



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:43 AM GMT

PDB ID : 2Y46
Title : Structure of the mixed-function P450 MycG in complex with mycinamicin IV
Authors : Li, S.; Kells, P.M.; Sherman, D.H.; Podust, L.M.
Deposited on : 2011-01-05
Resolution : 1.83 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

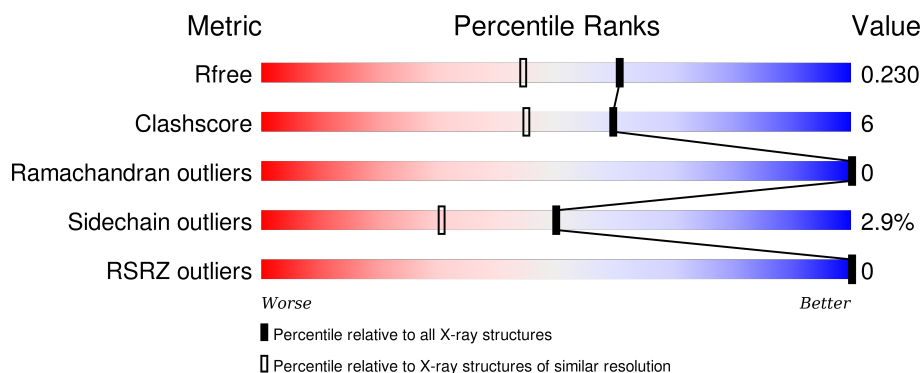
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.83 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	2634 (1.86-1.82)
Clashscore	102246	2862 (1.86-1.82)
Ramachandran outliers	100387	2831 (1.86-1.82)
Sidechain outliers	100360	2832 (1.86-1.82)
RSRZ outliers	91569	2639 (1.86-1.82)

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	417	 83% 9% • 6%
1	B	417	 85% 8% • 6%
1	C	417	 83% 10% • 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
5	GOL	A	1400	-	-	-	X
5	GOL	B	1399	-	-	-	X
5	GOL	C	1399	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 10665 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 P-450-LIKE PROTEIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	393	Total	C	N	O	S	0	7	0
			3131	1964	572	584	11			
1	B	393	Total	C	N	O	S	0	7	0
			3143	1971	576	585	11			
1	C	393	Total	C	N	O	S	0	6	0
			3136	1967	576	582	11			

There are 60 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q59523
A	-18	GLY	-	EXPRESSION TAG	UNP Q59523
A	-17	SER	-	EXPRESSION TAG	UNP Q59523
A	-16	SER	-	EXPRESSION TAG	UNP Q59523
A	-15	HIS	-	EXPRESSION TAG	UNP Q59523
A	-14	HIS	-	EXPRESSION TAG	UNP Q59523
A	-13	HIS	-	EXPRESSION TAG	UNP Q59523
A	-12	HIS	-	EXPRESSION TAG	UNP Q59523
A	-11	HIS	-	EXPRESSION TAG	UNP Q59523
A	-10	HIS	-	EXPRESSION TAG	UNP Q59523
A	-9	SER	-	EXPRESSION TAG	UNP Q59523
A	-8	SER	-	EXPRESSION TAG	UNP Q59523
A	-7	GLY	-	EXPRESSION TAG	UNP Q59523
A	-6	LEU	-	EXPRESSION TAG	UNP Q59523
A	-5	VAL	-	EXPRESSION TAG	UNP Q59523
A	-4	PRO	-	EXPRESSION TAG	UNP Q59523
A	-3	ARG	-	EXPRESSION TAG	UNP Q59523
A	-2	GLY	-	EXPRESSION TAG	UNP Q59523
A	-1	SER	-	EXPRESSION TAG	UNP Q59523
A	0	HIS	-	EXPRESSION TAG	UNP Q59523
B	-19	MET	-	EXPRESSION TAG	UNP Q59523
B	-18	GLY	-	EXPRESSION TAG	UNP Q59523
B	-17	SER	-	EXPRESSION TAG	UNP Q59523

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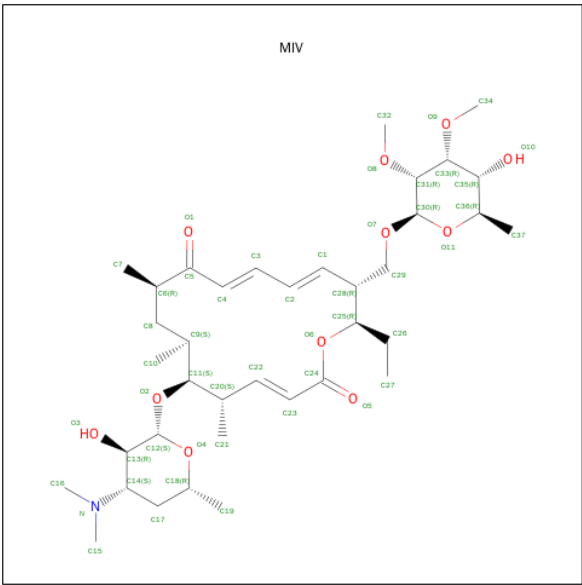
Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	EXPRESSION TAG	UNP Q59523
B	-15	HIS	-	EXPRESSION TAG	UNP Q59523
B	-14	HIS	-	EXPRESSION TAG	UNP Q59523
B	-13	HIS	-	EXPRESSION TAG	UNP Q59523
B	-12	HIS	-	EXPRESSION TAG	UNP Q59523
B	-11	HIS	-	EXPRESSION TAG	UNP Q59523
B	-10	HIS	-	EXPRESSION TAG	UNP Q59523
B	-9	SER	-	EXPRESSION TAG	UNP Q59523
B	-8	SER	-	EXPRESSION TAG	UNP Q59523
B	-7	GLY	-	EXPRESSION TAG	UNP Q59523
B	-6	LEU	-	EXPRESSION TAG	UNP Q59523
B	-5	VAL	-	EXPRESSION TAG	UNP Q59523
B	-4	PRO	-	EXPRESSION TAG	UNP Q59523
B	-3	ARG	-	EXPRESSION TAG	UNP Q59523
B	-2	GLY	-	EXPRESSION TAG	UNP Q59523
B	-1	SER	-	EXPRESSION TAG	UNP Q59523
B	0	HIS	-	EXPRESSION TAG	UNP Q59523
C	-19	MET	-	EXPRESSION TAG	UNP Q59523
C	-18	GLY	-	EXPRESSION TAG	UNP Q59523
C	-17	SER	-	EXPRESSION TAG	UNP Q59523
C	-16	SER	-	EXPRESSION TAG	UNP Q59523
C	-15	HIS	-	EXPRESSION TAG	UNP Q59523
C	-14	HIS	-	EXPRESSION TAG	UNP Q59523
C	-13	HIS	-	EXPRESSION TAG	UNP Q59523
C	-12	HIS	-	EXPRESSION TAG	UNP Q59523
C	-11	HIS	-	EXPRESSION TAG	UNP Q59523
C	-10	HIS	-	EXPRESSION TAG	UNP Q59523
C	-9	SER	-	EXPRESSION TAG	UNP Q59523
C	-8	SER	-	EXPRESSION TAG	UNP Q59523
C	-7	GLY	-	EXPRESSION TAG	UNP Q59523
C	-6	LEU	-	EXPRESSION TAG	UNP Q59523
C	-5	VAL	-	EXPRESSION TAG	UNP Q59523
C	-4	PRO	-	EXPRESSION TAG	UNP Q59523
C	-3	ARG	-	EXPRESSION TAG	UNP Q59523
C	-2	GLY	-	EXPRESSION TAG	UNP Q59523
C	-1	SER	-	EXPRESSION TAG	UNP Q59523
C	0	HIS	-	EXPRESSION TAG	UNP Q59523

- 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 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
2	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 3 is MYCINAMICIN IV (three-letter code: MIV) (formula: C₃₇H₆₁NO₁₁).



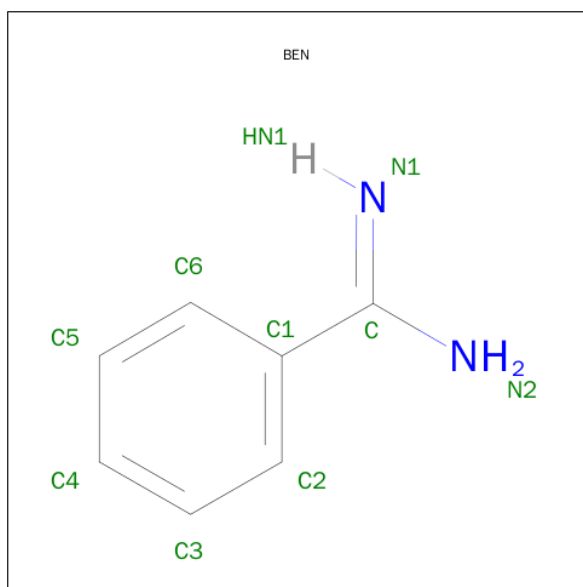
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			49	37	1	11		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			49	37	1	11		
3	C	1	Total	C	N	O	0	0
			49	37	1	11		

- Molecule 4 is BENZAMIDINE (three-letter code: BEN) (formula: C₇H₈N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	N	0	0
			9	7	2		
4	B	1	Total	C	N	0	0
			9	7	2		
4	C	1	Total	C	N	0	0
			9	7	2		

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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


- Molecule 6 is water.

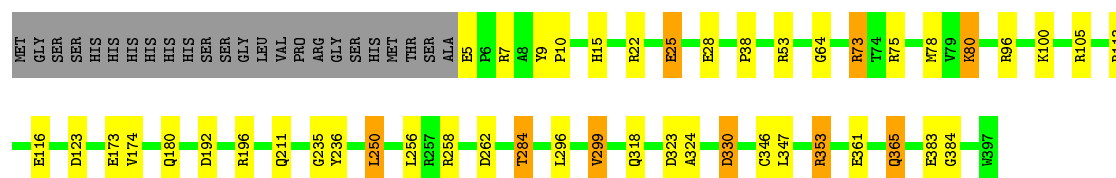
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	292	Total	O	0	0
			292	292		
6	B	313	Total	O	0	0
			313	313		
6	C	311	Total	O	0	0
			311	311		

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.

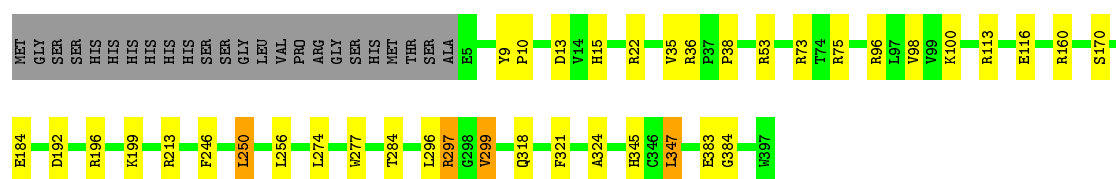
• Molecule 1: P-450-LIKE PROTEIN

Chain A: 




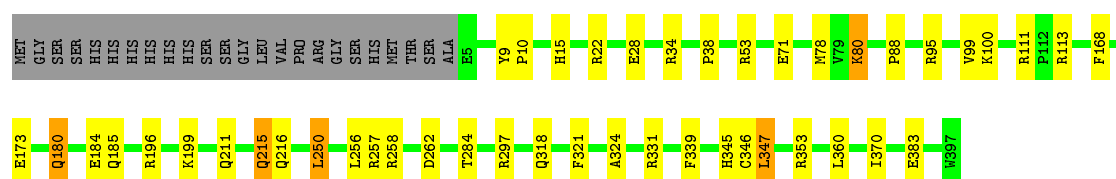
• Molecule 1: P-450-LIKE PROTEIN

Chain B: 



• Molecule 1: P-450-LIKE PROTEIN

Chain C: 



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	58.27Å 101.01Å 441.53Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	220.77 – 1.83 55.19 – 1.83	Depositor EDS
% Data completeness (in resolution range)	82.8 (220.77-1.83) 82.7 (55.19-1.83)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 1.83Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.157 , 0.233 0.157 , 0.230	Depositor DCC
R_{free} test set	4822 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.167	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 21.1	EDS
Estimated twinning fraction	0.479 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.479 for 1/2*h+1/2*k,3/2*h-1/2*k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Outliers	1 of 95597 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	10665	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 6.48% 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, BEN, HEM, MIV

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	1.12	4/3197 (0.1%)	0.95	8/4351 (0.2%)
1	B	1.10	4/3209 (0.1%)	0.94	6/4365 (0.1%)
1	C	1.10	7/3202 (0.2%)	0.92	4/4356 (0.1%)
All	All	1.11	15/9608 (0.2%)	0.94	18/13072 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	28	GLU	CB-CG	-6.87	1.39	1.52
1	A	28	GLU	CG-CD	6.82	1.62	1.51
1	C	28	GLU	CB-CG	-6.53	1.39	1.52
1	C	28	GLU	CG-CD	6.38	1.61	1.51
1	C	28	GLU	CD-OE1	6.28	1.32	1.25
1	C	53	ARG	CG-CD	6.26	1.67	1.51
1	C	339	PHE	CE1-CZ	5.96	1.48	1.37
1	C	321	PHE	CE1-CZ	5.43	1.47	1.37
1	A	25	GLU	CB-CG	-5.35	1.42	1.52
1	C	168	PHE	CE1-CZ	5.35	1.47	1.37
1	B	35	VAL	CB-CG2	5.35	1.64	1.52
1	B	98	VAL	CB-CG1	5.34	1.64	1.52
1	B	321	PHE	CE1-CZ	5.28	1.47	1.37
1	A	64	GLY	N-CA	5.27	1.53	1.46
1	B	277	TRP	CE3-CZ3	5.03	1.47	1.38

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	347	LEU	CB-CG-CD2	-8.81	96.02	111.00
1	B	96	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	B	297	ARG	NE-CZ-NH2	-6.85	116.87	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	22	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	A	330[A]	ASP	CB-CG-OD1	6.20	123.88	118.30
1	A	330[B]	ASP	CB-CG-OD1	6.20	123.88	118.30
1	A	73	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	C	331	ARG	NE-CZ-NH1	-5.99	117.31	120.30
1	A	353	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	B	160	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B	13	ASP	CB-CG-OD1	5.46	123.21	118.30
1	A	7	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	C	111	ARG	NE-CZ-NH2	-5.15	117.73	120.30
1	A	7	ARG	NE-CZ-NH2	-5.13	117.73	120.30
1	B	73	ARG	NE-CZ-NH1	5.13	122.87	120.30
1	C	22	ARG	NE-CZ-NH1	5.13	122.86	120.30
1	C	28	GLU	CG-CD-OE1	5.04	128.37	118.30
1	A	123	ASP	CB-CG-OD1	5.02	122.82	118.30

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	3131	0	3095	40	0
1	B	3143	0	3116	24	0
1	C	3136	0	3115	40	0
2	A	43	0	30	4	0
2	B	43	0	30	1	0
2	C	43	0	30	1	0
3	A	49	0	61	1	0
3	B	49	0	61	2	0
3	C	49	0	61	0	0
4	A	9	0	7	0	0
4	B	9	0	7	0	0
4	C	9	0	7	2	0
5	A	12	0	16	1	0
5	B	12	0	16	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	C	12	0	16	0	0
6	A	292	0	0	9	0
6	B	313	0	0	6	1
6	C	311	0	0	9	0
All	All	10665	0	9668	110	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 6.

All (110) 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:78:MET:HE2	1:A:80:LYS:CE	1.57	1.35
1:A:78:MET:HE2	1:A:80:LYS:NZ	1.59	1.18
1:A:284:THR:HG22	6:A:2007:HOH:O	1.43	1.17
1:C:78:MET:HE2	1:C:80:LYS:CE	1.77	1.13
1:C:78:MET:CE	1:C:80:LYS:HZ1	1.62	1.10
1:A:78:MET:HE2	1:A:80:LYS:HE3	1.27	1.10
1:C:78:MET:HE2	1:C:80:LYS:HE3	1.28	1.08
1:A:78:MET:CE	1:A:80:LYS:NZ	2.24	1.00
1:C:78:MET:CE	1:C:80:LYS:NZ	2.25	0.99
1:C:78:MET:HE2	1:C:80:LYS:NZ	1.81	0.94
1:C:250:LEU:HD12	1:C:256:LEU:HG	1.51	0.92
1:A:78:MET:CE	1:A:80:LYS:HZ1	1.83	0.89
1:C:78:MET:HE2	1:C:80:LYS:HZ1	1.38	0.87
1:A:5:GLU:O	6:A:2003:HOH:O	1.96	0.84
1:A:78:MET:CE	1:A:80:LYS:CE	2.51	0.83
1:C:9:TYR:OH	6:C:2007:HOH:O	1.98	0.81
1:C:78:MET:CE	1:C:80:LYS:CE	2.61	0.78
1:B:9:TYR:OH	6:B:2009:HOH:O	2.01	0.77
1:C:78:MET:HE1	1:C:80:LYS:NZ	2.00	0.76
1:C:284:THR:OG1	6:C:2007:HOH:O	2.05	0.74
1:A:284:THR:CG2	6:A:2007:HOH:O	2.15	0.73
1:A:78:MET:HE2	1:A:80:LYS:HZ1	1.38	0.71
1:A:78:MET:CE	1:A:80:LYS:HE3	2.16	0.71
1:C:345[B]:HIS:HE1	6:C:2281:HOH:O	1.74	0.70
1:A:9:TYR:OH	6:A:2007:HOH:O	2.10	0.64
1:B:15:HIS:HE1	1:B:383:GLU:OE2	1.81	0.64
1:A:192[B]:ASP:O	1:A:196:ARG:HG2	1.99	0.62
1:A:15:HIS:HE1	1:A:383:GLU:OE2	1.82	0.62
1:A:250:LEU:HD22	1:A:256:LEU:HG	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:258:ARG:NH1	1:C:262:ASP:OD2	2.32	0.62
1:B:53:ARG:CD	6:B:2072:HOH:O	2.48	0.61
5:B:1400:GOL:H12	6:B:2160:HOH:O	2.02	0.60
1:B:250:LEU:CD2	1:B:256:LEU:HG	2.32	0.60
1:B:284:THR:OG1	6:B:2009:HOH:O	2.14	0.60
1:C:15:HIS:HE1	1:C:383:GLU:OE2	1.85	0.59
1:C:347:LEU:HD12	1:C:347:LEU:C	2.23	0.58
1:B:22:ARG:HH11	1:B:22:ARG:HG2	1.68	0.57
1:C:78:MET:HE1	1:C:80:LYS:HZ1	1.53	0.57
1:C:180:GLN:O	1:C:184:GLU:HG3	2.04	0.56
1:B:345[A]:HIS:HE1	6:B:2281:HOH:O	1.88	0.55
1:A:353:ARG:HD2	6:A:2264:HOH:O	2.06	0.55
1:A:38:PRO:HD2	1:A:73:ARG:O	2.06	0.55
1:A:347:LEU:C	1:A:347:LEU:HD12	2.27	0.54
5:A:1399:GOL:H12	6:A:2162:HOH:O	2.07	0.54
1:B:53:ARG:HD3	6:B:2072:HOH:O	2.08	0.53
1:C:250:LEU:CD1	1:C:256:LEU:HG	2.33	0.53
1:B:113:ARG:HD2	1:B:116:GLU:OE1	2.10	0.52
4:C:1398:BEN:N1	6:C:2310:HOH:O	2.34	0.51
1:A:53:ARG:CD	6:A:2079:HOH:O	2.57	0.51
4:C:1398:BEN:N2	6:C:2311:HOH:O	2.33	0.51
1:A:318:GLN:NE2	1:A:324:ALA:H	2.10	0.49
1:C:250:LEU:HD22	1:C:360:LEU:HD22	1.94	0.49
1:C:9:TYR:CG	1:C:10:PRO:HA	2.47	0.49
1:B:347:LEU:HD23	1:B:347:LEU:C	2.33	0.49
1:C:257:ARG:NH2	1:C:370:ILE:O	2.39	0.49
1:C:250:LEU:CD2	1:C:360:LEU:HD22	2.43	0.49
1:A:318:GLN:HE22	1:A:324:ALA:H	1.59	0.49
1:A:113:ARG:HD2	1:A:116:GLU:OE1	2.13	0.49
1:B:9:TYR:O	1:B:38:PRO:HD3	2.13	0.49
1:B:100:LYS:HE3	1:B:213:ARG:O	2.12	0.49
1:A:296:LEU:O	1:A:299:VAL:HG13	2.12	0.49
2:B:450:HEM:HBC2	2:B:450:HEM:HMC2	1.95	0.48
1:A:78:MET:CE	1:A:80:LYS:HZ3	2.24	0.47
1:B:9:TYR:CG	1:B:10:PRO:HA	2.49	0.47
1:B:318:GLN:NE2	1:B:324:ALA:H	2.13	0.46
2:A:450:HEM:HMC2	2:A:450:HEM:HBC2	1.97	0.46
1:C:95:ARG:O	1:C:99:VAL:HG22	2.15	0.46
1:B:192[B]:ASP:O	1:B:196:ARG:HG3	2.15	0.46
1:C:297:ARG:HD3	1:C:297:ARG:HA	1.80	0.45
1:C:346:CYS:HB2	2:C:450:HEM:NA	2.32	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:LEU:CD2	1:A:256:LEU:HG	2.43	0.45
1:A:15:HIS:CE1	1:A:383:GLU:OE2	2.68	0.45
1:C:196:ARG:HA	1:C:199:LYS:HE2	1.98	0.45
1:C:318:GLN:NE2	1:C:324:ALA:H	2.15	0.44
1:A:78:MET:HE1	1:A:80:LYS:NZ	2.21	0.44
1:C:113:ARG:HD2	1:C:113:ARG:HA	1.80	0.44
1:B:296:LEU:O	1:B:299:VAL:HG13	2.17	0.44
1:A:53:ARG:HD3	6:A:2079:HOH:O	2.17	0.44
1:A:346:CYS:HB2	2:A:450:HEM:NA	2.33	0.44
1:A:192[A]:ASP:O	1:A:196:ARG:HG2	2.17	0.44
1:A:174:VAL:O	3:A:460:MIV:H161	2.18	0.43
1:C:353:ARG:HD2	6:C:2280:HOH:O	2.18	0.43
1:B:9:TYR:CD1	1:B:10:PRO:HA	2.54	0.43
1:A:9:TYR:CD1	1:A:10:PRO:HA	2.54	0.43
1:B:22:ARG:CG	1:B:22:ARG:HH11	2.31	0.43
1:C:297:ARG:O	6:C:2227:HOH:O	2.22	0.43
1:C:318:GLN:HE22	1:C:324:ALA:H	1.66	0.43
1:C:71:GLU:OE1	1:C:78:MET:HE3	2.19	0.42
1:B:246:PHE:CE1	1:B:274:LEU:HB3	2.55	0.42
1:B:318:GLN:HE22	1:B:324:ALA:H	1.66	0.42
1:A:235:GLY:HA2	2:A:450:HEM:C2C	2.55	0.42
1:B:250:LEU:HD23	1:B:256:LEU:HG	2.01	0.42
1:A:361:GLU:O	1:A:365:GLN:HB2	2.19	0.42
1:C:9:TYR:O	1:C:38:PRO:HD3	2.21	0.41
1:B:75:ARG:HD2	1:B:384:GLY:O	2.21	0.41
1:C:215:GLN:HG3	6:C:2093:HOH:O	2.19	0.41
1:C:34:ARG:HD2	1:C:34:ARG:HA	1.94	0.41
1:A:9:TYR:CG	1:A:10:PRO:HA	2.55	0.41
1:B:170:SER:HA	3:B:460:MIV:H212	2.03	0.41
1:A:323:ASP:HA	1:C:88:PRO:HB2	2.03	0.41
1:C:9:TYR:CD1	1:C:10:PRO:HA	2.55	0.40
1:C:199:LYS:HG2	1:C:199:LYS:H	1.73	0.40
3:B:460:MIV:C1	3:B:460:MIV:C24	2.99	0.40
1:A:258:ARG:NH1	1:A:262:ASP:OD2	2.54	0.40
1:B:113:ARG:HA	1:B:113:ARG:HD2	1.93	0.40
1:A:346:CYS:HA	2:A:450:HEM:CHA	2.51	0.40
1:C:215:GLN:O	1:C:216:GLN:HB2	2.22	0.40
1:C:185[A]:GLN:NE2	6:C:2171:HOH:O	2.53	0.40
1:A:53:ARG:NE	6:A:2079:HOH:O	2.53	0.40
1:A:75:ARG:HD2	1:A:384:GLY:O	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:B:2041:HOH:O	6:B:2228:HOH:O[4_555]	2.19	0.01

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	398/417 (95%)	385 (97%)	13 (3%)	0	100	100
1	B	398/417 (95%)	388 (98%)	10 (2%)	0	100	100
1	C	397/417 (95%)	386 (97%)	11 (3%)	0	100	100
All	All	1193/1251 (95%)	1159 (97%)	34 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	327/346 (94%)	312 (95%)	15 (5%)	33	13
1	B	329/346 (95%)	323 (98%)	6 (2%)	66	52
1	C	329/346 (95%)	321 (98%)	8 (2%)	57	39
All	All	985/1038 (95%)	956 (97%)	29 (3%)	50	30

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	GLU
1	A	80	LYS
1	A	96	ARG
1	A	100	LYS
1	A	105	ARG
1	A	173	GLU
1	A	180	GLN
1	A	211	GLN
1	A	236	TYR
1	A	250	LEU
1	A	284	THR
1	A	299	VAL
1	A	330[A]	ASP
1	A	330[B]	ASP
1	A	365	GLN
1	B	36	ARG
1	B	184	GLU
1	B	199	LYS
1	B	250	LEU
1	B	297	ARG
1	B	299	VAL
1	C	80	LYS
1	C	100	LYS
1	C	173	GLU
1	C	180	GLN
1	C	211	GLN
1	C	215	GLN
1	C	250	LEU
1	C	347	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	130	GLN
1	A	180	GLN
1	A	185	GLN
1	A	211	GLN
1	A	318	GLN
1	A	320	GLN
1	B	15	HIS
1	B	130	GLN
1	B	318	GLN

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Mol	Chain	Res	Type
1	C	15	HIS
1	C	211	GLN
1	C	215	GLN
1	C	318	GLN
1	C	320	GLN
1	C	335	GLN
1	C	365	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 ⓘ

15 ligands are modelled in this entry.

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	$\# Z > 2$
4	BEN	A	1398	-	9,9,9	0.75	0	9,11,11	0.96	0
5	GOL	A	1399	-	5,5,5	0.44	0	5,5,5	2.34	1 (20%)
5	GOL	A	1400	-	5,5,5	1.12	0	5,5,5	1.73	1 (20%)
2	HEM	A	450	1,6	30,50,50	2.56	12 (40%)	24,82,82	2.45	7 (29%)
3	MIV	A	460	-	50,51,51	1.08	1 (2%)	58,71,71	1.44	9 (15%)
4	BEN	B	1398	-	9,9,9	0.75	0	9,11,11	0.97	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GOL	B	1399	-	5,5,5	0.99	0	5,5,5	1.78	1 (20%)
5	GOL	B	1400	-	5,5,5	0.42	0	5,5,5	1.58	1 (20%)
2	HEM	B	450	1,6	30,50,50	2.39	12 (40%)	24,82,82	2.58	9 (37%)
3	MIV	B	460	-	50,51,51	0.99	2 (4%)	58,71,71	1.52	10 (17%)
4	BEN	C	1398	-	9,9,9	0.66	0	9,11,11	0.74	0
5	GOL	C	1399	-	5,5,5	0.89	0	5,5,5	1.48	1 (20%)
5	GOL	C	1400	-	5,5,5	0.41	0	5,5,5	1.09	0
2	HEM	C	450	1,6	30,50,50	2.69	11 (36%)	24,82,82	2.51	8 (33%)
3	MIV	C	460	-	50,51,51	1.04	2 (4%)	58,71,71	1.56	10 (17%)

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 Torsions and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	BEN	A	1398	-	-	0/4/4/4	0/1/1/1
5	GOL	A	1399	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1400	-	-	0/4/4/4	0/0/0/0
2	HEM	A	450	1,6	-	0/10/54/54	0/0/8/8
3	MIV	A	460	-	-	0/55/91/91	0/2/3/3
4	BEN	B	1398	-	-	0/4/4/4	0/1/1/1
5	GOL	B	1399	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1400	-	-	0/4/4/4	0/0/0/0
2	HEM	B	450	1,6	-	0/10/54/54	0/0/8/8
3	MIV	B	460	-	-	0/55/91/91	0/2/3/3
4	BEN	C	1398	-	-	0/4/4/4	0/1/1/1
5	GOL	C	1399	-	-	0/4/4/4	0/0/0/0
5	GOL	C	1400	-	-	0/4/4/4	0/0/0/0
2	HEM	C	450	1,6	-	0/10/54/54	0/0/8/8
3	MIV	C	460	-	-	0/55/91/91	0/2/3/3

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	450	HEM	C3B-C4B	-9.67	1.43	1.51
2	C	450	HEM	C3B-C4B	-8.62	1.44	1.51
2	B	450	HEM	C3B-C4B	-8.21	1.44	1.51
2	C	450	HEM	C3D-C4D	-7.33	1.42	1.51
2	B	450	HEM	C3D-C4D	-4.44	1.45	1.51
2	A	450	HEM	C3D-C4D	-4.17	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	450	HEM	C2C-C1C	-3.93	1.45	1.52
2	A	450	HEM	C2C-C1C	-3.71	1.45	1.52
2	B	450	HEM	C2C-C1C	-3.46	1.46	1.52
2	B	450	HEM	C2D-C1D	-2.29	1.44	1.51
2	C	450	HEM	C2D-C1D	-2.18	1.44	1.51
2	A	450	HEM	C2D-C1D	-2.05	1.45	1.51
3	B	460	MIV	C29-C28	2.02	1.54	1.52
2	B	450	HEM	CAA-C2A	2.02	1.55	1.52
2	C	450	HEM	CAA-C2A	2.05	1.55	1.52
2	B	450	HEM	CHC-C1C	2.06	1.41	1.36
2	A	450	HEM	C3C-CAC	2.07	1.55	1.51
2	A	450	HEM	FE-NB	2.08	2.08	1.97
2	B	450	HEM	FE-ND	2.20	2.09	1.97
2	C	450	HEM	CHD-C4C	2.23	1.41	1.36
2	C	450	HEM	FE-ND	2.30	2.09	1.97
2	A	450	HEM	C3B-CAB	2.31	1.55	1.51
2	A	450	HEM	FE-ND	2.38	2.10	1.97
2	C	450	HEM	FE-NB	2.40	2.10	1.97
2	A	450	HEM	CAA-C2A	2.47	1.56	1.52
2	B	450	HEM	CMA-C3A	2.50	1.56	1.51
2	A	450	HEM	CMA-C3A	2.52	1.56	1.51
3	C	460	MIV	O9-C33	2.52	1.49	1.42
2	C	450	HEM	C3C-CAC	2.52	1.56	1.51
2	B	450	HEM	FE-NB	2.55	2.11	1.97
2	B	450	HEM	C3C-CAC	2.56	1.56	1.51
2	C	450	HEM	CMA-C3A	2.60	1.57	1.51
2	B	450	HEM	C4C-NC	2.84	1.39	1.36
2	A	450	HEM	C4C-NC	2.90	1.39	1.36
2	A	450	HEM	C1C-NC	3.01	1.39	1.36
2	C	450	HEM	C1C-NC	3.29	1.40	1.36
2	B	450	HEM	C1C-NC	3.46	1.40	1.36
3	C	460	MIV	O6-C24	4.10	1.43	1.34
3	B	460	MIV	O6-C24	4.17	1.43	1.34
3	A	460	MIV	O6-C24	5.01	1.45	1.34

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1399	GOL	C3-C2-C1	-5.11	91.10	111.12
3	B	460	MIV	C2-C3-C4	-4.21	115.32	124.66
3	B	460	MIV	O6-C24-O5	-3.54	117.79	123.30
3	C	460	MIV	O6-C24-O5	-3.50	117.85	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1400	GOL	C3-C2-C1	-3.44	97.61	111.12
3	B	460	MIV	C35-C33-C31	-3.35	104.05	111.44
2	A	450	HEM	C3B-CAB-CBB	-3.26	119.46	124.46
3	C	460	MIV	C2-C3-C4	-3.23	117.49	124.66
2	C	450	HEM	C3B-CAB-CBB	-3.06	119.76	124.46
3	B	460	MIV	C21-C20-C22	-2.89	102.99	110.07
3	C	460	MIV	C28-C1-C2	-2.88	118.82	125.35
3	A	460	MIV	C21-C20-C22	-2.78	103.27	110.07
3	A	460	MIV	C2-C3-C4	-2.57	118.95	124.66
2	B	450	HEM	C3B-CAB-CBB	-2.51	120.61	124.46
3	A	460	MIV	C28-C1-C2	-2.51	119.67	125.35
3	A	460	MIV	O6-C24-O5	-2.49	119.42	123.30
3	B	460	MIV	C28-C1-C2	-2.46	119.77	125.35
3	B	460	MIV	C13-C14-N	-2.34	104.09	110.62
2	C	450	HEM	CMA-C3A-C4A	-2.25	124.64	128.36
3	C	460	MIV	C35-C33-C31	-2.24	106.49	111.44
2	B	450	HEM	C3B-C4B-NB	-2.10	107.61	111.63
2	B	450	HEM	CBD-CAD-C3D	-2.05	107.60	113.55
3	C	460	MIV	O3-C13-C14	2.03	113.47	109.82
3	A	460	MIV	O4-C18-C17	2.16	112.53	109.09
3	A	460	MIV	C15-N-C16	2.22	117.45	110.43
3	B	460	MIV	O6-C24-C23	2.29	117.09	111.42
3	C	460	MIV	O8-C31-C33	2.46	115.11	108.94
3	B	460	MIV	O3-C13-C12	2.48	115.45	110.02
3	A	460	MIV	O8-C31-C33	2.50	115.20	108.94
2	B	450	HEM	C2D-C3D-C4D	2.62	105.95	101.50
3	B	460	MIV	O8-C31-C33	2.73	115.77	108.94
3	B	460	MIV	O4-C18-C17	2.77	113.52	109.09
2	A	450	HEM	C2D-C3D-C4D	2.79	106.24	101.50
5	C	1399	GOL	O2-C2-C1	2.91	121.98	108.65
2	C	450	HEM	C2D-C3D-C4D	2.92	106.45	101.50
3	C	460	MIV	C34-O9-C33	2.92	122.84	114.59
2	A	450	HEM	CAD-C3D-C4D	3.11	123.44	112.47
3	C	460	MIV	O9-C33-C35	3.19	117.53	110.21
5	A	1400	GOL	O2-C2-C1	3.25	123.53	108.65
3	C	460	MIV	O4-C18-C17	3.28	114.34	109.09
2	B	450	HEM	CAD-C3D-C4D	3.29	124.07	112.47
2	C	450	HEM	CMD-C2D-C3D	3.32	129.04	114.35
3	A	460	MIV	C34-O9-C33	3.35	124.04	114.59
3	A	460	MIV	O9-C33-C35	3.42	118.06	110.21
2	C	450	HEM	CAD-C3D-C4D	3.46	124.68	112.47
5	B	1399	GOL	O2-C2-C3	3.49	124.64	108.65

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	450	HEM	CMD-C2D-C3D	3.88	131.52	114.35
2	B	450	HEM	CMD-C2D-C3D	3.95	131.81	114.35
3	C	460	MIV	O9-C33-C31	4.01	118.98	108.94
2	A	450	HEM	CMC-C2C-C3C	5.00	129.02	116.53
2	C	450	HEM	CMC-C2C-C3C	5.05	129.13	116.53
2	A	450	HEM	CMB-C2B-C3B	5.08	129.20	116.53
2	C	450	HEM	CMB-C2B-C3B	5.35	129.88	116.53
2	C	450	HEM	CAD-C3D-C2D	5.40	128.75	113.22
2	B	450	HEM	CMB-C2B-C3B	5.49	130.24	116.53
2	B	450	HEM	CMC-C2C-C3C	5.51	130.27	116.53
2	B	450	HEM	CAD-C3D-C2D	5.83	129.98	113.22
2	A	450	HEM	CAD-C3D-C2D	5.94	130.31	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1399	GOL	1	0
2	A	450	HEM	4	0
3	A	460	MIV	1	0
5	B	1400	GOL	1	0
2	B	450	HEM	1	0
3	B	460	MIV	2	0
4	C	1398	BEN	2	0
2	C	450	HEM	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	393/417 (94%)	-0.58	0 100 100	9, 20, 36, 44	0
1	B	393/417 (94%)	-0.58	0 100 100	10, 20, 37, 44	0
1	C	393/417 (94%)	-0.58	0 100 100	9, 20, 36, 49	0
All	All	1179/1251 (94%)	-0.58	0 100 100	9, 20, 37, 49	0

There are no RSRZ outliers to report.

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, 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
5	GOL	C	1399	6/6	0.92	0.14	9.62	14,22,23,23	0
5	GOL	B	1399	6/6	0.95	0.12	5.41	13,21,24,24	0
5	GOL	A	1400	6/6	0.96	0.10	2.66	14,19,20,21	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
3	MIV	A	460	49/49	0.94	0.12	1.73	26,32,43,44	0
3	MIV	B	460	49/49	0.94	0.11	1.58	25,30,42,44	0
3	MIV	C	460	49/49	0.93	0.10	1.48	26,30,42,43	0
4	BEN	A	1398	9/9	0.96	0.09	1.31	37,37,37,39	9
4	BEN	B	1398	9/9	0.96	0.09	1.31	37,37,37,39	9
5	GOL	C	1400	6/6	0.97	0.08	0.81	22,24,24,26	0
5	GOL	B	1400	6/6	0.97	0.07	0.02	25,28,28,28	0
2	HEM	A	450	43/43	0.99	0.07	-0.21	9,11,14,16	0
2	HEM	B	450	43/43	0.99	0.07	-0.22	9,11,14,16	0
2	HEM	C	450	43/43	0.99	0.07	-0.42	9,10,14,17	0
5	GOL	A	1399	6/6	0.97	0.06	-0.66	24,25,26,26	0
4	BEN	C	1398	9/9	0.97	0.07	-	27,28,29,30	9

6.5 Other polymers

There are no such residues in this entry.