wwPDB X-ray Structure Validation Summary Report (i)

Feb 19, 2016 – 11:00 PM 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)

This is a wwPDB X-ray Structure Validation Summary Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

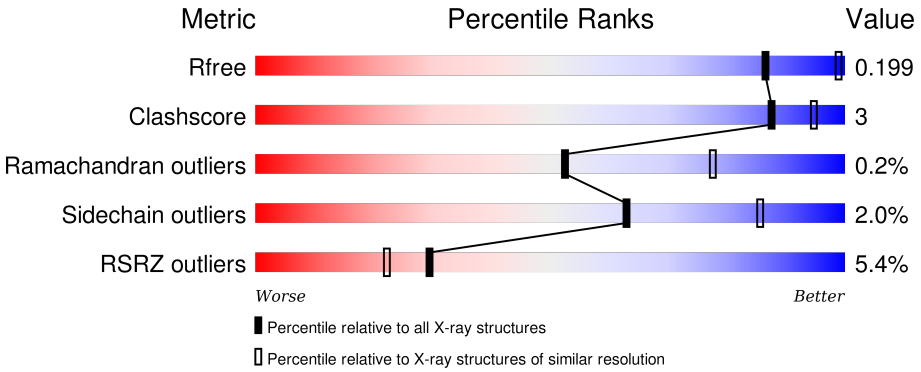
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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% ·

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	K	B	2013	-	-	-	X
4	K	C	2012	-	-	-	X

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	B	1	Total Ni 1 1	0	0
2	A	1	Total Ni 1 1	0	0
2	D	1	Total Ni 1 1	0	0
2	C	1	Total Ni 1 1	0	0

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

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

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

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

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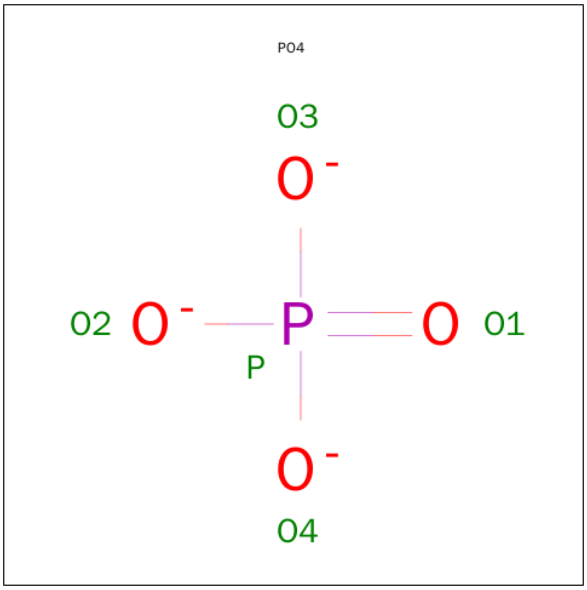
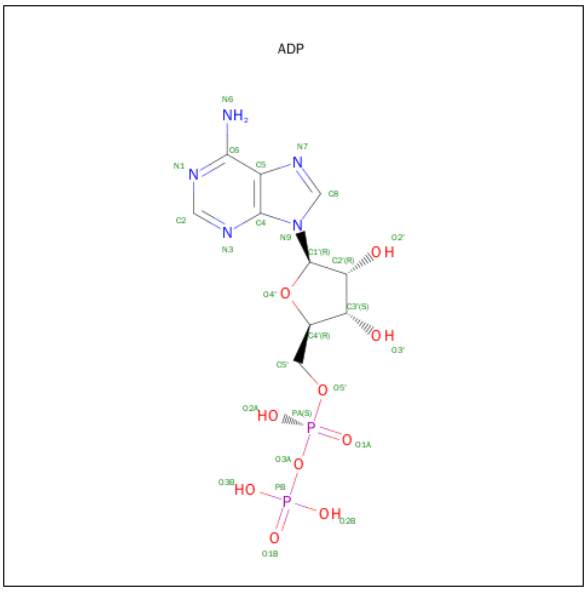
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	4	Total K 4 4	0	0

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



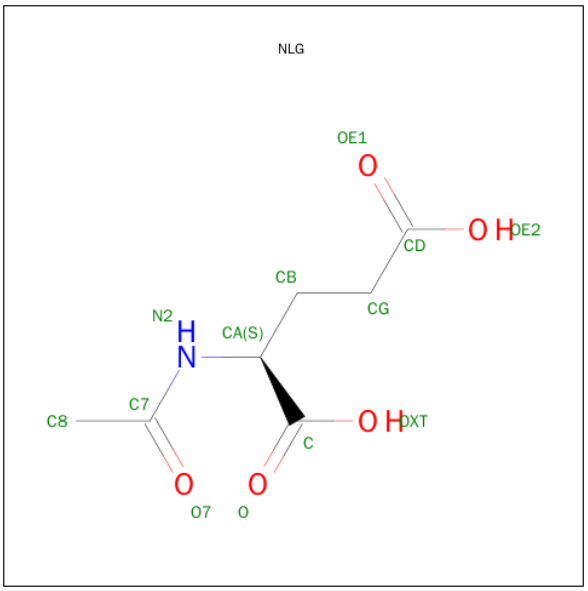
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0
5	C	1	Total O P 5 4 1	0	0
5	D	1	Total O P 5 4 1	0	0

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



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: $C_7H_{11}NO_5$).

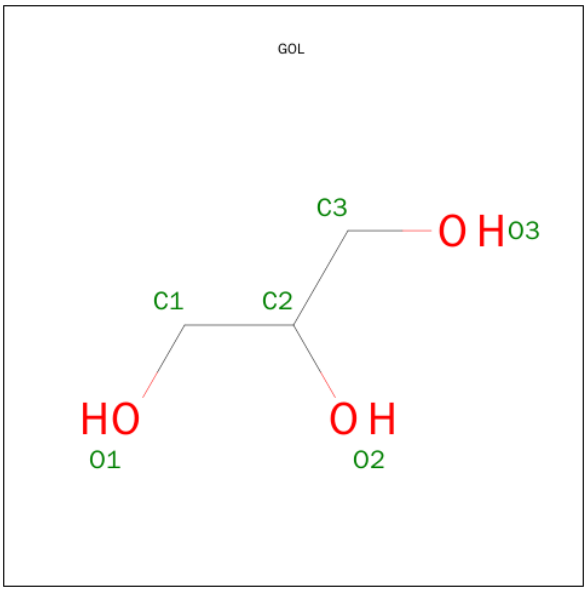


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	1	Total C N O 13 7 1 5	0	0
7	B	1	Total C N O 13 7 1 5	0	0
7	C	1	Total C N O 13 7 1 5	0	0
7	D	1	Total C N O 13 7 1 5	0	0

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

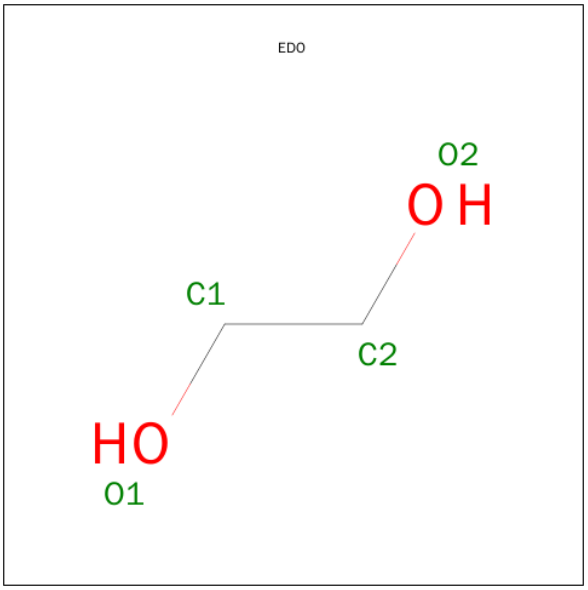
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Cl 1 1	0	0
8	A	1	Total Cl 1 1	0	0
8	D	1	Total Cl 1 1	0	0

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



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

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



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

- Molecule 11 is water.

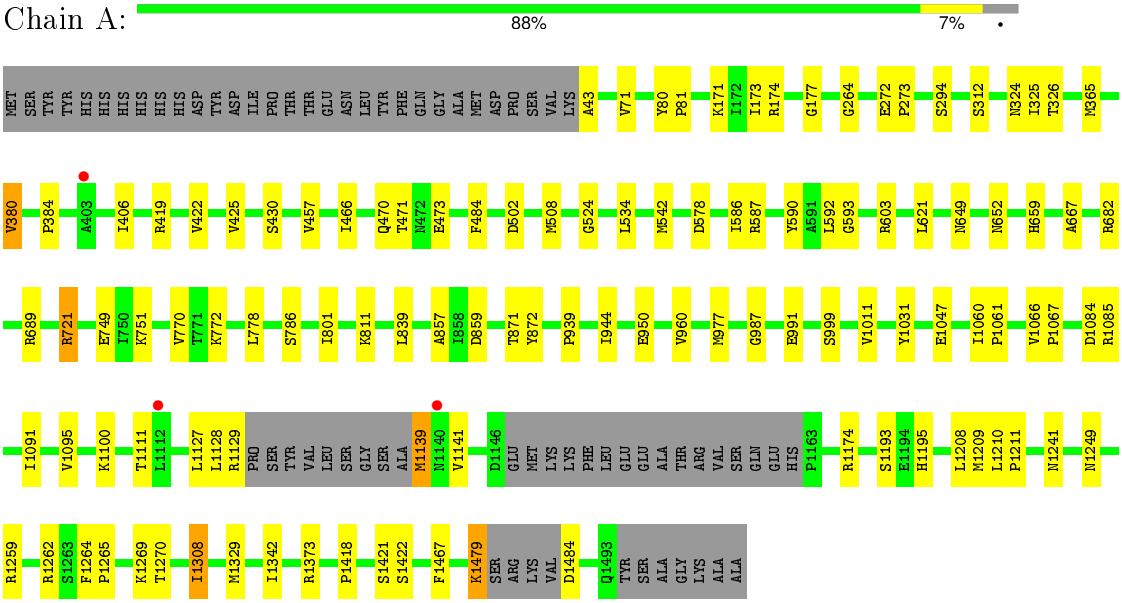
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	264	Total O 264 264	0	0
11	B	79	Total O 79 79	0	0
11	C	65	Total O 65 65	0	0
11	D	232	Total O 232 232	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

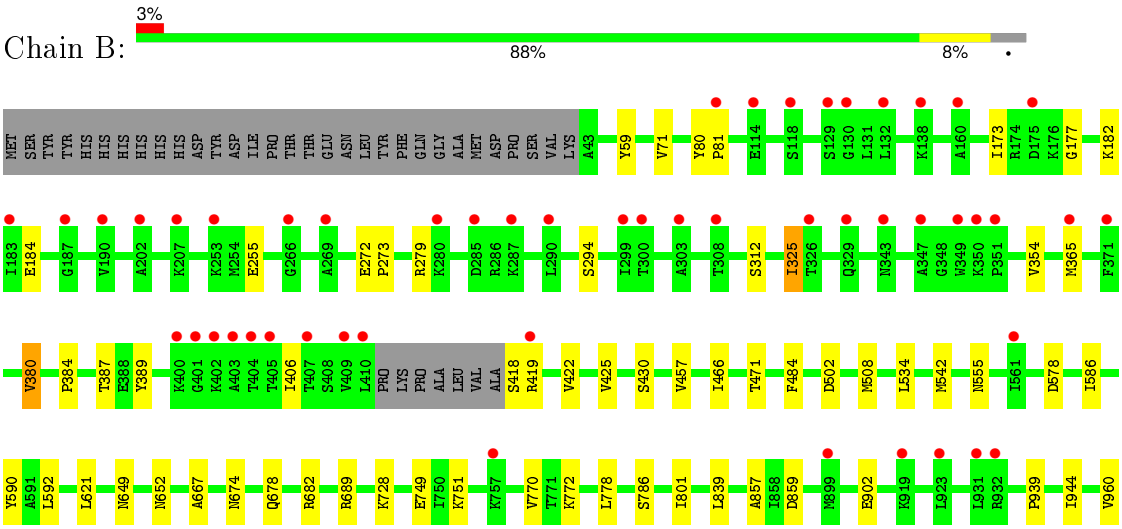
- Molecule 1: Carbamoyl-phosphate synthase [ammonia], mitochondrial

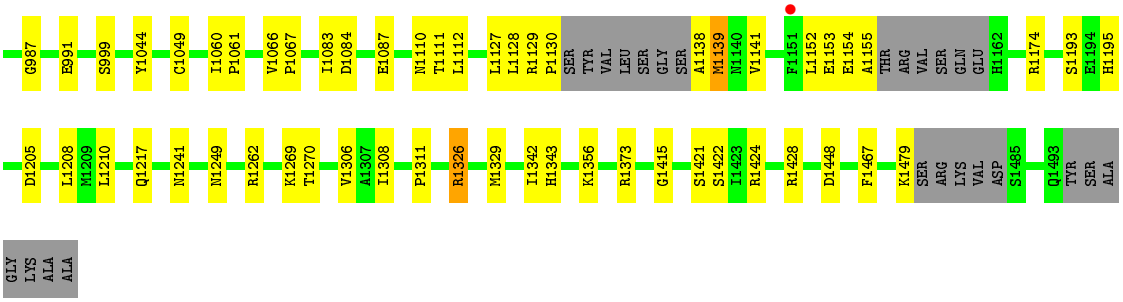
Chain A:



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

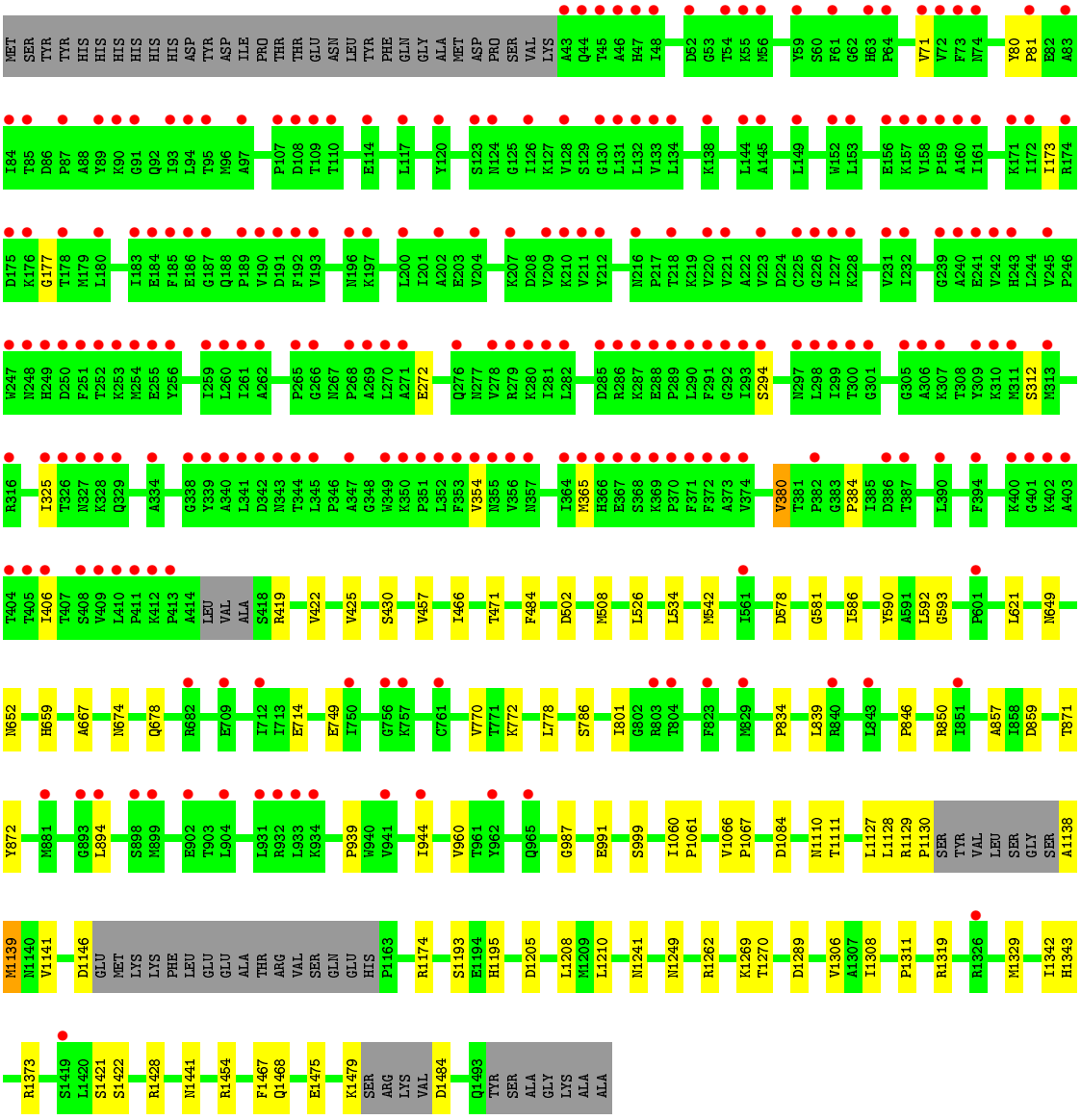
Chain B:





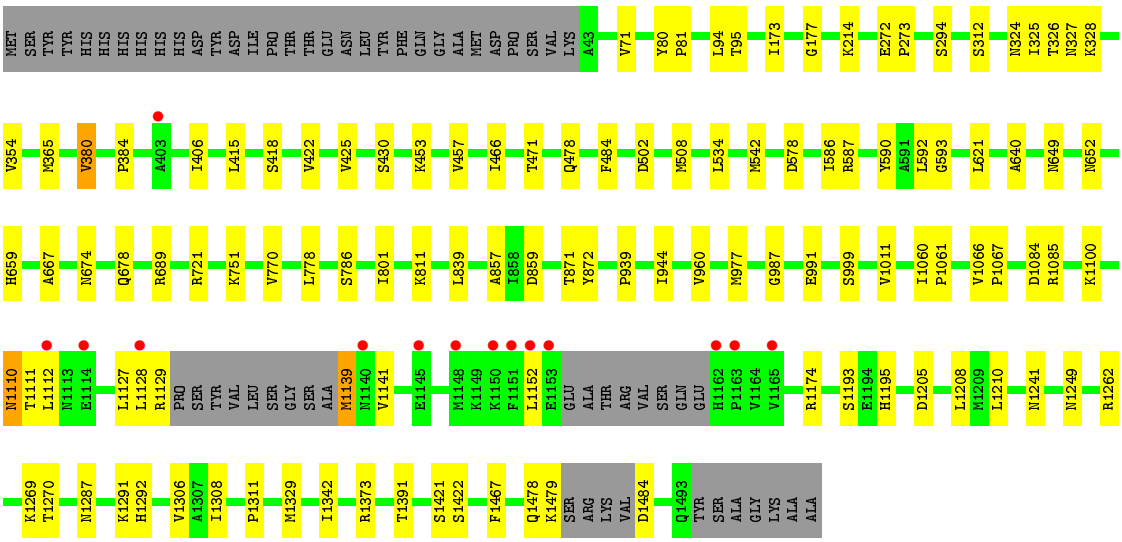
• Molecule 1: Carbamoyl-phosphate synthase [ammonia], mitochondrial

Chain C:



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

Chain D:


MET SER TYR TYR HIS HIS HIS HIS HIS ASP TYR ASP ILE PRO THR THR GLU ASN LEU TYR PHE GLN GLY ALA MET ASP PRO SER VAL LYS A43 V71 Y80 P81 L94 T95 I173 G177 K214 E272 P273 S294 S312 N324 I325 T326 N327 K328
V354 M365 V380 P384 A403 I406 L415 S418 V422 V425 S430 K453 V457 I466 T471 Q478 F484 D502 M508 L534 M542 D578 I586 R587 Y590 A591 L592 G593 L621 A640 N649 N652
H659 A667 N674 Q678 R689 R721 K751 V770 L778 S786 I801 K811 L839 A857 I868 D859 T871 Y872 P939 I944 V960 M977 G987 E991 S999 V1011 I1060 P1061 V1066 P1067 D1084 R1085 K1100
N1110 T1111 L1112 N1113 E1114 L1127 L1128 R1129 PRO SER TYR VAL LEU SER GLY SER ALA M1139 N1140 V1141 E1145 M1148 K1149 K1150 F1151 L1152 E1153 GLU ALA THR ARG VAL SER GLN GLU H1162 P1163 V1164 V1165 R1174 S1193 E1194 H1195 D1205 L1208 M1209 L1210 N1241 N1249 R1262
K1269 T1270 N1287 K1291 H1292 V1306 A1307 I1308 P1311 M1329 I1342 R1373 T1391 S1421 S1422 F1467 Q1478 K1479 SER ARG LYS VAL D1484 Q1493 TYR SER ALA GLY LYS ALA ALA

4 Data and refinement statistics (i)

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) 88.8 (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	8965 reflections (5.28%)	DCC
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 , 14.1	EDS
Estimated twinning fraction	0.035 for h,-k,-h-l 0.247 for -h,k,-l 0.030 for -h,-k,h+l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 178644 reflections	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 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: GOL, MG, ADP, CL, K, EDO, PO4, NLG, NI

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.

The worst 5 of 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

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	63	0
1	B	11018	0	11072	57	0

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

The worst 5 of 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:CG	1:A:419[B]:ARG:HH11	1.72	1.03
1:A:419[B]:ARG:HG3	1:A:419[B]:ARG:HH11	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

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 (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	1416/1489 (95%)	1367 (96%)	46 (3%)	3 (0%)	52	77
1	B	1416/1489 (95%)	1375 (97%)	38 (3%)	3 (0%)	52	77
1	C	1412/1489 (95%)	1369 (97%)	41 (3%)	2 (0%)	56	81
1	D	1423/1489 (96%)	1379 (97%)	42 (3%)	2 (0%)	56	81
All	All	5667/5956 (95%)	5490 (97%)	167 (3%)	10 (0%)	52	77

5 of 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

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	1210/1266 (96%)	1187 (98%)	23 (2%)	65	86
1	B	1212/1266 (96%)	1185 (98%)	27 (2%)	60	83
1	C	1208/1266 (95%)	1184 (98%)	24 (2%)	63	85
1	D	1217/1266 (96%)	1192 (98%)	25 (2%)	61	85
All	All	4847/5064 (96%)	4748 (98%)	99 (2%)	63	85

5 of 99 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	1356	LYS
1	C	652	ASN
1	D	1249	ASN
1	B	1422	SER
1	C	272	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 14 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	1243	GLN
1	C	1249	ASN
1	D	1110	ASN
1	C	1103	GLN
1	D	1103	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\| > 2$
5	PO4	A	2007	3,4	4,4,4	0.95	0	6,6,6	0.25	0
6	ADP	A	2008	3	24,29,29	1.31	4 (16%)	23,45,45	1.92	6 (26%)
6	ADP	A	2009	3	24,29,29	1.04	2 (8%)	23,45,45	1.79	2 (8%)
7	NLG	A	2010	-	6,12,12	0.85	0	6,15,15	1.29	1 (16%)
9	GOL	A	2015	-	5,5,5	0.84	0	5,5,5	0.81	0
10	EDO	A	2016	-	3,3,3	0.46	0	2,2,2	0.37	0
5	PO4	B	2007	3,4	4,4,4	0.71	0	6,6,6	0.24	0
6	ADP	B	2008	3	24,29,29	1.18	2 (8%)	23,45,45	2.00	3 (13%)
6	ADP	B	2009	3	24,29,29	1.07	3 (12%)	23,45,45	1.73	3 (13%)
7	NLG	B	2010	-	6,12,12	0.36	0	6,15,15	0.87	0
5	PO4	C	2007	3,4	4,4,4	0.71	0	6,6,6	0.26	0
6	ADP	C	2008	3	24,29,29	1.03	2 (8%)	23,45,45	2.30	5 (21%)
6	ADP	C	2009	3	24,29,29	1.16	2 (8%)	23,45,45	1.74	3 (13%)
7	NLG	C	2010	-	6,12,12	0.34	0	6,15,15	0.72	0
5	PO4	D	2007	3,4	4,4,4	0.96	0	6,6,6	0.26	0
6	ADP	D	2008	3	24,29,29	1.36	4 (16%)	23,45,45	1.93	6 (26%)
6	ADP	D	2009	3	24,29,29	1.06	1 (4%)	23,45,45	1.60	1 (4%)
7	NLG	D	2010	-	6,12,12	0.81	0	6,15,15	1.80	2 (33%)
9	GOL	D	2015	-	5,5,5	0.65	0	5,5,5	0.92	0

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
5	PO4	A	2007	3,4	-	0/0/0/0	0/0/0/0
6	ADP	A	2008	3	-	0/12/32/32	0/3/3/3
6	ADP	A	2009	3	-	0/12/32/32	0/3/3/3
7	NLG	A	2010	-	-	0/7/13/13	0/0/0/0
9	GOL	A	2015	-	-	0/4/4/4	0/0/0/0
10	EDO	A	2016	-	-	0/1/1/1	0/0/0/0
5	PO4	B	2007	3,4	-	0/0/0/0	0/0/0/0
6	ADP	B	2008	3	-	0/12/32/32	0/3/3/3
6	ADP	B	2009	3	-	0/12/32/32	0/3/3/3
7	NLG	B	2010	-	-	0/7/13/13	0/0/0/0
5	PO4	C	2007	3,4	-	0/0/0/0	0/0/0/0
6	ADP	C	2008	3	-	0/12/32/32	0/3/3/3
6	ADP	C	2009	3	-	0/12/32/32	0/3/3/3
7	NLG	C	2010	-	-	0/7/13/13	0/0/0/0
5	PO4	D	2007	3,4	-	0/0/0/0	0/0/0/0
6	ADP	D	2008	3	-	0/12/32/32	0/3/3/3
6	ADP	D	2009	3	-	0/12/32/32	0/3/3/3
7	NLG	D	2010	-	-	0/7/13/13	0/0/0/0
9	GOL	D	2015	-	-	0/4/4/4	0/0/0/0

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	2008	ADP	O4'-C4'	-2.67	1.38	1.45
6	A	2008	ADP	O4'-C4'	-2.27	1.39	1.45
6	A	2008	ADP	C2'-C1'	-2.22	1.50	1.53
6	B	2009	ADP	O4'-C1'	2.16	1.44	1.41
6	D	2008	ADP	C2-N1	2.21	1.38	1.33

The worst 5 of 32 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	2008	ADP	N3-C2-N1	-8.67	122.06	128.87
6	B	2008	ADP	N3-C2-N1	-7.61	122.89	128.87
6	A	2009	ADP	N3-C2-N1	-7.01	123.37	128.87
6	B	2009	ADP	N3-C2-N1	-6.37	123.87	128.87
6	D	2008	ADP	N3-C2-N1	-6.13	124.06	128.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 10 short contacts:

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

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, 95^{th} 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%)	-0.50	3 (0%) 95 95	12, 24, 47, 94	3 (0%)
1	B	1426/1489 (95%)	0.10	52 (3%) 46 38	19, 55, 87, 116	3 (0%)
1	C	1421/1489 (95%)	0.74	237 (16%) 2 1	20, 64, 144, 172	3 (0%)
1	D	1430/1489 (96%)	-0.49	14 (0%) 84 81	12, 24, 48, 113	3 (0%)
All	All	5699/5956 (95%)	-0.04	306 (5%) 29 22	12, 34, 111, 172	12 (0%)

The worst 5 of 306 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	404	THR	12.7
1	C	403	ALA	10.7
1	C	343	ASN	9.3
1	C	268	PRO	9.3
1	C	368	SER	8.8

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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} 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	LLDF	B-factors(Å^2)	Q<0.9
4	K	C	2012	1/1	0.92	0.24	9.67	75,75,75,75	0
4	K	B	2013	1/1	0.98	0.23	4.99	61,61,61,61	0
9	GOL	D	2015	6/6	0.98	0.16	1.25	30,34,37,38	0
4	K	B	2006	1/1	0.99	0.23	1.00	65,65,65,65	0
7	NLG	A	2010	13/13	0.96	0.16	0.84	17,18,19,21	0
7	NLG	D	2010	13/13	0.98	0.15	0.67	20,21,24,25	0
10	EDO	A	2016	4/4	0.94	0.16	0.31	39,40,40,41	0
3	MG	D	2002	1/1	0.97	0.14	0.26	13,13,13,13	0
5	PO4	A	2007	5/5	0.99	0.12	-0.35	11,12,12,13	0
4	K	C	2005	1/1	0.96	0.18	-0.39	45,45,45,45	0
6	ADP	C	2009	27/27	0.96	0.14	-0.47	28,31,37,38	0
7	NLG	B	2010	13/13	0.96	0.12	-0.57	16,23,25,26	0
7	NLG	C	2010	13/13	0.96	0.12	-0.65	18,22,25,26	0
6	ADP	B	2009	27/27	0.96	0.13	-0.81	24,28,35,37	0
6	ADP	A	2008	27/27	0.98	0.11	-0.90	7,8,11,12	0
5	PO4	D	2007	5/5	1.00	0.11	-0.90	11,11,13,14	0
6	ADP	D	2008	27/27	0.98	0.11	-0.90	7,7,10,10	0
6	ADP	C	2008	27/27	0.95	0.14	-0.92	26,29,36,38	0
2	NI	C	2001	1/1	0.89	0.18	-1.02	56,56,56,56	0
9	GOL	A	2015	6/6	0.95	0.11	-1.07	26,29,29,29	0
6	ADP	A	2009	27/27	0.96	0.12	-1.34	28,31,46,47	0
4	K	A	2005	1/1	0.99	0.11	-1.45	31,31,31,31	0
3	MG	A	2002	1/1	0.98	0.11	-1.67	13,13,13,13	0
5	PO4	B	2007	5/5	0.96	0.11	-1.77	26,26,29,29	0
3	MG	C	2002	1/1	0.97	0.07	-1.98	20,20,20,20	0
6	ADP	D	2009	27/27	0.97	0.09	-1.99	27,31,44,45	0
6	ADP	B	2008	27/27	0.97	0.10	-2.04	25,29,32,32	0
4	K	C	2004	1/1	0.95	0.09	-2.20	44,44,44,44	0
4	K	D	2004	1/1	0.99	0.09	-2.44	8,8,8,8	0
4	K	C	2006	1/1	0.83	0.12	-2.49	78,78,78,78	0
4	K	B	2004	1/1	0.98	0.05	-2.49	39,39,39,39	0
5	PO4	C	2007	5/5	0.97	0.07	-2.76	32,34,34,35	0
4	K	D	2006	1/1	0.99	0.08	-3.01	53,53,53,53	0
4	K	A	2004	1/1	0.99	0.08	-3.11	9,9,9,9	0
4	K	A	2014	1/1	0.99	0.04	-3.30	24,24,24,24	0
4	K	D	2013	1/1	0.99	0.04	-3.38	18,18,18,18	0
3	MG	D	2011	1/1	0.92	0.05	-3.64	34,34,34,34	0
4	K	D	2014	1/1	0.99	0.04	-3.94	37,37,37,37	0
4	K	B	2005	1/1	0.98	0.06	-4.28	42,42,42,42	0
2	NI	D	2001	1/1	0.99	0.07	-4.28	34,34,34,34	0
2	NI	B	2001	1/1	0.98	0.06	-4.30	75,75,75,75	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	K	A	2013	1/1	0.98	0.05	-4.48	32,32,32,32	0
3	MG	B	2002	1/1	0.95	0.08	-4.96	21,21,21,21	0
4	K	D	2005	1/1	0.98	0.07	-6.14	30,30,30,30	0
4	K	A	2006	1/1	0.98	0.06	-7.34	46,46,46,46	0
2	NI	A	2001	1/1	1.00	0.04	-8.76	34,34,34,34	0
3	MG	C	2011	1/1	0.98	0.04	-	41,41,41,41	0
3	MG	A	2011	1/1	0.93	0.05	-	41,41,41,41	0
8	CL	D	2012	1/1	0.99	0.11	-	26,26,26,26	0
3	MG	A	2003	1/1	0.97	0.09	-	9,9,9,9	0
3	MG	C	2003	1/1	0.92	0.05	-	20,20,20,20	0
3	MG	B	2011	1/1	0.94	0.05	-	15,15,15,15	0
3	MG	B	2003	1/1	0.94	0.07	-	35,35,35,35	0
3	MG	D	2003	1/1	0.98	0.11	-	13,13,13,13	0
8	CL	B	2012	1/1	0.96	0.09	-	43,43,43,43	0
8	CL	A	2012	1/1	0.99	0.06	-	31,31,31,31	0

6.5 Other polymers (i)

There are no such residues in this entry.