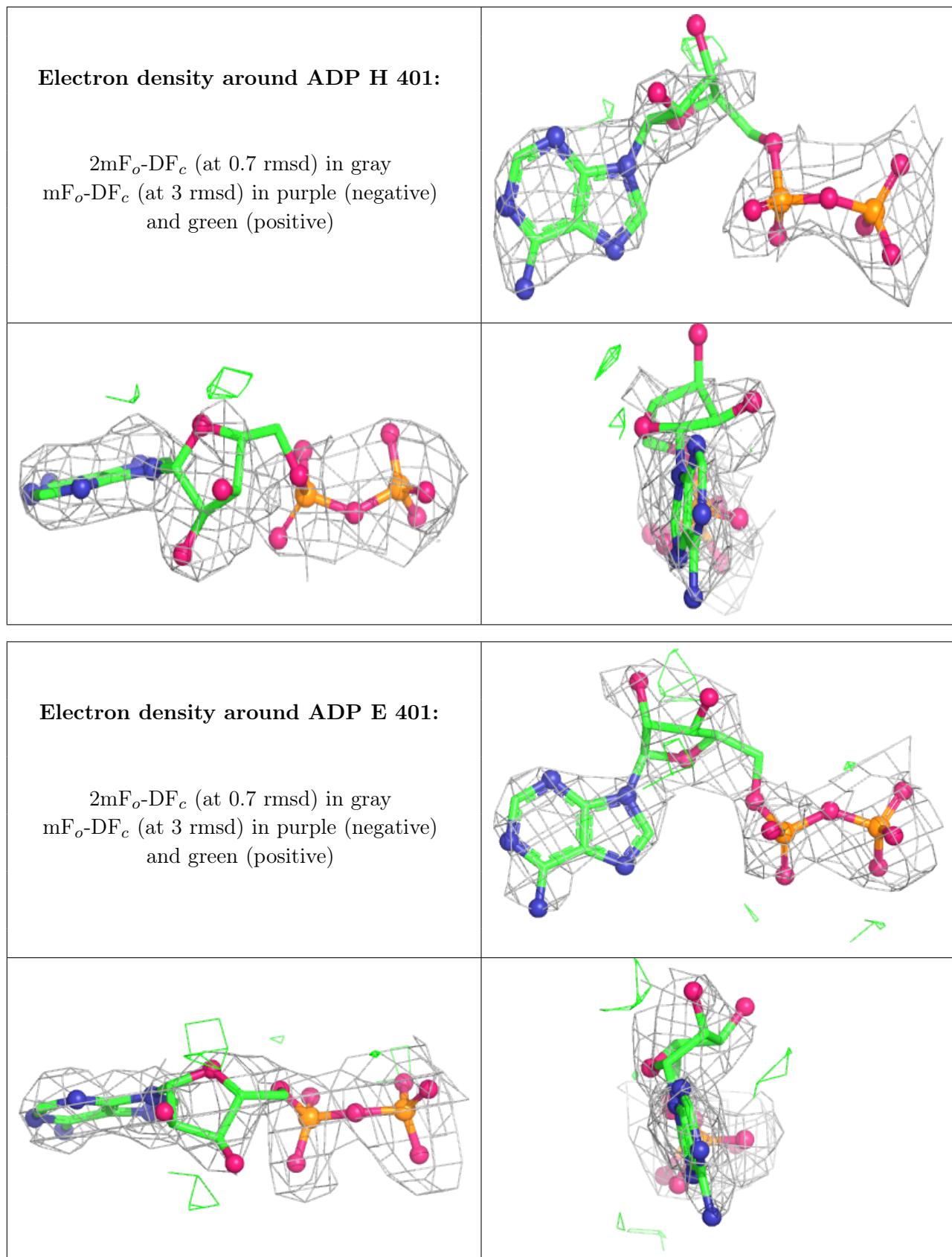












## 6.5 Other polymers [\(i\)](#)

There are no such residues in this entry.