



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 14, 2016 – 02:46 PM EDT

PDB ID : 5SYK
Title : Crystal structure of B. pseudomallei KatG treated with hydrogen peroxide
Authors : Loewen, P.C.
Deposited on : 2016-08-11
Resolution : 1.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027939
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-20027939

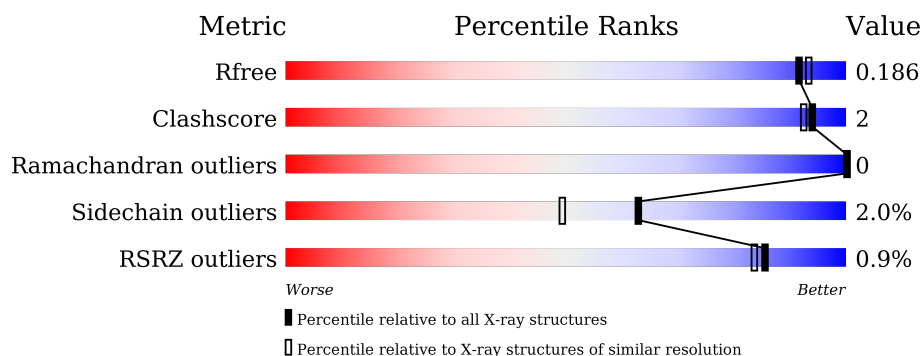
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	4533 (1.80-1.80)
Clashscore	102246	5383 (1.80-1.80)
Ramachandran outliers	100387	5320 (1.80-1.80)
Sidechain outliers	100360	5319 (1.80-1.80)
RSRZ outliers	91569	4547 (1.80-1.80)

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	728	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 88% 10% .. </div> </div>
1	B	728	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> % 86% 10% .. </div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MRD	A	805	-	-	-	X
7	MPD	B	805	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12673 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 Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	8	0
			5544	3501	988	1041	14			
1	B	713	Total	C	N	O	S	0	5	0
			5532	3493	987	1038	14			

- 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		

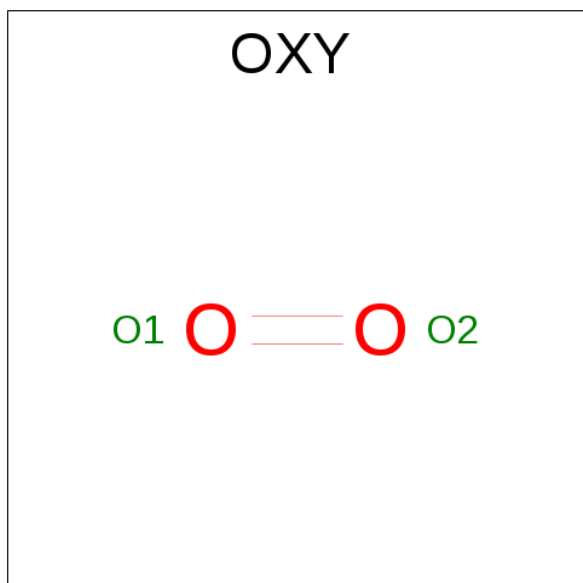
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total Na 1 1	0	0
3	A	1	Total Na 1 1	0	0

- Molecule 4 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

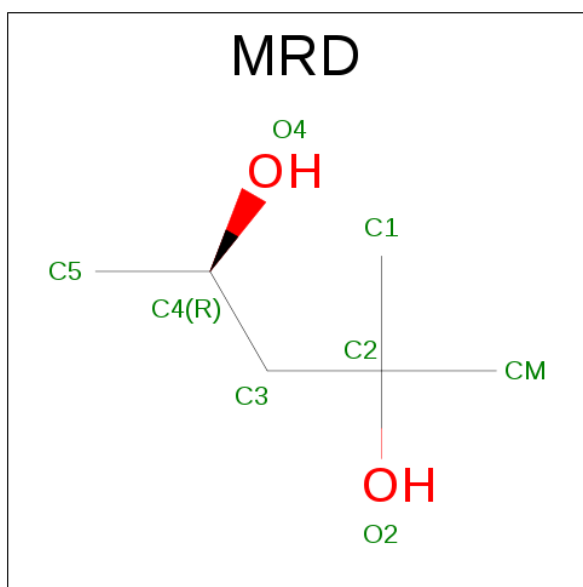
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	A	1	Total Cl 1 1	0	0

- Molecule 5 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂).



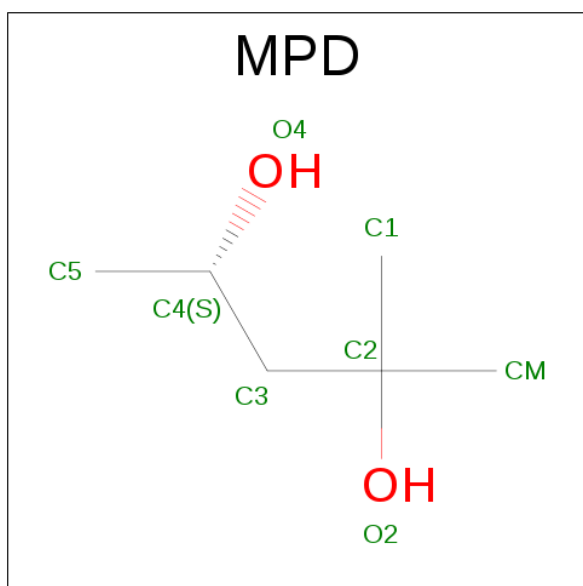
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 2 2	0	0
5	B	1	Total O 2 2	0	0

- Molecule 6 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula: C₆H₁₄O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	C	O	0	0
			8	6	2		

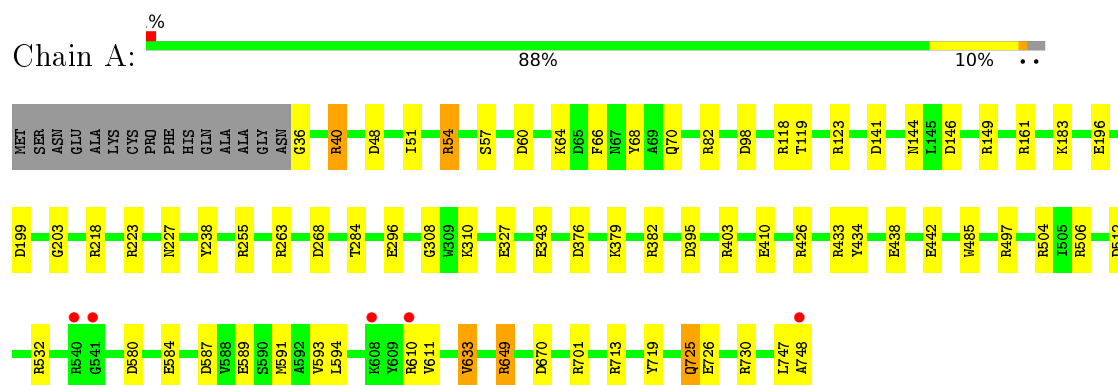
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	740	Total 740	O 740	0	0
8	B	747	Total 747	O 747	0	0

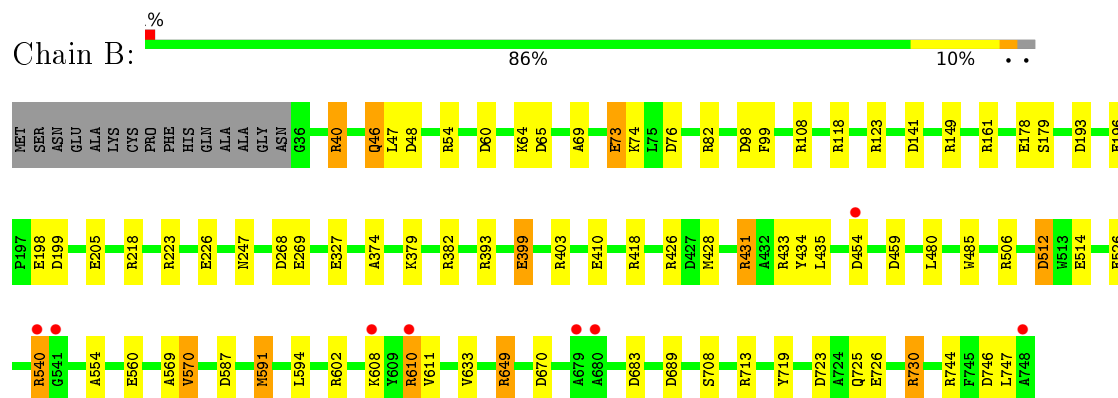
3 Residue-property plots [i](#)

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 ($\text{RSRZ} > 2$). 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: Catalase-peroxidase



• Molecule 1: Catalase-peroxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.72Å 116.20Å 174.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 48.37 – 1.80	Depositor EDS
% Data completeness (in resolution range)	94.7 (20.00-1.80) 94.7 (48.37-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.98 (at 1.81Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.148 , 0.179 0.160 , 0.186	Depositor DCC
R_{free} test set	8868 reflections (5.22%)	DCC
Wilson B-factor (Å ²)	19.4	Xtriage
Anisotropy	0.321	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12673	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 3.16% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: TOX, OXY, CL, NA, MPD, MRD, HEM

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	1.31	24/5690 (0.4%)	1.21	46/7732 (0.6%)
1	B	1.32	23/5668 (0.4%)	1.23	56/7702 (0.7%)
All	All	1.32	47/11358 (0.4%)	1.22	102/15434 (0.7%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	2
All	All	0	3

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	198	GLU	CD-OE2	9.35	1.35	1.25
1	A	343	GLU	CD-OE1	7.97	1.34	1.25
1	B	726	GLU	CD-OE2	7.87	1.34	1.25
1	B	514	GLU	CD-OE2	-7.62	1.17	1.25
1	A	57	SER	CB-OG	7.19	1.51	1.42
1	A	726	GLU	CG-CD	7.13	1.62	1.51
1	B	269	GLU	CD-OE2	-7.04	1.18	1.25
1	A	725	GLN	CG-CD	7.01	1.67	1.51
1	B	410	GLU	CG-CD	6.89	1.62	1.51
1	B	327	GLU	CG-CD	6.82	1.62	1.51
1	A	532	ARG	NE-CZ	-6.74	1.24	1.33
1	A	426[A]	ARG	CZ-NH2	6.65	1.41	1.33
1	A	426[B]	ARG	CZ-NH2	6.65	1.41	1.33
1	B	526	GLU	CD-OE1	6.60	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	205	GLU	CD-OE1	6.53	1.32	1.25
1	A	327	GLU	CD-OE1	6.46	1.32	1.25
1	A	748	ALA	N-CA	6.28	1.58	1.46
1	A	442	GLU	CD-OE2	-6.24	1.18	1.25
1	B	418	ARG	CZ-NH1	-6.23	1.25	1.33
1	B	196	GLU	CG-CD	6.15	1.61	1.51
1	B	746	ASP	CB-CG	6.14	1.64	1.51
1	B	512	ASP	CB-CG	6.03	1.64	1.51
1	A	584	GLU	CG-CD	6.00	1.60	1.51
1	A	70	GLN	CG-CD	5.99	1.64	1.51
1	B	512	ASP	CG-OD2	5.92	1.39	1.25
1	B	196	GLU	CB-CG	-5.88	1.41	1.52
1	A	196	GLU	CB-CG	-5.83	1.41	1.52
1	A	296	GLU	CD-OE1	-5.81	1.19	1.25
1	B	708	SER	CB-OG	-5.79	1.34	1.42
1	A	196	GLU	CG-CD	5.76	1.60	1.51
1	B	65	ASP	CB-CG	5.62	1.63	1.51
1	A	343	GLU	CG-CD	5.60	1.60	1.51
1	A	36	GLY	N-CA	5.46	1.54	1.46
1	B	602	ARG	CZ-NH2	-5.46	1.25	1.33
1	A	255	ARG	CD-NE	5.41	1.55	1.46
1	B	725	GLN	CD-NE2	5.40	1.46	1.32
1	B	399	GLU	CD-OE1	5.31	1.31	1.25
1	A	68	TYR	CZ-OH	5.28	1.46	1.37
1	A	308	GLY	N-CA	5.18	1.53	1.46
1	B	193	ASP	CB-CG	5.18	1.62	1.51
1	A	203	GLY	C-O	5.15	1.31	1.23
1	B	485	TRP	CE3-CZ3	5.08	1.47	1.38
1	B	179	SER	CA-CB	5.07	1.60	1.52
1	B	689	ASP	CG-OD2	-5.05	1.13	1.25
1	A	485	TRP	CE3-CZ3	5.04	1.47	1.38
1	A	410	GLU	CD-OE2	5.04	1.31	1.25
1	A	434	TYR	CE1-CZ	-5.04	1.32	1.38

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	591	MET	CG-SD-CE	-15.09	76.05	100.20
1	A	532	ARG	NE-CZ-NH2	-12.78	113.91	120.30
1	B	149	ARG	NE-CZ-NH1	11.03	125.82	120.30
1	B	393	ARG	NE-CZ-NH2	-11.01	114.80	120.30
1	B	713	ARG	NE-CZ-NH1	9.89	125.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	649	ARG	NE-CZ-NH1	9.89	125.24	120.30
1	A	426[A]	ARG	NE-CZ-NH1	-9.71	115.45	120.30
1	A	426[B]	ARG	NE-CZ-NH1	-9.71	115.45	120.30
1	A	403[A]	ARG	NE-CZ-NH1	-9.70	115.45	120.30
1	A	403[B]	ARG	NE-CZ-NH1	-9.70	115.45	120.30
1	A	713	ARG	NE-CZ-NH1	9.49	125.04	120.30
1	B	108	ARG	NE-CZ-NH2	-9.46	115.57	120.30
1	A	713	ARG	NE-CZ-NH2	-9.43	115.59	120.30
1	B	40	ARG	NE-CZ-NH1	8.97	124.78	120.30
1	B	506	ARG	NE-CZ-NH1	8.81	124.70	120.30
1	A	382	ARG	NE-CZ-NH2	-8.75	115.92	120.30
1	A	48	ASP	CB-CG-OD1	8.71	126.14	118.30
1	B	713	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	B	649	ARG	NE-CZ-NH1	8.34	124.47	120.30
1	B	82	ARG	NE-CZ-NH2	-8.29	116.15	120.30
1	B	73	GLU	OE1-CD-OE2	8.25	133.20	123.30
1	A	40	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	A	60	ASP	CB-CG-OD2	-8.22	110.90	118.30
1	B	382	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	B	730	ARG	NE-CZ-NH1	8.13	124.37	120.30
1	B	218	ARG	NE-CZ-NH2	-8.10	116.25	120.30
1	A	587	ASP	CB-CG-OD1	8.07	125.56	118.30
1	B	268	ASP	CB-CG-OD1	8.02	125.52	118.30
1	A	670	ASP	CB-CG-OD2	-7.83	111.25	118.30
1	B	98	ASP	CB-CG-OD1	-7.72	111.35	118.30
1	A	730	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	B	587	ASP	CB-CG-OD1	7.41	124.97	118.30
1	B	123	ARG	NE-CZ-NH1	7.37	123.99	120.30
1	B	649	ARG	NE-CZ-NH2	-7.28	116.66	120.30
1	B	683	ASP	CB-CG-OD1	7.23	124.81	118.30
1	B	226	GLU	OE1-CD-OE2	-7.21	114.65	123.30
1	B	161	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	B	683	ASP	CB-CG-OD2	-7.13	111.89	118.30
1	B	218	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	A	649	ARG	NE-CZ-NH2	-7.09	116.75	120.30
1	B	76	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	B	433	ARG	NE-CZ-NH2	-7.05	116.78	120.30
1	A	149	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	B	433	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	A	506	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	B	454	ASP	CB-CG-OD1	6.72	124.35	118.30
1	A	376	ASP	CB-CG-OD2	-6.67	112.30	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161	ARG	NE-CZ-NH2	6.60	123.60	120.30
1	A	434	TYR	CB-CG-CD1	6.50	124.90	121.00
1	A	54	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	B	382	ARG	CG-CD-NE	-6.45	98.26	111.80
1	B	434	TYR	CB-CG-CD1	6.41	124.85	121.00
1	B	48	ASP	CB-CG-OD1	6.39	124.05	118.30
1	B	82	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	A	263	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	B	54	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	B	570	VAL	CG1-CB-CG2	-6.21	100.97	110.90
1	B	379	LYS	CA-CB-CG	6.19	127.02	113.40
1	B	744	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	A	580	ASP	CB-CG-OD1	-6.13	112.78	118.30
1	A	497	ARG	NE-CZ-NH1	6.09	123.35	120.30
1	B	60	ASP	CB-CG-OD2	-6.07	112.83	118.30
1	A	701	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	B	123	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	218	ARG	NE-CZ-NH1	5.95	123.28	120.30
1	A	433	ARG	NE-CZ-NH1	5.95	123.27	120.30
1	A	218	ARG	NE-CZ-NH2	-5.88	117.36	120.30
1	A	268	ASP	CB-CG-OD1	5.84	123.56	118.30
1	A	395	ASP	CB-CG-OD1	5.84	123.55	118.30
1	A	438	GLU	OE1-CD-OE2	5.76	130.21	123.30
1	B	428	MET	CA-CB-CG	-5.71	103.59	113.30
1	A	512	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	B	426[A]	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	B	426[B]	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	B	418	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	A	82	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	B	149	ARG	NE-CZ-NH2	-5.59	117.51	120.30
1	B	723	ASP	CB-CG-OD2	5.57	123.32	118.30
1	B	410	GLU	OE1-CD-OE2	-5.54	116.65	123.30
1	A	382	ARG	CG-CD-NE	-5.50	100.24	111.80
1	B	689	ASP	CB-CG-OD1	5.50	123.25	118.30
1	B	730	ARG	NE-CZ-NH2	-5.41	117.59	120.30
1	A	310	LYS	CD-CE-NZ	-5.39	99.31	111.70
1	B	431	ARG	NE-CZ-NH1	-5.36	117.62	120.30
1	B	560	GLU	OE1-CD-OE2	5.35	129.72	123.30
1	A	255	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	A	433	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	123	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	A	183	LYS	CD-CE-NZ	5.30	123.89	111.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	54	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	A	66	PHE	CG-CD2-CE2	-5.25	115.02	120.80
1	A	343	GLU	CG-CD-OE2	-5.22	107.86	118.30
1	B	268	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	B	459	ASP	CB-CG-OD1	5.15	122.94	118.30
1	B	730	ARG	CA-CB-CG	5.14	124.71	113.40
1	A	98	ASP	CB-CG-OD2	5.13	122.92	118.30
1	A	343	GLU	CG-CD-OE1	5.13	128.56	118.30
1	B	410	GLU	CG-CD-OE1	5.12	128.55	118.30
1	A	51	ILE	CG1-CB-CG2	-5.11	100.15	111.40
1	B	670	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	B	435	LEU	CB-CG-CD1	-5.07	102.38	111.00
1	A	670	ASP	CB-CG-OD1	5.02	122.81	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	747	LEU	Peptide
1	B	199	ASP	Mainchain
1	B	747	LEU	Peptide

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	5544	0	5364	15	0
1	B	5532	0	5348	21	0
2	A	43	0	30	1	0
2	B	43	0	30	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	2	0	0	0	0
5	B	2	0	0	0	0
6	A	8	0	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	B	8	0	14	1	0
8	A	740	0	0	3	0
8	B	747	0	0	5	0
All	All	12673	0	10800	39	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 2.

All (39) 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:569:ALA:O	1:B:570:VAL:HG23	1.76	0.85
1:A:119[B]:THR:HG21	8:A:937:HOH:O	1.77	0.83
1:A:633[B]:VAL:CG2	1:A:719:TYR:CZ	2.73	0.72
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.75	0.70
1:B:247:ASN:HB2	8:B:1538:HOH:O	1.91	0.69
1:B:610:ARG:HG2	1:B:611:VAL:HG23	1.75	0.69
1:B:569:ALA:O	1:B:570:VAL:CG2	2.41	0.68
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	1.78	0.65
6:A:805:MRD:H1C2	6:A:805:MRD:O4	1.97	0.65
1:B:512:ASP:OD1	8:B:903:HOH:O	2.15	0.63
1:B:69:ALA:O	1:B:73:GLU:HG2	2.00	0.62
1:A:633[B]:VAL:HG21	1:A:719:TYR:CZ	2.38	0.58
1:B:399:GLU:OE1	1:B:403[B]:ARG:NH1	2.39	0.56
1:A:633[B]:VAL:HG23	1:A:719:TYR:CE1	2.41	0.55
1:B:633[A]:VAL:HG21	1:B:719:TYR:CZ	2.42	0.54
1:A:589:GLU:HG2	8:A:1096:HOH:O	2.10	0.52
1:B:610:ARG:H	1:B:610:ARG:HD2	1.77	0.49
1:A:633[B]:VAL:CG2	1:A:719:TYR:CE1	2.96	0.49
1:A:591:MET:SD	1:A:594:LEU:HD12	2.52	0.49
1:B:610:ARG:HG2	1:B:611:VAL:N	2.29	0.47
7:B:805:MPD:O2	7:B:805:MPD:O4	2.31	0.47
1:B:633[A]:VAL:HG23	1:B:719:TYR:CE1	2.50	0.46
6:A:805:MRD:C1	6:A:805:MRD:O4	2.62	0.46
1:B:46:GLN:HE21	1:B:47:LEU:H	1.62	0.46
1:A:610:ARG:HG3	1:A:611:VAL:HG23	1.97	0.45
1:B:431:ARG:HD2	8:B:1472:HOH:O	2.15	0.45
1:B:633[A]:VAL:CG2	1:B:719:TYR:CE1	3.00	0.45
1:B:591:MET:SD	1:B:594:LEU:HD12	2.57	0.45
1:A:119[B]:THR:CG2	1:A:593:VAL:HG11	2.46	0.44
1:B:431:ARG:CD	8:B:1472:HOH:O	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:ARG:NE	1:A:199:ASP:OD2	2.51	0.44
1:B:540:ARG:HA	1:B:540:ARG:CZ	2.48	0.43
1:B:178:GLU:OE1	8:B:904:HOH:O	2.22	0.42
1:A:144:ASN:HA	1:A:146:ASP:OD1	2.19	0.42
1:A:504:ARG:HD2	8:A:935:HOH:O	2.21	0.41
1:A:284:THR:HG22	2:A:801:HEM:HAA1	2.03	0.41
1:B:99:PHE:CD2	1:B:374:ALA:HA	2.57	0.40
1:B:480:LEU:HD22	1:B:554:ALA:HB1	2.01	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	717/728 (98%)	707 (99%)	10 (1%)	0	100	100
1	B	714/728 (98%)	705 (99%)	9 (1%)	0	100	100
All	All	1431/1456 (98%)	1412 (99%)	19 (1%)	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	556/560 (99%)	545 (98%)	11 (2%)	63	49

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	553/560 (99%)	541 (98%)	12 (2%)	60	45
All	All	1109/1120 (99%)	1086 (98%)	23 (2%)	63	47

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	64	LYS
1	A	118	ARG
1	A	141	ASP
1	A	223	ARG
1	A	227	ASN
1	A	379	LYS
1	A	633[A]	VAL
1	A	633[B]	VAL
1	A	649	ARG
1	A	725	GLN
1	B	40	ARG
1	B	46	GLN
1	B	64	LYS
1	B	74	LYS
1	B	118	ARG
1	B	141	ASP
1	B	223	ARG
1	B	540	ARG
1	B	608	LYS
1	B	610	ARG
1	B	649	ARG
1	B	730	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	227	ASN
1	A	247	ASN
1	B	46	GLN
1	B	227	ASN
1	B	247	ASN
1	B	650	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

4 non-standard protein/DNA/RNA residues 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
1	TOX	A	111[A]	2	10,17,18	3.50	2 (20%)	9,23,25	1.45	2 (22%)
1	TOX	A	111[B]	-	10,17,18	3.50	2 (20%)	9,23,25	1.45	2 (22%)
1	TOX	B	111[A]	2	10,17,18	3.49	7 (70%)	9,23,25	2.17	3 (33%)
1	TOX	B	111[B]	-	10,17,18	3.49	7 (70%)	9,23,25	2.17	3 (33%)

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
1	TOX	A	111[A]	2	-	0/3/8/10	0/2/2/2
1	TOX	A	111[B]	-	-	0/3/8/10	0/2/2/2
1	TOX	B	111[A]	2	-	0/3/8/10	0/2/2/2
1	TOX	B	111[B]	-	-	0/3/8/10	0/2/2/2

All (18) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111[A]	TOX	CD1-NE1	-10.29	1.29	1.39
1	A	111[B]	TOX	CD1-NE1	-10.29	1.29	1.39
1	B	111[A]	TOX	CD1-NE1	-6.85	1.32	1.39
1	B	111[B]	TOX	CD1-NE1	-6.85	1.32	1.39
1	B	111[A]	TOX	CZ2-CE2	-4.84	1.31	1.41
1	B	111[B]	TOX	CZ2-CE2	-4.84	1.31	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111[A]	TOX	CB-CA	-3.76	1.45	1.53
1	B	111[B]	TOX	CB-CA	-3.76	1.45	1.53
1	B	111[A]	TOX	CE3-CD2	-3.39	1.35	1.42
1	B	111[B]	TOX	CE3-CD2	-3.39	1.35	1.42
1	B	111[A]	TOX	CZ3-CH2	2.08	1.43	1.38
1	B	111[B]	TOX	CZ3-CH2	2.08	1.43	1.38
1	A	111[A]	TOX	O-C	2.13	1.29	1.19
1	A	111[B]	TOX	O-C	2.13	1.29	1.19
1	B	111[A]	TOX	O-C	2.85	1.33	1.19
1	B	111[B]	TOX	O-C	2.85	1.33	1.19
1	B	111[A]	TOX	CD2-CE2	3.04	1.45	1.41
1	B	111[B]	TOX	CD2-CE2	3.04	1.45	1.41

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111[A]	TOX	CB-CG-CD1	-3.90	123.15	127.97
1	B	111[B]	TOX	CB-CG-CD1	-3.90	123.15	127.97
1	B	111[A]	TOX	CZ2-CE2-CD2	-3.36	116.36	120.58
1	B	111[B]	TOX	CZ2-CE2-CD2	-3.36	116.36	120.58
1	A	111[A]	TOX	CZ2-CE2-CD2	-2.83	117.03	120.58
1	A	111[B]	TOX	CZ2-CE2-CD2	-2.83	117.03	120.58
1	B	111[A]	TOX	CH2-CZ2-CE2	2.29	124.11	119.28
1	B	111[B]	TOX	CH2-CZ2-CE2	2.29	124.11	119.28
1	A	111[A]	TOX	CE3-CD2-CE2	2.32	122.16	119.83
1	A	111[B]	TOX	CE3-CD2-CE2	2.32	122.16	119.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 4 are monoatomic - leaving 6 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	801	1	24,50,50	1.98	7 (29%)	16,82,82	2.23	6 (37%)
5	OXY	A	804	-	1,1,1	0.06	0	0,0,0	0.00	-
6	MRD	A	805	-	6,7,7	0.36	0	6,10,10	1.90	1 (16%)
2	HEM	B	801	1	24,50,50	3.53	5 (20%)	16,82,82	2.00	7 (43%)
5	OXY	B	804	-	1,1,1	0.47	0	0,0,0	0.00	-
7	MPD	B	805	-	6,7,7	0.29	0	6,10,10	2.32	1 (16%)

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	801	1	-	0/6/54/54	0/0/8/8
5	OXY	A	804	-	-	0/0/0/0	0/0/0/0
6	MRD	A	805	-	-	0/5/5/5	0/0/0/0
2	HEM	B	801	1	-	0/6/54/54	0/0/8/8
5	OXY	B	804	-	-	0/0/0/0	0/0/0/0
7	MPD	B	805	-	-	0/5/5/5	0/0/0/0

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C1B-NB	-8.53	1.25	1.36
2	B	801	HEM	C3B-C2B	-8.43	1.29	1.40
2	B	801	HEM	C1C-NC	-5.38	1.29	1.36
2	B	801	HEM	C3C-C2C	-3.77	1.35	1.40
2	A	801	HEM	C3B-CAB	-3.50	1.40	1.47
2	A	801	HEM	C4C-NC	-2.31	1.33	1.36
2	A	801	HEM	CAD-C3D	-2.16	1.49	1.52
2	A	801	HEM	CMA-C3A	2.36	1.56	1.51
2	A	801	HEM	C4D-ND	3.06	1.40	1.36
2	A	801	HEM	CAA-C2A	3.31	1.57	1.52
2	A	801	HEM	C1C-NC	5.92	1.44	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C4C-NC	9.96	1.50	1.36

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	CAA-CBA-CGA	-4.67	103.70	112.78
6	A	805	MRD	CM-C2-C1	-3.31	102.52	110.41
2	B	801	HEM	CAA-CBA-CGA	-3.17	106.62	112.78
2	A	801	HEM	C3C-CAC-CBC	-3.11	120.15	126.40
2	A	801	HEM	C3B-CAB-CBB	-2.78	120.82	126.40
2	B	801	HEM	C3B-CAB-CBB	-2.57	121.23	126.40
2	B	801	HEM	CMD-C2D-C1D	-2.41	124.22	128.31
2	A	801	HEM	CMA-C3A-C4A	-2.26	124.47	128.31
2	B	801	HEM	CMA-C3A-C4A	-2.26	124.47	128.31
2	B	801	HEM	CBD-CAD-C3D	2.36	116.61	112.47
2	B	801	HEM	CBA-CAA-C2A	2.40	116.71	112.49
2	B	801	HEM	CAD-CBD-CGD	3.14	118.89	112.78
2	A	801	HEM	CBD-CAD-C3D	3.26	118.20	112.47
2	A	801	HEM	CMB-C2B-C3B	3.34	131.62	125.09
7	B	805	MPD	CM-C2-C1	5.10	122.58	110.41

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	HEM	1	0
6	A	805	MRD	2	0
7	B	805	MPD	1	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 ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	712/728 (97%)	-0.63	5 (0%) 89 87	13, 20, 38, 82	0
1	B	712/728 (97%)	-0.62	8 (1%) 82 80	13, 20, 37, 89	0
All	All	1424/1456 (97%)	-0.63	13 (0%) 85 83	13, 20, 37, 89	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	9.5
1	B	748	ALA	8.1
1	A	540	ARG	3.3
1	B	610	ARG	3.1
1	B	541	GLY	2.9
1	A	541	GLY	2.8
1	A	610	ARG	2.7
1	B	540	ARG	2.7
1	A	608	LYS	2.6
1	B	680	ALA	2.4
1	B	679	ALA	2.3
1	B	608	LYS	2.2
1	B	454	ASP	2.2

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

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
1	TOX	A	111[A]	16/17	0.98	0.08	-	13,14,21,22	1
1	TOX	A	111[B]	16/17	0.98	0.08	-	13,14,17,22	1
1	TOX	B	111[A]	16/17	0.98	0.10	-	11,15,21,23	1
1	TOX	B	111[B]	16/17	0.98	0.10	-	11,15,18,23	1

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
6	MRD	A	805	8/8	0.94	0.14	5.82	48,59,65,65	0
7	MPD	B	805	8/8	0.90	0.13	2.40	49,56,60,60	0
2	HEM	A	801	43/43	0.99	0.08	0.33	12,15,17,18	0
2	HEM	B	801	43/43	0.99	0.09	0.29	13,15,16,19	0
3	NA	B	802	1/1	0.99	0.05	-1.31	16,16,16,16	0
4	CL	B	803	1/1	0.98	0.06	-2.24	31,31,31,31	0
4	CL	A	803	1/1	0.99	0.05	-2.92	33,33,33,33	0
3	NA	A	802	1/1	1.00	0.04	-4.77	16,16,16,16	0
5	OXY	B	804	2/2	0.92	0.12	-	31,31,31,32	0
5	OXY	A	804	2/2	0.93	0.20	-	39,39,39,41	0

6.5 Other polymers [i](#)

There are no such residues in this entry.