



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 29, 2016 – 05:35 PM EDT

PDB ID : 5SX1
Title : Crystal structure of D141E variant of B. pseudomallei KatG
Authors : Loewen, P.C.
Deposited on : 2016-08-09
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

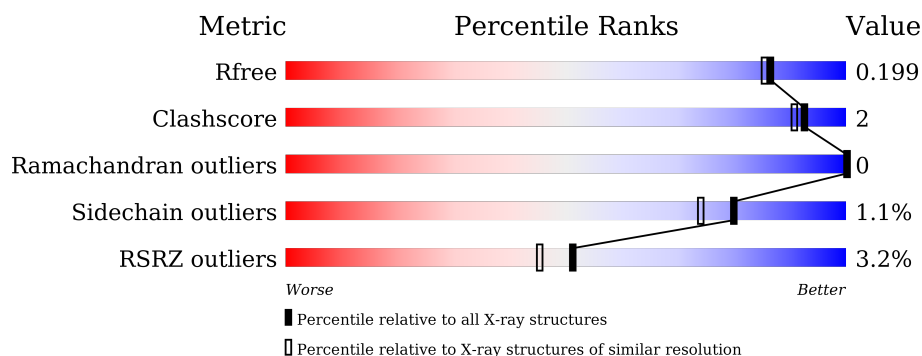
1 Overall quality at a glance

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>4%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>..</div> </div> </div>
1	B	728	<div> <div>3%</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
4	OXY	A	804	-	-	-	X
4	OXY	B	804	-	-	-	X
4	OXY	B	807	-	-	-	X
5	MPD	B	805	-	-	-	X

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 12789 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
			5532	3497	985	1036	14			
1	B	713	Total	C	N	O	S	0	6	0
			5528	3491	983	1040	14			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	141	GLU	ASP	engineered mutation	UNP Q3JNW6
B	141	GLU	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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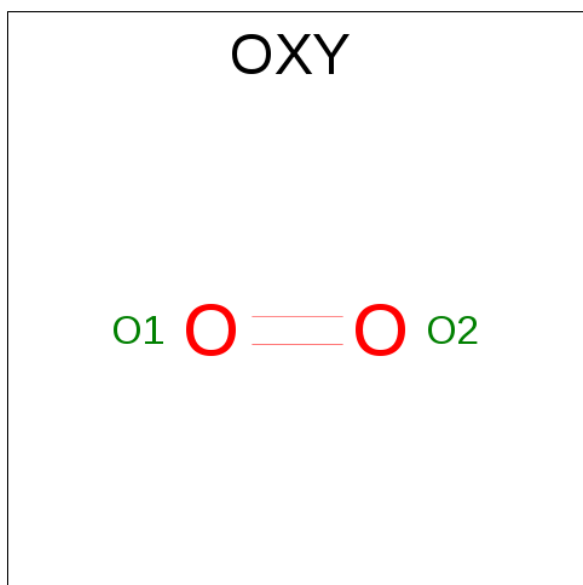
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	Fe	N	O	
			43	34	1	4	4	
							0	0

- 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

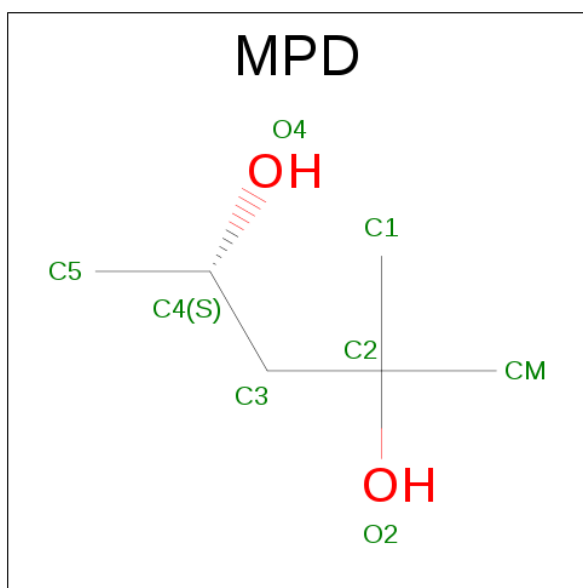
- Molecule 4 is OXYGEN MOLECULE (three-letter code: OXY) (formula: O₂).



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

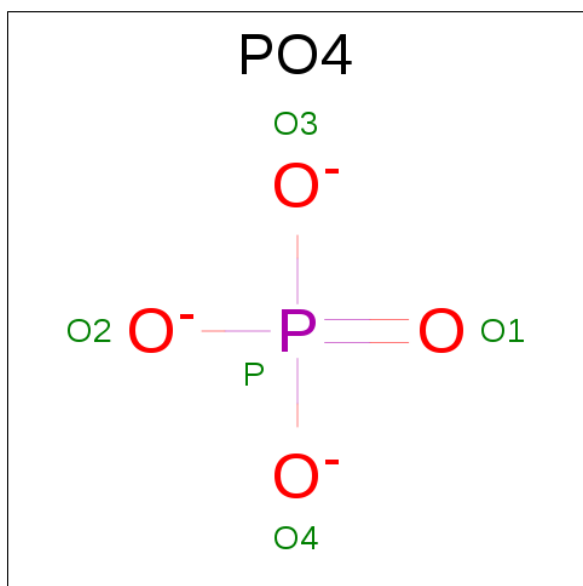
- Molecule 5 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:

C₆H₁₄O₂).



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

- Molecule 6 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

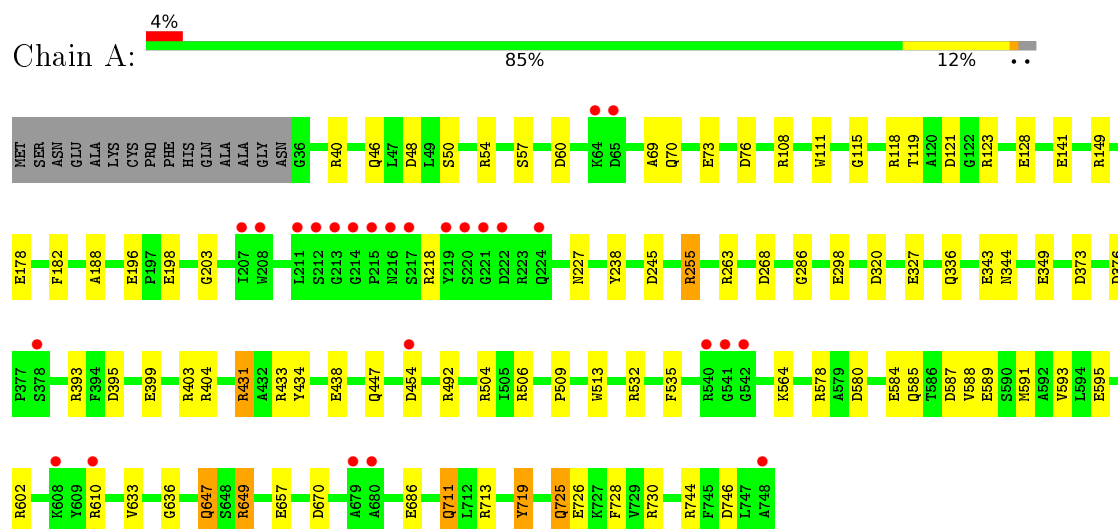
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	819	Total	O	0	0
			819	819		
7	B	778	Total	O	0	0
			778	778		

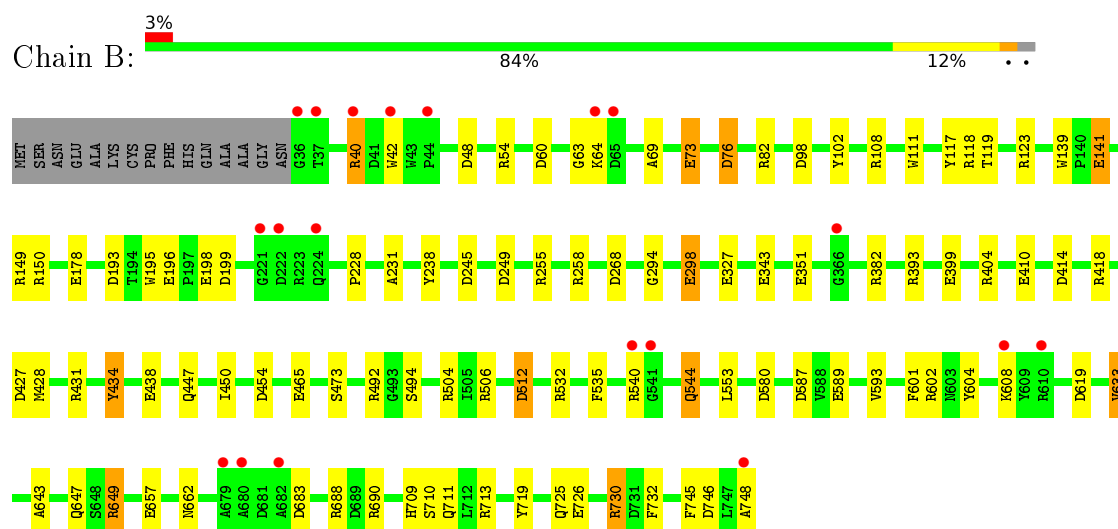
3 Residue-property plots [i](#)

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	100.74Å 116.20Å 175.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.80 29.17 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.1 (20.00-1.80) 99.2 (29.17-1.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.81 (at 1.80Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.155 , 0.191 0.167 , 0.199	Depositor DCC
R_{free} test set	9287 reflections (5.19%)	DCC
Wilson B-factor (Å ²)	18.6	Xtriage
Anisotropy	0.098	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 44.9	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	0.96	EDS
Total number of atoms	12789	wwPDB-VP
Average B, all atoms (Å ²)	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.49% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: PO4, NA, MPD, OXY, 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	1.60	57/5690 (1.0%)	1.38	54/7734 (0.7%)
1	B	1.56	49/5696 (0.9%)	1.39	62/7743 (0.8%)
All	All	1.58	106/11386 (0.9%)	1.38	116/15477 (0.7%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	2

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	726	GLU	CG-CD	10.47	1.67	1.51
1	A	725	GLN	CG-CD	9.34	1.72	1.51
1	A	584	GLU	CG-CD	9.28	1.65	1.51
1	B	410	GLU	CG-CD	9.24	1.65	1.51
1	A	141	GLU	CG-CD	8.71	1.65	1.51
1	A	438	GLU	CD-OE2	8.69	1.35	1.25
1	B	726	GLU	CG-CD	8.49	1.64	1.51
1	A	141	GLU	CD-OE1	8.43	1.34	1.25
1	A	327	GLU	CD-OE1	8.03	1.34	1.25
1	A	532	ARG	CD-NE	-7.97	1.32	1.46
1	B	532	ARG	CD-NE	-7.82	1.33	1.46
1	A	434	TYR	CG-CD1	-7.50	1.29	1.39
1	B	410	GLU	CD-OE2	7.49	1.33	1.25
1	B	730	ARG	CZ-NH1	7.34	1.42	1.33
1	A	399	GLU	CD-OE2	7.30	1.33	1.25
1	B	141	GLU	CD-OE1	7.24	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	50	SER	CB-OG	-7.22	1.32	1.42
1	B	298	GLU	CD-OE2	7.17	1.33	1.25
1	B	198	GLU	CG-CD	6.87	1.62	1.51
1	B	196	GLU	CB-CG	-6.82	1.39	1.52
1	A	298	GLU	CG-CD	6.80	1.62	1.51
1	B	82	ARG	CZ-NH2	-6.80	1.24	1.33
1	A	434	TYR	CE1-CZ	-6.80	1.29	1.38
1	B	512	ASP	CG-OD2	6.79	1.41	1.25
1	B	42	TRP	CE3-CZ3	6.69	1.49	1.38
1	B	434	TYR	CG-CD1	-6.66	1.30	1.39
1	A	719	TYR	CE1-CZ	6.54	1.47	1.38
1	B	294	GLY	C-O	6.49	1.34	1.23
1	A	141	GLU	CD-OE2	6.48	1.32	1.25
1	A	70	GLN	CG-CD	6.42	1.65	1.51
1	B	327	GLU	CD-OE2	6.42	1.32	1.25
1	B	410	GLU	CD-OE1	6.38	1.32	1.25
1	B	63	GLY	N-CA	6.24	1.55	1.46
1	B	601	PHE	CD2-CE2	6.19	1.51	1.39
1	B	544	GLN	CD-OE1	6.18	1.37	1.24
1	A	349	GLU	CD-OE2	-6.11	1.19	1.25
1	A	196	GLU	CG-CD	6.11	1.61	1.51
1	A	454	ASP	CB-CG	6.09	1.64	1.51
1	A	584	GLU	CD-OE2	6.09	1.32	1.25
1	B	532	ARG	NE-CZ	-6.08	1.25	1.33
1	A	57	SER	CB-OG	6.06	1.50	1.42
1	A	535	PHE	CG-CD1	-6.05	1.29	1.38
1	A	504	ARG	CZ-NH1	-6.02	1.25	1.33
1	A	399	GLU	CG-CD	-6.01	1.43	1.51
1	B	343	GLU	CD-OE2	6.01	1.32	1.25
1	A	589	GLU	CD-OE2	5.97	1.32	1.25
1	A	393	ARG	CZ-NH2	5.96	1.40	1.33
1	B	465	GLU	CD-OE1	5.95	1.32	1.25
1	B	602	ARG	CZ-NH2	-5.95	1.25	1.33
1	A	513	TRP	CE2-CZ2	-5.94	1.29	1.39
1	A	336	GLN	CD-NE2	5.89	1.47	1.32
1	A	198	GLU	CG-CD	5.85	1.60	1.51
1	B	418	ARG	CZ-NH1	-5.85	1.25	1.33
1	A	434	TYR	CE2-CZ	-5.81	1.31	1.38
1	B	343	GLU	CD-OE1	5.79	1.32	1.25
1	A	141	GLU	CB-CG	5.76	1.63	1.52
1	B	494	SER	CB-OG	5.73	1.49	1.42
1	A	203	GLY	C-O	5.71	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	128	GLU	CG-CD	5.68	1.60	1.51
1	A	327	GLU	CG-CD	5.67	1.60	1.51
1	A	636	GLY	N-CA	5.67	1.54	1.46
1	A	344	ASN	C-O	5.65	1.34	1.23
1	B	746	ASP	CB-CG	5.64	1.63	1.51
1	B	178	GLU	CG-CD	5.58	1.60	1.51
1	A	532	ARG	NE-CZ	-5.53	1.25	1.33
1	A	349	GLU	CD-OE1	-5.51	1.19	1.25
1	A	649	ARG	CZ-NH1	5.49	1.40	1.33
1	A	728	PHE	CG-CD2	-5.47	1.30	1.38
1	B	399	GLU	CD-OE1	5.46	1.31	1.25
1	A	343	GLU	CD-OE1	5.46	1.31	1.25
1	B	544	GLN	CG-CD	5.46	1.63	1.51
1	B	657	GLU	CD-OE2	5.46	1.31	1.25
1	A	245	ASP	CG-OD1	5.45	1.37	1.25
1	B	102	TYR	CE2-CZ	-5.45	1.31	1.38
1	A	686	GLU	CG-CD	5.45	1.60	1.51
1	B	141	GLU	CG-CD	5.45	1.60	1.51
1	B	434	TYR	CE2-CZ	-5.43	1.31	1.38
1	B	102	TYR	CD2-CE2	5.39	1.47	1.39
1	A	711	GLN	CG-CD	5.39	1.63	1.51
1	B	473	SER	CB-OG	5.38	1.49	1.42
1	A	726	GLU	CD-OE2	5.36	1.31	1.25
1	B	139	TRP	CZ3-CH2	5.35	1.48	1.40
1	B	198	GLU	CD-OE1	5.34	1.31	1.25
1	B	73	GLU	CD-OE1	5.32	1.31	1.25
1	B	535	PHE	CG-CD1	-5.29	1.30	1.38
1	B	195	TRP	CE3-CZ3	5.25	1.47	1.38
1	B	710	SER	CB-OG	-5.24	1.35	1.42
1	A	182	PHE	CG-CD1	5.22	1.46	1.38
1	A	286	GLY	N-CA	5.21	1.53	1.46
1	A	647	GLN	CG-CD	5.19	1.62	1.51
1	A	595	GLU	CD-OE1	5.19	1.31	1.25
1	B	438	GLU	CD-OE2	5.19	1.31	1.25
1	A	532	ARG	CZ-NH2	-5.18	1.26	1.33
1	A	115	GLY	CA-C	5.18	1.60	1.51
1	B	730	ARG	CZ-NH2	5.16	1.39	1.33
1	A	657	GLU	CD-OE1	5.16	1.31	1.25
1	A	399	GLU	CD-OE1	5.12	1.31	1.25
1	B	231	ALA	CA-CB	5.09	1.63	1.52
1	A	434	TYR	CD1-CE1	5.09	1.47	1.39
1	A	198	GLU	CD-OE1	5.09	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	193	ASP	CB-CG	5.08	1.62	1.51
1	A	178	GLU	CG-CD	5.07	1.59	1.51
1	B	604	TYR	CE2-CZ	-5.07	1.31	1.38
1	B	643	ALA	N-CA	-5.04	1.36	1.46
1	B	196	GLU	CG-CD	5.01	1.59	1.51
1	A	580	ASP	CB-CG	5.01	1.62	1.51

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	532	ARG	NE-CZ-NH2	-28.86	105.87	120.30
1	B	532	ARG	NE-CZ-NH2	-24.47	108.07	120.30
1	A	532	ARG	NE-CZ-NH1	18.16	129.38	120.30
1	B	532	ARG	NE-CZ-NH1	16.26	128.43	120.30
1	B	108	ARG	NE-CZ-NH1	12.72	126.66	120.30
1	B	713	ARG	NE-CZ-NH2	-12.10	114.25	120.30
1	B	713	ARG	NE-CZ-NH1	11.85	126.23	120.30
1	A	713	ARG	NE-CZ-NH1	11.82	126.21	120.30
1	A	713	ARG	NE-CZ-NH2	-11.52	114.54	120.30
1	B	393	ARG	NE-CZ-NH2	-10.76	114.92	120.30
1	A	649	ARG	NE-CZ-NH2	-10.49	115.06	120.30
1	A	149	ARG	NE-CZ-NH1	10.34	125.47	120.30
1	B	108	ARG	NE-CZ-NH2	-10.19	115.20	120.30
1	A	602	ARG	NE-CZ-NH2	-10.07	115.26	120.30
1	B	123	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	B	149	ARG	NE-CZ-NH2	-9.20	115.70	120.30
1	B	649	ARG	NE-CZ-NH1	9.15	124.88	120.30
1	B	619	ASP	CB-CG-OD1	-8.86	110.33	118.30
1	B	149	ARG	NE-CZ-NH1	8.80	124.70	120.30
1	B	633	VAL	CG1-CB-CG2	-8.77	96.87	110.90
1	A	649	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	A	60	ASP	CB-CG-OD2	-8.57	110.58	118.30
1	B	512	ASP	CB-CG-OD1	-8.56	110.60	118.30
1	A	108	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	A	670	ASP	CB-CG-OD2	-8.33	110.80	118.30
1	B	649	ARG	NE-CZ-NH2	-8.29	116.16	120.30
1	A	584	GLU	OE1-CD-OE2	-8.23	113.42	123.30
1	B	532	ARG	CD-NE-CZ	8.16	135.02	123.60
1	A	48	ASP	CB-CG-OD1	8.11	125.60	118.30
1	B	82	ARG	NE-CZ-NH1	8.11	124.36	120.30
1	B	434	TYR	CB-CG-CD1	8.00	125.80	121.00
1	A	532	ARG	CD-NE-CZ	7.96	134.75	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	602	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	A	492	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	A	108	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	A	506	ARG	NE-CZ-NH1	7.67	124.13	120.30
1	B	726	GLU	OE1-CD-OE2	-7.60	114.18	123.30
1	B	580	ASP	CB-CG-OD1	-7.47	111.58	118.30
1	A	433	ARG	NE-CZ-NH2	-7.45	116.58	120.30
1	B	732	PHE	CB-CG-CD1	-7.40	115.62	120.80
1	A	587	ASP	CB-CG-OD1	7.34	124.91	118.30
1	B	73	GLU	OE1-CD-OE2	7.32	132.08	123.30
1	A	149	ARG	NE-CZ-NH2	-7.25	116.67	120.30
1	A	578	ARG	NE-CZ-NH1	7.23	123.92	120.30
1	B	76	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	B	690	ARG	NE-CZ-NH2	7.18	123.89	120.30
1	A	434	TYR	CB-CG-CD1	7.18	125.31	121.00
1	B	48	ASP	CB-CG-OD1	7.02	124.61	118.30
1	B	504	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	B	60	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	B	427	ASP	CB-CG-OD1	-6.97	112.03	118.30
1	A	40	ARG	NE-CZ-NH1	6.95	123.78	120.30
1	B	506	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	A	255	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	A	504	ARG	NE-CZ-NH1	6.77	123.68	120.30
1	A	395	ASP	CB-CG-OD1	6.75	124.38	118.30
1	B	382	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	B	123	ARG	NE-CZ-NH2	-6.71	116.94	120.30
1	B	512	ASP	CB-CG-OD2	6.64	124.28	118.30
1	A	263	ARG	NE-CZ-NH2	-6.60	117.00	120.30
1	A	376	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	A	60	ASP	CB-CG-OD1	6.55	124.20	118.30
1	B	587	ASP	CB-CG-OD1	6.52	124.17	118.30
1	B	48	ASP	CB-CG-OD2	-6.44	112.50	118.30
1	B	258	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	B	98	ASP	CB-CG-OD1	-6.42	112.52	118.30
1	B	150	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	A	218	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	B	404	ARG	NE-CZ-NH1	6.35	123.48	120.30
1	A	188	ALA	N-CA-CB	6.24	118.83	110.10
1	A	255	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	B	198	GLU	OE1-CD-OE2	-6.18	115.88	123.30
1	B	688	ARG	NE-CZ-NH1	6.15	123.37	120.30
1	B	553	LEU	CB-CG-CD1	-6.09	100.64	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	249	ASP	CB-CG-OD2	6.08	123.77	118.30
1	A	123	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	373	ASP	CB-CG-OD1	5.96	123.66	118.30
1	B	198	GLU	CG-CD-OE1	5.95	130.20	118.30
1	A	121	ASP	CB-CG-OD1	5.94	123.65	118.30
1	A	320	ASP	CB-CG-OD1	-5.93	112.96	118.30
1	A	454	ASP	CB-CG-OD2	5.92	123.63	118.30
1	A	48	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	A	726	GLU	OE1-CD-OE2	-5.87	116.25	123.30
1	B	683	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	A	532	ARG	CG-CD-NE	-5.83	99.56	111.80
1	B	268	ASP	CB-CG-OD1	5.71	123.44	118.30
1	B	532	ARG	CG-CD-NE	-5.68	99.86	111.80
1	B	82	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	268	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	A	54	ARG	CB-CA-C	-5.65	99.11	110.40
1	B	454	ASP	CB-CG-OD1	5.64	123.38	118.30
1	B	504	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	B	40	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	B	245	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	A	198	GLU	CG-CD-OE1	5.46	129.22	118.30
1	B	619	ASP	CB-CG-OD2	5.45	123.21	118.30
1	B	492	ARG	NE-CZ-NH1	5.43	123.02	120.30
1	A	404	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	450	ILE	CA-CB-CG1	-5.34	100.85	111.00
1	B	745	PHE	CB-CG-CD1	-5.31	117.08	120.80
1	B	54	ARG	NE-CZ-NH2	-5.29	117.66	120.30
1	B	748	ALA	N-CA-CB	5.27	117.47	110.10
1	B	60	ASP	CB-CG-OD1	5.26	123.04	118.30
1	A	403	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	76	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	A	730	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	414	ASP	CB-CG-OD2	5.20	122.98	118.30
1	A	54	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	A	141	GLU	OE1-CD-OE2	-5.18	117.09	123.30
1	A	588	VAL	CG1-CB-CG2	5.16	119.15	110.90
1	A	744	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	438	GLU	OE1-CD-OE2	5.13	129.46	123.30
1	B	54	ARG	CB-CA-C	-5.11	100.18	110.40
1	B	255	ARG	NE-CZ-NH1	5.06	122.83	120.30
1	B	351	GLU	OE1-CD-OE2	5.05	129.35	123.30
1	A	431	ARG	NE-CZ-NH2	5.03	122.82	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	117	TYR	Sidechain
1	B	199	ASP	Mainchain

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	5532	0	5363	15	0
1	B	5528	0	5339	23	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	4	0	0	0	0
4	B	6	0	0	1	0
5	A	16	0	28	3	0
5	B	8	0	14	4	0
6	A	5	0	0	0	0
6	B	5	0	0	0	0
7	A	819	0	0	8	1
7	B	778	0	0	11	1
All	All	12789	0	10804	44	1

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 (44) 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:255:ARG:NH2	7:A:903:HOH:O	2.05	0.89
1:B:119:THR:HG21	7:B:1017:HOH:O	1.74	0.85
1:B:76:ASP:OD2	7:B:901:HOH:O	2.02	0.77
1:A:119:THR:HG21	7:A:1101:HOH:O	1.89	0.71
1:B:512:ASP:OD1	7:B:902:HOH:O	2.14	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:647:GLN:HG2	7:A:1488:HOH:O	1.98	0.64
1:B:111:TRP:HZ3	1:B:238:TYR:HH	1.46	0.63
1:B:141:GLU:OE2	4:B:807:OXY:O1	2.18	0.60
1:B:76:ASP:OD1	7:B:903:HOH:O	2.17	0.60
5:B:805:MPD:H52	5:B:805:MPD:CM	2.31	0.60
5:A:805:MPD:CM	5:A:805:MPD:O4	2.51	0.59
1:B:662:ASN:H	1:B:725:GLN:HE22	1.53	0.55
1:B:540:ARG:HA	1:B:540:ARG:NE	2.23	0.54
1:B:512:ASP:HB2	7:B:1396:HOH:O	2.07	0.53
1:A:69:ALA:O	1:A:73:GLU:HG3	2.08	0.53
1:A:711:GLN:OE1	7:A:905:HOH:O	2.18	0.51
1:B:647:GLN:HG2	7:B:1138:HOH:O	2.12	0.50
5:B:805:MPD:H52	5:B:805:MPD:HM1	1.94	0.50
1:B:431:ARG:CD	7:B:1497:HOH:O	2.59	0.50
1:B:633:VAL:CG2	1:B:719:TYR:CZ	2.95	0.50
1:A:119:THR:HG23	1:A:593:VAL:HG11	1.94	0.49
1:A:633[A]:VAL:CG2	1:A:719:TYR:CZ	2.96	0.49
1:A:746:ASP:HB3	7:A:1531:HOH:O	2.12	0.49
1:A:111:TRP:HZ3	1:A:238:TYR:HH	1.57	0.48
1:A:564:LYS:HE2	7:A:1478:HOH:O	2.13	0.48
1:B:431:ARG:HD2	1:B:447:GLN:OE1	2.14	0.48
5:A:806:MPD:H11	5:A:806:MPD:H53	1.97	0.47
1:B:730:ARG:HD2	7:B:1495:HOH:O	2.15	0.46
1:B:69:ALA:O	1:B:73:GLU:HG2	2.16	0.45
1:B:709:HIS:CE1	1:B:711[B]:GLN:HB2	2.51	0.45
1:A:585[A]:GLN:NE2	7:A:931:HOH:O	2.50	0.45
1:B:428[B]:MET:HE2	1:B:434:TYR:CD1	2.52	0.45
1:A:509:PRO:HD2	1:A:591:MET:HG2	2.00	0.43
1:B:589:GLU:HG2	7:B:944:HOH:O	2.18	0.43
1:A:431:ARG:HD2	1:A:447:GLN:OE1	2.18	0.42
1:B:725:GLN:NE2	7:B:931:HOH:O	2.53	0.42
1:B:119:THR:HG23	1:B:593:VAL:HG11	2.01	0.42
1:B:540:ARG:CA	1:B:540:ARG:NE	2.82	0.42
1:A:46:GLN:NE2	1:B:298:GLU:O	2.53	0.41
5:A:806:MPD:HM2	7:A:1025:HOH:O	2.18	0.41
1:B:431:ARG:HD2	7:B:1497:HOH:O	2.21	0.41
1:A:633[A]:VAL:HG22	1:A:719:TYR:CZ	2.55	0.41
5:B:805:MPD:H52	5:B:805:MPD:HM2	2.02	0.41
5:B:805:MPD:C5	5:B:805:MPD:CM	2.97	0.40

All (1) 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)
7:A:1321:HOH:O	7:B:1069:HOH:O[2_444]	2.11	0.09

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	716/728 (98%)	710 (99%)	6 (1%)	0	100	100
1	B	717/728 (98%)	708 (99%)	9 (1%)	0	100	100
All	All	1433/1456 (98%)	1418 (99%)	15 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	555/561 (99%)	550 (99%)	5 (1%)	84	80
1	B	556/561 (99%)	549 (99%)	7 (1%)	76	68
All	All	1111/1122 (99%)	1099 (99%)	12 (1%)	80	74

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	118	ARG
1	A	227	ASN
1	A	610	ARG

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Mol	Chain	Res	Type
1	A	649	ARG
1	A	725	GLN
1	B	40	ARG
1	B	64	LYS
1	B	118	ARG
1	B	228	PRO
1	B	544	GLN
1	B	608	LYS
1	B	649	ARG

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

Mol	Chain	Res	Type
1	A	227	ASN
1	A	247	ASN
1	A	711	GLN
1	B	55	HIS
1	B	227	ASN
1	B	650	HIS
1	B	725	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 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	2.28	6 (25%)	16,82,82	2.22	7 (43%)
4	OXY	A	803	-	1,1,1	0.25	0	0,0,0	0.00	-
4	OXY	A	804	-	1,1,1	0.35	0	0,0,0	0.00	-
5	MPD	A	805	-	6,7,7	0.61	0	6,10,10	1.45	2 (33%)
5	MPD	A	806	-	6,7,7	0.98	0	6,10,10	1.45	1 (16%)
6	PO4	A	807	-	4,4,4	1.75	1 (25%)	6,6,6	0.35	0
2	HEM	B	801	1,4	24,50,50	1.88	6 (25%)	16,82,82	1.94	5 (31%)
4	OXY	B	803	-	1,1,1	0.49	0	0,0,0	0.00	-
4	OXY	B	804	2	1,1,1	0.06	0	0,0,0	0.00	-
5	MPD	B	805	-	6,7,7	0.61	0	6,10,10	1.44	1 (16%)
6	PO4	B	806	-	4,4,4	1.56	1 (25%)	6,6,6	0.40	0
4	OXY	B	807	-	1,1,1	0.47	0	0,0,0	0.00	-

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
4	OXY	A	804	-	-	0/0/0/0	0/0/0/0
5	MPD	A	805	-	-	0/5/5/5	0/0/0/0
5	MPD	A	806	-	-	0/5/5/5	0/0/0/0
6	PO4	A	807	-	-	0/0/0/0	0/0/0/0
2	HEM	B	801	1,4	-	0/6/54/54	0/0/8/8
4	OXY	B	803	-	-	0/0/0/0	0/0/0/0
4	OXY	B	804	2	-	0/0/0/0	0/0/0/0
5	MPD	B	805	-	-	0/5/5/5	0/0/0/0
6	PO4	B	806	-	-	0/0/0/0	0/0/0/0
4	OXY	B	807	-	-	0/0/0/0	0/0/0/0

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	801	HEM	CAD-C3D	-5.51	1.44	1.52
2	B	801	HEM	C3B-C2B	-4.70	1.34	1.40
2	A	801	HEM	C1C-NC	-4.00	1.31	1.36
2	B	801	HEM	C1B-NB	-3.68	1.31	1.36
2	B	801	HEM	C1C-NC	-3.67	1.31	1.36
2	B	801	HEM	C3C-C2C	-3.36	1.36	1.40
6	A	807	PO4	P-O4	-3.01	1.44	1.53
2	B	801	HEM	CMD-C2D	-2.66	1.46	1.51
6	B	806	PO4	P-O3	-2.48	1.46	1.53
2	A	801	HEM	CMD-C2D	-2.38	1.46	1.51
2	B	801	HEM	CMC-C2C	-2.12	1.46	1.51
2	A	801	HEM	C1B-NB	-2.01	1.34	1.36
2	A	801	HEM	C4C-NC	4.17	1.42	1.36
2	A	801	HEM	C4D-ND	5.87	1.44	1.36

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	CAA-CBA-CGA	-4.59	103.86	112.78
2	B	801	HEM	CAA-CBA-CGA	-3.75	105.48	112.78
2	B	801	HEM	C3B-CAB-CBB	-3.21	119.94	126.40
2	A	801	HEM	CMA-C3A-C4A	-3.05	123.12	128.31
5	A	806	MPD	CM-C2-C1	-2.88	103.55	110.41
2	A	801	HEM	C3C-CAC-CBC	-2.58	121.21	126.40
5	A	805	MPD	CM-C2-C1	-2.12	105.34	110.41
5	A	805	MPD	O2-C2-C1	2.00	115.38	108.01
2	A	801	HEM	CMC-C2C-C3C	2.26	129.51	125.09
2	A	801	HEM	CMA-C3A-C2A	2.30	130.04	125.24
2	B	801	HEM	CMD-C2D-C3D	2.36	130.17	125.24
2	B	801	HEM	CBD-CAD-C3D	2.39	116.65	112.47
2	B	801	HEM	CAD-CBD-CGD	2.53	117.71	112.78
5	B	805	MPD	CM-C2-C1	2.55	116.50	110.41
2	A	801	HEM	CAD-CBD-CGD	2.65	117.94	112.78
2	A	801	HEM	CBD-CAD-C3D	3.95	119.41	112.47

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	805	MPD	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	806	MPD	2	0
5	B	805	MPD	4	0
4	B	807	OXY	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	713/728 (97%)	-0.33	26 (3%) 46 40	11, 19, 44, 78	0
1	B	713/728 (97%)	-0.43	19 (2%) 58 53	11, 18, 39, 87	0
All	All	1426/1456 (97%)	-0.38	45 (3%) 51 45	11, 19, 41, 87	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	748	ALA	7.6
1	A	748	ALA	7.3
1	A	222	ASP	5.1
1	A	221	GLY	5.1
1	A	220	SER	5.0
1	A	540	ARG	4.7
1	A	215	PRO	4.4
1	B	610	ARG	4.2
1	A	213	GLY	4.0
1	A	541	GLY	3.8
1	A	219	TYR	3.6
1	B	541	GLY	3.6
1	B	608	LYS	3.5
1	A	224	GLN	3.5
1	A	217	SER	3.4
1	A	211	LEU	3.4
1	B	679	ALA	3.3
1	B	222	ASP	3.2
1	A	454	ASP	3.2
1	A	216	ASN	3.2
1	A	610	ARG	3.1
1	B	540	ARG	3.0
1	B	65[A]	ASP	3.0
1	A	212	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	207	ILE	2.8
1	A	64	LYS	2.8
1	A	65	ASP	2.8
1	B	680	ALA	2.8
1	A	608	LYS	2.8
1	A	214	GLY	2.7
1	B	42	TRP	2.6
1	B	40	ARG	2.6
1	B	44	PRO	2.6
1	A	680	ALA	2.5
1	B	64	LYS	2.4
1	A	679	ALA	2.4
1	A	378	SER	2.4
1	B	36	GLY	2.3
1	A	542	GLY	2.2
1	B	224	GLN	2.2
1	A	208	TRP	2.2
1	B	37	THR	2.1
1	B	366	GLY	2.1
1	B	682	ALA	2.1
1	B	221	GLY	2.1

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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
4	OXY	A	804	2/2	0.84	0.20	7.24	33,33,33,44	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
5	MPD	B	805	8/8	0.87	0.17	6.40	53,59,65,66	0
4	OXY	B	804	2/2	0.87	0.19	6.17	39,39,39,50	0
4	OXY	B	807	2/2	0.93	0.15	3.85	30,30,30,38	0
5	MPD	A	805	8/8	0.87	0.15	2.00	52,62,73,74	0
2	HEM	A	801	43/43	0.99	0.13	1.18	12,14,19,19	0
2	HEM	B	801	43/43	0.99	0.10	0.14	11,13,15,18	0
3	NA	A	802	1/1	0.99	0.05	-1.22	17,17,17,17	0
3	NA	B	802	1/1	0.99	0.04	-2.62	15,15,15,15	0
4	OXY	A	803	2/2	0.98	0.14	-	35,35,35,44	0
6	PO4	A	807	5/5	0.97	0.16	-	41,51,56,62	0
6	PO4	B	806	5/5	0.95	0.16	-	42,48,49,61	0
4	OXY	B	803	2/2	0.98	0.11	-	25,25,25,41	0
5	MPD	A	806	8/8	0.91	0.16	-	33,38,50,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.