



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 05:21 AM EDT

PDB ID : 5SXR / pdb_00005sxr
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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.015 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.50

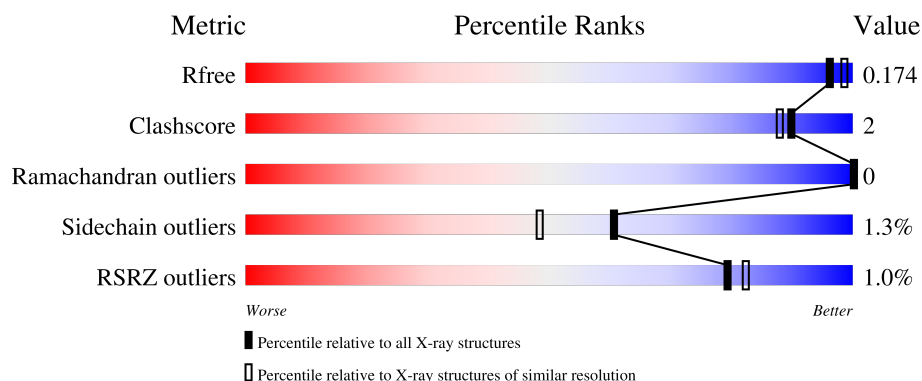
1 Overall quality at a glance

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}	180053	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	
1	B	728	

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	-	-

2 Entry composition [i](#)

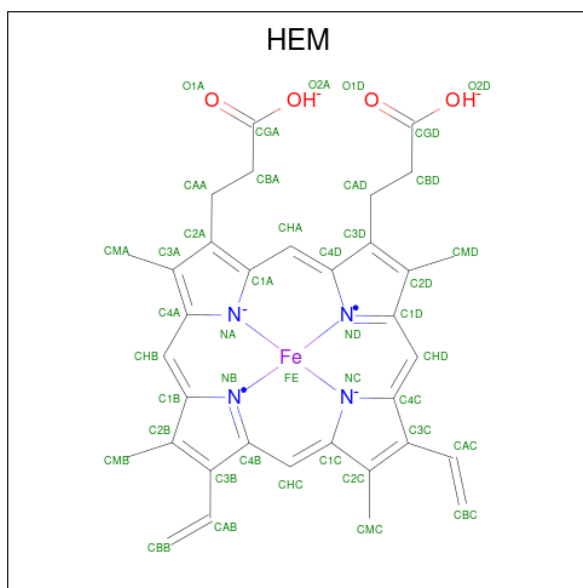
There are 9 unique types of molecules in this entry. The entry contains 12809 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Catalase-peroxidase.

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

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



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

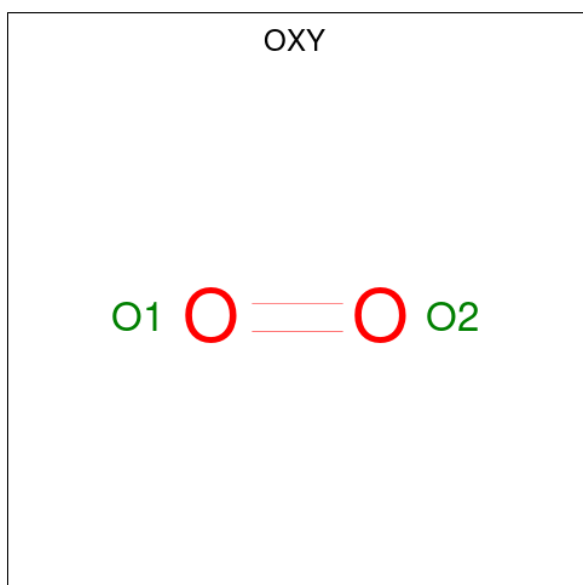
- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

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

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 5 is OXYGEN MOLECULE (CCD ID: OXY) (formula: O₂).



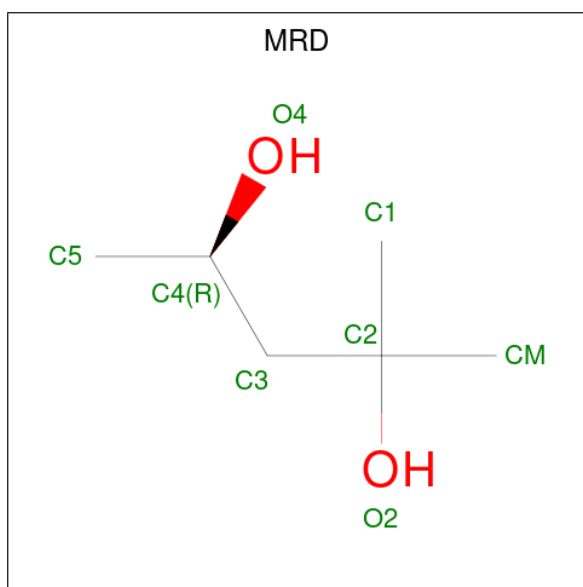
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			2	2		
5	B	1	Total	O	0	0
			2	2		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C₆H₁₄O₂).



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 (CCD ID: MRD) (formula: $C_6H_{14}O_2$).



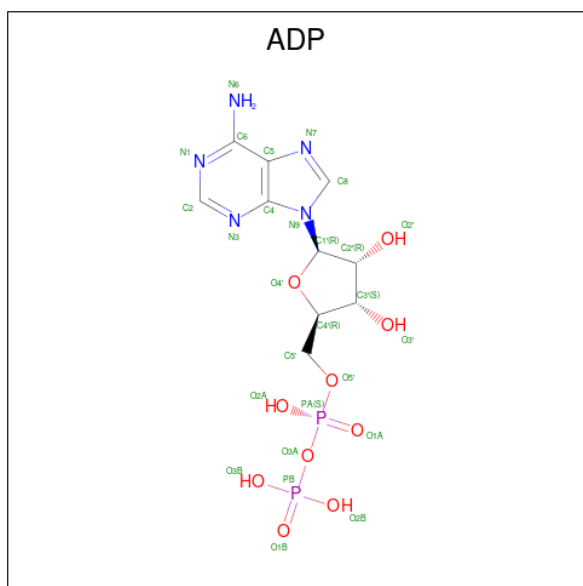
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			8	6	2		

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

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: 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		

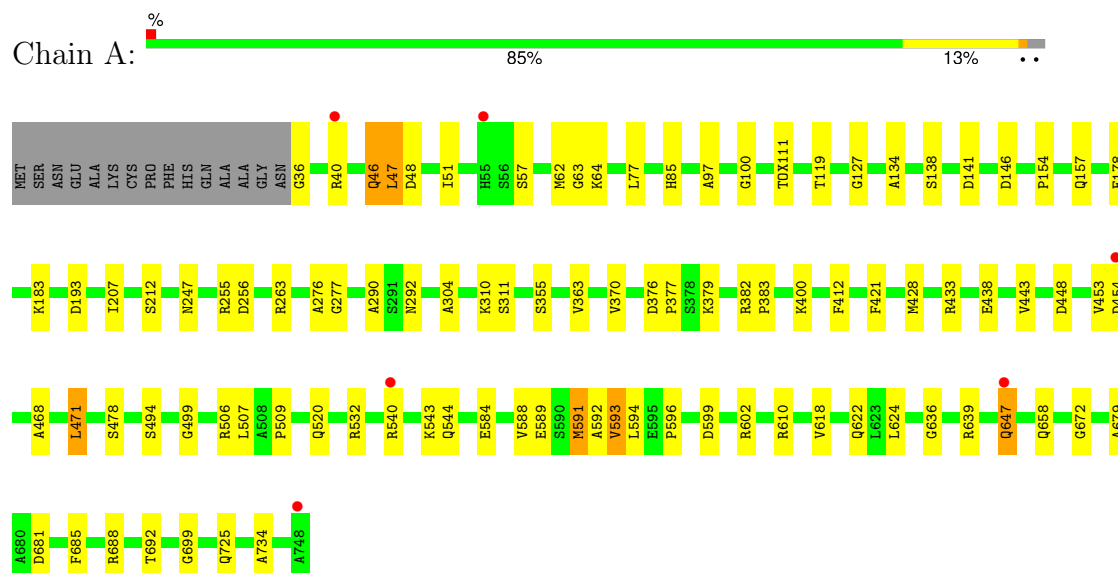
- Molecule 9 is water.

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

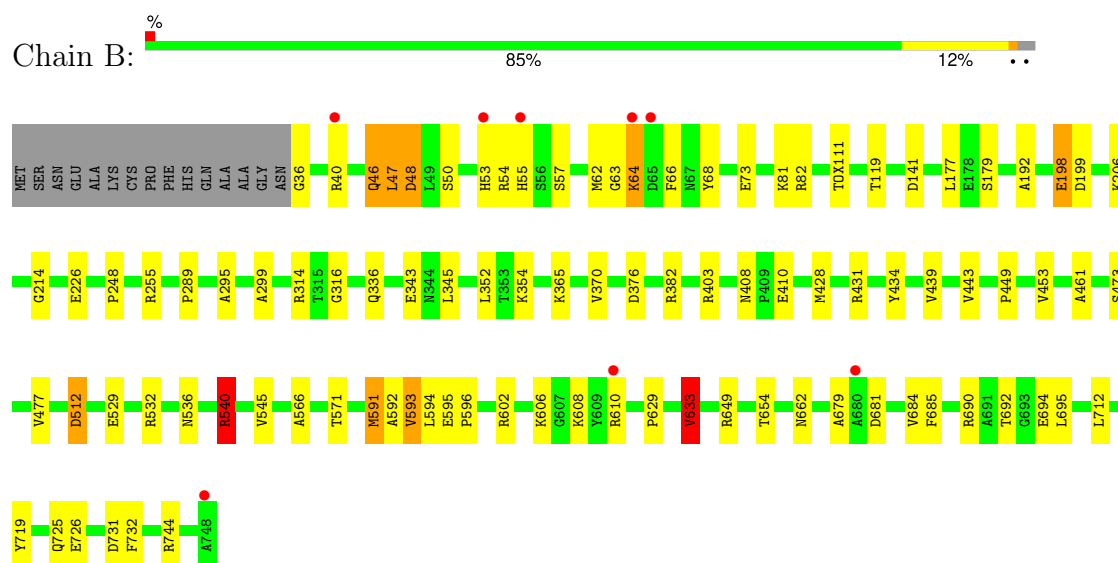
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Catalase-peroxidase



• Molecule 1: Catalase-peroxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	100.58Å 114.92Å 174.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.69 20.00 – 1.69	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-1.69) 99.8 (20.00-1.69)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 ²)	20.1	Xtriage
Anisotropy	0.041	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 44.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	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 ²)	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.*

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, NA, OXY, HEM, ADP, CL, MRD, MPD

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	1.78	76/5685 (1.3%)	1.42	21/7724 (0.3%)
1	B	1.78	70/5670 (1.2%)	1.43	31/7706 (0.4%)
All	All	1.78	146/11355 (1.3%)	1.43	52/15430 (0.3%)

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 (146) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	73	GLU	CD-OE2	13.69	1.51	1.25
1	A	532	ARG	NE-CZ	-12.20	1.19	1.33
1	B	63	GLY	N-CA	9.27	1.57	1.45
1	A	255	ARG	CD-NE	9.27	1.59	1.46
1	B	248	PRO	CA-C	-9.23	1.44	1.52
1	B	540	ARG	C-O	9.16	1.35	1.23
1	B	512	ASP	CG-OD2	9.07	1.42	1.25
1	B	408	ASN	CA-CB	-8.20	1.44	1.53
1	A	688	ARG	CA-C	-8.19	1.43	1.52
1	B	593	VAL	CA-C	-8.07	1.42	1.52
1	B	47	LEU	CB-CG	-7.98	1.37	1.53
1	A	63	GLY	N-CA	7.94	1.56	1.45
1	A	448	ASP	CA-CB	7.80	1.58	1.52
1	B	681	ASP	CA-C	7.80	1.61	1.52
1	B	36	GLY	N-CA	7.79	1.58	1.45
1	B	453	VAL	C-O	-7.42	1.15	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	692	THR	CA-C	-7.40	1.42	1.52
1	B	477	VAL	CA-C	-7.35	1.43	1.52
1	A	47	LEU	CB-CG	-7.30	1.38	1.53
1	A	471	LEU	CA-C	7.05	1.62	1.52
1	A	255	ARG	NE-CZ	6.95	1.40	1.33
1	B	596	PRO	CA-CB	-6.95	1.46	1.54
1	A	540	ARG	C-O	6.83	1.32	1.23
1	B	431	ARG	CD-NE	6.82	1.55	1.46
1	B	370	VAL	N-CA	-6.81	1.39	1.46
1	B	73	GLU	CG-CD	6.80	1.69	1.52
1	A	127	GLY	C-O	6.76	1.31	1.24
1	A	134	ALA	CA-C	-6.72	1.45	1.53
1	B	694	GLU	CA-C	6.71	1.61	1.52
1	A	685	PHE	N-CA	-6.65	1.37	1.46
1	B	532	ARG	NE-CZ	-6.61	1.25	1.33
1	A	591	MET	SD-CE	-6.61	1.63	1.79
1	A	207	ILE	N-CA	-6.59	1.38	1.46
1	B	591	MET	SD-CE	-6.53	1.63	1.79
1	A	725	GLN	CD-NE2	6.51	1.47	1.33
1	A	639	ARG	N-CA	6.50	1.54	1.46
1	B	299	ALA	CA-C	-6.41	1.44	1.52
1	B	654	THR	N-CA	-6.39	1.37	1.45
1	A	247	ASN	CG-ND2	-6.38	1.19	1.33
1	B	695	LEU	C-O	-6.36	1.16	1.24
1	B	82	ARG	CZ-NH2	-6.28	1.25	1.33
1	A	193	ASP	C-O	6.16	1.31	1.23
1	A	363	VAL	C-O	6.11	1.30	1.24
1	B	73	GLU	CA-CB	6.10	1.64	1.53
1	B	592	ALA	CA-C	-6.09	1.44	1.52
1	B	46	GLN	N-CA	6.04	1.53	1.45
1	A	454	ASP	CB-CG	6.01	1.67	1.52
1	B	255	ARG	CD-NE	6.01	1.54	1.46
1	B	376	ASP	N-CA	6.01	1.53	1.46
1	B	179	SER	C-O	6.00	1.31	1.24
1	B	461	ALA	CA-C	5.98	1.60	1.52
1	B	192	ALA	N-CA	5.96	1.53	1.46
1	A	647	GLN	CG-CD	5.94	1.67	1.52
1	B	370	VAL	C-O	-5.94	1.17	1.24
1	A	382	ARG	CA-C	5.93	1.60	1.52
1	B	68	TYR	N-CA	5.92	1.53	1.46
1	A	591	MET	CA-C	5.88	1.60	1.52
1	A	507	LEU	CA-C	-5.87	1.45	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	726	GLU	CB-CG	5.82	1.70	1.52
1	A	468	ALA	N-CA	5.81	1.53	1.46
1	A	443	VAL	CA-C	-5.77	1.45	1.52
1	B	536	ASN	N-CA	-5.76	1.39	1.46
1	B	198	GLU	CD-OE2	5.75	1.36	1.25
1	B	545	VAL	C-O	5.74	1.30	1.24
1	B	690	ARG	CD-NE	-5.74	1.38	1.46
1	A	699	GLY	N-CA	5.71	1.51	1.45
1	A	376	ASP	N-CA	5.64	1.53	1.46
1	B	214	GLY	C-N	5.62	1.40	1.33
1	B	81	LYS	N-CA	5.61	1.53	1.46
1	A	212	SER	CA-C	5.60	1.60	1.53
1	A	679	ALA	N-CA	5.60	1.53	1.46
1	B	289	PRO	N-CA	-5.60	1.40	1.47
1	A	383	PRO	CA-C	-5.59	1.45	1.52
1	A	622	GLN	CA-C	5.59	1.60	1.52
1	A	146	ASP	N-CA	-5.58	1.39	1.46
1	B	352	LEU	CA-C	-5.58	1.45	1.52
1	A	183	LYS	CA-CB	5.57	1.60	1.53
1	B	365	LYS	N-CA	5.55	1.52	1.46
1	B	726	GLU	CD-OE1	5.55	1.35	1.25
1	A	100	GLY	C-O	-5.54	1.16	1.23
1	B	53	HIS	N-CA	5.53	1.52	1.46
1	A	543	LYS	C-O	-5.52	1.17	1.23
1	B	606	LYS	N-CA	5.52	1.53	1.46
1	B	684	VAL	N-CA	-5.50	1.40	1.46
1	B	316	GLY	N-CA	5.49	1.53	1.45
1	A	311	SER	CA-C	5.49	1.59	1.52
1	A	596	PRO	CA-CB	-5.47	1.48	1.54
1	B	382	ARG	CA-C	5.45	1.59	1.53
1	A	658	GLN	CD-NE2	-5.44	1.21	1.33
1	A	310	LYS	C-N	-5.44	1.26	1.33
1	A	355	SER	CA-CB	5.42	1.59	1.53
1	B	434	TYR	CA-C	-5.35	1.45	1.52
1	A	154	PRO	C-O	5.34	1.30	1.24
1	A	370	VAL	CA-C	5.34	1.60	1.52
1	A	584	GLU	C-O	-5.33	1.17	1.24
1	B	343	GLU	CA-C	-5.31	1.46	1.52
1	B	692	THR	N-CA	5.30	1.52	1.45
1	A	36	GLY	N-CA	5.30	1.54	1.45
1	B	731	ASP	N-CA	-5.29	1.39	1.46
1	A	453	VAL	C-O	-5.29	1.17	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	178	GLU	CD-OE1	-5.28	1.15	1.25
1	B	685	PHE	CA-C	-5.27	1.46	1.52
1	A	688	ARG	CZ-NH2	-5.25	1.26	1.33
1	B	566	ALA	C-O	-5.24	1.17	1.24
1	B	679	ALA	N-CA	5.24	1.52	1.46
1	B	608	LYS	N-CA	5.24	1.52	1.46
1	A	692	THR	N-CA	5.23	1.53	1.46
1	A	734	ALA	C-O	5.22	1.30	1.24
1	B	602	ARG	CZ-NH2	-5.20	1.26	1.33
1	A	681	ASP	CA-C	5.20	1.58	1.52
1	A	593	VAL	CA-CB	5.19	1.61	1.54
1	B	443	VAL	CA-C	-5.19	1.46	1.52
1	A	499	GLY	C-O	5.18	1.29	1.23
1	A	400	LYS	N-CA	-5.17	1.40	1.46
1	A	478	SER	CA-CB	5.16	1.61	1.53
1	B	571	THR	CA-CB	5.15	1.61	1.53
1	B	314	ARG	CA-C	-5.15	1.48	1.53
1	A	157	GLN	C-O	5.14	1.30	1.24
1	B	336	GLN	CA-C	-5.13	1.46	1.52
1	A	277	GLY	CA-C	-5.12	1.46	1.52
1	A	672	GLY	C-O	5.12	1.29	1.24
1	A	602	ARG	CZ-NH2	-5.11	1.26	1.33
1	B	712	LEU	C-O	5.10	1.30	1.24
1	B	449	PRO	CA-C	5.10	1.58	1.52
1	A	412	PHE	C-O	5.09	1.29	1.24
1	A	438	GLU	CD-OE1	-5.09	1.15	1.25
1	A	593	VAL	CA-C	-5.09	1.46	1.52
1	A	77	LEU	N-CA	-5.08	1.40	1.46
1	A	255	ARG	CG-CD	5.06	1.67	1.52
1	A	256	ASP	CB-CG	5.06	1.64	1.52
1	B	473	SER	C-O	-5.06	1.17	1.24
1	B	596	PRO	C-O	5.06	1.27	1.24
1	B	596	PRO	C-N	-5.05	1.27	1.33
1	A	421	PHE	N-CA	5.05	1.52	1.46
1	A	599	ASP	CA-C	-5.05	1.47	1.53
1	A	377	PRO	C-O	-5.05	1.17	1.24
1	A	292	ASN	CA-C	5.04	1.59	1.52
1	A	276	ALA	CA-C	-5.04	1.46	1.52
1	A	506	ARG	N-CA	5.04	1.52	1.46
1	A	97	ALA	C-O	5.04	1.29	1.24
1	B	73	GLU	CB-CG	5.03	1.67	1.52
1	A	636	GLY	N-CA	5.02	1.52	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	439	VAL	CA-C	-5.01	1.48	1.53
1	B	177	LEU	N-CA	-5.01	1.40	1.46
1	A	494	SER	CA-CB	-5.01	1.45	1.53
1	A	138	SER	CA-C	-5.00	1.46	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	596	PRO	CB-CA-C	8.64	119.12	111.87
1	B	46	GLN	N-CA-C	-8.57	99.22	110.53
1	B	73	GLU	CG-CD-OE2	8.38	137.68	118.40
1	A	46	GLN	N-CA-C	-7.67	100.41	110.53
1	B	595	GLU	O-C-N	7.42	127.91	121.30
1	B	382	ARG	CG-CD-NE	-7.10	96.38	112.00
1	B	596	PRO	CB-CA-C	6.99	117.74	111.87
1	B	48	ASP	N-CA-C	6.87	119.94	108.20
1	A	47	LEU	N-CA-CB	-6.54	100.19	110.06
1	B	206	LYS	CG-CD-CE	6.39	125.99	111.30
1	A	57	SER	N-CA-C	-6.38	104.76	112.54
1	B	57	SER	N-CA-C	-6.38	104.76	112.54
1	B	62	MET	CA-C-N	-6.34	112.00	121.01
1	B	62	MET	C-N-CA	-6.34	112.00	121.01
1	B	73	GLU	CG-CD-OE1	-6.25	104.03	118.40
1	A	48	ASP	N-CA-C	6.02	118.49	108.20
1	A	624	LEU	N-CA-C	6.01	120.22	113.01
1	B	726	GLU	CG-CD-OE1	5.98	132.15	118.40
1	A	263	ARG	NE-CZ-NH2	-5.97	113.83	119.20
1	B	46	GLN	CA-CB-CG	5.94	125.98	114.10
1	A	255	ARG	CD-NE-CZ	5.93	132.70	124.40
1	A	46	GLN	CA-CB-CG	5.92	125.93	114.10
1	A	592	ALA	N-CA-C	5.77	118.31	111.33
1	A	382	ARG	CG-CD-NE	-5.77	99.31	112.00
1	A	62	MET	CA-C-N	-5.73	113.61	121.06
1	A	62	MET	C-N-CA	-5.73	113.61	121.06
1	B	47	LEU	N-CA-CB	-5.72	101.43	110.06
1	A	520	GLN	CB-CG-CD	5.70	122.29	112.60
1	B	744	ARG	NE-CZ-NH2	-5.59	114.17	119.20
1	A	478	SER	N-CA-C	5.58	117.04	111.07
1	A	532	ARG	NE-CZ-NH2	-5.56	114.19	119.20
1	B	382	ARG	CD-NE-CZ	5.54	132.15	124.40
1	B	633[A]	VAL	CG1-CB-CG2	-5.49	98.73	110.80
1	B	633[B]	VAL	CG1-CB-CG2	-5.49	98.73	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	382	ARG	CD-NE-CZ	5.42	131.98	124.40
1	B	529	GLU	N-CA-C	-5.39	105.56	111.82
1	B	46	GLN	CB-CG-CD	5.38	121.75	112.60
1	B	345	LEU	O-C-N	5.37	127.81	122.12
1	B	410	GLU	CB-CG-CD	5.37	121.72	112.60
1	B	66	PHE	CA-C-N	-5.34	115.27	122.86
1	B	66	PHE	C-N-CA	-5.34	115.27	122.86
1	B	732	PHE	N-CA-C	-5.23	105.49	111.14
1	B	354	LYS	CG-CD-CE	5.17	123.19	111.30
1	A	692	THR	N-CA-C	5.17	119.73	113.38
1	B	295	ALA	O-C-N	5.14	129.19	122.87
1	B	529	GLU	CB-CG-CD	5.11	121.28	112.60
1	A	304	ALA	N-CA-C	-5.10	106.89	113.01
1	A	507	LEU	O-C-N	-5.07	116.96	122.84
1	B	596	PRO	O-C-N	-5.05	119.14	122.73
1	B	410	GLU	CG-CD-OE1	5.05	130.01	118.40
1	B	428	MET	CA-CB-CG	-5.04	104.01	114.10
1	A	588	VAL	N-CA-C	5.00	115.72	110.62

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	16	0
1	B	5531	0	5347	19	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	40	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 (40) 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:O4	7:A:806:MRD:C1	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:HE3	1:B:64:LYS:HA	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:A:591:MET:HE2	1:A:591:MET:HB2	1.78	0.46
1:B:662:ASN:H	1:B:725:GLN:HE22	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:48:ASP:CG	1:B:50[A]:SER:HG	2.24	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:HD23	1:A:471:LEU:HA	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:HA	1:B:540:ARG:CZ	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:H5C3	7:B:806:MRD:H1C2	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 symmetry 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 ⓘ

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%)	549 (99%)	6 (1%)	65	54
1	B	554/560 (99%)	545 (98%)	9 (2%)	55	41
All	All	1109/1120 (99%)	1094 (99%)	15 (1%)	61	46

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

Mol	Chain	Res	Type
1	A	40	ARG
1	A	46	GLN
1	A	64	LYS
1	A	141	ASP
1	A	379	LYS
1	A	610	ARG
1	B	40	ARG
1	B	46	GLN
1	B	64	LYS
1	B	141	ASP
1	B	540	ARG
1	B	610	ARG
1	B	633[A]	VAL
1	B	633[B]	VAL
1	B	649	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	70	GLN
1	A	227	ASN
1	A	520	GLN
1	A	544	GLN

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Mol	Chain	Res	Type
1	A	647	GLN
1	A	737	ASN
1	B	55	HIS
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[B]	-	14,17,18	2.34	5 (35%)	12,23,25	2.66	5 (41%)
1	TOX	B	111[B]	-	14,17,18	2.10	6 (42%)	12,23,25	2.06	3 (25%)
1	TOX	B	111[A]	-	14,17,18	2.10	6 (42%)	12,23,25	2.06	3 (25%)
1	TOX	A	111[A]	2	14,17,18	2.34	5 (35%)	12,23,25	2.66	5 (41%)

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[B]	-	-	2/5/8/10	0/2/2/2
1	TOX	B	111[B]	-	-	2/5/8/10	0/2/2/2
1	TOX	B	111[A]	-	-	2/5/8/10	0/2/2/2
1	TOX	A	111[A]	2	-	2/5/8/10	0/2/2/2

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	111[A]	TOX	O1-NE1	5.15	1.45	1.39
1	A	111[B]	TOX	O1-NE1	5.15	1.45	1.39
1	B	111[A]	TOX	CZ2-CE2	-4.05	1.33	1.39
1	B	111[B]	TOX	CZ2-CE2	-4.05	1.33	1.39
1	B	111[A]	TOX	O-C	3.97	1.35	1.20
1	B	111[B]	TOX	O-C	3.97	1.35	1.20
1	A	111[A]	TOX	O-C	3.93	1.34	1.20
1	A	111[B]	TOX	O-C	3.93	1.34	1.20
1	A	111[A]	TOX	CD2-CE2	3.45	1.45	1.41
1	A	111[B]	TOX	CD2-CE2	3.45	1.45	1.41
1	B	111[A]	TOX	CD1-CG	3.27	1.43	1.36
1	B	111[B]	TOX	CD1-CG	3.27	1.43	1.36
1	A	111[A]	TOX	CB-CA	2.84	1.59	1.53
1	A	111[B]	TOX	CB-CA	2.84	1.59	1.53
1	A	111[A]	TOX	CA-N	-2.40	1.41	1.48
1	A	111[B]	TOX	CA-N	-2.40	1.41	1.48
1	B	111[A]	TOX	CA-N	-2.38	1.41	1.48
1	B	111[B]	TOX	CA-N	-2.38	1.41	1.48
1	B	111[A]	TOX	O1-NE1	2.37	1.42	1.39
1	B	111[B]	TOX	O1-NE1	2.37	1.42	1.39
1	B	111[A]	TOX	CH2-CZ3	2.04	1.42	1.38
1	B	111[B]	TOX	CH2-CZ3	2.04	1.42	1.38

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	111[A]	TOX	CZ2-CE2-CD2	-5.29	116.05	121.95
1	A	111[B]	TOX	CZ2-CE2-CD2	-5.29	116.05	121.95
1	A	111[A]	TOX	CE2-CD2-CG	-4.98	102.81	107.39
1	A	111[B]	TOX	CE2-CD2-CG	-4.98	102.81	107.39
1	B	111[A]	TOX	CD2-CG-CD1	-4.40	102.35	106.34
1	B	111[B]	TOX	CD2-CG-CD1	-4.40	102.35	106.34
1	A	111[A]	TOX	CZ2-CE2-NE1	3.73	135.32	129.37
1	A	111[B]	TOX	CZ2-CE2-NE1	3.73	135.32	129.37
1	B	111[A]	TOX	CE3-CD2-CG	-3.23	129.04	133.85
1	B	111[B]	TOX	CE3-CD2-CG	-3.23	129.04	133.85
1	A	111[A]	TOX	CD2-CG-CD1	2.86	108.94	106.34
1	A	111[B]	TOX	CD2-CG-CD1	2.86	108.94	106.34
1	B	111[A]	TOX	CZ2-CE2-CD2	-2.19	119.51	121.95
1	B	111[B]	TOX	CZ2-CE2-CD2	-2.19	119.51	121.95
1	A	111[A]	TOX	CH2-CZ2-CE2	2.03	122.37	118.28
1	A	111[B]	TOX	CH2-CZ2-CE2	2.03	122.37	118.28

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	A	111[B]	TOX	N-CA-CB-CG
1	A	111[B]	TOX	C-CA-CB-CG
1	B	111[A]	TOX	N-CA-CB-CG
1	B	111[A]	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 oligosaccharides 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	B	801	1	50,50,50	2.39	18 (36%)	67,82,82	1.86	19 (28%)
5	OXY	B	804	-	1,1,1	0.88	0	-		
5	OXY	A	804	-	1,1,1	0.50	0	-		
6	MPD	A	805	-	7,7,7	0.92	0	9,10,10	1.38	2 (22%)
7	MRD	A	806	-	7,7,7	0.45	0	9,10,10	2.32	4 (44%)
8	ADP	B	808	-	28,29,29	3.12	10 (35%)	43,45,45	2.77	19 (44%)
7	MRD	B	806	-	7,7,7	0.90	0	9,10,10	1.08	0
2	HEM	A	801	1	50,50,50	1.69	11 (22%)	67,82,82	1.82	16 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	MPD	B	805	-	7,7,7	0.86	0	9,10,10	1.54	2 (22%)
6	MPD	B	807	-	7,7,7	0.81	0	9,10,10	1.90	3 (33%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	HEM	B	801	1	-	2/14/54/54	-
6	MPD	A	805	-	-	1/5/5/5	-
7	MRD	A	806	-	-	5/5/5/5	-
8	ADP	B	808	-	-	5/16/32/32	0/3/3/3
7	MRD	B	806	-	-	5/5/5/5	-
2	HEM	A	801	1	-	3/14/54/54	-
6	MPD	B	805	-	-	3/5/5/5	-
6	MPD	B	807	-	-	2/5/5/5	-

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	808	ADP	PA-O3A	11.34	1.71	1.59
2	B	801	HEM	C1C-NC	-7.64	1.25	1.39
2	B	801	HEM	C4A-NA	-5.86	1.28	1.39
8	B	808	ADP	C2-N3	5.78	1.44	1.33
2	B	801	HEM	C4C-NC	5.50	1.50	1.39
8	B	808	ADP	C5-C4	5.10	1.48	1.39
2	B	801	HEM	C1D-ND	-4.96	1.29	1.38
2	A	801	HEM	C1D-ND	-4.25	1.30	1.38
8	B	808	ADP	C8-N7	3.63	1.38	1.31
2	B	801	HEM	FE-NB	3.52	2.05	1.94
2	A	801	HEM	FE-NC	3.47	2.06	1.95
8	B	808	ADP	C6-N6	3.43	1.43	1.34
2	A	801	HEM	FE-NB	3.42	2.05	1.94
8	B	808	ADP	O2'-C2'	3.22	1.50	1.43
8	B	808	ADP	PA-O5'	3.15	1.71	1.59
2	A	801	HEM	C4B-NB	-3.08	1.32	1.38
2	B	801	HEM	CHD-C4C	-3.01	1.32	1.38
2	B	801	HEM	C1A-NA	2.99	1.45	1.39
2	A	801	HEM	FE-NA	2.98	2.05	1.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	HEM	C4B-NB	-2.88	1.33	1.38
2	B	801	HEM	C3C-C4C	-2.87	1.41	1.46
2	B	801	HEM	C3B-C4B	2.69	1.50	1.44
2	B	801	HEM	C3D-C2D	2.62	1.42	1.36
2	A	801	HEM	C3C-C2C	2.53	1.42	1.37
8	B	808	ADP	C2'-C1'	2.50	1.61	1.53
2	A	801	HEM	C1D-C2D	2.48	1.49	1.44
2	B	801	HEM	C2A-C3A	-2.47	1.32	1.38
2	B	801	HEM	C4D-ND	2.47	1.44	1.40
8	B	808	ADP	C2-N1	2.47	1.38	1.33
2	A	801	HEM	O2A-CGA	-2.36	1.23	1.30
2	B	801	HEM	CHC-C1C	2.35	1.43	1.38
2	A	801	HEM	C1A-NA	-2.28	1.35	1.39
2	B	801	HEM	CHA-C1A	-2.28	1.34	1.39
2	B	801	HEM	CMB-C2B	2.26	1.55	1.50
2	A	801	HEM	C4D-ND	2.22	1.44	1.40
8	B	808	ADP	C8-N9	2.21	1.41	1.37
2	A	801	HEM	CBD-CGD	2.12	1.55	1.50
2	B	801	HEM	C4D-C3D	-2.11	1.41	1.45
2	B	801	HEM	O1D-CGD	2.02	1.28	1.22

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	808	ADP	N6-C6-N1	6.46	132.78	118.38
8	B	808	ADP	N3-C2-N1	-6.32	119.01	128.58
2	A	801	HEM	C2D-C1D-ND	5.60	116.38	109.90
2	B	801	HEM	C3C-C2C-C1C	-5.53	101.81	107.05
8	B	808	ADP	N3-C4-N9	5.52	136.56	127.17
8	B	808	ADP	C4-N9-C8	5.52	111.53	105.74
8	B	808	ADP	C5-C6-N6	-5.37	109.98	123.29
7	A	806	MRD	CM-C2-C1	-4.78	99.91	110.63
8	B	808	ADP	C5-C4-N3	-4.21	120.93	126.72
2	A	801	HEM	CHD-C1D-C2D	-4.12	118.52	125.03
2	A	801	HEM	C3B-C2B-C1B	4.10	109.49	106.41
2	A	801	HEM	C1D-C2D-C3D	-4.09	102.68	106.98
2	B	801	HEM	CHC-C1C-C2C	-4.07	117.02	125.49
2	A	801	HEM	O1D-CGD-CBD	-4.02	110.36	123.09
2	B	801	HEM	C3B-C2B-C1B	3.95	109.38	106.41
6	B	807	MPD	CM-C2-C3	3.74	126.34	110.20
2	B	801	HEM	C2C-C1C-NC	3.74	116.56	109.64
8	B	808	ADP	O4'-C1'-C2'	3.63	114.39	106.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	806	MRD	C1-C2-C3	3.62	125.83	110.20
8	B	808	ADP	N9-C8-N7	-3.56	108.88	113.94
2	A	801	HEM	C1B-NB-C4B	3.51	109.37	105.21
8	B	808	ADP	C2-N1-C6	3.45	124.40	118.73
8	B	808	ADP	O2B-PB-O3A	3.42	116.10	104.64
8	B	808	ADP	C2-N3-C4	3.40	120.14	111.83
2	A	801	HEM	C4B-C3B-C2B	-3.37	104.19	107.28
2	B	801	HEM	C4C-C3C-C2C	3.28	109.66	106.81
6	A	805	MPD	CM-C2-C1	-3.15	103.57	110.63
8	B	808	ADP	O3A-PB-O1B	-3.13	94.58	111.04
2	A	801	HEM	C2B-C1B-NB	-3.12	106.25	109.84
2	B	801	HEM	C4B-C3B-C2B	-3.11	104.42	107.28
2	A	801	HEM	O2A-CGA-CBA	3.10	123.80	114.00
2	B	801	HEM	CBA-CAA-C2A	3.09	121.09	112.53
8	B	808	ADP	C5-C4-N9	-3.03	102.51	105.81
2	B	801	HEM	CHA-C1A-NA	2.95	129.21	123.86
2	B	801	HEM	O2A-CGA-O1A	2.94	130.88	123.33
6	B	805	MPD	C1-C2-C3	2.90	122.70	110.20
2	A	801	HEM	CAA-CBA-CGA	-2.89	106.00	113.67
2	B	801	HEM	CHB-C4A-NA	-2.88	118.64	123.86
2	B	801	HEM	CMD-C2D-C1D	2.76	129.35	125.03
2	B	801	HEM	C3A-C4A-NA	2.76	114.56	110.14
2	B	801	HEM	CMC-C2C-C1C	2.76	129.58	124.73
2	A	801	HEM	CHC-C4B-NB	2.64	127.27	124.42
8	B	808	ADP	O2A-PA-O3A	-2.62	100.20	107.27
2	B	801	HEM	O1A-CGA-CBA	-2.60	114.83	123.09
8	B	808	ADP	C3'-C2'-C1'	-2.59	96.56	101.46
2	A	801	HEM	O1A-CGA-CBA	-2.54	115.03	123.09
2	A	801	HEM	CMD-C2D-C1D	2.49	128.92	125.03
8	B	808	ADP	C4'-O4'-C1'	-2.41	104.15	109.47
2	A	801	HEM	CMB-C2B-C1B	-2.31	121.42	125.03
8	B	808	ADP	O2B-PB-O1B	2.29	119.77	110.83
7	A	806	MRD	O2-C2-CM	2.26	115.03	107.99
2	A	801	HEM	O2D-CGD-CBD	2.23	121.04	114.00
2	B	801	HEM	CAD-C3D-C4D	2.22	128.56	124.70
2	B	801	HEM	CHA-C4D-ND	-2.21	121.64	124.37
6	B	805	MPD	O2-C2-C1	-2.20	101.12	107.99
2	A	801	HEM	C4D-ND-C1D	-2.20	102.60	105.21
7	A	806	MRD	O2-C2-C3	-2.17	101.15	109.27
2	B	801	HEM	C2D-C1D-ND	2.15	112.39	109.90
6	A	805	MPD	O4-C4-C3	-2.13	102.87	111.35
2	B	801	HEM	CHD-C4C-C3C	2.12	128.78	125.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	808	ADP	C5-N7-C8	2.11	106.77	103.45
2	B	801	HEM	CMB-C2B-C1B	-2.07	121.79	125.03
8	B	808	ADP	O2'-C2'-C1'	2.04	117.14	110.10
6	B	807	MPD	O2-C2-C3	-2.02	101.71	109.27
6	B	807	MPD	CM-C2-C1	-2.01	106.13	110.63

There are no chirality outliers.

All (26) torsion outliers are listed below:

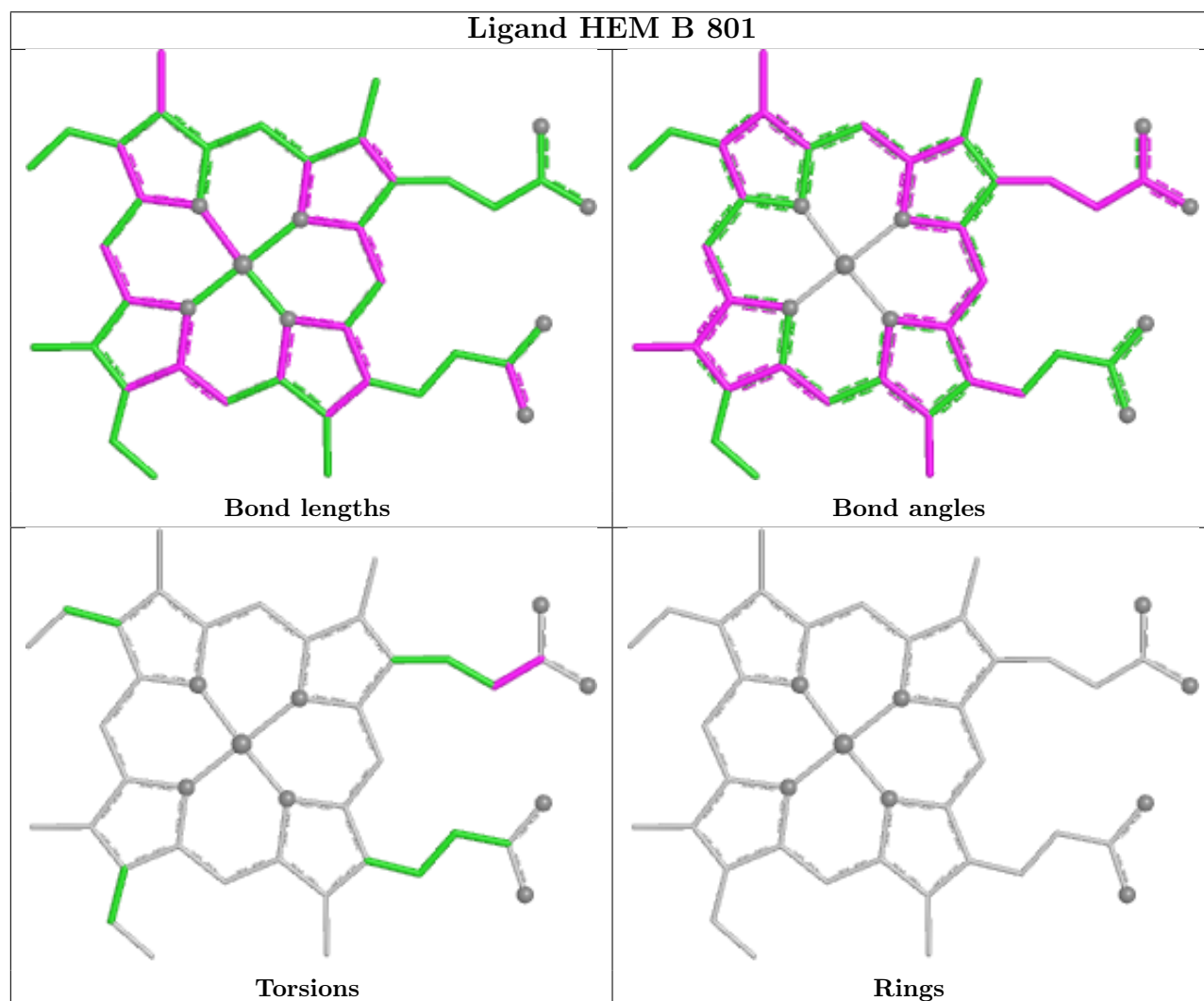
Mol	Chain	Res	Type	Atoms
6	B	805	MPD	C1-C2-C3-C4
7	A	806	MRD	O2-C2-C3-C4
7	B	806	MRD	C1-C2-C3-C4
7	B	806	MRD	C2-C3-C4-O4
7	B	806	MRD	C2-C3-C4-C5
8	B	808	ADP	PA-O3A-PB-O3B
8	B	808	ADP	C5'-O5'-PA-O1A
8	B	808	ADP	O4'-C4'-C5'-O5'
8	B	808	ADP	C3'-C4'-C5'-O5'
6	A	805	MPD	O2-C2-C3-C4
6	B	805	MPD	O2-C2-C3-C4
7	B	806	MRD	O2-C2-C3-C4
6	B	807	MPD	C2-C3-C4-O4
7	A	806	MRD	C2-C3-C4-O4
6	B	805	MPD	CM-C2-C3-C4
7	A	806	MRD	C1-C2-C3-C4
7	A	806	MRD	CM-C2-C3-C4
7	B	806	MRD	CM-C2-C3-C4
7	A	806	MRD	C2-C3-C4-C5
2	A	801	HEM	CAA-CBA-CGA-O2A
2	B	801	HEM	CAA-CBA-CGA-O2A
2	A	801	HEM	CAA-CBA-CGA-O1A
2	B	801	HEM	CAA-CBA-CGA-O1A
8	B	808	ADP	PA-O3A-PB-O1B
6	B	807	MPD	C1-C2-C3-C4
2	A	801	HEM	CAD-CBD-CGD-O2D

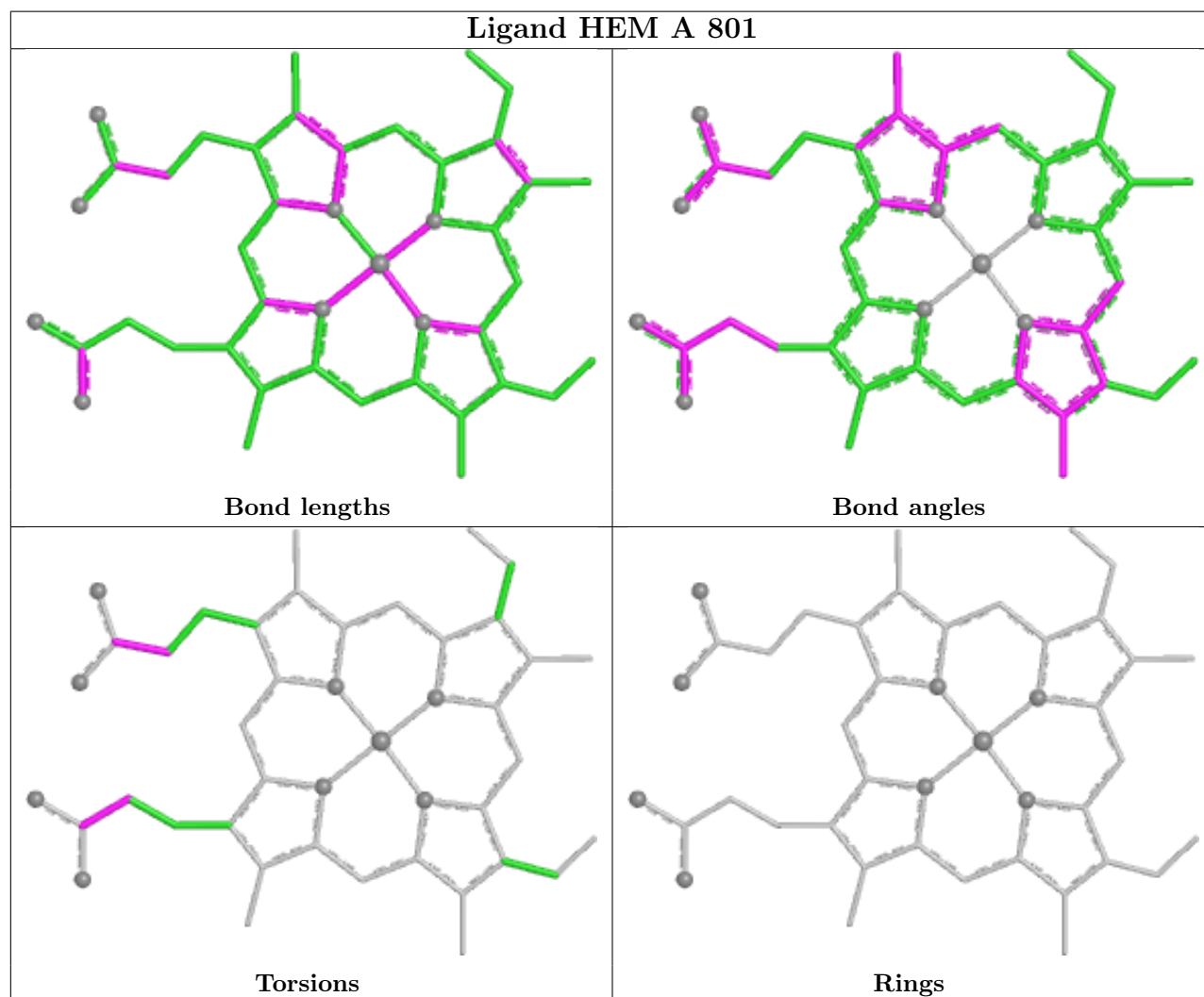
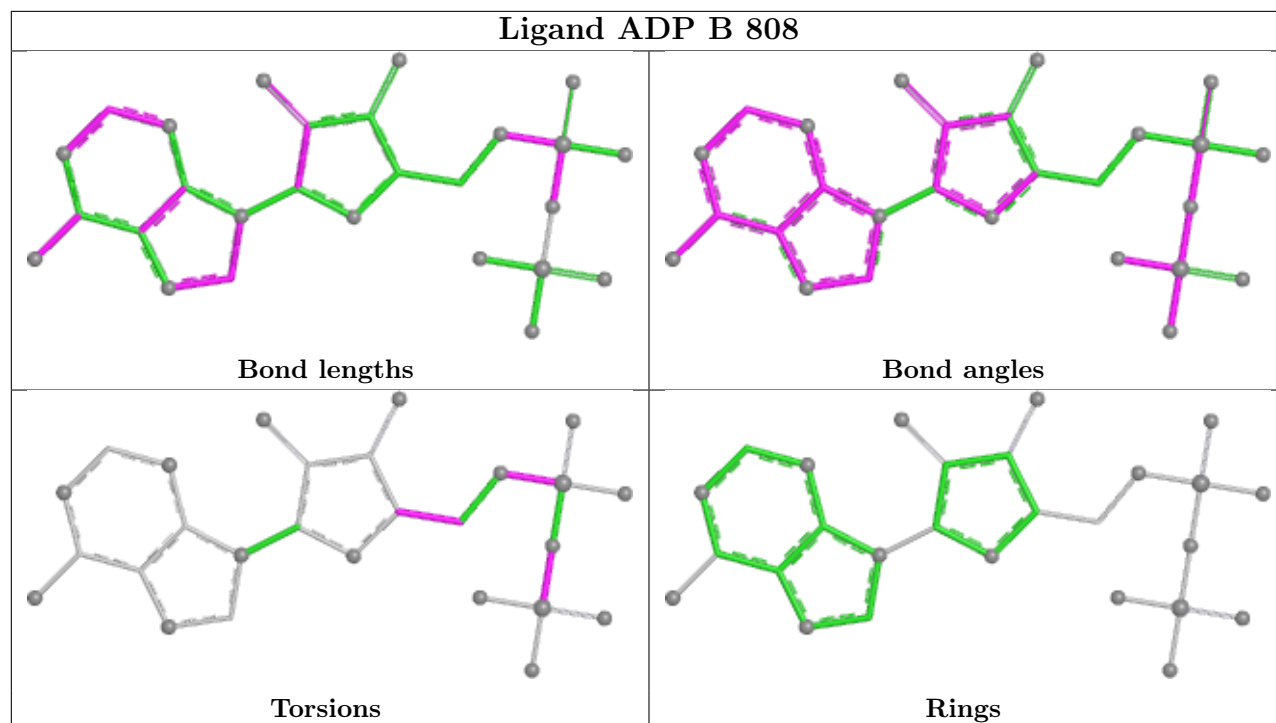
There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	806	MRD	4	0
7	B	806	MRD	3	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.42	6 (0%) 82 85	9, 21, 38, 79	6 (0%)
1	B	712/728 (97%)	-0.49	8 (1%) 78 81	10, 19, 37, 77	5 (0%)
All	All	1424/1456 (97%)	-0.46	14 (0%) 79 82	9, 20, 38, 79	11 (0%)

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	748	ALA	4.3
1	B	55	HIS	3.8
1	B	748	ALA	3.7
1	A	647	GLN	3.0
1	B	680	ALA	3.0
1	A	55	HIS	2.9
1	B	65	ASP	2.6
1	A	454	ASP	2.5
1	B	610	ARG	2.4
1	B	40	ARG	2.3
1	A	40	ARG	2.3
1	B	64	LYS	2.2
1	A	540	ARG	2.0
1	B	53	HIS	2.0

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, 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	B-factors($\text{\AA}^2$)	Q<0.9
1	TOX	A	111[A]	16/17	0.98	0.04	14,15,18,18	2
1	TOX	A	111[B]	16/17	0.98	0.04	14,15,18,18	2
1	TOX	B	111[A]	16/17	0.98	0.04	13,14,16,20	2
1	TOX	B	111[B]	16/17	0.98	0.04	13,14,16,20	2

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

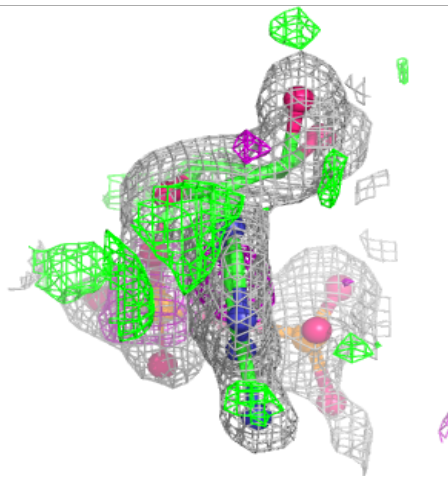
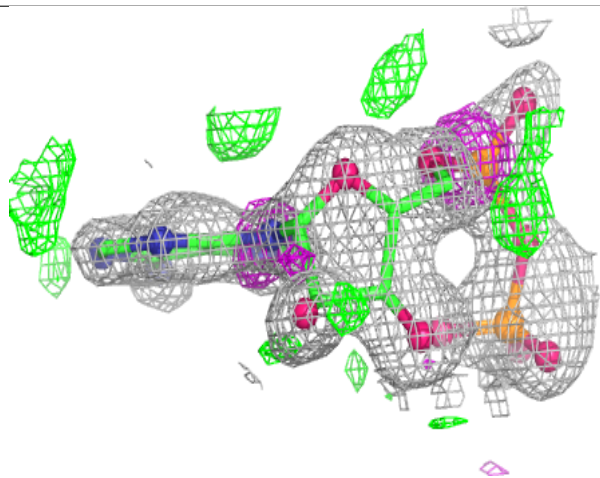
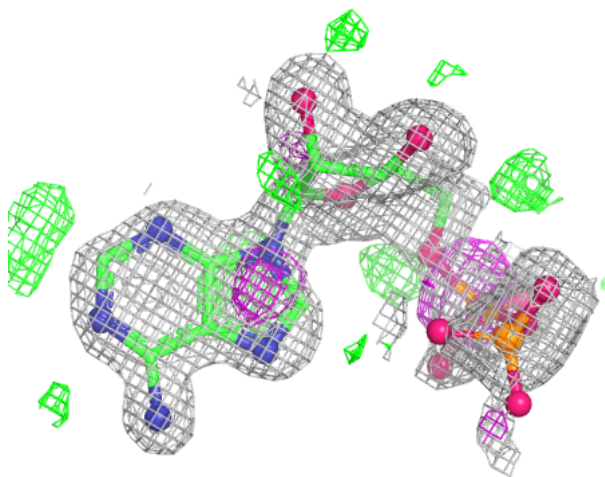
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MRD	B	806	8/8	0.77	0.21	44,62,74,75	0
6	MPD	B	807	8/8	0.80	0.16	46,52,54,59	0
8	ADP	B	808	27/27	0.87	0.12	26,32,66,69	27
7	MRD	A	806	8/8	0.88	0.14	45,53,61,65	0
6	MPD	A	805	8/8	0.90	0.10	38,44,51,52	0
6	MPD	B	805	8/8	0.91	0.13	44,46,56,66	0
5	OXY	A	804	2/2	0.92	0.18	33,33,33,39	0
5	OXY	B	804	2/2	0.92	0.19	28,28,28,30	0
4	CL	A	803	1/1	0.97	0.10	31,31,31,31	0
4	CL	B	803	1/1	0.97	0.07	32,32,32,32	0
2	HEM	B	801	43/43	0.99	0.04	13,14,16,18	0
3	NA	B	802	1/1	0.99	0.04	17,17,17,17	0
2	HEM	A	801	43/43	0.99	0.04	14,16,19,20	0
3	NA	A	802	1/1	1.00	0.05	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.

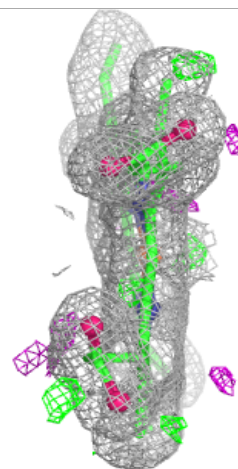
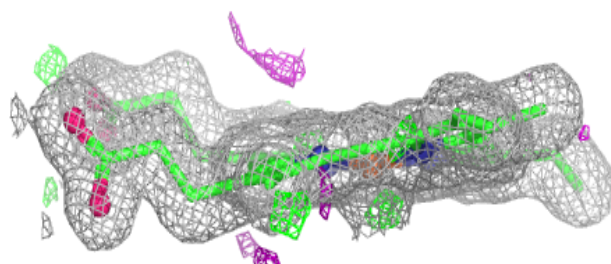
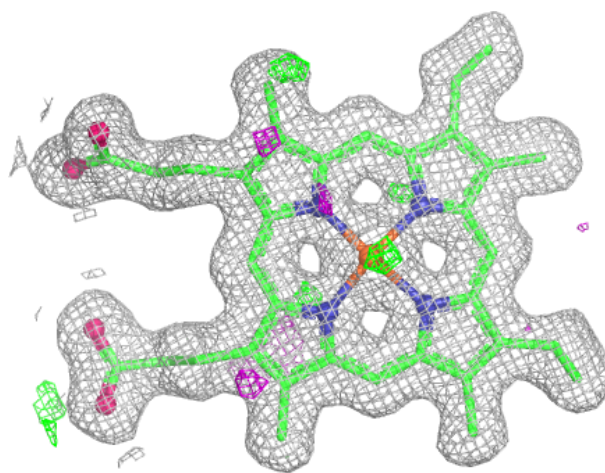
Electron density around ADP B 808:

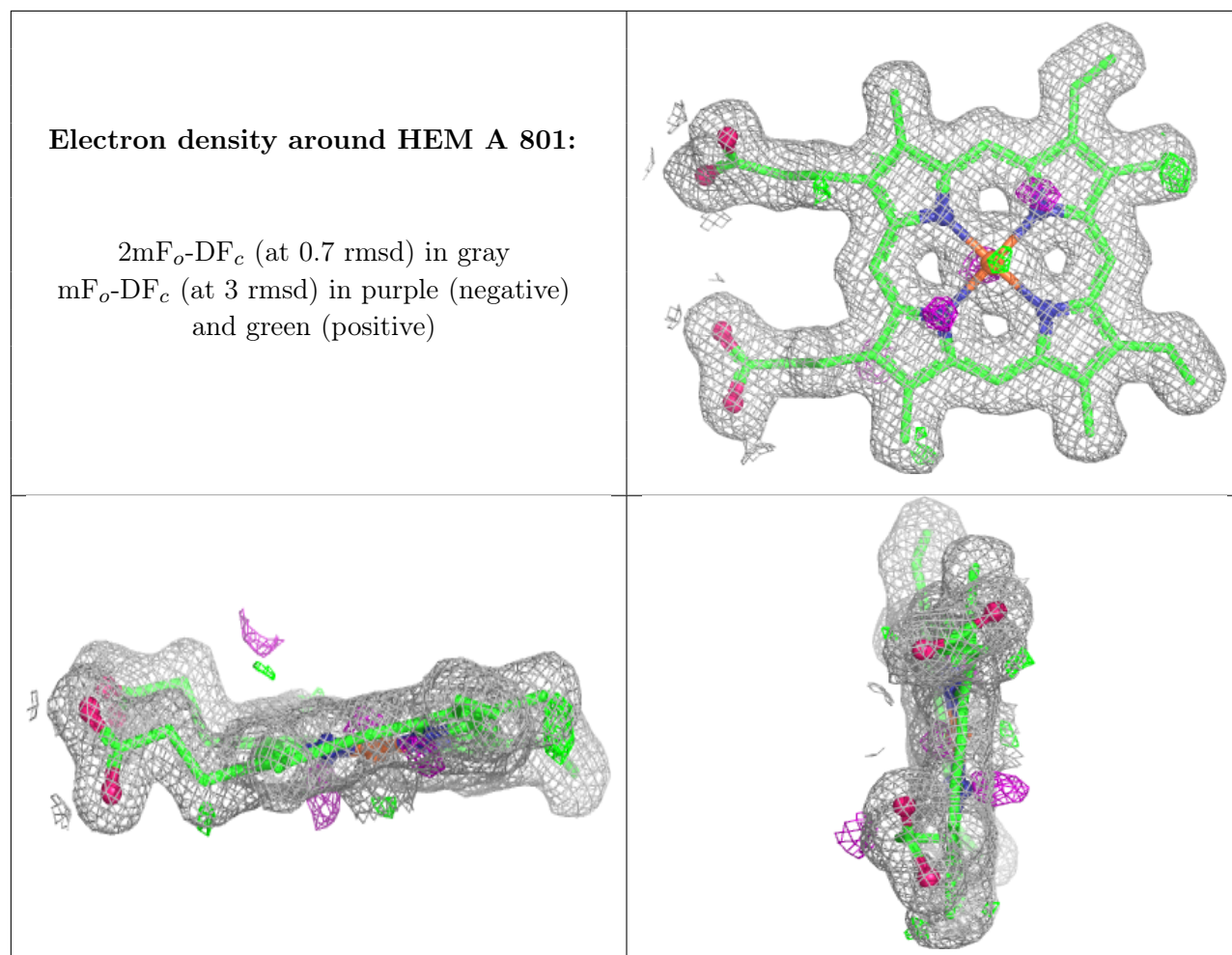
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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.