



Full wwPDB X-ray Structure Validation Report ⓘ

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 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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

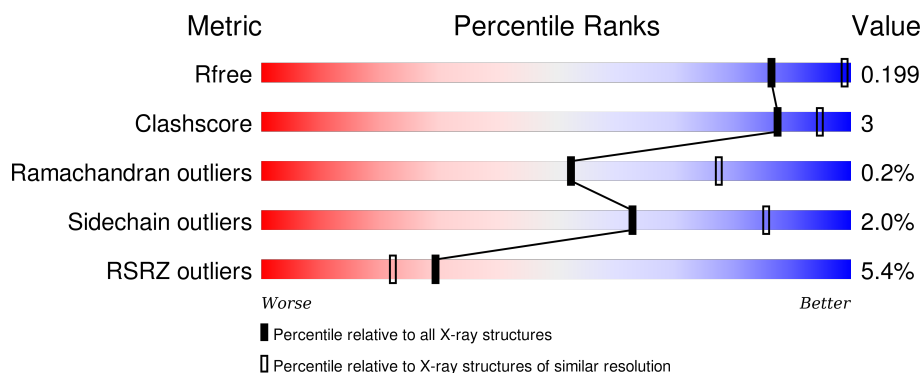
1 Overall quality at a glance

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 $\leq 5\%$. 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	<div> <div></div> <div>88%7%•</div> </div>
1	B	1489	<div> <div>3%</div> <div>88%8%•</div> </div>
1	C	1489	<div> <div>16%</div> <div>88%7%5%</div> </div>
1	D	1489	<div> <div>%</div> <div>88%8%•</div> </div>

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).

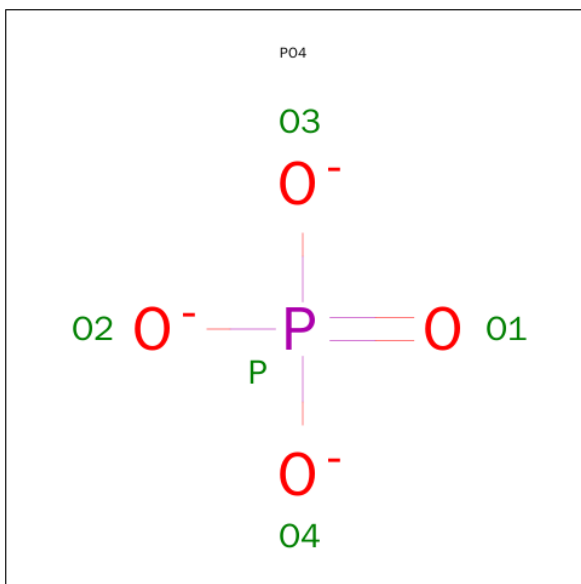
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	4	Total K 4 4	0	0
4	A	5	Total K 5 5	0	0
4	D	5	Total K 5 5	0	0

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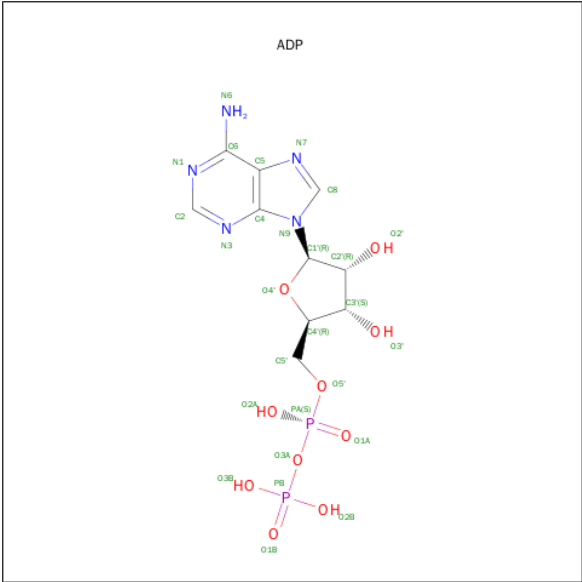
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	4	Total K 4 4	0	0

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



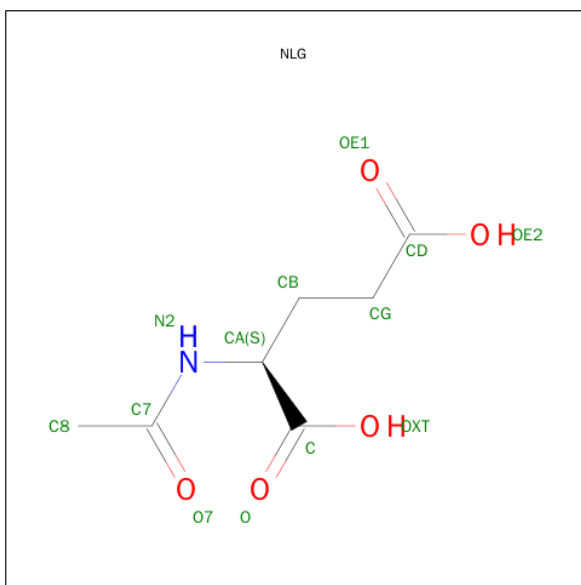
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O P 5 4 1	0	0
5	B	1	Total O P 5 4 1	0	0
5	C	1	Total O P 5 4 1	0	0
5	D	1	Total O P 5 4 1	0	0

- 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: C₇H₁₁NO₅).

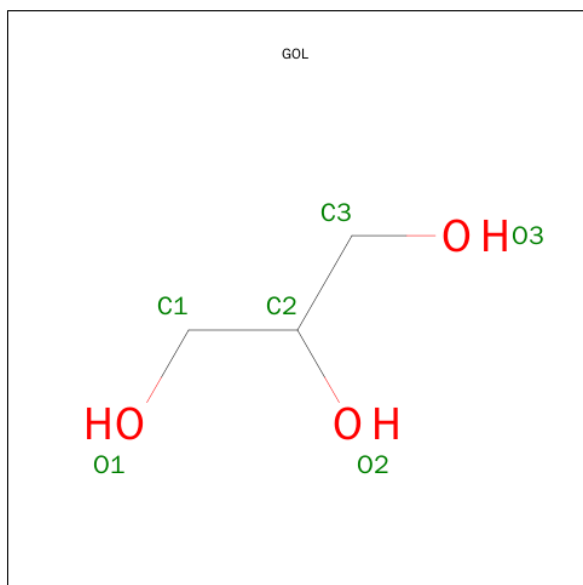


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total 13	C 7	N 1	O 5	0	0
7	B	1	Total 13	C 7	N 1	O 5	0	0
7	C	1	Total 13	C 7	N 1	O 5	0	0
7	D	1	Total 13	C 7	N 1	O 5	0	0

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

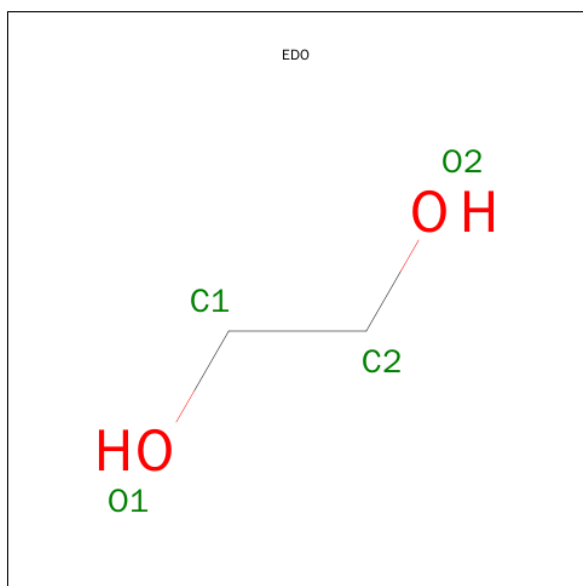
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	B	1	Total Cl 1 1	0	0
8	A	1	Total Cl 1 1	0	0
8	D	1	Total Cl 1 1	0	0

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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 (three-letter code: EDO) (formula: $C_2H_6O_2$).



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

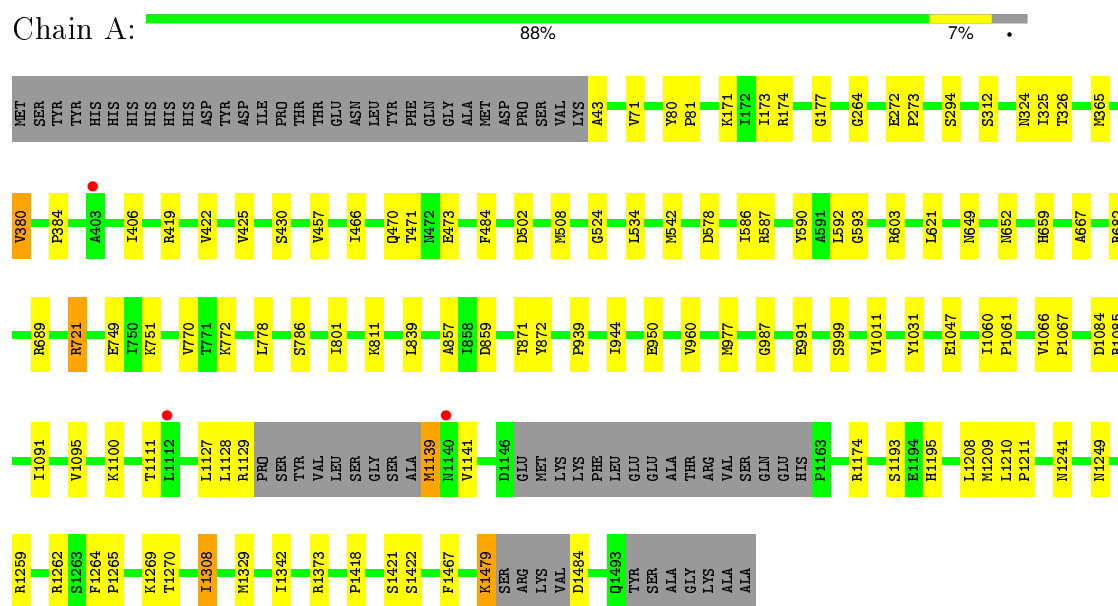
- Molecule 11 is water.

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

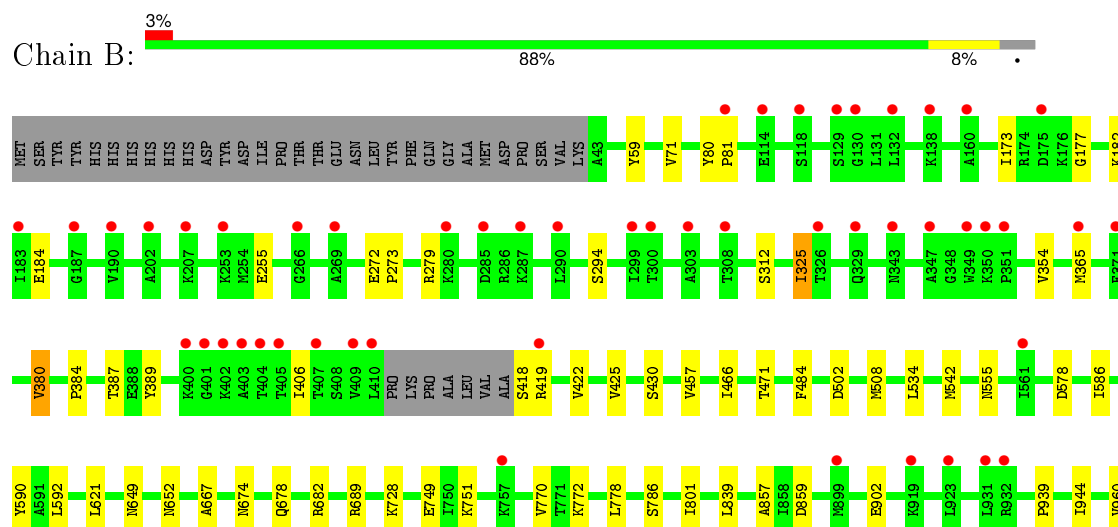
3 Residue-property plots

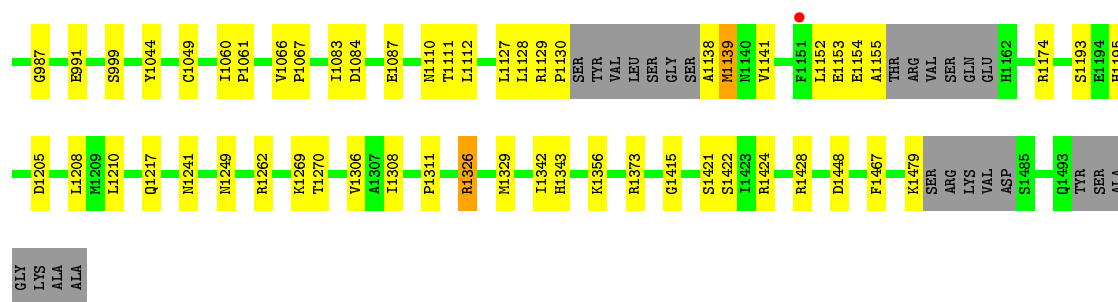
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

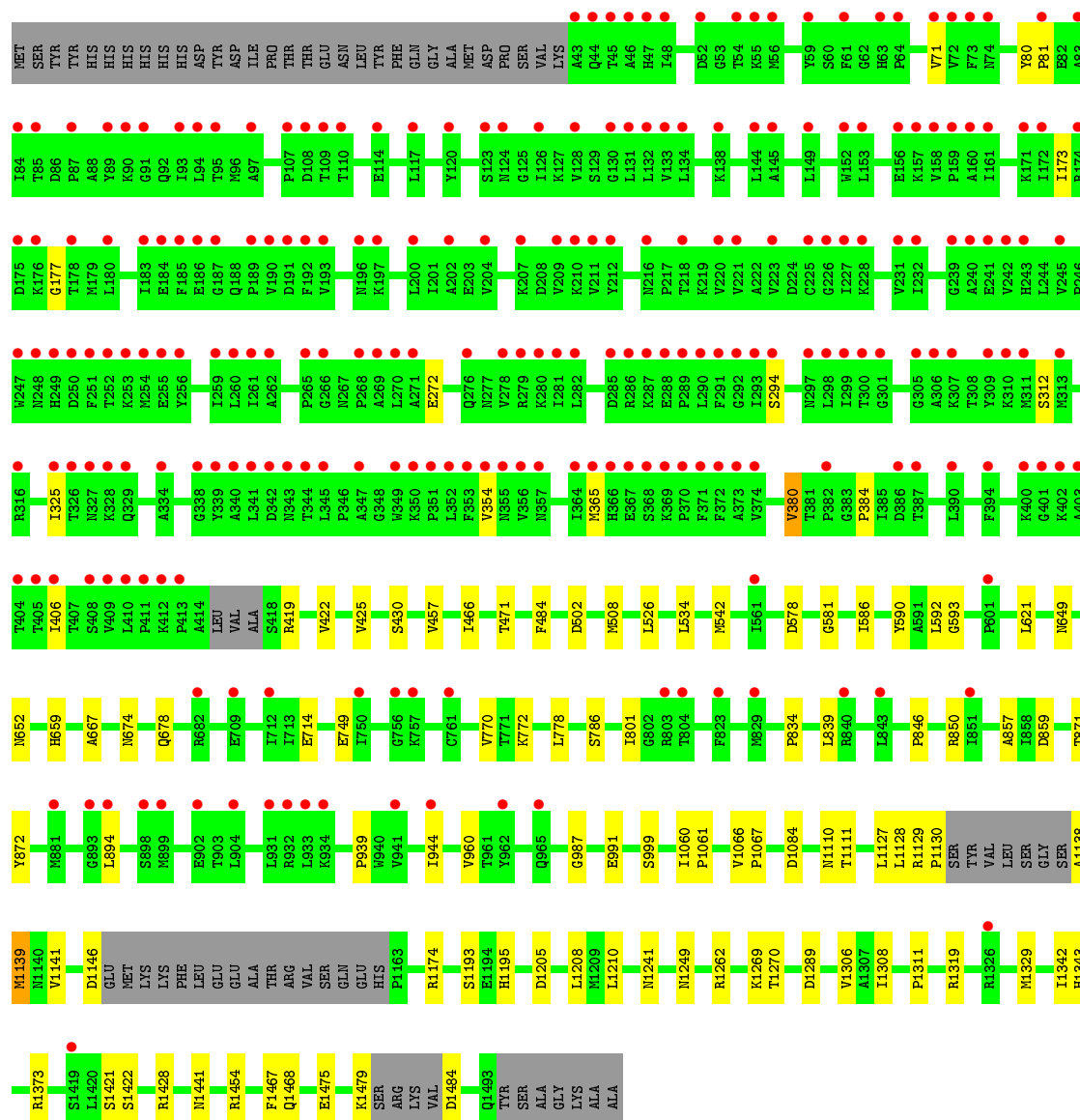
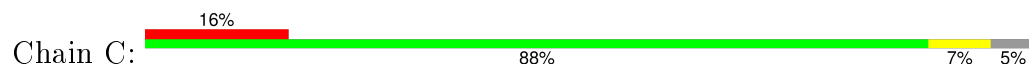


- Molecule 1: Carbamoyl-phosphate synthase [ammonia], mitochondrial

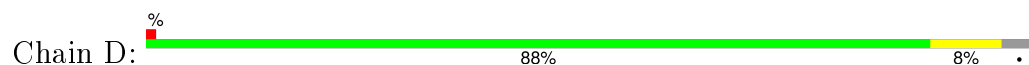


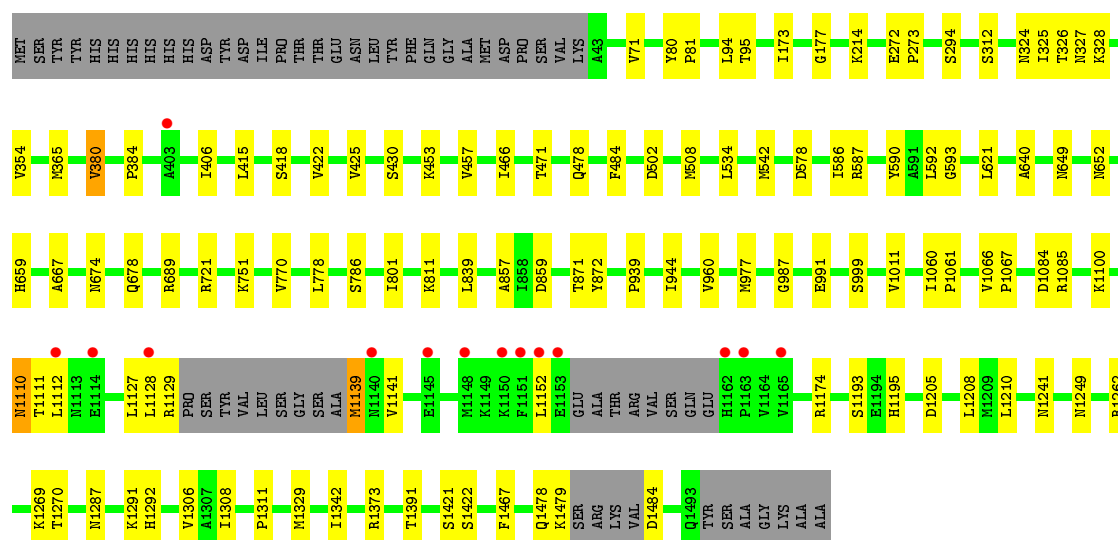


- Molecule 1: Carbamoyl-phosphate synthase [ammonia], mitochondrial



- 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 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
$\langle I/\sigma(I) \rangle$ 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 (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	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ 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.

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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

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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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: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
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:1127:LEU:HD23	1:B:1141:VAL:HG22	1.69	0.72
1:B:939:PRO:HB2	1:B:960:VAL:HG13	1.71	0.72
1:A:419[B]:ARG:NH1	1:A:419[B]:ARG:CG	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:D:1129:ARG:HG3	1:D:1139:MET:HG2	1.88	0.54
1:A:471:THR:OG1	1:A:1269:LYS:NZ	2.41	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:HD12	1:D:592:LEU:C	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:770:VAL:HG12	1:A:801:ILE:HG12	1.93	0.51
1:A:473:GLU:OE1	10:A:2016:EDO:C1	2.59	0.51
1:D:587:ARG:NH1	6:D:2008:ADP:O1A	2.43	0.51
1:B:667:ALA:HB3	1:B:770:VAL:HG22	1.93	0.51
1:A:80:TYR:CG	1:A:81:PRO:HD3	2.46	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:C	1:A:592:LEU:HD12	2.32	0.50
1:B:1195:HIS:CD2	1:B:1208:LEU:CD2	2.95	0.50
1:B:425:VAL:HG23	1:B:457:VAL:CG1	2.42	0.50
1:A:1308:ILE:HD11	1:A:1342:ILE:HG13	1.94	0.50
1:B:1139:MET:O	1:B:1326:ARG:NH2	2.45	0.49
1:C:846:PRO:HG3	1:C:850:ARG:NH1	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1418:PRO:O	1:D:214:LYS:HE3	2.12	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:D:667:ALA:HB3	1:D:770:VAL:HG22	1.93	0.48
1:D:80:TYR:CG	1:D:81:PRO:HD3	2.47	0.48
1:A:542:MET:HG2	1:A:590:TYR:OH	2.12	0.48
1:D:365:MET:CB	1:D:406:ILE:HG21	2.40	0.48
6:D:2009:ADP:O2A	6:D:2009:ADP:O3B	2.31	0.48
1:C:80:TYR:CG	1:C:81:PRO:HD3	2.47	0.48
1:D:502:ASP:N	1:D:502:ASP:OD1	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:C:425:VAL:HG23	1:C:457:VAL:HG11	1.95	0.47
1:B:542:MET:HG2	1:B:590:TYR:OH	2.13	0.47
1:B:80:TYR:CG	1:B:81:PRO:HD3	2.49	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:D:1066:VAL:HB	1:D:1067:PRO:HD3	1.98	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: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:1110:ASN:ND2	1:D:1110:ASN:N	2.64	0.46
1:D:71:VAL:HG12	1:D:173:ILE:HD11	1.98	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:1060:ILE:HB	1:D:1061:PRO:HD3	1.98	0.45
1:D:586:ILE:HA	1:D:621:LEU:O	2.17	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:D:272:GLU:O	1:D:273:PRO:C	2.53	0.44
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:1205:ASP:O	1:C:1311:PRO:HG3	2.17	0.44
1:C:778:LEU:HD13	1:C:786:SER:HA	1.99	0.44
1:D:380:VAL:HG11	1:D:384:PRO:O	2.16	0.44
1:C:71:VAL:HG12	1:C:173:ILE:HD11	1.98	0.44
1:C:1060:ILE:HB	1:C:1061:PRO:HD3	2.00	0.44
1:C:380:VAL:HG11	1:C:384:PRO:O	2.18	0.44
1:A:1210:LEU:HD23	1:A:1270:THR:HG21	2.00	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:D:1127:LEU:HD22	1:D:1139:MET:CE	2.48	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: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: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: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: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:C:987:GLY:HA2	1:C:1329:MET:CE	2.49	0.43
1:B:1044:TYR:CD1	1:B:1049:CYS:HB2	2.54	0.43
1:A:1060:ILE:HB	1:A:1061:PRO:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:593:GLY:HA2	1:C:659:HIS:CE1	2.54	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: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:A:71:VAL:HG12	1:A:173:ILE:HD11	2.00	0.43
1:D:987:GLY:HA2	1:D:1329:MET:CE	2.49	0.42
1:D:1127:LEU:HD22	1:D:1139:MET:HE2	2.01	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:1391:THR:OG1	7:D:2010:NLG:OE2	2.26	0.42
1:B:255:GLU:HG2	1:B:255:GLU:O	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:C:1210:LEU:HD23	1:C:1270:THR:HG21	2.02	0.42
1:B:839:LEU:HD21	1:B:857:ALA:HA	2.01	0.42
1:C:871:THR:O	1:C:872:TYR:HB2	2.19	0.42
1:C:991:GLU:HG3	1:C:1262:ARG:HB2	2.01	0.42
1:B:674:ASN:O	1:B:678:GLN:HG2	2.20	0.42
1:A:1211:PRO:HB2	1:B:1217:GLN:OE1	2.20	0.42
1:B:1152:LEU:O	1:B:1155:ALA:N	2.51	0.42
1:A:466:ILE:HD12	1:A:484:PHE:CE1	2.55	0.42
1:D:977:MET:HA	1:D:1011:VAL:O	2.20	0.42
1:D:811:LYS:HE2	11:D:2287:HOH:O	2.19	0.42
1:B:419:ARG:NH1	1:B:749:GLU:OE1	2.51	0.42
1:A:502:ASP:N	1:A:502:ASP:OD1	2.47	0.42
1:C:839:LEU:HD21	1:C:857:ALA:HA	2.01	0.42
1:B:1152:LEU:C	1:B:1154:GLU:N	2.73	0.42
1:D:94:LEU:HD12	1:D:95:THR:N	2.34	0.42
1:B:1373:ARG:HB3	1:B:1467:PHE:CZ	2.54	0.42
1:D:1306:VAL:HG21	1:D:1342:ILE:HD13	2.02	0.42
1:B:682:ARG:HD2	1:B:682:ARG:HA	1.84	0.42
1:A:1066:VAL:HB	1:A:1067:PRO:HD3	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:B:728:LYS:HA	1:B:728:LYS:HD3	1.96	0.41
1:A:524:GLY:HA2	11:A:2325:HOH:O	2.19	0.41
1:D:1373:ARG:HB3	1:D:1467:PHE:CZ	2.54	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:586:ILE:HA	1:B:621:LEU:O	2.21	0.41
1:C:1066:VAL:HB	1:C:1067:PRO:HD3	2.02	0.41
1:B:1415:GLY:HA2	11:B:2176:HOH:O	2.19	0.41
1:B:991:GLU:HG3	1:B:1262:ARG:CB	2.50	0.41
1:D:415:LEU:HB3	1:D:640:ALA:O	2.20	0.41
1:D:324:ASN:OD1	1:D:326:THR:HB	2.21	0.41
1:A:721:ARG:NH2	5:A:2007:PO4:O4	2.47	0.41
1:C:1306:VAL:HG21	1:C:1342:ILE:HD13	2.02	0.41
1:A:1479:LYS:HD2	1:A:1479:LYS:HA	1.95	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:D:1205:ASP:O	1:D:1311:PRO:HG3	2.21	0.41
1:C:325:ILE:HD11	1:C:354:VAL:HB	2.03	0.41
1:D:1291:LYS:HE3	1:D:1292:HIS:NE2	2.36	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:B:272:GLU:O	1:B:273:PRO:C	2.59	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: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:A:1259:ARG:NE	11:A:2144:HOH:O	2.51	0.41
1:D:674:ASN:O	1:D:678:GLN:HG2	2.21	0.41
1:C:991:GLU:HG3	1:C:1262:ARG:CB	2.51	0.40
1:A:1091:ILE:O	1:A:1095:VAL:HG23	2.21	0.40
9:D:2015:GOL:C1	11:D:2152:HOH:O	2.69	0.40
1:C:674:ASN:O	1:C:678:GLN:HG2	2.22	0.40
1:B:325:ILE:HD11	1:B:354:VAL:HB	2.02	0.40
1:D:1110:ASN:HD22	1:D:1110:ASN:N	2.19	0.40
1:A:682:ARG:HA	1:A:682:ARG:HD2	1.80	0.40
1:B:1130:PRO:HD2	1:B:1138:ALA:O	2.21	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%)	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

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%)	65	86

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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

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

Some 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 carbohydrates 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$
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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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

All (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
6	B	2008	ADP	C2-N3	2.22	1.36	1.32
6	B	2009	ADP	C2-N3	2.27	1.36	1.32
6	C	2008	ADP	O4'-C1'	2.28	1.44	1.41
6	D	2008	ADP	C5-C4	2.44	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	2009	ADP	O4'-C1'	2.53	1.44	1.41
6	A	2008	ADP	O4'-C1'	2.55	1.44	1.41
6	C	2009	ADP	C2-N3	2.59	1.36	1.32
6	D	2008	ADP	C2-N3	2.67	1.36	1.32
6	A	2008	ADP	C2-N1	2.80	1.39	1.33
6	C	2008	ADP	C5-C4	2.81	1.46	1.40
6	B	2009	ADP	C5-C4	2.95	1.47	1.40
6	A	2009	ADP	C5-C4	3.06	1.47	1.40
6	C	2009	ADP	C5-C4	3.10	1.47	1.40
6	B	2008	ADP	C5-C4	3.33	1.48	1.40
6	D	2009	ADP	C5-C4	3.48	1.48	1.40

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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
6	C	2009	ADP	N3-C2-N1	-6.11	124.07	128.87
6	D	2009	ADP	N3-C2-N1	-6.08	124.10	128.87
6	A	2008	ADP	N3-C2-N1	-5.20	124.79	128.87
6	C	2008	ADP	C1'-N9-C4	-3.00	123.45	126.81
6	D	2008	ADP	C1'-N9-C4	-2.51	124.00	126.81
6	A	2008	ADP	O5'-PA-O1A	-2.46	99.15	109.21
6	A	2008	ADP	C1'-N9-C4	-2.38	124.15	126.81
7	D	2010	NLG	O7-C7-C8	-2.34	117.77	122.07
6	B	2009	ADP	O3B-PB-O2B	2.01	114.81	107.44
6	C	2008	ADP	O3B-PB-O2B	2.01	114.81	107.44
6	C	2008	ADP	C2-N1-C6	2.02	122.37	118.77
6	A	2008	ADP	O2A-PA-O1A	2.05	123.25	112.56
6	A	2009	ADP	N6-C6-N1	2.08	122.01	118.52
6	B	2008	ADP	O3B-PB-O2B	2.22	115.60	107.44
6	B	2009	ADP	O3B-PB-O1B	2.38	118.40	110.63
6	D	2008	ADP	O2A-PA-O3A	2.41	115.61	105.27
6	D	2008	ADP	O3B-PB-O1B	2.60	119.11	110.63
6	D	2008	ADP	O3B-PB-O2B	2.68	117.28	107.44
6	C	2009	ADP	O3B-PB-O1B	2.71	119.47	110.63
7	A	2010	NLG	C-CA-N2	2.95	118.81	112.93
6	C	2008	ADP	C4'-O4'-C1'	2.96	112.78	109.64
6	A	2008	ADP	O3B-PB-O1B	3.01	120.43	110.63

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
6	D	2008	ADP	N6-C6-N1	3.02	123.58	118.52
6	A	2008	ADP	C4'-O4'-C1'	3.04	112.86	109.64
7	D	2010	NLG	CB-CA-N2	3.05	114.69	109.92
6	C	2009	ADP	N6-C6-N1	3.18	123.86	118.52
6	B	2008	ADP	N6-C6-N1	3.43	124.27	118.52

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 [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	-0.50	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%)

All (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
1	C	130	GLY	8.7
1	C	405	THR	8.6
1	C	225	CYS	8.5
1	C	131	LEU	8.0
1	C	192	PHE	7.9
1	C	183	ILE	7.6
1	C	401	GLY	7.5
1	C	309	TYR	7.5
1	C	176	LYS	7.4
1	C	227	ILE	6.8
1	B	371	PHE	6.8
1	C	338	GLY	6.8
1	C	46	ALA	6.7
1	C	413	PRO	6.7
1	C	291	PHE	6.6
1	C	260	LEU	6.6

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Mol	Chain	Res	Type	RSRZ
1	C	240	ALA	6.5
1	C	253	LYS	6.3
1	C	349	TRP	6.3
1	C	354	VAL	6.2
1	C	364	ILE	6.1
1	C	356	VAL	6.0
1	C	299	ILE	5.9
1	C	293	ILE	5.7
1	C	406	ILE	5.7
1	C	251	PHE	5.7
1	C	371	PHE	5.6
1	C	255	GLU	5.6
1	C	369	LYS	5.5
1	C	245	VAL	5.5
1	C	174[A]	ARG	5.5
1	C	757	LYS	5.4
1	C	412	LYS	5.4
1	C	402	LYS	5.3
1	C	120	TYR	5.3
1	C	72	VAL	5.3
1	C	298	LEU	5.2
1	C	132	LEU	5.2
1	C	44	GLN	5.2
1	C	84	ILE	5.1
1	C	144	LEU	5.1
1	C	160	ALA	5.1
1	B	326	THR	5.0
1	C	301	GLY	5.0
1	C	286	ARG	4.9
1	C	372	PHE	4.9
1	C	48	ILE	4.8
1	C	59	TYR	4.8
1	C	374	VAL	4.8
1	C	307	LYS	4.7
1	C	145	ALA	4.7
1	C	340	ALA	4.7
1	C	209	VAL	4.7
1	C	269	ALA	4.6
1	C	287	LYS	4.6
1	C	353	PHE	4.6
1	C	270	LEU	4.6
1	C	355	ASN	4.6

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Mol	Chain	Res	Type	RSRZ
1	C	89	TYR	4.5
1	C	261	ILE	4.5
1	C	91	GLY	4.5
1	C	357	ASN	4.4
1	C	184	GLU	4.4
1	C	90	LYS	4.4
1	C	278	VAL	4.4
1	C	271	ALA	4.4
1	C	280	LYS	4.3
1	C	87	PRO	4.3
1	C	202	ALA	4.3
1	C	248	ASN	4.3
1	C	243	HIS	4.3
1	C	93	ILE	4.3
1	C	934	LYS	4.3
1	B	404	THR	4.2
1	C	342	ASP	4.2
1	C	190	VAL	4.2
1	C	221	VAL	4.1
1	C	56	MET	4.1
1	C	114	GLU	4.1
1	C	933	LEU	4.1
1	B	401	GLY	4.0
1	C	899	MET	4.0
1	C	352	LEU	4.0
1	B	187	GLY	4.0
1	B	266	GLY	4.0
1	C	351	PRO	4.0
1	C	334	ALA	3.9
1	C	187	GLY	3.9
1	C	226	GLY	3.9
1	C	339	TYR	3.9
1	C	328	LYS	3.9
1	B	410	LEU	3.8
1	C	367	GLU	3.8
1	C	193	VAL	3.8
1	C	387	THR	3.8
1	C	297	ASN	3.8
1	C	197	LYS	3.7
1	C	931	LEU	3.7
1	C	290	LEU	3.7
1	C	45	THR	3.7

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Mol	Chain	Res	Type	RSRZ
1	C	242	VAL	3.7
1	C	282	LEU	3.6
1	B	130	GLY	3.6
1	C	394	PHE	3.6
1	B	114	GLU	3.6
1	D	1153	GLU	3.6
1	C	329	GLN	3.6
1	C	152	TRP	3.6
1	C	756	GLY	3.6
1	C	823	PHE	3.6
1	C	210	LYS	3.6
1	C	159	PRO	3.6
1	C	288	GLU	3.6
1	C	157	LYS	3.6
1	C	134	LEU	3.6
1	C	366	HIS	3.5
1	B	269	ALA	3.5
1	C	191	ASP	3.5
1	C	185	PHE	3.5
1	B	403	ALA	3.5
1	C	218	THR	3.4
1	D	403	ALA	3.4
1	A	1112	LEU	3.4
1	C	95	THR	3.4
1	C	186	GLU	3.4
1	C	126	ILE	3.4
1	C	171	LYS	3.4
1	B	202	ALA	3.4
1	C	265	PRO	3.4
1	B	419	ARG	3.4
1	C	266	GLY	3.4
1	C	204	VAL	3.4
1	C	347	ALA	3.3
1	C	843	LEU	3.3
1	B	400	LYS	3.3
1	C	294	SER	3.3
1	C	63	HIS	3.3
1	C	285	ASP	3.2
1	C	73	PHE	3.2
1	B	351	PRO	3.2
1	C	109	THR	3.2
1	C	232	ILE	3.2

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Mol	Chain	Res	Type	RSRZ
1	C	386	ASP	3.2
1	C	279	ARG	3.2
1	C	52	ASP	3.1
1	C	292	GLY	3.1
1	B	350	LYS	3.1
1	C	276	GLN	3.1
1	C	211	VAL	3.1
1	B	405	THR	3.1
1	A	403	ALA	3.1
1	C	829	MET	3.0
1	C	904	LEU	3.0
1	C	840	ARG	3.0
1	B	81	PRO	3.0
1	B	207	LYS	3.0
1	C	300	THR	3.0
1	C	365	MET	3.0
1	C	247	TRP	3.0
1	C	311	MET	3.0
1	C	161	ILE	3.0
1	C	97	ALA	3.0
1	C	902	GLU	2.9
1	D	1152	LEU	2.9
1	B	285	ASP	2.9
1	D	1150	LYS	2.9
1	C	345	LEU	2.9
1	C	712	ILE	2.9
1	C	1326	ARG	2.9
1	C	341	LEU	2.9
1	C	804	THR	2.9
1	B	409	VAL	2.9
1	C	158	VAL	2.9
1	C	108	ASP	2.9
1	C	408	SER	2.9
1	C	64	PRO	2.9
1	C	410	LEU	2.9
1	C	306	ALA	2.9
1	C	327	ASN	2.9
1	C	196	ASN	2.8
1	C	409	VAL	2.8
1	B	253	LYS	2.8
1	C	71	VAL	2.8
1	C	893	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	250	ASP	2.8
1	B	402	LYS	2.8
1	C	189	PRO	2.8
1	C	962	TYR	2.8
1	D	1145	GLU	2.8
1	C	133	VAL	2.8
1	C	932	ARG	2.8
1	C	123	SER	2.8
1	C	350	LYS	2.8
1	C	110	THR	2.8
1	B	347	ALA	2.7
1	C	241	GLU	2.7
1	C	83	ALA	2.7
1	C	128	VAL	2.7
1	B	132	LEU	2.7
1	B	329	GLN	2.6
1	C	94	LEU	2.6
1	C	259	ILE	2.6
1	C	281	ILE	2.6
1	C	153	LEU	2.6
1	C	881	MET	2.6
1	C	85	THR	2.6
1	C	138	LYS	2.6
1	C	207	LYS	2.6
1	C	310	LYS	2.6
1	C	561	ILE	2.6
1	C	289	PRO	2.6
1	C	373	ALA	2.6
1	B	365	MET	2.6
1	B	287	LYS	2.5
1	C	223	VAL	2.5
1	B	118	SER	2.5
1	C	107	PRO	2.5
1	C	344	THR	2.5
1	C	216	ASN	2.5
1	C	252	THR	2.5
1	C	325	ILE	2.5
1	C	761	CYS	2.5
1	B	175	ASP	2.5
1	D	1148	MET	2.4
1	C	305	GLY	2.4
1	B	407	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	C	326	THR	2.4
1	D	1151	PHE	2.4
1	B	190	VAL	2.4
1	C	212	TYR	2.4
1	C	256	TYR	2.4
1	B	931	LEU	2.4
1	C	228	LYS	2.4
1	C	81	PRO	2.3
1	D	1140	ASN	2.3
1	C	941	VAL	2.3
1	C	965	GLN	2.3
1	C	382	PRO	2.3
1	C	43	ALA	2.3
1	C	231	VAL	2.3
1	B	561	ILE	2.3
1	C	178	THR	2.3
1	C	709	GLU	2.3
1	C	316	ARG	2.3
1	C	803	ARG	2.3
1	B	919	LYS	2.3
1	C	172	ILE	2.3
1	C	400	LYS	2.3
1	B	290	LEU	2.2
1	C	200	LEU	2.2
1	C	390	LEU	2.2
1	C	894	LEU	2.2
1	D	1162	HIS	2.2
1	C	262	ALA	2.2
1	C	239	GLY	2.2
1	C	124	ASN	2.2
1	B	183	ILE	2.2
1	C	220	VAL	2.2
1	C	74	ASN	2.2
1	B	308	THR	2.2
1	B	1151	PHE	2.2
1	C	851	ILE	2.2
1	C	601	PRO	2.2
1	C	55	LYS	2.2
1	B	343	ASN	2.2
1	C	944	ILE	2.2
1	C	156	GLU	2.2
1	C	175	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	313	MET	2.2
1	C	1419	SER	2.2
1	D	1165	VAL	2.2
1	B	757	LYS	2.2
1	C	249	HIS	2.2
1	C	411	PRO	2.2
1	C	61	PHE	2.2
1	B	299	ILE	2.1
1	B	280	LYS	2.1
1	D	1163	PRO	2.1
1	B	899	MET	2.1
1	D	1114	GLU	2.1
1	C	898	SER	2.1
1	B	129	SER	2.1
1	C	54	THR	2.1
1	C	254	MET	2.1
1	B	923	LEU	2.1
1	C	117	LEU	2.1
1	D	1112	LEU	2.1
1	C	370	PRO	2.1
1	C	149	LEU	2.1
1	C	750	ILE	2.1
1	C	47	HIS	2.0
1	A	1140	ASN	2.0
1	B	160	ALA	2.0
1	B	303	ALA	2.0
1	B	300	THR	2.0
1	C	682	ARG	2.0
1	B	138	LYS	2.0
1	B	349	TRP	2.0
1	D	1128	LEU	2.0
1	B	932	ARG	2.0
1	C	180	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 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, 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	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

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
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
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

There are no such residues in this entry.