



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 16, 2017 – 11:00 PM EDT

PDB ID : 5SW5
Title : Crystal structure of native catalase-peroxidase KatG at pH7.5
Authors : Loewen, P.C.
Deposited on : unknown
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

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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20029824
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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-20029824

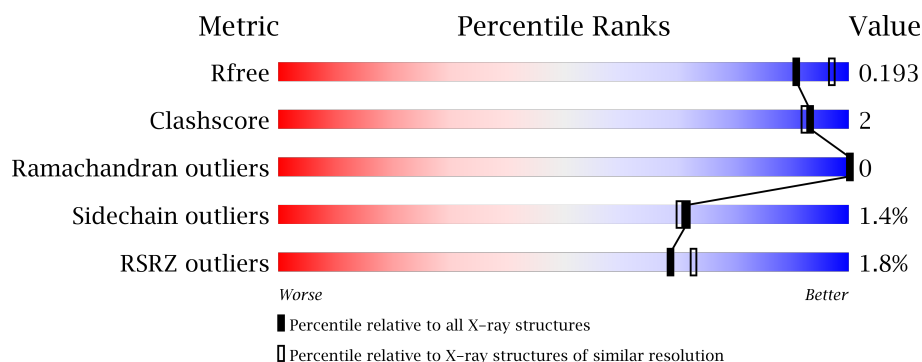
1 Overall quality at a glance ⓘ

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}	100719	1316 (2.04-2.04)
Clashscore	112137	1394 (2.04-2.04)
Ramachandran outliers	110173	1383 (2.04-2.04)
Sidechain outliers	110143	1383 (2.04-2.04)
RSRZ outliers	101464	1319 (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 ≥ 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>89%</div> <div>8%</div> <div>..</div> </div> </div>
1	B	728	<div> <div>2%</div> <div> <div></div> <div>88%</div> <div>9%</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
3	NA	A	802	-	-	-	X
6	MPD	B	805	-	-	-	X

2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 12638 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	5	0
			5549	3502	990	1043	14			
1	B	713	Total	C	N	O	S	0	10	0
			5583	3521	994	1054	14			

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

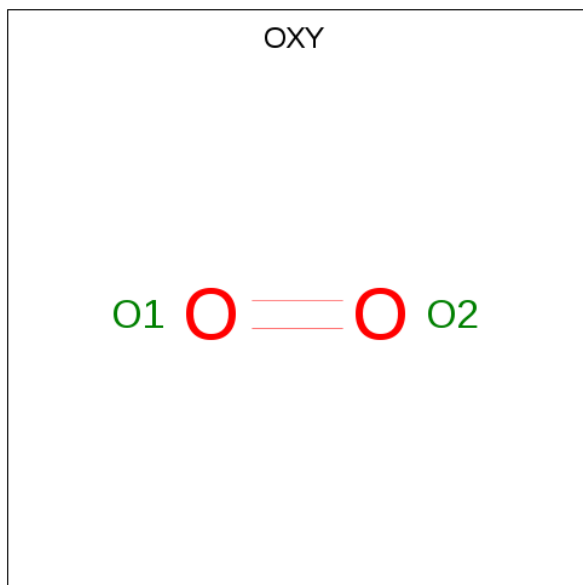


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

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

- Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂).



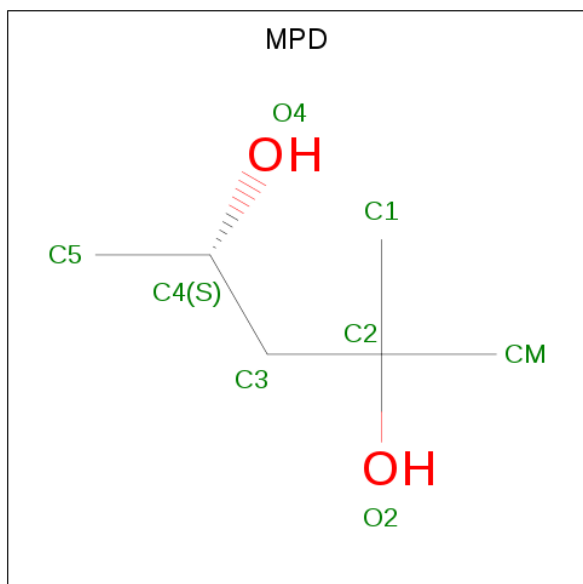
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			2	2		
4	B	1	Total	O	0	0
			2	2		

- Molecule 5 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: $C_6H_{14}O_2$).



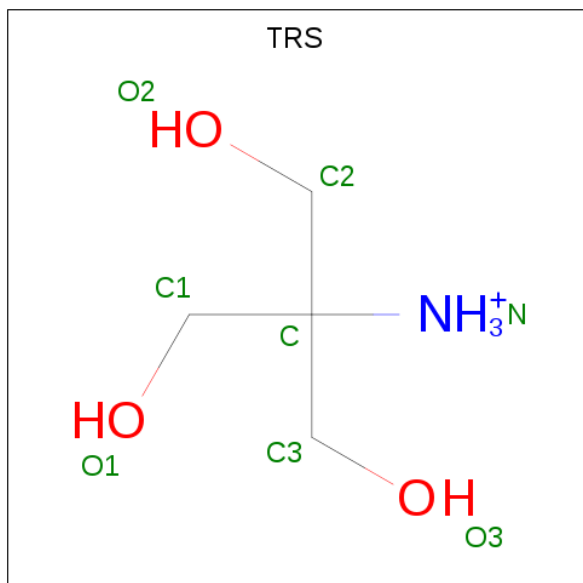
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		

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

- Molecule 7 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: $C_4H_{12}NO_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			8	4	1	3		
7	A	1	Total	C	N	O	0	0
			8	4	1	3		
7	A	1	Total	C	N	O	0	0
			8	4	1	3		
7	B	1	Total	C	N	O	0	0
			8	4	1	3		

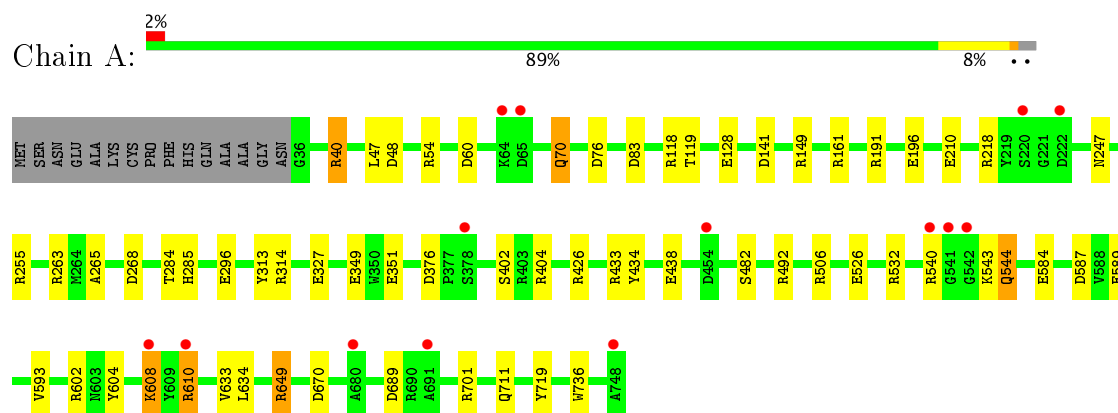
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	666	Total	O	0	0
			666	666		
8	B	682	Total	O	0	0
			682	682		

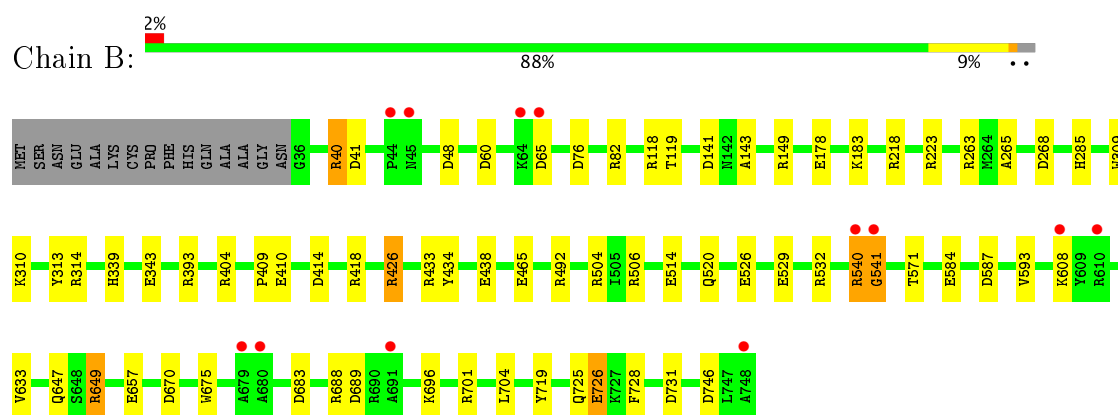
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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	100.34Å 114.85Å 174.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.05 19.93 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-2.05) 99.2 (19.93-2.05)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.97 (at 2.06Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.149 , 0.184 0.161 , 0.193	Depositor DCC
R_{free} test set	6350 reflections (5.31%)	DCC
Wilson B-factor (Å ²)	25.3	Xtriage
Anisotropy	0.033	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 52.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12638	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.83% 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, NA, PO4, MPD, HEM, TRS

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	1.28	20/5675 (0.4%)	1.17	45/7712 (0.6%)
1	B	1.27	18/5711 (0.3%)	1.15	44/7760 (0.6%)
All	All	1.27	38/11386 (0.3%)	1.16	89/15472 (0.6%)

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	410	GLU	CG-CD	9.28	1.65	1.51
1	B	514	GLU	CD-OE2	-7.93	1.17	1.25
1	B	725	GLN	CD-NE2	6.89	1.50	1.32
1	A	349	GLU	CD-OE2	-6.79	1.18	1.25
1	B	434	TYR	CE1-CZ	-6.53	1.30	1.38
1	A	438	GLU	CD-OE1	-6.40	1.18	1.25
1	B	726[A]	GLU	CG-CD	6.38	1.61	1.51
1	B	726[B]	GLU	CG-CD	6.38	1.61	1.51
1	B	343	GLU	CD-OE1	6.18	1.32	1.25
1	A	584	GLU	CG-CD	6.12	1.61	1.51
1	A	196	GLU	CD-OE1	-5.96	1.19	1.25
1	A	711	GLN	CG-CD	5.94	1.64	1.51
1	A	589	GLU	CD-OE2	5.74	1.31	1.25
1	A	296	GLU	CD-OE2	-5.73	1.19	1.25
1	B	410	GLU	CD-OE2	5.59	1.31	1.25
1	A	349	GLU	CD-OE1	-5.57	1.19	1.25
1	A	351	GLU	CD-OE2	-5.53	1.19	1.25
1	A	526	GLU	CD-OE1	-5.40	1.19	1.25
1	B	746	ASP	CB-CG	5.40	1.63	1.51
1	A	736	TRP	CG-CD1	-5.39	1.29	1.36
1	B	746	ASP	C-O	-5.30	1.13	1.23
1	A	402	SER	CB-OG	5.28	1.49	1.42
1	A	426[A]	ARG	CZ-NH2	5.26	1.39	1.33
1	A	426[B]	ARG	CZ-NH2	5.26	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	544	GLN	CD-OE1	5.24	1.35	1.24
1	B	726[A]	GLU	CB-CG	5.24	1.62	1.52
1	B	726[B]	GLU	CB-CG	5.24	1.62	1.52
1	B	675	TRP	CZ3-CH2	-5.22	1.31	1.40
1	A	247	ASN	CG-ND2	-5.21	1.19	1.32
1	B	526	GLU	CG-CD	5.20	1.59	1.51
1	B	285	HIS	C-O	5.13	1.33	1.23
1	A	285	HIS	C-O	5.12	1.33	1.23
1	B	529	GLU	CD-OE2	-5.09	1.20	1.25
1	A	604	TYR	CG-CD2	-5.08	1.32	1.39
1	B	438	GLU	CD-OE1	-5.08	1.20	1.25
1	A	327	GLU	CD-OE1	5.07	1.31	1.25
1	B	465	GLU	CD-OE1	5.05	1.31	1.25
1	A	482	SER	CB-OG	5.04	1.48	1.42

All (89) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	255[A]	ARG	NE-CZ-NH2	-11.87	114.36	120.30
1	A	255[B]	ARG	NE-CZ-NH2	-11.87	114.36	120.30
1	B	393	ARG	NE-CZ-NH2	-11.33	114.63	120.30
1	A	255[A]	ARG	NE-CZ-NH1	11.12	125.86	120.30
1	A	255[B]	ARG	NE-CZ-NH1	11.12	125.86	120.30
1	A	649	ARG	NE-CZ-NH1	9.21	124.91	120.30
1	A	587	ASP	CB-CG-OD1	8.73	126.16	118.30
1	A	532	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	B	82	ARG	NE-CZ-NH1	8.52	124.56	120.30
1	A	376	ASP	CB-CG-OD2	-8.21	110.91	118.30
1	B	506	ARG	NE-CZ-NH1	8.08	124.34	120.30
1	A	602	ARG	NE-CZ-NH1	7.71	124.15	120.30
1	B	649	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	B	149	ARG	NE-CZ-NH1	7.61	124.11	120.30
1	B	418	ARG	NE-CZ-NH1	7.59	124.10	120.30
1	A	40	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	A	426[A]	ARG	NE-CZ-NH1	-7.49	116.56	120.30
1	A	426[B]	ARG	NE-CZ-NH1	-7.49	116.56	120.30
1	B	149	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	B	404	ARG	NE-CZ-NH2	-7.47	116.56	120.30
1	A	649	ARG	NE-CZ-NH2	-7.46	116.57	120.30
1	A	506	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	B	506	ARG	NE-CZ-NH2	-7.44	116.58	120.30
1	A	218	ARG	NE-CZ-NH2	-7.37	116.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	504	ARG	NE-CZ-NH2	-7.35	116.62	120.30
1	B	48	ASP	CB-CG-OD1	7.28	124.86	118.30
1	B	433	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	A	76	ASP	CB-CG-OD2	-7.04	111.96	118.30
1	A	60	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	B	218	ARG	NE-CZ-NH2	-6.85	116.87	120.30
1	A	540	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	B	414	ASP	CB-CG-OD1	6.82	124.44	118.30
1	B	541	GLY	N-CA-C	-6.80	96.10	113.10
1	A	149	ARG	NE-CZ-NH1	6.79	123.69	120.30
1	A	210	GLU	OE1-CD-OE2	-6.75	115.20	123.30
1	A	689	ASP	CB-CG-OD2	-6.75	112.23	118.30
1	B	426[A]	ARG	NE-CZ-NH1	-6.74	116.93	120.30
1	B	426[B]	ARG	NE-CZ-NH1	-6.74	116.93	120.30
1	B	532	ARG	NE-CZ-NH2	-6.73	116.94	120.30
1	B	492	ARG	NE-CZ-NH1	6.72	123.66	120.30
1	B	404	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	B	726[A]	GLU	OE1-CD-OE2	-6.63	115.35	123.30
1	B	726[B]	GLU	OE1-CD-OE2	-6.63	115.35	123.30
1	B	587	ASP	CB-CG-OD1	6.57	124.21	118.30
1	A	433	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	B	689	ASP	CB-CG-OD1	6.50	124.15	118.30
1	A	268	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	B	65	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	B	268	ASP	CB-CG-OD2	-6.43	112.51	118.30
1	A	54	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	A	263	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	B	82	ARG	NE-CZ-NH2	-6.29	117.16	120.30
1	B	263	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	A	70	GLN	CA-CB-CG	6.20	127.05	113.40
1	A	60	ASP	CB-CG-OD1	6.18	123.87	118.30
1	B	434	TYR	CB-CG-CD1	6.17	124.70	121.00
1	A	191	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	A	263	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	434	TYR	CB-CG-CD1	6.02	124.61	121.00
1	A	48	ASP	CB-CG-OD1	6.01	123.71	118.30
1	A	670	ASP	CB-CG-OD2	-5.94	112.95	118.30
1	B	541	GLY	C-N-CA	-5.93	109.84	122.30
1	A	433	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	670	ASP	CB-CG-OD1	5.78	123.50	118.30
1	B	40	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	B	41	ASP	CB-CG-OD2	5.64	123.38	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	540	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	A	83	ASP	CB-CG-OD2	5.57	123.31	118.30
1	B	731	ASP	CB-CG-OD2	5.54	123.28	118.30
1	B	670	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	A	404	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	A	543	LYS	CD-CE-NZ	-5.44	99.20	111.70
1	A	689	ASP	CB-CG-OD1	5.43	123.18	118.30
1	B	310	LYS	CD-CE-NZ	-5.42	99.24	111.70
1	B	492	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	A	492	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	B	393	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	A	128	GLU	OE1-CD-OE2	-5.34	116.89	123.30
1	B	584	GLU	OE1-CD-OE2	-5.34	116.89	123.30
1	A	701	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	B	701	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	B	704	LEU	CB-CG-CD2	5.19	119.83	111.00
1	A	587	ASP	CB-CG-OD2	-5.15	113.67	118.30
1	A	610	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	B	60	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	634	LEU	CB-CG-CD2	-5.11	102.32	111.00
1	B	688	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	A	492	ARG	NE-CZ-NH1	5.02	122.81	120.30
1	B	683	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5549	0	5360	10	0
1	B	5583	0	5376	23	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	2	0	0	0	0
4	B	2	0	0	0	0
5	A	5	0	0	0	0
5	B	5	0	0	0	0
6	A	16	0	28	3	0
6	B	8	0	14	2	0
7	A	24	0	35	0	0
7	B	8	0	12	0	0
8	A	666	0	0	2	2
8	B	682	0	0	10	2
All	All	12638	0	10885	38	2

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 (38) 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:726[B]:GLU:OE1	8:B:903:HOH:O	1.62	1.13
1:B:726[B]:GLU:CD	8:B:903:HOH:O	1.93	1.07
1:B:571:THR:HG23	8:B:1113:HOH:O	1.66	0.94
1:B:119[B]:THR:HG21	8:B:935:HOH:O	1.68	0.93
6:A:805:MPD:CM	6:A:805:MPD:O4	2.25	0.83
6:B:805:MPD:H12	6:B:805:MPD:O4	1.80	0.81
6:A:805:MPD:HM1	6:A:805:MPD:O4	1.80	0.80
1:B:647:GLN:HG2	8:B:1147:HOH:O	1.81	0.79
1:B:520:GLN:HG3	8:B:958:HOH:O	1.88	0.72
1:B:76:ASP:OD1	8:B:904:HOH:O	2.13	0.66
6:B:805:MPD:O4	6:B:805:MPD:C1	2.44	0.65
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.83	0.62
1:B:696:LYS:HE2	8:B:937:HOH:O	2.00	0.61
1:A:633[A]:VAL:CG2	1:A:719:TYR:CZ	2.87	0.58
1:B:540:ARG:NH1	1:B:540:ARG:HA	2.18	0.57
1:B:119[B]:THR:HG23	1:B:593:VAL:HG11	1.91	0.52
1:B:540:ARG:CZ	1:B:540:ARG:HA	2.42	0.49
1:B:178:GLU:OE1	8:B:905:HOH:O	2.20	0.48
1:B:119[A]:THR:CG2	1:B:265:ALA:HB2	2.46	0.46
1:B:339:HIS:CD2	1:B:409:PRO:HB3	2.51	0.46
1:A:119[A]:THR:CG2	1:A:265:ALA:HB2	2.46	0.45
1:A:47:LEU:O	8:A:903:HOH:O	2.20	0.44
1:A:70:GLN:HE21	1:A:70:GLN:HB2	1.54	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:THR:HG22	2:A:801:HEM:HAA1	2.00	0.44
1:B:633[A]:VAL:HG22	1:B:719:TYR:CZ	2.53	0.44
6:A:806:MPD:HM1	8:A:1282:HOH:O	2.17	0.43
1:B:540:ARG:C	1:B:541:GLY:O	2.54	0.43
1:A:313:TYR:CE2	1:A:314:ARG:HD3	2.54	0.43
1:A:313:TYR:CZ	1:A:314:ARG:HD3	2.54	0.43
1:B:426[B]:ARG:HA	1:B:426[B]:ARG:HD2	1.88	0.43
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	2.01	0.41
1:B:633[B]:VAL:HG12	1:B:728:PHE:CD1	2.54	0.41
1:A:633[A]:VAL:HG22	1:A:719:TYR:CZ	2.56	0.41
1:A:608:LYS:HA	1:A:608:LYS:HD2	1.97	0.40
1:B:143:ALA:HA	1:B:309:TRP:CH2	2.56	0.40
1:B:313:TYR:CE2	1:B:314:ARG:HD3	2.56	0.40
1:B:657[A]:GLU:OE2	8:B:906:HOH:O	2.22	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1506:HOH:O	8:B:1527:HOH:O[4_445]	1.67	0.53
8:A:1325:HOH:O	8:B:1253:HOH:O[2_444]	1.93	0.27

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	715/728 (98%)	705 (99%)	10 (1%)	0	100	100
1	B	719/728 (99%)	708 (98%)	11 (2%)	0	100	100
All	All	1434/1456 (98%)	1413 (98%)	21 (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	554/560 (99%)	546 (99%)	8 (1%)	71	70
1	B	558/560 (100%)	551 (99%)	7 (1%)	73	72
All	All	1112/1120 (99%)	1097 (99%)	15 (1%)	71	72

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	40	ARG
1	A	118	ARG
1	A	141	ASP
1	A	161	ARG
1	A	544	GLN
1	A	608	LYS
1	A	610	ARG
1	A	649	ARG
1	B	40	ARG
1	B	118	ARG
1	B	141	ASP
1	B	183	LYS
1	B	223	ARG
1	B	608	LYS
1	B	649	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	247	ASN
1	A	711	GLN
1	B	227	ASN
1	B	339	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 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	1,2	12,17,18	2.43	8 (66%)	11,23,25	2.12	3 (27%)
1	TOX	B	111[A]	2	12,17,18	3.06	6 (50%)	11,23,25	2.14	4 (36%)
1	TOX	B	111[B]	-	12,17,18	3.06	6 (50%)	11,23,25	2.14	4 (36%)

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	1,2	-	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 (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111[A]	TOX	CD1-NE1	-4.24	1.35	1.39
1	B	111[B]	TOX	CD1-NE1	-4.24	1.35	1.39
1	A	111	TOX	CD1-NE1	-3.56	1.36	1.39
1	A	111	TOX	CE3-CD2	-2.69	1.36	1.42
1	A	111	TOX	CZ2-CE2	-2.18	1.36	1.41
1	B	111[A]	TOX	CE3-CD2	-2.02	1.38	1.42
1	B	111[B]	TOX	CE3-CD2	-2.02	1.38	1.42
1	A	111	TOX	CZ3-CE3	2.39	1.42	1.36
1	A	111	TOX	CH2-CZ2	2.46	1.42	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111[A]	TOX	CH2-CZ2	2.69	1.43	1.36
1	B	111[B]	TOX	CH2-CZ2	2.69	1.43	1.36
1	B	111[A]	TOX	CZ3-CE3	2.88	1.43	1.36
1	B	111[B]	TOX	CZ3-CE3	2.88	1.43	1.36
1	A	111	TOX	CZ3-CH2	3.01	1.45	1.38
1	A	111	TOX	O1-NE1	3.30	1.44	1.38
1	A	111	TOX	O-C	3.36	1.34	1.19
1	B	111[A]	TOX	O-C	4.97	1.41	1.19
1	B	111[B]	TOX	O-C	4.97	1.41	1.19
1	B	111[A]	TOX	O1-NE1	6.11	1.50	1.38
1	B	111[B]	TOX	O1-NE1	6.11	1.50	1.38

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111	TOX	O-C-CA	-4.46	112.71	125.02
1	B	111[A]	TOX	CZ3-CH2-CZ2	-3.89	114.90	120.45
1	B	111[B]	TOX	CZ3-CH2-CZ2	-3.89	114.90	120.45
1	B	111[A]	TOX	CZ2-CE2-CD2	-3.21	116.57	120.94
1	B	111[B]	TOX	CZ2-CE2-CD2	-3.21	116.57	120.94
1	A	111	TOX	CB-CG-CD1	-3.08	124.16	127.97
1	B	111[A]	TOX	O-C-CA	-2.88	117.05	125.02
1	B	111[B]	TOX	O-C-CA	-2.88	117.05	125.02
1	A	111	TOX	CZ2-CE2-CD2	-2.60	117.40	120.94
1	B	111[A]	TOX	CH2-CZ2-CE2	3.20	125.76	119.33
1	B	111[B]	TOX	CH2-CZ2-CE2	3.20	125.76	119.33

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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 2 are monoatomic - leaving 13 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	28,50,50	1.57	3 (10%)	17,82,82	2.20	7 (41%)
4	OXY	A	803	-	1,1,1	0.17	0	0,0,0	0.00	-
5	PO4	A	804	-	4,4,4	0.60	0	6,6,6	2.11	2 (33%)
6	MPD	A	805	-	7,7,7	0.71	0	9,10,10	2.09	3 (33%)
6	MPD	A	806	-	7,7,7	0.76	0	9,10,10	1.51	2 (22%)
7	TRS	A	807	-	7,7,7	1.64	1 (14%)	9,9,9	2.18	4 (44%)
7	TRS	A	808	-	7,7,7	1.28	1 (14%)	9,9,9	2.10	5 (55%)
7	TRS	A	809	-	7,7,7	1.26	1 (14%)	9,9,9	1.74	2 (22%)
2	HEM	B	801	1	28,50,50	1.71	5 (17%)	17,82,82	2.30	10 (58%)
4	OXY	B	803	-	1,1,1	0.32	0	0,0,0	0.00	-
5	PO4	B	804	-	4,4,4	0.98	0	6,6,6	1.90	1 (16%)
6	MPD	B	805	-	7,7,7	0.38	0	9,10,10	2.00	2 (22%)
7	TRS	B	806	-	7,7,7	1.58	2 (28%)	9,9,9	1.63	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
2	HEM	A	801	1	-	0/6/54/54	0/0/8/8
4	OXY	A	803	-	-	0/0/0/0	0/0/0/0
5	PO4	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	TRS	A	807	-	-	0/9/9/9	0/0/0/0
7	TRS	A	808	-	-	0/9/9/9	0/0/0/0
7	TRS	A	809	-	-	0/9/9/9	0/0/0/0
2	HEM	B	801	1	-	0/6/54/54	0/0/8/8
4	OXY	B	803	-	-	0/0/0/0	0/0/0/0
5	PO4	B	804	-	-	0/0/0/0	0/0/0/0
6	MPD	B	805	-	-	0/5/5/5	0/0/0/0
7	TRS	B	806	-	-	0/9/9/9	0/0/0/0

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C4D-ND	-5.62	1.30	1.36
2	A	801	HEM	C1B-NB	-4.40	1.31	1.36
2	B	801	HEM	C1B-NB	-3.99	1.32	1.36
2	B	801	HEM	CAA-C2A	-3.92	1.45	1.52
2	B	801	HEM	C4D-ND	-3.46	1.32	1.36
2	B	801	HEM	C4B-NB	-2.35	1.31	1.36
2	B	801	HEM	C1C-NC	-2.16	1.34	1.36
2	A	801	HEM	CAD-C3D	-2.10	1.48	1.52
7	B	806	TRS	O1-C1	2.15	1.49	1.42
7	A	809	TRS	C3-C	2.16	1.57	1.52
7	B	806	TRS	C2-C	2.27	1.58	1.52
7	A	808	TRS	C1-C	2.33	1.58	1.52
7	A	807	TRS	C1-C	2.71	1.59	1.52

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	805	MPD	CM-C2-C1	-4.53	100.31	110.42
2	A	801	HEM	CAA-CBA-CGA	-4.52	104.93	112.66
6	A	805	MPD	O4-C4-C3	-4.04	92.82	111.28
2	B	801	HEM	CMA-C3A-C4A	-3.72	122.75	128.46
5	A	804	PO4	O3-P-O1	-3.60	95.63	110.97
2	B	801	HEM	CAA-CBA-CGA	-3.29	107.03	112.66
7	A	809	TRS	C1-C-N	-3.26	100.80	107.73
2	A	801	HEM	CMA-C3A-C4A	-3.17	123.59	128.46
2	A	801	HEM	C1D-C2D-C3D	-3.10	104.84	107.00
7	A	808	TRS	C3-C-N	-2.81	101.75	107.73
7	B	806	TRS	C3-C-C2	-2.62	103.65	111.06
7	A	807	TRS	C3-C-C2	-2.52	103.92	111.06
7	A	807	TRS	C1-C-N	-2.47	102.47	107.73
6	B	805	MPD	O2-C2-C3	-2.46	100.12	109.88
2	B	801	HEM	C3C-C4C-NC	-2.21	106.78	110.94
7	A	807	TRS	O1-C1-C	-2.07	104.48	110.47
6	A	805	MPD	O2-C2-CM	-2.03	100.98	108.00
2	B	801	HEM	CAA-C2A-C3A	-2.02	123.23	129.00
2	B	801	HEM	CMD-C2D-C1D	-2.02	125.36	128.46
7	B	806	TRS	O3-C3-C	2.09	116.51	110.47
2	B	801	HEM	CMA-C3A-C2A	2.13	128.96	124.94
7	B	806	TRS	C2-C-N	2.13	112.26	107.73
7	A	808	TRS	C3-C-C1	2.14	117.13	111.06
7	A	808	TRS	O3-C3-C	2.19	116.81	110.47
2	A	801	HEM	CAD-CBD-CGD	2.21	116.44	112.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	806	MPD	C5-C4-C3	2.24	123.24	112.11
2	A	801	HEM	CBA-CAA-C2A	2.28	116.84	112.48
6	A	806	MPD	C1-C2-C3	2.41	122.05	110.08
2	A	801	HEM	CMA-C3A-C2A	2.41	129.48	124.94
7	A	809	TRS	C3-C-C1	2.48	118.08	111.06
2	B	801	HEM	CMB-C2B-C3B	2.57	129.65	124.89
5	B	804	PO4	O3-P-O1	2.58	121.97	110.97
6	A	805	MPD	CM-C2-C3	2.59	122.95	110.08
2	B	801	HEM	CMC-C2C-C3C	2.71	129.91	124.89
5	A	804	PO4	O4-P-O1	2.75	122.66	110.97
7	A	808	TRS	O1-C1-C	3.01	119.19	110.47
7	A	808	TRS	C1-C-N	3.12	114.36	107.73
2	B	801	HEM	CBD-CAD-C3D	3.29	118.75	112.47
2	A	801	HEM	CBD-CAD-C3D	3.82	119.75	112.47
2	B	801	HEM	CAD-CBD-CGD	4.12	119.70	112.66
7	A	807	TRS	C3-C-C1	4.49	123.80	111.06

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	801	HEM	1	0
6	A	805	MPD	2	0
6	A	806	MPD	1	0
6	B	805	MPD	2	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%)	-0.49	14 (1%) 65 70	18, 25, 41, 76	0
1	B	712/728 (97%)	-0.58	12 (1%) 70 74	17, 23, 39, 78	0
All	All	1424/1456 (97%)	-0.53	26 (1%) 69 73	17, 24, 41, 78	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	6.6
1	B	679	ALA	6.0
1	B	748	ALA	5.2
1	B	680	ALA	4.0
1	B	540	ARG	3.8
1	A	610	ARG	3.8
1	B	610	ARG	3.8
1	A	540	ARG	3.5
1	A	541	GLY	3.4
1	B	65	ASP	3.3
1	B	64	LYS	3.1
1	A	65	ASP	2.9
1	B	541	GLY	2.9
1	A	222	ASP	2.8
1	A	64	LYS	2.7
1	B	608	LYS	2.7
1	B	45	ASN	2.4
1	B	44	PRO	2.3
1	A	378	SER	2.3
1	A	680	ALA	2.3
1	A	691	ALA	2.2
1	A	542	GLY	2.2
1	A	220	SER	2.2
1	A	608	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	691	ALA	2.1
1	A	454	ASP	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	A	111	16/17	0.96	0.07	-	15,22,33,37	2
1	TOX	B	111[A]	16/17	0.96	0.07	-	18,21,26,30	2
1	TOX	B	111[B]	16/17	0.96	0.07	-	18,21,24,30	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
3	NA	A	802	1/1	0.99	0.10	2.98	23,23,23,23	0
6	MPD	B	805	8/8	0.90	0.12	2.57	50,53,59,60	0
6	MPD	A	805	8/8	0.92	0.14	1.88	59,64,68,71	0
7	TRS	A	808	8/8	0.90	0.12	1.65	33,36,40,45	0
7	TRS	A	809	8/8	0.77	0.25	1.52	48,56,60,71	0
7	TRS	A	807	8/8	0.90	0.20	1.18	43,47,50,53	0
3	NA	B	802	1/1	0.99	0.07	0.67	22,22,22,22	0
7	TRS	B	806	8/8	0.94	0.09	0.55	25,29,32,34	0
2	HEM	B	801	43/43	0.97	0.08	-0.42	17,19,21,26	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
2	HEM	A	801	43/43	0.97	0.07	-0.68	18,22,24,25	0
5	PO4	B	804	5/5	0.96	0.22	-	38,49,56,61	0
4	OXY	A	803	2/2	0.91	0.30	-	40,40,40,50	0
4	OXY	B	803	2/2	0.91	0.40	-	39,39,39,42	0
6	MPD	A	806	8/8	0.87	0.16	-	49,51,61,63	0
5	PO4	A	804	5/5	0.96	0.22	-	41,53,54,60	0

6.5 Other polymers [i](#)

There are no such residues in this entry.