



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 07:44 AM UTC

PDB ID : 5DOU / pdb_00005dou
Title : Crystal Structure of Human Carbamoyl phosphate synthetase I (CPS1),
ligand-bound form
Authors : de Cima, S.; Polo, L.M.; Fita, I.; Rubio, V.
Deposited on : 2015-09-11
Resolution : 2.60 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

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

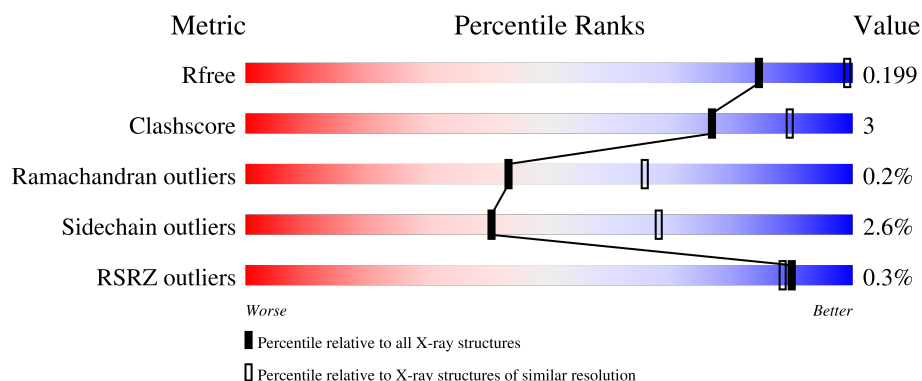
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	1489	
1	B	1489	
1	C	1489	
1	D	1489	

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 45021 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 synthase [ammonia], mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1422	Total	C	N	O	S	0	2	0
			10991	6980	1863	2090	58			
1	B	1426	Total	C	N	O	S	0	0	0
			11018	6997	1864	2098	59			
1	C	1421	Total	C	N	O	S	0	1	0
			10975	6969	1859	2089	58			
1	D	1430	Total	C	N	O	S	0	1	0
			11056	7023	1872	2102	59			

There are 112 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	12	MET	-	initiating methionine	UNP P31327
A	13	SER	-	expression tag	UNP P31327
A	14	TYR	-	expression tag	UNP P31327
A	15	TYR	-	expression tag	UNP P31327
A	16	HIS	-	expression tag	UNP P31327
A	17	HIS	-	expression tag	UNP P31327
A	18	HIS	-	expression tag	UNP P31327
A	19	HIS	-	expression tag	UNP P31327
A	20	HIS	-	expression tag	UNP P31327
A	21	HIS	-	expression tag	UNP P31327
A	22	ASP	-	expression tag	UNP P31327
A	23	TYR	-	expression tag	UNP P31327
A	24	ASP	-	expression tag	UNP P31327
A	25	ILE	-	expression tag	UNP P31327
A	26	PRO	-	expression tag	UNP P31327
A	27	THR	-	expression tag	UNP P31327
A	28	THR	-	expression tag	UNP P31327
A	29	GLU	-	expression tag	UNP P31327
A	30	ASN	-	expression tag	UNP P31327
A	31	LEU	-	expression tag	UNP P31327
A	32	TYR	-	expression tag	UNP P31327

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Chain	Residue	Modelled	Actual	Comment	Reference
A	33	PHE	-	expression tag	UNP P31327
A	34	GLN	-	expression tag	UNP P31327
A	35	GLY	-	expression tag	UNP P31327
A	36	ALA	-	expression tag	UNP P31327
A	37	MET	-	expression tag	UNP P31327
A	38	ASP	-	expression tag	UNP P31327
A	39	PRO	-	expression tag	UNP P31327
B	12	MET	-	initiating methionine	UNP P31327
B	13	SER	-	expression tag	UNP P31327
B	14	TYR	-	expression tag	UNP P31327
B	15	TYR	-	expression tag	UNP P31327
B	16	HIS	-	expression tag	UNP P31327
B	17	HIS	-	expression tag	UNP P31327
B	18	HIS	-	expression tag	UNP P31327
B	19	HIS	-	expression tag	UNP P31327
B	20	HIS	-	expression tag	UNP P31327
B	21	HIS	-	expression tag	UNP P31327
B	22	ASP	-	expression tag	UNP P31327
B	23	TYR	-	expression tag	UNP P31327
B	24	ASP	-	expression tag	UNP P31327
B	25	ILE	-	expression tag	UNP P31327
B	26	PRO	-	expression tag	UNP P31327
B	27	THR	-	expression tag	UNP P31327
B	28	THR	-	expression tag	UNP P31327
B	29	GLU	-	expression tag	UNP P31327
B	30	ASN	-	expression tag	UNP P31327
B	31	LEU	-	expression tag	UNP P31327
B	32	TYR	-	expression tag	UNP P31327
B	33	PHE	-	expression tag	UNP P31327
B	34	GLN	-	expression tag	UNP P31327
B	35	GLY	-	expression tag	UNP P31327
B	36	ALA	-	expression tag	UNP P31327
B	37	MET	-	expression tag	UNP P31327
B	38	ASP	-	expression tag	UNP P31327
B	39	PRO	-	expression tag	UNP P31327
C	12	MET	-	initiating methionine	UNP P31327
C	13	SER	-	expression tag	UNP P31327
C	14	TYR	-	expression tag	UNP P31327
C	15	TYR	-	expression tag	UNP P31327
C	16	HIS	-	expression tag	UNP P31327
C	17	HIS	-	expression tag	UNP P31327
C	18	HIS	-	expression tag	UNP P31327

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Chain	Residue	Modelled	Actual	Comment	Reference
C	19	HIS	-	expression tag	UNP P31327
C	20	HIS	-	expression tag	UNP P31327
C	21	HIS	-	expression tag	UNP P31327
C	22	ASP	-	expression tag	UNP P31327
C	23	TYR	-	expression tag	UNP P31327
C	24	ASP	-	expression tag	UNP P31327
C	25	ILE	-	expression tag	UNP P31327
C	26	PRO	-	expression tag	UNP P31327
C	27	THR	-	expression tag	UNP P31327
C	28	THR	-	expression tag	UNP P31327
C	29	GLU	-	expression tag	UNP P31327
C	30	ASN	-	expression tag	UNP P31327
C	31	LEU	-	expression tag	UNP P31327
C	32	TYR	-	expression tag	UNP P31327
C	33	PHE	-	expression tag	UNP P31327
C	34	GLN	-	expression tag	UNP P31327
C	35	GLY	-	expression tag	UNP P31327
C	36	ALA	-	expression tag	UNP P31327
C	37	MET	-	expression tag	UNP P31327
C	38	ASP	-	expression tag	UNP P31327
C	39	PRO	-	expression tag	UNP P31327
D	12	MET	-	initiating methionine	UNP P31327
D	13	SER	-	expression tag	UNP P31327
D	14	TYR	-	expression tag	UNP P31327
D	15	TYR	-	expression tag	UNP P31327
D	16	HIS	-	expression tag	UNP P31327
D	17	HIS	-	expression tag	UNP P31327
D	18	HIS	-	expression tag	UNP P31327
D	19	HIS	-	expression tag	UNP P31327
D	20	HIS	-	expression tag	UNP P31327
D	21	HIS	-	expression tag	UNP P31327
D	22	ASP	-	expression tag	UNP P31327
D	23	TYR	-	expression tag	UNP P31327
D	24	ASP	-	expression tag	UNP P31327
D	25	ILE	-	expression tag	UNP P31327
D	26	PRO	-	expression tag	UNP P31327
D	27	THR	-	expression tag	UNP P31327
D	28	THR	-	expression tag	UNP P31327
D	29	GLU	-	expression tag	UNP P31327
D	30	ASN	-	expression tag	UNP P31327
D	31	LEU	-	expression tag	UNP P31327
D	32	TYR	-	expression tag	UNP P31327

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Chain	Residue	Modelled	Actual	Comment	Reference
D	33	PHE	-	expression tag	UNP P31327
D	34	GLN	-	expression tag	UNP P31327
D	35	GLY	-	expression tag	UNP P31327
D	36	ALA	-	expression tag	UNP P31327
D	37	MET	-	expression tag	UNP P31327
D	38	ASP	-	expression tag	UNP P31327
D	39	PRO	-	expression tag	UNP P31327

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Ni 1 1	0	0
2	B	1	Total Ni 1 1	0	0
2	C	1	Total Ni 1 1	0	0
2	D	1	Total Ni 1 1	0	0

- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	3	Total Mg 3 3	0	0
3	B	3	Total Mg 3 3	0	0
3	C	3	Total Mg 3 3	0	0
3	D	3	Total Mg 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	4	Total K 4 4	0	0
4	C	4	Total K 4 4	0	0

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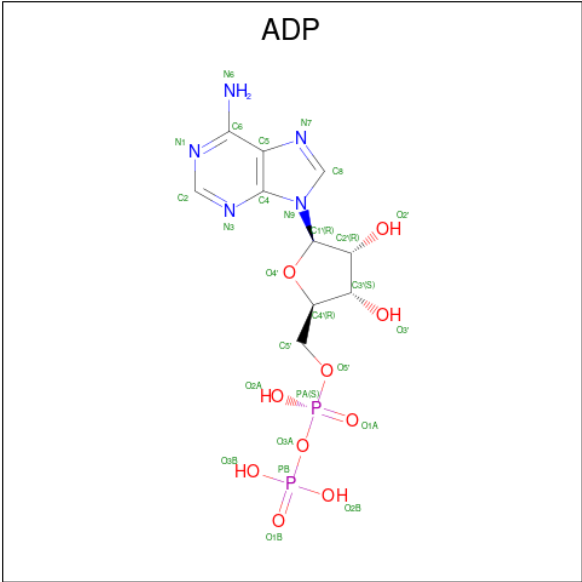
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	5	Total	K	0	0
			5	5		

- Molecule 5 is PHOSPHATE ION (CCD ID: PO4) (formula: O_4P).



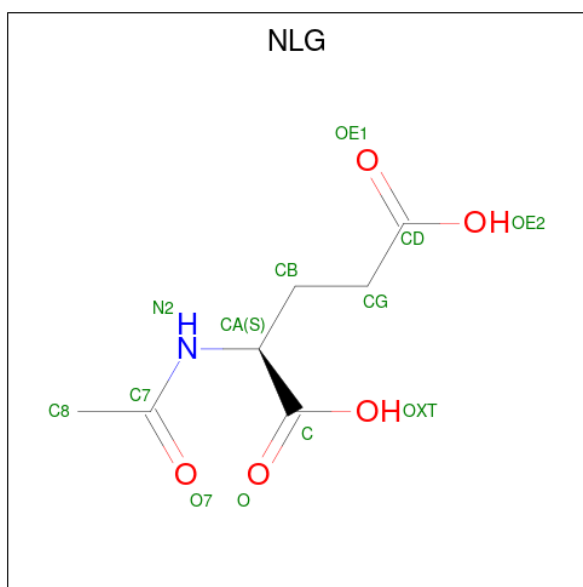
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	P	0	0
			5	4	1		
5	B	1	Total	O	P	0	0
			5	4	1		
5	C	1	Total	O	P	0	0
			5	4	1		
5	D	1	Total	O	P	0	0
			5	4	1		

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



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

- Molecule 7 is N-ACETYL-L-GLUTAMATE (CCD ID: NLG) (formula: C₇H₁₁NO₅).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			13	7	1	5		
7	B	1	Total	C	N	O	0	0
			13	7	1	5		
7	C	1	Total	C	N	O	0	0
			13	7	1	5		
7	D	1	Total	C	N	O	0	0
			13	7	1	5		

- Molecule 8 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

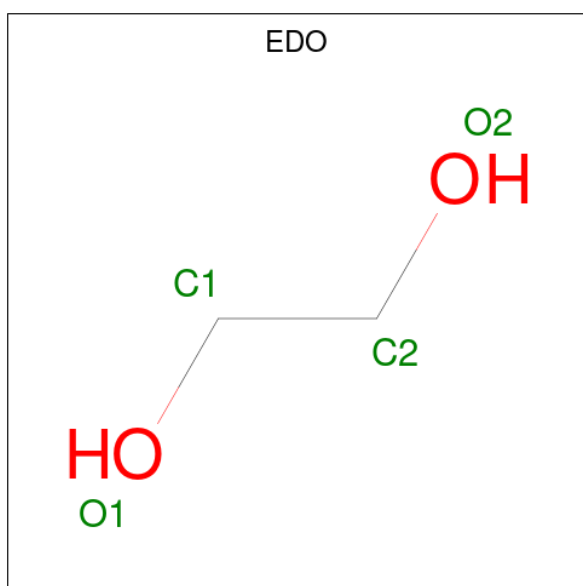
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	1	Total	Cl	0	0
			1	1		
8	B	1	Total	Cl	0	0
			1	1		
8	D	1	Total	Cl	0	0
			1	1		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	A	1	Total	C	O	0	0
			6	3	3		
9	D	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total	C	O	0	0
			4	2	2		

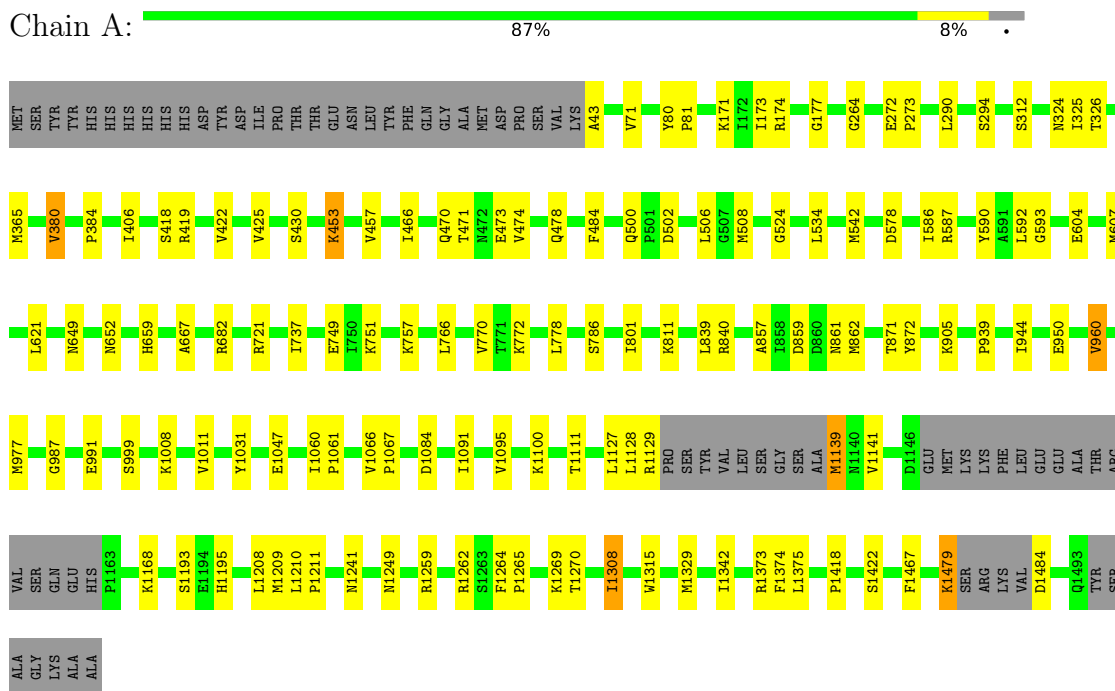
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	264	Total 264	O 264	0	0
11	B	79	Total 79	O 79	0	0
11	C	65	Total 65	O 65	0	0
11	D	232	Total 232	O 232	0	0

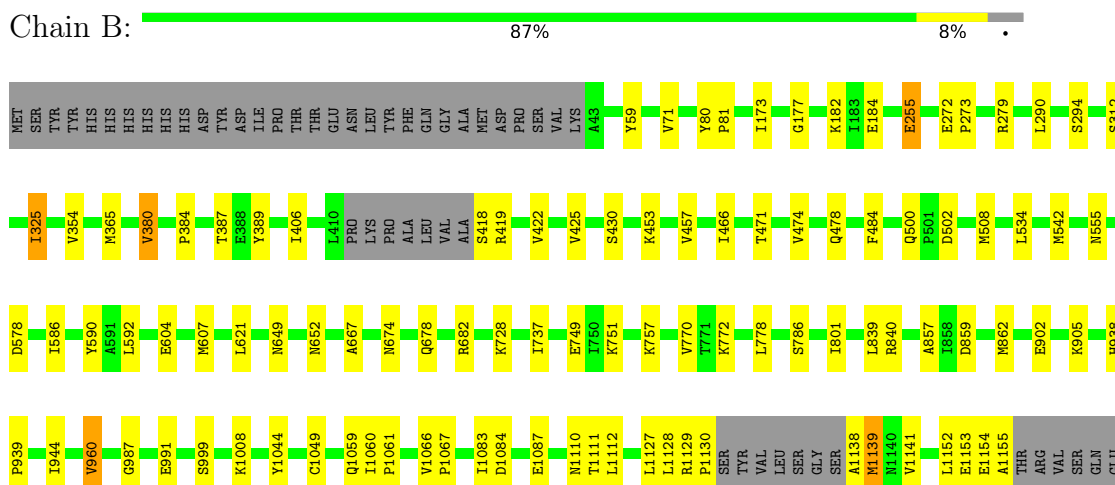
3 Residue-property plots [i](#)

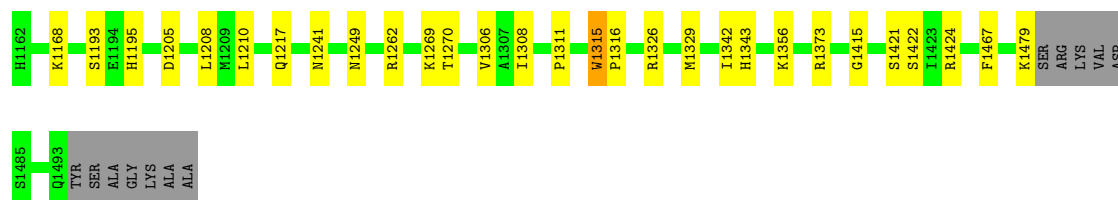
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Carbamoyl-phosphate synthase [ammonia], mitochondrial

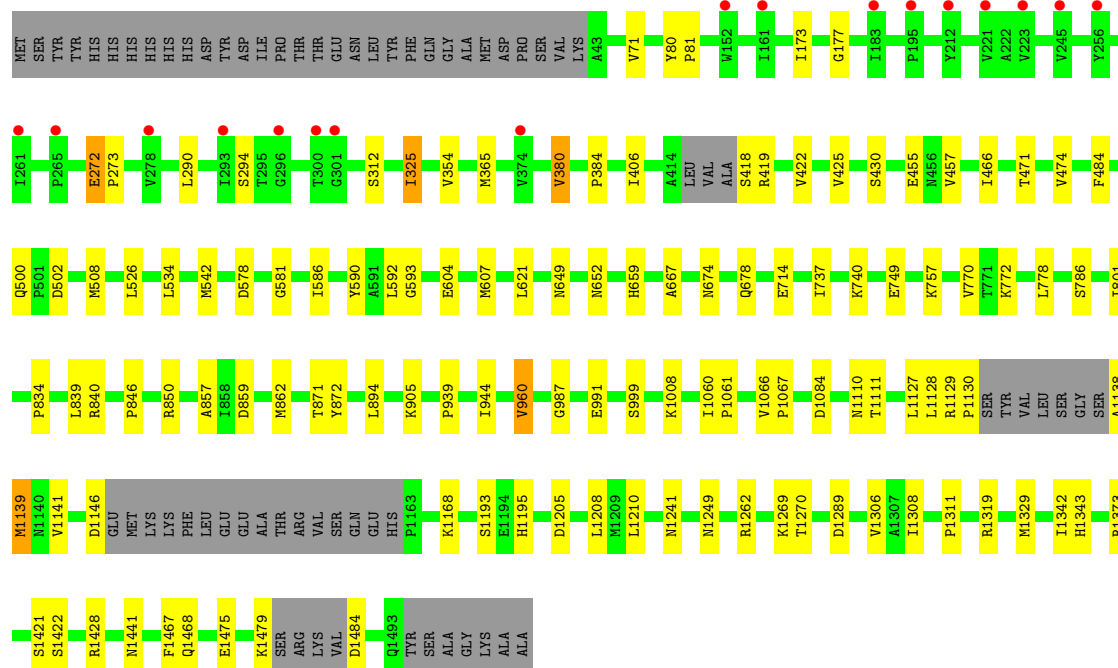
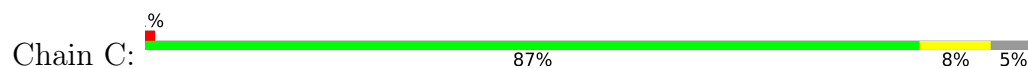


- Molecule 1: Carbamoyl-phosphate synthase [ammonia], mitochondrial

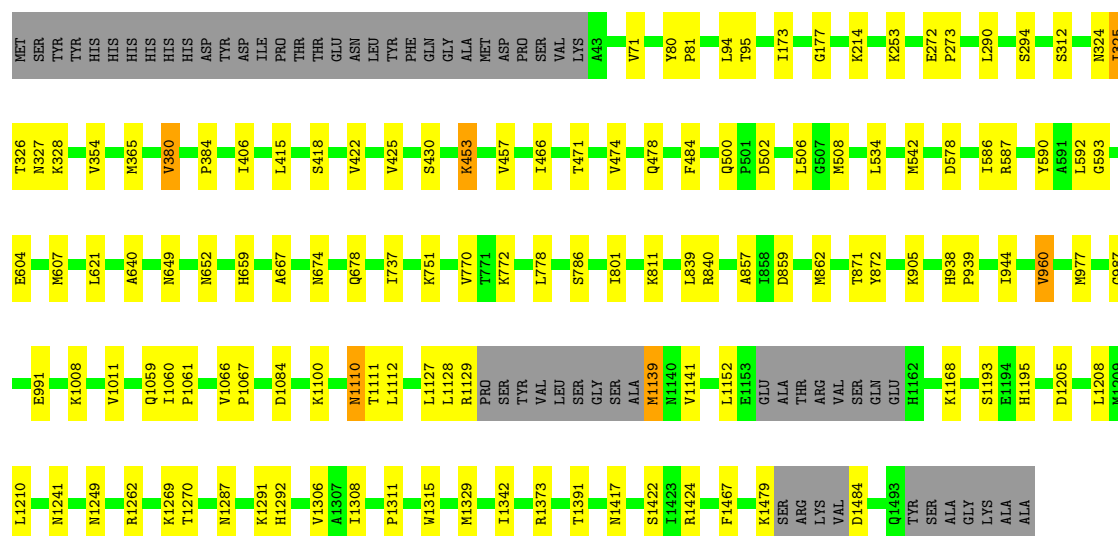
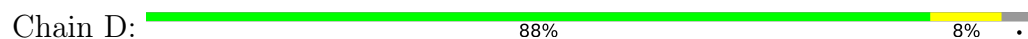




- Molecule 1: Carbamoyl-phosphate synthase [ammonia], mitochondrial



- Molecule 1: Carbamoyl-phosphate synthase [ammonia], mitochondrial



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	78.92Å 98.56Å 214.89Å 90.66° 98.65° 90.08°	Depositor
Resolution (Å)	40.00 – 2.60 40.00 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.7 (40.00-2.60) 87.6 (40.00-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.83 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.195 , 0.229 0.202 , 0.199	Depositor DCC
R_{free} test set	8965 reflections (4.55%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.535	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 14.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.035 for h,-k,-h-l 0.247 for -h,k,-l 0.030 for -h,-k,h+l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	45021	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.65% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: NI, NLG, GOL, EDO, PO4, K, MG, ADP, CL

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	0.89	1/11210 (0.0%)	0.90	4/15188 (0.0%)
1	B	0.70	1/11231 (0.0%)	0.85	5/15213 (0.0%)
1	C	0.68	1/11191 (0.0%)	0.84	2/15162 (0.0%)
1	D	0.88	1/11274 (0.0%)	0.90	5/15273 (0.0%)
All	All	0.79	4/44906 (0.0%)	0.87	16/60836 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	500	GLN	C-O	-5.63	1.21	1.23
1	C	500	GLN	C-O	-5.54	1.21	1.23
1	A	500	GLN	C-O	-5.18	1.21	1.23
1	D	500	GLN	C-O	-5.06	1.21	1.23

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1428	ARG	CB-CA-C	-6.08	101.08	110.81
1	D	1315	TRP	CA-C-N	-5.94	112.45	119.05
1	D	1315	TRP	C-N-CA	-5.94	112.45	119.05
1	D	474	VAL	N-CA-C	5.91	116.44	108.17
1	B	1315	TRP	CA-C-N	-5.88	112.53	119.05
1	B	1315	TRP	C-N-CA	-5.88	112.53	119.05
1	D	938	HIS	CA-C-N	-5.82	114.56	120.85
1	D	938	HIS	C-N-CA	-5.82	114.56	120.85
1	C	474	VAL	N-CA-C	5.78	116.62	108.36
1	A	861	ASN	N-CA-C	5.75	119.59	112.58
1	B	474	VAL	N-CA-C	5.29	115.93	108.36
1	B	938	HIS	CA-C-N	-5.28	115.29	120.52
1	B	938	HIS	C-N-CA	-5.28	115.29	120.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1315	TRP	CA-C-N	-5.24	113.23	119.05
1	A	1315	TRP	C-N-CA	-5.24	113.23	119.05
1	A	474	VAL	N-CA-C	5.21	116.48	108.71

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10991	0	11065	70	0
1	B	11018	0	11072	65	0
1	C	10975	0	11038	57	1
1	D	11056	0	11125	64	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	3	0	0	0	0
3	B	3	0	0	0	0
3	C	3	0	0	0	0
3	D	3	0	0	0	0
4	A	5	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	5	0	0	0	0
5	A	5	0	0	1	0
5	B	5	0	0	0	0
5	C	5	0	0	1	0
5	D	5	0	0	0	0
6	A	54	0	24	2	0
6	B	54	0	24	0	0
6	C	54	0	24	0	0
6	D	54	0	24	2	0
7	A	13	0	9	0	0
7	B	13	0	9	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	C	13	0	9	0	0
7	D	13	0	9	1	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	D	1	0	0	0	0
9	A	6	0	8	0	0
9	D	6	0	8	1	0
10	A	4	0	6	2	0
11	A	264	0	0	5	0
11	B	79	0	0	4	1
11	C	65	0	0	8	0
11	D	232	0	0	3	0
All	All	45021	0	44454	255	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 3.

All (255) 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:A:419[B]:ARG:HH11	1:A:419[B]:ARG:CG	1.72	1.03
1:A:419[B]:ARG:HH11	1:A:419[B]:ARG:HG3	0.86	1.03
1:A:419[B]:ARG:HG3	1:A:419[B]:ARG:NH1	1.67	0.98
1:C:419:ARG:NH1	1:C:749:GLU:OE1	1.97	0.98
1:C:894:LEU:O	11:C:2101:HOH:O	2.01	0.79
1:C:834:PRO:HB3	11:C:2106:HOH:O	1.83	0.77
1:C:1127:LEU:HD23	1:C:1141:VAL:HG22	1.67	0.76
1:A:365:MET:HB2	1:A:406:ILE:HG21	1.68	0.76
1:C:365:MET:HB2	1:C:406:ILE:HG21	1.68	0.76
1:B:365:MET:HB2	1:B:406:ILE:HG21	1.67	0.75
1:A:1127:LEU:HD23	1:A:1141:VAL:HG22	1.68	0.75
1:D:939:PRO:HB2	1:D:960:VAL:HG13	1.68	0.74
1:C:939:PRO:HB2	1:C:960:VAL:HG13	1.70	0.74
1:A:939:PRO:HB2	1:A:960:VAL:HG13	1.69	0.74
1:D:1127:LEU:HD23	1:D:1141:VAL:HG22	1.69	0.73
1:D:365:MET:HB2	1:D:406:ILE:HG21	1.69	0.72
1:B:939:PRO:HB2	1:B:960:VAL:HG13	1.71	0.72
1:B:1127:LEU:HD23	1:B:1141:VAL:HG22	1.69	0.72
1:A:419[B]:ARG:CG	1:A:419[B]:ARG:NH1	2.39	0.71
1:B:387:THR:HA	1:B:389:TYR:CE1	2.30	0.67
1:C:177:GLY:HA2	1:C:312:SER:HA	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1468:GLN:OE1	11:C:2102:HOH:O	2.13	0.65
1:B:279:ARG:NH2	11:B:2101:HOH:O	2.09	0.65
1:C:846:PRO:HA	1:C:850:ARG:HD3	1.79	0.65
1:B:177:GLY:HA2	1:B:312:SER:HA	1.79	0.64
1:D:177:GLY:HA2	1:D:312:SER:HA	1.80	0.64
1:C:581:GLY:HA2	11:C:2156:HOH:O	1.98	0.63
1:A:811:LYS:HE2	11:A:2340:HOH:O	1.97	0.63
1:A:177:GLY:HA2	1:A:312:SER:HA	1.81	0.62
1:C:714:GLU:OE2	5:C:2007:PO4:O3	2.19	0.61
1:B:592:LEU:C	1:B:592:LEU:HD12	2.28	0.58
1:C:1475:GLU:OE1	11:C:2103:HOH:O	2.17	0.58
1:C:1127:LEU:HD22	1:C:1139:MET:HE1	1.86	0.57
1:B:453:LYS:NZ	1:B:478:GLN:O	2.30	0.57
1:A:801:ILE:HD13	1:A:944:ILE:HD11	1.84	0.57
1:B:801:ILE:HD13	1:B:944:ILE:HD11	1.87	0.57
1:C:1129:ARG:HG3	1:C:1139:MET:HG2	1.86	0.57
1:A:1129:ARG:HG3	1:A:1139:MET:HG2	1.87	0.57
1:C:801:ILE:HD13	1:C:944:ILE:HD11	1.86	0.57
1:D:592:LEU:C	1:D:592:LEU:HD12	2.29	0.56
1:D:1127:LEU:HD22	1:D:1139:MET:HE1	1.86	0.56
1:A:453:LYS:NZ	1:A:478:GLN:O	2.29	0.56
1:A:470:GLN:NE2	11:A:2108:HOH:O	2.33	0.56
1:D:453:LYS:NZ	1:D:478:GLN:O	2.29	0.55
1:D:471:THR:OG1	1:D:1269:LYS:NZ	2.40	0.55
1:A:592:LEU:HD12	1:A:592:LEU:C	2.32	0.55
1:B:1129:ARG:HG3	1:B:1139:MET:HG2	1.87	0.55
1:A:419[B]:ARG:NH2	1:A:749:GLU:OE1	2.40	0.55
1:D:801:ILE:HD13	1:D:944:ILE:HD11	1.89	0.54
1:A:471:THR:OG1	1:A:1269:LYS:NZ	2.41	0.54
1:D:1129:ARG:HG3	1:D:1139:MET:HG2	1.88	0.54
1:C:592:LEU:HD12	1:C:592:LEU:C	2.33	0.53
1:B:365:MET:CB	1:B:406:ILE:HG21	2.39	0.53
1:C:770:VAL:HG12	1:C:801:ILE:HG12	1.91	0.53
1:D:770:VAL:HG12	1:D:801:ILE:HG12	1.91	0.52
1:A:43:ALA:HB1	11:A:2270:HOH:O	2.10	0.51
1:C:471:THR:OG1	1:C:1269:LYS:NZ	2.43	0.51
1:B:471:THR:OG1	1:B:1269:LYS:NZ	2.42	0.51
1:B:770:VAL:HG12	1:B:801:ILE:HG12	1.92	0.51
1:C:365:MET:CB	1:C:406:ILE:HG21	2.40	0.51
1:C:667:ALA:HB3	1:C:770:VAL:HG22	1.93	0.51
1:A:667:ALA:HB3	1:A:770:VAL:HG22	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:473:GLU:OE1	10:A:2016:EDO:C1	2.59	0.51
1:A:770:VAL:HG12	1:A:801:ILE:HG12	1.93	0.51
1:D:587:ARG:NH1	6:D:2008:ADP:O1A	2.43	0.51
1:A:80:TYR:CG	1:A:81:PRO:HD3	2.46	0.51
1:B:667:ALA:HB3	1:B:770:VAL:HG22	1.93	0.51
1:B:555:ASN:HA	11:B:2131:HOH:O	2.10	0.50
1:A:365:MET:CB	1:A:406:ILE:HG21	2.39	0.50
1:B:1195:HIS:CD2	1:B:1208:LEU:CD2	2.95	0.50
1:A:1308:ILE:HD11	1:A:1342:ILE:HG13	1.94	0.50
1:B:425:VAL:HG23	1:B:457:VAL:CG1	2.42	0.50
1:B:1139:MET:O	1:B:1326:ARG:NH2	2.45	0.49
1:A:1418:PRO:O	1:D:214:LYS:HE3	2.12	0.49
1:C:846:PRO:HG3	1:C:850:ARG:NH1	2.28	0.49
1:D:425:VAL:HG23	1:D:457:VAL:CG1	2.42	0.49
1:D:272:GLU:O	1:D:273:PRO:C	2.53	0.49
1:C:425:VAL:HG23	1:C:457:VAL:CG1	2.42	0.49
1:A:542:MET:HG2	1:A:590:TYR:OH	2.12	0.48
1:D:80:TYR:CG	1:D:81:PRO:HD3	2.47	0.48
1:D:667:ALA:HB3	1:D:770:VAL:HG22	1.93	0.48
1:C:80:TYR:CG	1:C:81:PRO:HD3	2.47	0.48
1:D:365:MET:CB	1:D:406:ILE:HG21	2.40	0.48
6:D:2009:ADP:O3B	6:D:2009:ADP:O2A	2.31	0.48
1:D:502:ASP:OD1	1:D:502:ASP:N	2.46	0.48
1:C:526:LEU:HB2	11:C:2149:HOH:O	2.14	0.48
1:A:425:VAL:HG23	1:A:457:VAL:CG1	2.44	0.48
1:A:840:ARG:NH1	1:A:862:MET:HE2	2.29	0.48
1:A:1209:MET:SD	1:A:1342:ILE:HD11	2.54	0.48
1:B:80:TYR:CG	1:B:81:PRO:HD3	2.49	0.47
1:B:542:MET:HG2	1:B:590:TYR:OH	2.13	0.47
1:C:425:VAL:HG23	1:C:457:VAL:HG11	1.95	0.47
1:C:542:MET:HG2	1:C:590:TYR:OH	2.14	0.47
1:B:425:VAL:HG23	1:B:457:VAL:HG11	1.96	0.47
1:A:272:GLU:O	1:A:273:PRO:C	2.53	0.47
1:D:593:GLY:HA2	1:D:659:HIS:CE1	2.50	0.47
1:A:593:GLY:HA2	1:A:659:HIS:CE1	2.49	0.47
1:B:1060:ILE:HB	1:B:1061:PRO:HD3	1.96	0.47
1:A:473:GLU:OE1	10:A:2016:EDO:O1	2.28	0.47
1:B:59:TYR:OH	1:B:902:GLU:OE1	2.32	0.47
1:B:840:ARG:NH1	1:B:862:MET:HE2	2.30	0.47
1:A:587:ARG:NH1	6:A:2008:ADP:O1A	2.48	0.47
1:D:542:MET:HG2	1:D:590:TYR:OH	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1152:LEU:C	1:B:1154:GLU:N	2.73	0.46
1:D:425:VAL:HG23	1:D:457:VAL:HG11	1.96	0.46
1:D:840:ARG:NH1	1:D:862:MET:HE2	2.30	0.46
1:D:991:GLU:HG3	1:D:1262:ARG:HB2	1.98	0.46
1:A:380:VAL:HG11	1:A:384:PRO:O	2.16	0.46
1:A:1031:TYR:OH	1:A:1047:GLU:OE2	2.25	0.46
1:C:840:ARG:NH1	1:C:862:MET:HE2	2.30	0.46
1:C:1343:HIS:NE2	11:C:2103:HOH:O	2.23	0.46
1:A:871:THR:O	1:A:872:TYR:HB2	2.15	0.46
1:C:1195:HIS:CD2	1:C:1208:LEU:CD2	2.98	0.46
1:D:1066:VAL:HB	1:D:1067:PRO:HD3	1.98	0.46
1:A:425:VAL:HG23	1:A:457:VAL:HG11	1.97	0.46
1:A:1195:HIS:CD2	1:A:1208:LEU:CD2	2.99	0.46
1:B:502:ASP:OD1	1:B:502:ASP:N	2.48	0.46
1:D:71:VAL:HG12	1:D:173:ILE:HD11	1.98	0.46
1:D:1110:ASN:N	1:D:1110:ASN:ND2	2.64	0.46
1:B:466:ILE:HD12	1:B:484:PHE:CE1	2.50	0.46
1:A:171:LYS:HA	1:A:174[B]:ARG:HD3	1.99	0.45
1:A:422:VAL:HG11	1:A:534:LEU:HD21	1.99	0.45
1:C:466:ILE:HD12	1:C:484:PHE:CE1	2.51	0.45
1:A:1373:ARG:HB3	1:A:1467:PHE:CZ	2.51	0.45
1:B:182:LYS:HE3	1:B:184:GLU:OE1	2.17	0.45
1:D:1195:HIS:CD2	1:D:1208:LEU:CD2	3.00	0.45
1:B:71:VAL:HG12	1:B:173:ILE:HD11	1.99	0.45
1:D:586:ILE:HA	1:D:621:LEU:O	2.17	0.45
1:D:1060:ILE:HB	1:D:1061:PRO:HD3	1.98	0.45
1:C:272:GLU:O	1:C:273:PRO:C	2.59	0.45
1:A:659:HIS:NE2	6:A:2008:ADP:O3B	2.47	0.45
1:C:422:VAL:HG11	1:C:534:LEU:HD21	1.99	0.45
1:B:1210:LEU:HD23	1:B:1270:THR:HG21	1.98	0.44
1:C:586:ILE:HA	1:C:621:LEU:O	2.18	0.44
1:C:778:LEU:HD13	1:C:786:SER:HA	1.99	0.44
1:C:1205:ASP:O	1:C:1311:PRO:HG3	2.17	0.44
1:C:71:VAL:HG12	1:C:173:ILE:HD11	1.98	0.44
1:D:380:VAL:HG11	1:D:384:PRO:O	2.16	0.44
1:C:1060:ILE:HB	1:C:1061:PRO:HD3	2.00	0.44
1:B:272:GLU:O	1:B:273:PRO:C	2.59	0.44
1:A:290:LEU:C	1:A:290:LEU:HD23	2.43	0.44
1:A:1210:LEU:HD23	1:A:1270:THR:HG21	2.00	0.44
1:C:380:VAL:HG11	1:C:384:PRO:O	2.18	0.44
1:B:1343:HIS:NE2	11:B:2103:HOH:O	2.23	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:466:ILE:HD12	1:D:484:PHE:CE1	2.53	0.44
1:D:778:LEU:HD13	1:D:786:SER:HA	2.00	0.44
1:B:422:VAL:HG11	1:B:534:LEU:HD21	1.99	0.43
1:B:1066:VAL:HB	1:B:1067:PRO:HD3	2.00	0.43
1:B:1083:ILE:O	1:B:1087:GLU:HG3	2.18	0.43
1:C:502:ASP:OD1	1:C:502:ASP:N	2.47	0.43
1:B:387:THR:HA	1:B:389:TYR:HE1	1.78	0.43
1:B:778:LEU:HD13	1:B:786:SER:HA	1.99	0.43
1:D:422:VAL:HG11	1:D:534:LEU:HD21	1.99	0.43
1:A:1418:PRO:O	1:D:214:LYS:CE	2.66	0.43
1:B:592:LEU:C	1:B:592:LEU:CD1	2.91	0.43
1:B:380:VAL:HG11	1:B:384:PRO:O	2.19	0.43
1:C:1373:ARG:HB3	1:C:1467:PHE:CZ	2.54	0.43
1:A:987:GLY:HA2	1:A:1329:MET:CE	2.49	0.43
1:A:991:GLU:HG3	1:A:1262:ARG:HB2	2.01	0.43
1:D:871:THR:O	1:D:872:TYR:HB2	2.19	0.43
1:D:1373:ARG:NH2	11:D:2136:HOH:O	2.52	0.43
1:A:1060:ILE:HB	1:A:1061:PRO:HD3	2.00	0.43
1:B:1044:TYR:CD1	1:B:1049:CYS:HB2	2.54	0.43
1:C:593:GLY:HA2	1:C:659:HIS:CE1	2.54	0.43
1:C:604:GLU:HA	1:C:607:MET:HE3	2.01	0.43
1:C:987:GLY:HA2	1:C:1329:MET:CE	2.49	0.43
1:D:592:LEU:C	1:D:592:LEU:CD1	2.91	0.43
1:C:1127:LEU:HD22	1:C:1139:MET:CE	2.48	0.43
1:B:991:GLU:HG3	1:B:1262:ARG:HB2	2.00	0.43
1:C:455:GLU:OE2	1:C:740:LYS:NZ	2.50	0.43
1:A:71:VAL:HG12	1:A:173:ILE:HD11	2.00	0.43
1:B:1205:ASP:O	1:B:1311:PRO:HG3	2.18	0.43
1:B:1306:VAL:HG21	1:B:1342:ILE:HD13	2.01	0.43
1:D:1210:LEU:HD23	1:D:1270:THR:HG21	2.00	0.43
1:B:1152:LEU:C	1:B:1154:GLU:H	2.28	0.42
1:D:987:GLY:HA2	1:D:1329:MET:CE	2.49	0.42
1:A:977:MET:HA	1:A:1011:VAL:O	2.19	0.42
1:D:604:GLU:HA	1:D:607:MET:HE3	2.01	0.42
1:D:839:LEU:HD21	1:D:857:ALA:HA	2.01	0.42
1:D:1391:THR:OG1	7:D:2010:NLG:OE2	2.26	0.42
1:B:255:GLU:O	1:B:255:GLU:HG2	2.19	0.42
1:A:506:LEU:HD12	1:A:506:LEU:C	2.44	0.42
1:A:586:ILE:HA	1:A:621:LEU:O	2.19	0.42
1:A:778:LEU:HD13	1:A:786:SER:HA	2.00	0.42
1:B:839:LEU:HD21	1:B:857:ALA:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1210:LEU:HD23	1:C:1270:THR:HG21	2.02	0.42
1:B:604:GLU:HA	1:B:607:MET:HE3	2.01	0.42
1:C:871:THR:O	1:C:872:TYR:HB2	2.19	0.42
1:A:1211:PRO:HB2	1:B:1217:GLN:OE1	2.20	0.42
1:B:674:ASN:O	1:B:678:GLN:HG2	2.20	0.42
1:B:1152:LEU:O	1:B:1155:ALA:N	2.51	0.42
1:C:991:GLU:HG3	1:C:1262:ARG:HB2	2.01	0.42
1:A:466:ILE:HD12	1:A:484:PHE:CE1	2.55	0.42
1:A:502:ASP:OD1	1:A:502:ASP:N	2.47	0.42
1:B:419:ARG:NH1	1:B:749:GLU:OE1	2.51	0.42
1:C:839:LEU:HD21	1:C:857:ALA:HA	2.01	0.42
1:D:811:LYS:HE2	11:D:2287:HOH:O	2.19	0.42
1:D:977:MET:HA	1:D:1011:VAL:O	2.20	0.42
1:A:1066:VAL:HB	1:A:1067:PRO:HD3	2.02	0.42
1:B:682:ARG:HA	1:B:682:ARG:HD2	1.84	0.42
1:B:1373:ARG:HB3	1:B:1467:PHE:CZ	2.54	0.42
1:D:94:LEU:HD12	1:D:95:THR:N	2.34	0.42
1:D:1306:VAL:HG21	1:D:1342:ILE:HD13	2.02	0.42
1:B:987:GLY:HA2	1:B:1329:MET:CE	2.50	0.42
1:D:290:LEU:HD23	1:D:290:LEU:C	2.45	0.42
1:C:1441:ASN:ND2	11:C:2116:HOH:O	2.53	0.41
1:D:325:ILE:HD11	1:D:354:VAL:HB	2.01	0.41
1:A:524:GLY:HA2	11:A:2325:HOH:O	2.19	0.41
1:B:728:LYS:HA	1:B:728:LYS:HD3	1.96	0.41
1:B:586:ILE:HA	1:B:621:LEU:O	2.21	0.41
1:B:1415:GLY:HA2	11:B:2176:HOH:O	2.19	0.41
1:C:1066:VAL:HB	1:C:1067:PRO:HD3	2.02	0.41
1:D:1373:ARG:HB3	1:D:1467:PHE:CZ	2.54	0.41
1:B:991:GLU:HG3	1:B:1262:ARG:CB	2.50	0.41
1:D:324:ASN:OD1	1:D:326:THR:HB	2.21	0.41
1:D:415:LEU:HB3	1:D:640:ALA:O	2.20	0.41
1:D:1417:ASN:OD1	1:D:1417:ASN:C	2.64	0.41
1:A:721:ARG:NH2	5:A:2007:PO4:O4	2.47	0.41
1:A:1479:LYS:HD2	1:A:1479:LYS:HA	1.95	0.41
1:C:1306:VAL:HG21	1:C:1342:ILE:HD13	2.02	0.41
1:D:506:LEU:HD12	1:D:506:LEU:C	2.46	0.41
1:B:1112:LEU:CD1	1:B:1152:LEU:HD12	2.51	0.41
1:C:290:LEU:C	1:C:290:LEU:HD23	2.45	0.41
1:A:991:GLU:HG3	1:A:1262:ARG:CB	2.50	0.41
1:C:325:ILE:HD11	1:C:354:VAL:HB	2.03	0.41
1:D:1127:LEU:HD22	1:D:1139:MET:CE	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1205:ASP:O	1:D:1311:PRO:HG3	2.21	0.41
1:D:1291:LYS:HE3	1:D:1292:HIS:NE2	2.36	0.41
1:A:324:ASN:OD1	1:A:326:THR:HB	2.21	0.41
1:A:1264:PHE:N	1:A:1265:PRO:CD	2.84	0.41
1:B:387:THR:HA	1:B:389:TYR:CD1	2.56	0.41
1:B:1315:TRP:O	1:B:1316:PRO:C	2.63	0.41
1:D:991:GLU:HG3	1:D:1262:ARG:CB	2.50	0.41
1:D:1112:LEU:CD1	1:D:1152:LEU:HD12	2.51	0.41
1:A:1259:ARG:NE	11:A:2144:HOH:O	2.51	0.41
1:D:80:TYR:N	1:D:81:PRO:CD	2.84	0.41
1:D:327:ASN:O	1:D:328:LYS:HB3	2.21	0.41
1:D:674:ASN:O	1:D:678:GLN:HG2	2.21	0.41
1:A:1091:ILE:O	1:A:1095:VAL:HG23	2.21	0.40
1:B:325:ILE:HD11	1:B:354:VAL:HB	2.02	0.40
1:B:1059:GLN:O	1:B:1060:ILE:C	2.64	0.40
1:C:674:ASN:O	1:C:678:GLN:HG2	2.22	0.40
1:C:991:GLU:HG3	1:C:1262:ARG:CB	2.51	0.40
9:D:2015:GOL:C1	11:D:2152:HOH:O	2.69	0.40
1:A:682:ARG:HD2	1:A:682:ARG:HA	1.80	0.40
1:B:1130:PRO:HD2	1:B:1138:ALA:O	2.21	0.40
1:D:1059:GLN:O	1:D:1060:ILE:C	2.65	0.40
1:D:1110:ASN:N	1:D:1110:ASN:HD22	2.19	0.40
1:A:604:GLU:HA	1:A:607:MET:HE3	2.02	0.40
1:C:1130:PRO:HD2	1:C:1138:ALA:O	2.21	0.40
1:A:174[A]:ARG:NE	1:A:950:GLU:O	2.55	0.40
1:A:592:LEU:C	1:A:592:LEU:CD1	2.94	0.40
1:A:839:LEU:HD21	1:A:857:ALA:HA	2.04	0.40
1:A:1374:PHE:O	1:A:1375:LEU:C	2.65	0.40
1:B:290:LEU:C	1:B:290:LEU:HD23	2.47	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:1289:ASP:OD2	11:B:2101:HOH:O[1_656]	2.10	0.10

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1416/1489 (95%)	1367 (96%)	46 (3%)	3 (0%)	43	66
1	B	1416/1489 (95%)	1375 (97%)	38 (3%)	3 (0%)	43	66
1	C	1412/1489 (95%)	1369 (97%)	41 (3%)	2 (0%)	48	70
1	D	1423/1489 (96%)	1379 (97%)	42 (3%)	2 (0%)	48	70
All	All	5667/5956 (95%)	5490 (97%)	167 (3%)	10 (0%)	43	66

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	1153	GLU
1	A	294	SER
1	A	380	VAL
1	B	294	SER
1	B	380	VAL
1	C	294	SER
1	C	380	VAL
1	D	294	SER
1	D	380	VAL
1	A	264	GLY

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	1210/1266 (96%)	1179 (97%)	31 (3%)	40	68

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1212/1266 (96%)	1180 (97%)	32 (3%)	40	68
1	C	1208/1266 (95%)	1176 (97%)	32 (3%)	40	68
1	D	1217/1266 (96%)	1185 (97%)	32 (3%)	40	68
All	All	4847/5064 (96%)	4720 (97%)	127 (3%)	40	68

All (127) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	325	ILE
1	A	418	SER
1	A	430	SER
1	A	453	LYS
1	A	508	MET
1	A	578	ASP
1	A	649	ASN
1	A	652	ASN
1	A	737	ILE
1	A	751	LYS
1	A	757	LYS
1	A	766	LEU
1	A	772	LYS
1	A	859	ASP
1	A	905	LYS
1	A	960	VAL
1	A	999	SER
1	A	1008	LYS
1	A	1084	ASP
1	A	1100	LYS
1	A	1111	THR
1	A	1128	LEU
1	A	1139	MET
1	A	1168	LYS
1	A	1193	SER
1	A	1241	ASN
1	A	1249	ASN
1	A	1308	ILE
1	A	1422	SER
1	A	1479	LYS
1	A	1484	ASP
1	B	255	GLU
1	B	325	ILE

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Mol	Chain	Res	Type
1	B	418	SER
1	B	430	SER
1	B	508	MET
1	B	578	ASP
1	B	649	ASN
1	B	652	ASN
1	B	737	ILE
1	B	751	LYS
1	B	757	LYS
1	B	772	LYS
1	B	859	ASP
1	B	905	LYS
1	B	960	VAL
1	B	999	SER
1	B	1008	LYS
1	B	1084	ASP
1	B	1110	ASN
1	B	1111	THR
1	B	1128	LEU
1	B	1139	MET
1	B	1168	LYS
1	B	1193	SER
1	B	1241	ASN
1	B	1249	ASN
1	B	1308	ILE
1	B	1356	LYS
1	B	1421	SER
1	B	1422	SER
1	B	1424	ARG
1	B	1479	LYS
1	C	272	GLU
1	C	325	ILE
1	C	418	SER
1	C	430	SER
1	C	508	MET
1	C	578	ASP
1	C	649	ASN
1	C	652	ASN
1	C	737	ILE
1	C	757	LYS
1	C	772	LYS
1	C	859	ASP

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Mol	Chain	Res	Type
1	C	905	LYS
1	C	960	VAL
1	C	999	SER
1	C	1008	LYS
1	C	1084	ASP
1	C	1110	ASN
1	C	1111	THR
1	C	1128	LEU
1	C	1139	MET
1	C	1146	ASP
1	C	1168	LYS
1	C	1193	SER
1	C	1241	ASN
1	C	1249	ASN
1	C	1308	ILE
1	C	1319	ARG
1	C	1421	SER
1	C	1422	SER
1	C	1479	LYS
1	C	1484	ASP
1	D	253	LYS
1	D	325	ILE
1	D	418	SER
1	D	430	SER
1	D	453	LYS
1	D	508	MET
1	D	578	ASP
1	D	649	ASN
1	D	652	ASN
1	D	737	ILE
1	D	751	LYS
1	D	772	LYS
1	D	859	ASP
1	D	905	LYS
1	D	960	VAL
1	D	1008	LYS
1	D	1084	ASP
1	D	1100	LYS
1	D	1110	ASN
1	D	1111	THR
1	D	1128	LEU
1	D	1139	MET

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Mol	Chain	Res	Type
1	D	1168	LYS
1	D	1193	SER
1	D	1241	ASN
1	D	1249	ASN
1	D	1287	ASN
1	D	1308	ILE
1	D	1422	SER
1	D	1424	ARG
1	D	1479	LYS
1	D	1484	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	456	ASN
1	A	465	ASN
1	A	674	ASN
1	A	1045	HIS
1	A	1059	GLN
1	A	1062	ASN
1	A	1103	GLN
1	A	1243	GLN
1	A	1359	GLN
1	A	1368	GLN
1	A	1416	GLN
1	A	1437	ASN
1	A	1449	ASN
1	A	1490	HIS
1	B	500	GLN
1	B	511	GLN
1	B	674	ASN
1	B	1045	HIS
1	B	1059	GLN
1	B	1103	GLN
1	B	1140	ASN
1	B	1292	HIS
1	B	1359	GLN
1	B	1368	GLN
1	B	1490	HIS
1	C	335	GLN
1	C	465	ASN
1	C	511	GLN

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Mol	Chain	Res	Type
1	C	674	ASN
1	C	1045	HIS
1	C	1059	GLN
1	C	1103	GLN
1	C	1243	GLN
1	C	1298	HIS
1	C	1359	GLN
1	C	1368	GLN
1	C	1382	HIS
1	C	1416	GLN
1	C	1437	ASN
1	C	1441	ASN
1	D	141	ASN
1	D	511	GLN
1	D	674	ASN
1	D	1059	GLN
1	D	1062	ASN
1	D	1103	GLN
1	D	1110	ASN
1	D	1140	ASN
1	D	1243	GLN
1	D	1257	ASN
1	D	1298	HIS
1	D	1359	GLN
1	D	1368	GLN
1	D	1382	HIS
1	D	1416	GLN
1	D	1437	ASN
1	D	1490	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 56 ligands modelled in this entry, 37 are monoatomic - leaving 19 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	NLG	A	2010	-	12,12,12	0.92	0	15,15,15	1.75	3 (20%)
9	GOL	A	2015	-	5,5,5	0.92	0	5,5,5	0.87	0
6	ADP	D	2008	3	28,29,29	1.72	6 (21%)	43,45,45	1.83	11 (25%)
6	ADP	A	2008	3	28,29,29	1.39	5 (17%)	43,45,45	2.05	14 (32%)
5	PO4	A	2007	4,3	4,4,4	1.16	0	6,6,6	1.01	0
6	ADP	D	2009	3	28,29,29	1.54	5 (17%)	43,45,45	1.88	7 (16%)
5	PO4	C	2007	4,3	4,4,4	0.95	0	6,6,6	0.89	0
7	NLG	D	2010	-	12,12,12	0.99	0	15,15,15	1.69	4 (26%)
6	ADP	B	2008	3	28,29,29	1.62	6 (21%)	43,45,45	1.74	9 (20%)
9	GOL	D	2015	-	5,5,5	0.73	0	5,5,5	0.95	0
6	ADP	A	2009	3	28,29,29	1.78	5 (17%)	43,45,45	1.78	7 (16%)
6	ADP	C	2008	3	28,29,29	1.37	5 (17%)	43,45,45	1.80	8 (18%)
10	EDO	A	2016	-	3,3,3	0.45	0	2,2,2	0.35	0
5	PO4	D	2007	4,3	4,4,4	1.17	0	6,6,6	1.11	0
6	ADP	B	2009	3	28,29,29	1.60	6 (21%)	43,45,45	1.95	8 (18%)
5	PO4	B	2007	4,3	4,4,4	1.02	0	6,6,6	0.81	0
7	NLG	B	2010	-	12,12,12	0.89	0	15,15,15	0.90	0
6	ADP	C	2009	3	28,29,29	1.64	5 (17%)	43,45,45	2.00	11 (25%)
7	NLG	C	2010	-	12,12,12	0.89	0	15,15,15	1.07	1 (6%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ADP	D	2009	3	-	5/16/32/32	0/3/3/3
6	ADP	B	2009	3	-	3/16/32/32	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	NLG	D	2010	-	-	2/13/13/13	-
6	ADP	A	2008	3	-	2/16/32/32	0/3/3/3
6	ADP	B	2008	3	-	1/16/32/32	0/3/3/3
7	NLG	C	2010	-	-	0/13/13/13	-
9	GOL	D	2015	-	-	4/4/4/4	-
6	ADP	A	2009	3	-	3/16/32/32	0/3/3/3
7	NLG	A	2010	-	-	4/13/13/13	-
7	NLG	B	2010	-	-	0/13/13/13	-
6	ADP	D	2008	3	-	3/16/32/32	0/3/3/3
6	ADP	C	2009	3	-	3/16/32/32	0/3/3/3
9	GOL	A	2015	-	-	4/4/4/4	-
6	ADP	C	2008	3	-	1/16/32/32	0/3/3/3
10	EDO	A	2016	-	-	1/1/1/1	-

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2009	ADP	PA-O3A	6.20	1.66	1.59
6	D	2009	ADP	C5-C4	5.19	1.48	1.39
6	B	2008	ADP	C5-C4	5.01	1.48	1.39
6	C	2009	ADP	C5-C4	4.71	1.47	1.39
6	A	2009	ADP	C5-C4	4.66	1.47	1.39
6	B	2009	ADP	C5-C4	4.52	1.47	1.39
6	C	2008	ADP	C5-C4	4.35	1.46	1.39
6	B	2009	ADP	PA-O3A	4.25	1.64	1.59
6	D	2008	ADP	C5-C4	3.88	1.46	1.39
6	D	2008	ADP	PA-O3A	3.88	1.63	1.59
6	C	2009	ADP	PA-O3A	3.48	1.63	1.59
6	B	2008	ADP	C5-N7	-3.13	1.33	1.39
6	D	2009	ADP	PA-O3A	3.11	1.62	1.59
6	A	2008	ADP	C2-N1	3.02	1.39	1.33
6	A	2008	ADP	C5-N7	-3.02	1.33	1.39
6	C	2009	ADP	C5-N7	-2.87	1.33	1.39
6	C	2009	ADP	C5-C6	2.86	1.48	1.41
6	D	2008	ADP	C5-N7	-2.84	1.33	1.39
6	A	2008	ADP	C5-C4	2.78	1.44	1.39
6	A	2009	ADP	C8-N7	2.74	1.36	1.31
6	D	2008	ADP	O4'-C4'	-2.73	1.38	1.45
6	C	2008	ADP	C8-N7	2.64	1.36	1.31
6	D	2009	ADP	C5-N7	-2.63	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	2008	ADP	C5-N7	-2.62	1.34	1.39
6	B	2009	ADP	C5-C6	2.61	1.48	1.41
6	B	2008	ADP	PA-O3A	2.61	1.62	1.59
6	D	2009	ADP	C5-C6	2.58	1.48	1.41
6	D	2009	ADP	C8-N7	2.55	1.36	1.31
6	A	2009	ADP	C5-N7	-2.54	1.34	1.39
6	B	2008	ADP	C4-N9	-2.43	1.32	1.37
6	D	2008	ADP	C2-N1	2.38	1.38	1.33
6	B	2009	ADP	C4-N9	-2.38	1.32	1.37
6	B	2009	ADP	C5-N7	-2.34	1.34	1.39
6	A	2008	ADP	O4'-C4'	-2.33	1.39	1.45
6	B	2008	ADP	C5-C6	2.23	1.47	1.41
6	B	2009	ADP	C8-N7	2.22	1.35	1.31
6	A	2009	ADP	C5-C6	2.18	1.47	1.41
6	C	2009	ADP	C8-N7	2.15	1.35	1.31
6	A	2008	ADP	C8-N7	2.09	1.35	1.31
6	C	2008	ADP	C4-N9	-2.08	1.33	1.37
6	C	2008	ADP	C5-C6	2.08	1.46	1.41
6	D	2008	ADP	C4-N9	-2.07	1.33	1.37
6	B	2008	ADP	C8-N7	2.02	1.35	1.31

All (83) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	2009	ADP	C5-C4-N3	-6.57	117.67	126.72
6	D	2009	ADP	C5-C4-N3	-6.52	117.74	126.72
6	C	2009	ADP	C5-C4-N3	-6.38	117.94	126.72
6	A	2009	ADP	C5-C4-N3	-6.03	118.42	126.72
6	A	2008	ADP	C5-C4-N3	-5.63	118.96	126.72
6	C	2009	ADP	N3-C4-N9	5.50	136.53	127.17
6	B	2009	ADP	N3-C4-N9	5.06	135.77	127.17
6	D	2008	ADP	N3-C4-N9	5.04	135.74	127.17
6	C	2008	ADP	C5-C4-N3	-4.97	119.87	126.72
6	D	2008	ADP	C5-C4-N3	-4.96	119.88	126.72
6	D	2009	ADP	N3-C4-N9	4.93	135.56	127.17
6	B	2008	ADP	C5-C4-N3	-4.93	119.93	126.72
6	A	2008	ADP	N3-C4-N9	4.73	135.21	127.17
6	B	2008	ADP	N3-C4-N9	4.72	135.20	127.17
6	A	2009	ADP	N3-C4-N9	4.65	135.07	127.17
6	C	2008	ADP	N3-C2-N1	-4.31	122.06	128.58
6	B	2009	ADP	C2-N3-C4	4.09	121.81	111.83
6	C	2008	ADP	C2-N3-C4	3.83	121.17	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	2009	ADP	C2-N3-C4	3.79	121.08	111.83
6	C	2009	ADP	C2-N3-C4	3.76	121.02	111.83
6	B	2008	ADP	N3-C2-N1	-3.76	122.89	128.58
6	A	2008	ADP	N9-C8-N7	-3.76	108.61	113.94
6	C	2008	ADP	N3-C4-N9	3.74	133.53	127.17
6	D	2009	ADP	C2-N3-C4	3.71	120.88	111.83
6	D	2009	ADP	C4-C5-N7	-3.66	106.40	110.58
6	D	2008	ADP	C5-C6-N6	-3.65	114.25	123.29
6	A	2008	ADP	C5-N7-C8	3.60	109.11	103.45
7	A	2010	NLG	C-CA-N2	3.55	118.81	110.57
7	A	2010	NLG	CB-CA-C	-3.46	102.14	110.35
6	A	2009	ADP	N3-C2-N1	-3.45	123.37	128.58
6	A	2008	ADP	C2-N3-C4	3.42	120.18	111.83
6	B	2008	ADP	C2-N3-C4	3.38	120.08	111.83
6	A	2008	ADP	C4-N9-C8	3.35	109.26	105.74
6	C	2009	ADP	C4-C5-N7	-3.32	106.78	110.58
6	B	2009	ADP	C4-C5-N7	-3.26	106.86	110.58
6	C	2009	ADP	C4-N9-C8	3.15	109.04	105.74
6	B	2009	ADP	N3-C2-N1	-3.11	123.87	128.58
7	D	2010	NLG	CB-CA-C	-3.11	102.98	110.35
6	D	2008	ADP	O2A-PA-O3A	3.08	115.61	107.27
6	D	2009	ADP	C5-N7-C8	3.07	108.27	103.45
6	B	2008	ADP	C4-N9-C8	3.01	108.90	105.74
6	D	2008	ADP	N3-C2-N1	-2.99	124.06	128.58
6	C	2009	ADP	N3-C2-N1	-2.98	124.07	128.58
6	D	2009	ADP	N3-C2-N1	-2.96	124.10	128.58
6	A	2008	ADP	C4-C5-N7	-2.96	107.20	110.58
6	C	2009	ADP	C5-N7-C8	2.86	107.94	103.45
6	A	2009	ADP	C4-C5-N7	-2.82	107.35	110.58
6	D	2008	ADP	C2-N3-C4	2.80	118.66	111.83
7	A	2010	NLG	OE1-CD-CG	-2.68	114.59	123.09
7	D	2010	NLG	OE2-CD-CG	2.66	122.41	114.00
6	B	2008	ADP	N6-C6-N1	2.65	124.27	118.38
6	D	2008	ADP	O3B-PB-O2B	2.53	117.28	107.80
6	A	2008	ADP	N3-C2-N1	-2.51	124.79	128.58
6	A	2008	ADP	O5'-PA-O1A	-2.47	99.15	108.94
6	D	2008	ADP	O3A-PA-O1A	-2.47	103.28	110.70
6	D	2008	ADP	O3A-PB-O1B	-2.47	98.06	111.04
6	A	2008	ADP	O3B-PB-O1B	2.46	120.43	110.83
6	C	2009	ADP	N6-C6-N1	2.46	123.86	118.38
6	C	2008	ADP	C4-C5-N7	-2.44	107.79	110.58
6	B	2009	ADP	C4-N9-C8	2.42	108.28	105.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	2010	NLG	O7-C7-C8	-2.41	117.77	122.05
6	A	2008	ADP	C5-C6-N6	-2.35	117.47	123.29
6	D	2008	ADP	N6-C6-N1	2.34	123.58	118.38
6	A	2008	ADP	O2A-PA-O1A	2.32	123.25	112.44
6	C	2009	ADP	N9-C8-N7	-2.30	110.68	113.94
6	A	2009	ADP	O2A-PA-O3A	2.27	113.42	107.27
6	C	2008	ADP	C6-C5-N7	2.22	136.38	132.09
6	A	2009	ADP	C5-N7-C8	2.22	106.94	103.45
6	C	2009	ADP	O3B-PB-O1B	2.22	119.47	110.83
6	C	2008	ADP	C2-N1-C6	2.22	122.37	118.73
6	C	2008	ADP	O2A-PA-O1A	2.21	122.72	112.44
6	B	2009	ADP	C5-N7-C8	2.20	106.91	103.45
6	A	2008	ADP	O2A-PA-O3A	2.18	113.16	107.27
6	B	2009	ADP	O2A-PA-O3A	2.17	113.12	107.27
7	D	2010	NLG	OE1-CD-CG	-2.16	116.25	123.09
6	D	2008	ADP	O3B-PB-O1B	2.12	119.11	110.83
6	A	2008	ADP	O3A-PB-O1B	-2.11	99.93	111.04
6	B	2008	ADP	C2-N1-C6	2.11	122.19	118.73
7	C	2010	NLG	OXT-C-CA	2.10	120.63	113.51
6	B	2008	ADP	O3B-PB-O2B	2.08	115.60	107.80
6	B	2008	ADP	C5-C6-N6	-2.08	118.14	123.29
6	C	2009	ADP	O2A-PA-O3A	2.05	112.81	107.27
6	D	2009	ADP	N9-C8-N7	-2.02	111.07	113.94

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	2009	ADP	PA-O3A-PB-O3B
6	B	2009	ADP	PA-O3A-PB-O3B
6	C	2009	ADP	C5'-O5'-PA-O1A
6	C	2009	ADP	C5'-O5'-PA-O2A
6	C	2009	ADP	C5'-O5'-PA-O3A
6	D	2008	ADP	PA-O3A-PB-O3B
6	D	2009	ADP	PA-O3A-PB-O3B
9	A	2015	GOL	O1-C1-C2-C3
9	D	2015	GOL	O1-C1-C2-C3
9	D	2015	GOL	C1-C2-C3-O3
7	A	2010	NLG	N2-CA-CB-CG
7	A	2010	NLG	C-CA-CB-CG
9	A	2015	GOL	C1-C2-C3-O3
9	A	2015	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
9	D	2015	GOL	O1-C1-C2-O2
9	D	2015	GOL	O2-C2-C3-O3
10	A	2016	EDO	O1-C1-C2-O2
6	D	2008	ADP	PA-O3A-PB-O2B
6	A	2008	ADP	PB-O3A-PA-O1A
6	A	2008	ADP	PB-O3A-PA-O2A
9	A	2015	GOL	O1-C1-C2-O2
7	A	2010	NLG	OE2-CD-CG-CB
6	A	2009	ADP	PA-O3A-PB-O1B
7	A	2010	NLG	OE1-CD-CG-CB
6	B	2009	ADP	PB-O3A-PA-O2A
6	C	2008	ADP	PB-O3A-PA-O2A
6	D	2008	ADP	PB-O3A-PA-O1A
6	D	2009	ADP	PB-O3A-PA-O1A
6	D	2009	ADP	PA-O3A-PB-O2B
6	A	2009	ADP	PB-O3A-PA-O1A
6	B	2008	ADP	PB-O3A-PA-O1A
6	D	2009	ADP	PB-O3A-PA-O2A
7	D	2010	NLG	OE1-CD-CG-CB
7	D	2010	NLG	OE2-CD-CG-CB
6	B	2009	ADP	PA-O3A-PB-O1B
6	D	2009	ADP	PA-O3A-PB-O1B

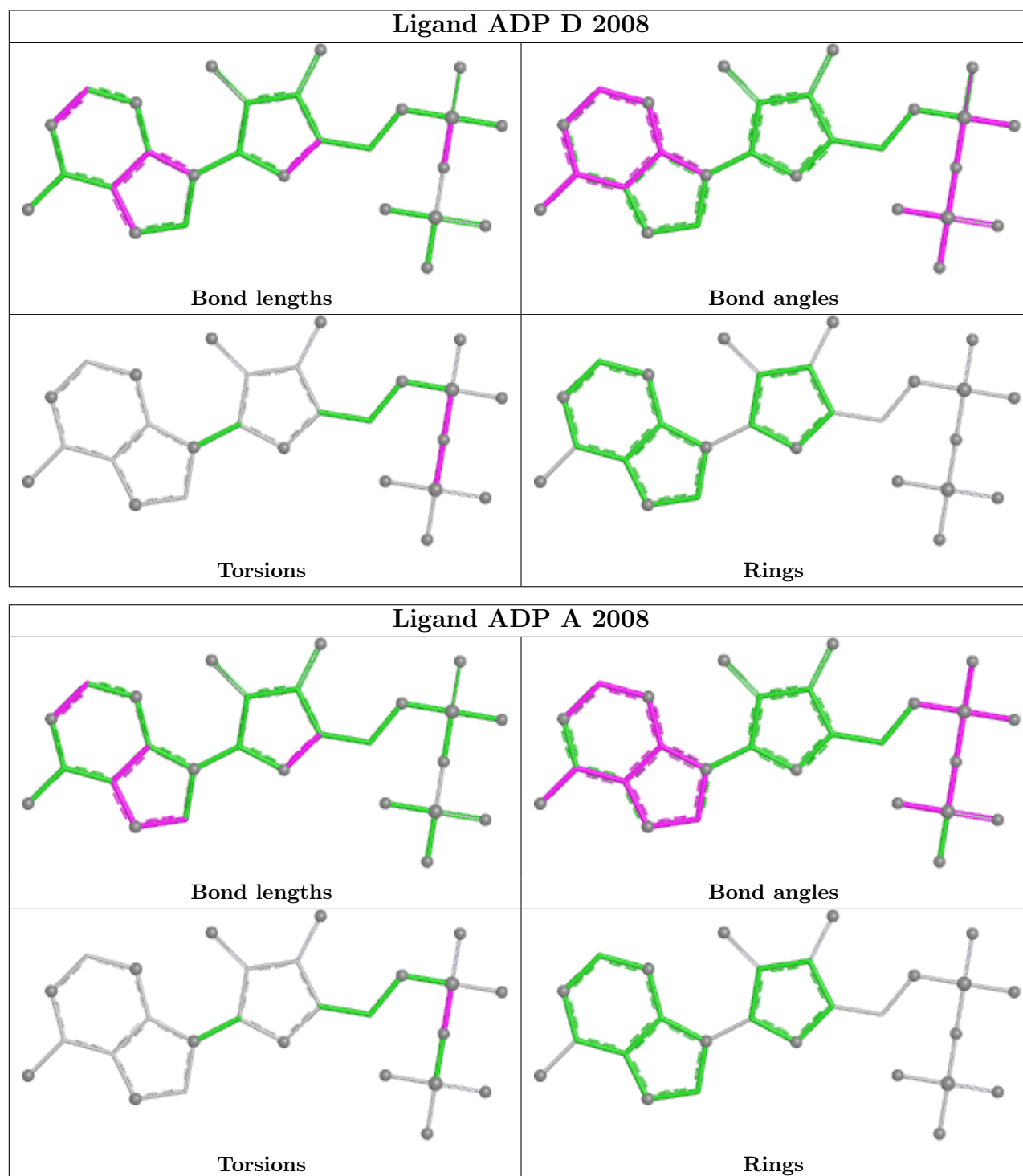
There are no ring outliers.

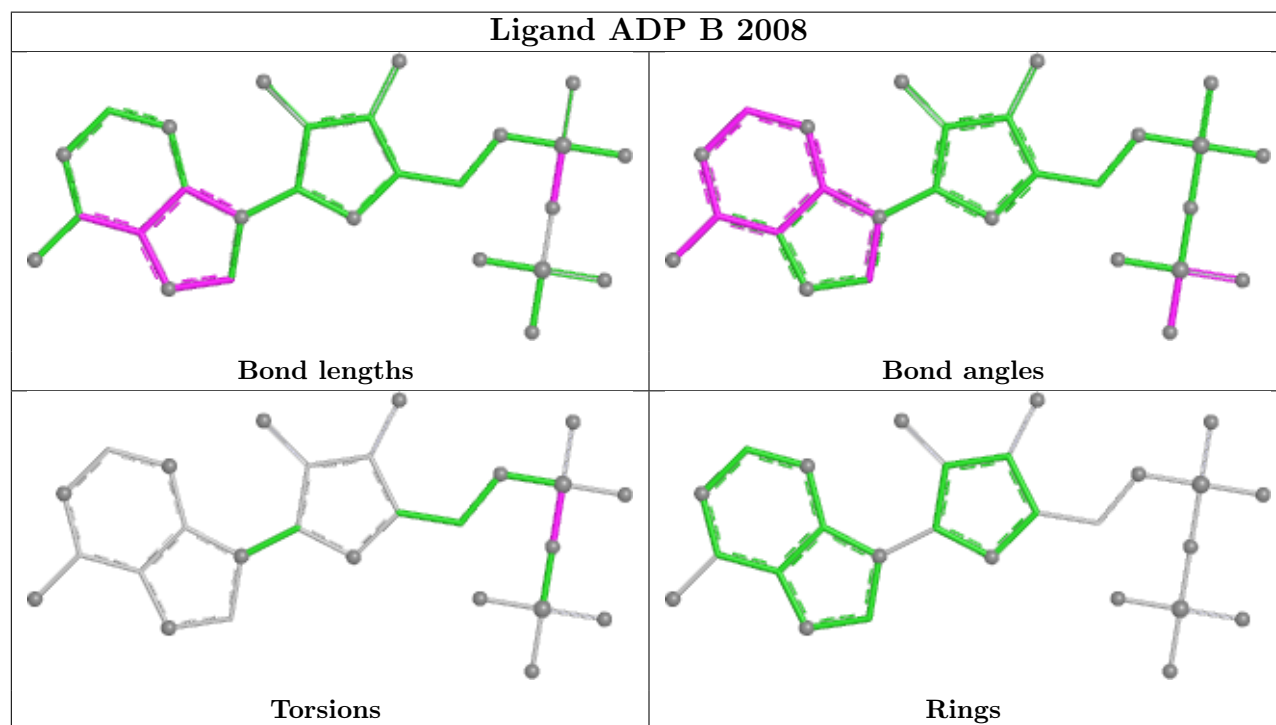
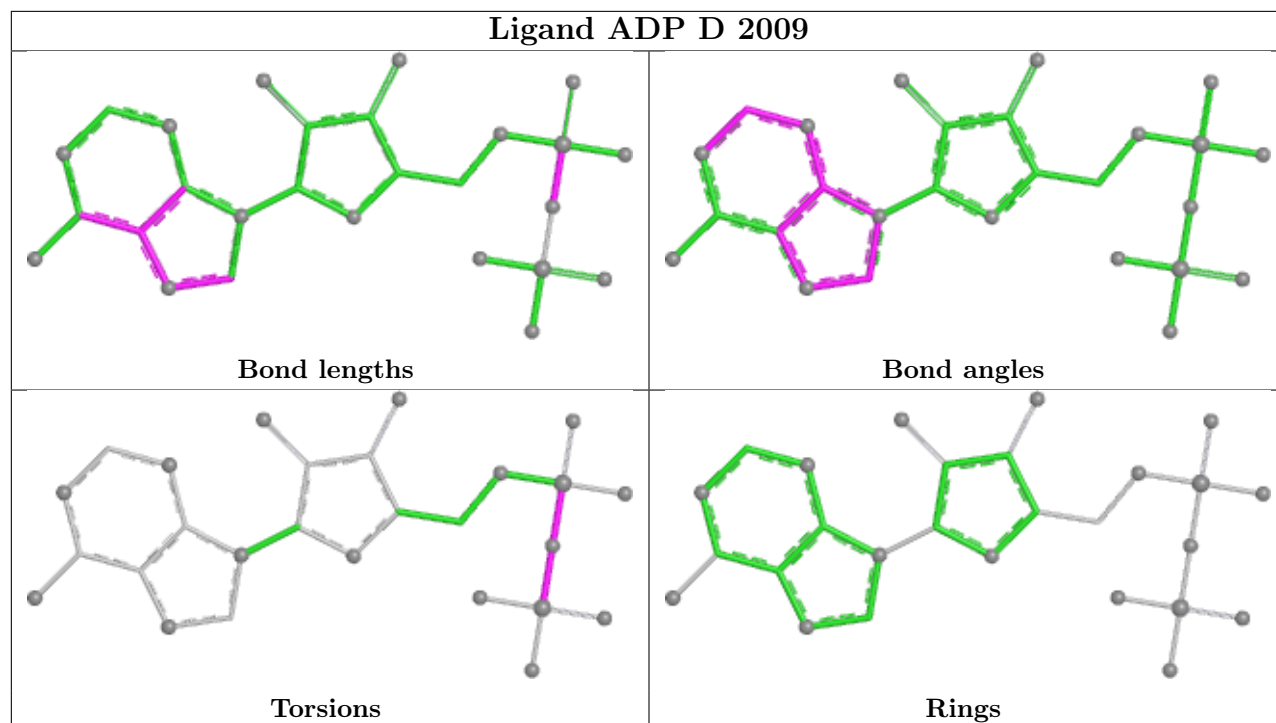
8 monomers are involved in 10 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	2008	ADP	1	0
6	A	2008	ADP	2	0
5	A	2007	PO4	1	0
6	D	2009	ADP	1	0
5	C	2007	PO4	1	0
7	D	2010	NLG	1	0
9	D	2015	GOL	1	0
10	A	2016	EDO	2	0

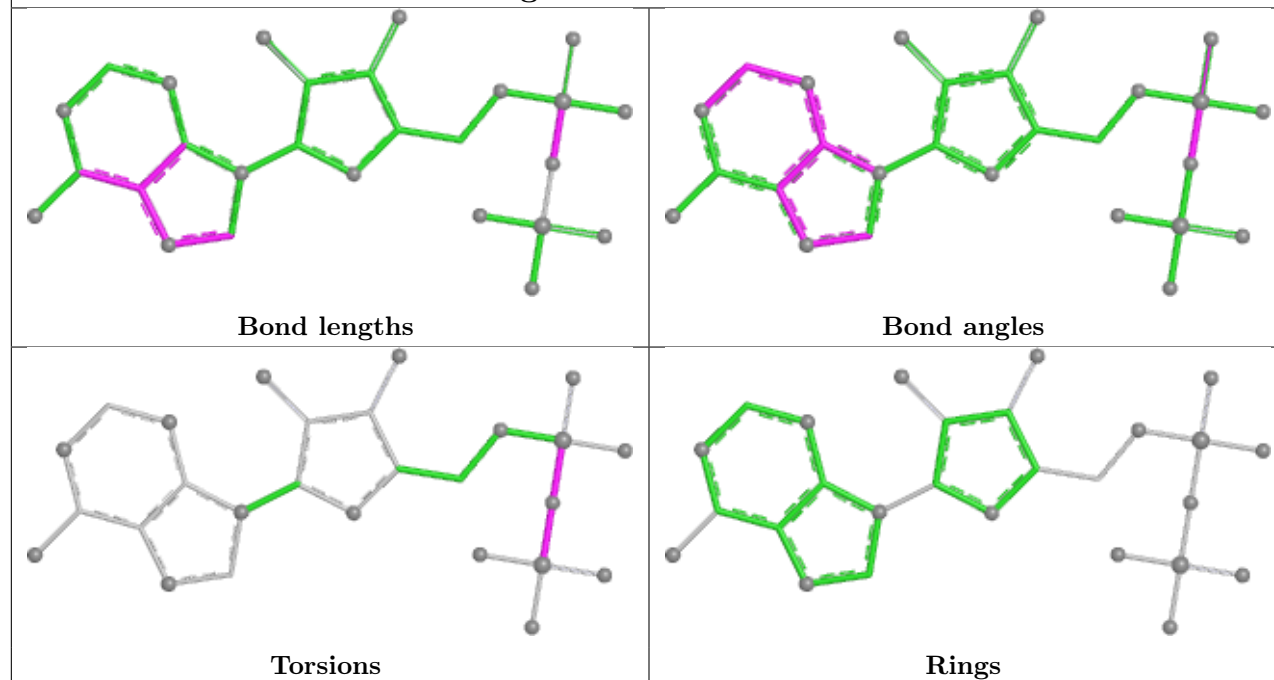
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

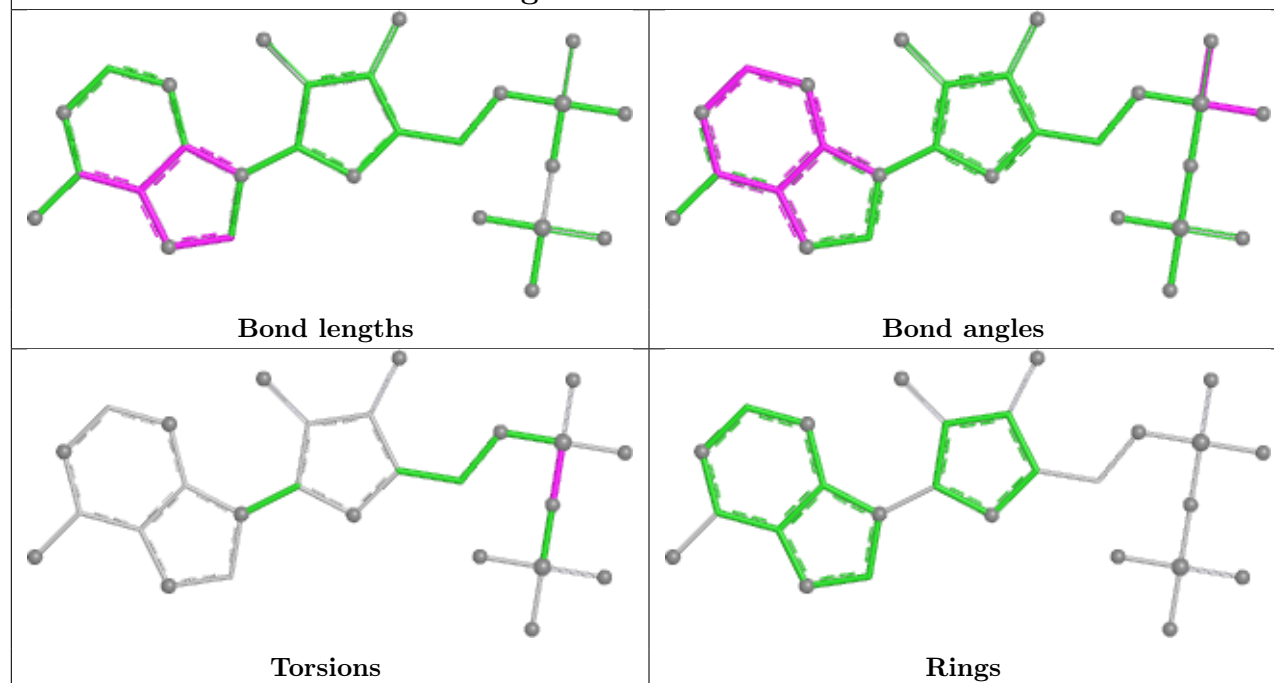


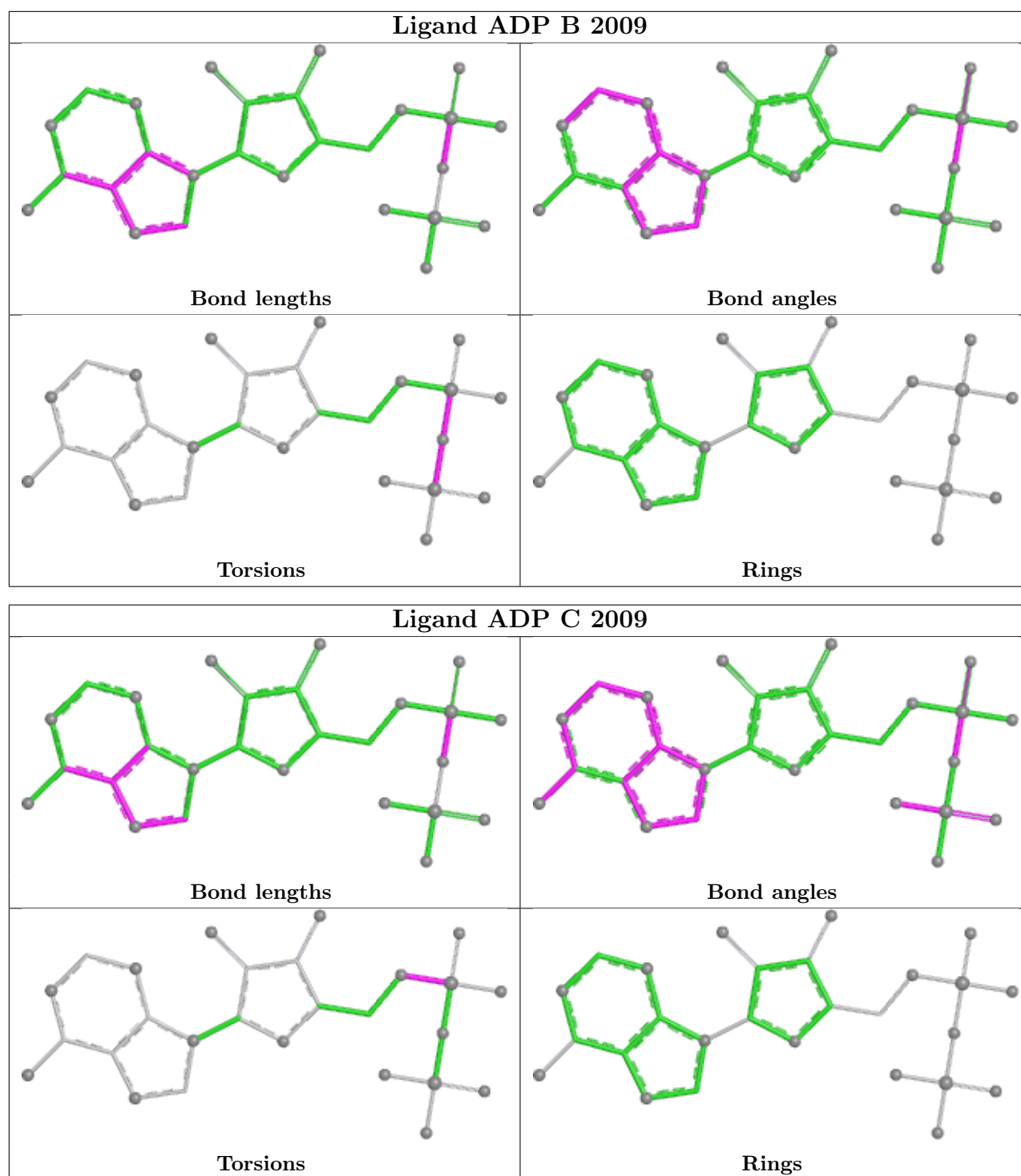


Ligand ADP A 2009



Ligand ADP C 2008





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(Å²)	Q<0.9	
1	A	1422/1489 (95%)	-1.70	0	100	100	12, 24, 47, 94	5 (0%)
1	B	1426/1489 (95%)	-1.30	0	100	100	15, 55, 87, 116	3 (0%)
1	C	1421/1489 (95%)	-0.81	17 (1%)	76	73	15, 64, 144, 172	4 (0%)
1	D	1430/1489 (96%)	-1.70	0	100	100	12, 24, 48, 113	4 (0%)
All	All	5699/5956 (95%)	-1.38	17 (0%)	90	88	12, 34, 111, 172	16 (0%)

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	221	VAL	3.9
1	C	183	ILE	3.7
1	C	301	GLY	2.8
1	C	245	VAL	2.7
1	C	278	VAL	2.7
1	C	265	PRO	2.7
1	C	212	TYR	2.6
1	C	161	ILE	2.6
1	C	256	TYR	2.5
1	C	300	THR	2.4
1	C	374	VAL	2.2
1	C	261	ILE	2.2
1	C	293	ILE	2.2
1	C	223	VAL	2.1
1	C	152	TRP	2.1
1	C	195	PRO	2.1
1	C	296	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 ⓘ

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($\text{\AA}^2$)	Q<0.9
2	NI	B	2001	1/1	0.99	0.03	75,75,75,75	0
2	NI	C	2001	1/1	0.99	0.05	56,56,56,56	0
3	MG	A	2011	1/1	0.99	0.02	41,41,41,41	0
3	MG	C	2011	1/1	0.99	0.01	41,41,41,41	0
3	MG	D	2011	1/1	0.99	0.02	34,34,34,34	0
4	K	A	2013	1/1	0.99	0.02	32,32,32,32	0
4	K	B	2004	1/1	0.99	0.03	39,39,39,39	0
4	K	B	2005	1/1	0.99	0.02	42,42,42,42	0
4	K	B	2013	1/1	0.99	0.06	61,61,61,61	0
4	K	C	2004	1/1	0.99	0.04	44,44,44,44	0
4	K	C	2006	1/1	0.99	0.03	78,78,78,78	0
4	K	C	2012	1/1	0.99	0.06	75,75,75,75	0
4	K	D	2005	1/1	0.99	0.03	30,30,30,30	0
4	K	D	2013	1/1	0.99	0.03	18,18,18,18	0
6	ADP	A	2009	27/27	0.99	0.02	28,31,46,47	0
6	ADP	C	2009	27/27	0.99	0.03	28,31,37,38	0
7	NLG	A	2010	13/13	0.99	0.03	17,18,19,21	0
7	NLG	C	2010	13/13	0.99	0.03	18,22,25,26	0
8	CL	D	2012	1/1	0.99	0.02	26,26,26,26	0
9	GOL	A	2015	6/6	0.99	0.04	26,29,29,29	0
9	GOL	D	2015	6/6	0.99	0.03	30,34,37,38	0
10	EDO	A	2016	4/4	0.99	0.04	39,40,40,41	0
3	MG	B	2002	1/1	1.00	0.02	21,21,21,21	0
4	K	B	2006	1/1	1.00	0.04	65,65,65,65	0
3	MG	B	2003	1/1	1.00	0.01	35,35,35,35	0
3	MG	B	2011	1/1	1.00	0.02	15,15,15,15	0
4	K	C	2005	1/1	1.00	0.07	45,45,45,45	0
3	MG	C	2002	1/1	1.00	0.02	20,20,20,20	0
3	MG	C	2003	1/1	1.00	0.01	20,20,20,20	0
4	K	D	2004	1/1	1.00	0.01	8,8,8,8	0
2	NI	D	2001	1/1	1.00	0.01	34,34,34,34	0
4	K	D	2006	1/1	1.00	0.03	53,53,53,53	0

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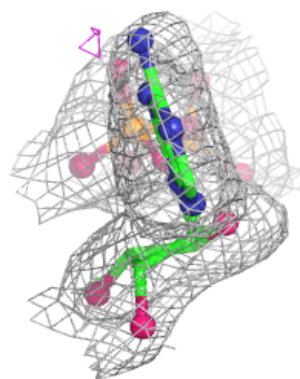
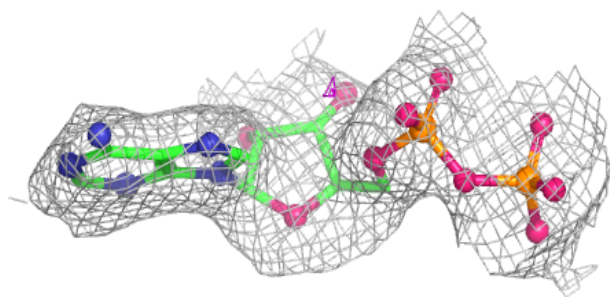
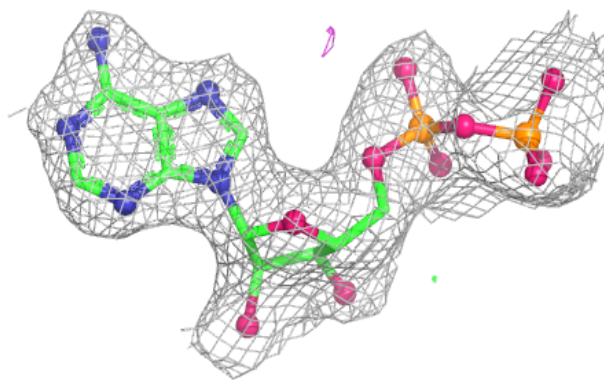
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	MG	D	2002	1/1	1.00	0.02	13,13,13,13	0
4	K	D	2014	1/1	1.00	0.01	37,37,37,37	0
5	PO4	A	2007	5/5	1.00	0.02	11,12,12,13	0
5	PO4	B	2007	5/5	1.00	0.02	26,26,29,29	0
5	PO4	C	2007	5/5	1.00	0.01	32,34,34,35	0
5	PO4	D	2007	5/5	1.00	0.01	11,11,13,14	0
6	ADP	A	2008	27/27	1.00	0.02	7,8,11,12	0
3	MG	D	2003	1/1	1.00	0.01	13,13,13,13	0
6	ADP	B	2008	27/27	1.00	0.02	25,29,32,32	0
6	ADP	B	2009	27/27	1.00	0.02	24,28,35,37	0
6	ADP	C	2008	27/27	1.00	0.02	26,29,36,38	0
3	MG	A	2002	1/1	1.00	0.01	13,13,13,13	0
6	ADP	D	2008	27/27	1.00	0.02	7,7,10,10	0
6	ADP	D	2009	27/27	1.00	0.02	27,31,44,45	0
4	K	A	2004	1/1	1.00	0.02	9,9,9,9	0
7	NLG	B	2010	13/13	1.00	0.03	16,23,25,26	0
4	K	A	2005	1/1	1.00	0.05	31,31,31,31	0
7	NLG	D	2010	13/13	1.00	0.04	20,21,24,25	0
8	CL	A	2012	1/1	1.00	0.01	31,31,31,31	0
8	CL	B	2012	1/1	1.00	0.04	43,43,43,43	0
4	K	A	2006	1/1	1.00	0.04	46,46,46,46	0
3	MG	A	2003	1/1	1.00	0.02	9,9,9,9	0
4	K	A	2014	1/1	1.00	0.03	24,24,24,24	0
2	NI	A	2001	1/1	1.00	0.01	34,34,34,34	0

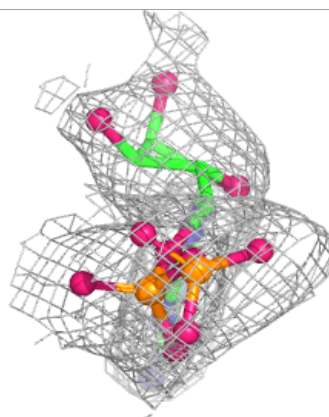
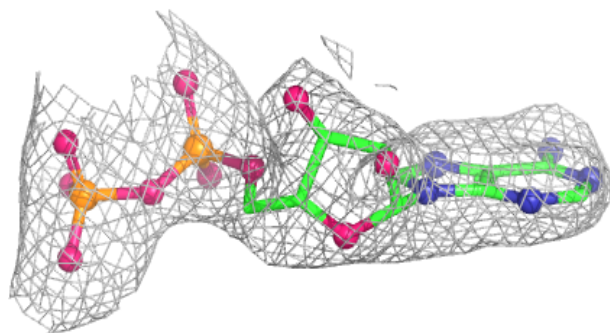
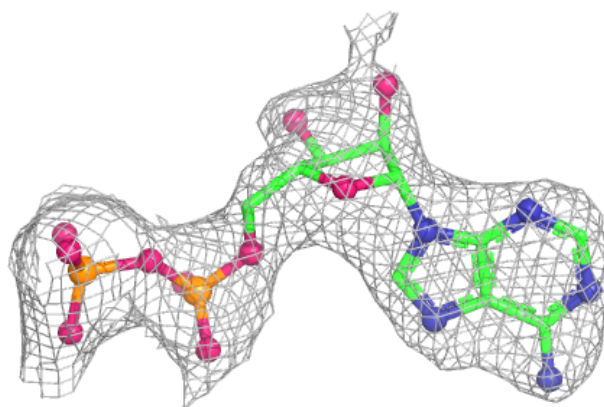
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP A 2009:

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

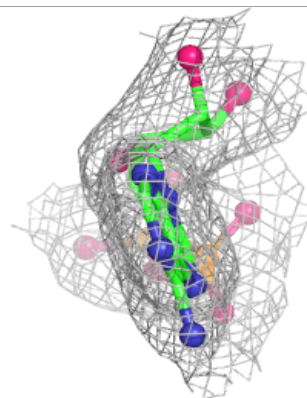
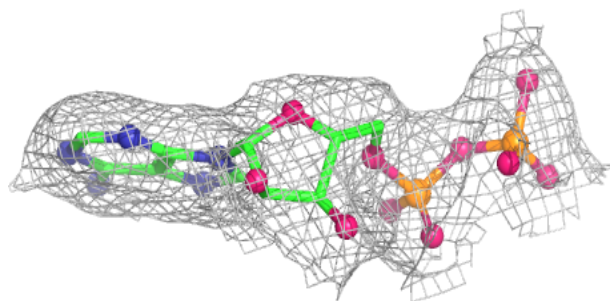
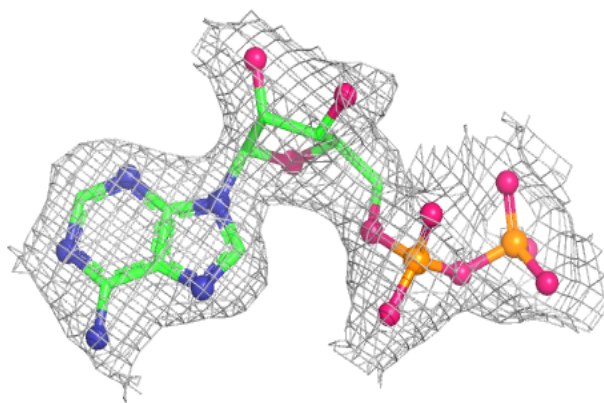
**Electron density around ADP C 2009:**

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

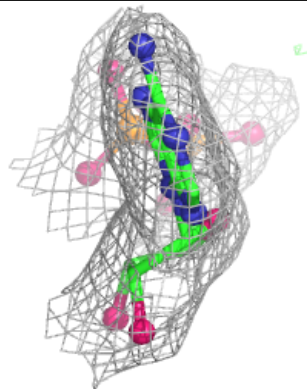
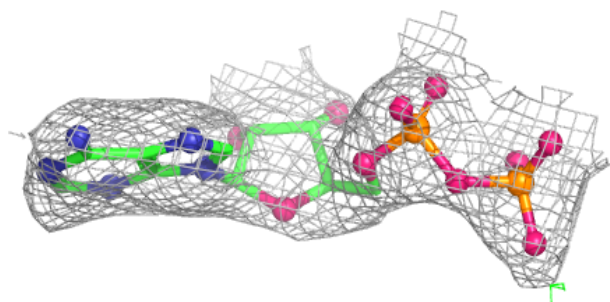
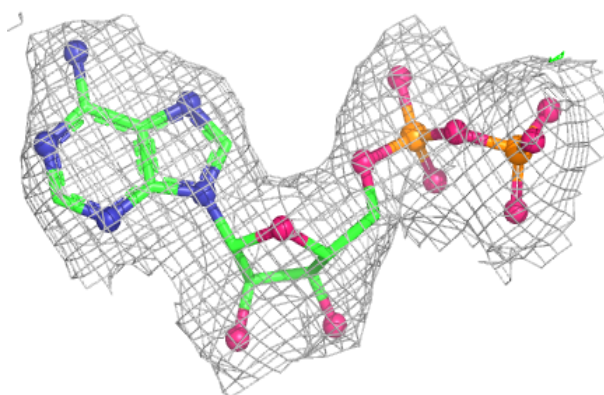


Electron density around ADP A 2008:

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

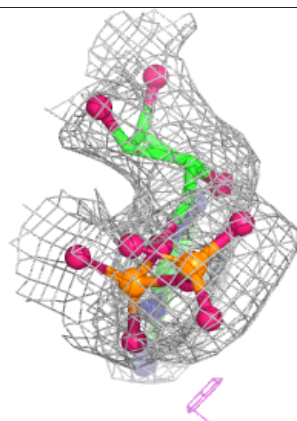
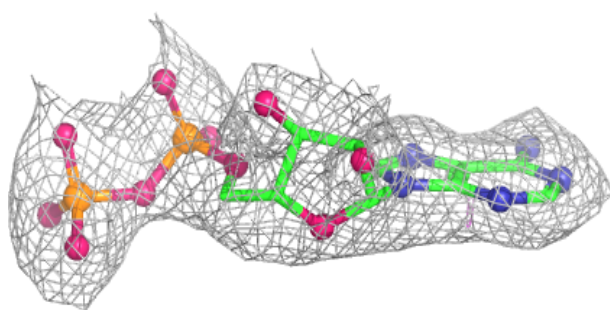
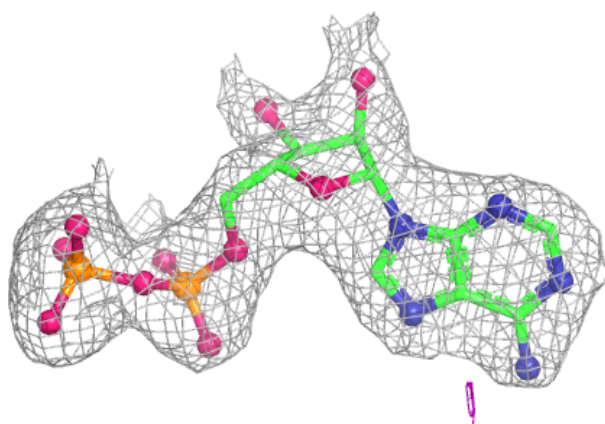
**Electron density around ADP B 2008:**

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and green (positive)

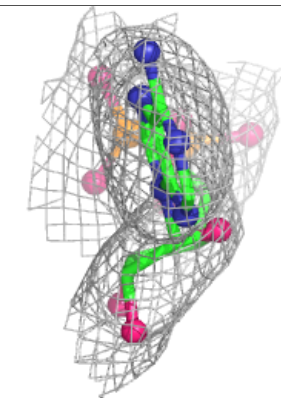
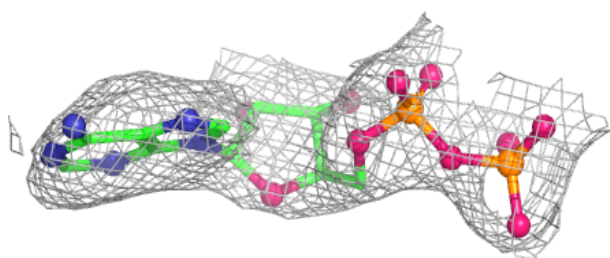
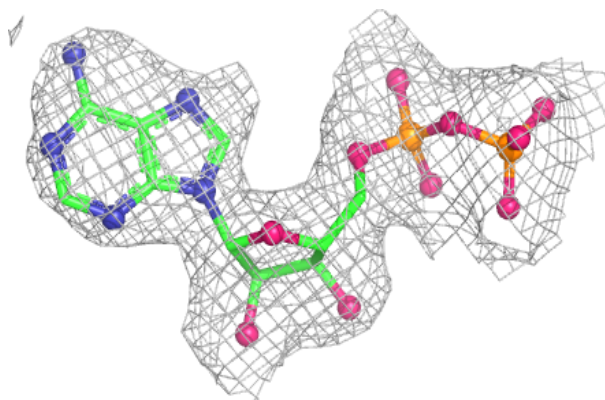


Electron density around ADP B 2009:

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

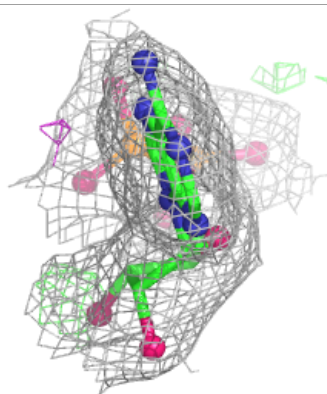
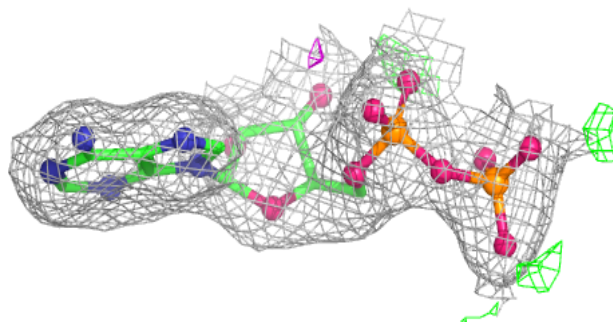
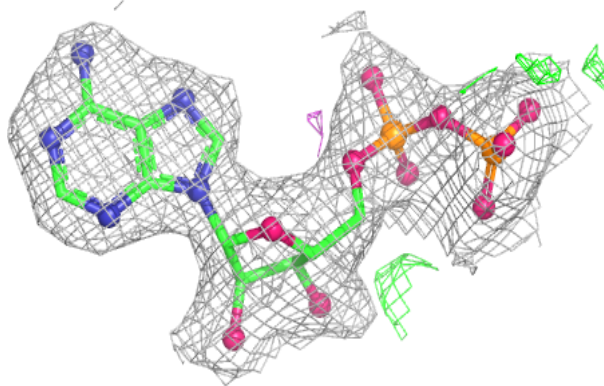
**Electron density around ADP C 2008:**

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

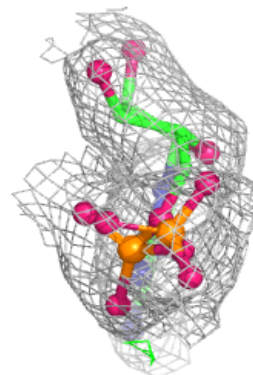
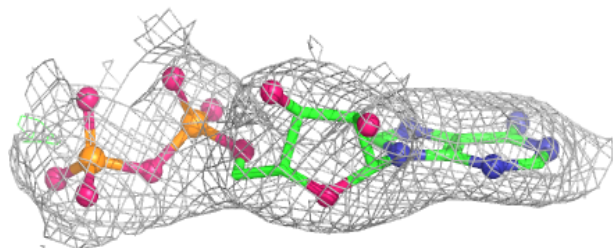
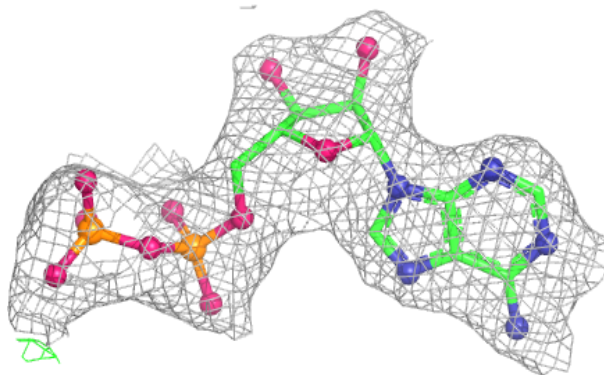


Electron density around ADP D 2008:

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

**Electron density around ADP D 2009:**

$2mF_o-DF_c$ (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.