



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 7, 2016 – 08:24 PM EDT

PDB ID : 5SYU
Title : Crystal structure of Burkholderia pseudomallei KatG E242Q variant
Authors : Loewen, P.C.
Deposited on : 2016-08-12
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

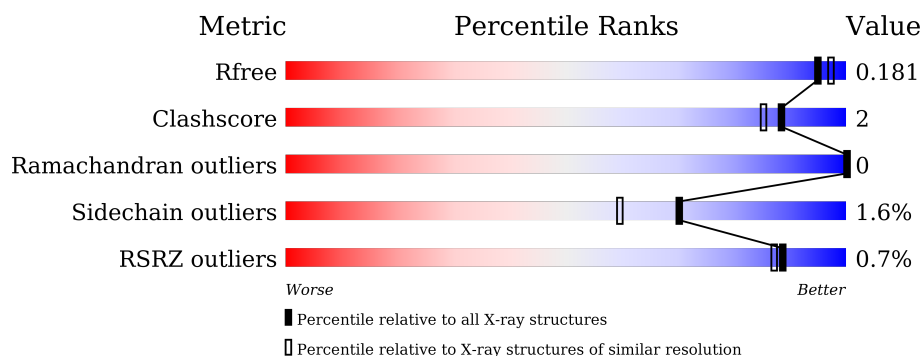
1 Overall quality at a glance

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;"> % 89% 8% .. </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;"> % 88% 8% .. </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	806	-	-	X	X
6	MPD	B	808	-	-	-	X

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.

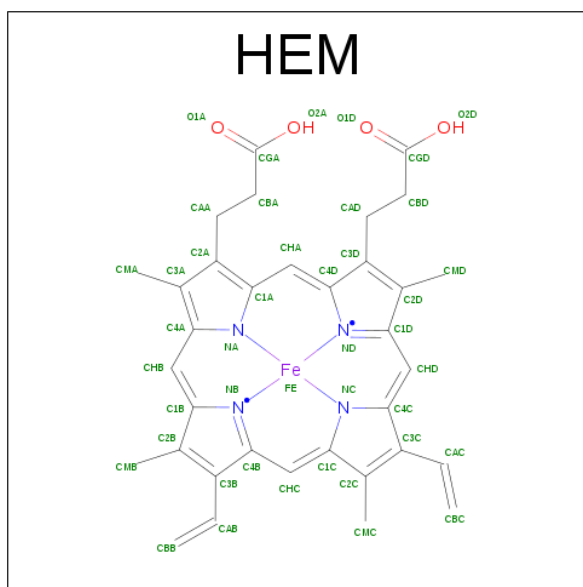
- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total 5540	C 3498	N 988	O 1040	S 14	0	6	0
1	B	713	Total 5560	C 3513	N 994	O 1039	S 14	0	10	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	242	GLN	GLU	engineered mutation	UNP Q3JNW6
B	242	GLN	GLU	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

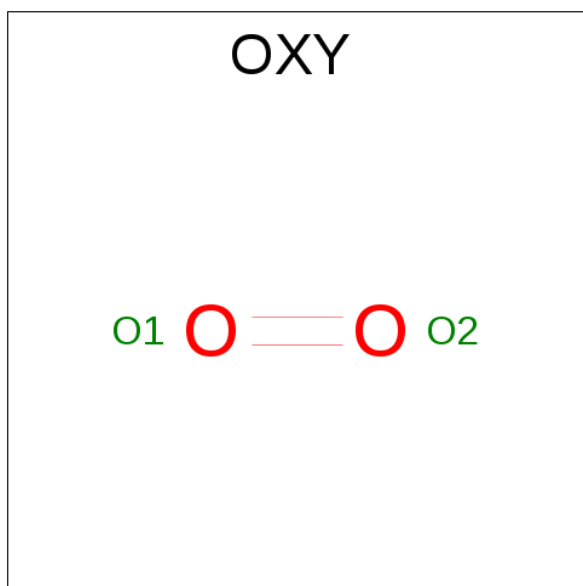
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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).

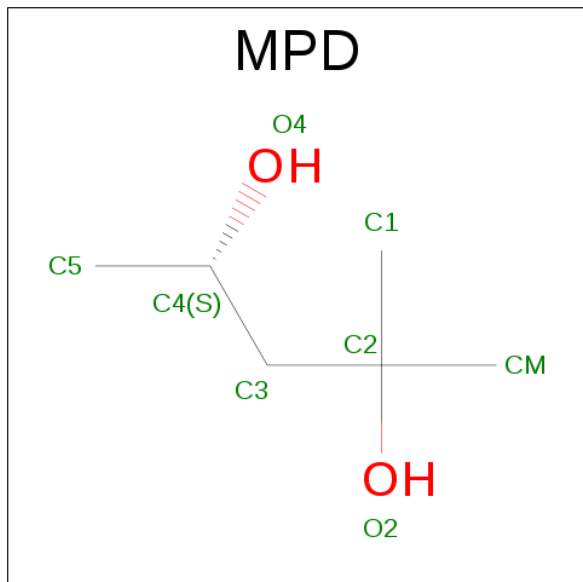
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl		
			1	1	0	0
4	A	1	Total	Cl		
			1	1	0	0

- 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		
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	B	1	Total	O	P	0	0
			5	4	1		

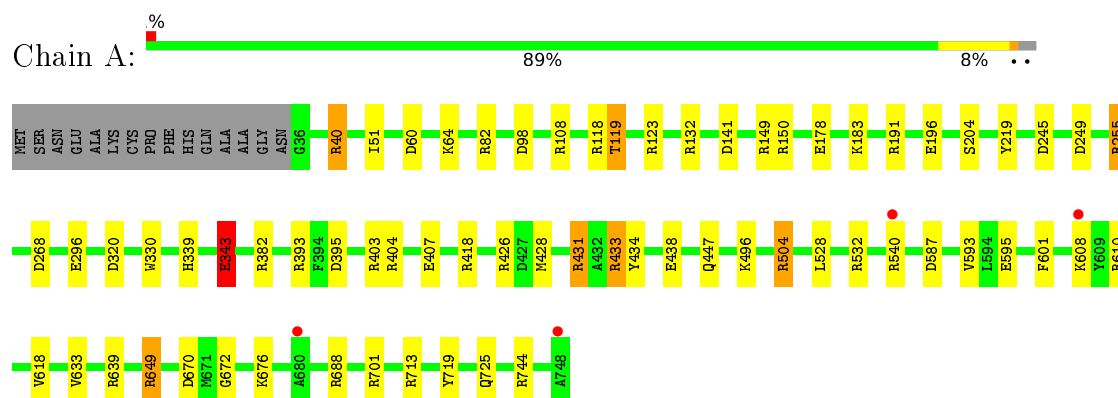
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	774	Total	O	0	0
			774	774		
8	B	733	Total	O	0	0
			733	733		

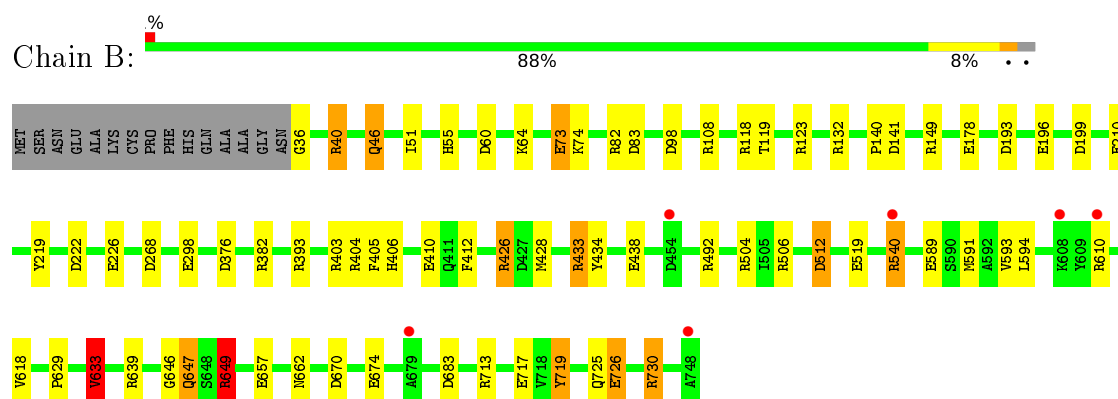
3 Residue-property plots [i](#)

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	101.00Å 113.67Å 174.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.65 – 1.80 47.66 – 1.80	Depositor EDS
% Data completeness (in resolution range)	89.1 (47.65-1.80) 89.1 (47.66-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 1.79Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.139 , 0.172 0.152 , 0.181	Depositor DCC
R_{free} test set	8195 reflections (5.20%)	DCC
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.364	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 45.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	12746	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 3.21% 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	1.33	24/5677 (0.4%)	1.25	52/7714 (0.7%)
1	B	1.37	26/5711 (0.5%)	1.26	55/7759 (0.7%)
All	All	1.35	50/11388 (0.4%)	1.26	107/15473 (0.7%)

All (50) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	726	GLU	CD-OE1	11.09	1.37	1.25
1	B	512	ASP	CB-CG	9.25	1.71	1.51
1	B	512	ASP	CG-OD2	9.08	1.46	1.25
1	B	36	GLY	N-CA	8.40	1.58	1.46
1	A	407	GLU	CD-OE1	7.84	1.34	1.25
1	B	73	GLU	CD-OE2	7.84	1.34	1.25
1	B	519	GLU	CD-OE2	7.69	1.34	1.25
1	A	532	ARG	NE-CZ	-7.54	1.23	1.33
1	A	434	TYR	CG-CD1	-7.37	1.29	1.39
1	B	226	GLU	CG-CD	7.09	1.62	1.51
1	B	426[A]	ARG	CZ-NH2	7.02	1.42	1.33
1	B	426[B]	ARG	CZ-NH2	7.02	1.42	1.33
1	A	407	GLU	CG-CD	6.72	1.62	1.51
1	B	657	GLU	CG-CD	6.68	1.61	1.51
1	B	589	GLU	CD-OE1	6.60	1.32	1.25
1	B	410	GLU	CG-CD	6.44	1.61	1.51
1	B	196	GLU	CG-CD	6.39	1.61	1.51
1	B	226	GLU	CB-CG	-6.32	1.40	1.52
1	B	674	GLU	CD-OE2	-6.18	1.18	1.25
1	A	219	TYR	CG-CD2	6.15	1.47	1.39
1	A	343[A]	GLU	CD-OE2	-6.10	1.19	1.25
1	A	343[B]	GLU	CD-OE2	-6.10	1.19	1.25
1	A	178	GLU	CD-OE2	-6.05	1.19	1.25
1	B	434	TYR	CG-CD1	-5.97	1.31	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	343[A]	GLU	CD-OE1	5.91	1.32	1.25
1	A	343[B]	GLU	CD-OE1	5.91	1.32	1.25
1	A	438	GLU	CD-OE2	-5.84	1.19	1.25
1	B	193	ASP	CB-CG	5.83	1.64	1.51
1	B	178	GLU	CG-CD	5.73	1.60	1.51
1	B	438	GLU	CD-OE1	-5.61	1.19	1.25
1	A	407	GLU	CD-OE2	5.60	1.31	1.25
1	B	210	GLU	CD-OE2	5.59	1.31	1.25
1	A	178	GLU	CG-CD	5.57	1.60	1.51
1	A	595	GLU	CD-OE2	5.56	1.31	1.25
1	A	196	GLU	CG-CD	5.53	1.60	1.51
1	A	119[A]	THR	CB-CG2	-5.52	1.34	1.52
1	A	119[B]	THR	CB-CG2	-5.52	1.34	1.52
1	B	492	ARG	CZ-NH2	5.45	1.40	1.33
1	B	46	GLN	CG-CD	5.45	1.63	1.51
1	A	719	TYR	CE2-CZ	5.36	1.45	1.38
1	B	717	GLU	CD-OE1	-5.32	1.19	1.25
1	B	219	TYR	CG-CD1	5.30	1.46	1.39
1	B	298	GLU	CD-OE2	5.27	1.31	1.25
1	A	672	GLY	C-O	5.24	1.32	1.23
1	B	82	ARG	CZ-NH2	-5.22	1.26	1.33
1	A	196	GLU	CB-CG	-5.18	1.42	1.52
1	A	330	TRP	CZ3-CH2	5.15	1.48	1.40
1	A	204	SER	CA-CB	5.13	1.60	1.52
1	A	418	ARG	CZ-NH2	-5.12	1.26	1.33
1	A	434	TYR	CE2-CZ	-5.11	1.31	1.38

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	ARG	NE-CZ-NH2	-12.91	113.84	120.30
1	B	512	ASP	CB-CG-OD2	11.35	128.51	118.30
1	A	404	ARG	NE-CZ-NH2	-11.14	114.73	120.30
1	A	108	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	B	512	ASP	CB-CG-OD1	-10.27	109.06	118.30
1	A	403	ARG	NE-CZ-NH1	9.90	125.25	120.30
1	B	670	ASP	CB-CG-OD1	9.53	126.88	118.30
1	B	82	ARG	NE-CZ-NH2	-9.46	115.57	120.30
1	B	633[A]	VAL	CG1-CB-CG2	-9.15	96.27	110.90
1	B	633[B]	VAL	CG1-CB-CG2	-9.15	96.27	110.90
1	B	376	ASP	CB-CG-OD2	-9.05	110.15	118.30
1	B	108	ARG	NE-CZ-NH1	8.91	124.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	649[A]	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	B	649[B]	ARG	NE-CZ-NH2	-8.57	116.02	120.30
1	A	149	ARG	NE-CZ-NH1	8.51	124.55	120.30
1	A	504	ARG	NE-CZ-NH1	8.24	124.42	120.30
1	A	431	ARG	NE-CZ-NH2	8.19	124.40	120.30
1	A	149	ARG	NE-CZ-NH2	-8.07	116.26	120.30
1	B	82	ARG	NE-CZ-NH1	8.00	124.30	120.30
1	A	434	TYR	CB-CG-CD1	7.82	125.69	121.00
1	A	268	ASP	CB-CG-OD1	7.75	125.27	118.30
1	B	108	ARG	NE-CZ-NH2	-7.61	116.49	120.30
1	B	405	PHE	CB-CG-CD1	7.50	126.05	120.80
1	A	504	ARG	NE-CZ-NH2	-7.49	116.56	120.30
1	B	123	ARG	NE-CZ-NH1	7.48	124.04	120.30
1	B	670	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	A	404	ARG	NE-CZ-NH1	7.34	123.97	120.30
1	A	713	ARG	NE-CZ-NH1	7.33	123.97	120.30
1	A	343[A]	GLU	CA-CB-CG	7.33	129.52	113.40
1	A	343[B]	GLU	CA-CB-CG	7.33	129.52	113.40
1	A	670	ASP	CB-CG-OD1	7.30	124.87	118.30
1	B	683	ASP	CB-CG-OD2	-7.20	111.82	118.30
1	B	683	ASP	CB-CG-OD1	7.04	124.63	118.30
1	A	82	ARG	NE-CZ-NH2	-6.96	116.82	120.30
1	A	82	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	B	40	ARG	NE-CZ-NH1	6.91	123.76	120.30
1	A	433	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	B	404	ARG	NE-CZ-NH1	6.71	123.66	120.30
1	B	405	PHE	CB-CG-CD2	-6.68	116.13	120.80
1	A	639	ARG	NE-CZ-NH1	6.62	123.61	120.30
1	A	688	ARG	NE-CZ-NH1	6.60	123.60	120.30
1	B	199	ASP	CB-CG-OD1	-6.56	112.39	118.30
1	B	713	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	A	123	ARG	NE-CZ-NH1	6.47	123.54	120.30
1	A	132	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	B	268	ASP	CB-CG-OD1	6.36	124.03	118.30
1	B	149	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	B	730[A]	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	B	730[B]	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	B	434	TYR	CB-CG-CD1	6.26	124.76	121.00
1	B	393	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	A	433	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	A	587	ASP	CB-CG-OD2	-6.07	112.83	118.30
1	B	719	TYR	CB-CG-CD1	-6.05	117.37	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	587	ASP	CB-CG-OD1	6.03	123.72	118.30
1	A	431	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	A	633	VAL	CG1-CB-CG2	-5.97	101.35	110.90
1	B	426[A]	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	B	426[B]	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	B	504	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	B	504	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	B	433	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	A	649	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	B	149	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	A	382	ARG	NE-CZ-NH1	5.83	123.21	120.30
1	B	98	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	255[A]	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	A	255[B]	ARG	NE-CZ-NH2	-5.79	117.40	120.30
1	B	540	ARG	NE-CZ-NH1	5.75	123.17	120.30
1	A	296	GLU	OE1-CD-OE2	5.74	130.19	123.30
1	B	412	PHE	CB-CG-CD1	5.73	124.81	120.80
1	B	222	ASP	CB-CG-OD1	-5.68	113.19	118.30
1	B	404	ARG	NE-CZ-NH2	-5.68	117.46	120.30
1	A	98	ASP	CB-CG-OD1	5.66	123.40	118.30
1	B	730[A]	ARG	CB-CA-C	5.64	121.69	110.40
1	B	730[B]	ARG	CB-CA-C	5.64	121.69	110.40
1	A	395	ASP	CB-CG-OD1	5.63	123.37	118.30
1	B	719	TYR	CB-CG-CD2	5.61	124.37	121.00
1	A	393	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	A	268	ASP	CB-CG-OD2	-5.54	113.32	118.30
1	B	382	ARG	NE-CZ-NH1	5.52	123.06	120.30
1	A	601	PHE	CB-CG-CD2	5.49	124.64	120.80
1	A	249	ASP	CB-CG-OD1	5.48	123.23	118.30
1	B	412	PHE	CB-CG-CD2	-5.46	116.98	120.80
1	A	676	LYS	CD-CE-NZ	-5.42	99.22	111.70
1	B	46	GLN	CB-CG-CD	5.38	125.58	111.60
1	A	40	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	B	60	ASP	CB-CG-OD2	-5.28	113.54	118.30
1	B	83	ASP	CB-CG-OD2	5.28	123.05	118.30
1	B	393	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	B	376	ASP	OD1-CG-OD2	5.26	133.30	123.30
1	B	639	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	B	726	GLU	CG-CD-OE2	-5.22	107.86	118.30
1	A	701	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	519	GLU	OE1-CD-OE2	5.17	129.51	123.30
1	A	320	ASP	CB-CG-OD1	-5.16	113.66	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	191	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	393	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	A	108	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	A	60	ASP	CB-CG-OD1	5.07	122.87	118.30
1	A	528	LEU	CB-CG-CD1	-5.05	102.41	111.00
1	B	132	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	A	150	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	744	ARG	NE-CZ-NH1	-5.03	117.78	120.30
1	A	496	LYS	CD-CE-NZ	-5.03	100.14	111.70
1	B	73	GLU	OE1-CD-OE2	5.02	129.33	123.30
1	A	245	ASP	CB-CG-OD1	5.01	122.81	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	5540	0	5358	13	0
1	B	5560	0	5399	31	0
2	A	43	0	30	0	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	16	0	28	3	0
6	B	24	0	42	12	0
7	B	5	0	0	0	0
8	A	774	0	0	6	0
8	B	733	0	0	10	0
All	All	12746	0	10887	55	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 (55) 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:506:ARG:HE	6:B:806:MPD:H12	1.30	0.95
1:B:730[A]:ARG:HD2	8:B:1503:HOH:O	1.67	0.93
6:B:808:MPD:H53	6:B:808:MPD:C1	2.06	0.83
1:A:119[B]:THR:HG21	8:A:1104:HOH:O	1.78	0.83
1:B:119[B]:THR:HG23	8:B:1065:HOH:O	1.81	0.81
6:B:806:MPD:H51	8:B:1285:HOH:O	1.81	0.80
6:B:808:MPD:H12	6:B:808:MPD:H53	1.62	0.80
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	1.65	0.78
1:A:593:VAL:HG13	8:A:995:HOH:O	1.87	0.74
6:A:806:MPD:O4	6:A:806:MPD:O2	2.04	0.74
1:B:540:ARG:CZ	1:B:540:ARG:HA	2.23	0.68
1:B:55:HIS:HD2	8:B:1209:HOH:O	1.77	0.67
1:B:73:GLU:OE2	8:B:902:HOH:O	2.11	0.67
1:B:540:ARG:NH1	1:B:540:ARG:HA	2.09	0.67
1:A:339:HIS:O	1:A:343[B]:GLU:HG3	1.96	0.66
1:B:512:ASP:OD1	8:B:904:HOH:O	2.15	0.65
6:B:806:MPD:H52	6:B:806:MPD:H11	1.79	0.65
1:B:119[B]:THR:HG22	1:B:593:VAL:HG21	1.80	0.64
1:B:633[A]:VAL:HG22	1:B:719:TYR:CZ	2.33	0.63
1:B:633[A]:VAL:HG22	1:B:719:TYR:CE2	2.32	0.63
6:B:807:MPD:HM2	6:B:807:MPD:H53	1.80	0.62
6:B:806:MPD:H13	8:B:1524:HOH:O	1.99	0.61
6:A:805:MPD:C5	6:A:805:MPD:H11	2.32	0.60
1:B:506:ARG:NE	6:B:806:MPD:H12	2.10	0.58
1:B:629:PRO:O	1:B:633[A]:VAL:HG23	2.04	0.58
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.87	0.57
1:A:51:ILE:HD11	1:A:618:VAL:HG12	1.87	0.56
6:B:806:MPD:C1	6:B:806:MPD:H52	2.35	0.56
1:B:506:ARG:HE	6:B:806:MPD:C1	2.12	0.55
1:A:426[A]:ARG:NH2	8:A:901:HOH:O	0.70	0.54
1:B:55:HIS:CD2	8:B:1209:HOH:O	2.57	0.54
1:B:512:ASP:HB2	8:B:1070:HOH:O	2.07	0.54
1:B:74:LYS:HA	1:B:74:LYS:HE2	1.89	0.54
1:A:540:ARG:NE	1:A:540:ARG:HA	2.25	0.51
1:B:662:ASN:H	1:B:725:GLN:HE22	1.59	0.51
1:B:426[A]:ARG:NE	8:B:903:HOH:O	2.13	0.49
1:B:647:GLN:HE21	1:B:647:GLN:H	1.60	0.49
1:B:647:GLN:HE21	1:B:647:GLN:N	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:428:MET:O	1:A:433:ARG:HD3	2.13	0.48
1:B:591:MET:SD	1:B:594:LEU:HD12	2.53	0.48
1:A:504:ARG:HD2	8:A:999:HOH:O	2.14	0.48
6:B:808:MPD:H53	6:B:808:MPD:H11	1.92	0.48
1:A:119[B]:THR:CG2	1:A:593:VAL:HG11	2.40	0.47
1:B:428:MET:O	1:B:433:ARG:HD3	2.15	0.47
6:A:805:MPD:H52	6:A:805:MPD:H11	1.98	0.45
1:B:646:GLY:C	1:B:647:GLN:HG2	2.36	0.45
1:B:51:ILE:HD11	1:B:618:VAL:HG12	1.99	0.45
1:B:140:PRO:HB3	6:B:808:MPD:H4	1.98	0.45
1:B:403[B]:ARG:HH12	1:B:406:HIS:HD2	1.62	0.45
1:B:649[A]:ARG:HD3	1:B:649[A]:ARG:HA	1.64	0.44
1:A:255[A]:ARG:HG3	8:A:1112:HOH:O	2.18	0.43
1:B:426[B]:ARG:HD2	1:B:426[B]:ARG:HA	1.84	0.41
1:B:726:GLU:CD	1:B:726:GLU:H	2.23	0.41
1:A:431:ARG:HD2	1:A:447:GLN:OE1	2.21	0.40
1:A:649:ARG:NH1	8:A:933:HOH:O	2.54	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	715/728 (98%)	703 (98%)	12 (2%)	0	100	100
1	B	719/728 (99%)	712 (99%)	7 (1%)	0	100	100
All	All	1434/1456 (98%)	1415 (99%)	19 (1%)	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%)	544 (98%)	10 (2%)	66	54
1	B	558/560 (100%)	547 (98%)	11 (2%)	63	49
All	All	1112/1120 (99%)	1091 (98%)	21 (2%)	70	52

All (21) 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	183	LYS
1	A	343[A]	GLU
1	A	343[B]	GLU
1	A	608	LYS
1	A	610	ARG
1	A	725	GLN
1	B	40	ARG
1	B	46	GLN
1	B	64	LYS
1	B	118	ARG
1	B	141	ASP
1	B	610	ARG
1	B	633[A]	VAL
1	B	633[B]	VAL
1	B	647	GLN
1	B	649[A]	ARG
1	B	649[B]	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN

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Mol	Chain	Res	Type
1	A	227	ASN
1	A	247	ASN
1	A	339	HIS
1	A	647	GLN
1	B	46	GLN
1	B	55	HIS
1	B	227	ASN
1	B	406	HIS
1	B	647	GLN
1	B	650	HIS
1	B	725	GLN
1	B	737	ASN

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	2.24	3 (30%)	9,23,25	2.67	5 (55%)
1	TOX	A	111[B]	-	10,17,18	2.24	3 (30%)	9,23,25	2.67	5 (55%)
1	TOX	B	111[A]	2	10,17,18	2.62	3 (30%)	9,23,25	2.07	4 (44%)
1	TOX	B	111[B]	-	10,17,18	2.62	3 (30%)	9,23,25	2.07	4 (44%)

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 (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111[A]	TOX	CD1-NE1	-7.13	1.32	1.39
1	B	111[B]	TOX	CD1-NE1	-7.13	1.32	1.39
1	A	111[B]	TOX	CD1-NE1	-4.27	1.35	1.39
1	A	111[A]	TOX	CD1-NE1	-4.27	1.35	1.39
1	A	111[B]	TOX	CE3-CD2	-3.48	1.35	1.42
1	A	111[A]	TOX	CE3-CD2	-3.48	1.35	1.42
1	B	111[A]	TOX	CE3-CD2	-2.00	1.38	1.42
1	B	111[B]	TOX	CE3-CD2	-2.00	1.38	1.42
1	B	111[A]	TOX	O-C	2.58	1.31	1.19
1	B	111[B]	TOX	O-C	2.58	1.31	1.19
1	A	111[B]	TOX	O-C	2.75	1.32	1.19
1	A	111[A]	TOX	O-C	2.75	1.32	1.19

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111[B]	TOX	CZ2-CE2-CD2	-3.93	115.65	120.58
1	A	111[A]	TOX	CZ2-CE2-CD2	-3.93	115.65	120.58
1	A	111[B]	TOX	CH2-CZ3-CE3	-3.42	115.51	120.45
1	A	111[A]	TOX	CH2-CZ3-CE3	-3.42	115.51	120.45
1	B	111[A]	TOX	CB-CG-CD1	-3.17	124.05	127.97
1	B	111[B]	TOX	CB-CG-CD1	-3.17	124.05	127.97
1	A	111[B]	TOX	CB-CG-CD1	-2.47	124.91	127.97
1	A	111[A]	TOX	CB-CG-CD1	-2.47	124.91	127.97
1	B	111[A]	TOX	CZ3-CE3-CD2	-2.33	117.65	120.88
1	B	111[B]	TOX	CZ3-CE3-CD2	-2.33	117.65	120.88
1	B	111[A]	TOX	CZ3-CH2-CZ2	-2.14	117.37	120.45
1	B	111[B]	TOX	CZ3-CH2-CZ2	-2.14	117.37	120.45
1	A	111[B]	TOX	CZ3-CH2-CZ2	3.44	125.42	120.45
1	A	111[A]	TOX	CZ3-CH2-CZ2	3.44	125.42	120.45
1	A	111[B]	TOX	CE3-CD2-CE2	3.93	123.78	119.83
1	A	111[A]	TOX	CE3-CD2-CE2	3.93	123.78	119.83
1	B	111[A]	TOX	CH2-CZ3-CE3	4.01	126.24	120.45
1	B	111[B]	TOX	CH2-CZ3-CE3	4.01	126.24	120.45

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	2.69	4 (16%)	16,82,82	2.13	6 (37%)
5	OXY	A	804	-	1,1,1	0.09	0	0,0,0	0.00	-
6	MPD	A	805	-	6,7,7	0.89	0	6,10,10	0.63	0
6	MPD	A	806	-	6,7,7	0.68	0	6,10,10	0.59	0
2	HEM	B	801	1	24,50,50	2.19	5 (20%)	16,82,82	1.86	7 (43%)
5	OXY	B	804	-	1,1,1	0.75	0	0,0,0	0.00	-
7	PO4	B	805	-	4,4,4	0.51	0	6,6,6	0.52	0
6	MPD	B	806	-	6,7,7	0.86	0	6,10,10	1.30	1 (16%)
6	MPD	B	807	-	6,7,7	0.72	0	6,10,10	1.91	1 (16%)
6	MPD	B	808	-	6,7,7	0.99	0	6,10,10	1.40	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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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	PO4	B	805	-	-	0/0/0/0	0/0/0/0
6	MPD	B	806	-	-	0/5/5/5	0/0/0/0
6	MPD	B	807	-	-	0/5/5/5	0/0/0/0
6	MPD	B	808	-	-	0/5/5/5	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	C4D-ND	-7.95	1.26	1.36
2	A	801	HEM	C1B-NB	-6.86	1.27	1.36
2	B	801	HEM	C1B-NB	-4.81	1.30	1.36
2	A	801	HEM	C1C-NC	-4.02	1.31	1.36
2	B	801	HEM	C1C-NC	-2.79	1.33	1.36
2	B	801	HEM	CAD-C3D	-2.36	1.49	1.52
2	B	801	HEM	CMA-C3A	2.50	1.56	1.51
2	A	801	HEM	C4C-NC	5.95	1.44	1.36
2	B	801	HEM	C4C-NC	7.80	1.47	1.36

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	807	MPD	O4-C4-C5	-4.34	87.81	109.47
2	A	801	HEM	CAA-CBA-CGA	-4.05	104.91	112.78
2	B	801	HEM	C3B-CAB-CBB	-4.03	118.28	126.40
2	A	801	HEM	CAA-C2A-C3A	-2.62	121.51	129.00
2	B	801	HEM	CAA-CBA-CGA	-2.50	107.92	112.78
2	B	801	HEM	C3C-C4C-NC	-2.42	106.38	110.94
6	B	806	MPD	CM-C2-C1	-2.14	105.31	110.41
2	A	801	HEM	CAD-CBD-CGD	2.01	116.69	112.78
2	B	801	HEM	CBD-CAD-C3D	2.05	116.07	112.47
2	A	801	HEM	CBD-CAD-C3D	2.10	116.14	112.47
2	B	801	HEM	C3B-C4B-NB	2.15	111.99	109.21
2	B	801	HEM	CBA-CAA-C2A	2.21	116.38	112.49
2	B	801	HEM	CMB-C2B-C3B	2.23	129.44	125.09
6	B	808	MPD	CM-C2-C1	2.32	115.94	110.41
2	A	801	HEM	CMB-C2B-C3B	2.89	130.73	125.09
2	A	801	HEM	CMC-C2C-C3C	4.38	133.65	125.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	805	MPD	2	0
6	A	806	MPD	1	0
6	B	806	MPD	7	0
6	B	807	MPD	1	0
6	B	808	MPD	4	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%)	-0.71	4 (0%) 90 88	13, 19, 37, 79	0
1	B	712/728 (97%)	-0.69	6 (0%) 87 85	14, 19, 36, 83	0
All	All	1424/1456 (97%)	-0.70	10 (0%) 89 87	13, 19, 37, 83	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	540	ARG	3.7
1	B	610	ARG	3.3
1	A	748	ALA	3.0
1	A	540	ARG	2.7
1	B	608	LYS	2.6
1	B	748	ALA	2.6
1	A	608	LYS	2.6
1	B	679	ALA	2.6
1	A	680	ALA	2.5
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(Å ²)	Q<0.9
1	TOX	A	111[B]	16/17	0.98	0.08	-	13,13,15,19	2
1	TOX	B	111[A]	16/17	0.98	0.12	-	12,14,19,21	2

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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	-	13,13,17,19	2
1	TOX	B	111[B]	16/17	0.98	0.12	-	12,14,17,21	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(\AA^2)	Q<0.9
6	MPD	A	806	8/8	0.89	0.19	16.28	55,66,73,75	0
6	MPD	B	806	8/8	0.92	0.14	6.90	38,46,47,47	0
6	MPD	B	808	8/8	0.87	0.15	5.28	44,56,66,73	0
6	MPD	B	807	8/8	0.94	0.13	1.92	27,35,43,48	0
2	HEM	B	801	43/43	0.99	0.10	0.47	13,15,17,18	0
2	HEM	A	801	43/43	0.99	0.07	0.06	12,14,15,17	0
4	CL	A	803	1/1	0.98	0.06	-1.24	33,33,33,33	0
4	CL	B	803	1/1	0.99	0.08	-1.30	32,32,32,32	0
3	NA	A	802	1/1	1.00	0.04	-2.02	16,16,16,16	0
3	NA	B	802	1/1	1.00	0.03	-2.47	15,15,15,15	0
6	MPD	A	805	8/8	0.90	0.16	-	35,40,49,51	0
5	OXY	A	804	2/2	0.96	0.11	-	33,33,33,34	0
7	PO4	B	805	5/5	0.97	0.17	-	37,50,51,53	0
5	OXY	B	804	2/2	0.92	0.14	-	28,28,28,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.