



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 14, 2026 – 04:36 PM UTC

PDB ID : 1M6V / pdb_00001m6v
Title : Crystal Structure of the G359F (small subunit) Point Mutant of Carbamoyl Phosphate Synthetase
Authors : Thoden, J.B.; Huang, X.; Raushel, F.M.; Holden, H.M.
Deposited on : 2002-07-17
Resolution : 2.10 Å(reported)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

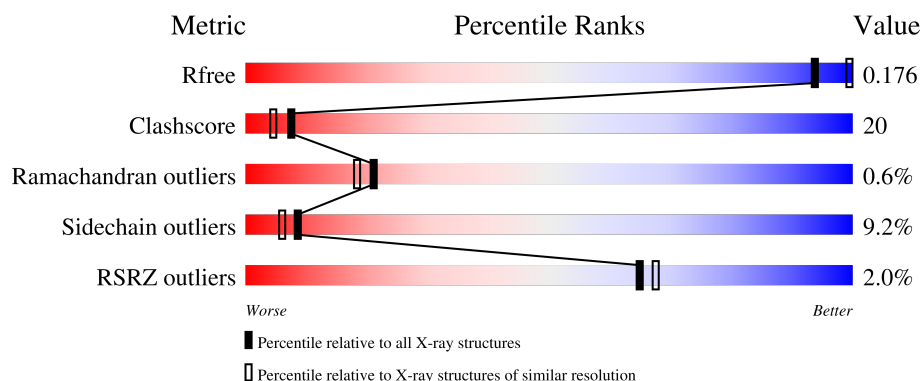
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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

Mol	Chain	Length	Quality of chain
1	A	1073	2% 64% 29% 5% .
1	C	1073	2% 64% 28% 7% .
1	E	1073	% 62% 31% 5% ..
1	G	1073	2% 56% 37% 6% .
2	B	382	4% 36% 49% 12% ...

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Mol	Chain	Length	Quality of chain
2	D	382	% 58% 35% 5% ••
2	F	382	% 47% 45% 5% ••
2	H	382	4% 40% 48% 9% ••

2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 48206 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 carbamoyl phosphate synthetase large chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1059	Total	C	N	O	S	0	6	0
			8190	5140	1425	1579	46			
1	C	1059	Total	C	N	O	S	0	5	0
			8196	5144	1431	1576	45			
1	E	1059	Total	C	N	O	S	0	6	0
			8189	5141	1426	1576	46			
1	G	1059	Total	C	N	O	S	0	6	0
			8197	5144	1428	1580	45			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	46	ASN	LEU	SEE REMARK 999	UNP P00968
C	46	ASN	LEU	SEE REMARK 999	UNP P00968
E	46	ASN	LEU	SEE REMARK 999	UNP P00968
G	46	ASN	LEU	SEE REMARK 999	UNP P00968

- Molecule 2 is a protein called carbamoyl-phosphate synthetase small chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	375	Total	C	N	O	S	0	1	0
			2871	1812	504	545	10			
2	D	375	Total	C	N	O	S	0	2	0
			2877	1814	507	546	10			
2	F	375	Total	C	N	O	S	0	3	0
			2880	1818	505	546	11			
2	H	375	Total	C	N	O	S	0	1	0
			2871	1812	504	545	10			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	183	GLN	GLU	SEE REMARK 999	UNP P00907
B	359	PHE	GLY	engineered mutation	UNP P00907
D	183	GLN	GLU	SEE REMARK 999	UNP P00907
D	359	PHE	GLY	engineered mutation	UNP P00907
F	183	GLN	GLU	SEE REMARK 999	UNP P00907
F	359	PHE	GLY	engineered mutation	UNP P00907
H	183	GLN	GLU	SEE REMARK 999	UNP P00907
H	359	PHE	GLY	engineered mutation	UNP P00907

- Molecule 3 is MANGANESE (II) ION (CCD ID: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Mn 3 3	0	0
3	C	3	Total Mn 3 3	0	0
3	E	3	Total Mn 3 3	0	0
3	G	3	Total Mn 3 3	0	0

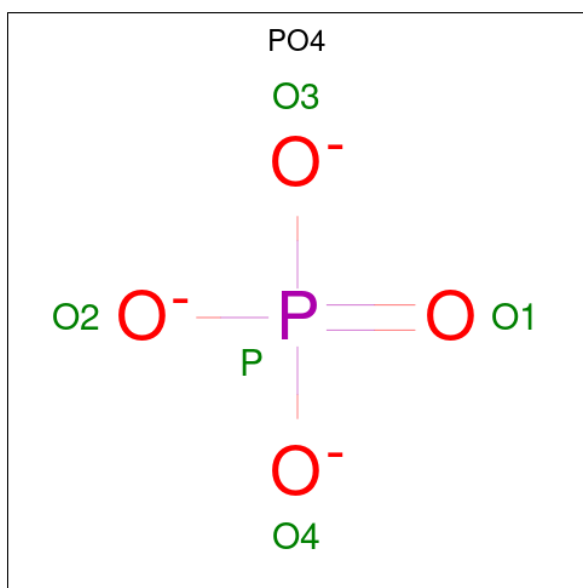
- Molecule 4 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	5	Total K 5 5	0	0
4	B	1	Total K 1 1	0	0
4	C	6	Total K 6 6	0	0
4	D	1	Total K 1 1	0	0
4	E	6	Total K 6 6	0	0
4	F	1	Total K 1 1	0	0
4	G	6	Total K 6 6	0	0

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

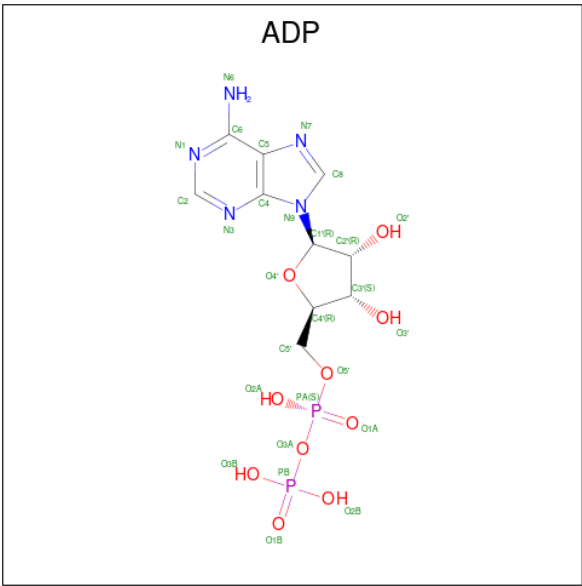
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	5	Total Cl 5 5	0	0
5	B	1	Total Cl 1 1	0	0
5	C	7	Total Cl 7 7	0	0
5	D	1	Total Cl 1 1	0	0
5	E	6	Total Cl 6 6	0	0
5	F	1	Total Cl 1 1	0	0
5	G	6	Total Cl 6 6	0	0
5	H	1	Total Cl 1 1	0	0

- Molecule 6 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



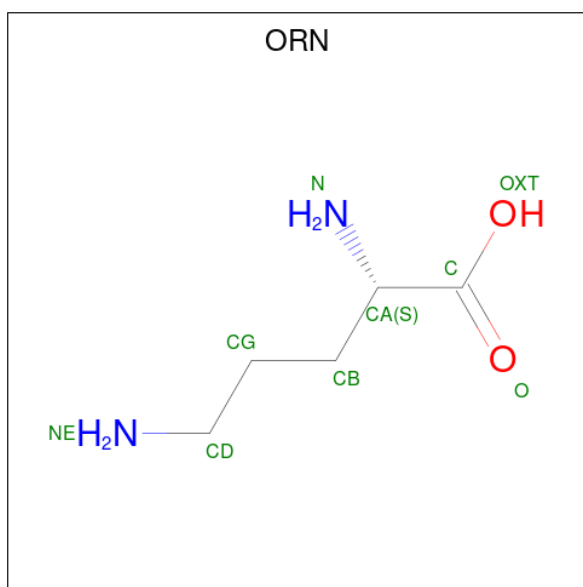
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O P 5 4 1	0	0
6	C	1	Total O P 5 4 1	0	0
6	E	1	Total O P 5 4 1	0	0
6	G	1	Total O P 5 4 1	0	0

- Molecule 7 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



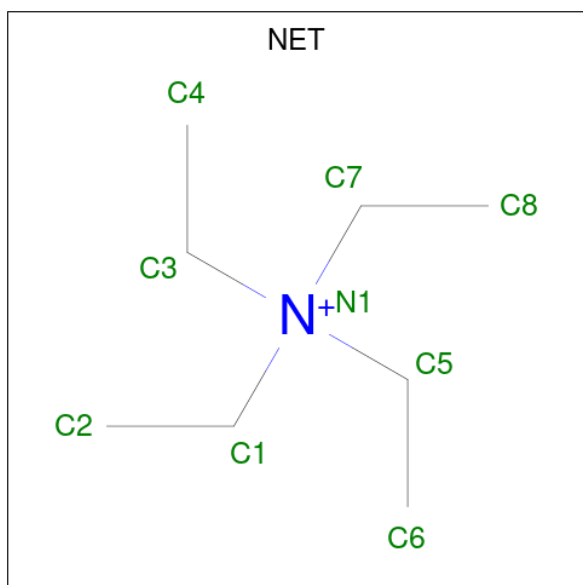
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
7	G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

- Molecule 8 is L-ornithine (CCD ID: ORN) (formula: C₅H₁₂N₂O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	A	1	Total	C	N	O	0	0
			9	5	2	2		
8	C	1	Total	C	N	O	0	0
			9	5	2	2		
8	E	1	Total	C	N	O	0	0
			9	5	2	2		
8	G	1	Total	C	N	O	0	0
			9	5	2	2		

- Molecule 9 is TETRAETHYLAMMONIUM ION (CCD ID: NET) (formula: C₈H₂₀N).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	A	1	Total C N 9 8 1	0	0
9	C	1	Total C N 9 8 1	0	0
9	E	1	Total C N 9 8 1	0	0
9	G	1	Total C N 9 8 1	0	0

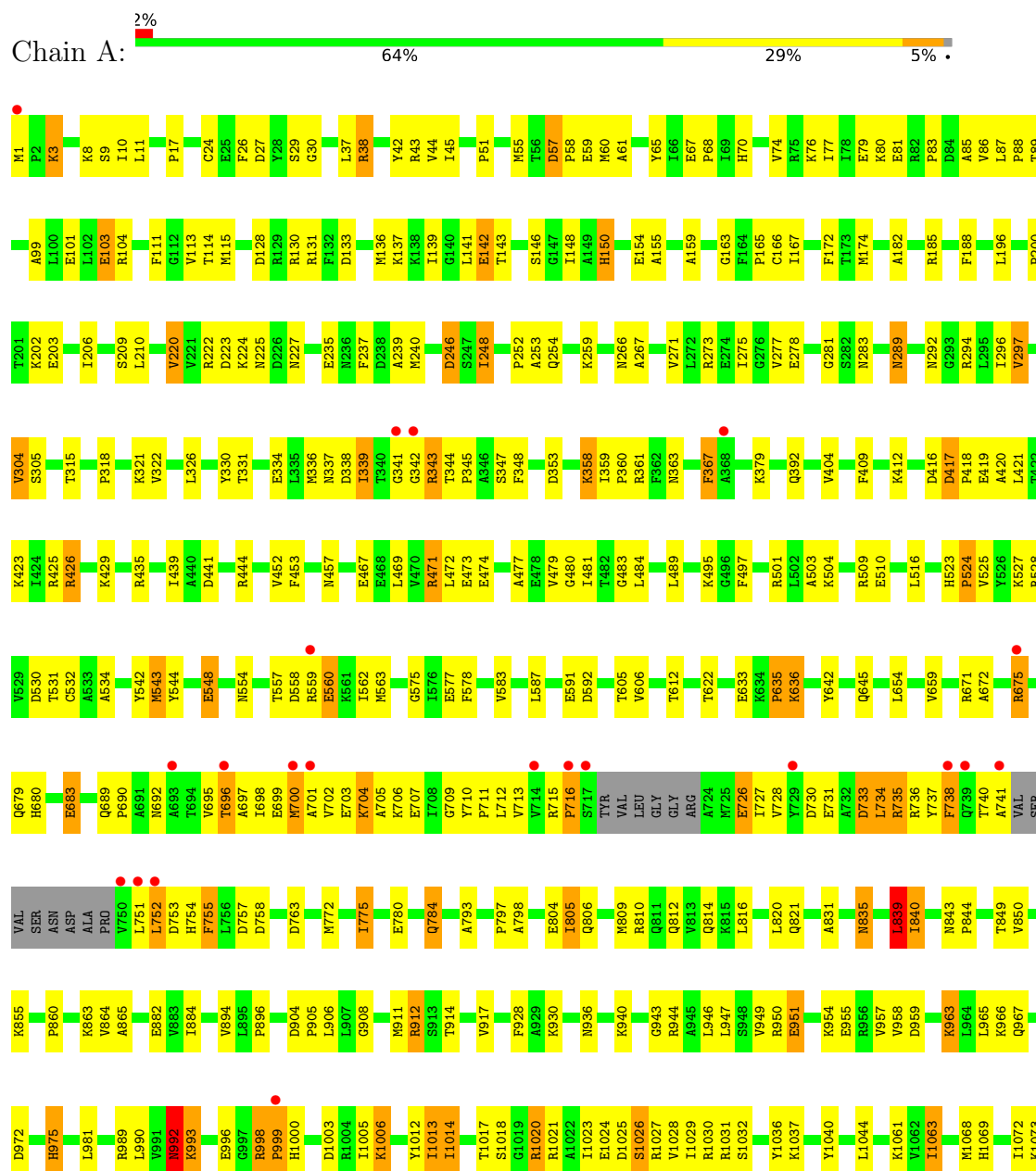
- Molecule 10 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	A	793	Total O 793 793	0	0
10	B	130	Total O 130 130	0	0
10	C	681	Total O 681 681	0	0
10	D	177	Total O 177 177	0	0
10	E	813	Total O 813 813	0	0
10	F	205	Total O 205 205	0	0
10	G	645	Total O 645 645	0	0
10	H	117	Total O 117 117	0	0

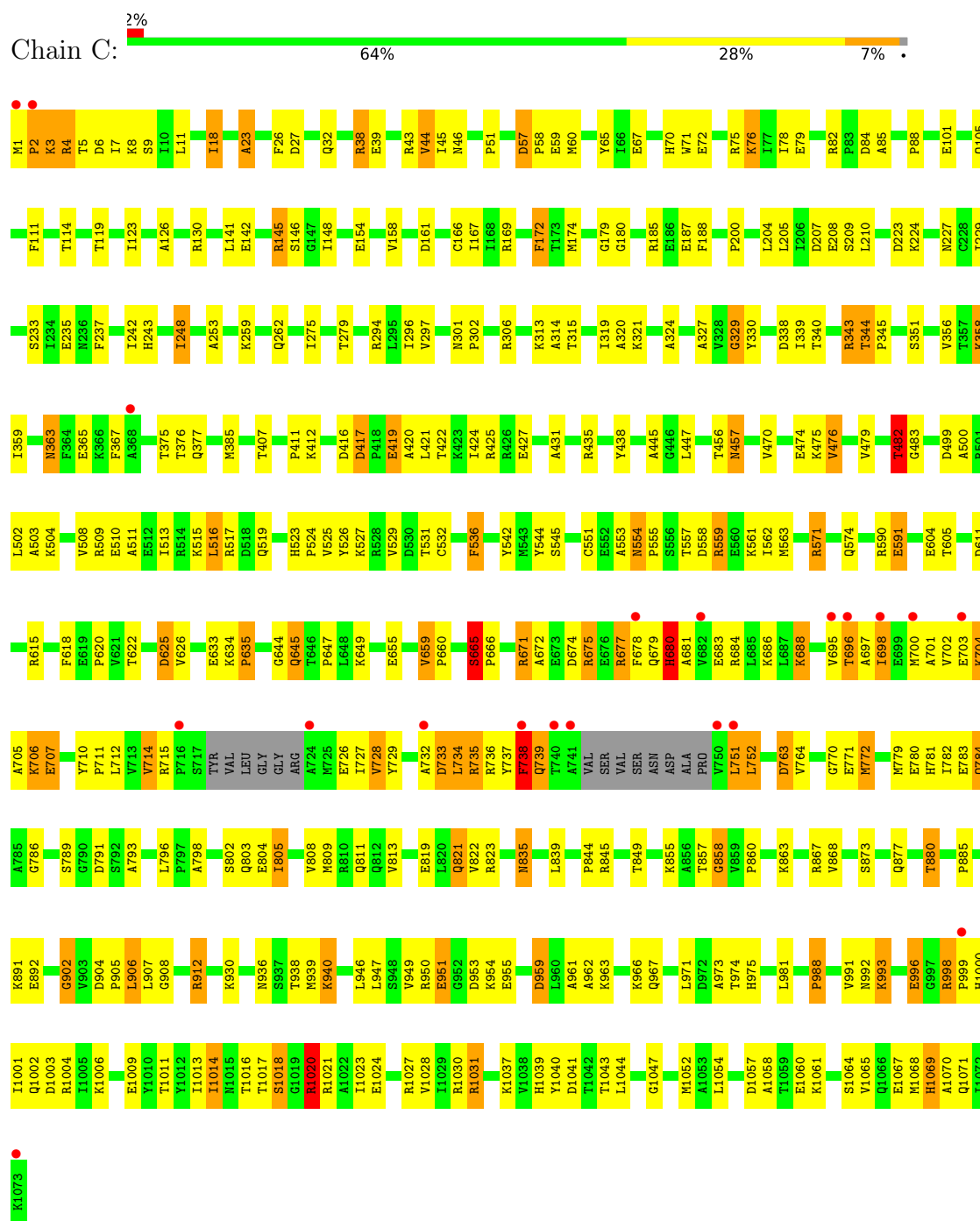
3 Residue-property plots

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

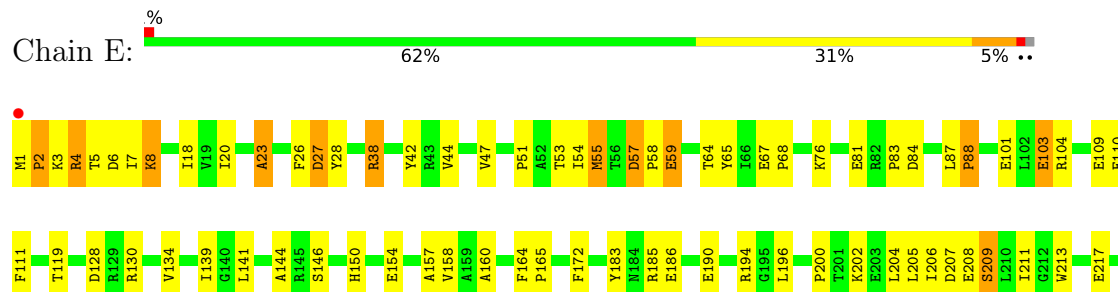
- Molecule 1: carbamoyl phosphate synthetase large chain

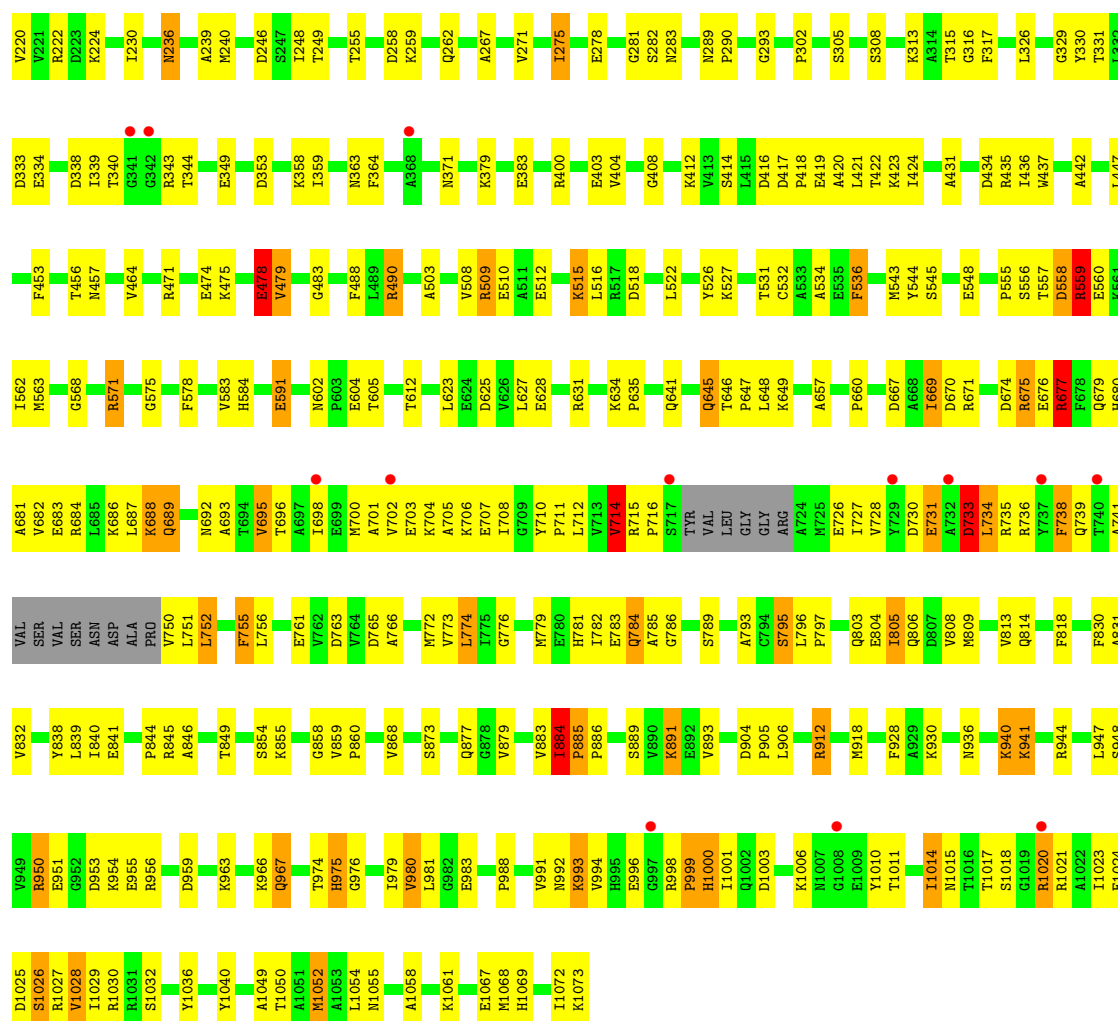


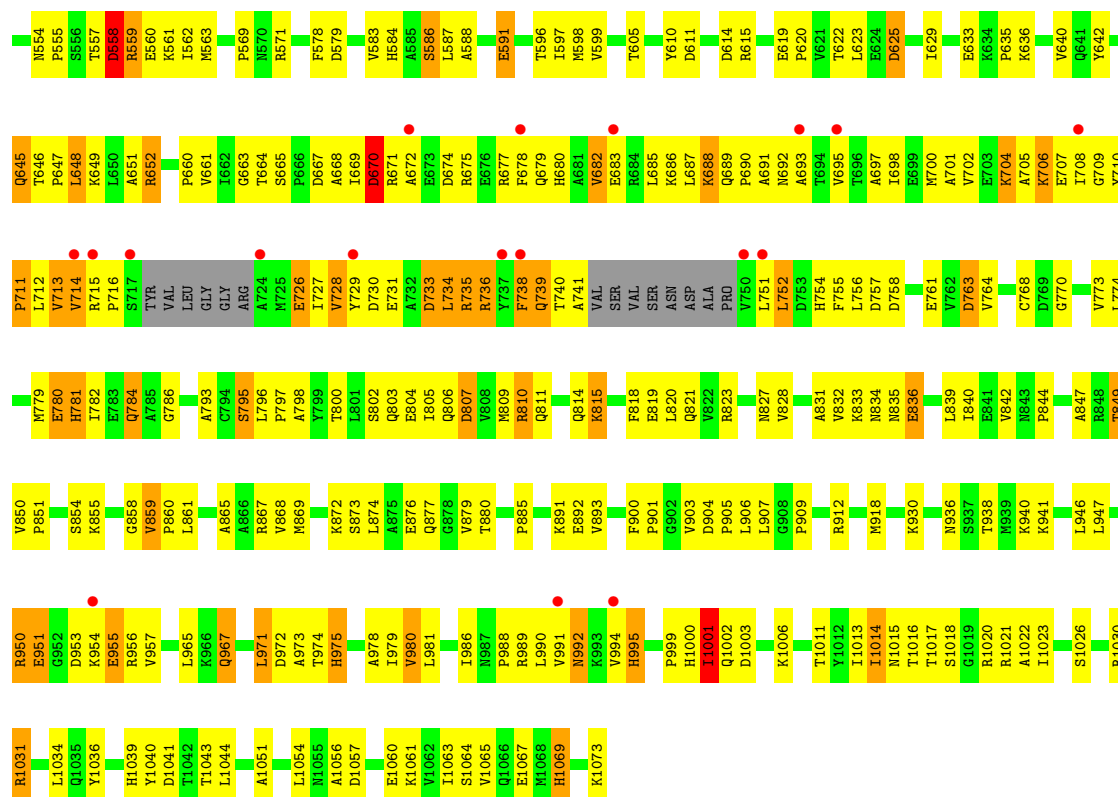
- Molecule 1: carbamoyl phosphate synthetase large chain



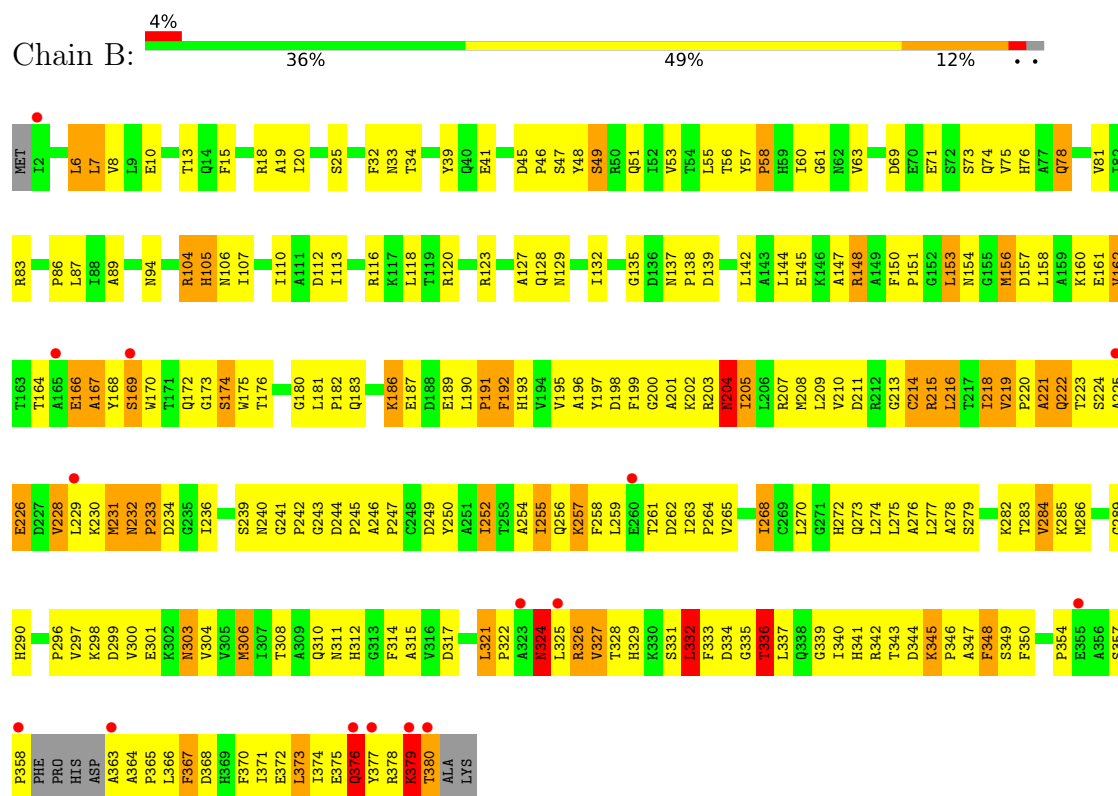
- Molecule 1: carbamoyl phosphate synthetase large chain



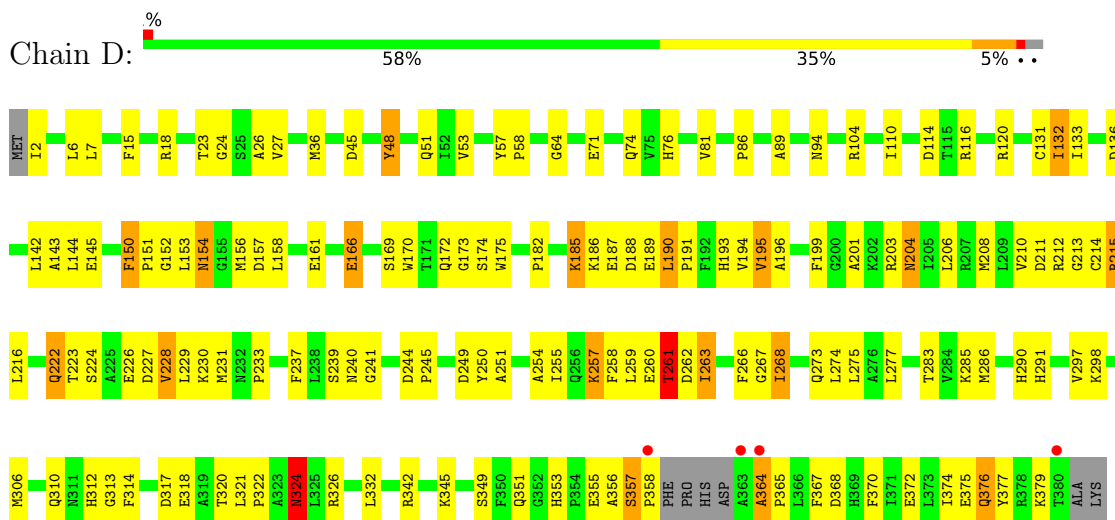




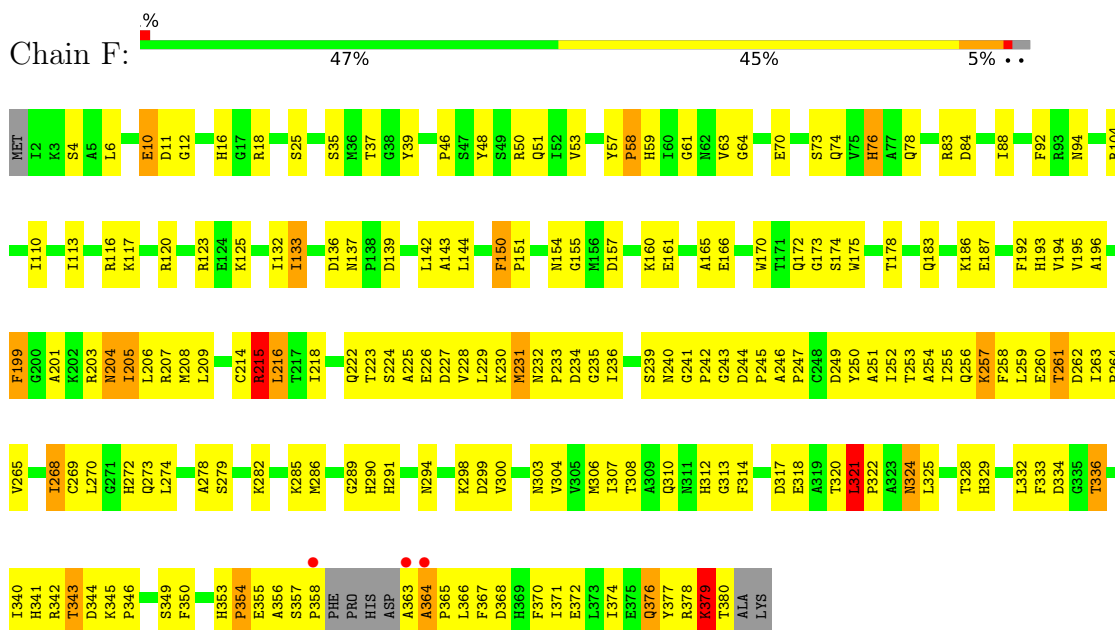
• Molecule 2: carbamoyl-phosphate synthetase small chain



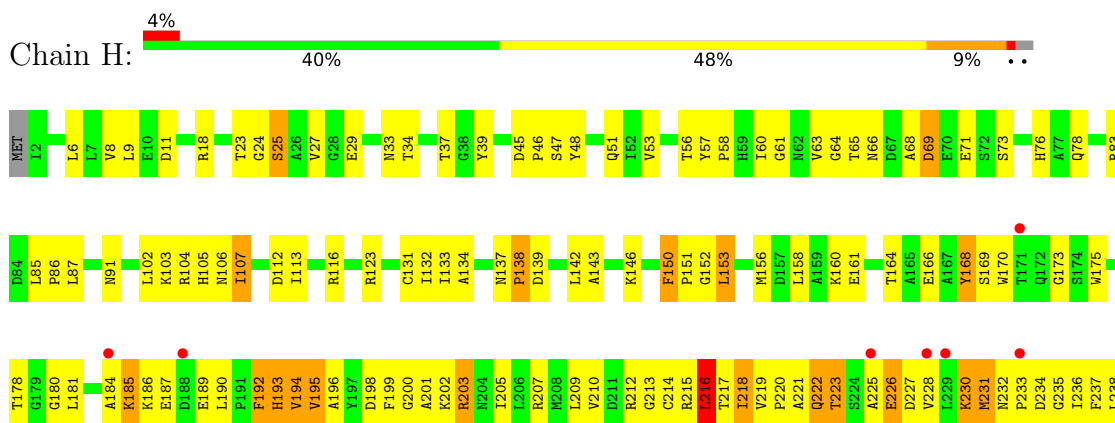
• Molecule 2: carbamoyl-phosphate synthetase small chain

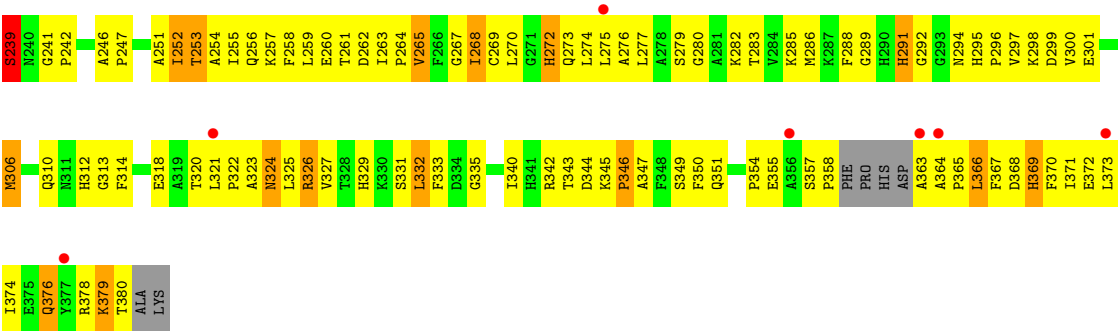


- Molecule 2: carbamoyl-phosphate synthetase small chain



- Molecule 2: carbamoyl-phosphate synthetase small chain





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	151.50Å 164.20Å 331.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.10 30.00 – 2.10	Depositor EDS
% Data completeness (in resolution range)	92.4 (30.00-2.10) 92.3 (30.00-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.78 (at 2.09Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.174 , 0.245 0.176 , 0.176	Depositor DCC
R_{free} test set	44498 reflections (9.99%)	wwPDB-VP
Wilson B-factor (Å ²)	25.4	Xtriage
Anisotropy	0.206	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 122.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	48206	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.78% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MN, PO4, NET, ADP, CL, K, ORN

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	1.20	2/8340 (0.0%)	1.64	90/11273 (0.8%)
1	C	1.19	4/8350 (0.0%)	1.65	94/11288 (0.8%)
1	E	1.19	2/8339 (0.0%)	1.63	91/11272 (0.8%)
1	G	1.16	2/8351 (0.0%)	1.65	79/11291 (0.7%)
2	B	1.12	0/2934	1.67	37/3981 (0.9%)
2	D	1.16	1/2944 (0.0%)	1.69	34/3996 (0.9%)
2	F	1.13	1/2951 (0.0%)	1.67	34/4003 (0.8%)
2	H	1.09	1/2934 (0.0%)	1.64	26/3981 (0.7%)
All	All	1.17	13/45143 (0.0%)	1.65	485/61085 (0.8%)

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
2	H	1	0

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

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	634	LYS	CA-C	-6.44	1.49	1.53
1	E	879	VAL	CA-C	-6.13	1.45	1.52
1	C	1069	HIS	ND1-CE1	-5.88	1.26	1.32
1	C	179	GLY	N-CA	5.73	1.49	1.44
1	A	683	GLU	CD-OE2	5.54	1.35	1.25

The worst 5 of 485 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	557	THR	CA-C-N	10.99	135.16	120.65
1	A	557	THR	C-N-CA	10.99	135.16	120.65
1	G	885	PRO	O-C-N	10.42	126.11	121.31
1	C	885	PRO	N-CA-CB	10.42	108.64	103.22
2	B	105	HIS	CA-CB-CG	-9.84	103.96	113.80

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	H	216	LEU	CA

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	8190	0	8213	248	0
1	C	8196	0	8236	252	0
1	E	8189	0	8219	270	0
1	G	8197	0	8218	348	0
2	B	2871	0	2850	225	0
2	D	2877	0	2852	111	0
2	F	2880	0	2859	161	0
2	H	2871	0	2850	213	0
3	A	3	0	0	0	0
3	C	3	0	0	0	0
3	E	3	0	0	0	0
3	G	3	0	0	0	0
4	A	5	0	0	1	0
4	B	1	0	0	0	0
4	C	6	0	0	1	0
4	D	1	0	0	0	0
4	E	6	0	0	1	0
4	F	1	0	0	0	0
4	G	6	0	0	0	0
5	A	5	0	0	0	0
5	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	7	0	0	1	0
5	D	1	0	0	1	0
5	E	6	0	0	0	0
5	F	1	0	0	0	0
5	G	6	0	0	1	0
5	H	1	0	0	0	0
6	A	5	0	0	0	0
6	C	5	0	0	0	0
6	E	5	0	0	0	0
6	G	5	0	0	0	0
7	A	54	0	24	3	0
7	C	54	0	24	1	0
7	E	54	0	24	1	0
7	G	54	0	24	0	0
8	A	9	0	11	0	0
8	C	9	0	11	2	0
8	E	9	0	11	1	0
8	G	9	0	11	2	0
9	A	9	0	20	3	0
9	C	9	0	20	1	0
9	E	9	0	20	0	0
9	G	9	0	20	0	0
10	A	793	0	0	25	0
10	B	130	0	0	3	0
10	C	681	0	0	14	0
10	D	177	0	0	2	0
10	E	813	0	0	19	0
10	F	205	0	0	10	0
10	G	645	0	0	15	0
10	H	117	0	0	6	0
All	All	48206	0	44517	1809	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 20.

The worst 5 of 1809 close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:4009:K:K	10:A:4434:HOH:O	1.26	1.26
2:H:133:ILE:HD12	2:H:143:ALA:HB2	1.28	1.15
2:D:187:GLU:HG2	2:D:215:ARG:HD2	1.25	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:228:VAL:HA	2:H:231:MET:HE2	1.30	1.11
2:B:187:GLU:HG2	2:B:215:ARG:HD2	1.30	1.11

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1059/1073 (99%)	993 (94%)	63 (6%)	3 (0%)	36	36
1	C	1060/1073 (99%)	997 (94%)	59 (6%)	4 (0%)	30	28
1	E	1059/1073 (99%)	1008 (95%)	46 (4%)	5 (0%)	24	22
1	G	1060/1073 (99%)	989 (93%)	64 (6%)	7 (1%)	18	15
2	B	372/382 (97%)	334 (90%)	31 (8%)	7 (2%)	6	3
2	D	373/382 (98%)	351 (94%)	21 (6%)	1 (0%)	36	36
2	F	374/382 (98%)	360 (96%)	11 (3%)	3 (1%)	16	12
2	H	372/382 (97%)	324 (87%)	40 (11%)	8 (2%)	5	2
All	All	5729/5820 (98%)	5356 (94%)	335 (6%)	38 (1%)	21	15

5 of 38 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	167	ALA
1	G	558	ASP
1	G	739	GLN
2	H	185	LYS
2	H	223	THR

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	871/878 (99%)	806 (92%)	65 (8%)	12	10
1	C	872/878 (99%)	799 (92%)	73 (8%)	10	7
1	E	871/878 (99%)	793 (91%)	78 (9%)	9	6
1	G	872/878 (99%)	794 (91%)	78 (9%)	9	6
2	B	306/311 (98%)	257 (84%)	49 (16%)	2	1
2	D	307/311 (99%)	283 (92%)	24 (8%)	11	9
2	F	308/311 (99%)	274 (89%)	34 (11%)	6	3
2	H	306/311 (98%)	268 (88%)	38 (12%)	4	2
All	All	4713/4756 (99%)	4274 (91%)	439 (9%)	8	6

5 of 439 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	422	THR
1	E	1020	ARG
2	H	379	LYS
1	G	1020	ARG
1	E	556	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 111 such sidechains are listed below:

Mol	Chain	Res	Type
2	D	324	ASN
2	H	351	GLN
1	E	987	ASN
2	H	324	ASN
1	G	1000	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 86 ligands modelled in this entry, 66 are monoatomic - leaving 20 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
8	ORN	E	4054	-	7,8,8	0.89	0	6,9,9	1.16	1 (16%)
7	ADP	E	4050	3,4	28,29,29	1.16	2 (7%)	43,45,45	0.83	2 (4%)
9	NET	G	4077	-	8,8,8	0.69	0	10,10,10	0.69	0
7	ADP	A	4001	3	28,29,29	1.40	6 (21%)	43,45,45	1.04	3 (6%)
7	ADP	C	4021	3	28,29,29	1.36	5 (17%)	43,45,45	0.95	3 (6%)
8	ORN	C	4031	-	7,8,8	0.99	0	6,9,9	0.80	0
6	PO4	G	4071	3	4,4,4	2.36	2 (50%)	6,6,6	1.14	0
9	NET	E	4055	-	8,8,8	0.68	0	10,10,10	0.65	0
6	PO4	E	4049	3	4,4,4	2.52	3 (75%)	6,6,6	0.79	0
7	ADP	G	4072	3,4	28,29,29	1.30	4 (14%)	43,45,45	0.92	0
6	PO4	C	4026	3	4,4,4	2.83	3 (75%)	6,6,6	1.08	0
8	ORN	A	4011	-	7,8,8	0.82	0	6,9,9	1.40	1 (16%)
9	NET	C	4032	-	8,8,8	0.60	0	10,10,10	0.73	0
7	ADP	G	4066	3	28,29,29	1.25	3 (10%)	43,45,45	1.28	5 (11%)
6	PO4	A	4006	3	4,4,4	2.16	2 (50%)	6,6,6	1.46	1 (16%)
7	ADP	C	4027	3,4	28,29,29	1.34	4 (14%)	43,45,45	1.14	3 (6%)
9	NET	A	4012	-	8,8,8	0.59	0	10,10,10	0.75	0
7	ADP	E	4044	3	28,29,29	1.50	1 (3%)	43,45,45	0.80	1 (2%)
8	ORN	G	4076	-	7,8,8	0.95	1 (14%)	6,9,9	0.91	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	ADP	A	4007	3,4	28,29,29	1.41	2 (7%)	43,45,45	0.91	1 (2%)

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
8	ORN	A	4011	-	-	3/8/8/8	-
9	NET	E	4055	-	-	0/12/12/12	-
9	NET	C	4032	-	-	2/12/12/12	-
7	ADP	G	4066	3	-	2/16/32/32	0/3/3/3
8	ORN	E	4054	-	-	5/8/8/8	-
7	ADP	C	4027	3,4	-	0/16/32/32	0/3/3/3
7	ADP	E	4050	3,4	-	3/16/32/32	0/3/3/3
9	NET	A	4012	-	-	0/12/12/12	-
7	ADP	A	4001	3	-	1/16/32/32	0/3/3/3
7	ADP	C	4021	3	-	1/16/32/32	0/3/3/3
7	ADP	A	4007	3,4	-	0/16/32/32	0/3/3/3
7	ADP	E	4044	3	-	2/16/32/32	0/3/3/3
7	ADP	G	4072	3,4	-	0/16/32/32	0/3/3/3
8	ORN	G	4076	-	-	6/8/8/8	-
9	NET	G	4077	-	-	0/12/12/12	-
8	ORN	C	4031	-	-	6/8/8/8	-

The worst 5 of 38 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	4044	ADP	PA-O3A	-6.01	1.53	1.59
7	A	4007	ADP	PA-O3A	-5.14	1.54	1.59
7	A	4001	ADP	PA-O3A	-3.91	1.55	1.59
6	C	4026	PO4	P-O2	-3.88	1.43	1.54
7	C	4027	ADP	O2'-C2'	3.64	1.52	1.43

The worst 5 of 21 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	4027	ADP	O2A-PA-O3A	3.50	116.74	107.27
7	G	4066	ADP	O3B-PB-O3A	-3.44	93.09	104.64
7	A	4001	ADP	C5-C6-N6	3.11	131.00	123.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	4066	ADP	O2'-C2'-C3'	2.91	121.14	111.82
7	G	4066	ADP	O4'-C1'-N9	-2.85	102.62	108.09

There are no chirality outliers.

5 of 31 torsion outliers are listed below:

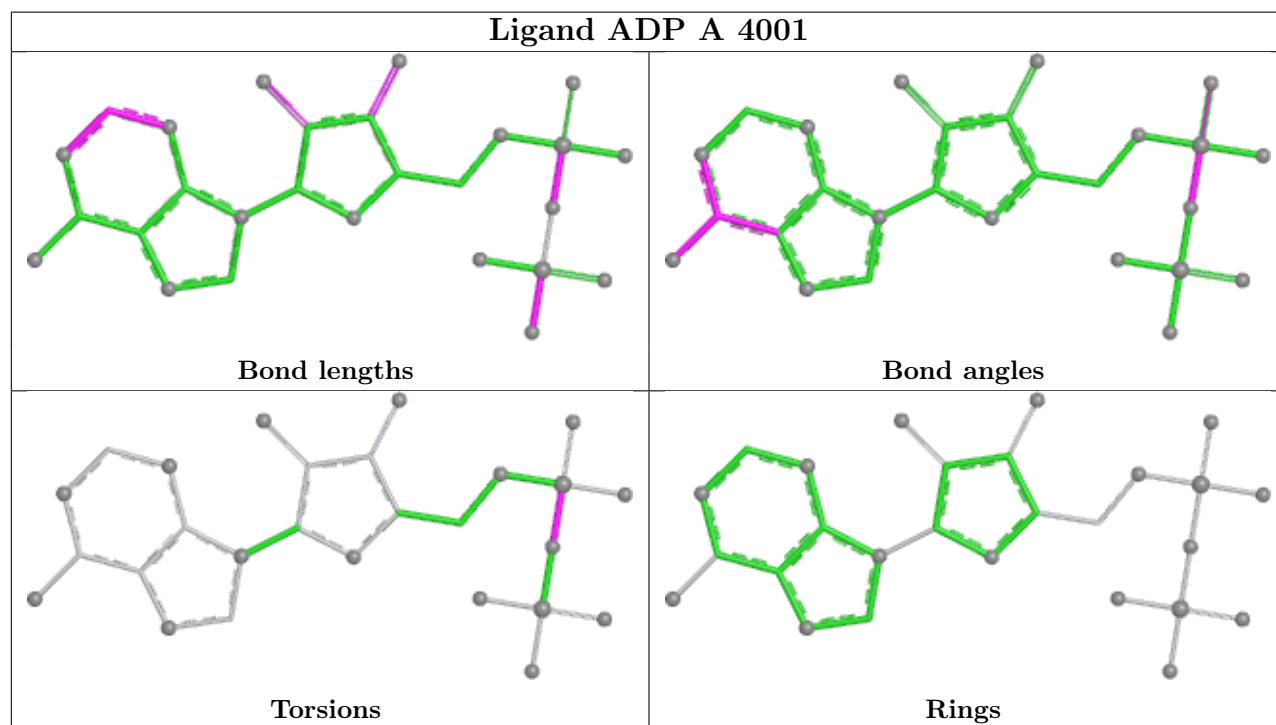
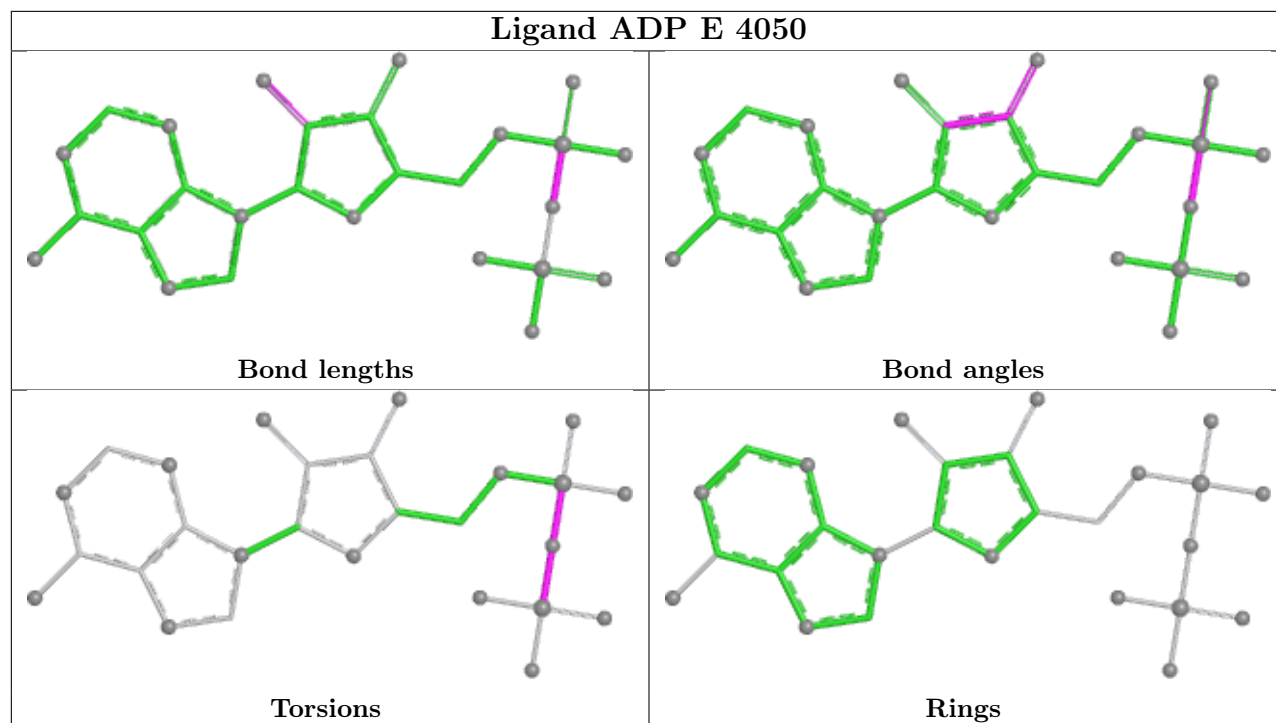
Mol	Chain	Res	Type	Atoms
7	E	4050	ADP	PA-O3A-PB-O3B
8	A	4011	ORN	N-CA-CB-CG
8	A	4011	ORN	C-CA-CB-CG
8	C	4031	ORN	N-CA-CB-CG
8	C	4031	ORN	C-CA-CB-CG

There are no ring outliers.

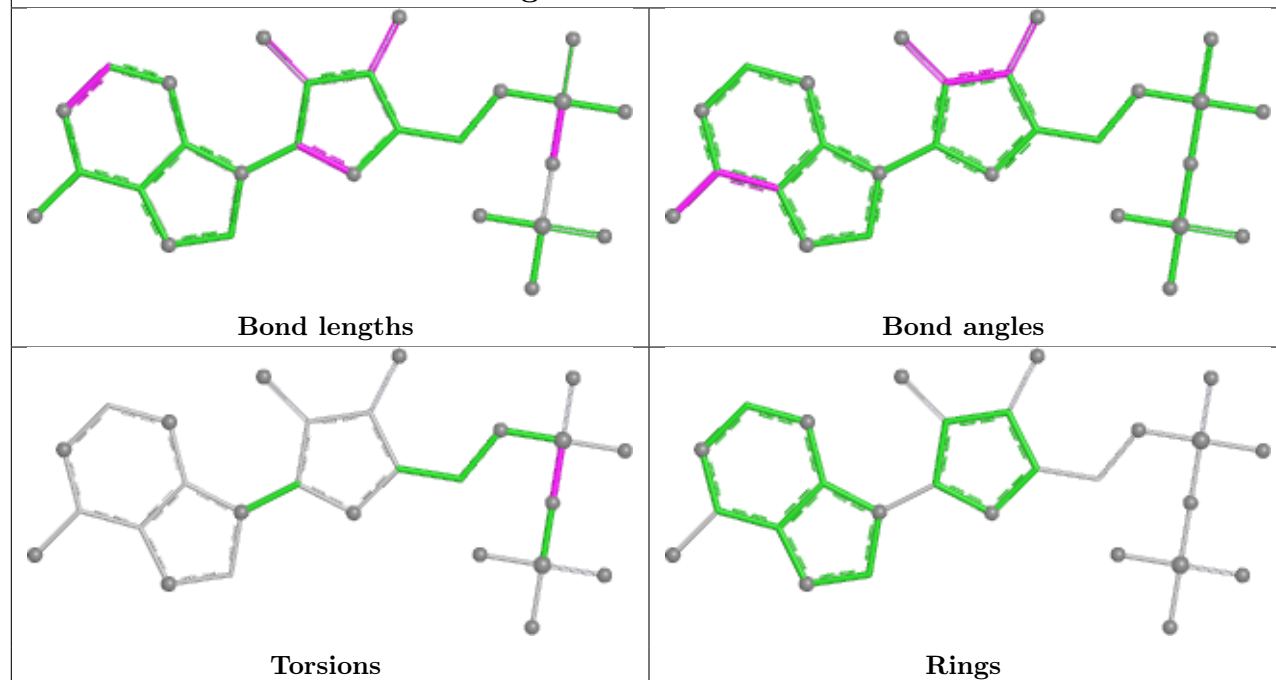
9 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	E	4054	ORN	1	0
7	E	4050	ADP	1	0
7	A	4001	ADP	1	0
8	C	4031	ORN	2	0
9	C	4032	NET	1	0
7	C	4027	ADP	1	0
9	A	4012	NET	3	0
8	G	4076	ORN	2	0
7	A	4007	ADP	2	0

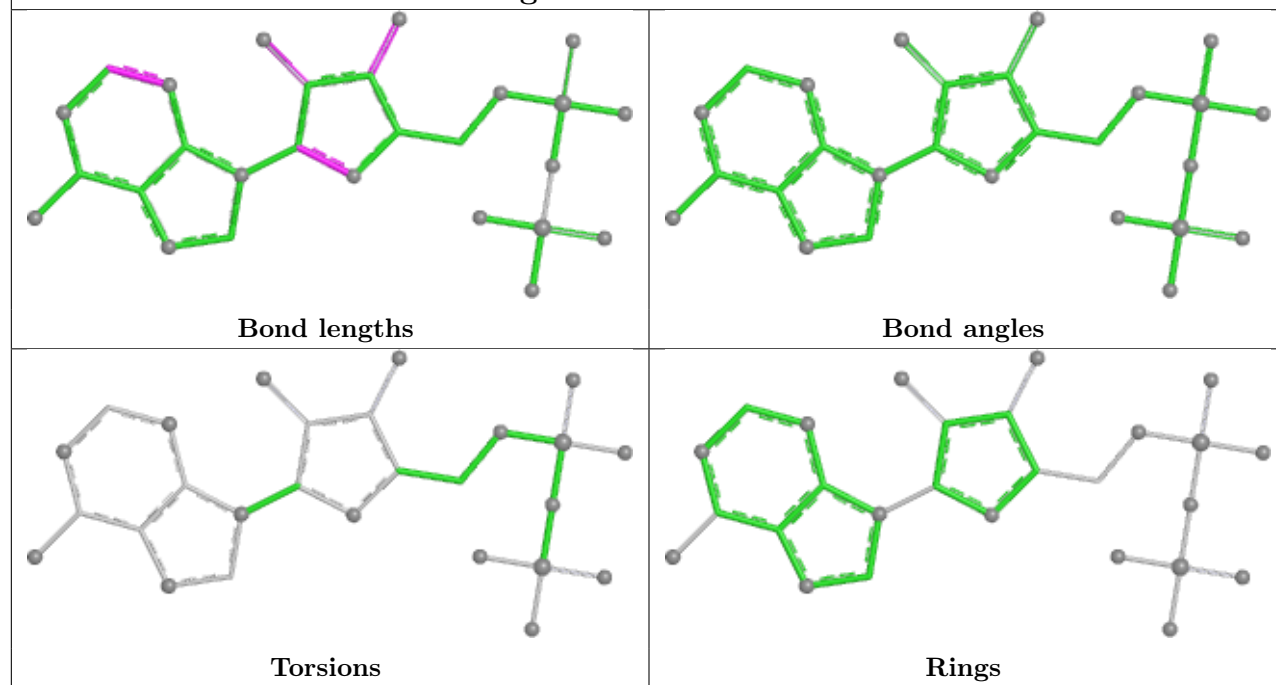
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



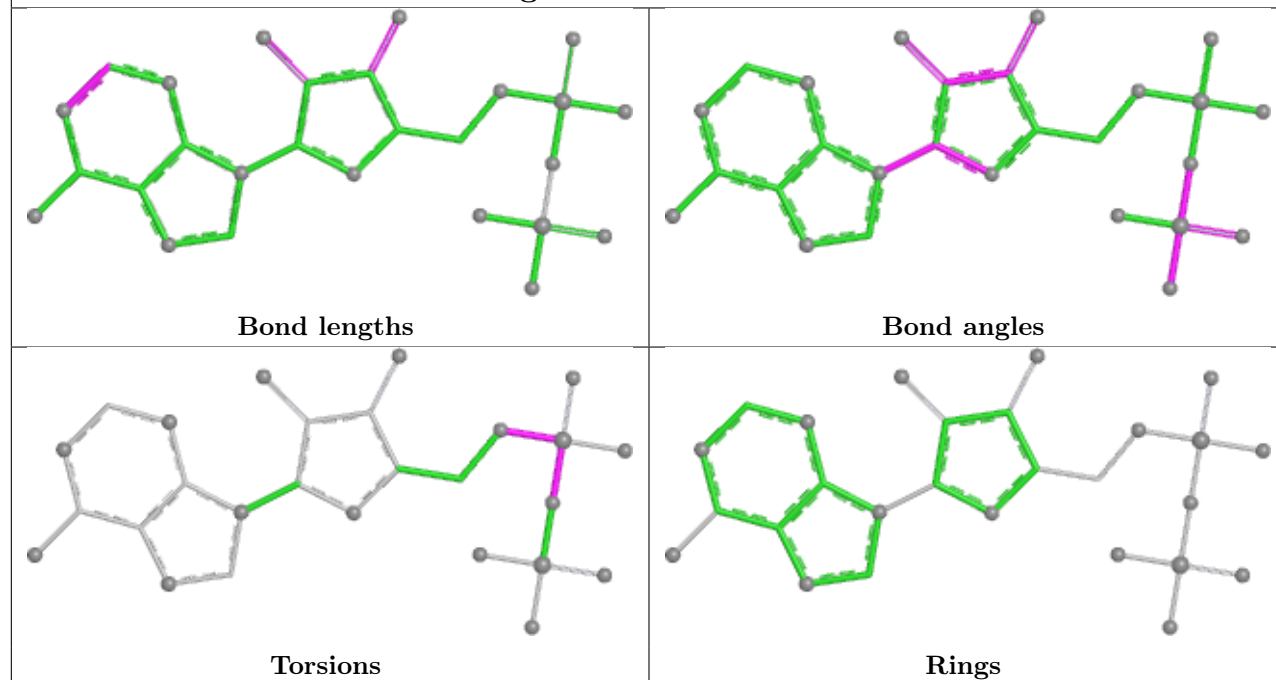
Ligand ADP C 4021



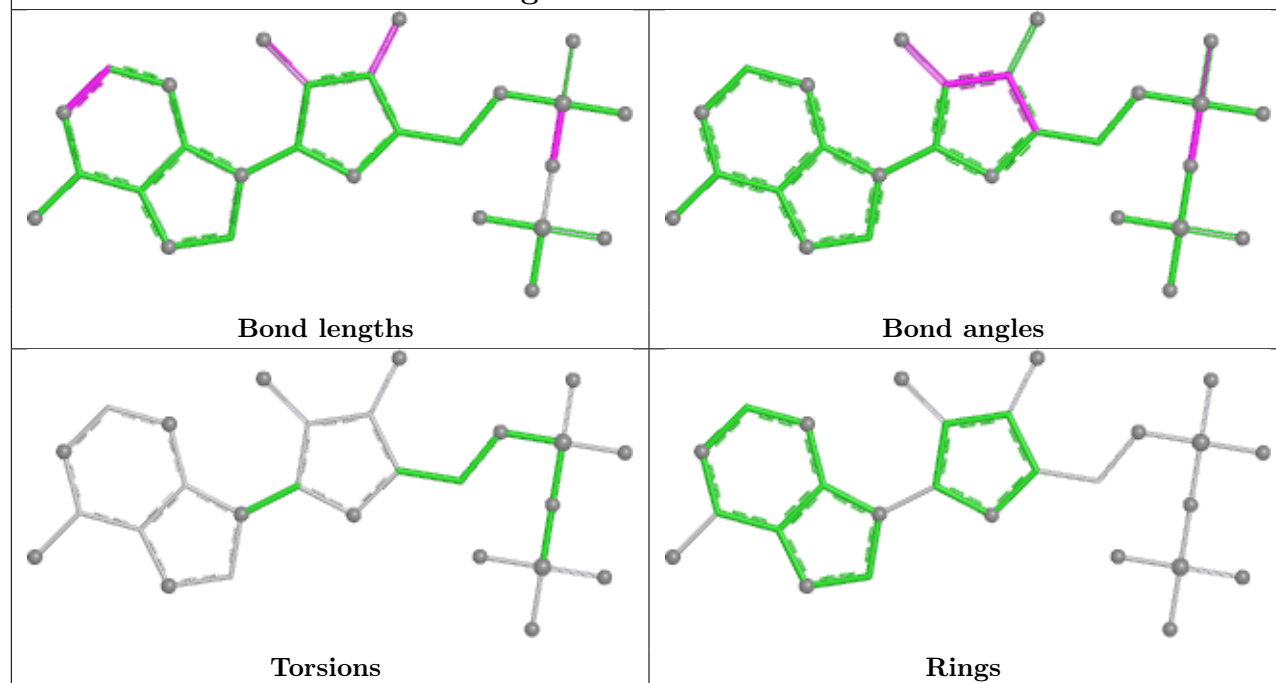
Ligand ADP G 4072

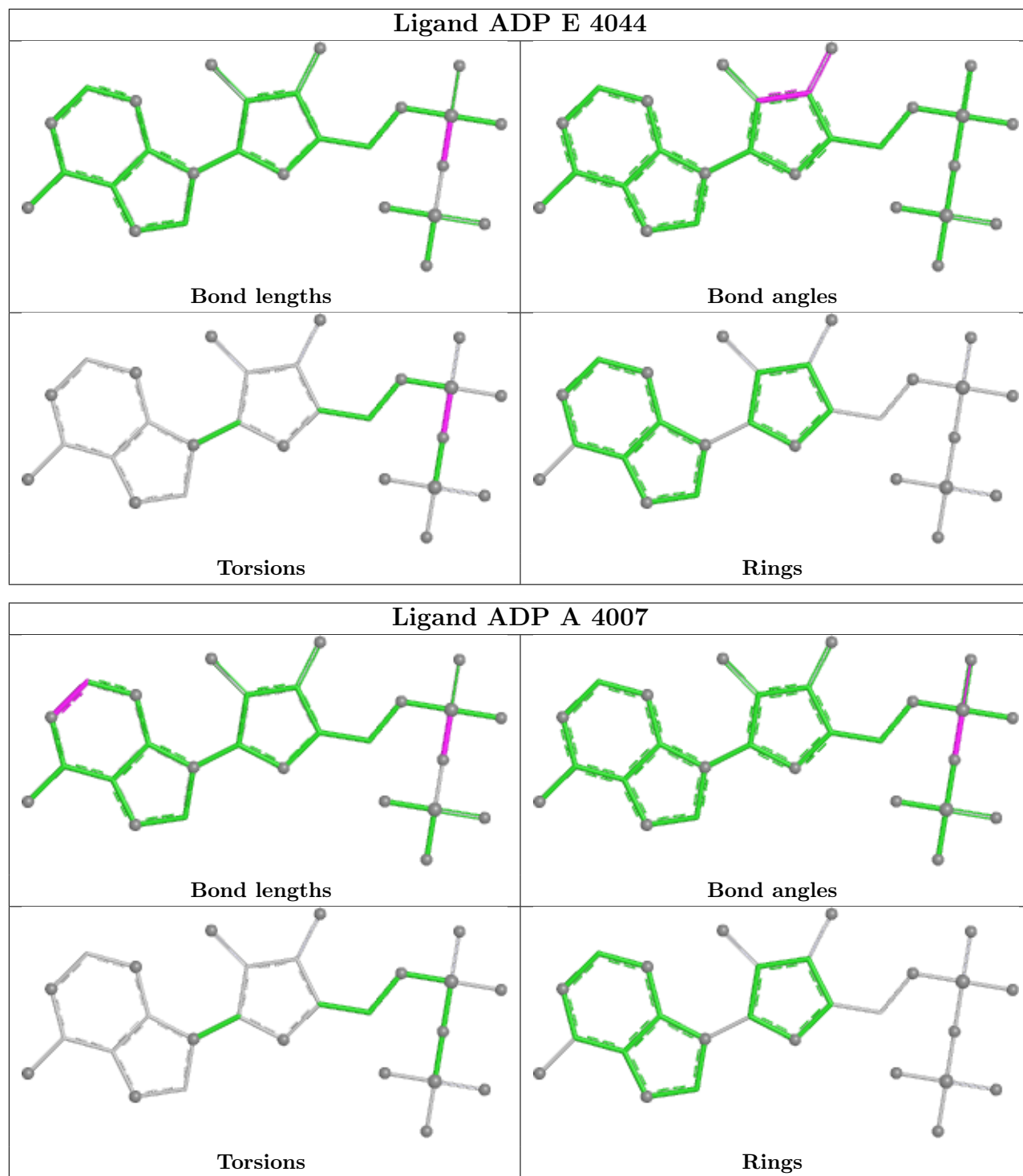


Ligand ADP G 4066



Ligand ADP C 4027





5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	1059/1073 (98%)	-0.58	21 (1%) 65 67	14, 29, 71, 100	6 (0%)
1	C	1059/1073 (98%)	-0.50	20 (1%) 66 69	14, 31, 76, 100	5 (0%)
1	E	1059/1073 (98%)	-0.62	14 (1%) 75 77	13, 27, 75, 100	6 (0%)
1	G	1059/1073 (98%)	-0.32	22 (2%) 63 66	17, 36, 81, 100	6 (0%)
2	B	375/382 (98%)	0.11	15 (4%) 42 44	21, 47, 84, 100	1 (0%)
2	D	375/382 (98%)	-0.36	4 (1%) 78 80	17, 33, 71, 100	2 (0%)
2	F	375/382 (98%)	-0.27	3 (0%) 82 84	15, 36, 76, 100	3 (0%)
2	H	375/382 (98%)	0.31	14 (3%) 45 47	26, 51, 90, 100	1 (0%)
All	All	5736/5820 (98%)	-0.39	113 (1%) 65 67	13, 33, 79, 100	30 (0%)

The worst 5 of 113 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	F	363	ALA	7.5
1	E	368	ALA	7.4
1	G	368	ALA	5.9
1	A	750	VAL	5.2
2	H	363	ALA	5.1

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
5	CL	C	4037	1/1	0.83	0.14	81,81,81,81	0
4	K	G	4074	1/1	0.90	0.11	86,86,86,86	0
5	CL	G	4081	1/1	0.91	0.13	75,75,75,75	0
5	CL	E	4060	1/1	0.93	0.08	56,56,56,56	0
5	CL	D	4043	1/1	0.93	0.11	80,80,80,80	0
5	CL	E	4063	1/1	0.94	0.07	59,59,59,59	0
8	ORN	A	4011	9/9	0.94	0.07	15,23,32,38	0
8	ORN	C	4031	9/9	0.94	0.09	19,26,46,57	0
4	K	G	4078	1/1	0.95	0.07	53,53,53,53	0
5	CL	G	4084	1/1	0.95	0.07	76,76,76,76	0
8	ORN	E	4054	9/9	0.95	0.07	17,28,35,38	0
8	ORN	G	4076	9/9	0.95	0.08	22,30,47,60	0
5	CL	A	4018	1/1	0.96	0.09	58,58,58,58	0
4	K	A	4013	1/1	0.96	0.07	55,55,55,55	0
5	CL	C	4040	1/1	0.96	0.07	59,59,59,59	0
9	NET	G	4077	9/9	0.96	0.06	23,28,36,42	0
7	ADP	G	4072	27/27	0.97	0.06	30,43,80,95	0
4	K	B	4014	1/1	0.97	0.06	42,42,42,42	0
4	K	C	4029	1/1	0.97	0.07	76,76,76,76	0
4	K	C	4034	1/1	0.97	0.06	51,51,51,51	0
4	K	E	4056	1/1	0.97	0.06	42,42,42,42	0
9	NET	A	4012	9/9	0.97	0.06	12,19,26,28	0
9	NET	C	4032	9/9	0.97	0.06	15,21,28,30	0
4	K	E	4057	1/1	0.97	0.06	55,55,55,55	0
5	CL	C	4039	1/1	0.98	0.06	45,45,45,45	0
5	CL	H	4085	1/1	0.98	0.06	52,52,52,52	0
7	ADP	A	4007	27/27	0.98	0.05	14,28,48,77	0
7	ADP	C	4027	27/27	0.98	0.05	16,33,62,83	0
7	ADP	E	4050	27/27	0.98	0.05	19,33,50,58	0
4	K	F	4058	1/1	0.98	0.04	39,39,39,39	0
5	CL	C	4041	1/1	0.98	0.03	27,27,27,27	0
4	K	D	4035	1/1	0.98	0.04	34,34,34,34	0
4	K	E	4052	1/1	0.98	0.05	61,61,61,61	0
5	CL	E	4061	1/1	0.98	0.04	41,41,41,41	0
4	K	C	4033	1/1	0.98	0.06	55,55,55,55	0
4	K	A	4009	1/1	0.98	0.10	80,80,80,80	0
9	NET	E	4055	9/9	0.98	0.06	12,19,31,35	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	CL	G	4083	1/1	0.98	0.07	58,58,58,58	0
5	CL	E	4062	1/1	0.99	0.04	48,48,48,48	0
4	K	G	4079	1/1	0.99	0.03	49,49,49,49	0
5	CL	E	4065	1/1	0.99	0.07	46,46,46,46	0
5	CL	G	4080	1/1	0.99	0.02	23,23,23,23	0
5	CL	A	4016	1/1	0.99	0.03	39,39,39,39	0
5	CL	G	4082	1/1	0.99	0.04	39,39,39,39	0
5	CL	A	4017	1/1	0.99	0.04	39,39,39,39	0
4	K	E	4053	1/1	0.99	0.03	23,23,23,23	0
5	CL	G	4086	1/1	0.99	0.04	47,47,47,47	0
5	CL	A	4020	1/1	0.99	0.07	45,45,45,45	0
6	PO4	A	4006	5/5	0.99	0.04	16,22,28,30	0
6	PO4	C	4026	5/5	0.99	0.03	14,15,19,24	0
6	PO4	E	4049	5/5	0.99	0.03	17,17,21,25	0
6	PO4	G	4071	5/5	0.99	0.03	15,16,17,32	0
7	ADP	A	4001	27/27	0.99	0.04	12,22,32,38	0
5	CL	B	4019	1/1	0.99	0.02	33,33,33,33	0
7	ADP	C	4021	27/27	0.99	0.04	12,19,24,45	0
5	CL	C	4036	1/1	0.99	0.03	26,26,26,26	0
7	ADP	E	4044	27/27	0.99	0.03	8,20,25,28	0
4	K	A	4010	1/1	0.99	0.02	21,21,21,21	0
7	ADP	G	4066	27/27	0.99	0.04	9,22,31,38	0
5	CL	C	4038	1/1	0.99	0.02	33,33,33,33	0
4	K	C	4025	1/1	0.99	0.02	25,25,25,25	0
4	K	A	4005	1/1	0.99	0.02	25,25,25,25	0
4	K	G	4070	1/1	0.99	0.02	30,30,30,30	0
5	CL	C	4042	1/1	0.99	0.03	45,45,45,45	0
4	K	E	4048	1/1	0.99	0.02	23,23,23,23	0
5	CL	E	4059	1/1	0.99	0.02	24,24,24,24	0
4	K	G	4075	1/1	0.99	0.03	37,37,37,37	0
4	K	C	4030	1/1	0.99	0.02	26,26,26,26	0
3	MN	C	4023	1/1	1.00	0.02	24,24,24,24	0
4	K	C	4024	1/1	1.00	0.01	19,19,19,19	0
3	MN	C	4028	1/1	1.00	0.02	39,39,39,39	0
3	MN	E	4045	1/1	1.00	0.03	24,24,24,24	0
3	MN	E	4046	1/1	1.00	0.02	21,21,21,21	0
5	CL	A	4015	1/1	1.00	0.02	23,23,23,23	0
3	MN	E	4051	1/1	1.00	0.02	36,36,36,36	0
3	MN	G	4067	1/1	1.00	0.02	25,25,25,25	0
5	CL	F	4064	1/1	1.00	0.02	33,33,33,33	0
3	MN	G	4068	1/1	1.00	0.01	22,22,22,22	0
4	K	E	4047	1/1	1.00	0.02	19,19,19,19	0

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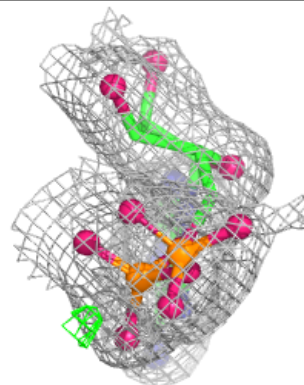
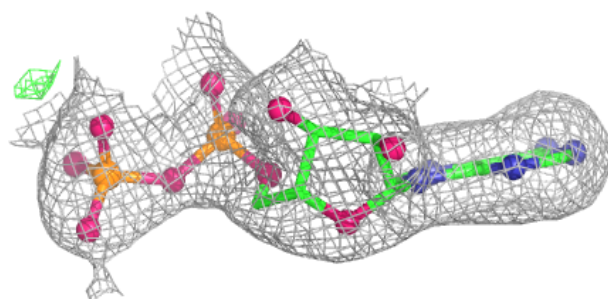
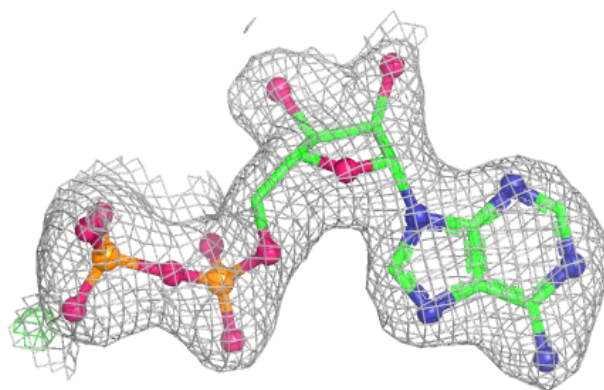
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MN	G	4073	1/1	1.00	0.02	49,49,49,49	0
4	K	A	4004	1/1	1.00	0.01	20,20,20,20	0
3	MN	A	4002	1/1	1.00	0.01	21,21,21,21	0
3	MN	A	4003	1/1	1.00	0.03	21,21,21,21	0
3	MN	A	4008	1/1	1.00	0.01	28,28,28,28	0
3	MN	C	4022	1/1	1.00	0.02	21,21,21,21	0
4	K	G	4069	1/1	1.00	0.02	24,24,24,24	0

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

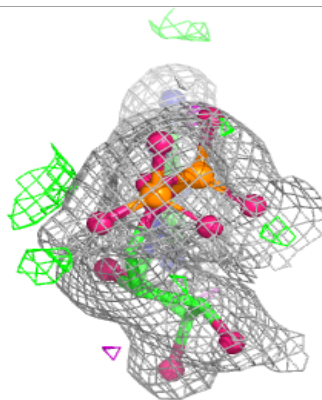
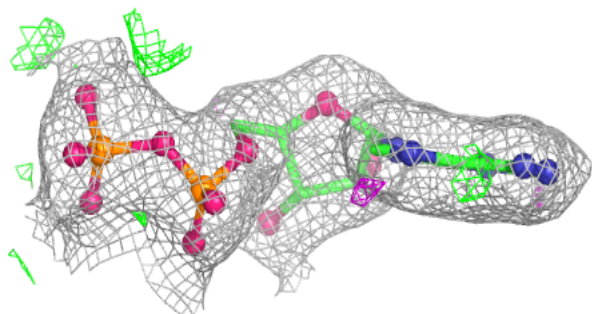
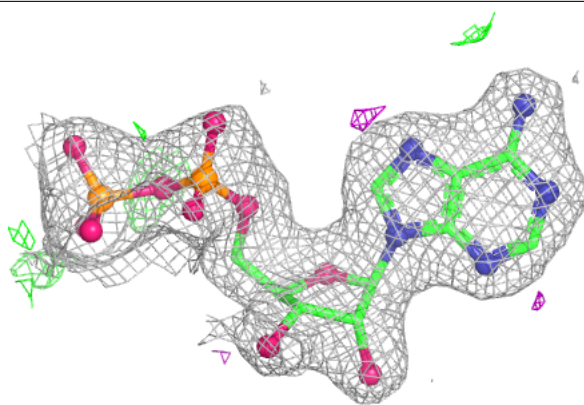
Electron density around ADP G 4072:

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

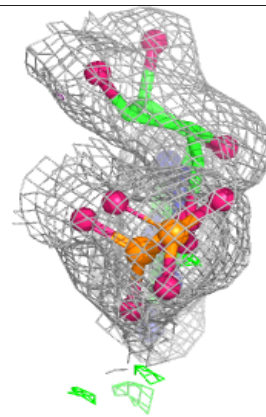
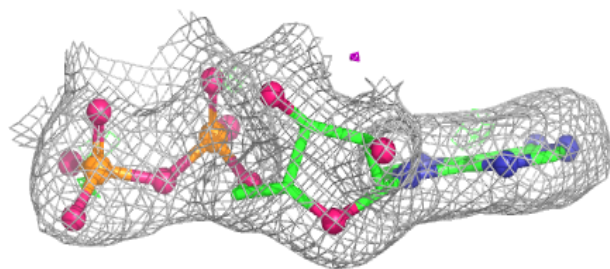
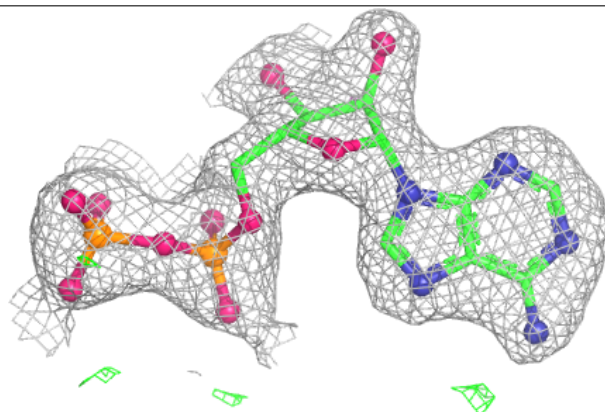


Electron density around ADP A 4007:

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

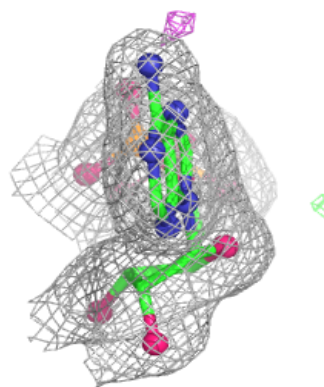
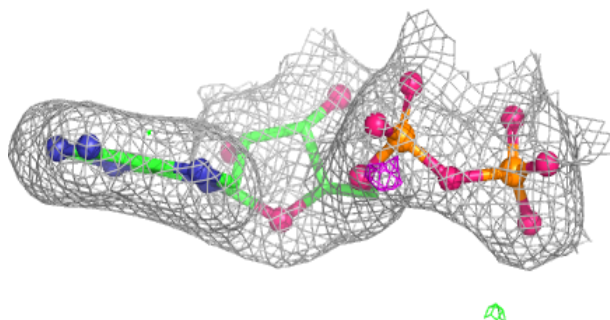
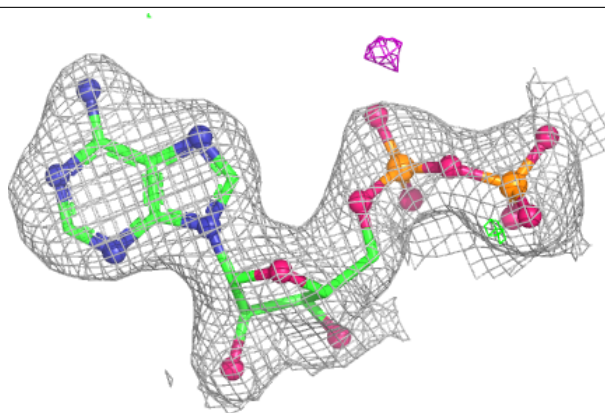
**Electron density around ADP C 4027:**

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

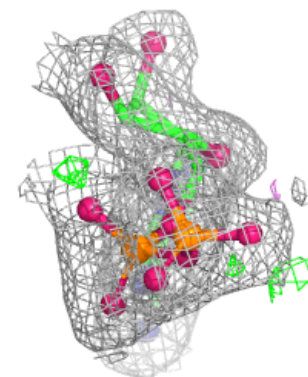
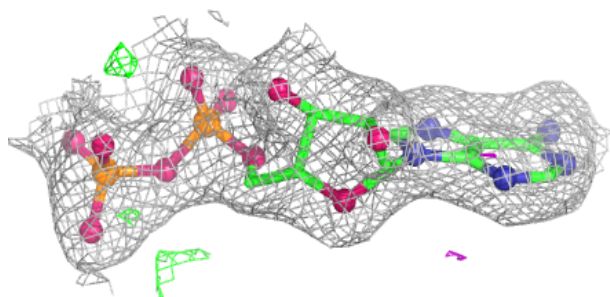
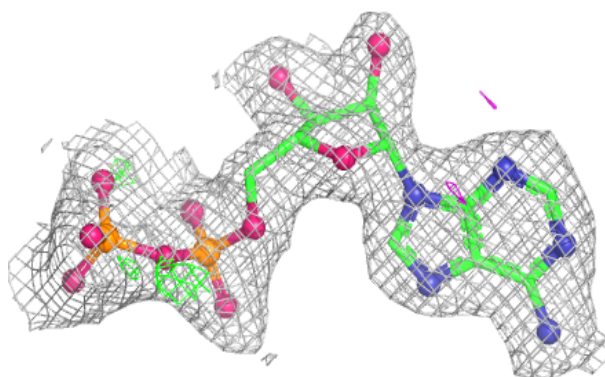


Electron density around ADP E 4050:

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

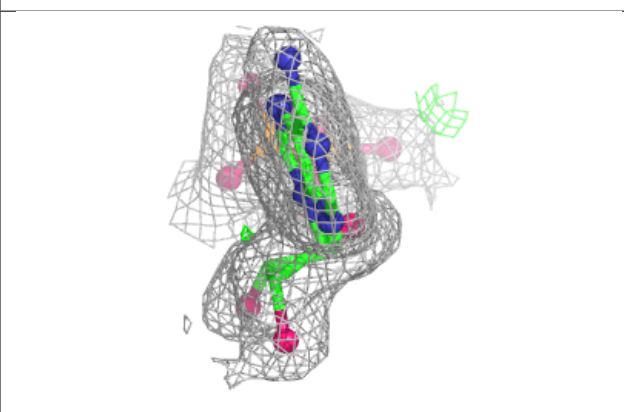
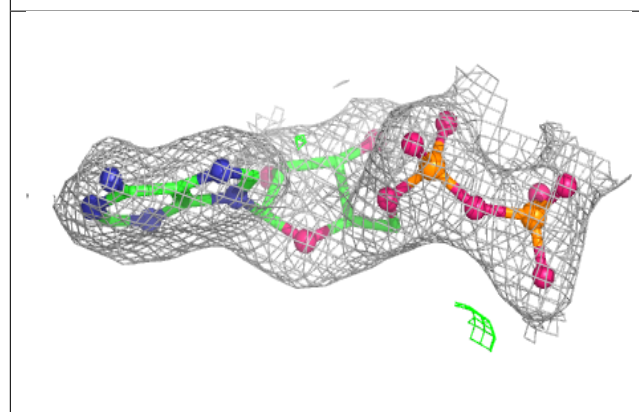
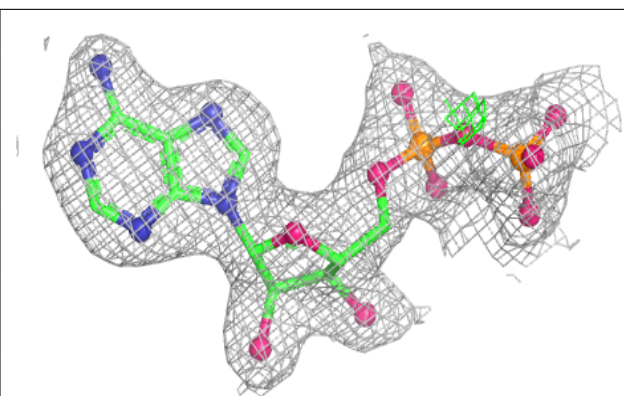
**Electron density around ADP A 4001:**

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

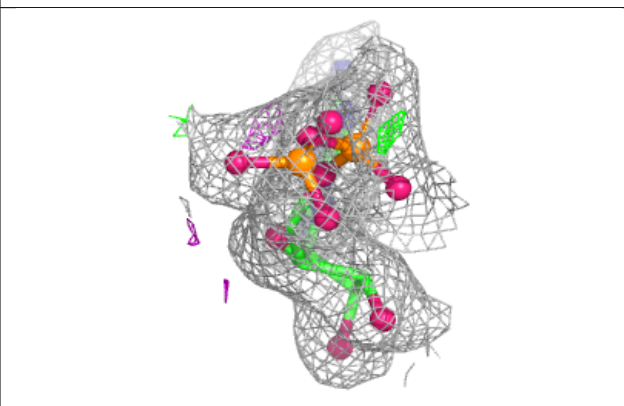
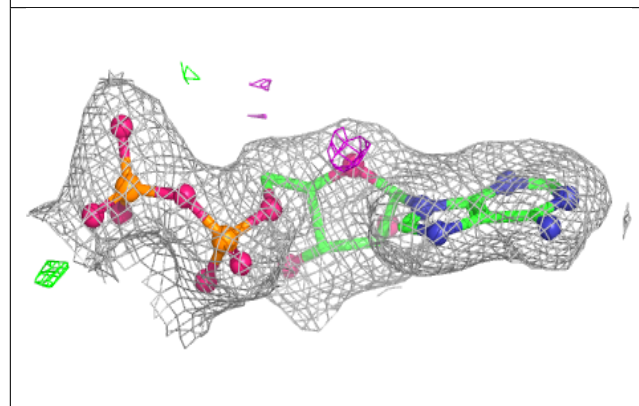
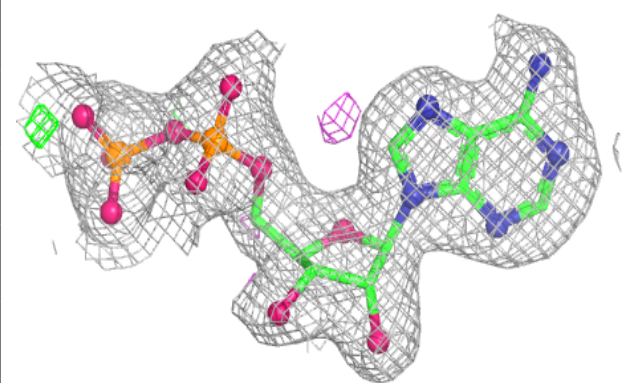


Electron density around ADP C 4021:

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

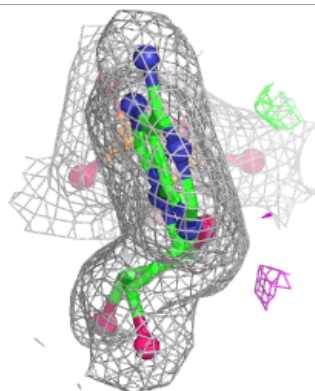
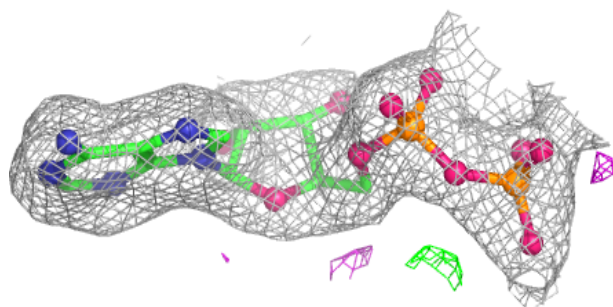
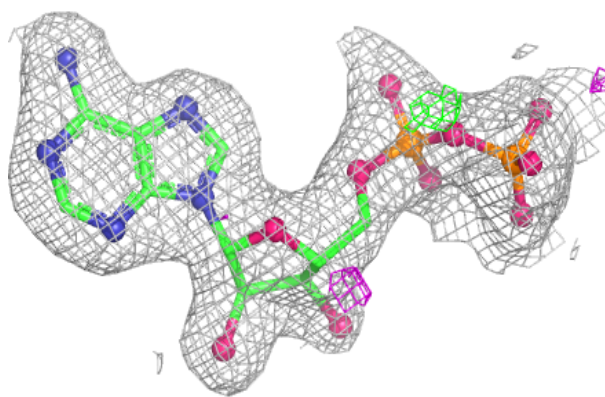
**Electron density around ADP E 4044:**

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



Electron density around ADP G 4066:

$2mF_o-DF_c$ (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.