



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 08:09 AM UTC

PDB ID : 5JHX / pdb_00005jhx
Title : Crystal Structure of Fungal MagKatG2 at pH 3.0
Authors : Gasselhuber, B.; Obinger, C.; Carpena, X.
Deposited on : 2016-04-21
Resolution : 1.40 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 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

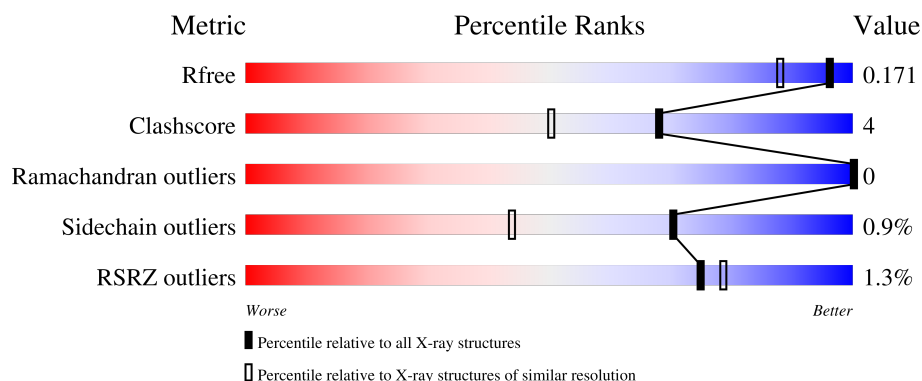
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.40 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	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (1.40-1.40)

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	764	
1	B	764	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	FLC	A	802[B]	-	X	-	-
3	FLC	B	1501[A]	-	-	X	-

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 13405 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.

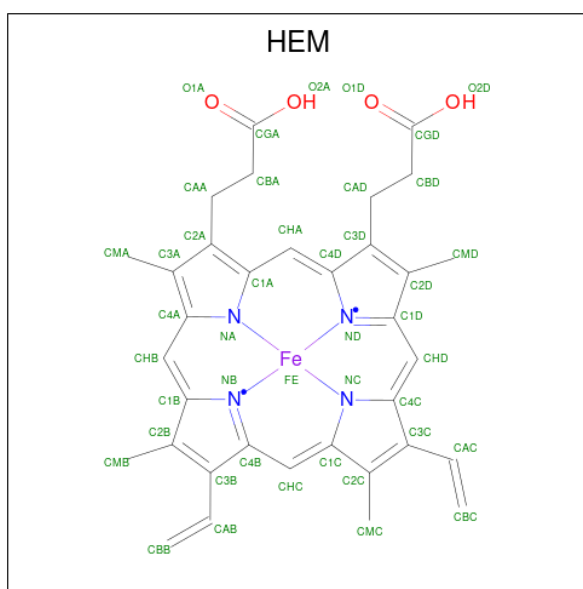
- Molecule 1 is a protein called Catalase-peroxidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	735	Total	C	N	O	S	0	15	0
			5726	3599	1003	1101	23			
1	B	734	Total	C	N	O	S	0	21	0
			5753	3623	1007	1101	22			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	23	MET	-	initiating methionine	UNP A4QUT2
B	23	MET	-	initiating methionine	UNP A4QUT2

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



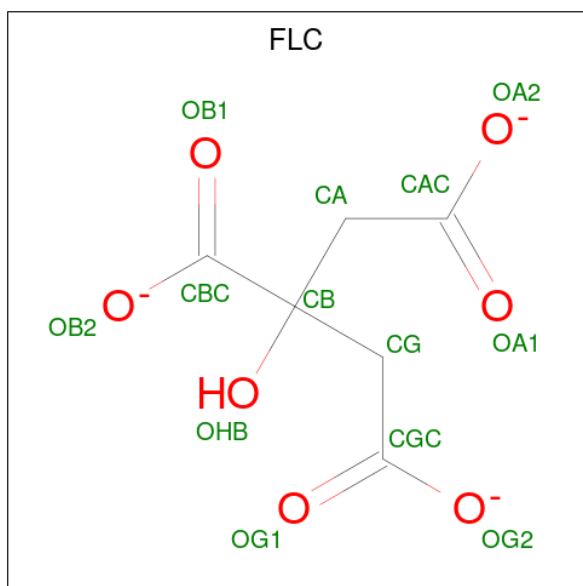
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

Continued on next page...

Continued from previous page...

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

- Molecule 3 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7^-$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	1
			26	12	14		
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	1
			26	12	14		
3	B	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		

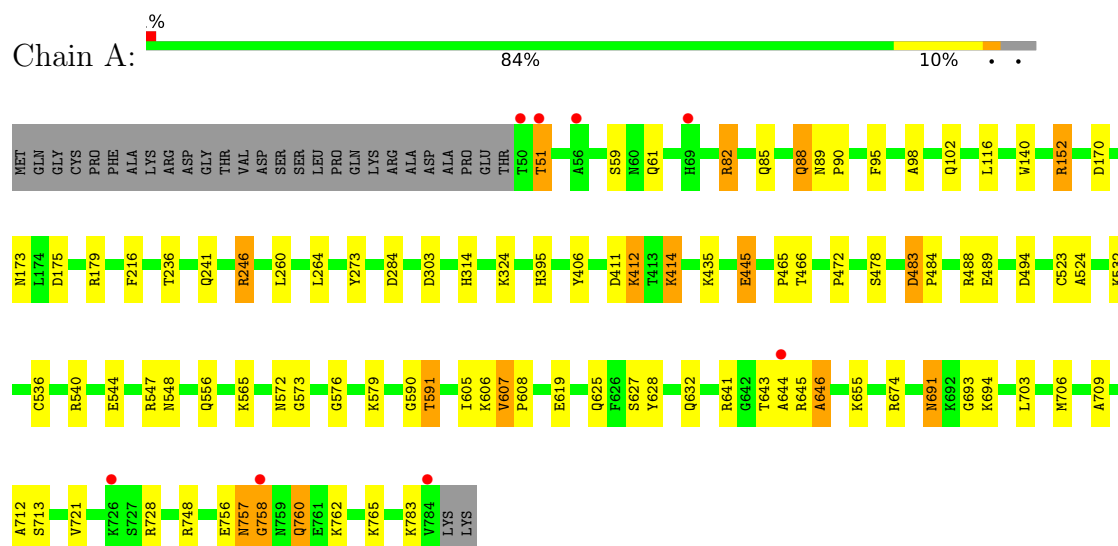
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	846	Total	O	0	0
			846	846		
4	B	903	Total	O	0	0
			903	903		

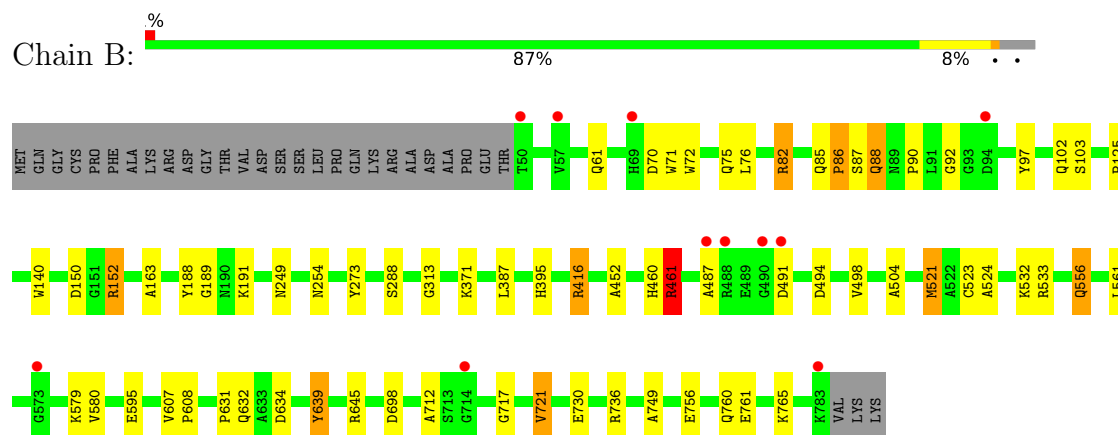
3 Residue-property plots [i](#)

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 2



• Molecule 1: Catalase-peroxidase 2



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	103.22Å 109.86Å 132.12Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 1.40 20.00 – 1.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (20.00-1.40) 99.8 (20.00-1.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.15 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.138 , 0.161 0.150 , 0.171	Depositor DCC
R_{free} test set	14720 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	13.4	Xtriage
Anisotropy	0.369	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 37.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	13405	wwPDB-VP
Average B, all atoms (Å ²)	17.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.08% 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: HEM, FLC

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	1.68	47/5905 (0.8%)	1.50	41/8014 (0.5%)
1	B	1.68	52/5953 (0.9%)	1.42	20/8076 (0.2%)
All	All	1.68	99/11858 (0.8%)	1.46	61/16090 (0.4%)

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	A	0	2
1	B	0	2
All	All	0	4

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	521	MET	SD-CE	-22.91	1.22	1.79
1	A	758	GLY	N-CA	16.34	1.68	1.45
1	B	607	VAL	N-CA	-13.97	1.35	1.46
1	A	644	ALA	C-O	10.12	1.35	1.24
1	A	241	GLN	CA-C	-10.03	1.48	1.53
1	A	152	ARG	NE-CZ	-9.05	1.23	1.33
1	B	461[A]	ARG	C-O	8.91	1.34	1.24
1	B	461[B]	ARG	C-O	8.91	1.34	1.24
1	A	757	ASN	C-O	-8.34	1.14	1.23
1	B	524	ALA	C-O	8.34	1.34	1.24
1	B	72	TRP	C-N	8.00	1.43	1.34
1	A	483	ASP	N-CA	7.74	1.51	1.46
1	A	758	GLY	CA-C	7.50	1.62	1.52
1	A	607	VAL	N-CA	-7.40	1.37	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	606	LYS	C-O	7.17	1.32	1.24
1	A	89	ASN	N-CA	-6.99	1.35	1.46
1	A	760	GLN	CA-C	6.96	1.61	1.52
1	B	249	ASN	N-CA	-6.95	1.38	1.46
1	A	591	THR	N-CA	-6.77	1.38	1.46
1	B	487	ALA	C-O	6.68	1.32	1.23
1	A	478	SER	CB-OG	-6.63	1.28	1.42
1	B	92	GLY	CA-C	-6.55	1.44	1.52
1	A	61	GLN	CA-C	-6.50	1.44	1.52
1	A	691	ASN	N-CA	6.46	1.54	1.46
1	B	90	PRO	N-CA	-6.46	1.38	1.47
1	B	721	VAL	N-CA	-6.34	1.39	1.46
1	A	324	LYS	N-CA	-6.27	1.38	1.45
1	A	284	ASP	C-O	-6.24	1.18	1.24
1	A	90	PRO	C-O	-6.21	1.16	1.24
1	A	646	ALA	CA-CB	-6.18	1.42	1.53
1	A	712	ALA	N-CA	-6.13	1.38	1.46
1	A	760	GLN	CA-CB	-6.09	1.43	1.53
1	A	465	PRO	CA-CB	6.05	1.62	1.53
1	B	523[A]	CYS	CA-C	6.05	1.60	1.52
1	B	523[B]	CYS	CA-C	6.05	1.60	1.52
1	B	639	TYR	C-O	-6.05	1.16	1.23
1	B	189	GLY	CA-C	-6.04	1.44	1.52
1	A	691	ASN	CA-C	6.01	1.60	1.52
1	A	762	LYS	N-CA	-6.00	1.39	1.46
1	A	236	THR	N-CA	6.00	1.53	1.46
1	B	561	LEU	CA-C	-5.99	1.45	1.52
1	B	288	SER	N-CA	-5.99	1.39	1.46
1	B	717	GLY	N-CA	5.94	1.54	1.45
1	A	605	ILE	C-O	-5.90	1.18	1.24
1	B	254	ASN	CA-C	-5.87	1.45	1.52
1	A	709	ALA	N-CA	-5.82	1.39	1.46
1	B	72	TRP	CZ3-CH2	-5.75	1.26	1.40
1	A	693	GLY	N-CA	5.75	1.53	1.45
1	A	590	GLY	C-O	5.74	1.30	1.23
1	A	303	ASP	N-CA	-5.74	1.39	1.46
1	B	416	ARG	CD-NE	-5.73	1.38	1.46
1	B	313	GLY	N-CA	-5.70	1.38	1.45
1	A	95	PHE	C-O	-5.66	1.17	1.23
1	A	216	PHE	CA-C	-5.64	1.45	1.52
1	B	72	TRP	N-CA	5.61	1.52	1.46
1	B	97	TYR	CA-CB	-5.60	1.44	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	547	ARG	C-O	-5.56	1.17	1.24
1	A	472	PRO	C-O	5.53	1.30	1.24
1	B	71	TRP	C-N	-5.51	1.26	1.33
1	B	498	VAL	CA-C	-5.49	1.45	1.52
1	A	90	PRO	CA-CB	5.48	1.61	1.53
1	B	491	ASP	C-O	5.48	1.30	1.23
1	A	706	MET	CA-C	-5.45	1.45	1.52
1	B	70	ASP	CA-C	-5.44	1.46	1.52
1	B	631	PRO	C-O	-5.44	1.18	1.23
1	A	748	ARG	CD-NE	-5.42	1.38	1.46
1	B	533	ARG	NE-CZ	-5.40	1.27	1.33
1	A	524	ALA	CA-C	-5.40	1.45	1.52
1	B	150	ASP	CA-C	-5.39	1.45	1.52
1	B	712	ALA	N-CA	-5.38	1.39	1.46
1	A	314	HIS	CE1-NE2	-5.36	1.27	1.32
1	B	152	ARG	NE-CZ	-5.34	1.27	1.33
1	B	452	ALA	CA-CB	-5.33	1.45	1.53
1	B	88[A]	GLN	CA-C	-5.30	1.45	1.52
1	B	88[B]	GLN	CA-C	-5.30	1.45	1.52
1	A	706	MET	N-CA	5.29	1.53	1.46
1	B	163	ALA	CA-CB	-5.27	1.45	1.53
1	A	98	ALA	CA-C	-5.27	1.46	1.52
1	B	72	TRP	CD2-CE2	-5.24	1.32	1.41
1	A	590	GLY	CA-C	-5.20	1.46	1.52
1	A	412	LYS	C-O	5.19	1.30	1.24
1	A	465	PRO	N-CA	-5.17	1.40	1.47
1	B	125	PRO	C-O	5.16	1.29	1.23
1	B	556	GLN	CA-CB	-5.14	1.45	1.53
1	A	758	GLY	C-O	5.14	1.31	1.24
1	B	595	GLU	CD-OE1	5.11	1.35	1.25
1	B	608	PRO	C-O	-5.10	1.18	1.23
1	B	760	GLN	CA-C	-5.10	1.46	1.52
1	B	632	GLN	CA-C	5.09	1.59	1.52
1	B	736	ARG	C-O	5.08	1.30	1.24
1	B	736	ARG	CA-C	-5.07	1.46	1.52
1	B	579	LYS	N-CA	5.07	1.52	1.45
1	B	580	VAL	C-N	-5.07	1.26	1.33
1	A	246	ARG	NE-CZ	-5.05	1.27	1.33
1	B	504	ALA	C-N	-5.05	1.27	1.33
1	B	86	PRO	C-O	-5.04	1.18	1.24
1	B	749	ALA	C-N	-5.02	1.27	1.33
1	B	494	ASP	CA-C	-5.00	1.45	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	703	LEU	CA-C	-5.00	1.46	1.52

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	757	ASN	CA-C-N	-16.11	104.27	123.44
1	A	757	ASN	C-N-CA	-16.11	104.27	123.44
1	A	757	ASN	O-C-N	-11.19	109.11	122.87
1	A	758	GLY	CA-C-O	10.52	128.71	119.56
1	B	82	ARG	NE-CZ-NH2	10.05	128.25	119.20
1	A	758	GLY	N-CA-C	9.04	124.37	113.79
1	A	540	ARG	NE-CZ-NH2	-8.97	111.13	119.20
1	A	88	GLN	O-C-N	-8.36	110.55	122.41
1	B	416	ARG	CG-CD-NE	-8.19	93.99	112.00
1	A	465	PRO	N-CA-CB	-7.98	95.89	103.39
1	B	70	ASP	O-C-N	-7.87	113.59	122.09
1	B	498	VAL	O-C-N	-7.86	114.25	121.87
1	B	82	ARG	NE-CZ-NH1	-7.70	113.80	121.50
1	B	532	LYS	CA-CB-CG	-7.28	99.55	114.10
1	B	152	ARG	NE-CZ-NH1	-7.20	114.30	121.50
1	A	88	GLN	CB-CA-C	6.94	123.05	109.72
1	A	82	ARG	NE-CZ-NH2	6.93	125.44	119.20
1	A	488	ARG	N-CA-C	6.84	119.66	110.35
1	A	88	GLN	CA-C-O	6.68	127.13	119.18
1	A	532	LYS	CA-CB-CG	-6.56	100.98	114.10
1	A	591	THR	CB-CA-C	6.48	121.06	110.88
1	A	579	LYS	CD-CE-NZ	6.45	132.54	111.90
1	B	71	TRP	CA-C-O	-6.44	113.59	120.42
1	A	540	ARG	NH1-CZ-NH2	6.25	127.43	119.30
1	A	608	PRO	CB-CA-C	-6.19	103.48	111.46
1	A	445	GLU	CB-CG-CD	-6.06	102.31	112.60
1	A	783	LYS	N-CA-C	6.03	119.54	109.95
1	A	544	GLU	CB-CG-CD	5.91	122.66	112.60
1	A	590	GLY	CA-C-N	5.78	127.96	120.44
1	A	590	GLY	C-N-CA	5.78	127.96	120.44
1	A	756	GLU	CB-CG-CD	5.66	122.22	112.60
1	A	757	ASN	CA-CB-CG	5.65	118.25	112.60
1	A	548	ASN	OD1-CG-ND2	5.64	128.24	122.60
1	B	561	LEU	O-C-N	-5.63	116.15	122.12
1	A	489	GLU	N-CA-C	-5.60	99.40	108.41
1	B	607	VAL	CA-C-N	-5.58	114.19	119.76
1	B	607	VAL	C-N-CA	-5.58	114.19	119.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	87	SER	CA-C-O	5.56	126.21	119.38
1	A	51	THR	N-CA-CB	5.53	118.02	110.38
1	B	71	TRP	O-C-N	5.50	128.42	122.15
1	B	461[A]	ARG	CA-C-O	5.50	127.45	121.02
1	B	461[B]	ARG	CA-C-O	5.50	127.45	121.02
1	A	82	ARG	NE-CZ-NH1	-5.46	116.03	121.50
1	B	524	ALA	CA-C-O	-5.42	114.67	120.42
1	A	152	ARG	NE-CZ-NH1	-5.39	116.11	121.50
1	A	494	ASP	CB-CG-OD1	5.38	130.78	118.40
1	A	241	GLN	O-C-N	-5.37	117.44	121.47
1	A	573	GLY	O-C-N	-5.33	116.63	122.65
1	A	628	TYR	CE1-CZ-CE2	5.24	130.78	120.30
1	A	406	TYR	N-CA-C	-5.20	103.23	109.72
1	A	532	LYS	CB-CG-CD	5.19	123.23	111.30
1	B	460	HIS	CA-C-N	5.16	129.40	121.19
1	B	460	HIS	C-N-CA	5.16	129.40	121.19
1	A	576	GLY	O-C-N	-5.13	115.47	122.55
1	B	188	TYR	CA-C-O	5.11	124.97	119.15
1	A	619	GLU	CG-CD-OE1	5.08	130.09	118.40
1	A	260	LEU	O-C-N	-5.07	116.70	122.93
1	A	179	ARG	NH1-CZ-NH2	5.06	125.87	119.30
1	B	698	ASP	CA-C-O	-5.04	114.41	120.10
1	A	88	GLN	N-CA-C	-5.00	107.18	113.28
1	A	645	ARG	NE-CZ-NH1	-5.00	116.50	121.50

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	572	ASN	Mainchain
1	A	674	ARG	Sidechain
1	B	461[A]	ARG	Mainchain
1	B	756	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	5726	0	5543	44	0
1	B	5753	0	5613	33	0
2	A	43	0	30	0	0
2	B	43	0	30	0	0
3	A	39	0	15	3	0
3	B	52	0	20	6	0
4	A	846	0	0	23	0
4	B	903	0	0	17	0
All	All	13405	0	11251	81	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 4.

All (81) 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:758:GLY:CA	1:A:758:GLY:N	1.68	1.53
1:A:523[A]:CYS:SG	4:A:1436:HOH:O	1.92	1.26
1:B:556:GLN:HG3	4:B:2173:HOH:O	1.56	1.03
1:A:757:ASN:C	1:A:758:GLY:CA	2.42	0.92
1:A:757:ASN:O	1:A:758:GLY:HA3	1.71	0.90
1:A:757:ASN:O	1:A:758:GLY:CA	2.24	0.84
1:B:152:ARG:NH2	4:B:1601:HOH:O	2.01	0.81
3:B:1501[A]:FLC:CGC	3:B:1501[A]:FLC:OA1	2.30	0.79
1:B:761:GLU:HG2	1:B:765:LYS:HE3	1.64	0.78
1:B:461[B]:ARG:HB2	4:B:2255:HOH:O	1.87	0.74
1:A:85:GLN:HG3	1:B:85[A]:GLN:OE1	1.86	0.74
1:A:395[A]:HIS:HB2	4:A:971:HOH:O	1.91	0.70
3:B:1501[A]:FLC:OA1	3:B:1501[A]:FLC:CG	2.40	0.69
1:A:625[A]:GLN:NE2	4:A:904:HOH:O	2.27	0.68
1:A:641[B]:ARG:NH2	4:A:905:HOH:O	2.27	0.67
1:B:371[B]:LYS:HD2	4:B:2328:HOH:O	1.93	0.66
1:B:371[A]:LYS:HE3	4:B:1993:HOH:O	1.97	0.65
1:B:152:ARG:NH1	4:B:1601:HOH:O	2.28	0.65
1:B:730:GLU:OE2	4:B:1602:HOH:O	2.13	0.65
1:B:152:ARG:CZ	4:B:1601:HOH:O	2.41	0.64
1:A:523[C]:CYS:HG	1:A:536:CYS:HG	1.44	0.64
1:A:641[B]:ARG:CZ	4:A:917:HOH:O	2.45	0.64
1:A:632[B]:GLN:HE22	1:A:643:THR:HG23	1.63	0.63
1:B:556:GLN:CG	4:B:2173:HOH:O	2.29	0.63
1:B:371[A]:LYS:HG3	4:B:1993:HOH:O	1.99	0.62
1:B:102[B]:GLN:OE1	4:B:1603:HOH:O	2.16	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:625[B]:GLN:NE2	4:A:908:HOH:O	2.33	0.61
3:B:1501[A]:FLC:CGC	3:B:1501[A]:FLC:CAC	2.81	0.58
1:B:461[B]:ARG:HG2	4:B:2255:HOH:O	2.03	0.58
1:B:521:MET:HA	1:B:521:MET:HE2	1.86	0.57
1:A:765:LYS:HG3	4:A:1202:HOH:O	2.02	0.57
1:B:721:VAL:HG13	1:B:730:GLU:HG3	1.85	0.57
1:B:75:GLN:HE21	1:B:76:LEU:H	1.53	0.56
1:B:461[B]:ARG:CB	4:B:2255:HOH:O	2.52	0.56
1:A:140:TRP:HZ3	1:A:273:TYR:HH	1.53	0.55
3:A:802[A]:FLC:OG2	3:A:802[A]:FLC:CBC	2.54	0.55
3:A:802[B]:FLC:OG2	3:A:802[B]:FLC:HA2	2.07	0.54
3:B:1501[A]:FLC:CAC	3:B:1501[A]:FLC:OG1	2.57	0.53
1:A:760:GLN:HB2	4:A:1511:HOH:O	2.08	0.53
1:A:88:GLN:OE1	1:B:82:ARG:HG2	2.09	0.53
1:A:641[B]:ARG:NH2	4:A:917:HOH:O	2.42	0.52
1:B:191[B]:LYS:HD2	4:B:2044:HOH:O	2.08	0.52
1:A:82:ARG:HG2	1:B:88[B]:GLN:OE1	2.10	0.52
1:A:591:THR:HG23	1:A:607:VAL:HG12	1.93	0.51
3:A:802[B]:FLC:OG2	3:A:802[B]:FLC:CA	2.58	0.51
1:A:116:LEU:C	1:A:116:LEU:HD23	2.37	0.49
1:A:627[A]:SER:OG	4:A:901:HOH:O	2.20	0.49
1:A:556:GLN:HG3	4:A:1554:HOH:O	2.12	0.49
1:B:85[B]:GLN:HB3	1:B:86:PRO:HD2	1.94	0.49
1:A:641[A]:ARG:NH1	4:A:909:HOH:O	2.34	0.48
1:B:395[B]:HIS:HB2	4:B:1743:HOH:O	2.11	0.48
1:A:395[A]:HIS:CB	4:A:971:HOH:O	2.53	0.48
1:A:565:LYS:HE3	4:A:911:HOH:O	2.14	0.47
1:B:103:SER:OG	1:B:191[A]:LYS:HD3	2.14	0.47
1:B:140:TRP:HZ3	1:B:273:TYR:HH	1.57	0.47
1:A:264:LEU:CD1	4:A:926:HOH:O	2.63	0.47
1:A:646:ALA:HB1	1:B:61[A]:GLN:HG3	1.96	0.47
1:A:565:LYS:NZ	4:A:911:HOH:O	2.36	0.46
1:A:691:ASN:HB3	1:A:694:LYS:HD2	1.97	0.46
1:A:59:SER:HA	1:B:645:ARG:O	2.16	0.46
1:A:523[C]:CYS:SG	1:A:536:CYS:SG	3.00	0.46
1:A:625[A]:GLN:OE1	4:A:902:HOH:O	2.21	0.46
1:A:646:ALA:CB	1:B:61[A]:GLN:HG3	2.46	0.46
1:B:371[A]:LYS:CD	4:B:1609:HOH:O	2.63	0.46
1:A:173:ASN:HA	1:A:175:ASP:OD1	2.16	0.45
1:A:246:ARG:NH2	4:A:926:HOH:O	2.49	0.44
1:B:634[A]:ASP:HB3	1:B:639:TYR:HB3	1.98	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:761:GLU:CG	1:B:765:LYS:HE3	2.41	0.44
1:A:411:ASP:OD2	1:A:414:LYS:HD2	2.18	0.44
1:A:565:LYS:CE	4:A:911:HOH:O	2.66	0.43
1:A:641[B]:ARG:NH2	4:A:923:HOH:O	2.46	0.43
1:A:152:ARG:NH2	4:A:907:HOH:O	2.31	0.42
1:B:387:LEU:HD11	1:B:395[B]:HIS:HB3	2.01	0.42
1:A:641[B]:ARG:CZ	4:A:905:HOH:O	2.64	0.41
1:A:483:ASP:N	1:A:484:PRO:HD3	2.34	0.41
3:B:1501[A]:FLC:OG1	3:B:1501[A]:FLC:CA	2.67	0.41
1:A:466[B]:THR:HG22	4:A:1206:HOH:O	2.21	0.41
3:B:1501[A]:FLC:OA1	3:B:1501[A]:FLC:HG1	2.19	0.41
1:A:713:SER:HB3	1:A:721[A]:VAL:HG23	2.02	0.40

There are no symmetry-related clashes.

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	749/764 (98%)	733 (98%)	16 (2%)	0	100	100
1	B	754/764 (99%)	736 (98%)	18 (2%)	0	100	100
All	All	1503/1528 (98%)	1469 (98%)	34 (2%)	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	594/606 (98%)	584 (98%)	10 (2%)	53	21
1	B	600/606 (99%)	599 (100%)	1 (0%)	87	71
All	All	1194/1212 (98%)	1183 (99%)	11 (1%)	70	44

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	THR
1	A	102[A]	GLN
1	A	102[B]	GLN
1	A	170	ASP
1	A	412	LYS
1	A	414	LYS
1	A	435	LYS
1	A	445	GLU
1	A	655	LYS
1	A	728	ARG
1	B	416	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	GLN
1	A	356	GLN
1	A	443	HIS
1	A	691	ASN
1	A	707	ASN
1	B	121	GLN
1	B	345	HIS
1	B	356	GLN
1	B	546	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

9 ligands 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	$\# Z > 2$
3	FLC	A	802[B]	-	12,12,12	1.91	4 (33%)	17,17,17	3.92	11 (64%)
3	FLC	A	803	-	12,12,12	1.08	1 (8%)	17,17,17	2.23	6 (35%)
3	FLC	B	1501[A]	-	12,12,12	1.07	1 (8%)	17,17,17	1.44	4 (23%)
3	FLC	B	1502	-	12,12,12	1.65	4 (33%)	17,17,17	1.83	5 (29%)
3	FLC	B	1503	-	12,12,12	2.32	5 (41%)	17,17,17	3.48	7 (41%)
3	FLC	A	802[A]	-	12,12,12	1.70	3 (25%)	17,17,17	1.74	3 (17%)
2	HEM	A	801	1,4	50,50,50	1.31	5 (10%)	67,82,82	1.59	10 (14%)
3	FLC	B	1501[B]	-	12,12,12	1.55	4 (33%)	17,17,17	1.55	3 (17%)
2	HEM	B	1500	1,4	50,50,50	1.33	6 (12%)	67,82,82	1.44	9 (13%)

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
3	FLC	A	802[B]	-	-	7/16/16/16	-
3	FLC	A	803	-	-	5/16/16/16	-
3	FLC	B	1501[A]	-	-	6/16/16/16	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FLC	B	1502	-	-	6/16/16/16	-
3	FLC	B	1503	-	-	4/16/16/16	-
3	FLC	A	802[A]	-	-	1/16/16/16	-
2	HEM	A	801	1,4	-	4/14/54/54	-
3	FLC	B	1501[B]	-	-	0/16/16/16	-
2	HEM	B	1500	1,4	-	3/14/54/54	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1503	FLC	CB-CBC	-4.94	1.48	1.53
2	A	801	HEM	FE-NB	4.01	2.07	1.94
3	A	802[B]	FLC	CB-CBC	4.00	1.57	1.53
3	B	1503	FLC	OHB-CB	3.79	1.50	1.43
2	B	1500	HEM	FE-NB	3.39	2.05	1.94
2	B	1500	HEM	C1C-C2C	-3.37	1.38	1.45
3	A	802[A]	FLC	OB1-CBC	3.12	1.31	1.22
2	B	1500	HEM	FE-NA	2.99	2.05	1.95
2	B	1500	HEM	FE-ND	2.96	2.04	1.94
2	B	1500	HEM	FE-NC	2.92	2.04	1.95
3	A	802[B]	FLC	CA-CB	-2.88	1.50	1.54
3	B	1503	FLC	OA2-CAC	-2.88	1.21	1.30
2	A	801	HEM	FE-ND	2.82	2.03	1.94
3	B	1502	FLC	CG-CB	2.75	1.57	1.54
3	A	802[A]	FLC	CG-CB	2.69	1.57	1.54
2	A	801	HEM	FE-NA	2.63	2.03	1.95
3	A	802[B]	FLC	OB2-CBC	-2.56	1.21	1.30
2	A	801	HEM	FE-NC	2.42	2.03	1.95
3	B	1503	FLC	OA1-CAC	2.41	1.30	1.22
3	A	802[A]	FLC	CB-CBC	2.37	1.55	1.53
3	B	1501[B]	FLC	CA-CB	2.30	1.56	1.54
3	B	1502	FLC	CA-CB	2.30	1.56	1.54
3	A	802[B]	FLC	CG-CB	-2.29	1.51	1.54
2	B	1500	HEM	C1A-NA	-2.28	1.35	1.39
2	A	801	HEM	C1B-NB	-2.22	1.36	1.40
3	B	1503	FLC	CG-CB	-2.20	1.51	1.54
3	A	803	FLC	OA1-CAC	2.18	1.29	1.22
3	B	1502	FLC	OA1-CAC	2.15	1.29	1.22
3	B	1501[B]	FLC	OB1-CBC	2.13	1.28	1.22
3	B	1501[B]	FLC	CB-CBC	2.11	1.55	1.53
3	B	1501[B]	FLC	OA2-CAC	-2.09	1.23	1.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1501[A]	FLC	OG2-CGC	-2.03	1.24	1.30
3	B	1502	FLC	OB1-CBC	2.00	1.28	1.22

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	802[B]	FLC	OHB-CB-CBC	11.92	125.86	108.96
3	B	1503	FLC	OHB-CB-CG	-9.66	87.34	109.38
3	B	1503	FLC	CG-CB-CBC	6.00	123.31	110.03
2	A	801	HEM	C3B-C4B-NB	-5.86	105.26	109.47
3	A	802[B]	FLC	OHB-CB-CG	-5.84	96.05	109.38
3	A	803	FLC	OB1-CBC-CB	-5.83	110.79	122.09
2	B	1500	HEM	C3B-C4B-NB	-5.56	105.47	109.47
3	A	802[B]	FLC	OHB-CB-CA	-4.54	99.03	109.38
3	A	802[A]	FLC	OB1-CBC-CB	4.44	130.69	122.09
3	B	1503	FLC	OHB-CB-CA	-4.43	99.27	109.38
2	A	801	HEM	CAA-CBA-CGA	-4.36	102.10	113.67
2	B	1500	HEM	CAA-CBA-CGA	-3.88	103.38	113.67
3	B	1503	FLC	OG1-CGC-CG	-3.65	112.60	122.95
3	B	1502	FLC	OB1-CBC-CB	-3.64	115.04	122.09
2	B	1500	HEM	CHD-C4C-NC	-3.51	120.63	124.45
3	B	1502	FLC	OHB-CB-CA	-3.50	101.38	109.38
3	A	803	FLC	OB2-CBC-CB	3.41	119.69	113.14
3	B	1501[B]	FLC	OA2-CAC-CA	3.40	125.13	114.35
3	B	1503	FLC	OG2-CGC-CG	3.36	125.00	114.35
2	A	801	HEM	C1D-C2D-C3D	3.35	110.51	106.98
2	A	801	HEM	C2D-C1D-ND	-3.34	106.04	109.90
3	B	1503	FLC	CG-CB-CA	3.20	117.53	109.31
3	A	803	FLC	OG1-CGC-CG	-3.19	113.92	122.95
3	A	802[B]	FLC	CG-CB-CA	3.17	117.46	109.31
3	B	1501[B]	FLC	OHB-CB-CG	-3.13	102.23	109.38
3	A	802[B]	FLC	OB1-CBC-CB	3.13	128.16	122.09
2	B	1500	HEM	O1D-CGD-CBD	-3.12	113.20	123.09
3	B	1501[A]	FLC	OB2-CBC-CB	3.09	119.07	113.14
3	A	802[B]	FLC	CB-CG-CGC	-3.04	105.61	113.92
3	A	802[B]	FLC	OB2-CBC-OB1	-2.97	114.35	123.86
2	A	801	HEM	C1B-NB-C4B	2.78	108.50	105.21
2	A	801	HEM	C4B-C3B-C2B	2.75	109.81	107.28
3	A	802[A]	FLC	OB2-CBC-OB1	-2.70	115.22	123.86
3	B	1502	FLC	CG-CB-CA	2.70	116.24	109.31
3	B	1501[A]	FLC	OB1-CBC-CB	-2.68	116.91	122.09
3	B	1501[B]	FLC	OA2-CAC-OA1	-2.63	116.56	123.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	801	HEM	CHC-C4B-C3B	2.61	130.28	125.07
3	A	802[A]	FLC	OHB-CB-CA	-2.59	103.47	109.38
2	A	801	HEM	C4D-ND-C1D	2.53	108.20	105.21
3	B	1502	FLC	OG1-CGC-CG	-2.48	115.94	122.95
2	B	1500	HEM	C3C-C2C-C1C	2.43	109.35	107.05
3	A	803	FLC	OG2-CGC-CG	2.38	121.89	114.35
2	B	1500	HEM	C1B-NB-C4B	2.35	108.00	105.21
2	B	1500	HEM	O2D-CGD-CBD	2.35	121.43	114.00
2	B	1500	HEM	C4C-C3C-C2C	-2.34	104.79	106.81
3	B	1502	FLC	OB2-CBC-CB	2.34	117.62	113.14
3	B	1501[A]	FLC	OHB-CB-CBC	-2.34	105.64	108.96
3	A	802[B]	FLC	OG1-CGC-CG	-2.33	116.34	122.95
2	B	1500	HEM	C4C-CHD-C1D	2.32	130.95	126.02
3	A	802[B]	FLC	OA1-CAC-CA	-2.30	116.44	122.95
2	A	801	HEM	CHC-C1C-NC	-2.29	121.96	124.45
3	A	803	FLC	OA1-CAC-CA	-2.26	116.55	122.95
3	A	802[B]	FLC	OB2-CBC-CB	2.22	117.39	113.14
2	A	801	HEM	CHD-C1D-ND	2.20	126.79	124.42
3	A	803	FLC	OHB-CB-CG	-2.19	104.39	109.38
3	B	1501[A]	FLC	CB-CG-CGC	2.19	119.90	113.92
3	A	802[B]	FLC	CB-CA-CAC	-2.03	108.37	113.92
3	B	1503	FLC	OA2-CAC-CA	2.03	120.77	114.35

There are no chirality outliers.

All (36) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	802[B]	FLC	CG-CB-CBC-OB1
3	A	802[B]	FLC	CG-CB-CBC-OB2
3	A	802[B]	FLC	OHB-CB-CBC-OB1
3	A	802[B]	FLC	OHB-CB-CBC-OB2
3	A	803	FLC	CG-CB-CBC-OB1
3	A	803	FLC	CG-CB-CBC-OB2
3	A	803	FLC	OHB-CB-CBC-OB1
3	A	803	FLC	OHB-CB-CBC-OB2
3	B	1501[A]	FLC	CA-CB-CG-CGC
3	B	1501[A]	FLC	CBC-CB-CG-CGC
3	B	1502	FLC	CG-CB-CBC-OB1
3	B	1502	FLC	CG-CB-CBC-OB2
3	B	1502	FLC	OHB-CB-CBC-OB1
3	B	1502	FLC	OHB-CB-CBC-OB2
3	B	1503	FLC	CBC-CB-CG-CGC

Continued on next page...

Continued from previous page...

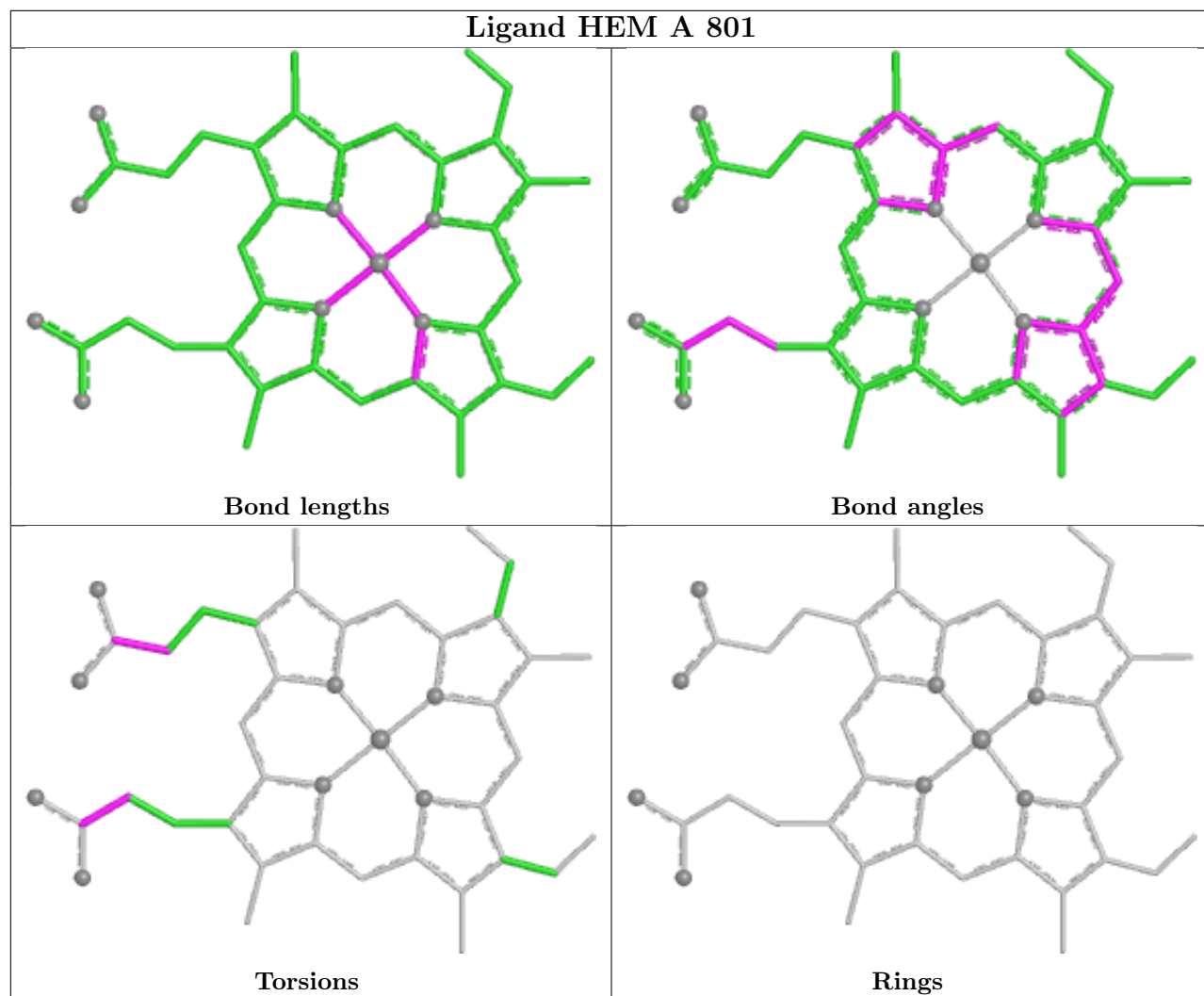
Mol	Chain	Res	Type	Atoms
3	B	1501[A]	FLC	OHB-CB-CG-CGC
3	B	1503	FLC	OHB-CB-CG-CGC
3	B	1503	FLC	CB-CG-CGC-OG1
3	B	1503	FLC	CB-CG-CGC-OG2
3	B	1502	FLC	CA-CB-CBC-OB2
3	B	1501[A]	FLC	CAC-CA-CB-OHB
3	B	1501[A]	FLC	CAC-CA-CB-CG
2	A	801	HEM	CAA-CBA-CGA-O2A
2	B	1500	HEM	CAA-CBA-CGA-O2A
3	B	1501[A]	FLC	CG-CB-CBC-OB2
2	A	801	HEM	CAA-CBA-CGA-O1A
2	B	1500	HEM	CAA-CBA-CGA-O1A
3	A	802[B]	FLC	OHB-CB-CG-CGC
3	A	803	FLC	CAC-CA-CB-OHB
3	B	1502	FLC	CAC-CA-CB-OHB
2	B	1500	HEM	CAD-CBD-CGD-O2D
3	A	802[A]	FLC	CB-CG-CGC-OG2
3	A	802[B]	FLC	CB-CG-CGC-OG1
2	A	801	HEM	CAD-CBD-CGD-O1D
2	A	801	HEM	CAD-CBD-CGD-O2D
3	A	802[B]	FLC	CB-CG-CGC-OG2

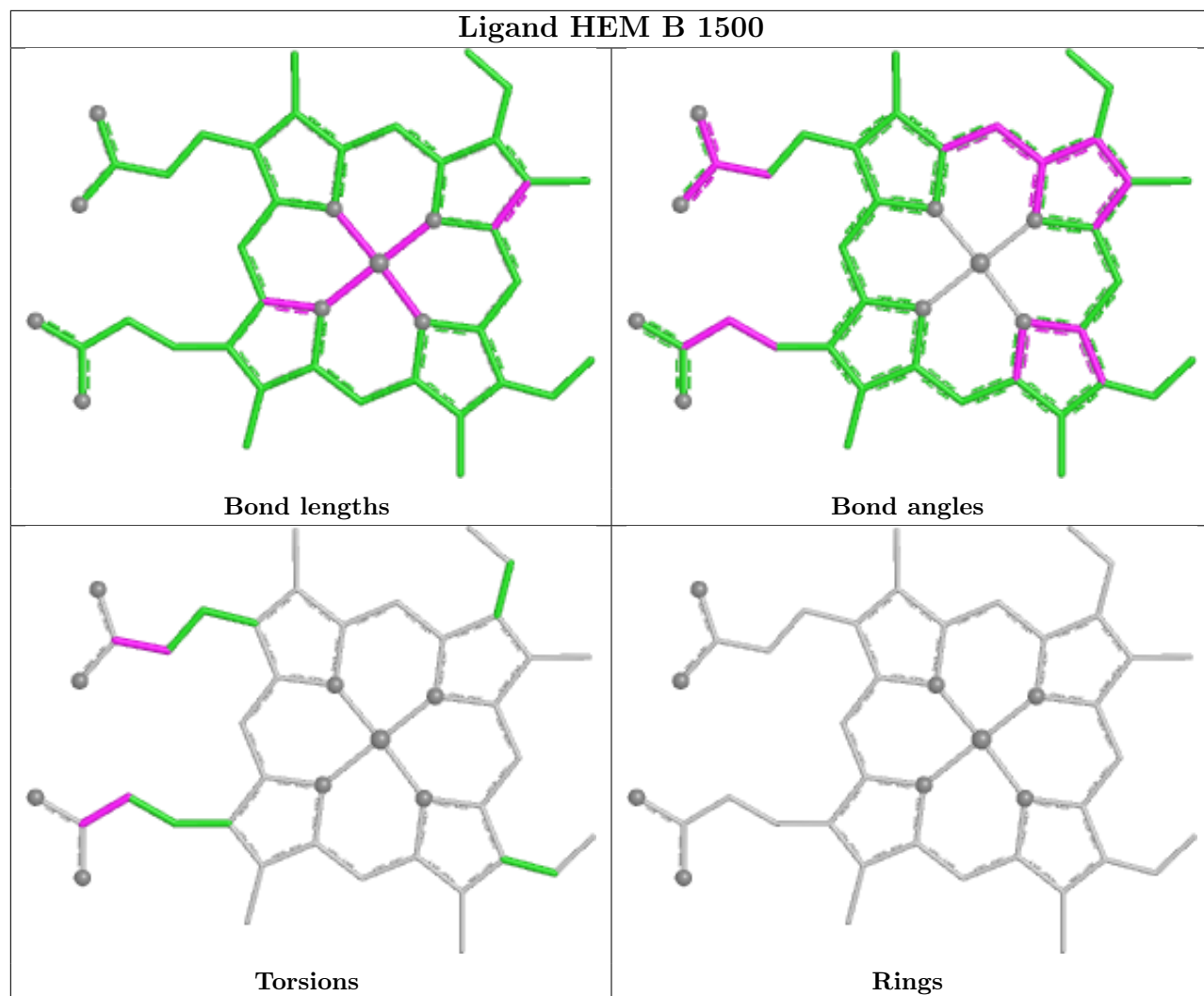
There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	802[B]	FLC	2	0
3	B	1501[A]	FLC	6	0
3	A	802[A]	FLC	1	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	735/764 (96%)	-0.35	8 (1%) 78 81	6, 14, 27, 81	15 (2%)
1	B	734/764 (96%)	-0.34	11 (1%) 72 75	8, 14, 27, 59	21 (2%)
All	All	1469/1528 (96%)	-0.35	19 (1%) 75 79	6, 14, 27, 81	36 (2%)

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	784	VAL	5.7
1	A	50	THR	5.0
1	B	50	THR	3.9
1	B	714	GLY	3.6
1	A	51	THR	3.5
1	A	56	ALA	3.4
1	A	758	GLY	3.2
1	B	783	LYS	3.1
1	A	644	ALA	3.1
1	A	69	HIS	2.3
1	B	57	VAL	2.3
1	B	487	ALA	2.3
1	B	491	ASP	2.3
1	B	490	GLY	2.1
1	B	69	HIS	2.1
1	B	573	GLY	2.1
1	B	488	ARG	2.1
1	B	94	ASP	2.1
1	A	726	LYS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

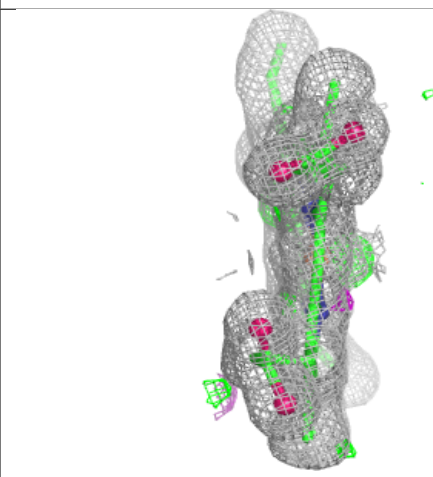
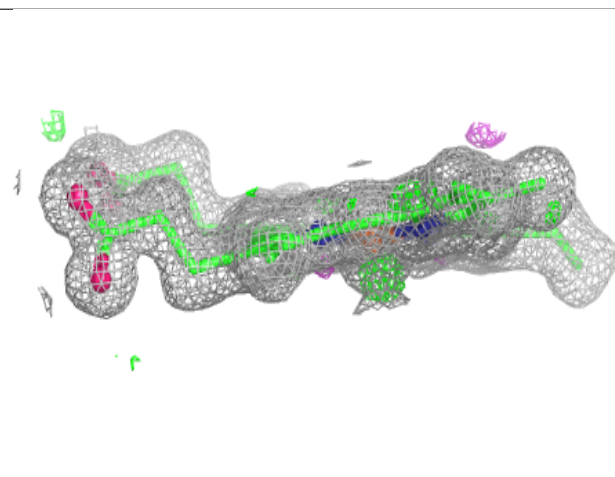
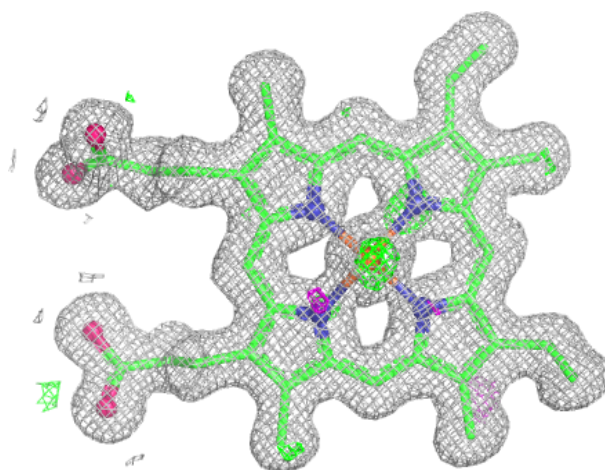
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

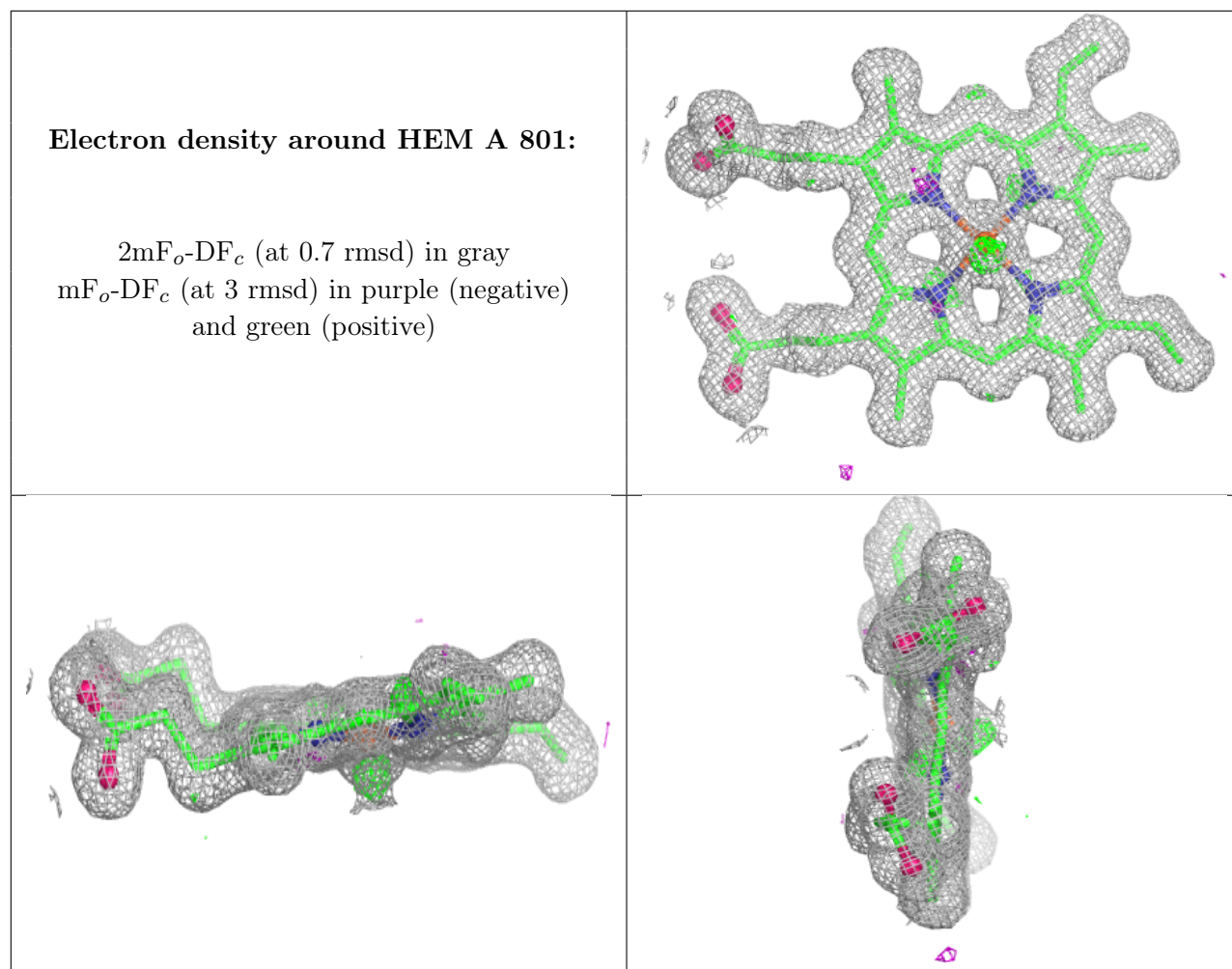
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	FLC	B	1501[A]	13/13	0.80	0.16	17,37,52,57	13
3	FLC	B	1501[B]	13/13	0.80	0.16	15,20,27,28	13
3	FLC	A	802[A]	13/13	0.84	0.13	12,18,28,29	13
3	FLC	A	802[B]	13/13	0.84	0.13	18,25,30,30	13
3	FLC	B	1502	13/13	0.86	0.11	17,25,36,40	13
3	FLC	A	803	13/13	0.89	0.10	17,25,31,35	13
3	FLC	B	1503	13/13	0.91	0.09	13,24,28,38	13
2	HEM	B	1500	43/43	0.99	0.04	9,10,11,13	0
2	HEM	A	801	43/43	0.99	0.04	8,10,11,12	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 1500:

$2mF_o-DF_c$ (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.