



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2016 – 10:28 PM EDT

PDB ID : 5SYH
Title : Structure of D141A variant of B. pseudomallei KatG
Authors : Loewen, P.C.
Deposited on : 2016-08-11
Resolution : 1.65 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

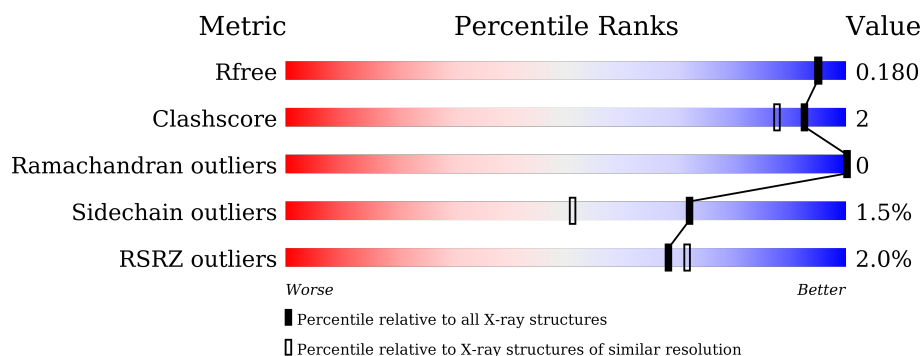
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.65 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	1226 (1.66-1.66)
Clashscore	102246	1323 (1.66-1.66)
Ramachandran outliers	100387	1295 (1.66-1.66)
Sidechain outliers	100360	1295 (1.66-1.66)
RSRZ outliers	91569	1227 (1.66-1.66)

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>2%</div> <div> <div></div> <div>86%</div> <div>11%</div> <div>..</div> </div> </div>
1	B	728	<div> <div>%</div> <div> <div></div> <div>84%</div> <div>12%</div> <div>..</div> </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	MPD	A	806	-	-	-	X
6	MPD	B	805	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12791 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.

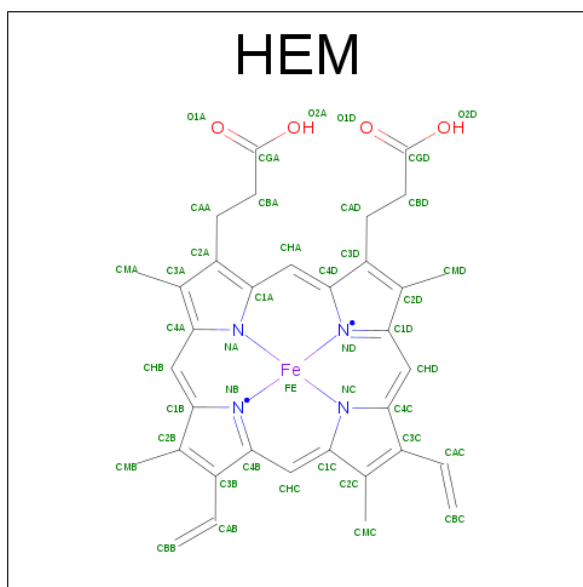
- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total	C	N	O	S	0	7	0
			5543	3500	991	1038	14			
1	B	713	Total	C	N	O	S	0	6	0
			5530	3496	982	1038	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	ALA	ASP	engineered mutation	UNP Q3JNW6
B	141	ALA	ASP	engineered mutation	UNP Q3JNW6

- 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		

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

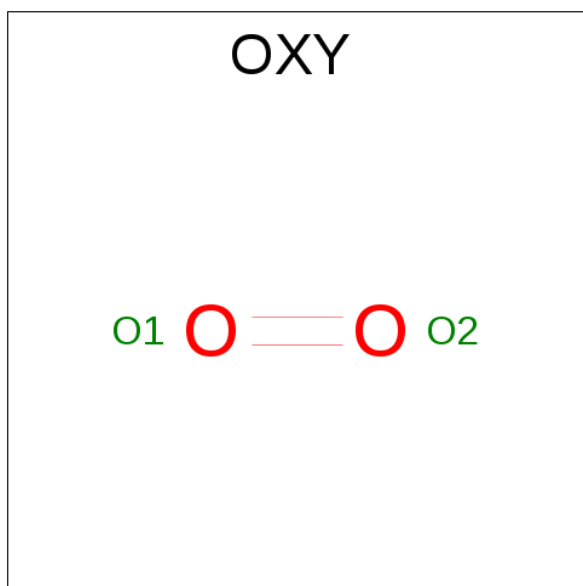
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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).

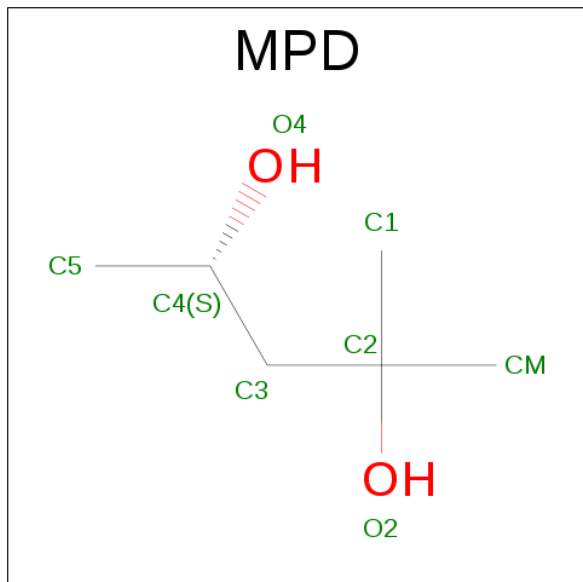
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl		
			1	1	0	0
4	A	1	Total	Cl		
			1	1	0	0

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



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

- Molecule 7 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).



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

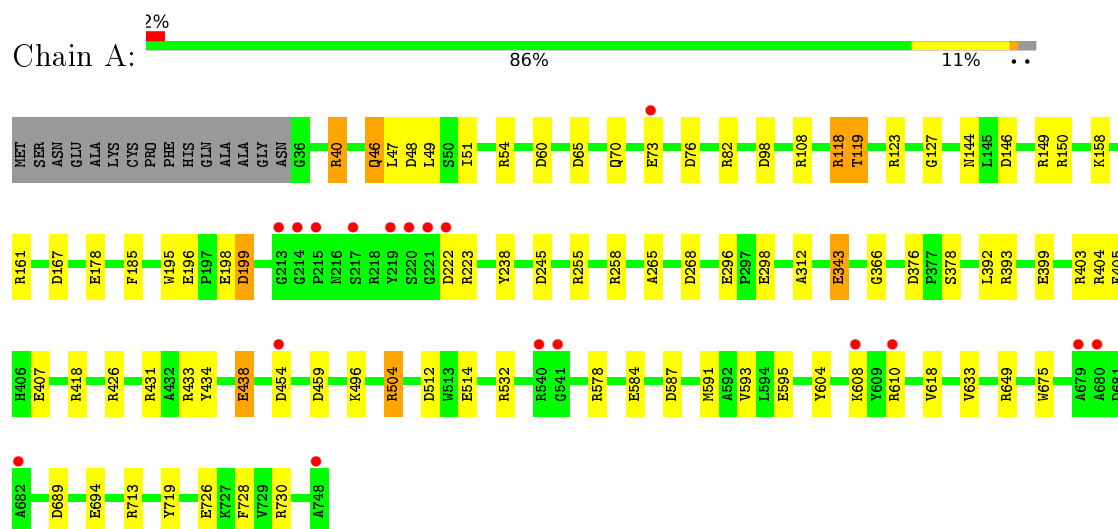
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	784	Total	O	0	0
			784	784		
8	B	798	Total	O	0	0
			798	798		

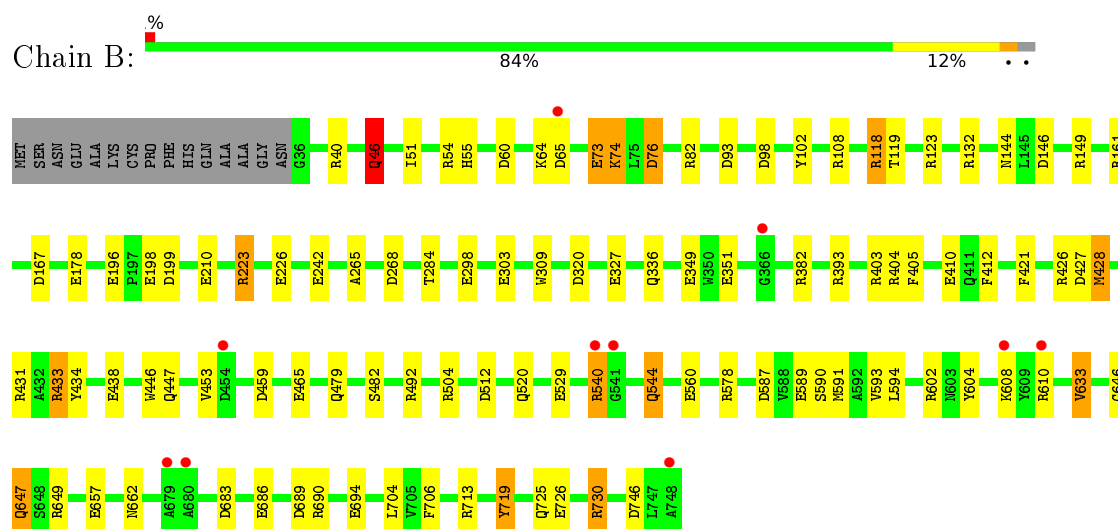
3 Residue-property plots [i](#)

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: 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	100.77Å 113.45Å 174.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.65 40.75 – 1.65	Depositor EDS
% Data completeness (in resolution range)	95.2 (20.00-1.65) 95.2 (40.75-1.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.40 (at 1.65Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.140 , 0.171 0.153 , 0.180	Depositor DCC
R_{free} test set	11378 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	18.5	Xtriage
Anisotropy	0.246	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 44.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12791	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.92% 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, PO4, MPD, 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	1.50	39/5691 (0.7%)	1.38	67/7732 (0.9%)
1	B	1.49	42/5673 (0.7%)	1.38	69/7711 (0.9%)
All	All	1.50	81/11364 (0.7%)	1.38	136/15443 (0.9%)

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

All (81) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	343	GLU	CD-OE1	15.39	1.42	1.25
1	B	198	GLU	CD-OE2	11.84	1.38	1.25
1	A	532	ARG	NE-CZ	-11.04	1.18	1.33
1	B	726	GLU	CG-CD	9.40	1.66	1.51
1	A	343	GLU	CG-CD	9.33	1.66	1.51
1	B	544	GLN	CD-OE1	8.65	1.43	1.24
1	A	584	GLU	CG-CD	8.65	1.65	1.51
1	A	407	GLU	CG-CD	8.54	1.64	1.51
1	A	196	GLU	CG-CD	8.26	1.64	1.51
1	B	210	GLU	CD-OE2	8.22	1.34	1.25
1	B	336	GLN	CG-CD	8.04	1.69	1.51
1	B	730	ARG	CZ-NH2	7.99	1.43	1.33
1	A	434	TYR	CB-CG	-7.86	1.39	1.51
1	A	407	GLU	CD-OE1	7.80	1.34	1.25
1	B	694	GLU	CD-OE2	7.67	1.34	1.25
1	B	196	GLU	CG-CD	7.61	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	694	GLU	CG-CD	7.12	1.62	1.51
1	A	694	GLU	CD-OE1	7.10	1.33	1.25
1	A	196	GLU	CB-CG	-7.08	1.38	1.52
1	A	198	GLU	CD-OE2	7.07	1.33	1.25
1	A	726	GLU	CG-CD	7.07	1.62	1.51
1	A	199	ASP	C-O	6.89	1.36	1.23
1	A	675	TRP	CE3-CZ3	6.58	1.49	1.38
1	B	482	SER	CA-CB	6.53	1.62	1.52
1	B	196	GLU	CB-CG	-6.51	1.39	1.52
1	B	529	GLU	CG-CD	6.51	1.61	1.51
1	A	378	SER	CB-OG	6.17	1.50	1.42
1	B	657	GLU	CG-CD	6.13	1.61	1.51
1	A	633	VAL	CB-CG1	-6.09	1.40	1.52
1	A	119[A]	THR	CB-CG2	-6.09	1.32	1.52
1	A	119[B]	THR	CB-CG2	-6.09	1.32	1.52
1	A	719	TYR	CG-CD1	-6.08	1.31	1.39
1	B	73	GLU	CD-OE2	6.08	1.32	1.25
1	A	185	PHE	CG-CD1	6.06	1.47	1.38
1	B	298	GLU	CG-CD	5.90	1.60	1.51
1	A	399	GLU	CD-OE2	5.88	1.32	1.25
1	B	403	ARG	CD-NE	5.88	1.56	1.46
1	B	226	GLU	CB-CG	-5.87	1.41	1.52
1	A	595	GLU	CD-OE2	5.81	1.32	1.25
1	A	604	TYR	CD2-CE2	5.80	1.48	1.39
1	B	604	TYR	CG-CD2	-5.79	1.31	1.39
1	B	730	ARG	CZ-NH1	5.78	1.40	1.33
1	B	465	GLU	CD-OE1	5.76	1.31	1.25
1	B	198	GLU	CD-OE1	5.76	1.31	1.25
1	B	65	ASP	CB-CG	5.74	1.63	1.51
1	A	223	ARG	CZ-NH1	5.70	1.40	1.33
1	A	426	ARG	CZ-NH2	5.69	1.40	1.33
1	B	438	GLU	CD-OE1	-5.68	1.19	1.25
1	A	178	GLU	CG-CD	5.68	1.60	1.51
1	A	438	GLU	CD-OE2	-5.62	1.19	1.25
1	B	351	GLU	CD-OE2	5.58	1.31	1.25
1	B	434	TYR	CB-CG	-5.58	1.43	1.51
1	B	602	ARG	CZ-NH1	-5.52	1.25	1.33
1	A	195	TRP	CE3-CZ3	5.50	1.47	1.38
1	A	298	GLU	CD-OE2	5.47	1.31	1.25
1	B	560	GLU	CD-OE2	5.45	1.31	1.25
1	B	649	ARG	CZ-NH1	5.45	1.40	1.33
1	B	590	SER	CB-OG	-5.44	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	532	ARG	CG-CD	5.43	1.65	1.51
1	B	446	TRP	CZ3-CH2	-5.40	1.31	1.40
1	B	223	ARG	CG-CD	-5.39	1.38	1.51
1	B	403	ARG	NE-CZ	5.35	1.40	1.33
1	A	514	GLU	CD-OE2	-5.34	1.19	1.25
1	B	102	TYR	CG-CD1	-5.32	1.32	1.39
1	A	73	GLU	CG-CD	5.32	1.59	1.51
1	A	454	ASP	CB-CG	5.30	1.62	1.51
1	A	127	GLY	CA-C	-5.20	1.43	1.51
1	B	309	TRP	CG-CD1	5.20	1.44	1.36
1	B	544	GLN	CG-CD	5.20	1.63	1.51
1	B	726	GLU	CB-CG	5.20	1.62	1.52
1	B	512	ASP	CB-CG	5.15	1.62	1.51
1	A	312	ALA	C-O	5.12	1.33	1.23
1	B	242	GLU	CD-OE1	5.11	1.31	1.25
1	B	453	VAL	C-O	-5.11	1.13	1.23
1	B	199	ASP	C-O	5.09	1.33	1.23
1	B	82	ARG	CZ-NH2	-5.09	1.26	1.33
1	A	376	ASP	N-CA	5.06	1.56	1.46
1	B	327	GLU	CD-OE2	5.05	1.31	1.25
1	A	343	GLU	N-CA	5.05	1.56	1.46
1	A	584	GLU	CD-OE2	5.01	1.31	1.25
1	B	746	ASP	CB-CG	5.01	1.62	1.51

All (136) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	149	ARG	NE-CZ-NH1	17.38	128.99	120.30
1	A	532	ARG	NE-CZ-NH2	-11.99	114.30	120.30
1	B	512	ASP	CB-CG-OD2	-11.13	108.28	118.30
1	B	434	TYR	CB-CG-CD1	11.12	127.67	121.00
1	A	393	ARG	NE-CZ-NH2	-10.18	115.21	120.30
1	B	403	ARG	NE-CZ-NH1	10.02	125.31	120.30
1	A	123	ARG	NE-CZ-NH1	9.74	125.17	120.30
1	A	343	GLU	CG-CD-OE1	9.69	137.69	118.30
1	B	649	ARG	NE-CZ-NH2	-9.65	115.47	120.30
1	A	403[A]	ARG	NE-CZ-NH2	-9.37	115.61	120.30
1	A	403[B]	ARG	NE-CZ-NH2	-9.37	115.61	120.30
1	B	633[A]	VAL	CG1-CB-CG2	-9.23	96.13	110.90
1	B	633[B]	VAL	CG1-CB-CG2	-9.23	96.13	110.90
1	B	108	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	A	434	TYR	CB-CG-CD1	8.99	126.39	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	504	ARG	NE-CZ-NH2	-8.86	115.87	120.30
1	A	238	TYR	CB-CG-CD2	8.80	126.28	121.00
1	A	713	ARG	NE-CZ-NH1	8.77	124.68	120.30
1	A	587	ASP	CB-CG-OD1	8.55	125.99	118.30
1	A	578	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	A	512	ASP	CB-CG-OD2	-8.50	110.65	118.30
1	A	433	ARG	NE-CZ-NH2	-8.50	116.05	120.30
1	A	76	ASP	CB-CG-OD2	-8.47	110.68	118.30
1	B	405	PHE	CB-CG-CD2	8.45	126.72	120.80
1	A	431	ARG	NE-CZ-NH2	8.37	124.48	120.30
1	B	730	ARG	NE-CZ-NH2	-8.36	116.12	120.30
1	A	431	ARG	NE-CZ-NH1	-8.31	116.15	120.30
1	A	407	GLU	OE1-CD-OE2	-8.23	113.43	123.30
1	A	150	ARG	NE-CZ-NH2	-8.16	116.22	120.30
1	B	713	ARG	NE-CZ-NH1	8.16	124.38	120.30
1	A	149	ARG	NE-CZ-NH1	8.07	124.33	120.30
1	A	689	ASP	CB-CG-OD2	-7.88	111.21	118.30
1	B	393	ARG	NE-CZ-NH2	-7.88	116.36	120.30
1	B	704[A]	LEU	CB-CG-CD1	-7.80	97.74	111.00
1	B	704[B]	LEU	CB-CG-CD1	-7.80	97.74	111.00
1	A	418	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	A	393	ARG	NE-CZ-NH1	7.62	124.11	120.30
1	B	123	ARG	NE-CZ-NH2	-7.61	116.49	120.30
1	A	404	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	B	683	ASP	CB-CG-OD2	-7.47	111.58	118.30
1	B	649	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	A	65	ASP	CB-CG-OD2	-7.39	111.65	118.30
1	A	496	LYS	CD-CE-NZ	-7.38	94.72	111.70
1	B	492	ARG	NE-CZ-NH2	-7.37	116.61	120.30
1	A	161[A]	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	A	161[B]	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	B	123	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	A	40	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	B	433	ARG	NE-CZ-NH2	-7.23	116.69	120.30
1	B	726	GLU	OE1-CD-OE2	-7.10	114.78	123.30
1	B	118	ARG	NE-CZ-NH2	-7.09	116.76	120.30
1	B	504	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	B	268	ASP	CB-CG-OD1	7.05	124.65	118.30
1	A	407	GLU	CG-CD-OE1	6.94	132.19	118.30
1	B	540	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	A	123	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	A	60	ASP	CB-CG-OD1	6.70	124.33	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	B	426	ARG	NE-CZ-NH1	-6.64	116.98	120.30
1	A	343	GLU	OE1-CD-OE2	-6.57	115.41	123.30
1	A	459	ASP	CB-CG-OD1	6.57	124.21	118.30
1	B	149	ARG	NE-CZ-NH2	-6.53	117.03	120.30
1	B	587	ASP	CB-CG-OD2	-6.50	112.44	118.30
1	B	427	ASP	CB-CG-OD2	-6.49	112.46	118.30
1	A	584	GLU	OE1-CD-OE2	-6.48	115.53	123.30
1	A	268	ASP	CB-CG-OD1	6.37	124.03	118.30
1	B	578	ARG	NE-CZ-NH1	6.37	123.48	120.30
1	B	587	ASP	CB-CG-OD1	6.36	124.02	118.30
1	B	404	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	A	238	TYR	CB-CG-CD1	-6.34	117.19	121.00
1	A	454	ASP	CB-CG-OD2	6.31	123.98	118.30
1	B	421	PHE	CB-CG-CD2	-6.31	116.38	120.80
1	A	98	ASP	CB-CG-OD2	6.30	123.97	118.30
1	B	382	ARG	NE-CZ-NH2	-6.28	117.16	120.30
1	B	76	ASP	CB-CG-OD2	-6.27	112.65	118.30
1	B	108	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	A	405	PHE	CB-CG-CD1	-6.26	116.42	120.80
1	A	48	ASP	CB-CG-OD1	6.24	123.92	118.30
1	A	404	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	B	320	ASP	CB-CG-OD1	-6.23	112.69	118.30
1	B	349	GLU	OE1-CD-OE2	-6.22	115.83	123.30
1	B	199	ASP	CB-CG-OD1	-6.21	112.71	118.30
1	A	694	GLU	CA-CB-CG	6.10	126.82	113.40
1	A	343	GLU	CG-CD-OE2	-6.09	106.12	118.30
1	B	686	GLU	OE1-CD-OE2	6.09	130.61	123.30
1	A	730	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	B	98	ASP	CB-CG-OD2	6.02	123.72	118.30
1	B	405	PHE	CB-CG-CD1	-6.00	116.60	120.80
1	B	719	TYR	CB-CG-CD2	-5.93	117.44	121.00
1	A	296	GLU	OE1-CD-OE2	5.92	130.40	123.30
1	A	719	TYR	CB-CG-CD2	-5.91	117.45	121.00
1	B	706	PHE	CB-CG-CD2	-5.88	116.69	120.80
1	B	132	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	A	108	ARG	NE-CZ-NH2	-5.77	117.42	120.30
1	A	532	ARG	NH1-CZ-NH2	5.76	125.74	119.40
1	B	393	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	A	49	LEU	CB-CG-CD1	-5.67	101.35	111.00
1	B	161	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	B	54	ARG	CG-CD-NE	-5.65	99.93	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	412	PHE	CB-CG-CD1	5.65	124.76	120.80
1	A	433	ARG	NE-CZ-NH1	5.61	123.10	120.30
1	B	60	ASP	CB-CG-OD2	-5.58	113.28	118.30
1	A	392	LEU	CB-CG-CD2	5.56	120.45	111.00
1	B	604	TYR	CB-CG-CD1	-5.55	117.67	121.00
1	B	428	MET	CA-CB-CG	-5.53	103.90	113.30
1	A	649	ARG	NE-CZ-NH1	-5.51	117.55	120.30
1	B	689	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	B	268	ASP	CB-CG-OD2	-5.47	113.37	118.30
1	A	70	GLN	CA-CB-CG	5.40	125.28	113.40
1	B	578	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	60	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	B	403	ARG	CD-NE-CZ	5.36	131.10	123.60
1	B	167	ASP	CB-CG-OD2	-5.36	113.48	118.30
1	B	459	ASP	CB-CG-OD1	5.35	123.12	118.30
1	A	167	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	A	245	ASP	CB-CG-OD1	5.34	123.11	118.30
1	B	434	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	A	108	ARG	NE-CZ-NH1	5.30	122.95	120.30
1	A	591	MET	CA-CB-CG	5.30	122.31	113.30
1	A	222	ASP	CB-CG-OD1	5.28	123.06	118.30
1	A	405	PHE	CB-CG-CD2	5.26	124.48	120.80
1	A	118	ARG	NE-CZ-NH2	-5.22	117.69	120.30
1	A	82	ARG	NE-CZ-NH2	-5.21	117.69	120.30
1	A	258	ARG	NE-CZ-NH1	5.19	122.90	120.30
1	B	303	GLU	CG-CD-OE1	5.18	128.67	118.30
1	B	746	ASP	CB-CG-OD2	5.18	122.96	118.30
1	B	226	GLU	OE1-CD-OE2	-5.17	117.10	123.30
1	B	223	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	B	198	GLU	CG-CD-OE1	-5.09	108.11	118.30
1	A	728	PHE	CB-CG-CD2	-5.08	117.25	120.80
1	B	93	ASP	CB-CG-OD2	5.07	122.86	118.30
1	A	578	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	B	46	GLN	CB-CG-CD	5.06	124.76	111.60
1	B	404	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	149	ARG	NH1-CZ-NH2	-5.01	113.89	119.40
1	A	46	GLN	CA-CB-CG	5.00	124.41	113.40

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	366	GLY	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	5543	0	5372	12	0
1	B	5530	0	5361	26	0
2	A	43	0	30	0	0
2	B	43	0	30	1	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	16	0	28	6	0
6	B	16	0	28	0	0
7	A	5	0	0	0	0
7	B	5	0	0	0	0
8	A	784	0	0	7	0
8	B	798	0	0	8	0
All	All	12791	0	10849	43	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 (43) 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:119[B]:THR:HG21	8:A:1028:HOH:O	1.68	0.94
1:A:438:GLU:OE2	8:A:901:HOH:O	1.97	0.80
1:B:119[B]:THR:HG23	8:B:1175:HOH:O	1.84	0.77
1:B:410:GLU:OE1	8:B:901:HOH:O	2.02	0.76
1:B:73:GLU:OE2	8:B:902:HOH:O	2.07	0.71
1:B:55:HIS:HD2	8:B:1328:HOH:O	1.72	0.71
1:B:540:ARG:CZ	1:B:540:ARG:HA	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:343:GLU:HG3	8:A:1494:HOH:O	1.91	0.70
1:B:662:ASN:H	1:B:725:GLN:HE22	1.41	0.68
6:A:806:MPD:HM1	6:A:806:MPD:O4	1.95	0.67
1:B:119[B]:THR:HG22	1:B:593:VAL:HG21	1.84	0.60
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.85	0.59
1:B:46:GLN:NE2	8:B:910:HOH:O	2.38	0.57
1:A:593:VAL:HG13	8:A:1030:HOH:O	2.05	0.57
6:A:806:MPD:O4	6:A:806:MPD:CM	2.52	0.56
1:B:633[A]:VAL:HG22	1:B:719:TYR:CZ	2.42	0.55
1:B:76:ASP:OD2	8:B:903:HOH:O	2.18	0.54
1:B:540:ARG:NH1	1:B:540:ARG:HA	2.25	0.52
1:B:591:MET:SD	1:B:594:LEU:HD12	2.50	0.51
1:B:178:GLU:OE1	8:B:904:HOH:O	2.19	0.51
1:B:633[A]:VAL:HG22	1:B:719:TYR:CE1	2.46	0.51
1:B:479:GLN:HE21	1:B:520[B]:GLN:NE2	2.11	0.48
1:A:144:ASN:HA	1:A:146:ASP:OD1	2.14	0.47
1:A:51:ILE:HD11	1:A:618:VAL:HG12	1.98	0.46
1:A:504:ARG:HD2	8:A:918:HOH:O	2.14	0.46
6:A:805:MPD:H53	6:A:805:MPD:H11	1.98	0.46
1:A:119[A]:THR:CG2	1:A:265:ALA:HB2	2.46	0.45
1:A:47:LEU:N	8:A:902:HOH:O	2.25	0.45
1:B:74:LYS:HD3	1:B:74:LYS:N	2.32	0.45
1:B:119[A]:THR:CG2	1:B:265:ALA:HB2	2.47	0.45
1:B:479:GLN:HE21	1:B:520[B]:GLN:HE22	1.66	0.44
1:B:730:ARG:HD2	8:B:1480:HOH:O	2.17	0.43
1:B:428:MET:O	1:B:433:ARG:HD3	2.19	0.43
1:B:431:ARG:HD2	1:B:447:GLN:OE1	2.19	0.43
1:A:158:LYS:HD2	6:A:805:MPD:H13	2.01	0.42
1:B:51:ILE:HG21	1:B:51:ILE:HD13	1.88	0.41
1:A:255[A]:ARG:HG2	8:A:1270:HOH:O	2.21	0.41
1:B:144:ASN:HA	1:B:146:ASP:OD1	2.21	0.41
1:B:284:THR:HG22	2:B:801:HEM:HAA1	2.03	0.41
6:A:805:MPD:C5	6:A:805:MPD:H11	2.50	0.40
1:B:646:GLY:C	1:B:647:GLN:HG2	2.40	0.40
6:A:806:MPD:HM1	6:A:806:MPD:HO4	1.85	0.40
1:A:54:ARG:NE	1:A:199:ASP:OD2	2.51	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	706 (98%)	11 (2%)	0	100	100
1	B	716/728 (98%)	704 (98%)	12 (2%)	0	100	100
All	All	1433/1456 (98%)	1410 (98%)	23 (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	555/559 (99%)	550 (99%)	5 (1%)	84	72
1	B	554/559 (99%)	543 (98%)	11 (2%)	63	38
All	All	1109/1118 (99%)	1093 (99%)	16 (1%)	72	53

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	46	GLN
1	A	118	ARG
1	A	608	LYS
1	A	610	ARG
1	B	46	GLN
1	B	64	LYS
1	B	74	LYS

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Mol	Chain	Res	Type
1	B	118	ARG
1	B	223	ARG
1	B	544	GLN
1	B	589	GLU
1	B	608	LYS
1	B	610	ARG
1	B	647	GLN
1	B	690	ARG

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	70	GLN
1	A	227	ASN
1	A	247	ASN
1	A	339	HIS
1	B	46	GLN
1	B	55	HIS
1	B	647	GLN
1	B	650	HIS
1	B	725	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 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	1	10,17,18	2.12	3 (30%)	9,23,25	2.51	4 (44%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	TOX	B	111	1	10,17,18	1.75	3 (30%)	9,23,25	2.92	6 (66%)

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	1	-	0/3/8/10	0/2/2/2
1	TOX	B	111	1	-	0/3/8/10	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111	TOX	CD1-NE1	-4.05	1.35	1.39
1	A	111	TOX	CE3-CD2	-3.79	1.34	1.42
1	A	111	TOX	CD1-NE1	-3.70	1.35	1.39
1	B	111	TOX	CE3-CD2	-2.12	1.37	1.42
1	B	111	TOX	O-C	2.43	1.31	1.19
1	A	111	TOX	O-C	2.67	1.32	1.19

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	111	TOX	O-C-CA	-4.70	113.11	125.72
1	A	111	TOX	CB-CG-CD1	-3.89	123.17	127.97
1	B	111	TOX	CB-CG-CD1	-3.36	123.82	127.97
1	A	111	TOX	O-C-CA	-3.28	116.94	125.72
1	A	111	TOX	CZ3-CE3-CD2	-3.02	116.69	120.88
1	B	111	TOX	CE3-CD2-CE2	-2.70	117.11	119.83
1	B	111	TOX	CZ3-CE3-CD2	-2.65	117.20	120.88
1	B	111	TOX	CH2-CZ3-CE3	3.03	124.82	120.45
1	B	111	TOX	CZ2-CE2-CD2	3.68	125.19	120.58
1	A	111	TOX	CE3-CD2-CE2	3.74	123.60	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 14 ligands modelled in this entry, 4 are monoatomic - leaving 10 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	1.23	1 (4%)	16,82,82	2.30	8 (50%)
5	OXY	A	804	-	1,1,1	0.17	0	0,0,0	0.00	-
6	MPD	A	805	-	6,7,7	1.05	0	6,10,10	1.52	1 (16%)
6	MPD	A	806	-	6,7,7	0.72	0	6,10,10	1.66	1 (16%)
7	PO4	A	807	-	4,4,4	0.58	0	6,6,6	0.24	0
2	HEM	B	801	1	24,50,50	1.89	6 (25%)	16,82,82	2.55	9 (56%)
5	OXY	B	804	-	1,1,1	0.31	0	0,0,0	0.00	-
6	MPD	B	805	-	6,7,7	1.13	0	6,10,10	1.99	2 (33%)
6	MPD	B	806	-	6,7,7	1.54	0	6,10,10	1.91	3 (50%)
7	PO4	B	807	-	4,4,4	1.46	1 (25%)	6,6,6	0.46	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	A	801	1	-	0/6/54/54	0/0/8/8
5	OXY	A	804	-	-	0/0/0/0	0/0/0/0
6	MPD	A	805	-	-	0/5/5/5	0/0/0/0
6	MPD	A	806	-	-	0/5/5/5	0/0/0/0
7	PO4	A	807	-	-	0/0/0/0	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
6	MPD	B	805	-	-	0/5/5/5	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	MPD	B	806	-	-	0/5/5/5	0/0/0/0
7	PO4	B	807	-	-	0/0/0/0	0/0/0/0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C3C-C2C	-4.96	1.34	1.40
2	B	801	HEM	C1B-NB	-3.65	1.31	1.36
2	A	801	HEM	C3C-C2C	-3.09	1.36	1.40
2	B	801	HEM	CMD-C2D	-2.98	1.45	1.51
2	B	801	HEM	C4C-NC	-2.69	1.33	1.36
7	B	807	PO4	P-O3	-2.23	1.46	1.53
2	B	801	HEM	CMB-C2B	2.07	1.56	1.51
2	B	801	HEM	C4D-ND	3.28	1.41	1.36

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	801	HEM	C3B-CAB-CBB	-4.85	116.64	126.40
2	A	801	HEM	C3B-CAB-CBB	-4.43	117.49	126.40
2	B	801	HEM	CMA-C3A-C4A	-4.08	121.37	128.31
2	B	801	HEM	CAA-C2A-C3A	-2.86	120.85	129.00
6	A	805	MPD	CM-C2-C1	-2.81	103.69	110.41
2	A	801	HEM	CAA-CBA-CGA	-2.40	108.11	112.78
6	B	805	MPD	O2-C2-C1	-2.06	100.44	108.01
2	A	801	HEM	C3C-CAC-CBC	2.06	130.54	126.40
2	B	801	HEM	CBA-CAA-C2A	2.07	116.13	112.49
6	B	806	MPD	CM-C2-C1	2.08	115.37	110.41
2	A	801	HEM	CMC-C2C-C3C	2.11	129.21	125.09
2	B	801	HEM	CAD-CBD-CGD	2.32	117.30	112.78
2	B	801	HEM	CMB-C2B-C3B	2.33	129.65	125.09
6	B	806	MPD	O2-C2-CM	2.38	116.76	108.01
2	A	801	HEM	CMB-C2B-C3B	2.43	129.84	125.09
2	B	801	HEM	CMC-C2C-C3C	2.57	130.11	125.09
6	B	806	MPD	O4-C4-C5	2.57	122.28	109.47
2	A	801	HEM	CBA-CAA-C2A	2.71	117.27	112.49
6	A	806	MPD	O4-C4-C5	2.78	123.36	109.47
2	B	801	HEM	CBD-CAD-C3D	2.93	117.61	112.47
2	A	801	HEM	CBD-CAD-C3D	3.67	118.91	112.47
2	A	801	HEM	CAD-CBD-CGD	3.73	120.05	112.78
6	B	805	MPD	CM-C2-C1	3.76	119.37	110.41
2	B	801	HEM	CMA-C3A-C2A	3.89	133.37	125.24

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	805	MPD	3	0
6	A	806	MPD	3	0
2	B	801	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 ⓘ

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%)	-0.39	18 (2%) 61 61	12, 19, 37, 77	0
1	B	712/728 (97%)	-0.47	10 (1%) 78 80	12, 18, 36, 79	0
All	All	1424/1456 (97%)	-0.43	28 (1%) 68 71	12, 18, 37, 79	0

All (28) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	5.7
1	A	541	GLY	5.0
1	A	540	ARG	4.7
1	B	540	ARG	4.4
1	A	610	ARG	4.2
1	B	679	ALA	4.2
1	B	748	ALA	4.2
1	A	215	PRO	4.1
1	A	608	LYS	3.8
1	B	608	LYS	3.8
1	A	454	ASP	3.8
1	B	610	ARG	3.6
1	B	541	GLY	3.6
1	A	213	GLY	3.6
1	A	679	ALA	3.3
1	A	222	ASP	3.1
1	B	454	ASP	2.9
1	A	680	ALA	2.9
1	A	221	GLY	2.8
1	A	217	SER	2.7
1	A	214	GLY	2.6
1	B	65	ASP	2.6
1	A	219	TYR	2.6
1	A	682	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	366	GLY	2.3
1	A	220	SER	2.2
1	A	73	GLU	2.1
1	B	680	ALA	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	TOX	B	111	16/17	0.98	0.10	-	12,13,18,21	2
1	TOX	A	111	16/17	0.98	0.11	-	11,14,21,22	2

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
6	MPD	A	806	8/8	0.87	0.16	8.71	52,64,66,67	0
6	MPD	B	805	8/8	0.89	0.13	3.71	42,44,53,55	0
2	HEM	A	801	43/43	0.99	0.09	0.71	11,13,17,22	0
2	HEM	B	801	43/43	0.99	0.10	0.51	12,13,16,20	0
3	NA	A	802	1/1	0.99	0.06	-1.43	15,15,15,15	0
3	NA	B	802	1/1	0.99	0.04	-2.18	15,15,15,15	0
4	CL	B	803	1/1	0.98	0.05	-2.19	33,33,33,33	0
4	CL	A	803	1/1	0.97	0.04	-2.71	33,33,33,33	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	MPD	A	805	8/8	0.92	0.12	-	37,43,53,53	0
5	OXY	B	804	2/2	0.89	0.15	-	31,31,31,39	0
5	OXY	A	804	2/2	0.96	0.11	-	33,33,33,39	0
7	PO4	B	807	5/5	0.94	0.20	-	34,48,55,56	0
7	PO4	A	807	5/5	0.77	0.24	-	42,60,78,79	0
6	MPD	B	806	8/8	0.74	0.31	-	49,67,71,74	0

6.5 Other polymers [i](#)

There are no such residues in this entry.