



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:55 PM GMT

PDB ID : 4AW3  
Title : Structure of the mixed-function P450 MycG F286V mutant in complex with mycinamicin V in P1 space group  
Authors : Li, S.; Tietz, D.R.; Rutaganira, F.U.; Kells, P.M.; Anzai, Y.; Kato, F.; Pochapsky, T.C.; Sherman, D.H.; Podust, L.M.  
Deposited on : 2012-05-30  
Resolution : 2.05 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](mailto: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

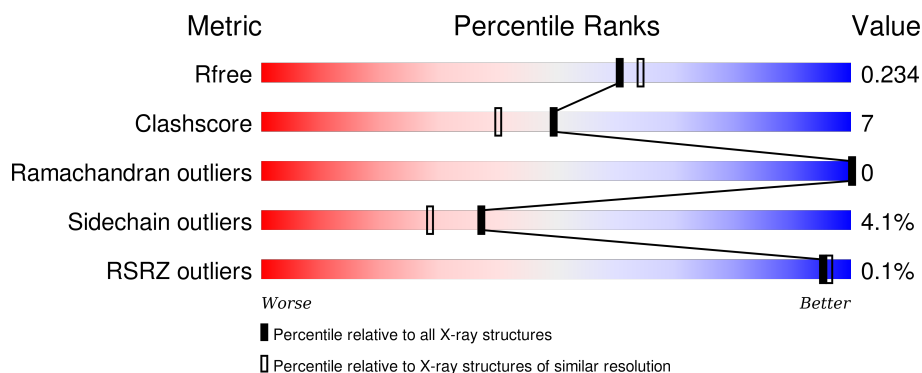
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 2.05 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	1192 (2.04-2.04)
Clashscore	102246	1269 (2.04-2.04)
Ramachandran outliers	100387	1258 (2.04-2.04)
Sidechain outliers	100360	1258 (2.04-2.04)
RSRZ outliers	91569	1194 (2.04-2.04)

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  $\geq 3$ , 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	 79% 15% 6%
1	B	417	 79% 15% 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
3	MYV	A	500[A]	-	-	-	X
3	MYV	A	500[B]	-	-	-	X
3	MYV	B	500[A]	-	-	-	X
3	MYV	B	500[B]	-	-	-	X
4	SO4	A	1398	-	-	-	X
4	SO4	A	1401	-	-	-	X
4	SO4	B	1400	-	-	X	-
5	GOL	B	1402	-	-	-	X

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 7065 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
			3122	1954	572	584	12			
1	B	393	Total	C	N	O	S	0	2	0
			3075	1930	563	571	11			

There are 42 discrepancies between the modelled and reference sequences:

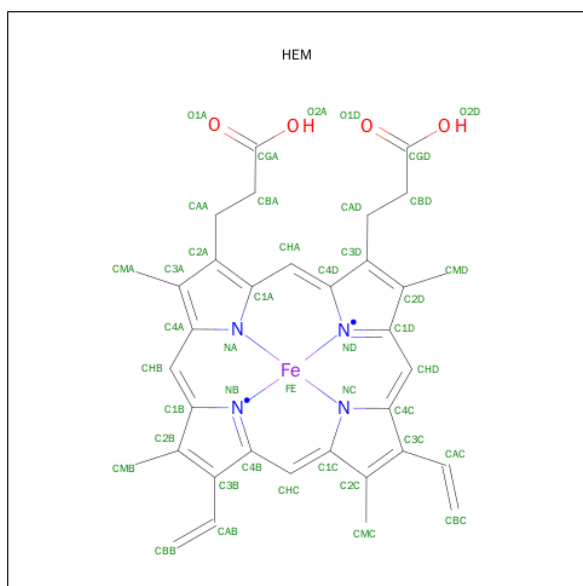
Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP Q59523
A	-18	GLY	-	EXPRESSION TAG	UNP Q59523
A	-17	SER	-	EXPRESSION TAG	UNP Q59523
A	-16	SER	-	EXPRESSION TAG	UNP Q59523
A	-15	HIS	-	EXPRESSION TAG	UNP Q59523
A	-14	HIS	-	EXPRESSION TAG	UNP Q59523
A	-13	HIS	-	EXPRESSION TAG	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
A	286	VAL	PHE	ENGINEERED MUTATION	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

*Continued on next page...*

Continued from previous page...

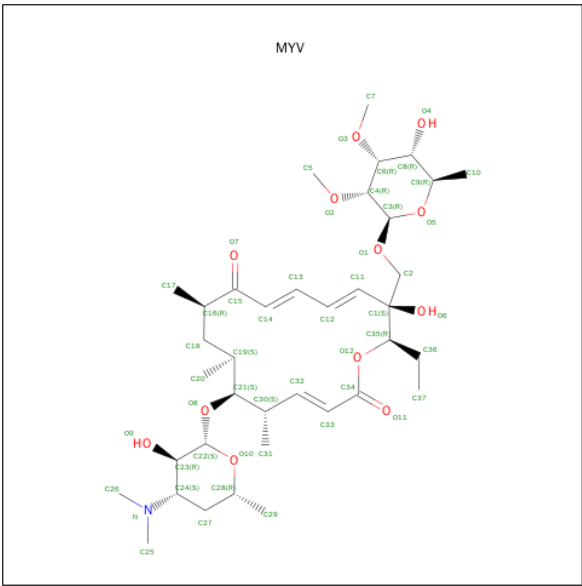
Chain	Residue	Modelled	Actual	Comment	Reference
B	-15	HIS	-	EXPRESSION TAG	UNP Q59523
B	-14	HIS	-	EXPRESSION TAG	UNP Q59523
B	-13	HIS	-	EXPRESSION TAG	UNP Q59523
B	-12	HIS	-	EXPRESSION TAG	UNP Q59523
B	-11	HIS	-	EXPRESSION TAG	UNP Q59523
B	-10	HIS	-	EXPRESSION TAG	UNP Q59523
B	-9	SER	-	EXPRESSION TAG	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
B	286	VAL	PHE	ENGINEERED MUTATION	UNP Q59523

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



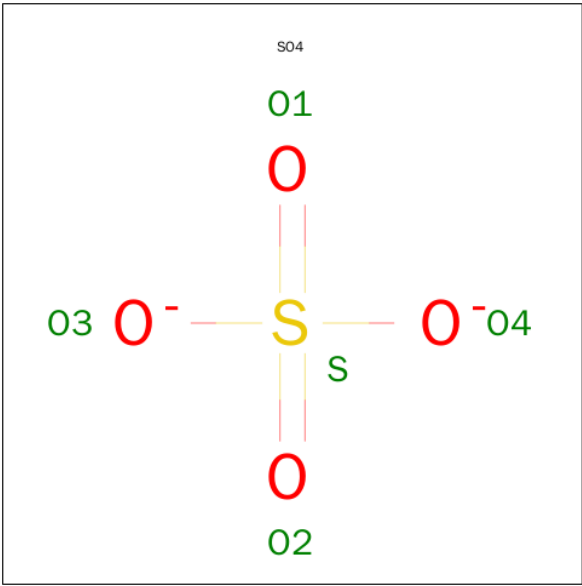
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is MYCINAMICIN V (three-letter code: MYV) (formula: C<sub>37</sub>H<sub>61</sub>NO<sub>12</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			100	74	2	24		
3	B	1	Total	C	N	O	0	1
			100	74	2	24		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	A	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0
4	B	1	Total O S 5 4 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

- Molecule 6 is water.


Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	273	Total 273	O 273	0	0
6	B	245	Total 245	O 245	0	0

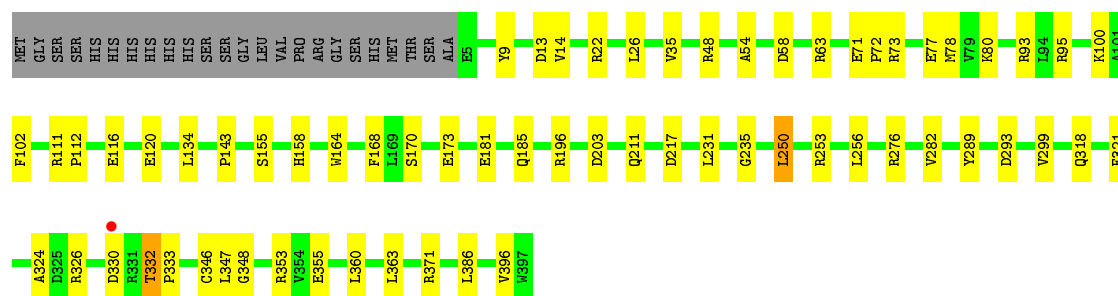


### 3 Residue-property plots


These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

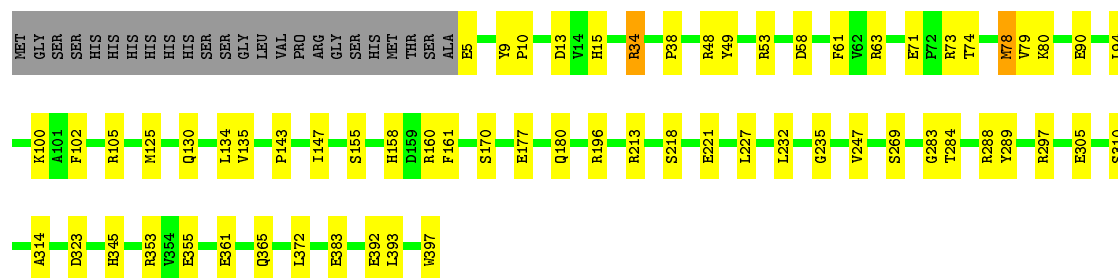
#### • Molecule 1: P-450-LIKE PROTEIN

Chain A: 



#### • Molecule 1: P-450-LIKE PROTEIN

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	55.45Å 56.11Å 76.42Å 90.43° 97.22° 102.11°	Depositor
Resolution (Å)	75.77 – 2.05 75.77 – 2.05	Depositor EDS
% Data completeness (in resolution range)	96.4 (75.77-2.05) 95.3 (75.77-2.05)	Depositor EDS
$R_{merge}$	0.17	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.81 (at 2.05Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.166 , 0.235 0.167 , 0.234	Depositor DCC
$R_{free}$ test set	2752 reflections (5.37%)	DCC
Wilson B-factor (Å <sup>2</sup> )	21.8	Xtriage
Anisotropy	0.333	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 48.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 54004 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7065	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.59% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, SO4, 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	1.09	1/3186 (0.0%)	1.03	13/4336 (0.3%)
1	B	1.05	2/3139 (0.1%)	0.94	3/4274 (0.1%)
All	All	1.07	3/6325 (0.0%)	0.99	16/8610 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	90	GLU	CG-CD	6.06	1.61	1.51
1	A	95	ARG	CB-CG	-5.04	1.39	1.52
1	B	221	GLU	CG-CD	5.03	1.59	1.51

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	63	ARG	NE-CZ-NH2	-7.69	116.46	120.30
1	A	253	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	B	63	ARG	NE-CZ-NH1	7.02	123.81	120.30
1	A	95	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	A	276	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	63	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	B	58	ASP	CB-CG-OD1	5.83	123.54	118.30
1	A	13	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	A	63	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	13	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	293	ASP	CB-CG-OD1	5.26	123.03	118.30
1	A	48	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	A	396	VAL	N-CA-C	-5.07	97.31	111.00
1	A	93	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	95	ARG	CG-CD-NE	-5.02	101.25	111.80
1	A	276	ARG	NE-CZ-NH1	5.01	122.81	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	3122	0	3083	37	0
1	B	3075	0	3053	44	0
2	A	43	0	30	4	0
2	B	43	0	30	1	0
3	A	100	0	122	7	0
3	B	100	0	122	10	0
4	A	20	0	0	0	0
4	B	20	0	0	3	0
5	A	12	0	16	1	0
5	B	12	0	16	3	0
6	A	273	0	0	5	0
6	B	245	0	0	10	0
All	All	7065	0	6472	93	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 (93) 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:48:ARG:NH2	6:B:2050:HOH:O	1.98	0.96
3:B:500[B]:MYV:H73C	3:B:500[B]:MYV:O4	1.78	0.83
3:B:500[B]:MYV:H72C	3:B:500[B]:MYV:HB	1.62	0.82
1:A:250:LEU:HD12	1:A:256:LEU:HG	1.61	0.81
1:B:5:GLU:HG2	6:B:2002:HOH:O	1.82	0.79
1:B:5:GLU:CG	6:B:2002:HOH:O	2.33	0.76
3:B:500[B]:MYV:H362	3:B:500[B]:MYV:H3	1.68	0.76
1:B:170:SER:HA	3:B:500[B]:MYV:H312	1.72	0.72
1:A:71:GLU:HG2	1:A:289:TYR:OH	1.94	0.67
1:B:345[A]:HIS:HE1	4:B:1400:SO4:O3	1.79	0.65
1:A:71:GLU:OE1	1:A:78[A]:MET:HE1	1.95	0.65

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:500[B]:MYV:O4	3:B:500[B]:MYV:C7	2.48	0.61
1:B:79:VAL:HG22	3:B:500[B]:MYV:H203	1.83	0.61
1:B:345[A]:HIS:CE1	4:B:1400:SO4:O3	2.55	0.60
1:B:345[B]:HIS:HE1	4:B:1401:SO4:O3	1.85	0.59
3:A:500[A]:MYV:C11	3:A:500[A]:MYV:C34	2.80	0.59
1:B:353:ARG:NH1	6:B:2219:HOH:O	2.13	0.58
1:B:15:HIS:HE1	1:B:383:GLU:OE2	1.86	0.58
1:A:111:ARG:HB3	1:A:112:PRO:HD3	1.85	0.58
1:A:250:LEU:CD1	1:A:256:LEU:HG	2.34	0.57
3:A:500[A]:MYV:O2	3:A:500[A]:MYV:H73C	2.05	0.57
1:B:53:ARG:NH1	6:B:2054:HOH:O	2.34	0.56
1:B:353:ARG:HD2	6:B:2219:HOH:O	2.06	0.55
1:B:213:ARG:HD3	1:B:218:SER:HB3	1.88	0.53
1:B:134:LEU:HD22	1:B:247:VAL:HG11	1.91	0.52
1:A:371:ARG:HD3	6:A:2187:HOH:O	2.08	0.52
1:A:235:GLY:HA2	2:A:450:HEM:C2C	2.45	0.51
1:A:116:GLU:O	1:A:120:GLU:HG3	2.09	0.51
1:B:9:TYR:CD1	1:B:10:PRO:HA	2.46	0.51
1:B:61:PHE:HB3	1:B:288:ARG:HB3	1.91	0.51
1:B:130:GLN:NE2	1:B:397:TRP:H	2.08	0.51
1:B:305:GLU:HG2	6:B:2031:HOH:O	2.11	0.49
1:A:170:SER:HA	3:A:500[A]:MYV:H312	1.93	0.49
1:A:143:PRO:HA	1:A:355:GLU:OE1	2.13	0.49
3:B:500[B]:MYV:O9	3:B:500[B]:MYV:H311	2.12	0.49
1:B:134:LEU:CD2	1:B:247:VAL:HG11	2.43	0.49
1:B:49:TYR:HA	1:B:314:ALA:HB1	1.94	0.48
1:A:318:GLN:HE22	1:A:324:ALA:H	1.61	0.48
1:A:348:GLY:HA3	2:A:450:HEM:C3C	2.49	0.48
1:A:386:LEU:CD1	3:A:500[B]:MYV:H372	2.45	0.47
1:B:235:GLY:HA2	2:B:450:HEM:C2C	2.50	0.47
3:B:500[B]:MYV:C9	3:B:500[B]:MYV:C7	2.92	0.47
1:A:386:LEU:HD13	3:A:500[B]:MYV:H372	1.97	0.47
1:B:196:ARG:NH2	6:B:2159:HOH:O	2.39	0.47
2:A:450:HEM:HBB2	2:A:450:HEM:HMB2	1.98	0.46
1:A:250:LEU:HD21	1:A:360:LEU:HD22	1.98	0.46
1:B:135:VAL:HG23	1:B:393:LEU:HB2	1.97	0.46
1:A:347:LEU:C	1:A:347:LEU:HD12	2.36	0.46
1:B:94:LEU:HD22	1:B:227:LEU:HD11	1.98	0.46
1:B:283:GLY:HA3	5:B:1402:GOL:H12	1.98	0.46
1:A:168:PHE:HB3	3:A:500[A]:MYV:H172	1.97	0.46
1:A:353:ARG:NH1	6:A:2240:HOH:O	2.11	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:13:ASP:OD2	1:B:15:HIS:HD2	1.98	0.45
1:A:332:THR:HG22	1:A:333:PRO:HA	1.98	0.45
1:B:5:GLU:HG3	6:B:2002:HOH:O	2.05	0.45
3:B:500[B]:MYV:C34	3:B:500[B]:MYV:C11	2.94	0.45
1:B:269:SER:HB2	6:B:2181:HOH:O	2.16	0.45
1:A:73:ARG:HA	5:A:1402:GOL:H11	1.99	0.45
1:B:71:GLU:HG2	1:B:289:TYR:OH	2.17	0.44
1:A:326:ARG:NH2	6:A:2225:HOH:O	2.42	0.44
1:A:54:ALA:O	1:A:58:ASP:HB2	2.18	0.44
1:A:77:GLU:OE1	6:A:2081:HOH:O	2.21	0.44
1:B:361:GLU:O	1:B:365:GLN:HB2	2.18	0.44
1:B:74:THR:HG23	5:B:1402:GOL:H11	2.00	0.43
1:A:155:SER:HA	1:A:158:HIS:CD2	2.53	0.43
1:A:363:LEU:HA	1:A:363:LEU:HD23	1.79	0.43
1:A:360:LEU:HA	1:A:360:LEU:HD23	1.69	0.43
1:B:73:ARG:HA	5:B:1402:GOL:H32	2.00	0.43
1:B:155:SER:HA	1:B:158:HIS:CD2	2.54	0.43
1:B:147:ILE:HG21	1:B:232:LEU:HA	2.00	0.43
1:B:48:ARG:HB3	1:B:48:ARG:HE	1.75	0.43
1:A:346:CYS:HA	2:A:450:HEM:CHA	2.49	0.43
3:B:500[B]:MYV:H23	3:B:500[B]:MYV:H263	1.72	0.43
1:B:15:HIS:CE1	1:B:383:GLU:OE2	2.69	0.43
1:B:143:PRO:HA	1:B:355:GLU:OE1	2.19	0.43
1:B:100:LYS:NZ	1:B:213:ARG:O	2.51	0.42
1:A:9:TYR:HB2	1:A:35:VAL:HB	2.01	0.42
1:B:34:ARG:HD2	1:B:34:ARG:HA	1.92	0.42
1:A:22:ARG:O	1:A:26:LEU:HG	2.20	0.42
1:A:231:LEU:HD21	1:A:347:LEU:HD11	2.02	0.42
1:B:372:LEU:HA	1:B:372:LEU:HD23	1.89	0.42
1:A:353:ARG:HD2	6:A:2240:HOH:O	2.19	0.41
1:B:9:TYR:O	1:B:38:PRO:HD3	2.20	0.41
3:A:500[B]:MYV:H23	3:A:500[B]:MYV:H263	1.76	0.41
1:A:164:TRP:HE1	1:A:185:GLN:NE2	2.18	0.41
1:A:321:PHE:O	1:A:324:ALA:HB2	2.20	0.41
1:A:14:VAL:HG12	1:A:282:VAL:HG22	2.03	0.41
1:A:100:LYS:HB2	1:A:100:LYS:HE3	1.94	0.41
1:B:147:ILE:HD11	1:B:235:GLY:HA3	2.03	0.41
1:B:284:THR:HG22	1:B:310:SER:HB2	2.02	0.41
1:B:78:MET:HB3	1:B:78:MET:HE2	1.82	0.40
1:A:78[A]:MET:HB3	1:A:78[A]:MET:HE2	1.88	0.40
1:A:71:GLU:HA	1:A:72:PRO:HD3	1.95	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	398/417 (95%)	386 (97%)	12 (3%)	0	100	100
1	B	393/417 (94%)	384 (98%)	9 (2%)	0	100	100
All	All	791/834 (95%)	770 (97%)	21 (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	326/346 (94%)	310 (95%)	16 (5%)	31	21
1	B	321/346 (93%)	308 (96%)	13 (4%)	38	29
All	All	647/692 (94%)	618 (96%)	29 (4%)	37	25

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

Mol	Chain	Res	Type
1	A	80	LYS
1	A	102	PHE
1	A	134	LEU
1	A	173	GLU
1	A	181	GLU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	196	ARG
1	A	203[A]	ASP
1	A	203[B]	ASP
1	A	211	GLN
1	A	217[A]	ASP
1	A	217[B]	ASP
1	A	250	LEU
1	A	299	VAL
1	A	330[A]	ASP
1	A	330[B]	ASP
1	A	332	THR
1	B	34	ARG
1	B	78	MET
1	B	80	LYS
1	B	102	PHE
1	B	105	ARG
1	B	125	MET
1	B	160	ARG
1	B	161	PHE
1	B	177	GLU
1	B	180	GLN
1	B	297	ARG
1	B	323	ASP
1	B	392	GLU

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	130	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	185	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 ⓘ

18 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	SO4	A	1398	-	4,4,4	0.20	0	6,6,6	0.28	0
4	SO4	A	1399	-	4,4,4	0.21	0	6,6,6	0.68	0
4	SO4	A	1400	-	4,4,4	0.25	0	6,6,6	0.56	0
4	SO4	A	1401	-	4,4,4	0.24	0	6,6,6	0.63	0
5	GOL	A	1402	-	5,5,5	0.57	0	5,5,5	1.34	1 (20%)
5	GOL	A	1403	-	5,5,5	0.63	0	5,5,5	0.86	0
2	HEM	A	450	1,6	30,50,50	1.93	9 (30%)	24,82,82	2.67	13 (54%)
3	MYV	A	500[A]	-	49,52,52	0.92	2 (4%)	60,74,74	1.67	10 (16%)
3	MYV	A	500[B]	-	49,52,52	0.92	2 (4%)	60,74,74	1.79	14 (23%)
4	SO4	B	1398	-	4,4,4	0.95	0	6,6,6	1.08	1 (16%)
4	SO4	B	1399	-	4,4,4	0.34	0	6,6,6	0.96	1 (16%)
4	SO4	B	1400	-	4,4,4	0.24	0	6,6,6	0.31	0
4	SO4	B	1401	-	4,4,4	0.26	0	6,6,6	0.29	0
5	GOL	B	1402	-	5,5,5	0.60	0	5,5,5	0.90	0
5	GOL	B	1403	-	5,5,5	0.28	0	5,5,5	0.68	0
2	HEM	B	450	1,6	30,50,50	2.58	10 (33%)	24,82,82	2.83	15 (62%)
3	MYV	B	500[A]	-	49,52,52	0.97	2 (4%)	60,74,74	1.62	10 (16%)
3	MYV	B	500[B]	-	49,52,52	0.99	3 (6%)	60,74,74	1.57	12 (20%)

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	SO4	A	1398	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1399	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1400	-	-	0/0/0/0	0/0/0/0
4	SO4	A	1401	-	-	0/0/0/0	0/0/0/0
5	GOL	A	1402	-	-	0/4/4/4	0/0/0/0
5	GOL	A	1403	-	-	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	500[A]	-	-	0/59/95/95	0/2/3/3
3	MYV	A	500[B]	-	-	0/59/95/95	0/2/3/3
4	SO4	B	1398	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1399	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1400	-	-	0/0/0/0	0/0/0/0
4	SO4	B	1401	-	-	0/0/0/0	0/0/0/0
5	GOL	B	1402	-	-	0/4/4/4	0/0/0/0
5	GOL	B	1403	-	-	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	500[A]	-	-	0/59/95/95	0/2/3/3
3	MYV	B	500[B]	-	-	0/59/95/95	0/2/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	450	HEM	C3B-C4B	-9.11	1.43	1.51
2	A	450	HEM	C3B-C4B	-4.46	1.47	1.51
2	B	450	HEM	C2C-C1C	-4.35	1.44	1.52
2	A	450	HEM	C2C-C1C	-3.72	1.45	1.52
2	B	450	HEM	C3D-C4D	-3.62	1.46	1.51
2	A	450	HEM	C3D-C4D	-3.18	1.47	1.51
3	B	500[A]	MYV	O12-C35	-3.17	1.40	1.46
3	B	500[B]	MYV	O12-C35	-2.89	1.41	1.46
2	B	450	HEM	C2B-C1B	-2.73	1.42	1.51
3	A	500[B]	MYV	O12-C35	-2.72	1.41	1.46
3	A	500[A]	MYV	O12-C35	-2.61	1.41	1.46
2	A	450	HEM	C2B-C1B	-2.02	1.45	1.51
2	B	450	HEM	FE-NB	2.00	2.08	1.97
2	A	450	HEM	C3C-CAC	2.05	1.55	1.51
3	B	500[B]	MYV	O1-C3	2.14	1.44	1.40
2	A	450	HEM	CHC-C1C	2.18	1.41	1.36
2	B	450	HEM	CMC-C2C	2.33	1.58	1.53
2	B	450	HEM	FE-ND	2.70	2.11	1.97

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	450	HEM	CAA-C2A	2.76	1.56	1.52
2	B	450	HEM	CMA-C3A	3.06	1.57	1.51
2	A	450	HEM	FE-NC	3.09	2.08	1.95
2	B	450	HEM	C1C-NC	3.76	1.40	1.36
2	B	450	HEM	FE-NC	3.80	2.10	1.95
2	A	450	HEM	FE-ND	3.83	2.17	1.97
3	A	500[B]	MYV	O12-C34	4.08	1.43	1.34
3	A	500[A]	MYV	O12-C34	4.22	1.43	1.34
3	B	500[A]	MYV	O12-C34	4.59	1.44	1.34
3	B	500[B]	MYV	O12-C34	4.80	1.44	1.34

All (77) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500[B]	MYV	C1-C11-C12	-6.27	116.02	126.18
2	B	450	HEM	C3B-CAB-CBB	-4.99	116.80	124.46
3	B	500[A]	MYV	C1-C11-C12	-4.98	118.11	126.18
3	B	500[A]	MYV	C12-C13-C14	-4.70	114.22	124.66
3	A	500[A]	MYV	C1-C11-C12	-4.64	118.67	126.18
3	B	500[B]	MYV	C1-C11-C12	-4.45	118.98	126.18
2	A	450	HEM	CBD-CAD-C3D	-4.28	101.09	113.55
3	A	500[B]	MYV	C7-O3-C6	-4.16	102.84	114.59
3	B	500[A]	MYV	O5-C9-C8	-4.13	102.38	109.53
2	A	450	HEM	CMA-C3A-C4A	-4.10	121.59	128.36
3	A	500[B]	MYV	O5-C9-C8	-3.75	103.03	109.53
3	B	500[B]	MYV	C12-C13-C14	-3.74	116.35	124.66
3	B	500[A]	MYV	C7-O3-C6	-3.69	104.16	114.59
2	B	450	HEM	CBD-CAD-C3D	-3.52	103.30	113.55
3	A	500[B]	MYV	O5-C3-O1	-3.48	101.67	110.05
2	B	450	HEM	C3B-C4B-NB	-3.48	104.98	111.63
3	A	500[B]	MYV	O12-C34-O11	-3.46	117.92	123.30
3	A	500[A]	MYV	C36-C35-C1	-3.45	108.33	115.17
3	A	500[B]	MYV	C6-C8-C9	-3.37	102.15	109.80
3	B	500[B]	MYV	O5-C9-C8	-3.32	103.77	109.53
3	A	500[A]	MYV	C27-C24-C23	-3.29	105.24	110.03
3	B	500[B]	MYV	C30-C21-C19	-3.13	108.40	115.73
3	A	500[A]	MYV	C12-C13-C14	-3.02	117.95	124.66
3	A	500[A]	MYV	O3-C6-C8	-2.98	103.35	110.21
3	A	500[A]	MYV	O12-C34-O11	-2.92	118.75	123.30
3	B	500[A]	MYV	C31-C30-C32	-2.80	103.20	110.07
3	B	500[B]	MYV	C35-O12-C34	-2.77	113.20	116.90
2	A	450	HEM	CBA-CAA-C2A	-2.69	107.71	112.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	500[A]	MYV	C20-C19-C21	-2.61	106.68	111.27
2	A	450	HEM	C3B-C4B-NB	-2.53	106.79	111.63
3	B	500[B]	MYV	C3-O5-C9	-2.51	109.37	113.64
3	B	500[A]	MYV	C22-O10-C28	-2.48	108.81	112.97
4	B	1398	SO4	O4-S-O3	-2.47	98.92	108.98
3	A	500[B]	MYV	C20-C19-C21	-2.44	106.96	111.27
2	B	450	HEM	CMA-C3A-C4A	-2.41	124.37	128.36
2	A	450	HEM	CAA-C2A-C1A	-2.36	124.45	127.01
3	A	500[B]	MYV	C12-C13-C14	-2.35	119.44	124.66
3	B	500[B]	MYV	O12-C34-O11	-2.35	119.64	123.30
3	B	500[A]	MYV	O5-C3-C4	-2.29	104.85	109.47
3	B	500[A]	MYV	C27-C24-N	-2.27	108.97	115.70
5	A	1402	GOL	O2-C2-C1	-2.26	98.29	108.65
3	A	500[B]	MYV	O2-C4-C6	-2.24	103.33	108.94
3	B	500[A]	MYV	C27-C24-C23	-2.20	106.82	110.03
3	B	500[B]	MYV	C27-C24-N	-2.13	109.41	115.70
3	B	500[B]	MYV	O3-C6-C4	-2.09	103.71	108.94
3	A	500[B]	MYV	C27-C24-N	-2.08	109.55	115.70
2	B	450	HEM	CAA-C2A-C1A	-2.03	124.80	127.01
3	A	500[B]	MYV	O4-C8-C9	2.03	114.59	109.84
2	B	450	HEM	C4B-CHC-C1C	2.07	129.28	125.82
3	A	500[B]	MYV	O10-C28-C27	2.16	112.55	109.09
4	B	1399	SO4	O2-S-O1	2.19	116.44	109.50
2	B	450	HEM	C3B-C4B-CHC	2.22	126.29	123.16
2	B	450	HEM	CMA-C3A-C2A	2.26	129.96	125.24
3	B	500[A]	MYV	O4-C8-C9	2.30	115.24	109.84
3	A	500[A]	MYV	O10-C28-C27	2.32	112.80	109.09
3	B	500[B]	MYV	O12-C34-C33	2.44	117.46	111.42
2	A	450	HEM	CMA-C3A-C2A	2.49	130.44	125.24
3	A	500[A]	MYV	O5-C9-C10	2.63	112.38	106.64
3	A	500[B]	MYV	C22-C23-C24	2.67	113.96	109.25
3	A	500[B]	MYV	O12-C34-C33	2.68	118.06	111.42
3	B	500[B]	MYV	C22-C23-C24	2.77	114.13	109.25
2	B	450	HEM	C2C-C1C-CHC	2.87	128.05	123.68
2	B	450	HEM	C2D-C3D-C4D	2.88	106.38	101.50
2	A	450	HEM	C2C-C1C-CHC	2.91	128.11	123.68
3	B	500[B]	MYV	O5-C9-C10	3.06	113.33	106.64
2	A	450	HEM	CMD-C2D-C3D	3.09	128.00	114.35
2	A	450	HEM	C2D-C3D-C4D	3.12	106.80	101.50
2	B	450	HEM	CMD-C2D-C3D	3.31	128.98	114.35
2	A	450	HEM	CMC-C2C-C3C	3.71	125.78	116.53
2	A	450	HEM	CAD-C3D-C2D	4.14	125.12	113.22

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	450	HEM	CMC-C2C-C3C	4.17	126.93	116.53
2	B	450	HEM	CAD-C3D-C4D	4.22	127.37	112.47
2	A	450	HEM	CAD-C3D-C4D	4.42	128.06	112.47
2	B	450	HEM	CAD-C3D-C2D	4.51	126.18	113.22
2	A	450	HEM	CMB-C2B-C3B	4.63	128.08	116.53
2	B	450	HEM	CMB-C2B-C3B	4.78	128.46	116.53
3	A	500[A]	MYV	C35-O12-C34	4.83	123.36	116.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1402	GOL	1	0
2	A	450	HEM	4	0
3	A	500[A]	MYV	4	0
3	A	500[B]	MYV	3	0
4	B	1400	SO4	2	0
4	B	1401	SO4	1	0
5	B	1402	GOL	3	0
2	B	450	HEM	1	0
3	B	500[B]	MYV	10	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	393/417 (94%)	-0.39	1 (0%) 94 95	9, 19, 34, 48	0
1	B	393/417 (94%)	-0.36	0 100 100	10, 21, 37, 51	0
All	All	786/834 (94%)	-0.38	1 (0%) 95 96	9, 20, 36, 51	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	330[A]	ASP	2.2

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
4	SO4	A	1398	5/5	0.94	0.20	7.28	58,59,60,60	0
3	MYV	B	500[B]	50/50	0.92	0.16	4.45	19,24,30,30	50

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MYV	A	500[A]	50/50	0.91	0.17	4.16	17,23,34,35	50
3	MYV	B	500[A]	50/50	0.92	0.16	3.76	5,17,29,31	50
5	GOL	B	1402	6/6	0.94	0.13	3.71	36,42,42,44	0
3	MYV	A	500[B]	50/50	0.91	0.17	3.26	6,25,36,37	50
4	SO4	A	1401	5/5	0.94	0.13	2.40	61,62,64,64	0
5	GOL	A	1402	6/6	0.92	0.11	1.34	45,45,47,48	0
4	SO4	A	1400	5/5	0.94	0.12	1.01	52,55,57,57	0
4	SO4	B	1398	5/5	0.99	0.11	0.71	25,25,28,31	0
5	GOL	B	1403	6/6	0.96	0.10	0.37	22,26,28,29	0
2	HEM	A	450	43/43	0.99	0.10	0.32	8,14,16,19	0
4	SO4	B	1399	5/5	0.96	0.12	0.30	60,60,61,63	0
2	HEM	B	450	43/43	0.98	0.10	0.22	8,13,17,23	0
5	GOL	A	1403	6/6	0.96	0.09	-0.73	20,23,28,29	0
4	SO4	B	1400	5/5	0.94	0.18	-	55,55,56,57	0
4	SO4	A	1399	5/5	0.95	0.21	-	50,53,54,55	0
4	SO4	B	1401	5/5	0.97	0.13	-	40,45,46,46	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.