



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 06:44 AM GMT

PDB ID : 2Y5N
Title : Structure of the mixed-function P450 MycG in complex with mycinamicin V
in P21 space group
Authors : Li, S.; Kells, P.M.; Sherman, D.H.; Podust, L.M.
Deposited on : 2011-01-15
Resolution : 1.62 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

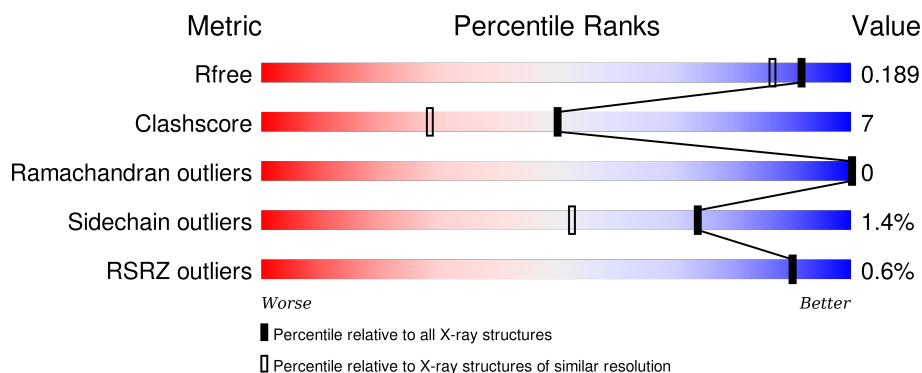
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.62 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	3202 (1.64-1.60)
Clashscore	102246	3500 (1.64-1.60)
Ramachandran outliers	100387	3411 (1.64-1.60)
Sidechain outliers	100360	3410 (1.64-1.60)
RSRZ outliers	91569	3207 (1.64-1.60)

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	417	
1	B	417	

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	GOL	A	1398	-	-	-	X
4	GOL	A	1399	-	-	-	X
4	GOL	A	1401	-	-	X	X
4	GOL	A	1404	-	-	-	X
4	GOL	A	1405	-	-	-	X
4	GOL	B	1399	-	-	-	X
4	GOL	B	1401	-	-	X	X
4	GOL	B	1402	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 7841 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	394	Total	C	N	O	S	0	12	0
			3206	2002	594	598	12			
1	B	400	Total	C	N	O	S	0	11	0
			3233	2021	595	603	14			

There are 40 discrepancies between the modelled and reference sequences:

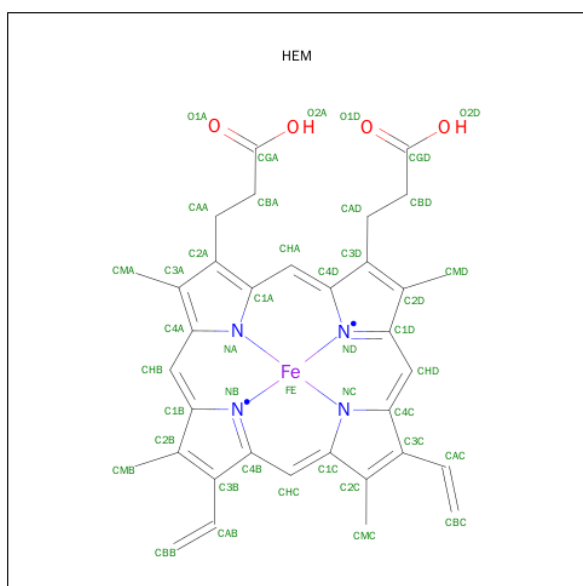
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q59523
A	-18	GLY	-	EXPRESSION TAG	UNP Q59523
A	-17	SER	-	EXPRESSION TAG	UNP Q59523
A	-16	SER	-	EXPRESSION TAG	UNP Q59523
A	-15	HIS	-	EXPRESSION TAG	UNP Q59523
A	-14	HIS	-	EXPRESSION TAG	UNP Q59523
A	-13	HIS	-	EXPRESSION TAG	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
B	-16	SER	-	EXPRESSION TAG	UNP Q59523
B	-15	HIS	-	EXPRESSION TAG	UNP Q59523

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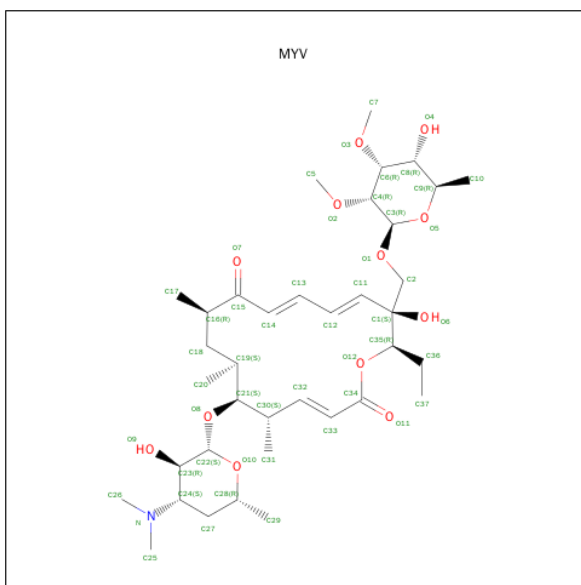
Chain	Residue	Modelled	Actual	Comment	Reference
B	-14	HIS	-	EXPRESSION TAG	UNP Q59523
B	-13	HIS	-	EXPRESSION TAG	UNP Q59523
B	-12	HIS	-	EXPRESSION TAG	UNP Q59523
B	-11	HIS	-	EXPRESSION TAG	UNP Q59523
B	-10	HIS	-	EXPRESSION TAG	UNP Q59523
B	-9	SER	-	EXPRESSION TAG	UNP Q59523
B	-8	SER	-	EXPRESSION TAG	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

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



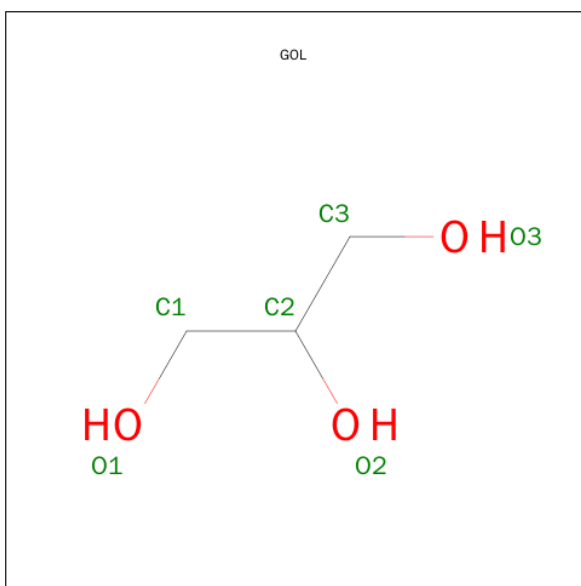
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is MYCINAMICIN V (three-letter code: MYV) (formula: $C_{37}H_{61}NO_{12}$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total 50	C 37	N 1	O 12	0	0
3	B	1	Total 50	C 37	N 1	O 12	0	0

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $\text{C}_3\text{H}_8\text{O}_3$).



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

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

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	584	Total	O	0	0
			584	584		
6	B	553	Total	O	0	0
			553	553		

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	82.75Å 57.43Å 101.93Å 90.00° 113.47° 90.00°	Depositor
Resolution (Å)	75.91 – 1.62 49.99 – 1.62	Depositor EDS
% Data completeness (in resolution range)	70.4 (75.91-1.62) 70.5 (49.99-1.62)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.54 (at 1.62Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, R_{free}	0.115 , 0.188 0.117 , 0.189	Depositor DCC
R_{free} test set	4037 reflections (5.36%)	DCC
Wilson B-factor (Å ²)	16.7	Xtriage
Anisotropy	0.108	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.1	EDS
Estimated twinning fraction	0.017 for h,-k,-h-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 79411 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.98	EDS
Total number of atoms	7841	wwPDB-VP
Average B, all atoms (Å ²)	18.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.96% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	3/3270 (0.1%)	0.97	15/4444 (0.3%)
1	B	1.14	7/3299 (0.2%)	1.09	10/4485 (0.2%)
All	All	1.13	10/6569 (0.2%)	1.03	25/8929 (0.3%)

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	28	GLU	CD-OE1	7.36	1.33	1.25
1	B	28	GLU	CG-CD	7.12	1.62	1.51
1	A	238	SER	CB-OG	6.83	1.51	1.42
1	A	95	ARG	CB-CG	-6.66	1.34	1.52
1	A	200	GLU	CD-OE1	6.45	1.32	1.25
1	B	353	ARG	CZ-NH2	-6.44	1.24	1.33
1	B	120	GLU	CG-CD	6.13	1.61	1.51
1	B	335	GLN	CG-CD	-5.85	1.37	1.51
1	B	321	PHE	CE2-CZ	5.60	1.48	1.37
1	B	28	GLU	CB-CG	-5.45	1.41	1.52

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	353	ARG	NE-CZ-NH1	25.20	132.90	120.30
1	B	353	ARG	NE-CZ-NH2	-23.42	108.59	120.30
1	A	250	LEU	CA-CB-CG	-9.21	94.12	115.30
1	B	353	ARG	CD-NE-CZ	7.52	134.13	123.60
1	B	53	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	A	213	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	B	53	ARG	NE-CZ-NH1	6.21	123.41	120.30
1	B	115	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	353	ARG	NE-CZ-NH2	-6.08	117.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	28	GLU	CG-CD-OE1	5.85	129.99	118.30
1	A	63	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	A	198[A]	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	A	198[B]	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	A	93	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	A	73	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	297	ARG	CG-CD-NE	-5.35	100.57	111.80
1	A	372	LEU	CB-CG-CD1	-5.30	101.98	111.00
1	A	145	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	95	ARG	CG-CD-NE	-5.21	100.87	111.80
1	A	140	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	B	84	LEU	CB-CG-CD1	5.15	119.75	111.00
1	A	288	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	297	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	63	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	111	ARG	NE-CZ-NH2	-5.01	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	3206	0	3187	31	0
1	B	3233	0	3211	54	0
2	A	43	0	30	2	0
2	B	43	0	30	3	0
3	A	50	0	61	1	0
3	B	50	0	61	5	0
4	A	48	0	64	10	0
4	B	30	0	40	11	0
5	A	1	0	0	0	0
6	A	584	0	0	14	0
6	B	553	0	0	6	0
All	All	7841	0	6684	94	0

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 7.

All (94) 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:B:75[B]:ARG:NH1	1:B:77:GLU:OE2	1.82	1.09
1:A:335:GLN:HG3	6:A:2505:HOH:O	1.57	1.03
1:A:181:GLU:HG2	6:A:2329:HOH:O	1.67	0.94
1:A:28[B]:GLU:HG2	1:A:29:THR:HG23	1.49	0.94
1:B:34:ARG:HH22	4:B:1401:GOL:C2	1.82	0.92
1:B:306:PRO:HD2	4:B:1401:GOL:C3	2.01	0.90
4:A:1401:GOL:C3	6:A:2578:HOH:O	2.21	0.89
1:B:34:ARG:HH22	4:B:1401:GOL:H2	1.38	0.88
4:A:1401:GOL:H11	6:A:2346:HOH:O	1.74	0.86
1:B:306:PRO:HD2	4:B:1401:GOL:H32	1.57	0.85
1:A:21:GLY:H	4:A:1399:GOL:H32	1.44	0.82
1:B:80:LYS:HE3	6:B:2171:HOH:O	1.81	0.80
4:A:1401:GOL:H31	6:A:2578:HOH:O	1.79	0.80
1:A:18[B]:THR:HG22	6:A:2020:HOH:O	1.85	0.76
1:B:284[A]:THR:HG21	1:B:310:SER:HB2	1.69	0.75
1:B:15:HIS:HE1	1:B:383:GLU:OE2	1.69	0.74
1:B:380:ARG:HD3	1:B:392:GLU:OE1	1.93	0.69
1:A:21:GLY:N	4:A:1399:GOL:H32	2.09	0.68
1:B:272:GLU:OE2	1:B:353:ARG:HD3	1.94	0.68
1:A:192:ASP:O	1:A:196:ARG:HG2	1.95	0.66
1:A:258[A]:ARG:NH1	1:A:262:ASP:OD2	2.28	0.66
1:A:198[B]:ARG:NH1	6:A:2351:HOH:O	2.27	0.66
1:B:380:ARG:NH1	1:B:392:GLU:OE2	2.31	0.63
1:A:15:HIS:HE1	1:A:383:GLU:OE2	1.80	0.63
1:A:215:GLN:HB2	6:A:2381:HOH:O	1.98	0.62
1:A:21:GLY:H	4:A:1399:GOL:C3	2.12	0.62
1:B:284[A]:THR:HG21	1:B:310:SER:CB	2.29	0.61
1:B:105[B]:ARG:CZ	1:B:105[B]:ARG:HB2	2.30	0.61
1:B:84:LEU:HD23	1:B:286[A]:PHE:CE1	2.38	0.58
1:B:284[A]:THR:O	1:B:308:LEU:HD22	2.03	0.58
1:B:75[B]:ARG:HH21	1:B:386:LEU:HD11	1.69	0.58
1:A:375:PRO:HB2	1:A:378[B]:GLN:HG2	1.85	0.57
1:B:0:HIS:HE1	6:B:2007:HOH:O	1.86	0.57
4:A:1401:GOL:H32	6:A:2578:HOH:O	1.90	0.56
1:B:386:LEU:HD13	3:B:460:MYV:H372	1.88	0.55
1:A:318:GLN:HE22	1:A:324:ALA:H	1.55	0.55
1:A:18[B]:THR:HG23	6:A:2037:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:318:GLN:NE2	1:A:324:ALA:H	2.05	0.54
1:B:75[B]:ARG:NH2	3:B:460:MYV:H32	2.23	0.54
1:A:380:ARG:HD3	1:A:392:GLU:OE1	2.07	0.54
1:B:284[A]:THR:OG1	1:B:308:LEU:HB3	2.08	0.53
1:A:283:GLY:H	4:A:1405:GOL:C1	2.21	0.53
1:B:42:GLU:O	4:B:1401:GOL:H31	2.07	0.53
1:B:75[B]:ARG:CZ	3:B:460:MYV:H32	2.39	0.52
1:B:240:THR:HG22	4:B:1399:GOL:H31	1.90	0.52
1:B:306:PRO:HD2	4:B:1401:GOL:H31	1.90	0.52
1:B:318:GLN:HE22	1:B:324:ALA:H	1.57	0.52
1:B:318:GLN:NE2	1:B:324:ALA:H	2.06	0.52
1:B:75[B]:ARG:NH2	1:B:386:LEU:HD11	2.25	0.51
1:B:348:GLY:HA3	2:B:450:HEM:C3C	2.46	0.51
1:B:160:ARG:NH2	6:B:2309:HOH:O	2.41	0.51
1:B:0:HIS:HD2	1:B:305:GLU:OE2	1.93	0.51
1:B:34:ARG:NH2	4:B:1401:GOL:O2	2.44	0.50
2:B:450:HEM:HBC2	2:B:450:HEM:HMC2	1.93	0.50
1:A:258[A]:ARG:NH2	6:A:2415:HOH:O	2.41	0.50
1:B:75[B]:ARG:HE	1:B:386:LEU:HD11	1.77	0.50
1:B:347:LEU:HD12	1:B:347:LEU:C	2.33	0.48
1:B:350:PRO:HD2	6:B:2496:HOH:O	2.13	0.48
1:B:9:TYR:OH	1:B:284[A]:THR:HG23	2.14	0.48
1:A:113:ARG:HD2	1:A:116:GLU:OE1	2.14	0.48
1:B:34:ARG:NH2	4:B:1401:GOL:H2	2.17	0.47
1:B:61:PHE:HB3	1:B:288:ARG:HB3	1.97	0.47
1:B:28:GLU:HG2	6:B:2081:HOH:O	2.14	0.46
4:A:1405:GOL:H2	6:A:2439:HOH:O	2.15	0.46
1:B:147:ILE:HG21	1:B:232:LEU:HA	1.97	0.46
2:A:450:HEM:HBC2	2:A:450:HEM:HMC2	1.97	0.46
4:B:1401:GOL:H11	6:B:2551:HOH:O	2.16	0.46
1:B:9:TYR:HB2	1:B:35:VAL:HB	1.98	0.46
1:A:196:ARG:H	1:A:196:ARG:HG2	1.65	0.46
1:B:49:TYR:HA	1:B:314:ALA:HB1	1.97	0.46
1:A:335:GLN:CG	6:A:2505:HOH:O	2.38	0.45
1:A:36[B]:ARG:HD3	6:A:2106:HOH:O	2.16	0.45
1:B:241:THR:HG23	4:B:1399:GOL:H2	1.98	0.44
2:B:450:HEM:CMC	2:B:450:HEM:HBC2	2.47	0.44
1:B:130:GLN:HE22	1:B:397:TRP:H	1.65	0.44
1:B:284[B]:THR:HB	1:B:310:SER:HA	1.99	0.44
1:A:190:MET:HA	1:A:190:MET:HE2	2.00	0.44
1:B:9:TYR:O	1:B:38:PRO:HD3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:170:SER:HA	3:B:460:MYV:H312	2.00	0.43
1:B:130:GLN:NE2	1:B:397:TRP:H	2.16	0.43
1:B:79:VAL:HG22	3:B:460:MYV:H203	2.01	0.43
1:A:235:GLY:HA2	2:A:450:HEM:C2C	2.54	0.42
1:A:258[A]:ARG:HH11	1:A:258[A]:ARG:HG2	1.85	0.42
1:A:241:THR:HG23	4:A:1402:GOL:H12	2.02	0.42
1:B:75[B]:ARG:NE	1:B:386:LEU:HD11	2.35	0.42
1:B:0:HIS:CD2	1:B:2:THR:HG22	2.56	0.41
1:A:176:ALA:O	1:A:180[B]:GLN:HG3	2.20	0.41
1:A:9:TYR:O	1:A:38:PRO:HD3	2.21	0.41
1:B:75[B]:ARG:HE	1:B:386:LEU:CG	2.34	0.41
1:B:84:LEU:HD23	1:B:286[A]:PHE:CZ	2.56	0.41
1:B:191:GLY:CA	1:B:225:LEU:HD21	2.50	0.41
1:A:374:ILE:HD11	1:A:379:LEU:HD23	2.03	0.40
1:A:179:MET:SD	3:A:460:MYV:H182	2.61	0.40
1:B:380:ARG:HH11	1:B:392:GLU:CD	2.23	0.40

There are no symmetry-related clashes.

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	404/417 (97%)	397 (98%)	7 (2%)	0	100	100
1	B	409/417 (98%)	397 (97%)	12 (3%)	0	100	100
All	All	813/834 (98%)	794 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	338/346 (98%)	332 (98%)	6 (2%)	66	40
1	B	340/346 (98%)	336 (99%)	4 (1%)	78	59
All	All	678/692 (98%)	668 (98%)	10 (2%)	74	49

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	28[A]	GLU
1	A	28[B]	GLU
1	A	102	PHE
1	A	196	ARG
1	A	250	LEU
1	A	297	ARG
1	B	3	SER
1	B	28	GLU
1	B	100	LYS
1	B	232	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	HIS
1	A	130	GLN
1	A	259	GLN
1	A	318	GLN
1	B	0	HIS
1	B	15	HIS
1	B	130	GLN
1	B	259	GLN
1	B	318	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 18 ligands modelled in this entry, 1 is monoatomic - leaving 17 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	$\# Z > 2$
4	GOL	A	1398	-	5,5,5	0.42	0	5,5,5	0.81	0
4	GOL	A	1399	-	5,5,5	0.36	0	5,5,5	1.60	1 (20%)
4	GOL	A	1400	-	5,5,5	0.54	0	5,5,5	1.44	1 (20%)
4	GOL	A	1401	-	5,5,5	0.36	0	5,5,5	0.94	0
4	GOL	A	1402	-	5,5,5	0.46	0	5,5,5	1.33	1 (20%)
4	GOL	A	1403	-	5,5,5	0.28	0	5,5,5	0.89	0
4	GOL	A	1404	-	5,5,5	0.68	0	5,5,5	1.48	1 (20%)
4	GOL	A	1405	-	5,5,5	0.76	0	5,5,5	1.19	1 (20%)
2	HEM	A	450	1,6	30,50,50	2.33	8 (26%)	24,82,82	2.51	9 (37%)
3	MYV	A	460	-	49,52,52	0.88	2 (4%)	60,74,74	1.29	5 (8%)
4	GOL	B	1398	-	5,5,5	0.75	0	5,5,5	1.44	2 (40%)
4	GOL	B	1399	-	5,5,5	0.94	0	5,5,5	2.00	2 (40%)
4	GOL	B	1400	-	5,5,5	0.46	0	5,5,5	0.82	0
4	GOL	B	1401	-	5,5,5	0.41	0	5,5,5	1.07	1 (20%)
4	GOL	B	1402	-	5,5,5	0.68	0	5,5,5	0.94	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	HEM	B	450	1,6	30,50,50	2.02	9 (30%)	24,82,82	2.59	12 (50%)
3	MYV	B	460	-	49,52,52	1.25	4 (8%)	60,74,74	1.31	8 (13%)

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
4	GOL	A	1398	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1399	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1400	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1401	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1402	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1403	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1404	-	-	0/4/4/4	0/0/0/0
4	GOL	A	1405	-	-	0/4/4/4	0/0/0/0
2	HEM	A	450	1,6	-	0/10/54/54	0/0/8/8
3	MYV	A	460	-	-	0/59/95/95	0/2/3/3
4	GOL	B	1398	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1399	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1400	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1401	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1402	-	-	0/4/4/4	0/0/0/0
2	HEM	B	450	1,6	-	0/10/54/54	0/0/8/8
3	MYV	B	460	-	-	0/59/95/95	0/2/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	450	HEM	C3B-C4B	-7.05	1.45	1.51
2	B	450	HEM	C3B-C4B	-6.11	1.46	1.51
2	A	450	HEM	C3D-C4D	-5.50	1.44	1.51
2	B	450	HEM	C3D-C4D	-4.73	1.45	1.51
2	A	450	HEM	C2C-C1C	-3.73	1.45	1.52
2	B	450	HEM	C2C-C1C	-3.34	1.46	1.52
2	B	450	HEM	C2D-C1D	-2.57	1.43	1.51
2	B	450	HEM	C2D-C3D	-2.07	1.48	1.54
2	A	450	HEM	C3C-CAC	2.13	1.55	1.51
2	B	450	HEM	C3C-CAC	2.13	1.55	1.51
2	B	450	HEM	FE-ND	2.20	2.09	1.97
3	A	460	MYV	O1-C3	2.29	1.44	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	460	MYV	O5-C3	2.30	1.47	1.41
2	A	450	HEM	CAA-C2A	2.32	1.56	1.52
2	B	450	HEM	C4C-NC	2.60	1.39	1.36
3	B	460	MYV	C12-C11	2.64	1.37	1.33
2	B	450	HEM	FE-NC	2.93	2.07	1.95
3	B	460	MYV	O1-C3	3.04	1.45	1.40
2	A	450	HEM	FE-NC	3.25	2.08	1.95
3	A	460	MYV	O12-C34	3.28	1.41	1.34
2	A	450	HEM	CMA-C3A	3.65	1.59	1.51
2	A	450	HEM	C1C-NC	3.72	1.40	1.36
3	B	460	MYV	O12-C34	5.79	1.47	1.34

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	460	MYV	C12-C13-C14	-3.56	116.75	124.66
3	B	460	MYV	C12-C13-C14	-3.54	116.81	124.66
3	B	460	MYV	C1-C11-C12	-3.07	121.21	126.18
3	B	460	MYV	C27-C24-N	-3.06	106.66	115.70
2	B	450	HEM	CBD-CAD-C3D	-2.99	104.85	113.55
2	A	450	HEM	C3B-CAB-CBB	-2.85	120.09	124.46
3	A	460	MYV	O5-C9-C8	-2.76	104.74	109.53
2	A	450	HEM	CBD-CAD-C3D	-2.67	105.79	113.55
2	B	450	HEM	CMA-C3A-C4A	-2.55	124.15	128.36
4	A	1400	GOL	O1-C1-C2	-2.53	97.91	110.18
2	B	450	HEM	CBA-CAA-C2A	-2.49	108.07	112.53
3	A	460	MYV	C36-C35-C1	-2.49	110.24	115.17
3	B	460	MYV	O8-C21-C30	-2.48	105.65	110.93
2	A	450	HEM	CBA-CAA-C2A	-2.45	108.14	112.53
4	B	1398	GOL	O2-C2-C3	-2.28	98.21	108.65
4	A	1402	GOL	C3-C2-C1	-2.17	102.63	111.12
4	B	1398	GOL	C3-C2-C1	2.01	118.99	111.12
2	B	450	HEM	C4B-CHC-C1C	2.01	129.19	125.82
4	B	1399	GOL	O3-C3-C2	2.03	120.03	110.18
4	A	1399	GOL	O3-C3-C2	2.06	120.19	110.18
4	A	1404	GOL	O2-C2-C3	2.09	118.22	108.65
4	B	1401	GOL	O3-C3-C2	2.16	120.67	110.18
4	A	1405	GOL	C3-C2-C1	2.19	119.72	111.12
3	B	460	MYV	C35-O12-C34	2.25	119.91	116.90
3	B	460	MYV	C17-C16-C18	2.28	115.98	111.42
3	B	460	MYV	O12-C35-C36	2.30	111.53	107.36
2	B	450	HEM	C2D-C3D-C4D	2.36	105.51	101.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	460	MYV	O10-C28-C29	2.40	111.86	106.78
2	A	450	HEM	C2C-C1C-CHC	2.41	127.34	123.68
3	B	460	MYV	O4-C8-C9	2.49	115.67	109.84
2	A	450	HEM	CMD-C2D-C3D	2.58	125.76	114.35
2	B	450	HEM	CMD-C2D-C3D	2.78	126.65	114.35
2	B	450	HEM	C2C-C1C-CHC	2.97	128.20	123.68
4	B	1399	GOL	O2-C2-C1	2.97	122.27	108.65
2	B	450	HEM	C3B-C4B-CHC	3.14	127.58	123.16
2	B	450	HEM	CAD-C3D-C2D	4.13	125.09	113.22
3	A	460	MYV	C35-O12-C34	4.16	122.46	116.90
2	A	450	HEM	CAD-C3D-C4D	4.51	128.39	112.47
2	A	450	HEM	CAD-C3D-C2D	4.66	126.62	113.22
2	B	450	HEM	CAD-C3D-C4D	4.78	129.34	112.47
2	B	450	HEM	CMC-C2C-C3C	4.84	128.62	116.53
2	B	450	HEM	CMB-C2B-C3B	4.89	128.74	116.53
2	A	450	HEM	CMC-C2C-C3C	5.20	129.50	116.53
2	A	450	HEM	CMB-C2B-C3B	5.48	130.21	116.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1399	GOL	3	0
4	A	1401	GOL	4	0
4	A	1402	GOL	1	0
4	A	1405	GOL	2	0
2	A	450	HEM	2	0
3	A	460	MYV	1	0
4	B	1399	GOL	2	0
4	B	1401	GOL	9	0
2	B	450	HEM	3	0
3	B	460	MYV	5	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [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	394/417 (94%)	-0.82	1 (0%) 94 94	9, 14, 25, 42	0
1	B	400/417 (95%)	-0.76	4 (1%) 84 84	8, 15, 26, 36	0
All	All	794/834 (95%)	-0.79	5 (0%) 90 90	8, 14, 26, 42	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	4	ALA	4.7
1	B	79	VAL	2.6
1	B	176	ALA	2.1
1	B	173	GLU	2.0
1	B	215	GLN	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, 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(\AA^2)	Q<0.9
4	GOL	B	1401	6/6	0.89	0.24	33.78	30,37,41,41	0
4	GOL	A	1405	6/6	0.88	0.25	22.75	32,35,37,37	0
4	GOL	B	1399	6/6	0.96	0.07	6.50	15,18,20,23	0
4	GOL	A	1398	6/6	0.96	0.09	5.39	17,23,25,28	0
4	GOL	A	1399	6/6	0.84	0.11	5.25	42,47,47,48	0
4	GOL	A	1401	6/6	0.75	0.13	4.33	42,49,52,52	0
4	GOL	B	1402	6/6	0.96	0.08	2.56	21,27,30,30	0
4	GOL	A	1404	6/6	0.98	0.07	2.32	13,13,16,16	0
3	MYV	B	460	50/50	0.90	0.17	1.75	17,20,25,26	50
4	GOL	B	1400	6/6	0.99	0.06	1.30	10,12,14,14	0
4	GOL	B	1398	6/6	0.97	0.06	0.96	14,19,20,29	0
3	MYV	A	460	50/50	0.98	0.07	0.48	11,15,21,23	0
2	HEM	A	450	43/43	0.99	0.06	0.42	6,9,11,16	0
4	GOL	A	1400	6/6	0.97	0.06	0.21	18,23,25,33	0
4	GOL	A	1403	6/6	0.97	0.07	-0.07	22,32,32,33	0
4	GOL	A	1402	6/6	0.98	0.05	-0.20	14,15,17,19	0
2	HEM	B	450	43/43	0.99	0.05	-0.32	6,9,12,16	0
5	MG	A	1406	1/1	0.99	0.04	-	24,24,24,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.