Full wwPDB X-ray Structure Validation Report

Nov 21, 2016 – 11:57 AM EST

PDB ID	:	5CX7
Title	:	Crystal Structure of PduOC:Heme Complex
Authors	:	Geremia, S.; Hickey, N.; Ortiz de Orue Lucana, D.
Deposited on	:	2015-07-28
Resolution	:	1.97 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 (i) symbol.

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

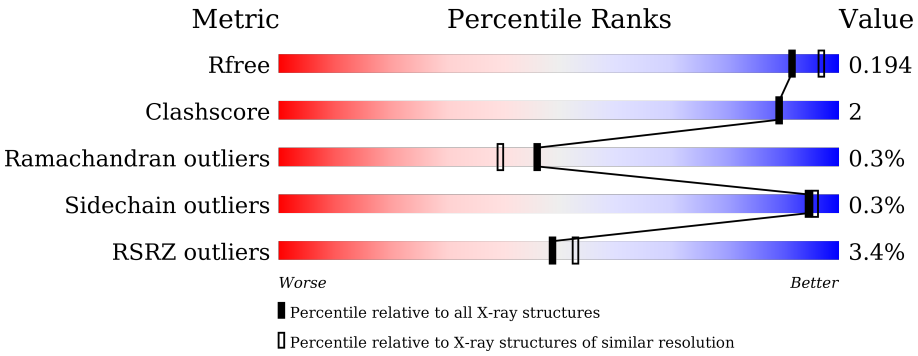
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20028320
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20028320

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 1.97 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	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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	147	89% 5% 6%
1	B	147	3% 90% · 6%
1	C	147	86% 7% · 6%
1	D	147	3% 88% 5% · 6%
1	E	147	89% · · 5%
1	F	147	3% 91% ·· 6%

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Mol	Chain	Length	Quality of chain
1	G	147	3% 90% 6%
1	H	147	2% 88% 5% 6%
1	I	147	5% 90% 6%
1	J	147	3% 90% 6%
1	K	147	% 88% 5% 6%
1	L	147	4% 90% 6%
1	M	147	9% 88% 6% 6%
1	N	147	5% 88% 5% 6%
1	O	147	3% 93% 6%
1	P	147	3% 88% 5% 6%

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
2	HEM	E	201	-	-	-	X
2	HEM	I	201	-	-	-	X
3	GOL	A	203	-	-	-	X
3	GOL	A	204	-	-	-	X
3	GOL	G	202	-	-	-	X
3	GOL	G	204	-	-	-	X
3	GOL	H	201	-	-	-	X
3	GOL	I	202	-	-	-	X
3	GOL	I	203	-	-	-	X
3	GOL	I	205	-	-	-	X
3	GOL	K	202	-	-	-	X
3	GOL	N	201	-	-	-	X
3	GOL	P	202	-	-	-	X
4	NA	A	205	-	-	-	X
4	NA	A	206	-	-	-	X
4	NA	B	202	-	-	-	X
4	NA	E	203	-	-	-	X
4	NA	F	202	-	-	-	X
4	NA	G	205	-	-	-	X
4	NA	H	203	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	NA	I	206	-	-	-	X
4	NA	M	204	-	-	-	X
4	NA	N	202	-	-	-	X
5	CL	J	203	-	-	-	X

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 18350 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 ATP:cob(I)alamin adenosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	138	Total	C	N	O	S	0	0	0
			1024	647	179	195	3			
1	B	138	Total	C	N	O	S	0	0	0
			1024	647	179	195	3			
1	C	138	Total	C	N	O	S	0	0	0
			1024	647	179	195	3			
1	D	138	Total	C	N	O	S	0	0	0
			1024	647	179	195	3			
1	E	139	Total	C	N	O	S	0	0	0
			1031	652	180	196	3			
1	F	138	Total	C	N	O	S	0	0	0
			1024	647	179	195	3			
1	G	138	Total	C	N	O	S	0	0	0
			1024	647	179	195	3			
1	H	138	Total	C	N	O	S	0	0	0
			1024	647	179	195	3			
1	I	138	Total	C	N	O	S	0	0	0
			1024	647	179	195	3			
1	J	138	Total	C	N	O	S	0	0	0
			1024	647	179	195	3			
1	K	138	Total	C	N	O	S	0	0	0
			1024	647	179	195	3			
1	L	138	Total	C	N	O	S	0	0	0
			1024	647	179	195	3			
1	M	138	Total	C	N	O	S	0	0	0
			1024	647	179	195	3			
1	N	138	Total	C	N	O	S	0	0	0
			1024	647	179	195	3			
1	O	138	Total	C	N	O	S	0	0	0
			1024	647	179	195	3			
1	P	138	Total	C	N	O	S	0	0	0
			1024	647	179	195	3			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	-	expression tag	UNP A0A0F0IPG3
A	2	ALA	-	expression tag	UNP A0A0F0IPG3
A	3	MET	-	expression tag	UNP A0A0F0IPG3
A	4	ALA	-	expression tag	UNP A0A0F0IPG3
B	1	GLY	-	expression tag	UNP A0A0F0IPG3
B	2	ALA	-	expression tag	UNP A0A0F0IPG3
B	3	MET	-	expression tag	UNP A0A0F0IPG3
B	4	ALA	-	expression tag	UNP A0A0F0IPG3
C	1	GLY	-	expression tag	UNP A0A0F0IPG3
C	2	ALA	-	expression tag	UNP A0A0F0IPG3
C	3	MET	-	expression tag	UNP A0A0F0IPG3
C	4	ALA	-	expression tag	UNP A0A0F0IPG3
D	1	GLY	-	expression tag	UNP A0A0F0IPG3
D	2	ALA	-	expression tag	UNP A0A0F0IPG3
D	3	MET	-	expression tag	UNP A0A0F0IPG3
D	4	ALA	-	expression tag	UNP A0A0F0IPG3
E	1	GLY	-	expression tag	UNP A0A0F0IPG3
E	2	ALA	-	expression tag	UNP A0A0F0IPG3
E	3	MET	-	expression tag	UNP A0A0F0IPG3
E	4	ALA	-	expression tag	UNP A0A0F0IPG3
F	1	GLY	-	expression tag	UNP A0A0F0IPG3
F	2	ALA	-	expression tag	UNP A0A0F0IPG3
F	3	MET	-	expression tag	UNP A0A0F0IPG3
F	4	ALA	-	expression tag	UNP A0A0F0IPG3
G	1	GLY	-	expression tag	UNP A0A0F0IPG3
G	2	ALA	-	expression tag	UNP A0A0F0IPG3
G	3	MET	-	expression tag	UNP A0A0F0IPG3
G	4	ALA	-	expression tag	UNP A0A0F0IPG3
H	1	GLY	-	expression tag	UNP A0A0F0IPG3
H	2	ALA	-	expression tag	UNP A0A0F0IPG3
H	3	MET	-	expression tag	UNP A0A0F0IPG3
H	4	ALA	-	expression tag	UNP A0A0F0IPG3
I	1	GLY	-	expression tag	UNP A0A0F0IPG3
I	2	ALA	-	expression tag	UNP A0A0F0IPG3
I	3	MET	-	expression tag	UNP A0A0F0IPG3
I	4	ALA	-	expression tag	UNP A0A0F0IPG3
J	1	GLY	-	expression tag	UNP A0A0F0IPG3
J	2	ALA	-	expression tag	UNP A0A0F0IPG3
J	3	MET	-	expression tag	UNP A0A0F0IPG3
J	4	ALA	-	expression tag	UNP A0A0F0IPG3
K	1	GLY	-	expression tag	UNP A0A0F0IPG3
K	2	ALA	-	expression tag	UNP A0A0F0IPG3

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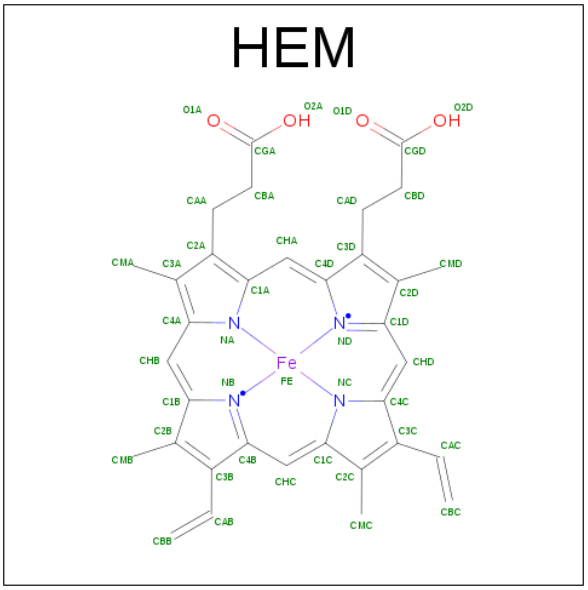
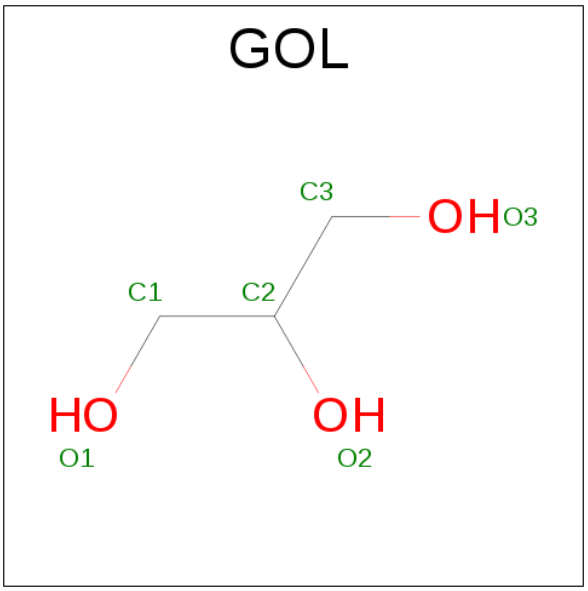
Chain	Residue	Modelled	Actual	Comment	Reference
K	3	MET	-	expression tag	UNP A0A0F0IPG3
K	4	ALA	-	expression tag	UNP A0A0F0IPG3
L	1	GLY	-	expression tag	UNP A0A0F0IPG3
L	2	ALA	-	expression tag	UNP A0A0F0IPG3
L	3	MET	-	expression tag	UNP A0A0F0IPG3
L	4	ALA	-	expression tag	UNP A0A0F0IPG3
M	1	GLY	-	expression tag	UNP A0A0F0IPG3
M	2	ALA	-	expression tag	UNP A0A0F0IPG3
M	3	MET	-	expression tag	UNP A0A0F0IPG3
M	4	ALA	-	expression tag	UNP A0A0F0IPG3
N	1	GLY	-	expression tag	UNP A0A0F0IPG3
N	2	ALA	-	expression tag	UNP A0A0F0IPG3
N	3	MET	-	expression tag	UNP A0A0F0IPG3
N	4	ALA	-	expression tag	UNP A0A0F0IPG3
O	1	GLY	-	expression tag	UNP A0A0F0IPG3
O	2	ALA	-	expression tag	UNP A0A0F0IPG3
O	3	MET	-	expression tag	UNP A0A0F0IPG3
O	4	ALA	-	expression tag	UNP A0A0F0IPG3
P	1	GLY	-	expression tag	UNP A0A0F0IPG3
P	2	ALA	-	expression tag	UNP A0A0F0IPG3
P	3	MET	-	expression tag	UNP A0A0F0IPG3
P	4	ALA	-	expression tag	UNP A0A0F0IPG3

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	E	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	G	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	I	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	K	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	M	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	O	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



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

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	D	1	Total	C	O	0	0
			6	3	3		
3	E	1	Total	C	O	0	0
			6	3	3		
3	F	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	G	1	Total	C	O	0	0
			6	3	3		
3	H	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	I	1	Total	C	O	0	0
			6	3	3		
3	J	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		
3	K	1	Total	C	O	0	0
			6	3	3		
3	M	1	Total	C	O	0	0
			6	3	3		
3	N	1	Total	C	O	0	0
			6	3	3		
3	O	1	Total	C	O	0	0
			6	3	3		
3	P	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	P	1	Total Na 1 1	0	0
4	G	1	Total Na 1 1	0	0
4	J	2	Total Na 2 2	0	0
4	D	1	Total Na 1 1	0	0
4	E	1	Total Na 1 1	0	0
4	H	2	Total Na 2 2	0	0
4	B	1	Total Na 1 1	0	0
4	I	2	Total Na 2 2	0	0
4	A	2	Total Na 2 2	0	0
4	N	1	Total Na 1 1	0	0
4	L	1	Total Na 1 1	0	0
4	F	1	Total Na 1 1	0	0
4	M	2	Total Na 2 2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	J	1	Total Cl 1 1	0	0
5	I	1	Total Cl 1 1	0	0
5	D	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	H	1	Total Mg 1 1	0	0
6	P	1	Total Mg 1 1	0	0

- Molecule 7 is water.

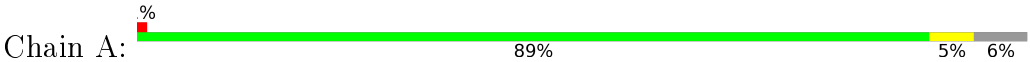
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	123	Total O 123 123	0	0
7	B	87	Total O 87 87	0	0
7	C	109	Total O 109 109	0	0
7	D	85	Total O 85 85	0	0
7	E	108	Total O 108 108	0	0
7	F	76	Total O 76 76	0	0
7	G	103	Total O 103 103	0	0
7	H	102	Total O 102 102	0	0
7	I	83	Total O 83 83	0	0
7	J	71	Total O 71 71	0	0
7	K	100	Total O 100 100	0	0
7	L	72	Total O 72 72	0	0
7	M	62	Total O 62 62	0	0
7	N	72	Total O 72 72	0	0
7	O	88	Total O 88 88	0	0
7	P	100	Total O 100 100	0	0

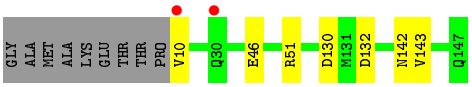
3 Residue-property plots (i)

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: ATP:cob(I)alamin adenosyltransferase

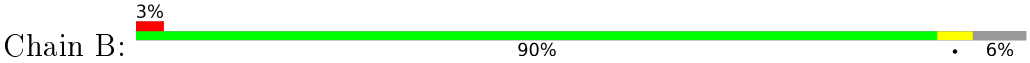
Chain A:

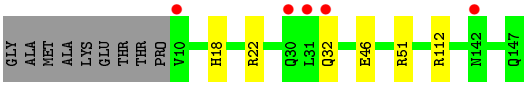




- Molecule 1: ATP:cob(I)alamin adenosyltransferase

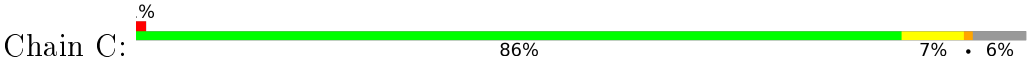
Chain B:

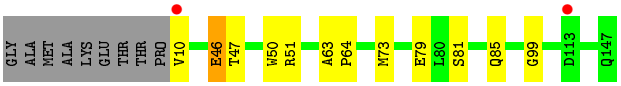




- Molecule 1: ATP:cob(I)alamin adenosyltransferase

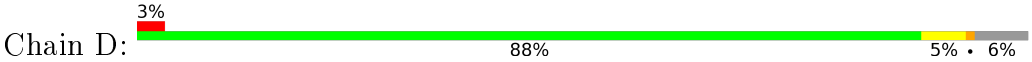
Chain C:

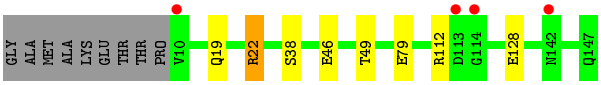




- Molecule 1: ATP:cob(I)alamin adenosyltransferase

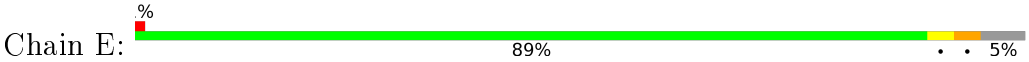
Chain D:

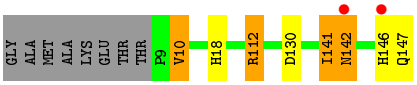




- Molecule 1: ATP:cob(I)alamin adenosyltransferase

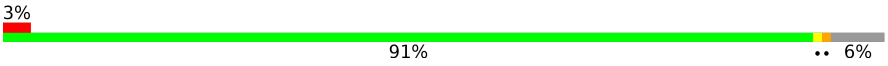
Chain E:

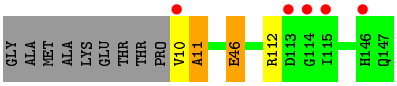




- Molecule 1: ATP:cob(I)alamin adenosyltransferase

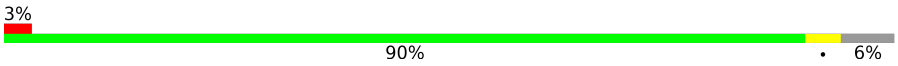
Chain F:

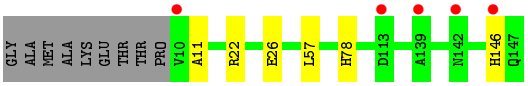




• Molecule 1: ATP:cob(I)alamin adenosyltransferase

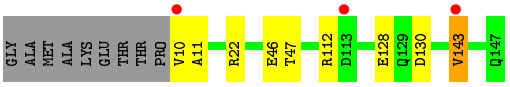
Chain G:





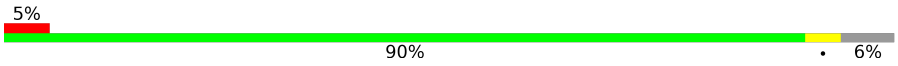
• Molecule 1: ATP:cob(I)alamin adenosyltransferase

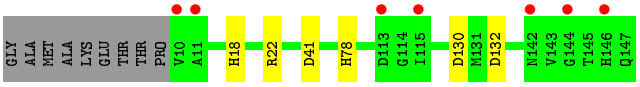
Chain H:



• Molecule 1: ATP:cob(I)alamin adenosyltransferase

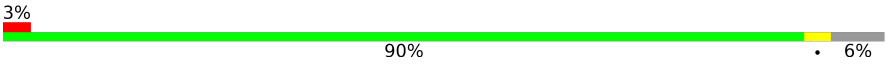
Chain I:

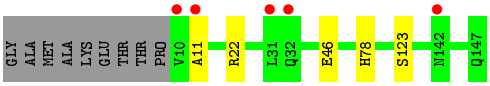




• Molecule 1: ATP:cob(I)alamin adenosyltransferase

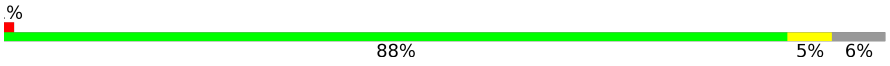
Chain J:

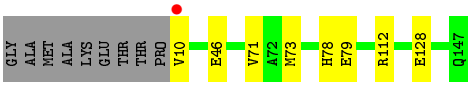




• Molecule 1: ATP:cob(I)alamin adenosyltransferase

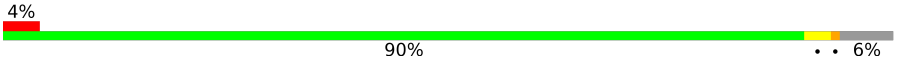
Chain K:





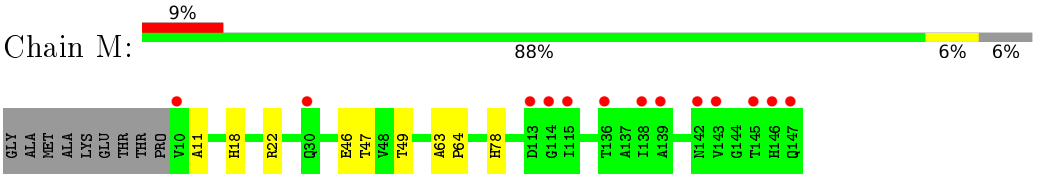
• Molecule 1: ATP:cob(I)alamin adenosyltransferase

Chain L:



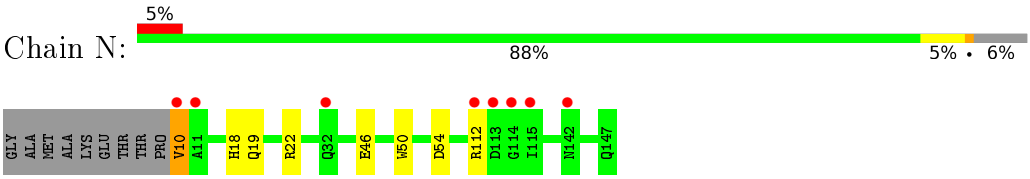
• Molecule 1: ATP:cob(I)alamin adenosyltransferase

Chain M:



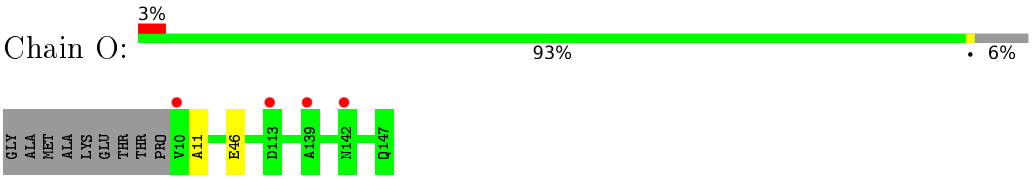
• Molecule 1: ATP:cob(I)alamin adenosyltransferase

Chain N:



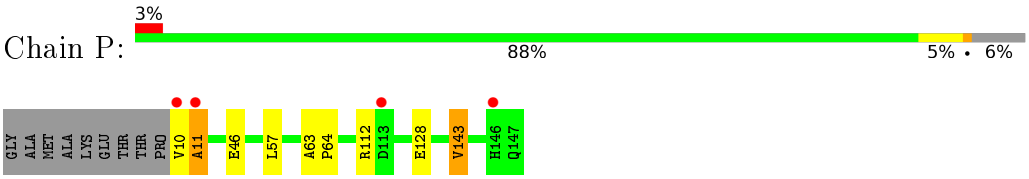
• Molecule 1: ATP:cob(I)alamin adenosyltransferase

Chain O:



• Molecule 1: ATP:cob(I)alamin adenosyltransferase

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	71.30Å 130.12Å 120.75Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	33.07 – 1.97 33.07 – 1.97	Depositor EDS
% Data completeness (in resolution range)	98.0 (33.07-1.97) 99.9 (33.07-1.97)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.26 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.158 , 0.186 0.167 , 0.194	Depositor DCC
R_{free} test set	7911 reflections (5.38%)	DCC
Wilson B-factor (Å^2)	20.0	Xtriage
Anisotropy	0.079	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.41 , 61.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.52$, $< L^2 > = 0.36$	Xtriage
Estimated twinning fraction	0.138 for h,-k,-l	Xtriage
Reported twinning fraction	0.204 for H, K, L 0.796 for -H, -K, L	Depositor
Outliers	0 of 155209 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	18350	wwPDB-VP
Average B, all atoms (Å^2)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.85% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, MG, NA, HEM, CL

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.09	0/1043	0.99	5/1421 (0.4%)
1	B	0.86	0/1043	0.84	2/1421 (0.1%)
1	C	1.04	2/1043 (0.2%)	1.01	5/1421 (0.4%)
1	D	0.93	2/1043 (0.2%)	0.95	5/1421 (0.4%)
1	E	1.05	2/1051 (0.2%)	1.02	5/1432 (0.3%)
1	F	0.87	1/1043 (0.1%)	0.84	1/1421 (0.1%)
1	G	0.92	0/1043	0.83	0/1421
1	H	0.93	1/1043 (0.1%)	0.89	3/1421 (0.2%)
1	I	0.91	0/1043	0.87	3/1421 (0.2%)
1	J	0.80	0/1043	0.78	0/1421
1	K	0.98	4/1043 (0.4%)	1.02	5/1421 (0.4%)
1	L	0.80	0/1043	0.83	1/1421 (0.1%)
1	M	0.79	0/1043	0.80	0/1421
1	N	0.86	0/1043	0.88	3/1421 (0.2%)
1	O	0.79	0/1043	0.82	0/1421
1	P	0.92	2/1043 (0.2%)	0.89	2/1421 (0.1%)
All	All	0.91	14/16696 (0.1%)	0.89	40/22747 (0.2%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	46	GLU	CD-OE2	8.51	1.35	1.25
1	K	79	GLU	CD-OE1	8.46	1.34	1.25
1	E	142	ASN	N-CA	8.34	1.63	1.46
1	C	79	GLU	CD-OE2	-7.87	1.17	1.25
1	D	79	GLU	CD-OE2	-7.01	1.18	1.25
1	K	79	GLU	CD-OE2	-6.85	1.18	1.25
1	D	46	GLU	CD-OE2	-6.43	1.18	1.25
1	K	128	GLU	CD-OE1	-5.88	1.19	1.25
1	P	46	GLU	CD-OE2	5.66	1.31	1.25
1	H	128	GLU	CD-OE1	5.53	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	128	GLU	CD-OE2	-5.50	1.19	1.25
1	F	46	GLU	CD-OE2	5.49	1.31	1.25
1	E	10	VAL	C-O	-5.45	1.12	1.23
1	P	128	GLU	CD-OE1	5.36	1.31	1.25

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	128	GLU	OE1-CD-OE2	-14.08	106.40	123.30
1	C	46	GLU	OE1-CD-OE2	9.41	134.59	123.30
1	C	46	GLU	CG-CD-OE1	-9.29	99.72	118.30
1	K	73	MET	CG-SD-CE	8.54	113.86	100.20
1	D	46	GLU	CG-CD-OE2	-7.72	102.85	118.30
1	E	130	ASP	CB-CG-OD1	7.58	125.12	118.30
1	C	73	MET	CG-SD-CE	7.07	111.51	100.20
1	N	10	VAL	CB-CA-C	6.80	124.33	111.40
1	A	143	VAL	CA-CB-CG2	6.72	120.98	110.90
1	I	132	ASP	CB-CG-OD2	6.63	124.27	118.30
1	E	112	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	E	112	ARG	CG-CD-NE	-6.42	98.32	111.80
1	D	22	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	D	46	GLU	CG-CD-OE1	6.25	130.81	118.30
1	N	22	ARG	CB-CG-CD	-6.04	95.91	111.60
1	K	112	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	E	141	ILE	CA-C-N	5.69	129.71	117.20
1	B	51	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	D	128	GLU	OE1-CD-OE2	-5.56	116.62	123.30
1	H	130	ASP	CB-CG-OD1	5.50	123.25	118.30
1	C	51	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	H	143	VAL	N-CA-C	-5.37	96.51	111.00
1	A	130	ASP	CB-CG-OD2	-5.35	113.49	118.30
1	N	19	GLN	CG-CD-OE1	-5.30	110.99	121.60
1	L	142	ASN	CB-CA-C	5.30	121.00	110.40
1	P	143	VAL	N-CA-C	-5.27	96.76	111.00
1	K	79	GLU	CG-CD-OE1	5.26	128.82	118.30
1	E	112	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	I	130	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	K	10	VAL	CA-CB-CG2	5.19	118.69	110.90
1	D	112	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	C	10	VAL	CA-CB-CG2	5.17	118.65	110.90
1	P	112	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	A	10	VAL	CA-CB-CG2	5.16	118.64	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	112	ARG	NE-CZ-NH2	-5.13	117.74	120.30
1	A	132	ASP	CB-CG-OD2	5.09	122.88	118.30
1	F	112	ARG	NE-CZ-NH1	5.04	122.82	120.30
1	A	51	ARG	NE-CZ-NH1	5.01	122.81	120.30
1	I	41	ASP	CB-CG-OD1	5.01	122.81	118.30
1	B	112	ARG	NE-CZ-NH2	-5.01	117.80	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	1024	0	1025	1	0
1	B	1024	0	1025	3	0
1	C	1024	0	1025	6	0
1	D	1024	0	1025	7	0
1	E	1031	0	1033	6	0
1	F	1024	0	1025	3	0
1	G	1024	0	1025	6	0
1	H	1024	0	1025	5	0
1	I	1024	0	1025	4	0
1	J	1024	0	1025	4	0
1	K	1024	0	1025	3	0
1	L	1024	0	1025	3	0
1	M	1024	0	1025	5	0
1	N	1024	0	1025	6	0
1	O	1024	0	1025	1	0
1	P	1024	0	1025	2	0
2	A	43	0	30	2	0
2	C	43	0	30	7	0
2	E	43	0	30	3	0
2	G	43	0	30	4	0
2	I	43	0	30	5	0
2	K	43	0	30	2	0
2	M	43	0	30	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	O	43	0	30	3	0
3	A	18	0	24	0	0
3	B	6	0	8	0	0
3	C	6	0	8	0	0
3	D	12	0	16	0	0
3	E	6	0	7	0	0
3	F	6	0	8	0	0
3	G	18	0	24	1	0
3	H	6	0	8	0	0
3	I	24	0	32	1	0
3	J	6	0	8	1	0
3	K	18	0	24	0	0
3	M	6	0	8	0	0
3	N	6	0	8	0	0
3	O	6	0	8	0	0
3	P	6	0	8	0	0
4	A	2	0	0	0	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
4	E	1	0	0	0	0
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	H	2	0	0	0	0
4	I	2	0	0	0	0
4	J	2	0	0	0	0
4	L	1	0	0	0	0
4	M	2	0	0	0	0
4	N	1	0	0	0	0
4	P	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
5	I	1	0	0	0	0
5	J	1	0	0	0	0
6	H	1	0	0	0	0
6	P	1	0	0	0	0
7	A	123	0	0	1	2
7	B	87	0	0	2	0
7	C	109	0	0	3	0
7	D	85	0	0	2	0
7	E	108	0	0	0	2
7	F	76	0	0	3	0
7	G	103	0	0	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	H	102	0	0	4	0
7	I	83	0	0	1	0
7	J	71	0	0	2	0
7	K	100	0	0	2	0
7	L	72	0	0	1	0
7	M	62	0	0	1	0
7	N	72	0	0	2	0
7	O	88	0	0	1	0
7	P	100	0	0	0	0
All	All	18350	0	16847	82	2

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 2.

All (82) 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:G:57:LEU:HD22	7:G:392:HOH:O	1.47	1.14
1:H:22:ARG:HG3	7:H:317:HOH:O	1.63	0.97
1:M:46:GLU:OE2	1:M:49:THR:OG1	1.86	0.92
2:G:201:HEM:HBC2	2:G:201:HEM:HHD	1.62	0.81
1:G:26:GLU:HG3	7:G:343:HOH:O	1.81	0.79
1:I:18:HIS:CE1	1:I:22:ARG:HD2	2.18	0.79
1:N:46:GLU:HG3	7:N:307:HOH:O	1.83	0.78
1:D:49:THR:HG23	7:D:353:HOH:O	1.84	0.77
1:O:46:GLU:HG3	7:O:302:HOH:O	1.83	0.77
1:C:81:SER:HB3	7:C:302:HOH:O	1.83	0.77
2:O:201:HEM:HMC2	2:O:201:HEM:HBC2	1.72	0.71
1:M:18:HIS:CE1	1:M:22:ARG:HD2	2.24	0.71
1:A:46:GLU:HG3	7:A:301:HOH:O	1.91	0.70
2:C:201:HEM:HMD1	1:D:22:ARG:HH21	1.60	0.67
1:D:38:SER:HB2	7:D:353:HOH:O	1.95	0.66
1:F:46:GLU:HG3	7:F:301:HOH:O	1.96	0.64
2:M:201:HEM:HBB2	2:M:201:HEM:HHC	1.80	0.63
2:E:201:HEM:HBB2	2:E:201:HEM:HHC	1.79	0.63
1:B:18:HIS:CE1	1:B:22:ARG:HD2	2.34	0.62
1:E:141:ILE:O	1:E:142:ASN:HB2	2.00	0.62
2:I:201:HEM:HBB2	2:I:201:HEM:HHC	1.80	0.62
1:H:11:ALA:N	7:H:303:HOH:O	2.33	0.61
1:B:46:GLU:HG3	7:B:302:HOH:O	2.00	0.61
1:B:32:GLN:CD	7:B:304:HOH:O	2.40	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:26:GLU:HG3	7:L:356:HOH:O	2.03	0.59
2:A:201:HEM:HBB2	2:A:201:HEM:HHC	1.86	0.57
1:J:46:GLU:HG3	7:J:301:HOH:O	2.05	0.56
2:O:201:HEM:HBC2	2:O:201:HEM:CMC	2.34	0.56
1:D:19:GLN:HE22	1:D:22:ARG:HH11	1.51	0.56
1:C:50:TRP:CE3	2:C:201:HEM:HAB	2.42	0.54
2:I:201:HEM:HHD	2:I:201:HEM:HBC2	1.89	0.54
1:F:11:ALA:N	7:F:302:HOH:O	2.41	0.54
2:K:201:HEM:HBB2	2:K:201:HEM:HHC	1.89	0.54
3:G:202:GOL:H32	1:H:47:THR:HG23	1.90	0.52
2:O:201:HEM:HBB2	2:O:201:HEM:HHC	1.92	0.52
1:I:22:ARG:NH1	2:I:201:HEM:O1A	2.43	0.52
1:G:57:LEU:CD2	7:G:392:HOH:O	2.28	0.51
1:I:78:HIS:HD2	7:I:336:HOH:O	1.92	0.51
1:F:10:VAL:HG13	7:F:302:HOH:O	2.11	0.51
1:C:85:GLN:NE2	7:C:302:HOH:O	2.43	0.51
2:G:201:HEM:CBC	2:G:201:HEM:HHD	2.39	0.50
1:J:78:HIS:HD2	7:J:312:HOH:O	1.95	0.49
1:H:46:GLU:HG3	7:H:301:HOH:O	2.12	0.49
1:M:78:HIS:HD2	7:M:335:HOH:O	1.94	0.49
2:M:201:HEM:HAB	1:N:50:TRP:CE3	2.48	0.48
2:C:201:HEM:HBC2	2:C:201:HEM:HMC1	1.95	0.48
1:P:10:VAL:HG13	1:P:11:ALA:O	2.14	0.48
2:I:201:HEM:HBD2	1:J:22:ARG:CZ	2.45	0.47
2:C:201:HEM:HMD1	1:D:22:ARG:NH2	2.26	0.47
1:K:46:GLU:HG3	7:K:301:HOH:O	2.15	0.47
1:N:10:VAL:HG22	1:N:112:ARG:CD	2.44	0.47
3:I:203:GOL:C1	1:K:71:VAL:O	2.63	0.46
2:C:201:HEM:CMD	1:D:22:ARG:NH2	2.79	0.46
1:C:46:GLU:HG3	1:C:47:THR:N	2.28	0.46
2:E:201:HEM:HMC2	2:E:201:HEM:HBC2	1.97	0.46
1:C:99:GLY:HA2	7:C:317:HOH:O	2.17	0.45
1:G:146:HIS:CE1	7:G:341:HOH:O	2.70	0.45
1:N:10:VAL:HG22	1:N:112:ARG:HD2	1.97	0.45
2:M:201:HEM:HMC2	2:M:201:HEM:HBC2	1.98	0.44
1:E:18:HIS:CD2	2:E:201:HEM:NB	2.86	0.44
1:K:78:HIS:HD2	7:K:354:HOH:O	2.00	0.44
1:E:141:ILE:O	1:E:142:ASN:CB	2.59	0.44
1:E:146:HIS:ND1	1:E:147:GLN:O	2.52	0.43
1:G:78:HIS:HD2	7:G:344:HOH:O	2.01	0.43
1:M:46:GLU:HG3	1:M:47:THR:N	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:G:201:HEM:HBC2	2:G:201:HEM:CHD	2.37	0.43
2:A:201:HEM:HBC2	2:A:201:HEM:HMC2	2.01	0.42
2:M:201:HEM:NC	1:N:18:HIS:CD2	2.87	0.42
1:M:63:ALA:HB3	1:M:64:PRO:HD3	2.02	0.42
1:J:123:SER:HG	3:J:201:GOL:C3	2.33	0.42
2:K:201:HEM:HAA1	1:L:22:ARG:NH2	2.35	0.42
1:I:18:HIS:CD2	2:I:201:HEM:NC	2.88	0.41
2:C:201:HEM:CGD	1:D:22:ARG:HH22	2.31	0.41
1:E:10:VAL:HB	1:E:112:ARG:HD2	2.02	0.41
1:H:10:VAL:HG22	7:H:303:HOH:O	2.19	0.41
2:C:201:HEM:HMB2	2:C:201:HEM:HHB	1.78	0.41
1:E:10:VAL:HB	1:E:112:ARG:HB3	2.02	0.41
1:P:63:ALA:HB3	1:P:64:PRO:HD3	2.02	0.41
1:C:63:ALA:HB3	1:C:64:PRO:HD3	2.03	0.40
1:N:54:ASP:HA	7:N:354:HOH:O	2.21	0.40
1:G:22:ARG:HG2	2:G:201:HEM:HMB3	2.02	0.40
1:L:69:THR:OG1	1:L:101:VAL:HA	2.21	0.40

All (2) 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)
7:A:399:HOH:O	7:E:319:HOH:O[2_655]	2.13	0.07
7:A:407:HOH:O	7:E:371:HOH:O[2_655]	2.15	0.05

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	136/147 (92%)	136 (100%)	0	0	100	100
1	B	136/147 (92%)	136 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	136/147 (92%)	135 (99%)	1 (1%)	0	100	100
1	D	136/147 (92%)	135 (99%)	1 (1%)	0	100	100
1	E	137/147 (93%)	135 (98%)	2 (2%)	0	100	100
1	F	136/147 (92%)	135 (99%)	0	1 (1%)	26	17
1	G	136/147 (92%)	134 (98%)	1 (1%)	1 (1%)	26	17
1	H	136/147 (92%)	134 (98%)	2 (2%)	0	100	100
1	I	136/147 (92%)	135 (99%)	1 (1%)	0	100	100
1	J	136/147 (92%)	135 (99%)	0	1 (1%)	26	17
1	K	136/147 (92%)	135 (99%)	1 (1%)	0	100	100
1	L	136/147 (92%)	134 (98%)	1 (1%)	1 (1%)	26	17
1	M	136/147 (92%)	135 (99%)	0	1 (1%)	26	17
1	N	136/147 (92%)	134 (98%)	2 (2%)	0	100	100
1	O	136/147 (92%)	135 (99%)	0	1 (1%)	26	17
1	P	136/147 (92%)	134 (98%)	1 (1%)	1 (1%)	26	17
All	All	2177/2352 (93%)	2157 (99%)	13 (1%)	7 (0%)	46	39

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	P	11	ALA
1	F	11	ALA
1	O	11	ALA
1	G	11	ALA
1	J	11	ALA
1	L	11	ALA
1	M	11	ALA

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	106/112 (95%)	105 (99%)	1 (1%)	84 86
1	B	106/112 (95%)	106 (100%)	0	100 100
1	C	106/112 (95%)	106 (100%)	0	100 100
1	D	106/112 (95%)	106 (100%)	0	100 100
1	E	107/112 (96%)	107 (100%)	0	100 100
1	F	106/112 (95%)	106 (100%)	0	100 100
1	G	106/112 (95%)	106 (100%)	0	100 100
1	H	106/112 (95%)	105 (99%)	1 (1%)	84 86
1	I	106/112 (95%)	106 (100%)	0	100 100
1	J	106/112 (95%)	106 (100%)	0	100 100
1	K	106/112 (95%)	106 (100%)	0	100 100
1	L	106/112 (95%)	105 (99%)	1 (1%)	84 86
1	M	106/112 (95%)	106 (100%)	0	100 100
1	N	106/112 (95%)	106 (100%)	0	100 100
1	O	106/112 (95%)	106 (100%)	0	100 100
1	P	106/112 (95%)	104 (98%)	2 (2%)	65 65
All	All	1697/1792 (95%)	1692 (100%)	5 (0%)	94 96

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	142	ASN
1	H	143	VAL
1	L	142	ASN
1	P	57	LEU
1	P	143	VAL

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	142	ASN
1	B	78	HIS
1	D	19	GLN
1	F	78	HIS
1	G	78	HIS
1	G	135	GLN

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Mol	Chain	Res	Type
1	I	78	HIS
1	J	78	HIS
1	K	78	HIS
1	L	43	HIS
1	M	43	HIS
1	M	78	HIS
1	N	78	HIS
1	O	19	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 57 ligands modelled in this entry, 24 are monoatomic - leaving 33 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	$\#\|Z\| > 2$
2	HEM	A	201	1	24,50,50	1.30	3 (12%)	16,82,82	2.25	4 (25%)
3	GOL	A	202	-	5,5,5	0.64	0	5,5,5	2.09	2 (40%)
3	GOL	A	203	-	5,5,5	1.29	1 (20%)	5,5,5	1.33	0
3	GOL	A	204	-	5,5,5	0.34	0	5,5,5	0.52	0
3	GOL	B	201	-	5,5,5	0.69	0	5,5,5	0.73	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	HEM	C	201	1	24,50,50	1.09	3 (12%)	16,82,82	2.38	8 (50%)
3	GOL	C	202	-	5,5,5	0.60	0	5,5,5	1.74	2 (40%)
3	GOL	D	201	-	5,5,5	0.81	0	5,5,5	1.62	1 (20%)
3	GOL	D	202	-	5,5,5	0.30	0	5,5,5	1.24	0
2	HEM	E	201	1	24,50,50	1.19	3 (12%)	16,82,82	1.85	5 (31%)
3	GOL	E	202	-	5,5,5	0.71	0	5,5,5	1.61	1 (20%)
3	GOL	F	201	-	5,5,5	0.49	0	5,5,5	0.80	0
2	HEM	G	201	1	24,50,50	1.44	5 (20%)	16,82,82	2.11	5 (31%)
3	GOL	G	202	-	5,5,5	0.85	0	5,5,5	1.35	0
3	GOL	G	203	-	5,5,5	0.54	0	5,5,5	0.55	0
3	GOL	G	204	-	5,5,5	0.58	0	5,5,5	1.02	1 (20%)
3	GOL	H	201	-	5,5,5	1.03	0	5,5,5	1.08	0
2	HEM	I	201	1	24,50,50	1.24	2 (8%)	16,82,82	1.79	4 (25%)
3	GOL	I	202	-	5,5,5	0.88	0	5,5,5	1.52	1 (20%)
3	GOL	I	203	-	5,5,5	0.32	0	5,5,5	1.10	1 (20%)
3	GOL	I	204	-	5,5,5	0.61	0	5,5,5	0.46	0
3	GOL	I	205	-	5,5,5	1.00	0	5,5,5	2.00	1 (20%)
3	GOL	J	201	-	5,5,5	0.50	0	5,5,5	1.24	0
2	HEM	K	201	1	24,50,50	1.29	4 (16%)	16,82,82	2.15	7 (43%)
3	GOL	K	202	-	5,5,5	0.49	0	5,5,5	0.48	0
3	GOL	K	203	-	5,5,5	0.29	0	5,5,5	0.56	0
3	GOL	K	204	-	5,5,5	0.62	0	5,5,5	1.15	0
2	HEM	M	201	1	24,50,50	0.88	0	16,82,82	2.03	5 (31%)
3	GOL	M	202	-	5,5,5	0.46	0	5,5,5	0.67	0
3	GOL	N	201	-	5,5,5	0.33	0	5,5,5	0.61	0
2	HEM	O	201	1	24,50,50	1.21	3 (12%)	16,82,82	2.07	8 (50%)
3	GOL	O	202	-	5,5,5	0.56	0	5,5,5	1.41	1 (20%)
3	GOL	P	202	-	5,5,5	0.45	0	5,5,5	0.58	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
2	HEM	A	201	1	-	0/6/54/54	0/0/8/8
3	GOL	A	202	-	-	0/4/4/4	0/0/0/0
3	GOL	A	203	-	-	0/4/4/4	0/0/0/0
3	GOL	A	204	-	-	0/4/4/4	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	B	201	-	-	0/4/4/4	0/0/0/0
2	HEM	C	201	1	-	0/6/54/54	0/0/8/8
3	GOL	C	202	-	-	0/4/4/4	0/0/0/0
3	GOL	D	201	-	-	0/4/4/4	0/0/0/0
3	GOL	D	202	-	-	0/4/4/4	0/0/0/0
2	HEM	E	201	1	-	0/6/54/54	0/0/8/8
3	GOL	E	202	-	-	0/4/4/4	0/0/0/0
3	GOL	F	201	-	-	0/4/4/4	0/0/0/0
2	HEM	G	201	1	-	0/6/54/54	0/0/8/8
3	GOL	G	202	-	-	0/4/4/4	0/0/0/0
3	GOL	G	203	-	-	0/4/4/4	0/0/0/0
3	GOL	G	204	-	-	0/4/4/4	0/0/0/0
3	GOL	H	201	-	-	0/4/4/4	0/0/0/0
2	HEM	I	201	1	-	0/6/54/54	0/0/8/8
3	GOL	I	202	-	-	0/4/4/4	0/0/0/0
3	GOL	I	203	-	-	0/4/4/4	0/0/0/0
3	GOL	I	204	-	-	0/4/4/4	0/0/0/0
3	GOL	I	205	-	-	0/4/4/4	0/0/0/0
3	GOL	J	201	-	-	0/4/4/4	0/0/0/0
2	HEM	K	201	1	-	0/6/54/54	0/0/8/8
3	GOL	K	202	-	-	0/4/4/4	0/0/0/0
3	GOL	K	203	-	-	0/4/4/4	0/0/0/0
3	GOL	K	204	-	-	0/4/4/4	0/0/0/0
2	HEM	M	201	1	-	0/6/54/54	0/0/8/8
3	GOL	M	202	-	-	0/4/4/4	0/0/0/0
3	GOL	N	201	-	-	0/4/4/4	0/0/0/0
2	HEM	O	201	1	-	0/6/54/54	0/0/8/8
3	GOL	O	202	-	-	0/4/4/4	0/0/0/0
3	GOL	P	202	-	-	0/4/4/4	0/0/0/0

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	HEM	C1B-NB	-4.49	1.30	1.36
2	G	201	HEM	C3B-C2B	-3.58	1.35	1.40
2	K	201	HEM	C3B-C2B	-3.54	1.35	1.40
2	I	201	HEM	C3B-C2B	-2.97	1.36	1.40
2	E	201	HEM	C3B-C2B	-2.85	1.36	1.40
2	E	201	HEM	C4D-ND	-2.84	1.32	1.36
2	O	201	HEM	C3B-C2B	-2.54	1.37	1.40
2	K	201	HEM	C4C-NC	-2.52	1.33	1.36
2	C	201	HEM	C4A-CHB	-2.35	1.33	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	201	HEM	C1B-NB	-2.34	1.33	1.36
2	G	201	HEM	C4A-CHB	-2.31	1.33	1.40
2	K	201	HEM	C4A-CHB	-2.29	1.34	1.40
2	A	201	HEM	C3B-C2B	-2.26	1.37	1.40
2	C	201	HEM	C3B-C2B	-2.25	1.37	1.40
2	I	201	HEM	C4C-NC	-2.22	1.33	1.36
2	G	201	HEM	C3C-CAC	-2.03	1.43	1.47
2	C	201	HEM	C3C-CAC	2.03	1.51	1.47
2	G	201	HEM	CAA-C2A	2.04	1.55	1.52
2	A	201	HEM	C3C-CAC	2.14	1.52	1.47
2	O	201	HEM	CAA-C2A	2.20	1.55	1.52
2	K	201	HEM	CAA-C2A	2.30	1.55	1.52
3	A	203	GOL	O2-C2	2.36	1.50	1.43
2	O	201	HEM	CAD-C3D	2.51	1.55	1.52
2	G	201	HEM	CAD-C3D	3.09	1.56	1.52

All (57) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201	HEM	CBA-CAA-C2A	-5.48	102.86	112.49
3	I	205	GOL	C3-C2-C1	-4.26	93.09	111.06
2	M	201	HEM	CAD-CBD-CGD	-4.24	104.53	112.78
2	G	201	HEM	C3B-C4B-NB	-4.11	103.89	109.21
2	C	201	HEM	CAA-CBA-CGA	-4.08	104.85	112.78
2	A	201	HEM	CBD-CAD-C3D	-4.03	105.40	112.47
2	A	201	HEM	C3B-C4B-NB	-3.93	104.13	109.21
2	E	201	HEM	CBA-CAA-C2A	-3.91	105.62	112.49
2	G	201	HEM	C3C-C4C-NC	-3.74	103.88	110.94
2	O	201	HEM	CMA-C3A-C4A	-3.52	122.33	128.31
2	E	201	HEM	C3B-C4B-NB	-3.48	104.71	109.21
3	D	201	GOL	C3-C2-C1	-3.42	96.63	111.06
2	I	201	HEM	CBD-CAD-C3D	-3.21	106.84	112.47
3	A	202	GOL	O1-C1-C2	-3.13	94.10	109.97
3	E	202	GOL	C3-C2-C1	-3.10	97.99	111.06
2	M	201	HEM	CMA-C3A-C4A	-3.04	123.13	128.31
3	C	202	GOL	O1-C1-C2	-3.00	94.76	109.97
2	O	201	HEM	C3B-C4B-NB	-2.96	105.38	109.21
2	C	201	HEM	CAD-C3D-C2D	-2.74	121.17	129.00
2	C	201	HEM	C3C-C4C-NC	-2.73	105.80	110.94
2	K	201	HEM	CMD-C2D-C1D	-2.73	123.68	128.31
2	K	201	HEM	C3C-C4C-NC	-2.54	106.16	110.94
2	C	201	HEM	C3B-C4B-NB	-2.52	105.95	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	201	HEM	CMA-C3A-C4A	-2.51	124.05	128.31
2	I	201	HEM	C3C-C4C-NC	-2.39	106.44	110.94
2	K	201	HEM	C3C-CAC-CBC	-2.38	121.61	126.40
2	K	201	HEM	C3B-C4B-NB	-2.31	106.23	109.21
2	O	201	HEM	CAA-C2A-C3A	-2.26	122.54	129.00
2	E	201	HEM	CMA-C3A-C4A	-2.24	124.51	128.31
2	O	201	HEM	C3C-C4C-NC	-2.16	106.87	110.94
2	C	201	HEM	C3C-CAC-CBC	-2.11	122.16	126.40
2	E	201	HEM	CMD-C2D-C3D	2.02	129.46	125.24
3	G	204	GOL	O2-C2-C3	2.02	118.18	108.47
2	M	201	HEM	CBA-CAA-C2A	2.11	116.20	112.49
3	C	202	GOL	O2-C2-C3	2.12	118.66	108.47
3	I	203	GOL	O1-C1-C2	2.14	120.83	109.97
2	O	201	HEM	CMA-C3A-C2A	2.22	129.88	125.24
2	O	201	HEM	CMB-C2B-C3B	2.26	129.51	125.09
2	C	201	HEM	CMA-C3A-C2A	2.27	129.97	125.24
2	M	201	HEM	CMA-C3A-C2A	2.28	130.00	125.24
2	K	201	HEM	CMC-C2C-C3C	2.33	129.65	125.09
3	O	202	GOL	O2-C2-C3	2.48	120.38	108.47
2	O	201	HEM	CMC-C2C-C3C	2.55	130.08	125.09
2	A	201	HEM	C3B-CAB-CBB	2.56	131.54	126.40
2	M	201	HEM	CMB-C2B-C3B	2.62	130.22	125.09
3	A	202	GOL	O2-C2-C3	2.65	121.20	108.47
2	E	201	HEM	CMB-C2B-C3B	2.74	130.45	125.09
3	I	202	GOL	O2-C2-C1	2.91	122.44	108.47
2	I	201	HEM	CMC-C2C-C3C	2.99	130.94	125.09
2	G	201	HEM	CBA-CAA-C2A	3.01	117.78	112.49
2	C	201	HEM	CBD-CAD-C3D	3.11	117.92	112.47
2	G	201	HEM	CMC-C2C-C3C	3.19	131.33	125.09
2	K	201	HEM	CBA-CAA-C2A	3.25	118.21	112.49
2	I	201	HEM	CAA-CBA-CGA	3.42	119.43	112.78
2	O	201	HEM	CBD-CAD-C3D	3.45	118.52	112.47
2	K	201	HEM	CMB-C2B-C3B	4.51	133.91	125.09
2	C	201	HEM	CMB-C2B-C3B	4.70	134.28	125.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

11 monomers are involved in 33 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	201	HEM	2	0
2	C	201	HEM	7	0
2	E	201	HEM	3	0
2	G	201	HEM	4	0
3	G	202	GOL	1	0
2	I	201	HEM	5	0
3	I	203	GOL	1	0
3	J	201	GOL	1	0
2	K	201	HEM	2	0
2	M	201	HEM	4	0
2	O	201	HEM	3	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, 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	138/147 (93%)	-0.11	2 (1%)	78	80	9, 16, 26, 36	0
1	B	138/147 (93%)	0.18	5 (3%)	46	50	13, 20, 34, 51	0
1	C	138/147 (93%)	-0.11	2 (1%)	78	80	11, 15, 26, 48	0
1	D	138/147 (93%)	0.05	4 (2%)	55	58	11, 21, 36, 56	0
1	E	139/147 (94%)	-0.03	2 (1%)	78	80	10, 17, 31, 50	0
1	F	138/147 (93%)	0.13	5 (3%)	46	50	12, 19, 37, 59	0
1	G	138/147 (93%)	-0.09	5 (3%)	46	50	11, 17, 30, 41	0
1	H	138/147 (93%)	-0.03	3 (2%)	65	68	11, 17, 33, 50	0
1	I	138/147 (93%)	0.26	7 (5%)	32	36	12, 20, 38, 78	0
1	J	138/147 (93%)	0.34	5 (3%)	46	50	15, 24, 39, 63	0
1	K	138/147 (93%)	-0.08	1 (0%)	89	90	12, 17, 27, 44	0
1	L	138/147 (93%)	0.32	6 (4%)	39	43	16, 24, 43, 54	0
1	M	138/147 (93%)	0.44	13 (9%)	11	13	15, 25, 45, 54	0
1	N	138/147 (93%)	0.27	8 (5%)	26	30	15, 23, 44, 64	0
1	O	138/147 (93%)	0.10	4 (2%)	55	58	14, 21, 34, 54	0
1	P	138/147 (93%)	0.03	4 (2%)	55	58	12, 18, 34, 60	0
All	All	2209/2352 (93%)	0.10	76 (3%)	49	53	9, 19, 38, 78	0

All (76) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	I	10	VAL	9.5
1	N	10	VAL	7.6
1	P	10	VAL	7.6
1	F	10	VAL	7.4
1	J	10	VAL	6.6

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Mol	Chain	Res	Type	RSRZ
1	C	10	VAL	6.1
1	H	10	VAL	6.1
1	D	10	VAL	5.8
1	M	142	ASN	5.4
1	M	115	ILE	5.3
1	K	10	VAL	5.0
1	O	10	VAL	4.9
1	A	10	VAL	4.8
1	L	10	VAL	4.8
1	M	10	VAL	4.7
1	E	146	HIS	4.5
1	G	10	VAL	4.5
1	N	113	ASP	4.4
1	N	142	ASN	4.3
1	B	10	VAL	4.2
1	L	113	ASP	4.2
1	M	139	ALA	4.0
1	I	11	ALA	3.8
1	I	142	ASN	3.8
1	J	142	ASN	3.7
1	D	142	ASN	3.6
1	M	146	HIS	3.5
1	I	115	ILE	3.4
1	L	115	ILE	3.4
1	F	146	HIS	3.4
1	O	142	ASN	3.3
1	M	113	ASP	3.2
1	M	138	ILE	3.2
1	P	113	ASP	3.1
1	B	30	GLN	3.1
1	L	142	ASN	3.1
1	D	113	ASP	3.1
1	F	115	ILE	3.1
1	I	113	ASP	3.0
1	H	143	VAL	3.0
1	B	142	ASN	3.0
1	G	142	ASN	3.0
1	I	146	HIS	2.9
1	O	113	ASP	2.9
1	B	32	GLN	2.8
1	N	32	GLN	2.8
1	I	144	GLY	2.8

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Mol	Chain	Res	Type	RSRZ
1	N	115	ILE	2.8
1	F	114	GLY	2.7
1	D	114	GLY	2.7
1	G	113	ASP	2.6
1	P	11	ALA	2.6
1	L	114	GLY	2.5
1	M	147	GLN	2.5
1	C	113	ASP	2.5
1	J	11	ALA	2.5
1	O	139	ALA	2.5
1	J	32	GLN	2.4
1	N	114	GLY	2.4
1	P	146	HIS	2.4
1	B	31	LEU	2.4
1	F	113	ASP	2.4
1	J	31	LEU	2.3
1	H	113	ASP	2.3
1	A	30	GLN	2.3
1	M	136	THR	2.2
1	M	143	VAL	2.2
1	M	114	GLY	2.2
1	N	112	ARG	2.1
1	G	139	ALA	2.1
1	G	146	HIS	2.1
1	M	30	GLN	2.1
1	M	145	THR	2.1
1	E	142	ASN	2.1
1	L	144	GLY	2.1
1	N	11	ALA	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

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	NA	I	206	1/1	0.96	0.22	20.61	51,51,51,51	0
3	GOL	H	201	6/6	0.89	0.20	8.05	20,24,33,42	0
4	NA	F	202	1/1	0.98	0.18	7.93	45,45,45,45	0
4	NA	A	206	1/1	0.91	0.16	6.81	54,54,54,54	0
3	GOL	A	203	6/6	0.84	0.25	6.19	31,32,36,38	0
4	NA	B	202	1/1	0.88	0.16	5.44	46,46,46,46	0
4	NA	G	205	1/1	0.95	0.16	5.20	46,46,46,46	0
3	GOL	I	202	6/6	0.75	0.29	5.11	30,36,39,46	0
4	NA	A	205	1/1	0.97	0.14	4.50	45,45,45,45	0
3	GOL	G	204	6/6	0.94	0.14	3.89	18,21,35,49	0
4	NA	H	203	1/1	0.96	0.13	3.74	49,49,49,49	0
3	GOL	I	203	6/6	0.94	0.19	3.73	22,35,46,48	0
2	HEM	I	201	43/43	0.90	0.27	2.75	32,46,64,69	0
2	HEM	E	201	43/43	0.93	0.22	2.58	26,34,58,69	0
3	GOL	I	205	6/6	0.89	0.17	2.56	17,20,23,27	0
4	NA	E	203	1/1	0.96	0.12	2.48	48,48,48,48	0
5	CL	J	203	1/1	0.96	0.12	2.47	48,48,48,48	0
4	NA	N	202	1/1	0.84	0.11	2.45	54,54,54,54	0
4	NA	M	204	1/1	0.98	0.12	2.41	47,47,47,47	0
3	GOL	P	202	6/6	0.93	0.13	2.39	21,21,26,37	0
3	GOL	G	202	6/6	0.88	0.18	2.35	28,34,36,40	0
3	GOL	A	204	6/6	0.82	0.20	2.32	44,45,50,50	0
3	GOL	K	202	6/6	0.90	0.17	2.16	25,29,34,39	0
3	GOL	N	201	6/6	0.92	0.13	2.04	26,29,34,43	0
2	HEM	M	201	43/43	0.92	0.17	1.96	37,45,63,68	0
3	GOL	K	204	6/6	0.94	0.12	1.94	21,24,25,26	0
4	NA	J	204	1/1	0.86	0.12	1.82	45,45,45,45	0
3	GOL	C	202	6/6	0.92	0.12	1.81	21,25,26,26	0
3	GOL	D	201	6/6	0.94	0.13	1.73	23,25,29,33	0
3	GOL	A	202	6/6	0.94	0.13	1.52	18,20,20,20	0
2	HEM	A	201	43/43	0.95	0.14	1.51	25,32,59,62	0
3	GOL	F	201	6/6	0.90	0.14	1.50	22,23,27,37	0
4	NA	M	203	1/1	0.93	0.11	1.38	40,40,40,40	0
3	GOL	M	202	6/6	0.94	0.12	1.29	21,24,27,32	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
4	NA	J	202	1/1	0.97	0.11	1.26	47,47,47,47	0
2	HEM	K	201	43/43	0.95	0.15	1.26	21,28,41,44	0
3	GOL	E	202	6/6	0.94	0.12	1.21	18,21,27,29	0
3	GOL	J	201	6/6	0.90	0.13	1.17	28,30,32,35	0
2	HEM	O	201	43/43	0.96	0.13	1.00	19,26,36,39	0
2	HEM	G	201	43/43	0.97	0.12	0.77	16,22,34,39	0
2	HEM	C	201	43/43	0.95	0.15	0.69	21,28,42,57	0
3	GOL	B	201	6/6	0.92	0.12	0.48	19,22,30,46	0
3	GOL	O	202	6/6	0.94	0.11	0.45	25,27,30,30	0
3	GOL	K	203	6/6	0.95	0.13	0.44	30,32,34,34	0
3	GOL	D	202	6/6	0.94	0.13	0.39	21,35,38,43	0
4	NA	I	208	1/1	0.92	0.09	0.38	46,46,46,46	0
3	GOL	G	203	6/6	0.89	0.15	0.37	33,40,41,42	0
4	NA	D	203	1/1	0.98	0.10	0.11	41,41,41,41	0
4	NA	P	201	1/1	0.75	0.14	-0.23	47,47,47,47	0
4	NA	H	204	1/1	0.93	0.12	-0.34	37,37,37,37	0
5	CL	C	203	1/1	0.88	0.08	-0.73	54,54,54,54	0
4	NA	L	201	1/1	0.95	0.07	-1.87	44,44,44,44	0
5	CL	D	204	1/1	0.96	0.06	-3.98	46,46,46,46	0
5	CL	I	207	1/1	0.97	0.04	-5.81	40,40,40,40	0
6	MG	H	202	1/1	0.91	0.26	-	31,31,31,31	0
6	MG	P	203	1/1	0.96	0.16	-	32,32,32,32	0
3	GOL	I	204	6/6	0.83	0.20	-	33,44,47,51	0

6.5 Other polymers

There are no such residues in this entry.