



# Full wwPDB X-ray Structure Validation Report ⓘ

May 19, 2020 – 01:12 am BST

PDB ID : 5SXR  
Title : Crystal structure of B. pseudomallei KatG with NAD bound  
Authors : Loewen, P.C.  
Deposited on : 2016-08-10  
Resolution : 1.69 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

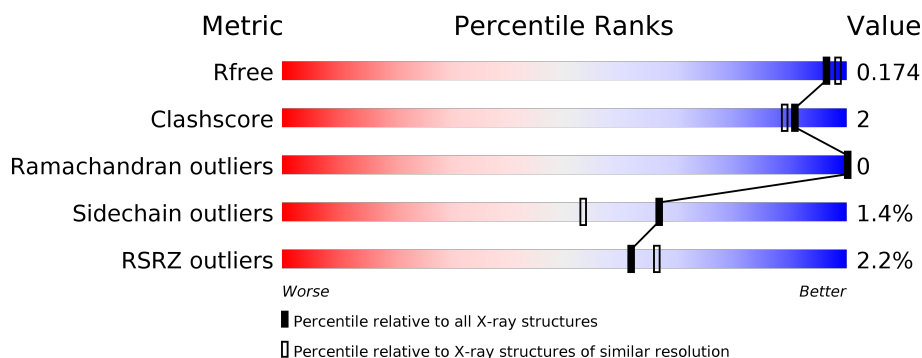
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.69 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))
$R_{free}$	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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>3%</div> <div> <div></div> <div>85%</div> <div>12%</div> <div>••</div> </div> </div>
1	B	728	<div> <div>2%</div> <div> <div></div> <div>87%</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
7	MRD	A	806	-	X	-	-

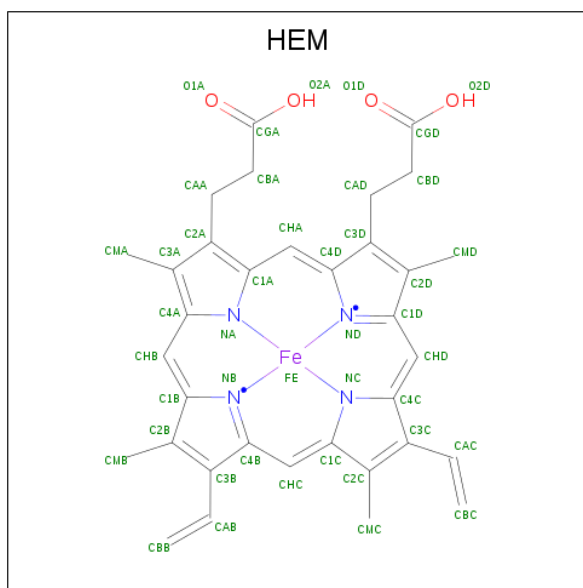


In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Catalase-peroxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	713	Total 5541	C 3497	N 990	O 1040	S 14	0	7	0
1	B	713	Total 5531	C 3493	N 984	O 1040	S 14	0	6	0

- 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 43	C 34	Fe 1	N 4	O 4	0	0
2	B	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

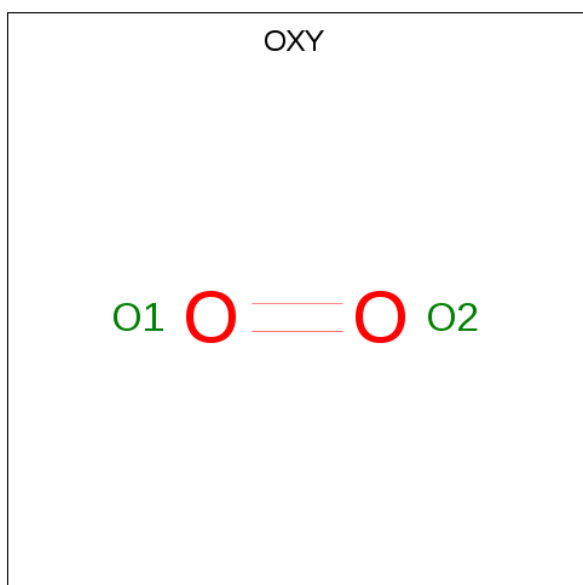
- Molecule 3 is SODIUM ION (three-letter code: NA) (formula: Na).

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: O<sub>2</sub>).



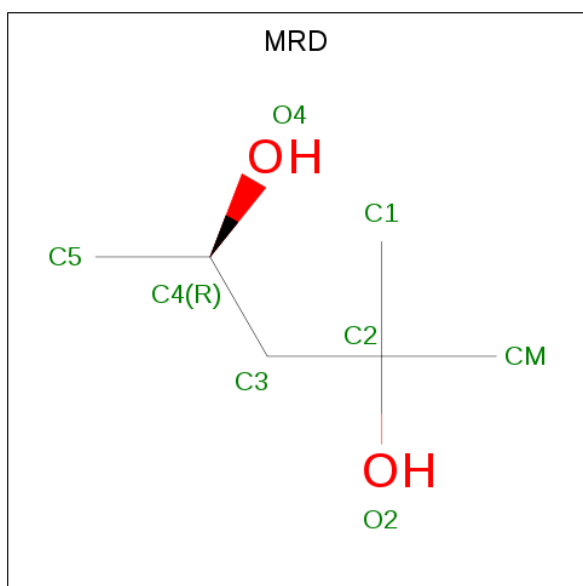
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total O 2 2	0	0
5	B	1	Total O 2 2	0	0

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



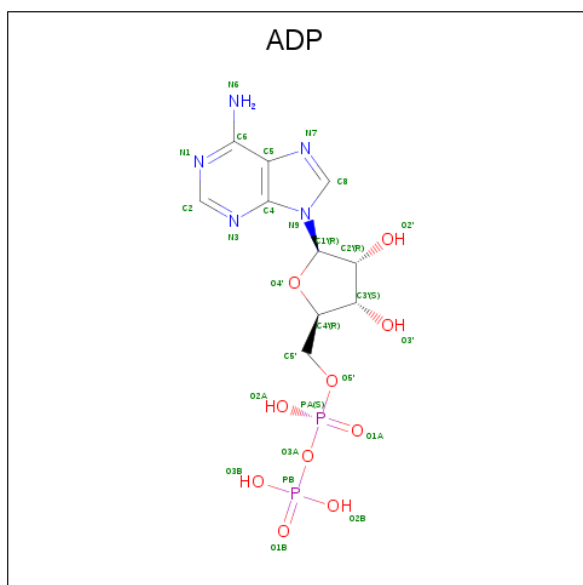
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		
6	B	1	Total	C	O	0	0
			8	6	2		

- Molecule 7 is (4R)-2-METHYLPENTANE-2,4-DIOL (three-letter code: MRD) (formula:  $C_6H_{14}O_2$ ).



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

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

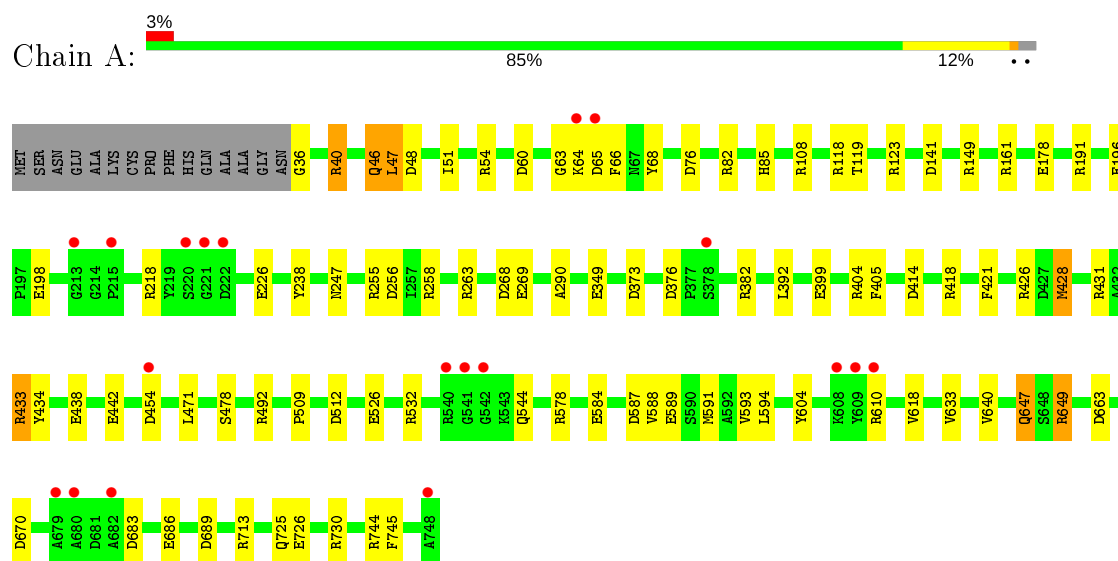
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	758	Total	O	0	0
			758	758		
9	B	818	Total	O	0	0
			818	818		

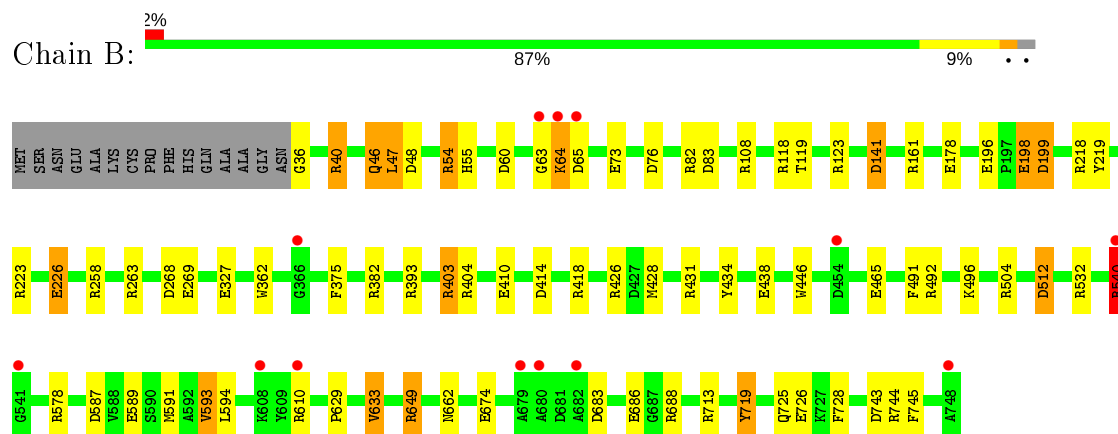
### 3 Residue-property plots [i](#)

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, $\alpha$ , $\beta$ , $\gamma$	100.58Å 114.92Å 174.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.69 37.87 – 1.69	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-1.69) 99.9 (37.87-1.69)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.75 (at 1.69Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, $R_{free}$	0.139 , 0.165 0.153 , 0.174	Depositor DCC
$R_{free}$ test set	11236 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.1	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 47.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	12809	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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, ADP, CL, NA, MPD, MRD, HEM

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	1.48	42/5685 (0.7%)	1.41	75/7724 (1.0%)
1	B	1.49	45/5670 (0.8%)	1.38	64/7706 (0.8%)
All	All	1.49	87/11355 (0.8%)	1.40	139/15430 (0.9%)

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

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

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	GLU	CD-OE2	23.38	1.51	1.25
1	B	73	GLU	CG-CD	11.39	1.69	1.51
1	A	532	ARG	NE-CZ	-10.32	1.19	1.33
1	A	426[A]	ARG	CZ-NH1	-9.82	1.20	1.33
1	A	426[B]	ARG	CZ-NH1	-9.82	1.20	1.33
1	B	198	GLU	CD-OE2	9.66	1.36	1.25
1	A	178	GLU	CD-OE1	-9.39	1.15	1.25
1	B	726	GLU	CB-CG	9.35	1.70	1.52
1	B	726	GLU	CD-OE1	9.31	1.35	1.25
1	A	438	GLU	CD-OE1	-9.07	1.15	1.25
1	A	426[A]	ARG	CZ-NH2	8.57	1.44	1.33
1	A	426[B]	ARG	CZ-NH2	8.57	1.44	1.33
1	B	426[A]	ARG	CZ-NH2	8.16	1.43	1.33
1	B	426[B]	ARG	CZ-NH2	8.16	1.43	1.33
1	B	73	GLU	CB-CG	8.11	1.67	1.52
1	A	196	GLU	CG-CD	8.01	1.64	1.51

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	36	GLY	N-CA	7.98	1.58	1.46
1	A	726	GLU	CG-CD	7.88	1.63	1.51
1	B	63	GLY	N-CA	7.78	1.57	1.46
1	A	255	ARG	CD-NE	7.51	1.59	1.46
1	B	196	GLU	CG-CD	7.50	1.63	1.51
1	B	512	ASP	CG-OD2	7.49	1.42	1.25
1	A	454	ASP	CB-CG	7.30	1.67	1.51
1	A	633	VAL	CB-CG1	-7.29	1.37	1.52
1	B	410	GLU	CG-CD	7.14	1.62	1.51
1	B	726	GLU	CG-CD	7.13	1.62	1.51
1	B	410	GLU	CD-OE1	7.04	1.33	1.25
1	B	226	GLU	CB-CG	-6.97	1.39	1.52
1	A	647	GLN	CG-CD	6.89	1.67	1.51
1	A	604	TYR	CE1-CZ	-6.87	1.29	1.38
1	A	686	GLU	CG-CD	6.86	1.62	1.51
1	A	63	GLY	N-CA	6.72	1.56	1.46
1	A	198	GLU	CD-OE2	6.58	1.32	1.25
1	A	434	TYR	CB-CG	-6.57	1.41	1.51
1	B	269	GLU	CD-OE2	-6.47	1.18	1.25
1	B	540	ARG	C-O	6.44	1.35	1.23
1	A	226	GLU	CG-CD	6.31	1.61	1.51
1	A	255	ARG	CG-CD	6.28	1.67	1.51
1	A	256	ASP	CB-CG	6.17	1.64	1.51
1	B	219	TYR	CE1-CZ	-6.12	1.30	1.38
1	B	438	GLU	CG-CD	6.07	1.61	1.51
1	B	446	TRP	CD2-CE2	6.04	1.48	1.41
1	B	196	GLU	CB-CG	-6.01	1.40	1.52
1	A	269	GLU	CD-OE2	-6.00	1.19	1.25
1	A	584	GLU	CG-CD	5.99	1.60	1.51
1	B	82	ARG	CZ-NH2	-5.97	1.25	1.33
1	B	674	GLU	CG-CD	5.95	1.60	1.51
1	A	178	GLU	CG-CD	5.92	1.60	1.51
1	B	589	GLU	CD-OE2	5.91	1.32	1.25
1	B	438	GLU	CD-OE1	-5.89	1.19	1.25
1	A	255	ARG	NE-CZ	5.88	1.40	1.33
1	B	327	GLU	CD-OE1	5.86	1.32	1.25
1	A	434	TYR	CG-CD1	-5.86	1.31	1.39
1	A	376	ASP	CB-CG	5.77	1.63	1.51
1	A	196	GLU	CB-CG	-5.75	1.41	1.52
1	B	46	GLN	CG-CD	5.73	1.64	1.51
1	B	512	ASP	CB-CG	5.64	1.63	1.51
1	A	725	GLN	CD-NE2	5.63	1.47	1.32

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	434	TYR	CE1-CZ	-5.61	1.31	1.38
1	A	478	SER	CA-CB	5.60	1.61	1.52
1	A	399	GLU	CD-OE2	5.60	1.31	1.25
1	B	532	ARG	NE-CZ	-5.59	1.25	1.33
1	A	418	ARG	CZ-NH1	-5.55	1.25	1.33
1	A	349	GLU	CD-OE2	-5.54	1.19	1.25
1	B	223	ARG	CG-CD	-5.50	1.38	1.51
1	B	431	ARG	CD-NE	5.50	1.55	1.46
1	A	512	ASP	CB-CG	5.49	1.63	1.51
1	B	178	GLU	CD-OE1	-5.40	1.19	1.25
1	A	442	GLU	CD-OE2	-5.37	1.19	1.25
1	A	36	GLY	N-CA	5.32	1.54	1.46
1	A	725	GLN	CG-CD	5.28	1.63	1.51
1	B	327	GLU	CD-OE2	5.24	1.31	1.25
1	B	593	VAL	CB-CG1	-5.23	1.41	1.52
1	B	362	TRP	CG-CD1	5.22	1.44	1.36
1	B	496	LYS	CE-NZ	-5.22	1.36	1.49
1	A	247	ASN	CG-ND2	-5.20	1.19	1.32
1	B	47	LEU	CB-CG	-5.19	1.37	1.52
1	B	465	GLU	CD-OE2	5.17	1.31	1.25
1	A	526	GLU	CD-OE1	-5.17	1.20	1.25
1	B	686	GLU	CG-CD	5.17	1.59	1.51
1	B	418	ARG	CZ-NH1	-5.14	1.26	1.33
1	A	438	GLU	CG-CD	5.12	1.59	1.51
1	B	465	GLU	CD-OE1	5.09	1.31	1.25
1	B	633[A]	VAL	CB-CG2	-5.08	1.42	1.52
1	B	633[B]	VAL	CB-CG2	-5.08	1.42	1.52
1	A	68	TYR	CG-CD2	-5.05	1.32	1.39
1	B	65	ASP	CB-CG	5.04	1.62	1.51

All (139) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	426[A]	ARG	NE-CZ-NH1	-22.07	109.27	120.30
1	A	426[B]	ARG	NE-CZ-NH1	-22.07	109.27	120.30
1	A	426[A]	ARG	NE-CZ-NH2	13.01	126.80	120.30
1	A	426[B]	ARG	NE-CZ-NH2	13.01	126.80	120.30
1	A	263	ARG	NE-CZ-NH2	-12.95	113.83	120.30
1	B	123	ARG	NE-CZ-NH1	12.30	126.45	120.30
1	B	744	ARG	NE-CZ-NH2	-12.27	114.17	120.30
1	A	532	ARG	NE-CZ-NH2	-12.21	114.19	120.30
1	B	512	ASP	CB-CG-OD1	-12.14	107.37	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	434	TYR	CB-CG-CD1	11.66	128.00	121.00
1	A	255	ARG	NE-CZ-NH1	11.06	125.83	120.30
1	B	713	ARG	NE-CZ-NH1	11.03	125.82	120.30
1	A	376	ASP	CB-CG-OD2	-10.79	108.59	118.30
1	B	393	ARG	NE-CZ-NH2	-10.04	115.28	120.30
1	B	73	GLU	CG-CD-OE2	9.69	137.68	118.30
1	B	76	ASP	CB-CG-OD2	-9.58	109.67	118.30
1	A	404	ARG	NE-CZ-NH2	-9.52	115.54	120.30
1	B	108	ARG	NE-CZ-NH1	9.41	125.00	120.30
1	B	434	TYR	CB-CG-CD1	9.36	126.61	121.00
1	B	649	ARG	NE-CZ-NH2	-9.31	115.65	120.30
1	B	82	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	A	649	ARG	NE-CZ-NH2	-9.21	115.69	120.30
1	A	404	ARG	NE-CZ-NH1	8.74	124.67	120.30
1	A	649	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	B	258	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	B	382	ARG	NE-CZ-NH2	-8.46	116.07	120.30
1	B	54	ARG	NE-CZ-NH1	8.22	124.41	120.30
1	A	54	ARG	NE-CZ-NH1	8.20	124.40	120.30
1	A	382	ARG	NE-CZ-NH2	-8.11	116.25	120.30
1	A	730	ARG	NE-CZ-NH1	8.11	124.35	120.30
1	B	532	ARG	NE-CZ-NH2	-8.04	116.28	120.30
1	B	263	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	B	83	ASP	CB-CG-OD2	7.75	125.28	118.30
1	B	54	ARG	NE-CZ-NH2	-7.75	116.43	120.30
1	B	48	ASP	CB-CG-OD1	7.75	125.27	118.30
1	B	578	ARG	NE-CZ-NH1	7.64	124.12	120.30
1	B	633[A]	VAL	CG1-CB-CG2	-7.60	98.73	110.90
1	B	633[B]	VAL	CG1-CB-CG2	-7.60	98.73	110.90
1	B	404	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	B	744	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	B	226	GLU	OE1-CD-OE2	-7.36	114.47	123.30
1	B	382	ARG	CG-CD-NE	-7.34	96.38	111.80
1	A	587	ASP	CB-CG-OD1	7.28	124.85	118.30
1	B	268	ASP	CB-CG-OD1	7.25	124.83	118.30
1	A	76	ASP	CB-CG-OD2	-7.19	111.83	118.30
1	B	674	GLU	OE1-CD-OE2	7.17	131.90	123.30
1	B	73	GLU	CG-CD-OE1	-7.13	104.03	118.30
1	B	108	ARG	NE-CZ-NH2	-7.13	116.74	120.30
1	A	60	ASP	CB-CG-OD2	-7.11	111.90	118.30
1	A	60	ASP	CB-CG-OD1	7.06	124.66	118.30
1	B	726	GLU	CG-CD-OE1	6.92	132.15	118.30

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	663	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	A	405	PHE	CB-CG-CD1	-6.70	116.11	120.80
1	A	670	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	B	745	PHE	CB-CG-CD1	-6.64	116.15	120.80
1	A	149	ARG	NE-CZ-NH1	6.63	123.61	120.30
1	A	433	ARG	NE-CZ-NH2	-6.59	117.00	120.30
1	B	743	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	B	728	PHE	CB-CG-CD1	-6.52	116.24	120.80
1	A	40	ARG	NE-CZ-NH1	6.50	123.55	120.30
1	A	255	ARG	CD-NE-CZ	6.50	132.70	123.60
1	A	454	ASP	CB-CG-OD2	6.48	124.13	118.30
1	B	60	ASP	CB-CG-OD1	6.44	124.10	118.30
1	A	744	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	A	48	ASP	CB-CG-OD1	6.40	124.06	118.30
1	B	683	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	A	414	ASP	CB-CG-OD1	-6.36	112.57	118.30
1	B	382	ARG	NE-CZ-NH1	6.30	123.45	120.30
1	B	60	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	A	713	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	A	713	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	B	40	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	B	141	ASP	CB-CG-OD1	6.18	123.86	118.30
1	A	431	ARG	NE-CZ-NH2	6.16	123.38	120.30
1	B	404	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	382	ARG	CD-NE-CZ	6.11	132.15	123.60
1	A	421	PHE	CB-CG-CD2	-6.09	116.53	120.80
1	B	649	ARG	NE-CZ-NH1	6.04	123.32	120.30
1	A	123	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	A	382	ARG	CD-NE-CZ	5.99	131.98	123.60
1	A	382	ARG	CG-CD-NE	-5.95	99.31	111.80
1	B	578	ARG	NE-CZ-NH2	-5.93	117.33	120.30
1	A	376	ASP	OD1-CG-OD2	5.90	134.52	123.30
1	B	410	GLU	CG-CD-OE1	5.85	130.01	118.30
1	A	578	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	A	268	ASP	CB-CG-OD2	-5.79	113.09	118.30
1	B	587	ASP	CB-CG-OD1	5.72	123.45	118.30
1	B	46	GLN	CA-CB-CG	5.72	125.98	113.40
1	A	46	GLN	CA-CB-CG	5.70	125.93	113.40
1	A	633	VAL	CG1-CB-CG2	-5.68	101.81	110.90
1	A	373	ASP	CB-CG-OD1	5.67	123.40	118.30
1	A	588	VAL	CG1-CB-CG2	5.67	119.97	110.90
1	A	238	TYR	CB-CG-CD2	5.64	124.39	121.00

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	161[A]	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	161[B]	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	745	PHE	CB-CG-CD1	-5.63	116.86	120.80
1	A	492	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	191	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	B	540	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	B	199	ASP	CB-CG-OD1	-5.50	113.35	118.30
1	B	726	GLU	OE1-CD-OE2	-5.50	116.70	123.30
1	A	263	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	B	161	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	108	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	B	428	MET	CA-CB-CG	-5.46	104.01	113.30
1	B	512	ASP	CB-CG-OD2	5.46	123.22	118.30
1	B	123	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	A	392	LEU	CB-CG-CD1	-5.44	101.75	111.00
1	A	730	ARG	NE-CZ-NH2	-5.44	117.58	120.30
1	A	532	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	238	TYR	CB-CG-CD1	-5.41	117.75	121.00
1	A	434	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	A	405	PHE	CB-CG-CD2	5.35	124.54	120.80
1	B	504	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	B	414	ASP	CB-CG-OD1	-5.32	113.52	118.30
1	A	512	ASP	CB-CG-OD2	-5.29	113.53	118.30
1	A	218	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	A	226	GLU	OE1-CD-OE2	-5.28	116.97	123.30
1	A	640	VAL	CA-CB-CG2	5.25	118.78	110.90
1	A	82	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	B	403	ARG	NE-CZ-NH2	-5.24	117.68	120.30
1	A	744	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	A	683	ASP	CB-CG-OD1	5.22	123.00	118.30
1	A	689	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	B	434	TYR	CZ-CE2-CD2	5.19	124.47	119.80
1	B	218	ARG	NE-CZ-NH2	-5.19	117.71	120.30
1	A	178	GLU	OE1-CD-OE2	5.17	129.50	123.30
1	B	492	ARG	NE-CZ-NH2	-5.17	117.72	120.30
1	B	688	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	258	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	A	686	GLU	OE1-CD-OE2	5.15	129.48	123.30
1	B	719	TYR	CB-CG-CD2	-5.13	117.92	121.00
1	A	47	LEU	N-CA-CB	-5.11	100.19	110.40
1	B	375	PHE	CB-CG-CD1	-5.11	117.22	120.80
1	B	491	PHE	CB-CG-CD2	-5.11	117.23	120.80

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	428	MET	CA-CB-CG	-5.09	104.65	113.30
1	A	66	PHE	CG-CD2-CE2	-5.05	115.25	120.80
1	A	584	GLU	OE1-CD-OE2	-5.04	117.25	123.30
1	A	65	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	199	ASP	Mainchain
1	B	226	GLU	Sidechain

## 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	5541	0	5356	15	0
1	B	5531	0	5347	18	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	8	0	14	0	0
6	B	16	0	28	0	0
7	A	8	0	14	4	0
7	B	8	0	14	3	0
8	B	27	0	12	0	0
9	A	758	0	0	7	1
9	B	818	0	0	8	1
All	All	12809	0	10845	38	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 (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:A:119[B]:THR:HG21	9:A:997:HOH:O	1.66	0.94
7:A:806:MRD:O4	7:A:806:MRD:H1C2	1.73	0.88
1:A:589:GLU:HG2	9:A:1375:HOH:O	1.77	0.82
1:B:119[B]:THR:HG22	1:B:593:VAL:HG21	1.64	0.80
1:B:119[B]:THR:HG23	9:B:1166:HOH:O	1.82	0.78
1:B:512:ASP:OD1	9:B:903:HOH:O	2.05	0.74
7:A:806:MRD:C1	7:A:806:MRD:O4	2.34	0.74
1:A:647:GLN:HG2	9:A:1390:HOH:O	1.89	0.71
1:B:47:LEU:O	9:B:904:HOH:O	2.10	0.67
1:B:64:LYS:HA	1:B:64:LYS:HE3	1.76	0.67
1:B:591:MET:SD	1:B:594:LEU:HD12	2.44	0.58
1:B:540:ARG:NE	1:B:540:ARG:HA	2.18	0.58
1:A:544:GLN:OE1	9:A:903:HOH:O	2.18	0.57
1:B:55:HIS:NE2	9:B:909:HOH:O	2.33	0.55
1:B:633[A]:VAL:CG2	1:B:719:TYR:CZ	2.92	0.52
1:A:119[B]:THR:HG23	1:A:593:VAL:HG11	1.92	0.52
1:A:591:MET:SD	1:A:594:LEU:HD12	2.52	0.49
1:A:593:VAL:HG13	9:A:943:HOH:O	2.14	0.48
1:A:290:ALA:CB	7:A:806:MRD:H5C3	2.43	0.48
1:B:633[A]:VAL:HG22	1:B:719:TYR:CZ	2.50	0.47
1:B:633[A]:VAL:HG22	1:B:719:TYR:CE1	2.50	0.47
1:B:662:ASN:H	1:B:725:GLN:HE22	1.62	0.46
1:B:629:PRO:O	1:B:633[A]:VAL:HG23	2.16	0.46
7:B:806:MRD:HMC1	9:B:1480:HOH:O	2.14	0.46
1:B:55:HIS:CD2	9:B:909:HOH:O	2.68	0.46
1:B:55:HIS:CE1	1:B:198:GLU:OE1	2.70	0.45
1:A:51:ILE:HD11	1:A:618:VAL:HG12	2.00	0.44
1:A:471:LEU:HA	1:A:471:LEU:HD23	1.91	0.43
1:A:509:PRO:HD2	1:A:591:MET:HG2	2.01	0.43
1:A:47:LEU:N	9:A:911:HOH:O	2.42	0.43
1:A:428:MET:O	1:A:433:ARG:HD3	2.18	0.43
1:B:540:ARG:CZ	1:B:540:ARG:HA	2.48	0.43
1:B:403:ARG:NH1	9:B:923:HOH:O	2.50	0.42
7:B:806:MRD:H5C2	9:B:1697:HOH:O	2.20	0.42
1:A:85:HIS:HD2	9:A:1496:HOH:O	2.01	0.42
1:A:290:ALA:HB1	7:A:806:MRD:H5C3	2.03	0.41
7:B:806:MRD:H1C2	7:B:806:MRD:H5C3	2.03	0.41
1:B:54:ARG:HB3	1:B:55:HIS:CD2	2.56	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:1045:HOH:O	9:B:1087:HOH:O[2_444]	1.89	0.31

## 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%)	706 (99%)	10 (1%)	0	100	100
1	B	715/728 (98%)	705 (99%)	10 (1%)	0	100	100
All	All	1431/1456 (98%)	1411 (99%)	20 (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	555/560 (99%)	548 (99%)	7 (1%)	69	56
1	B	554/560 (99%)	546 (99%)	8 (1%)	67	53
All	All	1109/1120 (99%)	1094 (99%)	15 (1%)	67	53

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

Mol	Chain	Res	Type
1	A	40	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	46	GLN
1	A	64	LYS
1	A	118	ARG
1	A	141	ASP
1	A	610	ARG
1	A	649	ARG
1	B	40	ARG
1	B	46	GLN
1	B	64	LYS
1	B	118	ARG
1	B	141	ASP
1	B	540	ARG
1	B	610	ARG
1	B	649	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	227	ASN
1	A	247	ASN
1	A	544	GLN
1	B	46	GLN
1	B	55	HIS
1	B	227	ASN
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](#)

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	2.16	4 (40%)	10,23,25	1.59	1 (10%)
1	TOX	B	111[A]	-	10,17,18	2.27	4 (40%)	10,23,25	1.62	3 (30%)
1	TOX	A	111[B]	-	10,17,18	2.16	4 (40%)	10,23,25	1.59	1 (10%)
1	TOX	B	111[B]	-	10,17,18	2.27	4 (40%)	10,23,25	1.62	3 (30%)

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	-	2/4/8/10	0/2/2/2
1	TOX	B	111[A]	-	-	2/4/8/10	0/2/2/2
1	TOX	A	111[B]	-	-	2/4/8/10	0/2/2/2
1	TOX	B	111[B]	-	-	2/4/8/10	0/2/2/2

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	111[A]	TOX	CZ2-CE2	-3.89	1.33	1.41
1	B	111[B]	TOX	CZ2-CE2	-3.89	1.33	1.41
1	B	111[A]	TOX	O-C	3.79	1.35	1.19
1	B	111[B]	TOX	O-C	3.79	1.35	1.19
1	A	111[A]	TOX	O-C	3.75	1.34	1.19
1	A	111[B]	TOX	O-C	3.75	1.34	1.19
1	A	111[A]	TOX	CD1-NE1	-3.19	1.36	1.39
1	A	111[B]	TOX	CD1-NE1	-3.19	1.36	1.39
1	B	111[A]	TOX	CD1-NE1	-3.16	1.36	1.39
1	B	111[B]	TOX	CD1-NE1	-3.16	1.36	1.39
1	A	111[A]	TOX	CB-CA	2.76	1.59	1.53
1	A	111[B]	TOX	CB-CA	2.76	1.59	1.53
1	A	111[A]	TOX	CA-N	-2.25	1.41	1.48
1	A	111[B]	TOX	CA-N	-2.25	1.41	1.48
1	B	111[A]	TOX	CA-N	-2.24	1.41	1.48
1	B	111[B]	TOX	CA-N	-2.24	1.41	1.48

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111[A]	TOX	CZ2-CE2-CD2	-3.59	116.05	120.94
1	A	111[B]	TOX	CZ2-CE2-CD2	-3.59	116.05	120.94
1	B	111[A]	TOX	CE3-CD2-CG	-2.93	129.04	134.42
1	B	111[B]	TOX	CE3-CD2-CG	-2.93	129.04	134.42
1	B	111[A]	TOX	CZ3-CE3-CD2	-2.46	117.49	120.89
1	B	111[B]	TOX	CZ3-CE3-CD2	-2.46	117.49	120.89
1	B	111[A]	TOX	CB-CG-CD2	2.15	129.59	126.25
1	B	111[B]	TOX	CB-CG-CD2	2.15	129.59	126.25

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	111[A]	TOX	N-CA-CB-CG
1	A	111[A]	TOX	C-CA-CB-CG
1	B	111[A]	TOX	N-CA-CB-CG
1	B	111[A]	TOX	C-CA-CB-CG
1	A	111[B]	TOX	N-CA-CB-CG
1	A	111[B]	TOX	C-CA-CB-CG
1	B	111[B]	TOX	N-CA-CB-CG
1	B	111[B]	TOX	C-CA-CB-CG

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
5	OXY	A	804	-	1,1,1	0.61	0	-		
7	MRD	B	806	-	7,7,7	0.85	0	9,10,10	1.09	0
6	MPD	B	807	-	7,7,7	0.80	0	9,10,10	1.86	3 (33%)
7	MRD	A	806	-	7,7,7	0.43	0	9,10,10	2.36	4 (44%)
8	ADP	B	808	-	24,29,29	2.41	8 (33%)	29,45,45	2.79	9 (31%)
5	OXY	B	804	-	1,1,1	1.03	0	-		
2	HEM	B	801	1	27,50,50	1.80	6 (22%)	17,82,82	2.21	6 (35%)
2	HEM	A	801	1	27,50,50	1.05	2 (7%)	17,82,82	2.38	8 (47%)
6	MPD	A	805	-	7,7,7	0.89	0	9,10,10	1.42	2 (22%)
6	MPD	B	805	-	7,7,7	0.82	0	9,10,10	1.51	2 (22%)

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
7	MRD	B	806	-	-	5/5/5/5	-
6	MPD	B	807	-	-	1/5/5/5	-
7	MRD	A	806	-	-	5/5/5/5	-
8	ADP	B	808	-	-	5/12/32/32	0/3/3/3
2	HEM	B	801	1	-	0/6/54/54	-
2	HEM	A	801	1	-	0/6/54/54	-
6	MPD	A	805	-	-	0/5/5/5	-
6	MPD	B	805	-	-	3/5/5/5	-

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	808	ADP	C2-N3	7.50	1.44	1.32
8	B	808	ADP	C2'-C1'	4.99	1.61	1.53
2	B	801	HEM	C1A-NA	4.41	1.45	1.36
2	B	801	HEM	C4A-NA	-3.68	1.28	1.36
2	B	801	HEM	C1D-ND	-3.42	1.29	1.36
8	B	808	ADP	O2'-C2'	3.37	1.50	1.43
8	B	808	ADP	PA-O5'	3.07	1.71	1.59
2	B	801	HEM	C3B-C2B	-2.88	1.36	1.40
2	A	801	HEM	C1D-ND	-2.74	1.30	1.36
8	B	808	ADP	C5-C4	2.74	1.48	1.40
8	B	808	ADP	C6-N6	2.45	1.43	1.34

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C1A-CHA	-2.41	1.34	1.41
8	B	808	ADP	C2-N1	2.37	1.38	1.33
2	A	801	HEM	C4B-CHC	-2.24	1.34	1.41
8	B	808	ADP	C8-N7	2.22	1.38	1.34
2	B	801	HEM	C1C-C2C	2.04	1.47	1.42

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	808	ADP	N6-C6-N1	6.84	132.78	118.57
8	B	808	ADP	C5-C6-N6	-6.83	109.98	120.35
2	A	801	HEM	C1D-C2D-C3D	-6.20	102.68	107.00
8	B	808	ADP	N3-C2-N1	-6.19	119.01	128.68
7	A	806	MRD	CM-C2-C1	-5.12	99.91	110.57
8	B	808	ADP	O4'-C1'-C2'	5.11	114.39	106.93
2	B	801	HEM	CBA-CAA-C2A	4.66	121.09	112.49
2	A	801	HEM	CAA-CBA-CGA	-3.98	106.00	112.67
2	B	801	HEM	C4C-C3C-C2C	3.95	109.66	106.90
6	B	807	MPD	CM-C2-C3	3.52	126.34	109.96
8	B	808	ADP	O2B-PB-O3A	3.42	116.10	104.64
7	A	806	MRD	C1-C2-C3	3.41	125.83	109.96
6	A	805	MPD	CM-C2-C1	-3.36	103.57	110.57
8	B	808	ADP	C2-N1-C6	3.30	124.40	118.75
2	B	801	HEM	CMA-C3A-C4A	-3.28	123.42	128.46
8	B	808	ADP	O3A-PB-O1B	-3.00	94.58	111.19
2	B	801	HEM	C1D-C2D-C3D	-2.99	104.92	107.00
8	B	808	ADP	C3'-C2'-C1'	-2.93	96.56	100.98
6	B	805	MPD	C1-C2-C3	2.74	122.70	109.96
2	A	801	HEM	C4A-C3A-C2A	-2.68	105.13	107.00
2	A	801	HEM	CBA-CAA-C2A	2.63	117.33	112.49
2	B	801	HEM	CMA-C3A-C2A	2.60	129.85	124.94
2	A	801	HEM	C4C-C3C-C2C	-2.37	105.25	106.90
2	A	801	HEM	CMA-C3A-C2A	2.33	129.33	124.94
8	B	808	ADP	O2B-PB-O1B	2.32	119.77	110.68
7	A	806	MRD	O2-C2-C3	-2.30	101.15	109.80
2	A	801	HEM	CBD-CAD-C3D	2.20	116.53	112.48
6	B	805	MPD	O2-C2-C1	-2.17	101.12	108.08
7	A	806	MRD	O2-C2-CM	2.17	115.03	108.08
6	B	807	MPD	O2-C2-C3	-2.15	101.71	109.80
6	B	807	MPD	CM-C2-C1	-2.13	106.13	110.57
6	A	805	MPD	O4-C4-C3	-2.10	102.87	111.36
2	B	801	HEM	C3C-C4C-NC	-2.08	107.02	110.94

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	CMB-C2B-C3B	2.03	128.47	124.68

There are no chirality outliers.

All (19) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	806	MRD	C1-C2-C3-C4
7	B	806	MRD	O2-C2-C3-C4
7	B	806	MRD	C2-C3-C4-O4
7	A	806	MRD	O2-C2-C3-C4
8	B	808	ADP	PA-O3A-PB-O3B
8	B	808	ADP	C5'-O5'-PA-O1A
8	B	808	ADP	O4'-C4'-C5'-O5'
6	B	805	MPD	C1-C2-C3-C4
6	B	805	MPD	O2-C2-C3-C4
8	B	808	ADP	C3'-C4'-C5'-O5'
7	B	806	MRD	C2-C3-C4-C5
7	A	806	MRD	C2-C3-C4-C5
6	B	807	MPD	C2-C3-C4-O4
7	A	806	MRD	C2-C3-C4-O4
7	B	806	MRD	CM-C2-C3-C4
7	A	806	MRD	C1-C2-C3-C4
7	A	806	MRD	CM-C2-C3-C4
6	B	805	MPD	CM-C2-C3-C4
8	B	808	ADP	PA-O3A-PB-O1B

There are no ring outliers.

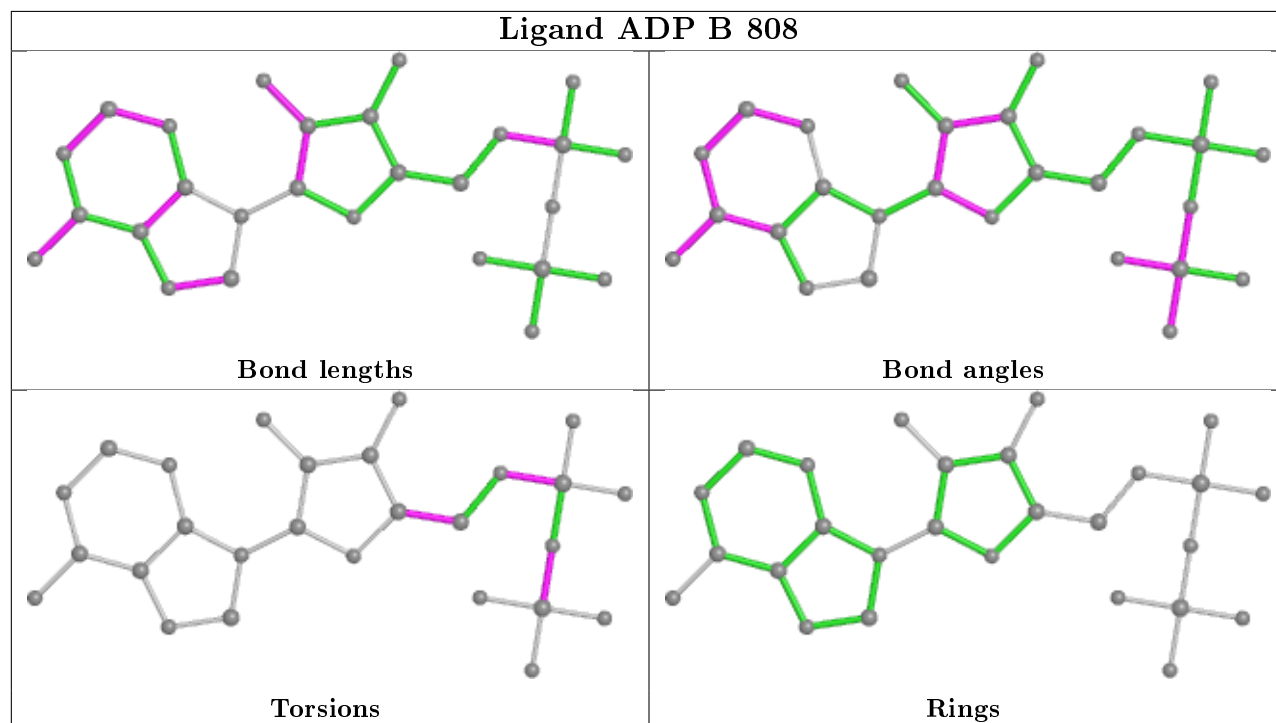
2 monomers are involved in 7 short contacts:

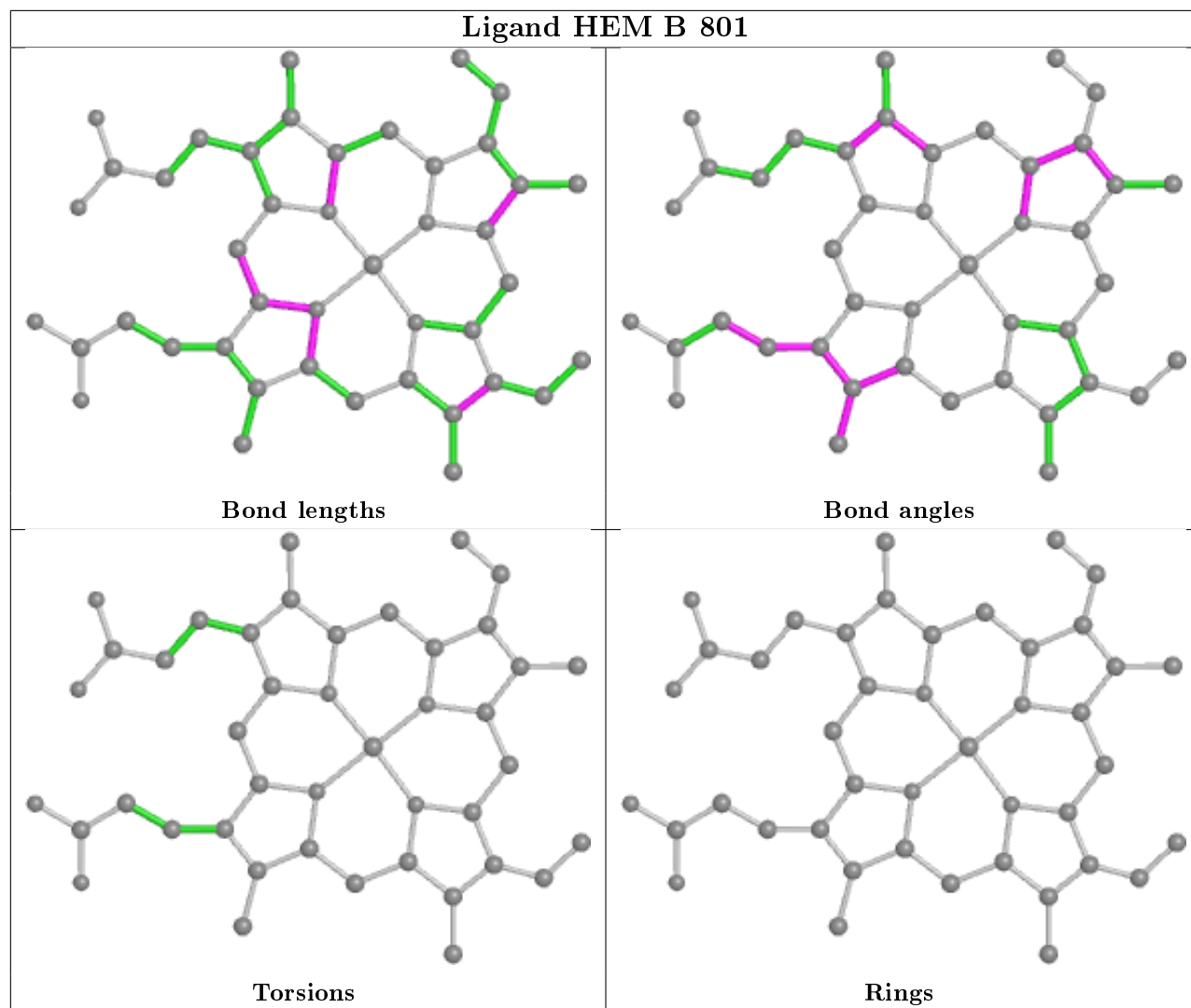
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	B	806	MRD	3	0
7	A	806	MRD	4	0

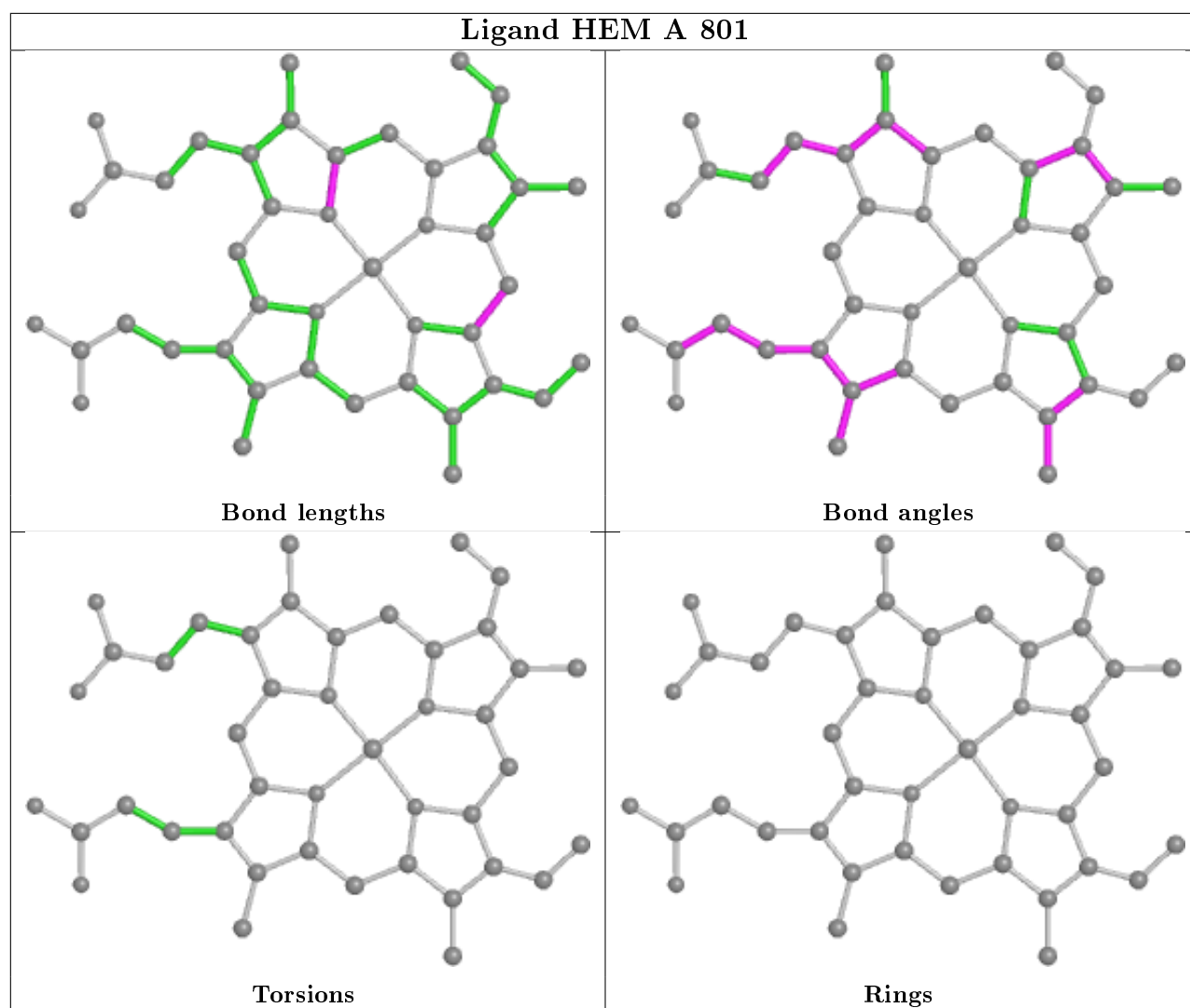
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and



any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







## 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	712/728 (97%)	-0.37	19 (2%) 54 58	14, 21, 38, 79	0
1	B	712/728 (97%)	-0.40	13 (1%) 68 72	14, 19, 37, 77	0
All	All	1424/1456 (97%)	-0.38	32 (2%) 62 66	14, 20, 38, 79	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	6.0
1	B	679	ALA	5.2
1	A	540	ARG	4.9
1	B	748	ALA	4.9
1	A	610	ARG	4.6
1	B	610	ARG	4.3
1	B	680	ALA	4.1
1	B	541	GLY	3.9
1	A	608	LYS	3.9
1	B	540	ARG	3.8
1	A	541	GLY	3.8
1	B	608	LYS	3.5
1	A	680	ALA	3.5
1	A	454	ASP	3.5
1	A	679	ALA	3.4
1	B	65	ASP	3.4
1	A	215	PRO	3.0
1	A	542	GLY	3.0
1	B	454	ASP	2.8
1	A	220	SER	2.6
1	B	64	LYS	2.6
1	A	65	ASP	2.6
1	A	378	SER	2.5
1	B	682	ALA	2.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	609	TYR	2.4
1	B	366	GLY	2.4
1	A	221	GLY	2.2
1	B	63	GLY	2.2
1	A	64	LYS	2.2
1	A	213	GLY	2.2
1	A	682	ALA	2.1
1	A	222	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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors(Å <sup>2</sup> )	Q<0.9
1	TOX	A	111[A]	16/17	0.97	0.16	14,15,18,18	2
1	TOX	A	111[B]	16/17	0.97	0.16	14,15,18,18	2
1	TOX	B	111[A]	16/17	0.98	0.13	13,14,16,20	2
1	TOX	B	111[B]	16/17	0.98	0.13	13,14,16,20	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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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.

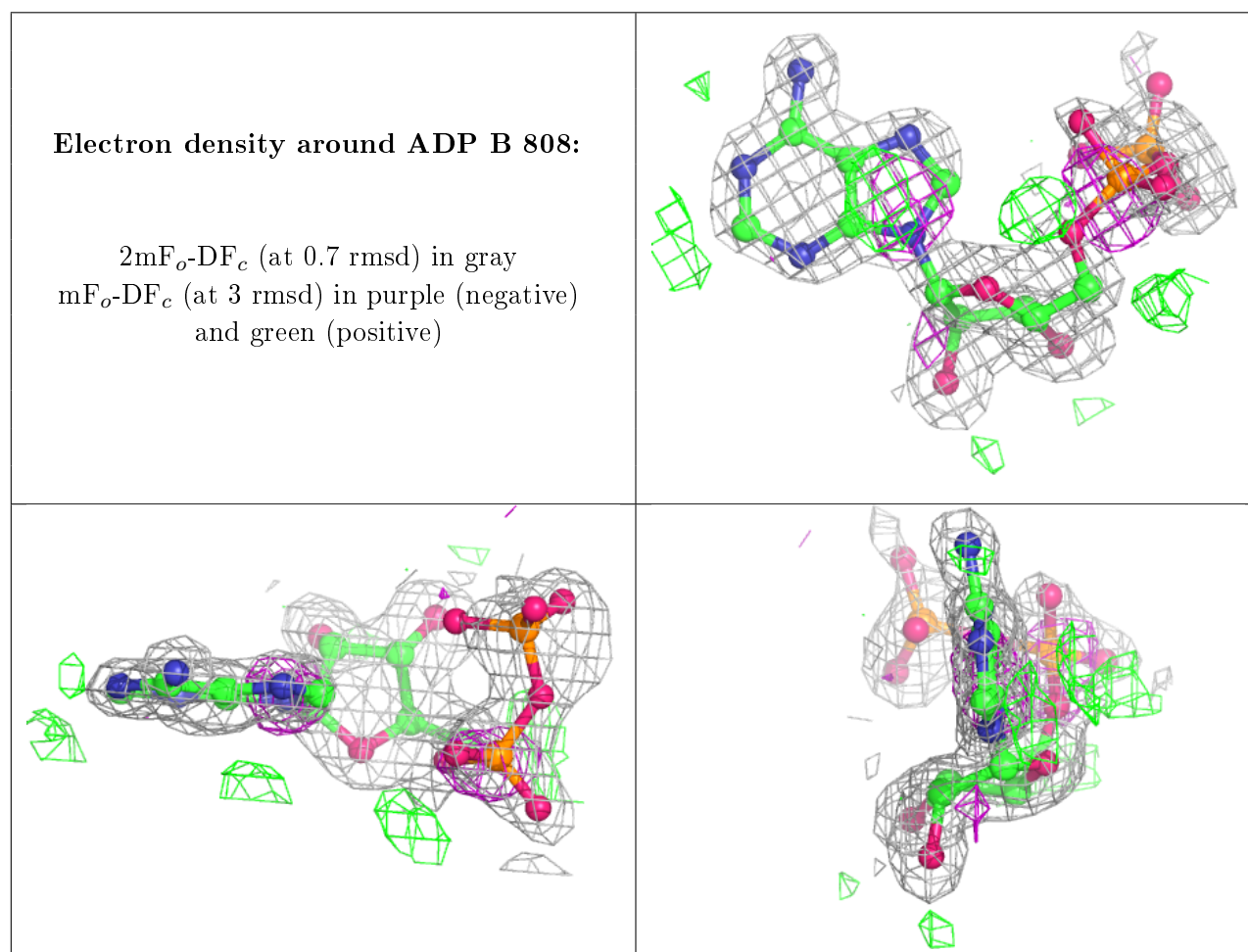
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
6	MPD	B	807	8/8	0.76	0.24	46,52,54,59	0
8	ADP	B	808	27/27	0.84	0.19	26,32,66,69	27
7	MRD	B	806	8/8	0.86	0.17	44,62,74,75	0
7	MRD	A	806	8/8	0.90	0.15	45,53,61,65	0
6	MPD	A	805	8/8	0.91	0.17	38,44,51,52	0
5	OXY	A	804	2/2	0.93	0.12	33,33,33,39	0

*Continued on next page...*

*Continued from previous page...*

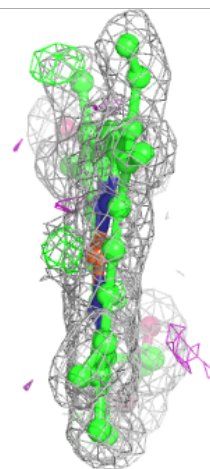
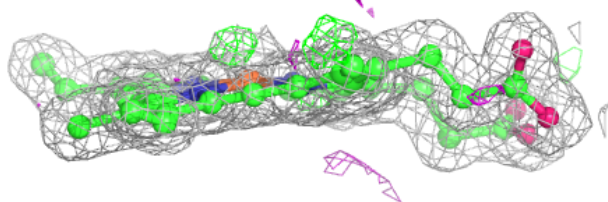
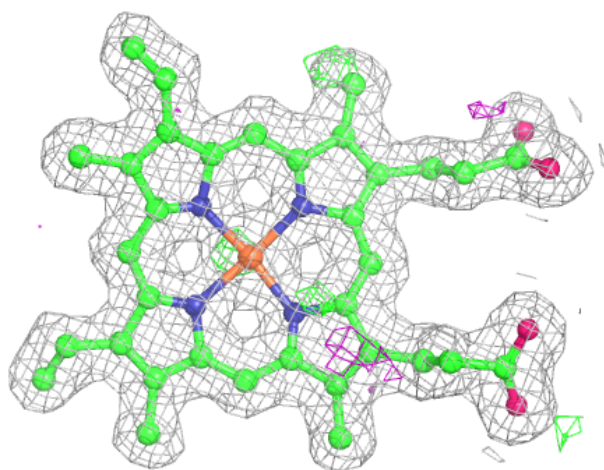
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	MPD	B	805	8/8	0.93	0.14	44,46,56,66	0
5	OXY	B	804	2/2	0.95	0.12	28,28,28,30	0
4	CL	B	803	1/1	0.97	0.06	32,32,32,32	0
2	HEM	B	801	43/43	0.99	0.11	13,14,16,18	0
2	HEM	A	801	43/43	0.99	0.10	14,16,19,20	0
3	NA	B	802	1/1	0.99	0.05	17,17,17,17	0
4	CL	A	803	1/1	0.99	0.03	31,31,31,31	0
3	NA	A	802	1/1	1.00	0.03	16,16,16,16	0

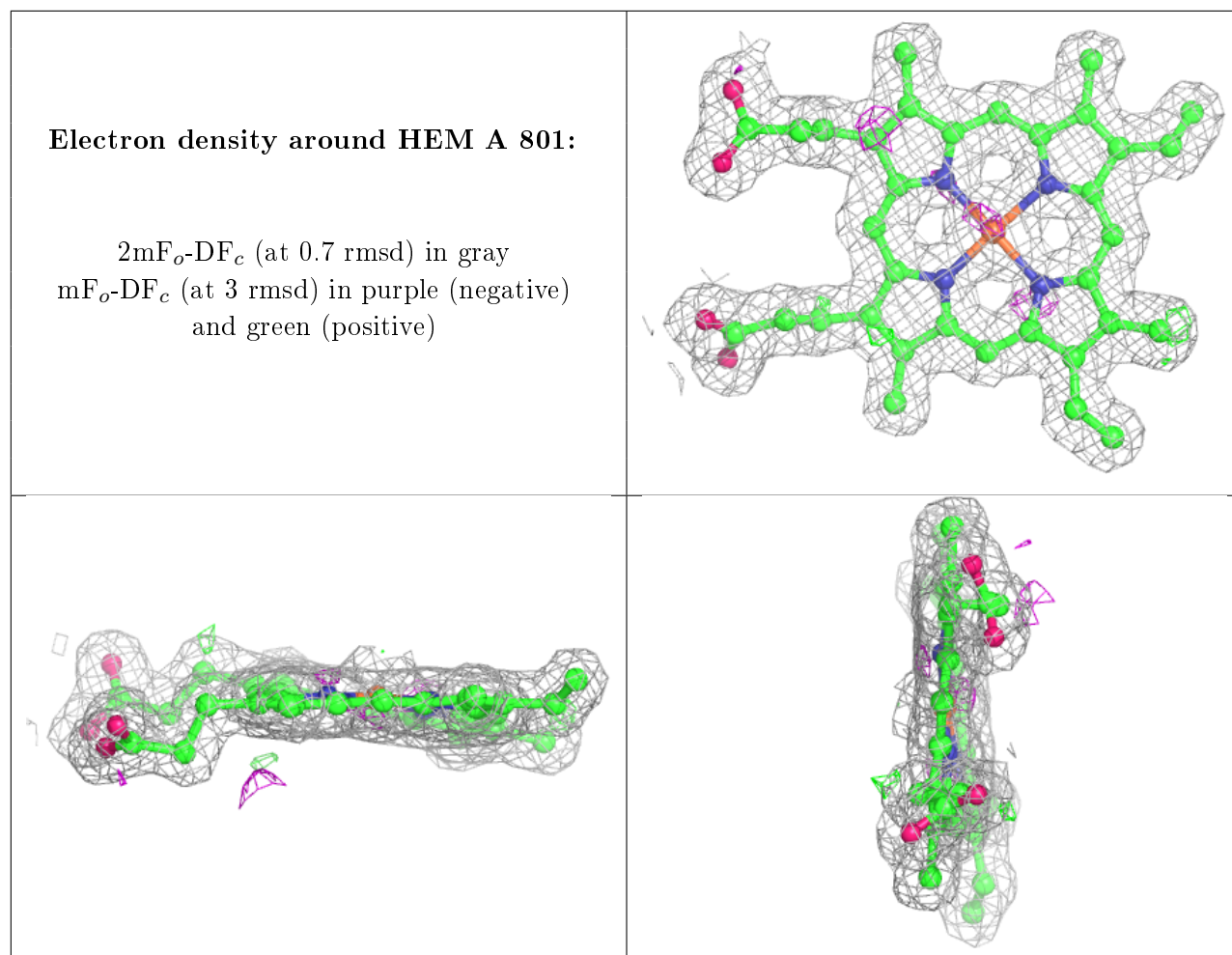
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



**Electron density around HEM B 801:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





## 6.5 Other polymers [i](#)

There are no such residues in this entry.