WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Jan 4, 2024 – 06:13 am GMT

PDB ID	:	5DOU
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)

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

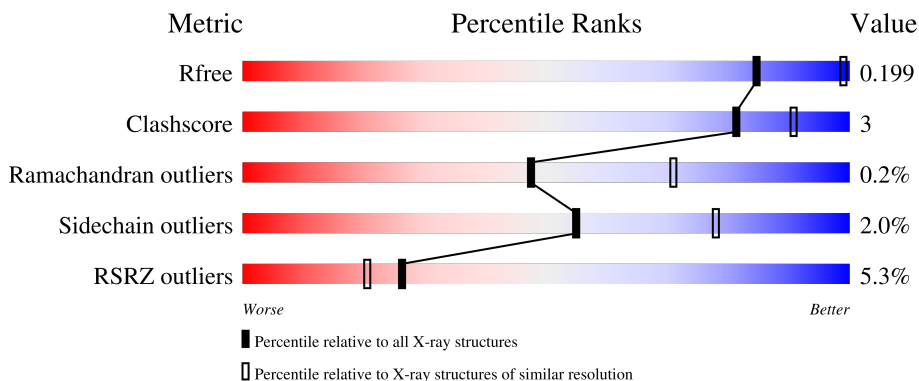|		
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

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	Percentile Ranks	Value
Rfree		0.199
Clashscore		3
Ramachandran outliers		0.2%
Sidechain outliers		2.0%
RSRZ outliers		5.3%

Worse ← → *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R$_{free}$	130704	3163 (2.60-2.60)
Clashscore	141614	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)
RSRZ outliers	127900	3104 (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 <=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	88% 7% •
1	B	1489	3% / 88% 8% •
1	C	1489	16% / 88% 7% 5%
1	D	1489	.% / 88% 8% •

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 (three-letter code: NI) (formula: Ni).

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

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 4 is POTASSIUM ION (three-letter code: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total 5	K 5	0	0
4	B	4	Total 4	K 4	0	0
4	C	4	Total 4	K 4	0	0

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

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).
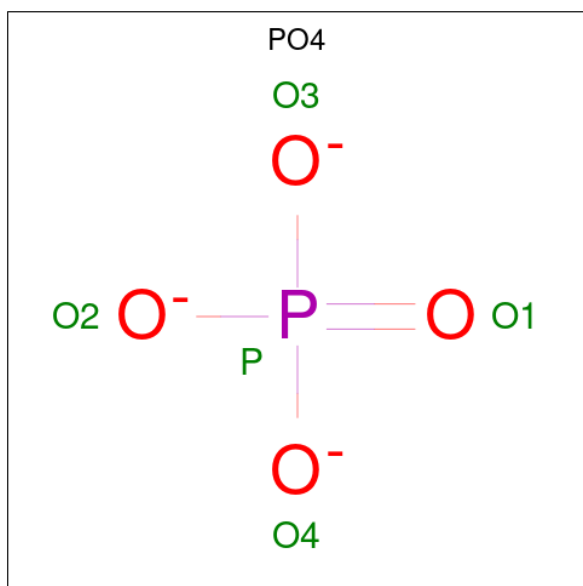
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total O P 5 4 1			0	0
5	B	1	Total O P 5 4 1			0	0
5	C	1	Total O P 5 4 1			0	0
5	D	1	Total O P 5 4 1			0	0

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

ADP
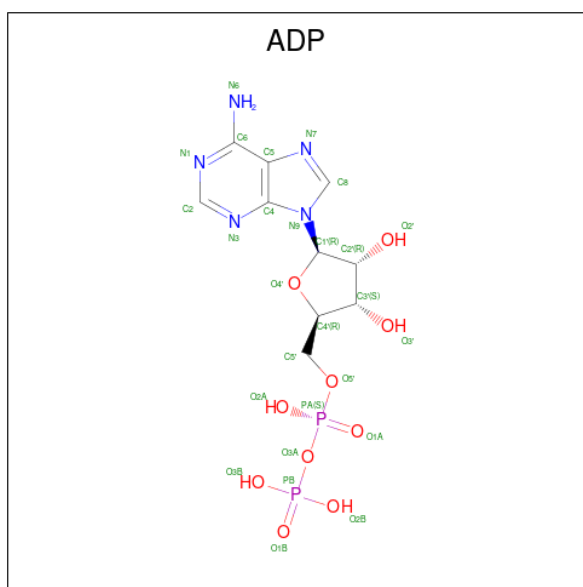
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
6	D	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 (three-letter code: NLG) (formula: $C_7H_{11}NO_5$).
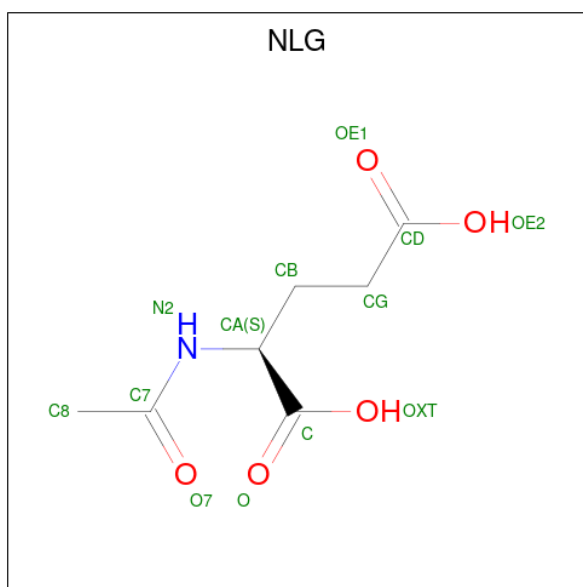
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total 13	C 7	N 1	O 5	0	0
7	B	1	Total 13	C 7	N 1	O 5	0	0
7	C	1	Total 13	C 7	N 1	O 5	0	0
7	D	1	Total 13	C 7	N 1	O 5	0	0

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL

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

- Molecule 10 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).

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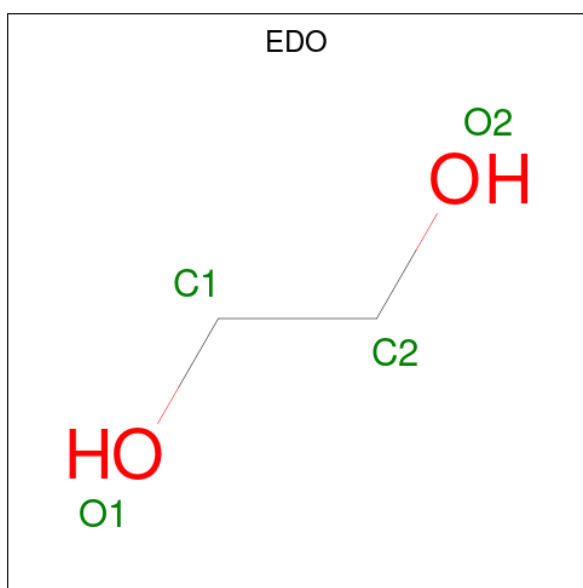
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total 4	C 2	O 2	0	0

- 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 ⓘ

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.

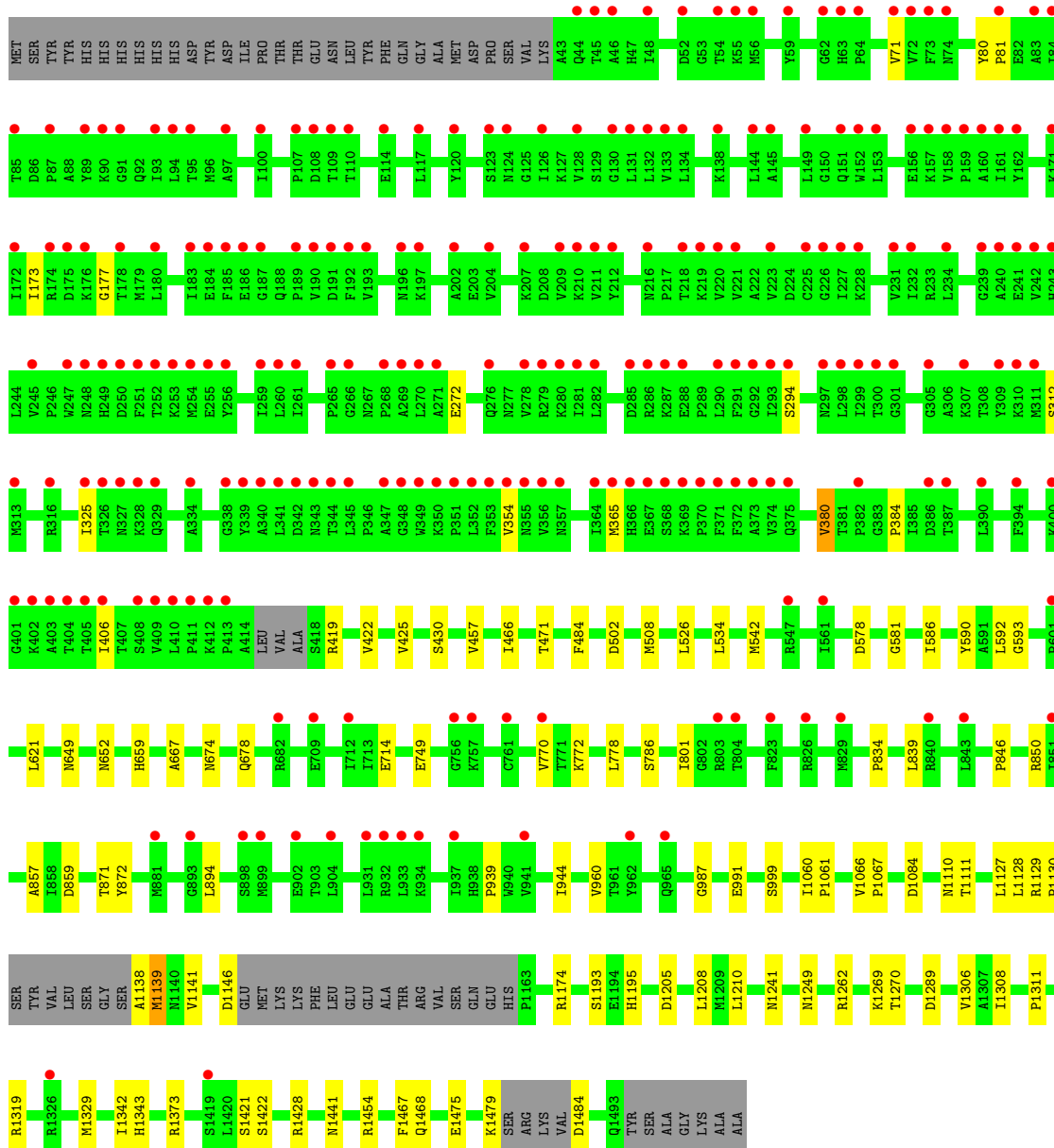- Molecule 1: Carbamoyl-phosphate synthase [ammonia], mitochondrial
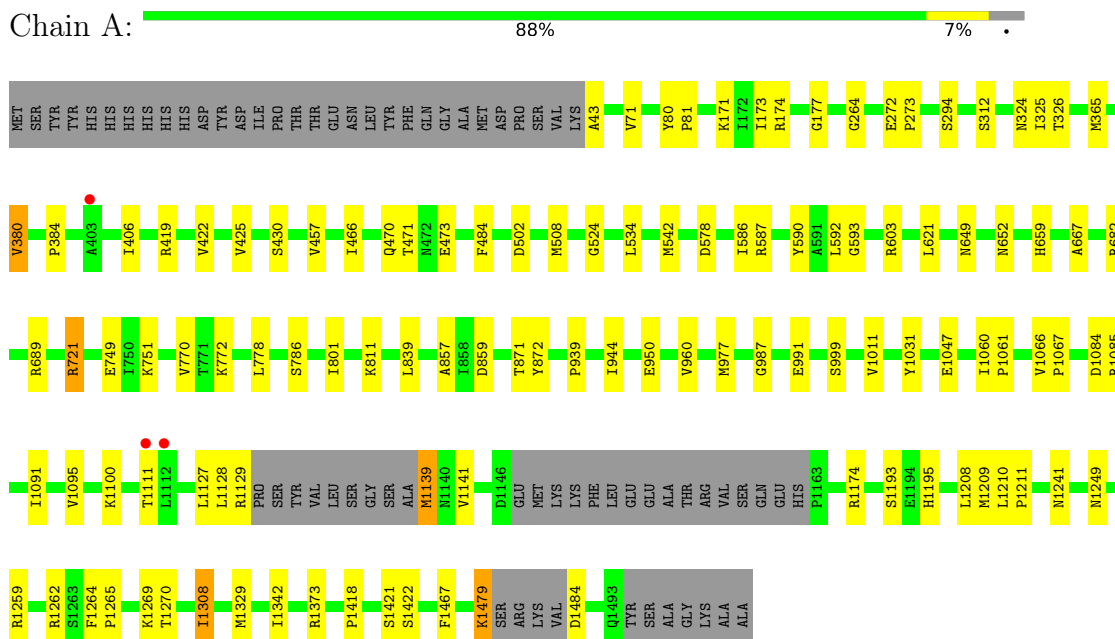
Chain A:
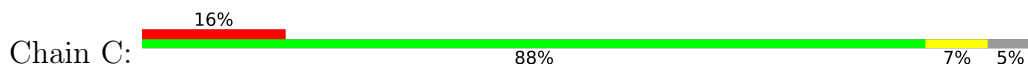

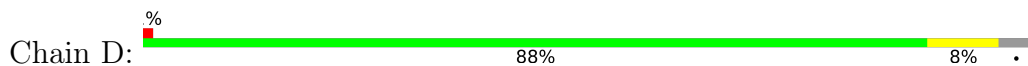- Molecule 1: Carbamoyl-phosphate synthase [ammonia], mitochondrial

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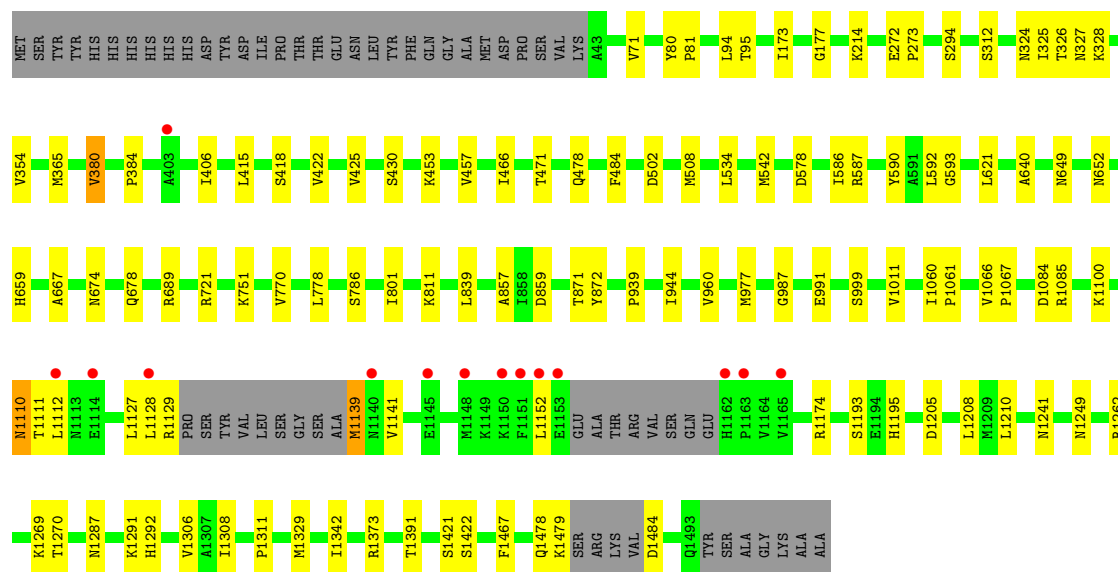
• Molecule 1: Carbamoyl-phosphate synthase [ammonia], mitochondrial

Chain C:

16%

88%   7%   5%

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

Chain D:

%

88%   8%   •
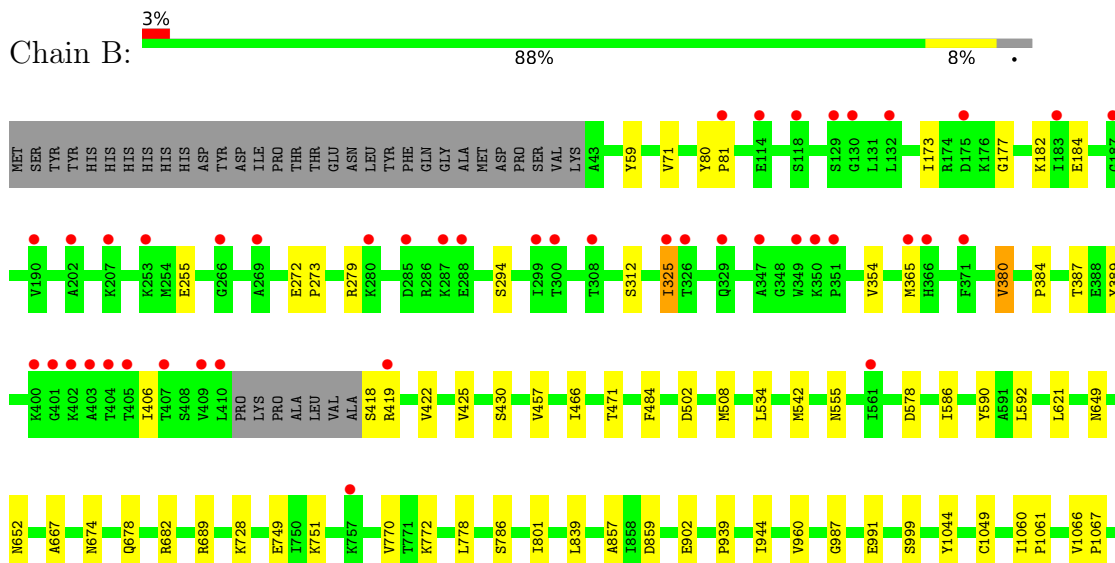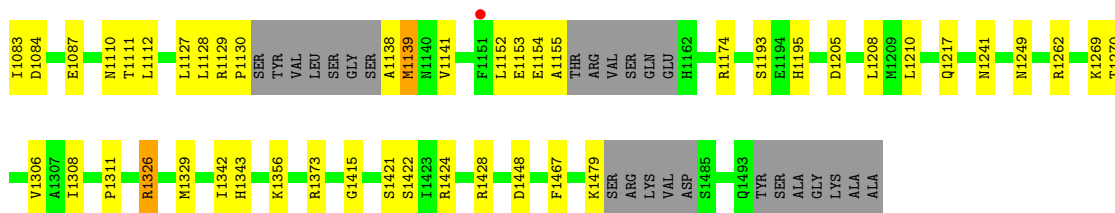
4 Data and refinement statistics ⓘ

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 39.98 – 2.60	Depositor EDS
% Data completeness (in resolution range)	90.7 (40.00-2.60) 87.6 (39.98-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.08	Depositor
$< I/\sigma(I) >$ [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	8964 reflections (5.02%)	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 , 14.2	EDS
L-test for twinning[2]	$< |L| > = 0.45, < L^2 > = 0.27$	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	0.93	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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.65	0/11210	0.71	6/15188 (0.0%)
1	B	0.51	0/11231	0.67	4/15213 (0.0%)
1	C	0.48	0/11191	0.66	4/15162 (0.0%)
1	D	0.64	0/11274	0.71	5/15273 (0.0%)
All	All	0.58	0/44906	0.69	19/60836 (0.0%)

There are no bond length outliers.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	1174	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	D	689	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	A	689	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	B	1428	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	A	1174	ARG	NE-CZ-NH2	-6.02	117.29	120.30
1	A	721	ARG	NE-CZ-NH2	6.02	123.31	120.30
1	D	721	ARG	NE-CZ-NH2	5.87	123.23	120.30
1	A	1085	ARG	NE-CZ-NH1	5.79	123.20	120.30
1	D	1174	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	B	1174	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	603	ARG	NE-CZ-NH2	5.65	123.13	120.30
1	B	1174	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	A	1174	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	C	1174	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	B	689	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	1319	ARG	NE-CZ-NH1	-5.38	117.61	120.30
1	D	1174	ARG	NE-CZ-NH1	5.24	122.92	120.30
1	D	1085	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	C	1454	ARG	NE-CZ-NH1	-5.02	117.79	120.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10991	0	11065	63	0
1	B	11018	0	11072	57	0
1	C	10975	0	11038	51	1
1	D	11056	0	11125	57	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
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

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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	227	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 (227) 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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:1475:GLU:OE1	11:C:2103:HOH:O	2.17	0.58
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:453:LYS:NZ	1:D:478:GLN:O	2.29	0.56
1:A:470:GLN:NE2	11:A:2108:HOH:O	2.33	0.56
1:D:471:THR:OG1	1:D:1269:LYS:NZ	2.40	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:B:592:LEU:C	1:B:592:LEU:HD12	2.28	0.54
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: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:D:592:LEU:C	1:D:592:LEU:HD12	2.29	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: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
1:B:471:THR:OG1	1:B:1269:LYS:NZ	2.42	0.51
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:A:592:LEU:HD12	1:A:592:LEU:C	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:592:LEU:HD12	1:C:592:LEU:C	2.33	0.48
1:A:425:VAL:HG23	1:A:457:VAL:CG1	2.44	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: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: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
1:D:425:VAL:HG23	1:D:457:VAL:HG11	1.96	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:D:272:GLU:O	1:D:273:PRO:C	2.53	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: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
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:D:1127:LEU:HD22	1:D:1139:MET:CE	2.48	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:987:GLY:HA2	1:C:1329:MET:CE	2.49	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:A:71:VAL:HG12	1:A:173:ILE:HD11	2.00	0.43
1:A:272:GLU:O	1:A:273:PRO:C	2.53	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: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:839:LEU:HD21	1:D:857:ALA:HA	2.01	0.42
1:D:1127:LEU:HD22	1:D:1139:MET:HE2	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: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
1:C:1210:LEU:HD23	1:C:1270:THR:HG21	2.02	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:1152:LEU:C	1:B:1154:GLU:N	2.73	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:1112:LEU:CD1	1:B:1152:LEU:HD12	2.51	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: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:272:GLU:O	1:B:273:PRO:C	2.59	0.41
1:B:387:THR:HA	1:B:389:TYR:CD1	2.56	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: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:1110:ASN:N	1:D:1110:ASN:HD22	2.19	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:839:LEU:HD21	1:A:857:ALA:HA	2.04	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%)	47	71
1	B	1416/1489 (95%)	1375 (97%)	38 (3%)	3 (0%)	47	71
1	C	1412/1489 (95%)	1369 (97%)	41 (3%)	2 (0%)	51	75
1	D	1423/1489 (96%)	1379 (97%)	42 (3%)	2 (0%)	51	75
All	All	5667/5956 (95%)	5490 (97%)	167 (3%)	10 (0%)	47	71

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%)	1187 (98%)	23 (2%)	57	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	1212/1266 (96%)	1185 (98%)	27 (2%)	52	76
1	C	1208/1266 (95%)	1184 (98%)	24 (2%)	55	78
1	D	1217/1266 (96%)	1192 (98%)	25 (2%)	53	77
All	All	4847/5064 (96%)	4748 (98%)	99 (2%)	55	78

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	325	ILE
1	A	430	SER
1	A	508	MET
1	A	578	ASP
1	A	649	ASN
1	A	652	ASN
1	A	751	LYS
1	A	772	LYS
1	A	859	ASP
1	A	999	SER
1	A	1084	ASP
1	A	1100	LYS
1	A	1111	THR
1	A	1128	LEU
1	A	1139	MET
1	A	1193	SER
1	A	1241	ASN
1	A	1249	ASN
1	A	1308	ILE
1	A	1421	SER
1	A	1422	SER
1	A	1479	LYS
1	A	1484	ASP
1	B	325	ILE
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	751	LYS
1	B	772	LYS
1	B	859	ASP

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Mol	Chain	Res	Type
1	B	999	SER
1	B	1084	ASP
1	B	1110	ASN
1	B	1111	THR
1	B	1128	LEU
1	B	1139	MET
1	B	1193	SER
1	B	1241	ASN
1	B	1249	ASN
1	B	1308	ILE
1	B	1326	ARG
1	B	1356	LYS
1	B	1421	SER
1	B	1422	SER
1	B	1424	ARG
1	B	1448	ASP
1	B	1479	LYS
1	C	272	GLU
1	C	430	SER
1	C	508	MET
1	C	578	ASP
1	C	649	ASN
1	C	652	ASN
1	C	772	LYS
1	C	859	ASP
1	C	999	SER
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	1193	SER
1	C	1241	ASN
1	C	1249	ASN
1	C	1308	ILE
1	C	1421	SER
1	C	1422	SER
1	C	1428	ARG
1	C	1479	LYS
1	C	1484	ASP
1	D	418	SER

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Mol	Chain	Res	Type
1	D	430	SER
1	D	508	MET
1	D	578	ASP
1	D	649	ASN
1	D	652	ASN
1	D	751	LYS
1	D	859	ASP
1	D	999	SER
1	D	1084	ASP
1	D	1100	LYS
1	D	1110	ASN
1	D	1111	THR
1	D	1128	LEU
1	D	1139	MET
1	D	1193	SER
1	D	1241	ASN
1	D	1249	ASN
1	D	1287	ASN
1	D	1308	ILE
1	D	1421	SER
1	D	1422	SER
1	D	1478	GLN
1	D	1479	LYS
1	D	1484	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	465	ASN
1	A	1243	GLN
1	A	1359	GLN
1	B	1103	GLN
1	C	465	ASN
1	C	1103	GLN
1	C	1243	GLN
1	C	1249	ASN
1	C	1359	GLN
1	C	1441	ASN
1	D	1103	GLN
1	D	1110	ASN
1	D	1243	GLN
1	D	1359	GLN

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 monosaccharides 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	$\#|Z| > 2$
9	GOL	D	2015	-	5,5,5	0.70	0	5,5,5	0.91	0
6	ADP	C	2009	3	24,29,29	1.17	2 (8%)	29,45,45	1.30	4 (13%)
10	EDO	A	2016	-	3,3,3	0.48	0	2,2,2	0.32	0
6	ADP	C	2008	3	24,29,29	1.01	2 (8%)	29,45,45	1.44	4 (13%)
5	PO4	D	2007	3,4	4,4,4	1.13	0	6,6,6	1.08	0
6	ADP	A	2009	3	24,29,29	1.01	2 (8%)	29,45,45	1.13	1 (3%)
7	NLG	A	2010	-	12,12,12	0.89	0	15,15,15	1.73	3 (20%)
6	ADP	D	2009	3	24,29,29	1.02	1 (4%)	29,45,45	1.42	4 (13%)
7	NLG	D	2010	-	12,12,12	0.96	0	15,15,15	1.66	4 (26%)
9	GOL	A	2015	-	5,5,5	0.88	0	5,5,5	0.83	0
5	PO4	C	2007	3,4	4,4,4	0.91	0	6,6,6	0.85	0
6	ADP	D	2008	3	24,29,29	1.38	3 (12%)	29,45,45	1.50	6 (20%)
7	NLG	C	2010	-	12,12,12	0.86	0	15,15,15	1.06	1 (6%)
7	NLG	B	2010	-	12,12,12	0.86	0	15,15,15	0.90	0
5	PO4	A	2007	3,4	4,4,4	1.12	0	6,6,6	0.98	0
6	ADP	B	2008	3	24,29,29	1.16	2 (8%)	29,45,45	1.37	5 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
6	ADP	B	2009	3	24,29,29	1.06	3 (12%)	29,45,45	1.27	3 (10%)
5	PO4	B	2007	3,4	4,4,4	0.97	0	6,6,6	0.78	0
6	ADP	A	2008	3	24,29,29	1.36	5 (20%)	29,45,45	1.45	6 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
9	GOL	D	2015	-	-	4/4/4/4	-
6	ADP	A	2008	3	-	2/12/32/32	0/3/3/3
6	ADP	D	2008	3	-	3/12/32/32	0/3/3/3
7	NLG	C	2010	-	-	0/13/13/13	-
6	ADP	C	2009	3	-	3/12/32/32	0/3/3/3
10	EDO	A	2016	-	-	1/1/1/1	-
7	NLG	B	2010	-	-	0/13/13/13	-
6	ADP	A	2009	3	-	3/12/32/32	0/3/3/3
7	NLG	A	2010	-	-	4/13/13/13	-
6	ADP	D	2009	3	-	5/12/32/32	0/3/3/3
6	ADP	B	2009	3	-	4/12/32/32	0/3/3/3
7	NLG	D	2010	-	-	2/13/13/13	-
6	ADP	C	2008	3	-	1/12/32/32	0/3/3/3
9	GOL	A	2015	-	-	4/4/4/4	-
6	ADP	B	2008	3	-	1/12/32/32	0/3/3/3

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	2008	ADP	C2-N3	2.97	1.36	1.32
6	A	2008	ADP	C2-N1	2.90	1.39	1.33
6	C	2009	ADP	C2-N3	2.88	1.36	1.32
6	D	2009	ADP	C5-C4	2.80	1.48	1.40
6	A	2008	ADP	O4'-C1'	2.72	1.44	1.41
6	D	2008	ADP	O4'-C4'	-2.72	1.38	1.45
6	A	2009	ADP	O4'-C1'	2.70	1.44	1.41
6	B	2008	ADP	C5-C4	2.68	1.48	1.40
6	B	2009	ADP	C2-N3	2.53	1.36	1.32
6	C	2009	ADP	C5-C4	2.48	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	2008	ADP	C2-N3	2.48	1.36	1.32
6	C	2008	ADP	O4'-C1'	2.45	1.44	1.41
6	A	2009	ADP	C5-C4	2.44	1.47	1.40
6	A	2008	ADP	C2'-C1'	-2.41	1.50	1.53
6	B	2009	ADP	C5-C4	2.35	1.47	1.40
6	B	2009	ADP	O4'-C1'	2.33	1.44	1.41
6	A	2008	ADP	O4'-C4'	-2.32	1.39	1.45
6	D	2008	ADP	C2-N1	2.29	1.38	1.33
6	C	2008	ADP	C5-C4	2.23	1.46	1.40
6	A	2008	ADP	C2-N3	2.15	1.35	1.32

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	2008	ADP	N3-C2-N1	-4.23	122.06	128.68
6	D	2008	ADP	C5-C6-N6	-4.02	114.25	120.35
6	B	2008	ADP	N3-C2-N1	-3.70	122.89	128.68
7	A	2010	NLG	C-CA-N2	3.49	118.81	110.55
7	A	2010	NLG	CB-CA-C	-3.40	102.14	110.35
6	A	2009	ADP	N3-C2-N1	-3.40	123.37	128.68
6	D	2009	ADP	PA-O3A-PB	-3.21	121.81	132.83
6	B	2009	ADP	N3-C2-N1	-3.08	123.87	128.68
7	D	2010	NLG	CB-CA-C	-3.06	102.98	110.35
6	D	2008	ADP	N3-C2-N1	-2.96	124.06	128.68
6	C	2009	ADP	N3-C2-N1	-2.95	124.07	128.68
6	D	2009	ADP	N3-C2-N1	-2.93	124.10	128.68
6	D	2009	ADP	C4-C5-N7	-2.88	106.40	109.40
6	D	2009	ADP	C3'-C2'-C1'	2.80	105.20	100.98
6	B	2008	ADP	N6-C6-N1	2.74	124.27	118.57
7	A	2010	NLG	OE1-CD-CG	-2.64	114.59	123.08
7	D	2010	NLG	OE2-CD-CG	2.61	122.41	114.03
6	C	2009	ADP	N6-C6-N1	2.54	123.86	118.57
6	A	2008	ADP	O5'-PA-O1A	-2.54	99.15	109.07
6	D	2008	ADP	O3B-PB-O2B	2.52	117.28	107.64
6	C	2009	ADP	C4-C5-N7	-2.51	106.78	109.40
6	A	2008	ADP	O3B-PB-O1B	2.49	120.43	110.68
6	A	2008	ADP	N3-C2-N1	-2.49	124.79	128.68
6	B	2009	ADP	C4-C5-N7	-2.44	106.86	109.40
6	C	2008	ADP	C3'-C2'-C1'	2.42	104.62	100.98
6	B	2008	ADP	C3'-C2'-C1'	2.41	104.61	100.98
6	D	2008	ADP	N6-C6-N1	2.41	123.58	118.57
6	D	2008	ADP	O3A-PB-O1B	-2.37	98.06	111.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	D	2010	NLG	O7-C7-C8	-2.31	117.77	122.06
6	C	2009	ADP	O3B-PB-O1B	2.25	119.47	110.68
6	A	2008	ADP	O2A-PA-O1A	2.23	123.25	112.24
6	B	2009	ADP	C3'-C2'-C1'	2.19	104.27	100.98
7	C	2010	NLG	OXT-C-CA	2.18	120.63	113.40
6	D	2008	ADP	O3B-PB-O1B	2.15	119.11	110.68
7	D	2010	NLG	OE1-CD-CG	-2.13	116.25	123.08
6	C	2008	ADP	O2A-PA-O1A	2.12	122.72	112.24
6	C	2008	ADP	C2-N1-C6	2.11	122.37	118.75
6	A	2008	ADP	C4-C5-N7	-2.11	107.20	109.40
6	B	2008	ADP	O3B-PB-O2B	2.08	115.60	107.64
6	A	2008	ADP	O3A-PB-O1B	-2.03	99.93	111.19
6	B	2008	ADP	C2-N1-C6	2.01	122.19	118.75

There are no chirality outliers.

All (37) 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
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
6	A	2009	ADP	PA-O3A-PB-O1B
7	A	2010	NLG	OE2-CD-CG-CB
7	A	2010	NLG	OE1-CD-CG-CB

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Mol	Chain	Res	Type	Atoms
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	OE2-CD-CG-CB
7	D	2010	NLG	OE1-CD-CG-CB
6	B	2009	ADP	C5'-O5'-PA-O1A
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
9	D	2015	GOL	1	0
10	A	2016	EDO	2	0
6	D	2009	ADP	1	0
7	D	2010	NLG	1	0
5	C	2007	PO4	1	0
6	D	2008	ADP	1	0
5	A	2007	PO4	1	0
6	A	2008	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 then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand ADP C 2009

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP C 2008

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP A 2009

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP D 2009

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP D 2008

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP B 2008

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP B 2009

Bond lengths

Bond angles

Torsions

Rings

Ligand ADP A 2008

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1422/1489 (95%)	-0.51	3 (0%)	95	95	12, 24, 47, 94	3 (0%)
1	B	1426/1489 (95%)	0.08	45 (3%)	47	40	19, 55, 87, 116	3 (0%)
1	C	1421/1489 (95%)	0.72	239 (16%)	1	1	20, 64, 144, 172	3 (0%)
1	D	1430/1489 (96%)	-0.51	14 (0%)	82	80	12, 24, 48, 113	3 (0%)
All	All	5699/5956 (95%)	-0.05	301 (5%)	26	20	12, 34, 111, 172	12 (0%)

All (301) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	404	THR	13.0
1	C	343	ASN	9.5
1	C	403	ALA	9.5
1	C	368	SER	9.0
1	C	130	GLY	8.6
1	C	268	PRO	8.5
1	C	131	LEU	8.2
1	C	338	GLY	8.2
1	C	405	THR	8.1
1	C	176	LYS	7.9
1	C	192	PHE	7.8
1	C	183	ILE	7.7
1	C	225	CYS	7.7
1	C	309	TYR	7.3
1	C	401	GLY	7.3
1	C	227	ILE	7.1
1	C	413	PRO	6.7
1	C	291	PHE	6.6
1	C	349	TRP	6.6
1	C	260	LEU	6.6
1	B	371	PHE	6.5

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Mol	Chain	Res	Type	RSRZ
1	C	240	ALA	6.5
1	C	46	ALA	6.3
1	C	354	VAL	6.1
1	C	356	VAL	6.0
1	C	364	ILE	5.9
1	C	253	LYS	5.9
1	C	251	PHE	5.8
1	C	406	ILE	5.6
1	C	293	ILE	5.6
1	C	287	LYS	5.6
1	C	255	GLU	5.5
1	C	299	ILE	5.5
1	C	84	ILE	5.5
1	C	245	VAL	5.4
1	C	369	LYS	5.4
1	C	402	LYS	5.4
1	C	412	LYS	5.4
1	C	132	LEU	5.4
1	C	371	PHE	5.4
1	C	757	LYS	5.4
1	C	72	VAL	5.3
1	C	174[A]	ARG	5.3
1	C	160	ALA	5.3
1	C	286	ARG	5.2
1	C	91	GLY	5.2
1	C	144	LEU	5.2
1	C	120	TYR	5.1
1	C	340	ALA	5.0
1	C	44	GLN	4.9
1	C	209	VAL	4.9
1	C	48	ILE	4.9
1	C	934	LYS	4.8
1	C	374	VAL	4.8
1	C	87	PRO	4.7
1	C	307	LYS	4.7
1	C	261	ILE	4.7
1	C	221	VAL	4.6
1	C	372	PHE	4.6
1	C	89	TYR	4.6
1	C	899	MET	4.6
1	C	59	TYR	4.5
1	C	933	LEU	4.5

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Mol	Chain	Res	Type	RSRZ
1	C	355	ASN	4.5
1	C	269	ALA	4.5
1	C	352	LEU	4.5
1	C	184	GLU	4.4
1	B	404	THR	4.4
1	C	197	LYS	4.4
1	C	357	ASN	4.4
1	C	298	LEU	4.4
1	C	145	ALA	4.4
1	C	56	MET	4.3
1	C	248	ASN	4.3
1	B	326	THR	4.3
1	C	190	VAL	4.2
1	B	403	ALA	4.2
1	C	353	PHE	4.2
1	C	93	ILE	4.2
1	C	342	ASP	4.2
1	C	242	VAL	4.2
1	C	288	GLU	4.1
1	C	280	LYS	4.1
1	B	187	GLY	4.1
1	C	187	GLY	4.0
1	C	351	PRO	4.0
1	C	243	HIS	4.0
1	C	114	GLU	4.0
1	C	282	LEU	3.9
1	C	334	ALA	3.9
1	C	328	LYS	3.9
1	B	266	GLY	3.8
1	C	367	GLU	3.8
1	C	297	ASN	3.8
1	B	401	GLY	3.8
1	C	366	HIS	3.8
1	C	285	ASP	3.8
1	B	410	LEU	3.8
1	C	278	VAL	3.8
1	C	271	ALA	3.7
1	C	157	LYS	3.7
1	C	387	THR	3.7
1	C	204	VAL	3.7
1	C	90	LYS	3.7
1	C	152	TRP	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	45	THR	3.7
1	C	301	GLY	3.6
1	C	210	LYS	3.6
1	C	159	PRO	3.6
1	C	191	ASP	3.6
1	C	202	ALA	3.6
1	C	83	ALA	3.5
1	B	130	GLY	3.5
1	C	294	SER	3.5
1	C	218	THR	3.5
1	C	186	GLU	3.5
1	C	63	HIS	3.5
1	C	329	GLN	3.5
1	D	403	ALA	3.5
1	C	185	PHE	3.5
1	C	823	PHE	3.5
1	B	351	PRO	3.5
1	C	339	TYR	3.5
1	D	1153	GLU	3.5
1	C	226	GLY	3.5
1	C	266	GLY	3.5
1	C	161	ILE	3.5
1	C	276	GLN	3.4
1	B	269	ALA	3.4
1	A	1112	LEU	3.4
1	C	931	LEU	3.4
1	B	419	ARG	3.4
1	C	394	PHE	3.3
1	C	270	LEU	3.3
1	C	290	LEU	3.3
1	B	114	GLU	3.3
1	C	292	GLY	3.3
1	B	207	LYS	3.3
1	C	211	VAL	3.3
1	C	171	LYS	3.3
1	C	347	ALA	3.3
1	B	400	LYS	3.2
1	C	126	ILE	3.2
1	D	1152	LEU	3.2
1	C	712	ILE	3.2
1	C	97	ALA	3.2
1	C	73	PHE	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	193	VAL	3.2
1	B	347	ALA	3.2
1	B	402	LYS	3.1
1	C	52	ASP	3.1
1	C	756	GLY	3.1
1	C	232	ILE	3.1
1	C	345	LEU	3.1
1	C	108	ASP	3.1
1	C	95	THR	3.1
1	A	403	ALA	3.1
1	C	265	PRO	3.1
1	C	109	THR	3.1
1	C	904	LEU	3.1
1	C	365	MET	3.0
1	C	247	TRP	3.0
1	C	134	LEU	3.0
1	C	341	LEU	3.0
1	C	252	THR	3.0
1	C	300	THR	3.0
1	D	1145	GLU	3.0
1	C	189	PRO	3.0
1	C	281	ILE	2.9
1	C	840	ARG	2.9
1	C	843	LEU	2.9
1	C	153	LEU	2.9
1	C	133	VAL	2.9
1	C	327	ASN	2.9
1	C	259	ILE	2.9
1	C	344	THR	2.9
1	C	279	ARG	2.9
1	C	311	MET	2.8
1	C	138	LYS	2.8
1	C	123	SER	2.8
1	B	81	PRO	2.8
1	B	202	ALA	2.8
1	C	94	LEU	2.8
1	C	386	ASP	2.8
1	C	196	ASN	2.8
1	B	409	VAL	2.8
1	B	405	THR	2.8
1	C	110	THR	2.8
1	C	410	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	158	VAL	2.8
1	C	71	VAL	2.8
1	B	253	LYS	2.8
1	C	207	LYS	2.8
1	C	241	GLU	2.7
1	C	409	VAL	2.7
1	B	287	LYS	2.7
1	C	941	VAL	2.7
1	C	390	LEU	2.7
1	C	932	ARG	2.7
1	C	962	TYR	2.7
1	B	329	GLN	2.7
1	C	1326	ARG	2.7
1	C	350	LYS	2.7
1	C	829	MET	2.6
1	C	804	THR	2.6
1	C	408	SER	2.6
1	B	280	LYS	2.6
1	C	326	THR	2.6
1	D	1150	LYS	2.6
1	D	1148	MET	2.6
1	B	407	THR	2.6
1	C	107	PRO	2.6
1	C	803	ARG	2.6
1	C	85	THR	2.6
1	C	561	ILE	2.6
1	B	350	LYS	2.5
1	B	349	TRP	2.5
1	C	128	VAL	2.5
1	C	223	VAL	2.5
1	C	62	GLY	2.5
1	C	902	GLU	2.5
1	B	365	MET	2.5
1	C	547	ARG	2.5
1	C	216	ASN	2.5
1	B	285	ASP	2.5
1	C	250	ASP	2.5
1	C	682	ARG	2.5
1	C	1419	SER	2.5
1	B	299	ILE	2.4
1	B	118	SER	2.4
1	D	1151	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	881	MET	2.4
1	B	325	ILE	2.4
1	B	132	LEU	2.4
1	B	561	ILE	2.4
1	B	190	VAL	2.4
1	C	761	CYS	2.4
1	B	175	ASP	2.4
1	C	64	PRO	2.4
1	C	74	ASN	2.4
1	C	316	ARG	2.4
1	C	400	LYS	2.4
1	C	212	TYR	2.3
1	C	965	GLN	2.3
1	C	373	ALA	2.3
1	C	375	GLN	2.3
1	D	1140	ASN	2.3
1	C	55	LYS	2.3
1	C	310	LYS	2.3
1	B	366	HIS	2.3
1	C	382	PRO	2.3
1	C	220	VAL	2.3
1	C	709	GLU	2.3
1	C	228	LYS	2.3
1	B	1151	PHE	2.3
1	C	156	GLU	2.3
1	C	175	ASP	2.3
1	D	1128	LEU	2.3
1	C	256	TYR	2.3
1	C	180	LEU	2.2
1	C	231	VAL	2.2
1	C	239	GLY	2.2
1	C	893	GLY	2.2
1	C	149	LEU	2.2
1	C	172	ILE	2.2
1	C	325	ILE	2.2
1	C	770	VAL	2.2
1	C	254	MET	2.2
1	C	348	GLY	2.2
1	C	898	SER	2.2
1	C	370	PRO	2.2
1	C	305	GLY	2.2
1	B	183	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	826	ARG	2.2
1	C	81	PRO	2.2
1	A	1111	THR	2.2
1	C	937	ILE	2.1
1	D	1162	HIS	2.1
1	C	178	THR	2.1
1	C	124	ASN	2.1
1	B	757	LYS	2.1
1	C	219	LYS	2.1
1	C	249	HIS	2.1
1	C	411	PRO	2.1
1	B	300	THR	2.1
1	C	601	PRO	2.1
1	C	313	MET	2.1
1	B	129	SER	2.1
1	D	1165	VAL	2.1
1	D	1163	PRO	2.1
1	C	117	LEU	2.1
1	C	100	ILE	2.1
1	C	54	THR	2.1
1	C	151	GLN	2.0
1	D	1112	LEU	2.0
1	C	162	TYR	2.0
1	B	288	GLU	2.0
1	C	851	ILE	2.0
1	D	1114	GLU	2.0
1	B	308	THR	2.0
1	C	234	LEU	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	C	2003	1/1	0.82	0.07	20,20,20,20	0
3	MG	B	2003	1/1	0.89	0.07	35,35,35,35	0
2	NI	C	2001	1/1	0.89	0.17	56,56,56,56	0
4	K	C	2006	1/1	0.91	0.09	78,78,78,78	0
4	K	C	2004	1/1	0.92	0.09	44,44,44,44	0
4	K	C	2012	1/1	0.92	0.23	75,75,75,75	0
10	EDO	A	2016	4/4	0.92	0.17	39,40,40,41	0
3	MG	A	2011	1/1	0.93	0.05	41,41,41,41	0
6	ADP	C	2008	27/27	0.94	0.13	26,29,36,38	0
3	MG	B	2011	1/1	0.94	0.05	15,15,15,15	0
3	MG	D	2002	1/1	0.95	0.14	13,13,13,13	0
4	K	C	2005	1/1	0.95	0.18	45,45,45,45	0
7	NLG	A	2010	13/13	0.95	0.15	17,18,19,21	0
9	GOL	A	2015	6/6	0.95	0.11	26,29,29,29	0
3	MG	D	2011	1/1	0.95	0.08	34,34,34,34	0
6	ADP	A	2009	27/27	0.96	0.11	28,31,46,47	0
6	ADP	B	2009	27/27	0.96	0.12	24,28,35,37	0
3	MG	C	2002	1/1	0.96	0.06	20,20,20,20	0
6	ADP	C	2009	27/27	0.96	0.14	28,31,37,38	0
3	MG	B	2002	1/1	0.96	0.08	21,21,21,21	0
7	NLG	B	2010	13/13	0.96	0.13	16,23,25,26	0
7	NLG	C	2010	13/13	0.96	0.13	18,22,25,26	0
5	PO4	B	2007	5/5	0.96	0.11	26,26,29,29	0
5	PO4	C	2007	5/5	0.96	0.08	32,34,34,35	0
3	MG	A	2002	1/1	0.97	0.11	13,13,13,13	0
6	ADP	B	2008	27/27	0.97	0.10	25,29,32,32	0
7	NLG	D	2010	13/13	0.97	0.15	20,21,24,25	0
8	CL	B	2012	1/1	0.97	0.10	43,43,43,43	0
6	ADP	D	2009	27/27	0.97	0.09	27,31,44,45	0
9	GOL	D	2015	6/6	0.97	0.15	30,34,37,38	0
4	K	A	2013	1/1	0.97	0.04	32,32,32,32	0
6	ADP	D	2008	27/27	0.98	0.11	7,7,10,10	0
4	K	D	2005	1/1	0.98	0.06	30,30,30,30	0
4	K	B	2005	1/1	0.98	0.04	42,42,42,42	0
4	K	B	2006	1/1	0.98	0.22	65,65,65,65	0
6	ADP	A	2008	27/27	0.98	0.11	7,8,11,12	0
4	K	B	2013	1/1	0.98	0.23	61,61,61,61	0
2	NI	B	2001	1/1	0.98	0.06	75,75,75,75	0
3	MG	D	2003	1/1	0.98	0.11	13,13,13,13	0
3	MG	A	2003	1/1	0.98	0.09	9,9,9,9	0
3	MG	C	2011	1/1	0.98	0.04	41,41,41,41	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($Å^2$)	Q<0.9
4	K	D	2006	1/1	0.99	0.10	53,53,53,53	0
4	K	D	2013	1/1	0.99	0.04	18,18,18,18	0
4	K	D	2014	1/1	0.99	0.05	37,37,37,37	0
5	PO4	A	2007	5/5	0.99	0.12	11,12,12,13	0
4	K	A	2006	1/1	0.99	0.09	46,46,46,46	0
2	NI	D	2001	1/1	0.99	0.07	34,34,34,34	0
4	K	A	2014	1/1	0.99	0.04	24,24,24,24	0
8	CL	A	2012	1/1	0.99	0.06	31,31,31,31	0
4	K	B	2004	1/1	0.99	0.05	39,39,39,39	0
8	CL	D	2012	1/1	0.99	0.12	26,26,26,26	0
4	K	A	2004	1/1	0.99	0.08	9,9,9,9	0
4	K	D	2004	1/1	0.99	0.09	8,8,8,8	0
4	K	A	2005	1/1	0.99	0.10	31,31,31,31	0
2	NI	A	2001	1/1	1.00	0.04	34,34,34,34	0
5	PO4	D	2007	5/5	1.00	0.11	11,11,13,14	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.
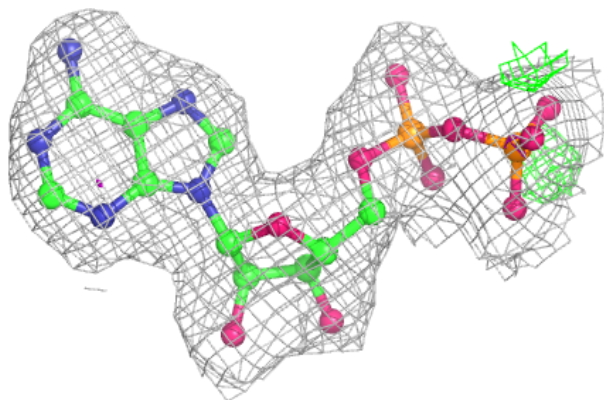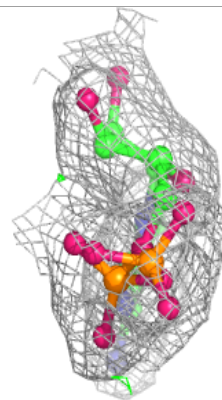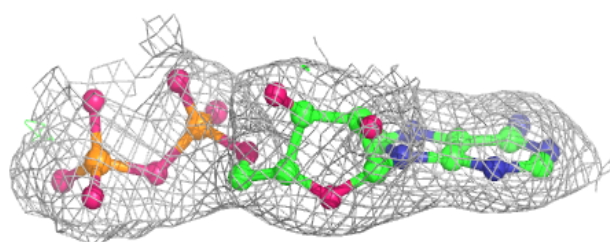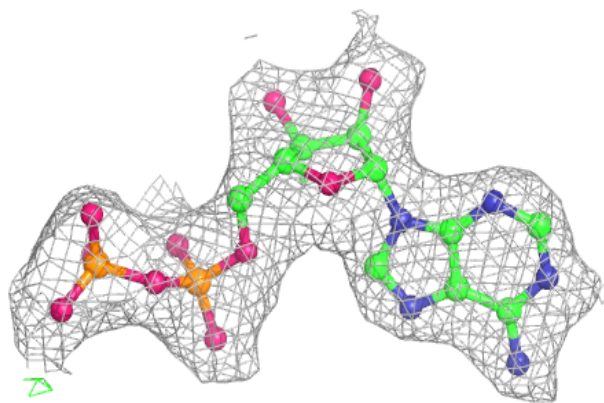

Electron density around ADP C 2008:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
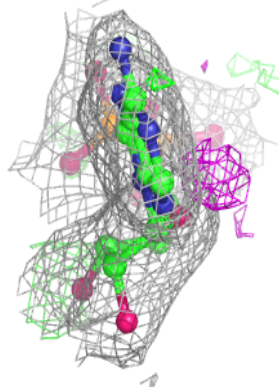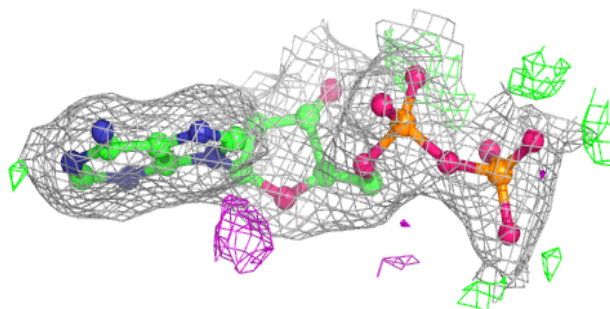mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
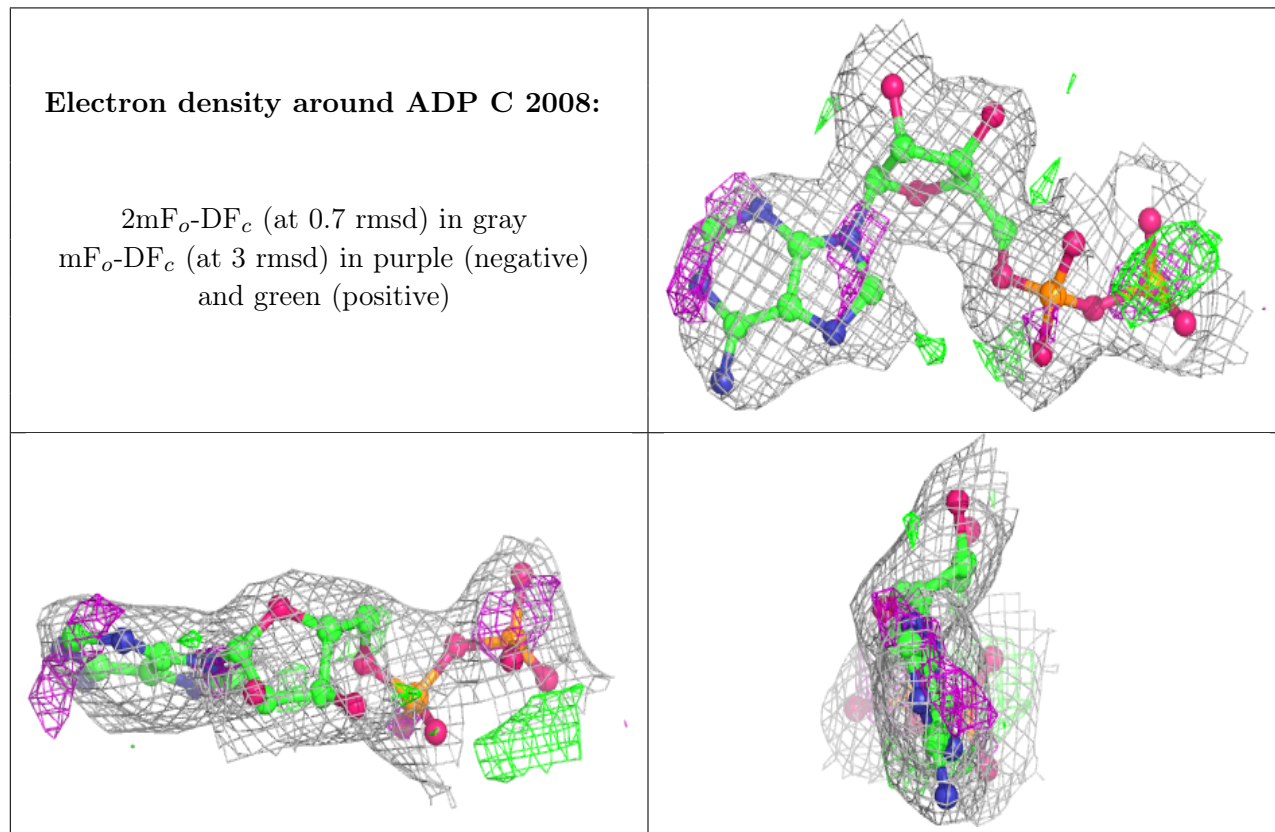
Electron density around ADP A 2009:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
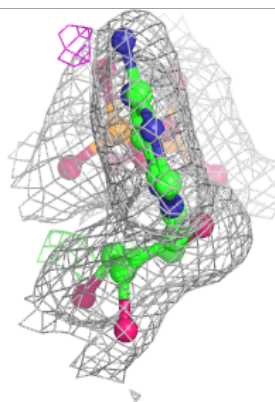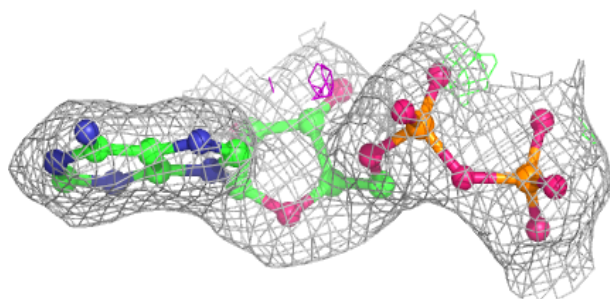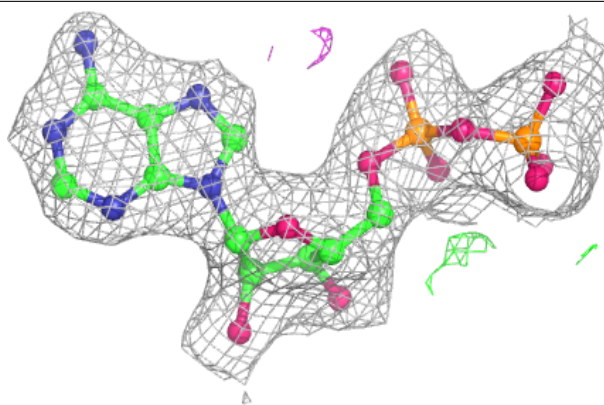
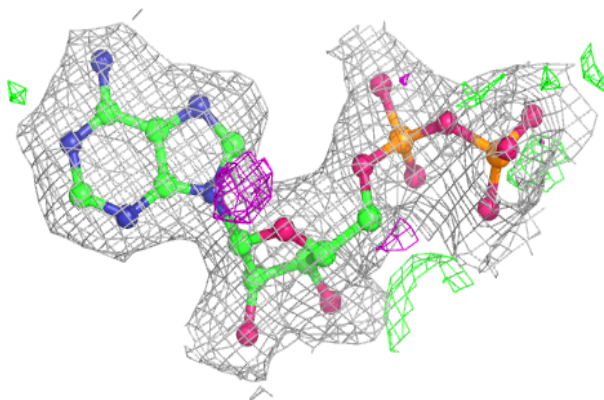Electron density around ADP B 2009:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
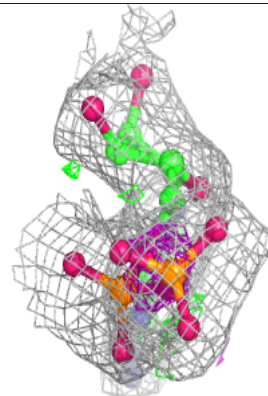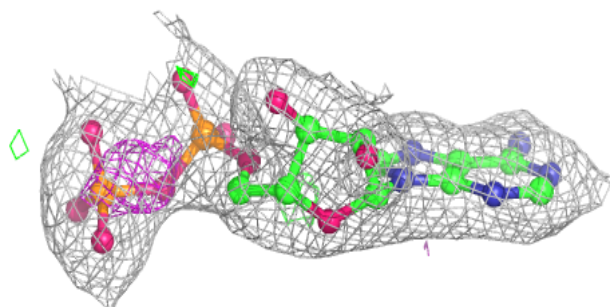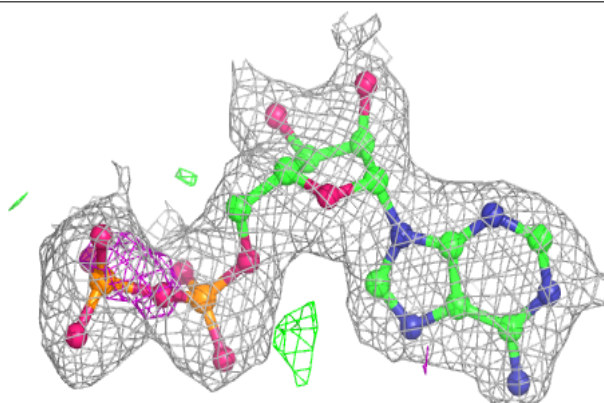
Electron density around ADP C 2009:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
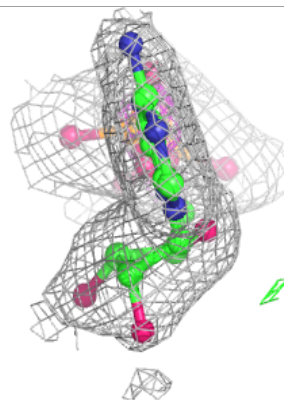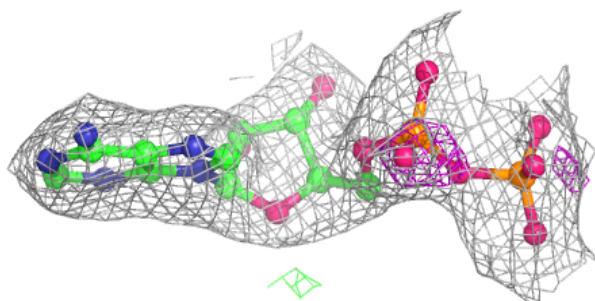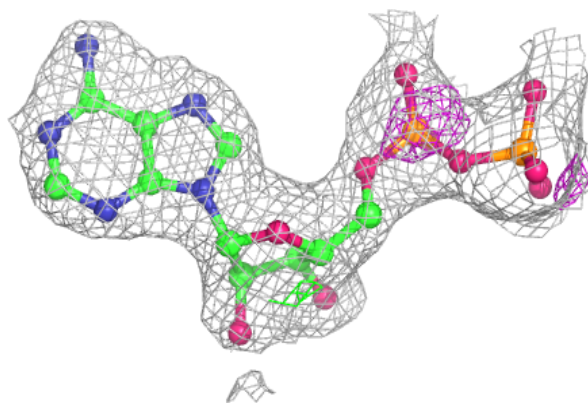
Electron density around ADP B 2008:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
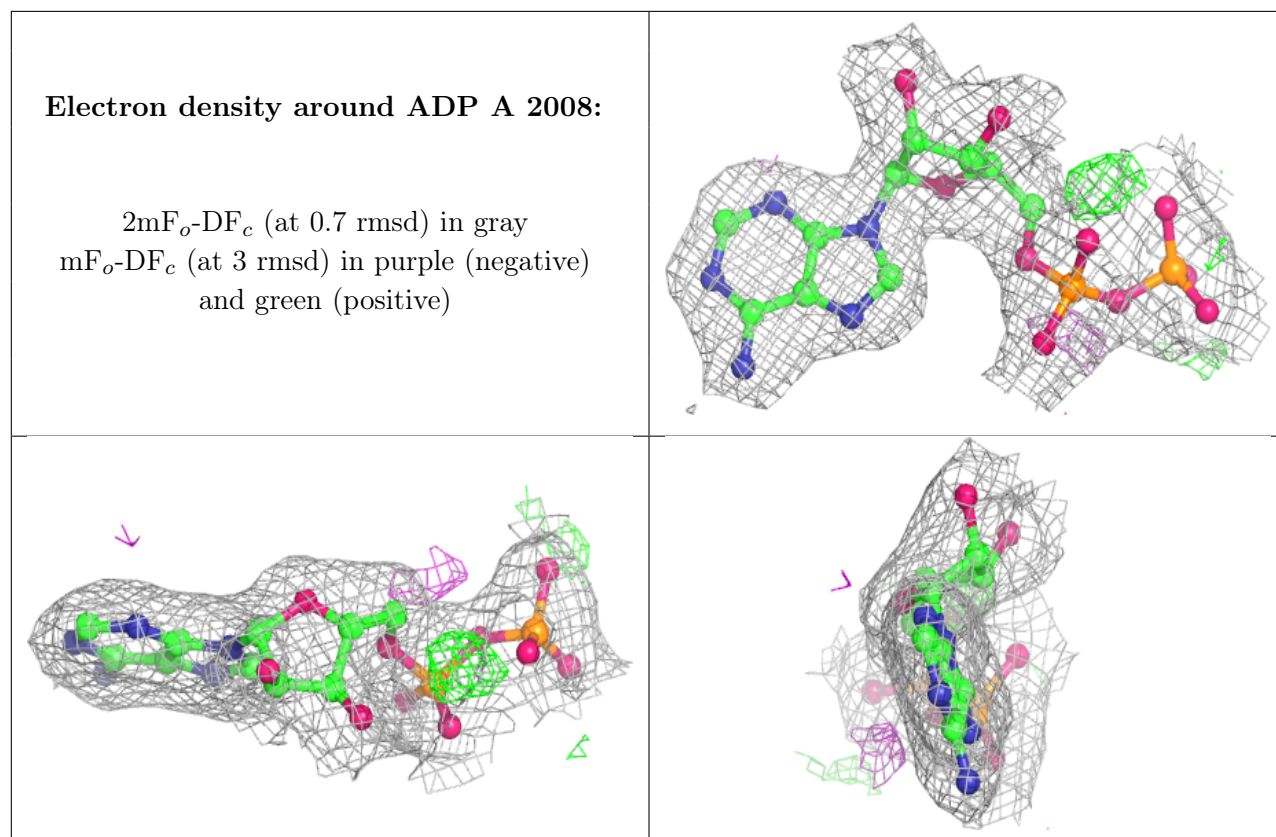mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
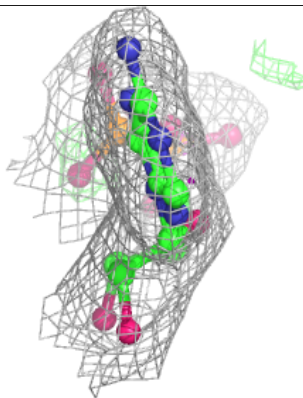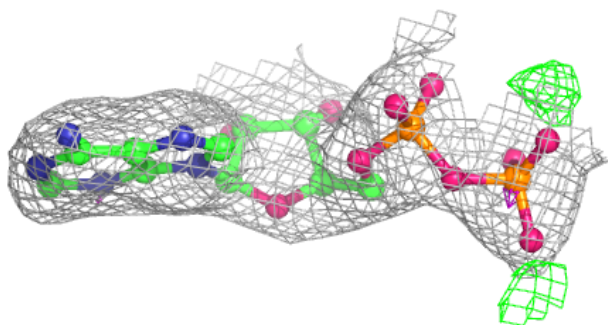
Electron density around ADP D 2009:

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

Electron density around ADP D 2008:

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

Electron density around ADP 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)

6.5 Other polymers ⓘ

There are no such residues in this entry.