



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 10:06 AM UTC

PDB ID : 3EH4 / pdb_00003eh4
Title : Structure of the reduced form of cytochrome ba3 oxidase from *Thermus thermophilus*
Authors : Liu, B.; Chen, Y.; Doukov, T.; Soltis, S.M.; Stout, D.; Fee, J.A.
Deposited on : 2008-09-11
Resolution : 2.90 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

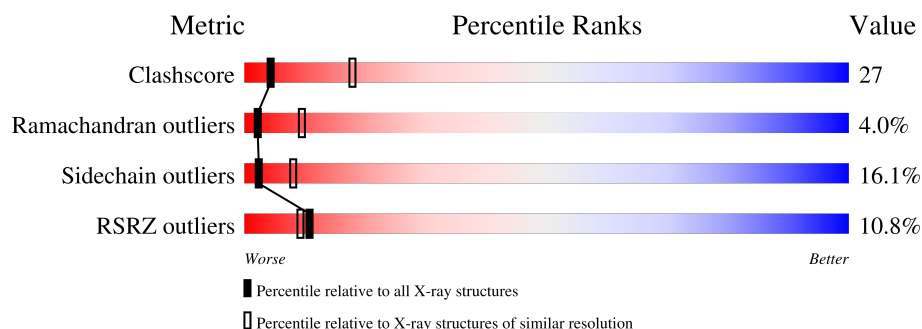
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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))
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	618	11% 40% 38% 10% • 10%
2	B	166	8% 51% 37% 10% •
3	C	33	3% 70% 21% 6% •

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	HAS	A	801	X	-	-	-

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 6143 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 Cytochrome c oxidase subunit 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	557	4409	2985	709	699	16	0	0	0

There are 58 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-55	SER	-	expression tag	UNP Q5SJ79
A	-54	GLU	-	expression tag	UNP Q5SJ79
A	-53	ILE	-	expression tag	UNP Q5SJ79
A	-52	SER	-	expression tag	UNP Q5SJ79
A	-51	ARG	-	expression tag	UNP Q5SJ79
A	-50	VAL	-	expression tag	UNP Q5SJ79
A	-49	TYR	-	expression tag	UNP Q5SJ79
A	-48	GLU	-	expression tag	UNP Q5SJ79
A	-47	ALA	-	expression tag	UNP Q5SJ79
A	-46	TYR	-	expression tag	UNP Q5SJ79
A	-45	PRO	-	expression tag	UNP Q5SJ79
A	-44	GLU	-	expression tag	UNP Q5SJ79
A	-43	LYS	-	expression tag	UNP Q5SJ79
A	-42	LYS	-	expression tag	UNP Q5SJ79
A	-41	ALA	-	expression tag	UNP Q5SJ79
A	-40	THR	-	expression tag	UNP Q5SJ79
A	-39	LEU	-	expression tag	UNP Q5SJ79
A	-38	TYR	-	expression tag	UNP Q5SJ79
A	-37	PHE	-	expression tag	UNP Q5SJ79
A	-36	LEU	-	expression tag	UNP Q5SJ79
A	-35	VAL	-	expression tag	UNP Q5SJ79
A	-34	LEU	-	expression tag	UNP Q5SJ79
A	-33	GLY	-	expression tag	UNP Q5SJ79
A	-32	PHE	-	expression tag	UNP Q5SJ79
A	-31	LEU	-	expression tag	UNP Q5SJ79
A	-30	ALA	-	expression tag	UNP Q5SJ79
A	-29	LEU	-	expression tag	UNP Q5SJ79

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-28	ILE	-	expression tag	UNP Q5SJ79
A	-27	VAL	-	expression tag	UNP Q5SJ79
A	-26	GLY	-	expression tag	UNP Q5SJ79
A	-25	SER	-	expression tag	UNP Q5SJ79
A	-24	LEU	-	expression tag	UNP Q5SJ79
A	-23	PHE	-	expression tag	UNP Q5SJ79
A	-22	GLY	-	expression tag	UNP Q5SJ79
A	-21	PRO	-	expression tag	UNP Q5SJ79
A	-20	PHE	-	expression tag	UNP Q5SJ79
A	-19	GLN	-	expression tag	UNP Q5SJ79
A	-18	ALA	-	expression tag	UNP Q5SJ79
A	-17	LEU	-	expression tag	UNP Q5SJ79
A	-16	ASN	-	expression tag	UNP Q5SJ79
A	-15	TYR	-	expression tag	UNP Q5SJ79
A	-14	GLY	-	expression tag	UNP Q5SJ79
A	-13	ASN	-	expression tag	UNP Q5SJ79
A	-12	VAL	-	expression tag	UNP Q5SJ79
A	-11	ASP	-	expression tag	UNP Q5SJ79
A	-10	ALA	-	expression tag	UNP Q5SJ79
A	-9	TYR	-	expression tag	UNP Q5SJ79
A	-8	PRO	-	expression tag	UNP Q5SJ79
A	-7	LEU	-	expression tag	UNP Q5SJ79
A	-6	LEU	-	expression tag	UNP Q5SJ79
A	-5	MET	-	expression tag	UNP Q5SJ79
A	-4	HIS	-	expression tag	UNP Q5SJ79
A	-3	HIS	-	expression tag	UNP Q5SJ79
A	-2	HIS	-	expression tag	UNP Q5SJ79
A	-1	HIS	-	expression tag	UNP Q5SJ79
A	0	HIS	-	expression tag	UNP Q5SJ79
A	1	HIS	-	expression tag	UNP Q5SJ79
A	258	ARG	LYS	engineered mutation	UNP Q5SJ79

- Molecule 2 is a protein called Cytochrome c oxidase subunit 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	166	Total	C	N	O	S	0	0	0
			1298	844	217	233	4			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	4	GLN	GLU	engineered mutation	UNP Q5SJ80

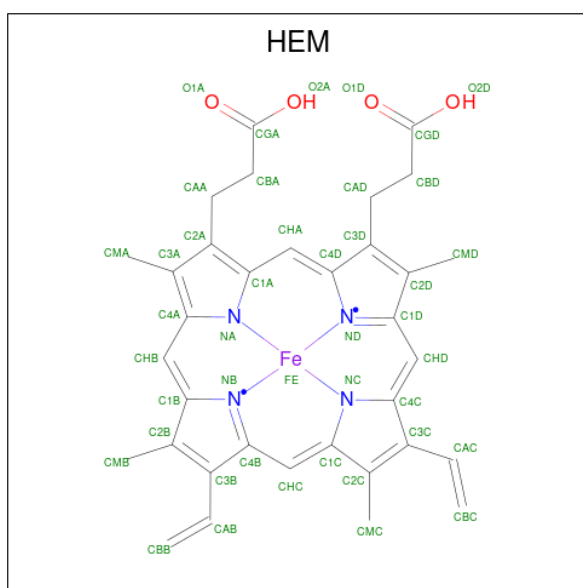
- Molecule 3 is a protein called Cytochrome c oxidase polypeptide 2A.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	33	Total	C	N	O	0	0	0
			259	179	39	41			

- Molecule 4 is COPPER (I) ION (CCD ID: CU1) (formula: Cu).

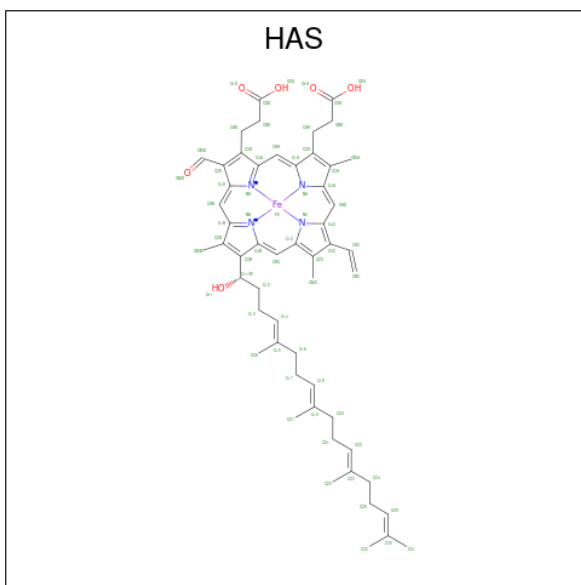
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Cu	0	0
			1	1		

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



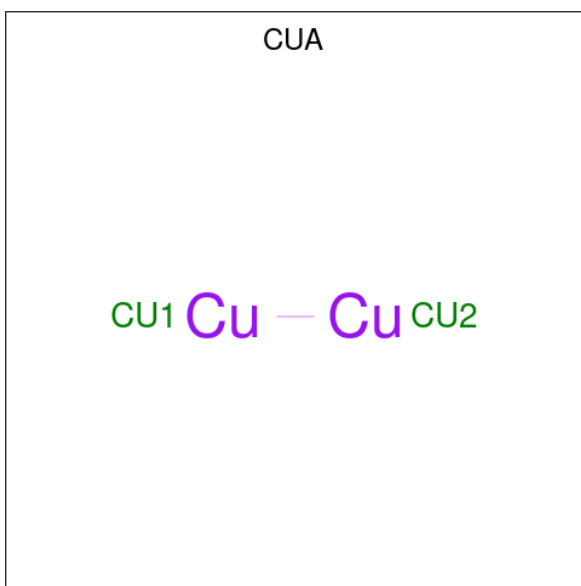
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 6 is HEME-AS (CCD ID: HAS) (formula: $C_{54}H_{64}FeN_4O_6$).



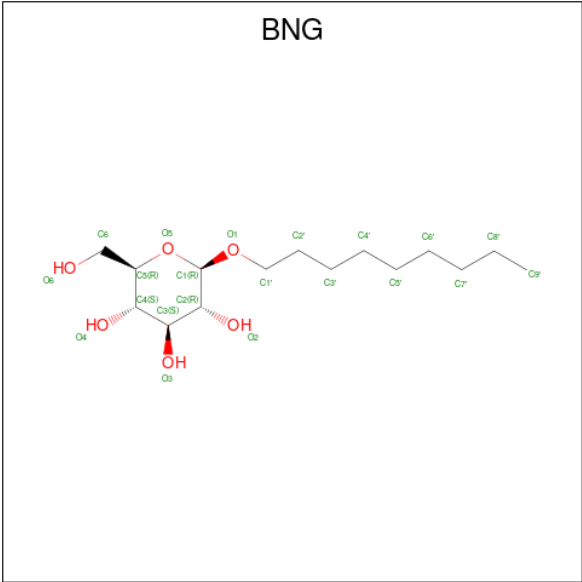
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total	C	Fe	N	O	0	0
			65	54	1	4	6		

- Molecule 7 is DINUCLEAR COPPER ION (CCD ID: CUA) (formula: Cu₂).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	Cu	0	0
			2	2		

- Molecule 8 is nonyl beta-D-glucopyranoside (CCD ID: BNG) (formula: C₁₅H₃₀O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total	C	O	0	0
			21	15	6		

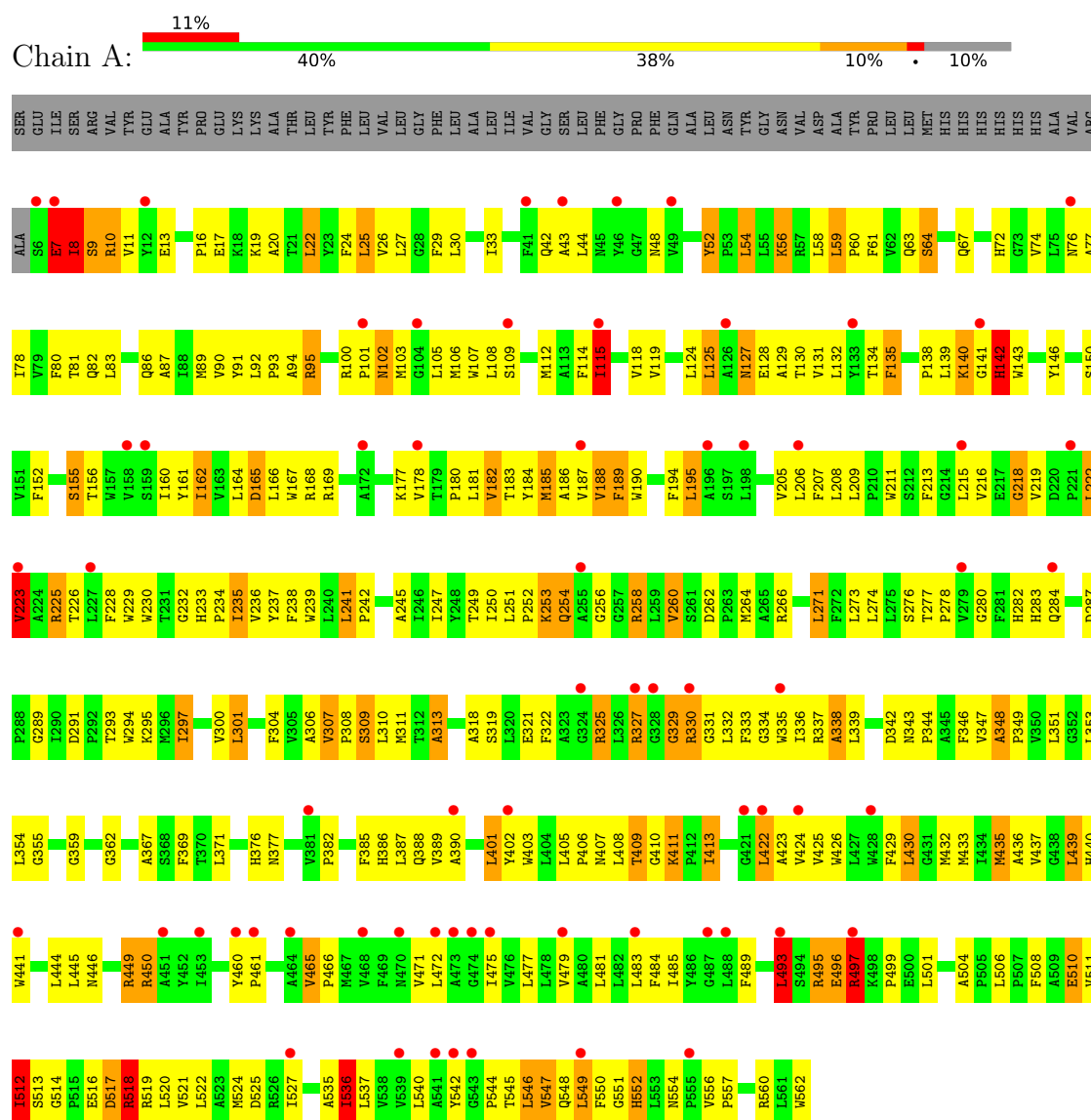
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	34	Total	O	0	0
			34	34		
9	B	10	Total	O	0	0
			10	10		
9	C	1	Total	O	0	0
			1	1		

3 Residue-property plots

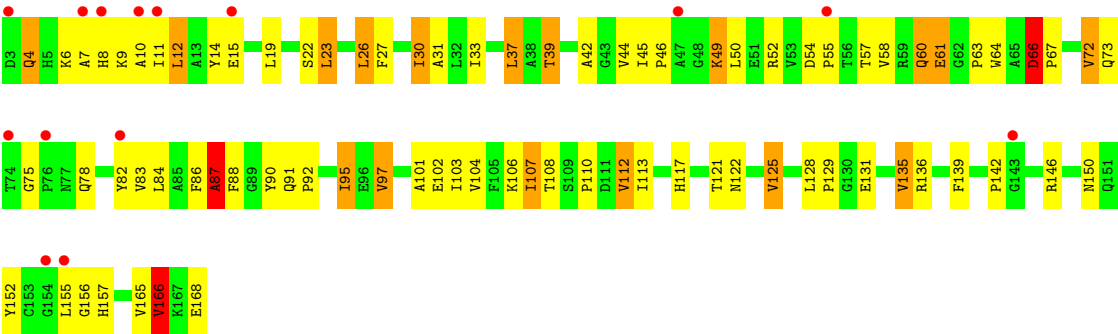
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cytochrome c oxidase subunit 1



• Molecule 2: Cytochrome c oxidase subunit 2





● Molecule 3: Cytochrome c oxidase polypeptide 2A



4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	120.85Å 120.85Å 150.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.96 – 2.90 19.96 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.96-2.90) 99.1 (19.96-2.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.34 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.268 (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	96.9	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 178.7	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	0.90	EDS
Total number of atoms	6143	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, HAS, BNG, CU1, CUA

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	1.30	15/4566 (0.3%)	1.42	40/6266 (0.6%)
2	B	1.32	8/1335 (0.6%)	1.42	12/1822 (0.7%)
3	C	1.44	2/265 (0.8%)	1.28	0/359
All	All	1.31	25/6166 (0.4%)	1.42	52/8447 (0.6%)

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	3
2	B	0	1
All	All	0	4

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	108	THR	CA-CB	7.20	1.64	1.53
1	A	52	TYR	CA-C	7.12	1.61	1.52
1	A	471	VAL	CA-CB	6.65	1.62	1.54
1	A	43	ALA	CA-CB	-6.37	1.43	1.53
1	A	209	LEU	CA-C	6.09	1.60	1.52
3	C	17	LEU	CA-C	6.05	1.60	1.52
1	A	223	VAL	CA-CB	5.93	1.61	1.54
1	A	338	ALA	N-CA	5.91	1.53	1.46
2	B	30	ILE	CA-CB	5.85	1.61	1.54
2	B	91	GLN	CA-C	5.73	1.57	1.52
2	B	135	VAL	C-O	-5.73	1.17	1.24
2	B	31	ALA	CA-CB	-5.66	1.44	1.53
1	A	413	ILE	CA-CB	5.65	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	42	GLN	C-O	5.60	1.30	1.24
2	B	90	TYR	N-CA	5.53	1.52	1.45
1	A	72	HIS	C-O	-5.40	1.17	1.24
1	A	115	ILE	CA-CB	5.40	1.62	1.54
2	B	72	VAL	CA-CB	5.35	1.61	1.54
3	C	17	LEU	C-O	5.19	1.30	1.24
1	A	80	PHE	N-CA	5.18	1.52	1.46
1	A	475	ILE	CA-CB	5.17	1.59	1.54
1	A	536	ILE	CA-CB	5.16	1.61	1.54
2	B	95	ILE	CA-CB	5.14	1.60	1.54
1	A	307	VAL	CA-CB	-5.12	1.47	1.54
1	A	249	THR	CA-C	5.03	1.58	1.52

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	ILE	N-CA-C	-9.78	100.34	111.00
1	A	348	ALA	CA-C-N	-8.01	111.39	120.04
1	A	348	ALA	C-N-CA	-8.01	111.39	120.04
1	A	8	ILE	N-CA-C	7.55	125.05	109.34
1	A	409	THR	CB-CA-C	-7.51	101.15	111.51
1	A	437	VAL	N-CA-C	-7.47	103.05	110.30
2	B	95	ILE	N-CA-C	-7.18	97.38	107.80
1	A	493	LEU	CA-CB-CG	7.16	141.36	116.30
1	A	44	LEU	N-CA-C	-7.11	103.61	111.36
2	B	165	VAL	CA-C-N	-6.83	114.24	123.12
2	B	165	VAL	C-N-CA	-6.83	114.24	123.12
1	A	293	THR	N-CA-C	-6.77	104.65	113.12
1	A	241	LEU	CA-C-N	-6.76	111.55	119.05
1	A	241	LEU	C-N-CA	-6.76	111.55	119.05
2	B	66	ASP	CA-C-N	6.69	126.37	119.82
2	B	66	ASP	C-N-CA	6.69	126.37	119.82
1	A	223	VAL	N-CA-C	6.42	116.56	110.53
1	A	322	PHE	N-CA-C	-6.41	104.37	111.36
1	A	319	SER	N-CA-C	6.39	118.04	111.14
1	A	249	THR	N-CA-C	6.26	121.99	113.97
1	A	209	LEU	CA-C-N	6.12	125.34	118.97
1	A	209	LEU	C-N-CA	6.12	125.34	118.97
1	A	291	ASP	N-CA-C	6.12	117.42	109.64
2	B	33	ILE	N-CA-C	-6.10	104.57	110.42
1	A	206	LEU	N-CA-C	5.98	118.59	111.71
1	A	401	LEU	N-CA-C	-5.95	106.06	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	496	GLU	N-CA-C	5.93	123.44	110.80
2	B	146	ARG	NE-CZ-NH1	-5.93	115.57	121.50
2	B	39	THR	N-CA-C	-5.89	100.00	108.60
2	B	97	VAL	N-CA-C	-5.88	104.37	109.19
2	B	166	VAL	CB-CA-C	5.86	119.51	110.96
1	A	260	VAL	N-CA-C	5.85	118.40	111.09
1	A	518	ARG	N-CA-C	5.85	117.45	111.14
1	A	313	ALA	N-CA-C	5.80	117.28	111.07
2	B	146	ARG	CB-CG-CD	-5.73	98.11	111.30
1	A	510	GLU	N-CA-C	-5.69	103.41	110.41
1	A	440	HIS	N-CA-C	-5.60	105.25	111.36
1	A	338	ALA	N-CA-C	5.48	119.07	112.38
1	A	271	LEU	N-CA-C	5.45	117.22	111.28
2	B	49	LYS	N-CA-C	5.42	118.08	110.23
1	A	517	ASP	N-CA-C	5.41	117.60	111.11
1	A	256	GLY	N-CA-C	-5.37	107.13	115.67
1	A	115	ILE	CB-CA-C	5.29	120.36	112.16
1	A	27	LEU	N-CA-C	-5.25	104.99	111.40
1	A	74	VAL	N-CA-C	5.21	115.65	110.23
1	A	295	LYS	N-CA-C	-5.21	105.28	111.69
1	A	189	PHE	CA-C-N	5.20	127.50	120.38
1	A	189	PHE	C-N-CA	5.20	127.50	120.38
1	A	218	GLY	N-CA-C	5.18	120.46	111.14
1	A	182	VAL	N-CA-CB	5.04	117.40	110.54
1	A	423	ALA	N-CA-C	-5.02	107.29	113.41
1	A	355	GLY	N-CA-C	-5.00	107.59	113.99

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	329	GLY	Peptide
1	A	52	TYR	Peptide
1	A	7	GLU	Peptide
2	B	87	ALA	Peptide

5.2 Too-close contacts [i](#)

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	4409	0	4516	282	0
2	B	1298	0	1282	62	0
3	C	259	0	279	10	0
4	A	1	0	0	0	0
5	A	43	0	30	8	0
6	A	65	0	61	7	0
7	B	2	0	0	0	0
8	C	21	0	30	1	0
9	A	34	0	0	15	0
9	B	10	0	0	2	0
9	C	1	0	0	1	0
All	All	6143	0	6198	331	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 27.

All (331) 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:233:HIS:NE2	1:A:237:TYR:HE2	1.02	1.46
1:A:140:LYS:HD2	9:A:580:HOH:O	1.42	1.19
1:A:233:HIS:NE2	1:A:237:TYR:CE2	1.85	1.15
1:A:258:ARG:HH11	1:A:258:ARG:HG3	1.12	1.14
2:B:84:LEU:HD11	2:B:110:PRO:HD3	1.27	1.14
1:A:108:LEU:O	1:A:112:MET:HB2	1.54	1.08
1:A:140:LYS:CD	9:A:580:HOH:O	1.98	1.07
1:A:59:LEU:HD23	1:A:61:PHE:HE1	1.20	1.04
1:A:59:LEU:HD23	1:A:61:PHE:CE1	1.96	0.99
1:A:195:LEU:HD11	1:A:535:ALA:HB2	1.47	0.97
1:A:489:PHE:HB3	1:A:493:LEU:HD13	1.49	0.94
1:A:103:MET:HE3	1:A:107:TRP:NE1	1.84	0.92
1:A:330:ARG:HH21	1:A:330:ARG:CG	1.84	0.90
1:A:223:VAL:HG12	1:A:549:LEU:HD13	1.53	0.90
1:A:260:VAL:HG21	2:B:11:ILE:HG21	1.56	0.88
1:A:92:LEU:HB3	1:A:182:VAL:HG11	1.55	0.87
2:B:22:SER:O	2:B:26:LEU:HD22	1.74	0.87
2:B:84:LEU:CD1	2:B:110:PRO:HD3	2.05	0.87
1:A:258:ARG:HG3	1:A:258:ARG:NH1	1.90	0.84
1:A:309:SER:HB2	9:A:565:HOH:O	1.75	0.84
1:A:518:ARG:O	1:A:522:LEU:HB2	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:24:PHE:HZ	1:A:109:SER:HG	1.23	0.83
1:A:103:MET:HE3	1:A:107:TRP:HE1	1.39	0.82
1:A:264:MET:SD	2:B:15:GLU:HG2	2.19	0.82
1:A:330:ARG:HH21	1:A:330:ARG:HG3	1.44	0.82
1:A:311:MET:HG2	9:B:178:HOH:O	1.80	0.81
1:A:207:PHE:HZ	1:A:550:PHE:HE2	1.28	0.81
1:A:329:GLY:HA2	1:A:330:ARG:NH2	1.95	0.81
1:A:188:VAL:HG12	1:A:273:LEU:HD22	1.62	0.80
2:B:92:PRO:HG2	2:B:95:ILE:HG12	1.62	0.80
1:A:146:TYR:HD2	1:A:208:LEU:HD13	1.46	0.79
1:A:160:ILE:HD13	1:A:194:PHE:HB2	1.63	0.79
1:A:346:PHE:O	1:A:349:PRO:HD2	1.82	0.79
1:A:233:HIS:CE1	1:A:237:TYR:HE2	1.99	0.78
2:B:88:PHE:CD2	2:B:156:GLY:HA3	2.19	0.77
1:A:233:HIS:CE1	1:A:237:TYR:CE2	2.72	0.76
1:A:258:ARG:HH11	1:A:258:ARG:CG	1.93	0.76
2:B:122:ASN:ND2	3:C:33:ARG:HB2	2.00	0.76
1:A:389:VAL:HB	6:A:801:HAS:HBC2	1.68	0.75
1:A:489:PHE:HB3	1:A:493:LEU:CD1	2.16	0.75
1:A:146:TYR:CE2	1:A:208:LEU:HD22	2.22	0.74
1:A:59:LEU:CD2	1:A:61:PHE:HE1	2.00	0.73
1:A:95:ARG:HA	1:A:95:ARG:HH21	1.50	0.73
1:A:551:GLY:O	1:A:552:HIS:ND1	2.23	0.72
1:A:146:TYR:CD2	1:A:208:LEU:HD13	2.24	0.72
1:A:29:PHE:CE2	1:A:484:PHE:HZ	2.07	0.72
1:A:518:ARG:HD2	9:A:585:HOH:O	1.89	0.71
1:A:64:SER:HB3	2:B:155:LEU:HD21	1.71	0.71
1:A:329:GLY:HA2	1:A:330:ARG:HG3	1.74	0.70
1:A:250:ILE:HD13	1:A:403:TRP:CH2	2.27	0.70
1:A:24:PHE:CZ	1:A:109:SER:OG	2.45	0.69
1:A:114:PHE:O	1:A:118:VAL:HG23	1.91	0.69
1:A:29:PHE:HE2	1:A:484:PHE:HZ	1.39	0.69
2:B:88:PHE:CG	2:B:156:GLY:HA3	2.27	0.69
2:B:73:GLN:NE2	2:B:75:GLY:O	2.25	0.69
1:A:188:VAL:HG12	1:A:273:LEU:CD2	2.23	0.68
1:A:518:ARG:HH21	1:A:518:ARG:HG3	1.59	0.68
1:A:236:VAL:HG12	1:A:239:TRP:CZ3	2.29	0.67
1:A:497:ARG:HG3	1:A:497:ARG:O	1.93	0.67
1:A:134:THR:O	1:A:135:PHE:C	2.38	0.67
1:A:211:TRP:HE1	1:A:218:GLY:HA2	1.60	0.66
1:A:511:VAL:O	1:A:511:VAL:HG12	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4:LYS:HB3	3:C:6:LYS:HG2	1.78	0.66
1:A:29:PHE:HE2	1:A:484:PHE:CZ	2.12	0.66
1:A:294:TRP:HZ2	1:A:544:PRO:HG2	1.61	0.66
1:A:24:PHE:HZ	1:A:109:SER:OG	1.77	0.65
1:A:514:GLY:HA3	2:B:8:HIS:NE2	2.12	0.65
1:A:390:ALA:HB1	1:A:432:MET:HE3	1.79	0.65
1:A:90:VAL:HG11	1:A:106:MET:HE3	1.78	0.64
1:A:232:GLY:O	1:A:235:ILE:HG22	1.97	0.64
1:A:82:GLN:NE2	1:A:86:GLN:OE1	2.28	0.64
1:A:103:MET:HE3	1:A:107:TRP:CD1	2.31	0.64
1:A:233:HIS:NE2	1:A:237:TYR:CD2	2.58	0.64
1:A:307:VAL:N	1:A:308:PRO:HD2	2.13	0.64
1:A:223:VAL:HG12	1:A:549:LEU:CD1	2.27	0.63
1:A:195:LEU:CD1	1:A:535:ALA:HB2	2.26	0.63
1:A:449:ARG:HH12	6:A:801:HAS:CGA	2.12	0.63
1:A:160:ILE:CD1	1:A:194:PHE:HB2	2.28	0.62
2:B:64:TRP:CD1	2:B:82:TYR:HB3	2.34	0.62
1:A:330:ARG:HG3	1:A:330:ARG:NH2	2.13	0.62
1:A:207:PHE:CZ	1:A:550:PHE:HE2	2.14	0.62
1:A:108:LEU:O	1:A:112:MET:CB	2.41	0.61
1:A:344:PRO:CA	1:A:422:LEU:HD23	2.30	0.61
1:A:242:PRO:O	1:A:245:ALA:HB3	2.01	0.61
1:A:479:VAL:O	1:A:483:LEU:HG	2.01	0.61
1:A:258:ARG:NH1	1:A:258:ARG:CG	2.55	0.61
1:A:103:MET:CE	1:A:107:TRP:HE1	2.12	0.61
1:A:521:VAL:HB	9:A:585:HOH:O	2.00	0.60
1:A:330:ARG:H	1:A:334:GLY:HA3	1.64	0.60
2:B:12:LEU:O	2:B:12:LEU:HG	2.01	0.60
1:A:139:LEU:HD23	2:B:112:VAL:HG11	1.84	0.60
1:A:235:ILE:HD11	9:A:594:HOH:O	2.01	0.59
1:A:253:LYS:HE3	1:A:253:LYS:O	2.02	0.59
1:A:93:PRO:CG	1:A:186:ALA:CB	2.79	0.59
1:A:226:THR:HG22	1:A:226:THR:O	2.01	0.59
1:A:140:LYS:O	1:A:562:TRP:HH2	1.85	0.59
1:A:557:PRO:O	9:A:583:HOH:O	2.17	0.59
1:A:19:LYS:HD2	1:A:107:TRP:HZ2	1.66	0.59
1:A:359:GLY:HA3	1:A:388:GLN:NE2	2.17	0.59
1:A:371:LEU:N	1:A:371:LEU:HD12	2.17	0.59
2:B:142:PRO:HA	2:B:166:VAL:HG22	1.83	0.59
1:A:211:TRP:CG	1:A:219:VAL:HG23	2.37	0.58
1:A:377:ASN:HB3	2:B:150:ASN:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:146:TYR:CD2	1:A:208:LEU:HB3	2.38	0.58
1:A:184:TYR:O	1:A:188:VAL:HG22	2.04	0.58
1:A:389:VAL:HG22	5:A:800:HEM:CBC	2.33	0.58
1:A:225:ARG:HD3	1:A:287:ASP:OD1	2.04	0.58
1:A:92:LEU:HB3	1:A:182:VAL:CG1	2.30	0.58
1:A:10:ARG:HA	1:A:13:GLU:HB2	1.85	0.57
1:A:130:THR:HG22	1:A:130:THR:O	2.03	0.57
1:A:266:ARG:HD2	1:A:524:MET:HE3	1.86	0.57
1:A:449:ARG:HD2	9:A:563:HOH:O	2.04	0.57
1:A:386:HIS:CD2	1:A:435:MET:HE1	2.40	0.57
2:B:42:ALA:O	2:B:45:ILE:HG13	2.05	0.56
1:A:93:PRO:HG2	1:A:186:ALA:CB	2.35	0.56
1:A:19:LYS:HD2	1:A:107:TRP:CZ2	2.41	0.56
1:A:132:LEU:HD13	1:A:450:ARG:CZ	2.34	0.56
1:A:260:VAL:CG2	2:B:11:ILE:HG21	2.33	0.56
1:A:33:ILE:HD12	1:A:485:ILE:HG12	1.88	0.56
1:A:207:PHE:HZ	1:A:550:PHE:CE2	2.17	0.56
1:A:294:TRP:CZ2	1:A:544:PRO:HG2	2.41	0.56
5:A:800:HEM:HMB2	5:A:800:HEM:HBB2	1.88	0.56
1:A:330:ARG:HH21	1:A:330:ARG:HG2	1.69	0.55
1:A:128:GLU:CD	1:A:560:ARG:HH22	2.15	0.55
1:A:435:MET:HG2	1:A:439:LEU:HD22	1.89	0.55
1:A:141:GLY:O	1:A:142:HIS:O	2.25	0.55
1:A:511:VAL:O	1:A:512:ILE:C	2.50	0.55
2:B:10:ALA:O	2:B:14:TYR:HD1	1.89	0.55
1:A:58:LEU:O	1:A:59:LEU:HD12	2.06	0.54
1:A:390:ALA:HB1	1:A:432:MET:CE	2.37	0.54
1:A:376:HIS:O	1:A:377:ASN:HB2	2.08	0.54
1:A:477:LEU:HB3	5:A:800:HEM:CBB	2.37	0.54
1:A:64:SER:CB	2:B:155:LEU:HD21	2.37	0.54
1:A:230:TRP:HZ3	1:A:546:LEU:CD1	2.20	0.54
1:A:93:PRO:HG3	1:A:186:ALA:CB	2.38	0.54
1:A:90:VAL:CG1	1:A:106:MET:HE3	2.38	0.53
1:A:101:PRO:O	1:A:102:ASN:C	2.50	0.53
1:A:178:VAL:HG13	1:A:525:ASP:OD1	2.07	0.53
1:A:282:HIS:CD2	1:A:283:HIS:CD2	2.97	0.53
1:A:477:LEU:HD12	5:A:800:HEM:HMB3	1.91	0.53
1:A:403:TRP:HZ3	1:A:506:LEU:HD22	1.74	0.53
1:A:518:ARG:HH21	1:A:518:ARG:CG	2.22	0.53
1:A:234:PRO:HG3	1:A:277:THR:HA	1.91	0.53
1:A:449:ARG:HG3	1:A:450:ARG:HG3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:161:TYR:CE2	1:A:165:ASP:HB2	2.44	0.52
1:A:313:ALA:HB2	6:A:801:HAS:H273	1.91	0.52
1:A:25:LEU:O	1:A:25:LEU:HD22	2.09	0.52
1:A:321:GLU:OE1	1:A:325:ARG:NH2	2.42	0.52
1:A:329:GLY:HA2	1:A:330:ARG:HH21	1.74	0.52
2:B:104:VAL:HG22	2:B:136:ARG:HG3	1.91	0.52
1:A:22:LEU:O	1:A:26:VAL:HG23	2.10	0.52
2:B:7:ALA:O	2:B:11:ILE:HD12	2.09	0.52
2:B:60:GLN:O	2:B:61:GLU:HB3	2.09	0.52
2:B:84:LEU:HD11	2:B:110:PRO:CD	2.19	0.52
1:A:103:MET:CE	1:A:107:TRP:NE1	2.67	0.51
1:A:138:PRO:HG2	2:B:129:PRO:HG2	1.91	0.51
1:A:7:GLU:HA	1:A:8:ILE:HG13	1.92	0.51
1:A:444:LEU:HA	9:C:35:HOH:O	2.10	0.51
2:B:52:ARG:HH21	2:B:131:GLU:HB2	1.75	0.51
1:A:181:LEU:HA	9:A:593:HOH:O	2.09	0.51
1:A:77:ALA:O	1:A:81:THR:OG1	2.28	0.51
1:A:140:LYS:HD3	9:A:580:HOH:O	1.87	0.51
2:B:97:VAL:O	2:B:166:VAL:HA	2.11	0.51
1:A:67:GLN:NE2	1:A:124:LEU:O	2.38	0.50
2:B:14:TYR:HD2	3:C:9:LEU:HD21	1.76	0.50
1:A:325:ARG:NH1	1:A:331:GLY:O	2.44	0.50
2:B:14:TYR:HE2	3:C:9:LEU:HD11	1.76	0.50
1:A:289:GLY:HA3	2:B:50:LEU:HD23	1.93	0.50
1:A:362:GLY:HA3	9:A:570:HOH:O	2.10	0.50
1:A:401:LEU:O	1:A:405:LEU:HB2	2.11	0.50
2:B:125:VAL:HG11	2:B:135:VAL:HG11	1.92	0.50
2:B:142:PRO:HA	2:B:166:VAL:CG2	2.42	0.50
1:A:91:TYR:CE1	1:A:95:ARG:HD3	2.47	0.50
1:A:152:PHE:O	1:A:155:SER:HB3	2.11	0.50
1:A:211:TRP:CD1	1:A:219:VAL:HG23	2.47	0.50
1:A:11:VAL:HG21	1:A:499:PRO:HB3	1.94	0.50
1:A:409:THR:O	1:A:411:LYS:N	2.44	0.50
2:B:101:ALA:O	2:B:103:ILE:HD12	2.12	0.50
1:A:20:ALA:HB2	1:A:103:MET:HE1	1.94	0.50
2:B:14:TYR:CD2	3:C:9:LEU:HD21	2.47	0.50
1:A:445:LEU:O	1:A:446:ASN:HB2	2.12	0.49
1:A:294:TRP:CH2	1:A:540:LEU:O	2.66	0.49
3:C:28:ALA:O	3:C:29:VAL:C	2.54	0.49
1:A:178:VAL:HG11	1:A:521:VAL:CG1	2.41	0.49
1:A:230:TRP:CZ3	1:A:546:LEU:HD11	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:TRP:HH2	1:A:540:LEU:O	1.95	0.49
1:A:134:THR:HG22	1:A:228:PHE:CZ	2.47	0.49
1:A:129:ALA:O	1:A:131:VAL:HG22	2.13	0.49
1:A:132:LEU:HD13	1:A:450:ARG:NE	2.27	0.49
1:A:146:TYR:O	1:A:150:SER:HB2	2.12	0.49
1:A:321:GLU:HA	1:A:335:TRP:CE3	2.48	0.49
1:A:54:LEU:HD13	1:A:58:LEU:HD22	1.94	0.49
1:A:344:PRO:CB	1:A:422:LEU:HD23	2.43	0.49
1:A:29:PHE:CE2	1:A:484:PHE:CZ	2.92	0.48
2:B:63:PRO:HB2	2:B:82:TYR:CD2	2.47	0.48
2:B:122:ASN:HD21	3:C:33:ARG:HB2	1.74	0.48
1:A:327:ARG:HD3	1:A:338:ALA:O	2.12	0.48
1:A:211:TRP:NE1	1:A:218:GLY:HA2	2.27	0.48
1:A:139:LEU:CD2	2:B:112:VAL:HG11	2.42	0.48
1:A:307:VAL:N	1:A:308:PRO:CD	2.76	0.48
1:A:266:ARG:CZ	1:A:521:VAL:HG13	2.44	0.48
1:A:226:THR:O	1:A:226:THR:CG2	2.62	0.48
1:A:233:HIS:C	1:A:233:HIS:CD2	2.90	0.48
1:A:17:GLU:OE1	1:A:100:ARG:HG3	2.14	0.47
1:A:233:HIS:HB3	1:A:234:PRO:CD	2.44	0.47
1:A:82:GLN:NE2	1:A:156:THR:HG23	2.30	0.47
1:A:139:LEU:HG	9:B:169:HOH:O	2.14	0.47
2:B:14:TYR:CE2	3:C:9:LEU:HD11	2.50	0.47
1:A:164:LEU:O	1:A:167:TRP:HB3	2.14	0.47
1:A:336:ILE:HG12	6:A:801:HAS:H311	1.95	0.47
2:B:83:VAL:O	2:B:107:ILE:HA	2.15	0.47
1:A:93:PRO:HG2	1:A:186:ALA:HB1	1.95	0.47
1:A:266:ARG:HD2	1:A:524:MET:CE	2.44	0.47
1:A:167:TRP:CZ2	1:A:527:ILE:HD12	2.50	0.47
2:B:54:ASP:OD1	2:B:57:THR:HG23	2.15	0.47
1:A:76:ASN:HB3	5:A:800:HEM:C3C	2.50	0.46
1:A:234:PRO:HD3	1:A:276:SER:O	2.16	0.46
1:A:406:PRO:CG	1:A:413:ILE:HD13	2.45	0.46
1:A:140:LYS:CE	9:A:579:HOH:O	2.63	0.46
1:A:407:ASN:ND2	1:A:504:ALA:O	2.48	0.46
1:A:332:LEU:HD23	1:A:333:PHE:CE2	2.51	0.46
1:A:406:PRO:HG3	1:A:413:ILE:HD13	1.97	0.46
1:A:460:TYR:N	1:A:461:PRO:CD	2.78	0.46
2:B:45:ILE:O	2:B:46:PRO:C	2.56	0.46
1:A:371:LEU:N	1:A:371:LEU:CD1	2.79	0.46
1:A:235:ILE:HA	1:A:238:PHE:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:GLU:C	1:A:511:VAL:HG23	2.41	0.46
1:A:307:VAL:O	1:A:311:MET:HG3	2.16	0.45
1:A:371:LEU:CD1	1:A:371:LEU:H	2.28	0.45
3:C:3:GLU:CD	3:C:4:LYS:H	2.24	0.45
1:A:247:ILE:HD13	1:A:353:LEU:HD11	1.98	0.45
1:A:146:TYR:HE2	1:A:208:LEU:HD22	1.74	0.45
1:A:56:LYS:O	1:A:60:PRO:HA	2.16	0.45
2:B:26:LEU:O	2:B:30:ILE:HG13	2.17	0.45
1:A:105:LEU:C	1:A:107:TRP:H	2.23	0.45
1:A:195:LEU:HD11	1:A:535:ALA:CB	2.33	0.45
1:A:300:VAL:HG22	2:B:30:ILE:HD13	1.98	0.45
2:B:86:PHE:O	2:B:88:PHE:N	2.50	0.45
1:A:93:PRO:HG3	1:A:186:ALA:HB2	1.99	0.45
1:A:401:LEU:HB2	1:A:402:TYR:CE2	2.52	0.45
1:A:91:TYR:CE2	1:A:408:LEU:HD21	2.51	0.45
1:A:407:ASN:OD1	1:A:407:ASN:O	2.34	0.45
1:A:178:VAL:HG11	1:A:521:VAL:HG11	1.99	0.45
1:A:190:TRP:HA	1:A:190:TRP:CE3	2.51	0.45
1:A:264:MET:HE3	2:B:12:LEU:HD12	1.99	0.45
1:A:187:VAL:HG11	1:A:527:ILE:HD13	1.99	0.44
1:A:237:TYR:O	1:A:241:LEU:HD13	2.17	0.44
1:A:250:ILE:O	1:A:254:GLN:HG2	2.17	0.44
1:A:61:PHE:CE2	1:A:125:LEU:HD23	2.53	0.44
1:A:140:LYS:NZ	9:A:579:HOH:O	2.29	0.44
1:A:222:LEU:HD23	2:B:52:ARG:HH12	1.82	0.44
1:A:348:ALA:HA	1:A:425:VAL:HG11	1.99	0.44
1:A:332:LEU:CD2	1:A:333:PHE:CE2	3.01	0.44
1:A:189:PHE:CE1	1:A:242:PRO:HD3	2.53	0.44
1:A:230:TRP:HA	1:A:542:TYR:OH	2.17	0.44
1:A:329:GLY:CA	1:A:330:ARG:HG3	2.46	0.44
1:A:138:PRO:O	1:A:139:LEU:C	2.60	0.44
1:A:63:GLN:HB2	1:A:127:ASN:ND2	2.32	0.44
1:A:140:LYS:NZ	1:A:211:TRP:CE2	2.76	0.44
1:A:465:VAL:CG1	9:A:589:HOH:O	2.66	0.44
1:A:187:VAL:CG1	1:A:527:ILE:HD13	2.48	0.43
1:A:229:TRP:O	1:A:230:TRP:C	2.60	0.43
1:A:344:PRO:HB3	1:A:422:LEU:HD23	2.00	0.43
2:B:103:ILE:HD13	2:B:139:PHE:HD1	1.83	0.43
1:A:387:LEU:HD23	1:A:387:LEU:HA	1.63	0.43
1:A:506:LEU:HD23	1:A:506:LEU:HA	1.59	0.43
1:A:517:ASP:O	1:A:521:VAL:HG23	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:THR:C	1:A:547:VAL:H	2.26	0.43
1:A:161:TYR:O	1:A:162:ILE:C	2.62	0.43
1:A:132:LEU:HG	2:B:152:TYR:CD2	2.53	0.43
1:A:297:ILE:O	1:A:301:LEU:HD23	2.18	0.43
1:A:556:VAL:CG1	2:B:55:PRO:HG3	2.48	0.43
2:B:37:LEU:HD12	2:B:37:LEU:HA	1.93	0.43
2:B:86:PHE:O	2:B:87:ALA:C	2.62	0.43
1:A:183:THR:O	1:A:187:VAL:HG23	2.19	0.43
1:A:277:THR:N	1:A:278:PRO:CD	2.82	0.43
1:A:367:ALA:HA	6:A:801:HAS:OMD	2.19	0.43
1:A:115:ILE:O	1:A:119:VAL:HG23	2.19	0.42
6:A:801:HAS:H253	6:A:801:HAS:H211	1.79	0.42
1:A:446:ASN:HD22	2:B:117:HIS:CE1	2.37	0.42
1:A:160:ILE:HG22	1:A:164:LEU:HD12	2.01	0.42
1:A:266:ARG:NH1	1:A:521:VAL:HG13	2.34	0.42
1:A:304:PHE:C	1:A:306:ALA:N	2.78	0.42
2:B:103:ILE:HD13	2:B:139:PHE:CD1	2.55	0.42
1:A:346:PHE:O	1:A:347:VAL:C	2.62	0.42
1:A:76:ASN:HB3	5:A:800:HEM:CAC	2.50	0.42
1:A:426:TRP:O	1:A:430:LEU:HD22	2.19	0.42
1:A:465:VAL:HG13	9:A:589:HOH:O	2.19	0.42
1:A:449:ARG:NH2	5:A:800:HEM:O2D	2.53	0.42
1:A:554:ASN:ND2	2:B:52:ARG:HB3	2.35	0.42
1:A:61:PHE:HD2	1:A:125:LEU:O	2.03	0.42
1:A:310:LEU:HD23	1:A:310:LEU:HA	1.71	0.42
1:A:343:ASN:O	1:A:346:PHE:N	2.52	0.42
1:A:382:PRO:HA	1:A:385:PHE:CE2	2.55	0.42
2:B:125:VAL:HG11	2:B:135:VAL:CG1	2.50	0.42
1:A:441:TRP:CG	8:C:804:BNG:H5'2	2.55	0.41
1:A:251:LEU:N	1:A:252:PRO:CD	2.83	0.41
1:A:518:ARG:HG3	1:A:518:ARG:NH2	2.29	0.41
1:A:547:VAL:C	1:A:549:LEU:H	2.28	0.41
2:B:66:ASP:HA	2:B:67:PRO:HD2	1.85	0.41
1:A:59:LEU:O	1:A:61:PHE:N	2.54	0.41
1:A:481:LEU:HD12	1:A:481:LEU:HA	1.85	0.41
5:A:800:HEM:HAC	5:A:800:HEM:HMC2	1.75	0.41
2:B:60:GLN:O	2:B:61:GLU:CB	2.68	0.41
1:A:82:GLN:HE21	1:A:86:GLN:CD	2.26	0.41
1:A:135:PHE:HD1	1:A:135:PHE:O	2.03	0.41
1:A:450:ARG:O	2:B:157:HIS:CD2	2.73	0.41
1:A:56:LYS:HE2	1:A:60:PRO:HA	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:141:GLY:H	1:A:146:TYR:HE1	1.68	0.41
1:A:402:TYR:N	1:A:402:TYR:CD2	2.89	0.41
1:A:435:MET:O	1:A:439:LEU:HB2	2.21	0.41
1:A:449:ARG:NH1	6:A:801:HAS:O2A	2.54	0.41
2:B:23:LEU:O	2:B:27:PHE:HD2	2.04	0.41
1:A:16:PRO:HG2	1:A:103:MET:HG2	2.01	0.41
1:A:351:LEU:HB3	1:A:429:PHE:CD2	2.55	0.41
1:A:371:LEU:HD12	1:A:371:LEU:H	1.83	0.41
1:A:465:VAL:N	1:A:466:PRO:HD2	2.36	0.41
1:A:545:THR:O	1:A:549:LEU:HB2	2.21	0.41
1:A:82:GLN:HG3	1:A:238:PHE:CE1	2.56	0.41
1:A:521:VAL:HA	1:A:524:MET:HE2	2.03	0.40
1:A:143:TRP:HB2	1:A:213:PHE:CD2	2.56	0.40
1:A:230:TRP:CZ3	1:A:546:LEU:CD1	3.02	0.40
1:A:537:LEU:HD23	1:A:537:LEU:HA	1.90	0.40
2:B:113:ILE:HA	2:B:129:PRO:HD3	2.03	0.40
1:A:8:ILE:CD1	1:A:9:SER:H	2.34	0.40
1:A:226:THR:HA	1:A:284:GLN:OE1	2.22	0.40
1:A:141:GLY:O	1:A:142:HIS:C	2.64	0.40
1:A:344:PRO:HA	1:A:422:LEU:HD23	2.01	0.40
1:A:433:MET:O	1:A:436:ALA:HB3	2.21	0.40
2:B:121:THR:HA	3:C:33:ARG:HB3	2.02	0.40
1:A:24:PHE:HD2	1:A:83:LEU:HD22	1.85	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	555/618 (90%)	444 (80%)	86 (16%)	25 (4%)	2 8
2	B	164/166 (99%)	147 (90%)	14 (8%)	3 (2%)	6 25

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	31/33 (94%)	25 (81%)	4 (13%)	2 (6%)	1	3
All	All	750/817 (92%)	616 (82%)	104 (14%)	30 (4%)	2	9

All (30) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ILE
1	A	142	HIS
1	A	410	GLY
1	A	497	ARG
1	A	508	PHE
1	A	512	ILE
2	B	4	GLN
2	B	61	GLU
1	A	162	ILE
1	A	546	LEU
1	A	552	HIS
2	B	87	ALA
1	A	102	ASN
1	A	135	PHE
1	A	185	MET
1	A	369	PHE
1	A	495	ARG
3	C	3	GLU
1	A	9	SER
1	A	280	GLY
1	A	496	GLU
1	A	94	ALA
1	A	205	VAL
1	A	318	ALA
1	A	536	ILE
1	A	87	ALA
1	A	169	ARG
1	A	411	LYS
1	A	180	PRO
3	C	29	VAL

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	453/503 (90%)	382 (84%)	71 (16%)	2	9
2	B	136/136 (100%)	112 (82%)	24 (18%)	2	6
3	C	26/26 (100%)	22 (85%)	4 (15%)	2	9
All	All	615/665 (92%)	516 (84%)	99 (16%)	2	8

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLU
1	A	8	ILE
1	A	10	ARG
1	A	22	LEU
1	A	25	LEU
1	A	30	LEU
1	A	48	ASN
1	A	54	LEU
1	A	56	LYS
1	A	59	LEU
1	A	64	SER
1	A	78	ILE
1	A	89	MET
1	A	95	ARG
1	A	115	ILE
1	A	125	LEU
1	A	127	ASN
1	A	140	LYS
1	A	142	HIS
1	A	155	SER
1	A	165	ASP
1	A	166	LEU
1	A	168	ARG
1	A	177	LYS
1	A	185	MET
1	A	188	VAL
1	A	195	LEU
1	A	215	LEU
1	A	216	VAL
1	A	222	LEU

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Mol	Chain	Res	Type
1	A	223	VAL
1	A	225	ARG
1	A	235	ILE
1	A	253	LYS
1	A	254	GLN
1	A	258	ARG
1	A	262	ASP
1	A	271	LEU
1	A	274	LEU
1	A	301	LEU
1	A	309	SER
1	A	325	ARG
1	A	327	ARG
1	A	330	ARG
1	A	337	ARG
1	A	339	LEU
1	A	342	ASP
1	A	354	LEU
1	A	422	LEU
1	A	424	VAL
1	A	430	LEU
1	A	435	MET
1	A	439	LEU
1	A	449	ARG
1	A	450	ARG
1	A	465	VAL
1	A	472	LEU
1	A	493	LEU
1	A	495	ARG
1	A	497	ARG
1	A	501	LEU
1	A	512	ILE
1	A	513	SER
1	A	516	GLU
1	A	518	ARG
1	A	519	ARG
1	A	520	LEU
1	A	536	ILE
1	A	547	VAL
1	A	548	GLN
1	A	549	LEU
2	B	4	GLN

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Mol	Chain	Res	Type
2	B	6	LYS
2	B	9	LYS
2	B	12	LEU
2	B	19	LEU
2	B	23	LEU
2	B	26	LEU
2	B	37	LEU
2	B	39	THR
2	B	44	VAL
2	B	49	LYS
2	B	58	VAL
2	B	60	GLN
2	B	66	ASP
2	B	72	VAL
2	B	78	GLN
2	B	102	GLU
2	B	106	LYS
2	B	107	ILE
2	B	112	VAL
2	B	125	VAL
2	B	128	LEU
2	B	166	VAL
2	B	168	GLU
3	C	3	GLU
3	C	6	LYS
3	C	13	LEU
3	C	24	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	ASN
1	A	76	ASN
1	A	127	ASN
1	A	254	GLN
1	A	298	HIS
1	A	407	ASN
1	A	446	ASN
1	A	470	ASN
2	B	5	HIS
2	B	69	GLN
2	B	77	ASN

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Mol	Chain	Res	Type
2	B	78	GLN
2	B	122	ASN
2	B	151	GLN
2	B	159	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 5 ligands modelled in this entry, 1 is monoatomic - leaving 4 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	HEM	A	800	1	50,50,50	2.30	15 (30%)	67,82,82	2.27	22 (32%)
8	BNG	C	804	-	21,21,21	1.13	1 (4%)	26,26,26	2.20	7 (26%)
6	HAS	A	801	1	72,72,72	2.49	26 (36%)	87,109,109	2.64	31 (35%)
7	CUA	B	802	2	0,1,1	-	-	-	-	-

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
5	HEM	A	800	1	-	2/14/54/54	-
8	BNG	C	804	-	-	7/12/32/32	0/1/1/1
6	HAS	A	801	1	1/1/8/18	6/42/82/82	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	800	HEM	FE-NC	7.58	2.20	1.95
5	A	800	HEM	C3D-C2D	7.32	1.52	1.36
6	A	801	HAS	CAC-C3C	-5.44	1.32	1.47
6	A	801	HAS	CHB-C1D	5.04	1.48	1.38
6	A	801	HAS	CHA-C4D	4.85	1.50	1.39
6	A	801	HAS	CHA-C1A	4.82	1.47	1.38
6	A	801	HAS	C2A-C3A	4.79	1.47	1.36
6	A	801	HAS	FE-ND	4.77	2.09	1.94
6	A	801	HAS	FE-NB	4.65	2.09	1.94
6	A	801	HAS	FE-NA	4.48	2.09	1.95
6	A	801	HAS	C2D-C3D	4.34	1.47	1.37
6	A	801	HAS	C1D-ND	-4.31	1.32	1.40
6	A	801	HAS	CHC-C1C	4.19	1.48	1.39
6	A	801	HAS	FE-NC	4.15	2.08	1.95
6	A	801	HAS	CHD-C4A	4.10	1.46	1.38
5	A	800	HEM	FE-NA	-3.82	1.82	1.95
5	A	800	HEM	CAB-C3B	3.63	1.57	1.47
6	A	801	HAS	CHC-C4B	3.60	1.45	1.38
6	A	801	HAS	C4A-NA	-3.55	1.32	1.39
5	A	800	HEM	CMB-C2B	3.51	1.58	1.50
8	C	804	BNG	O1-C1	3.31	1.45	1.40
6	A	801	HAS	C4D-C3D	-3.21	1.39	1.45
5	A	800	HEM	CAC-C3C	3.20	1.55	1.47
6	A	801	HAS	C11-C3B	-3.19	1.47	1.51
6	A	801	HAS	CMD-C2D	3.05	1.52	1.45
6	A	801	HAS	CHB-C1B	3.04	1.46	1.39
5	A	800	HEM	CMA-C3A	3.04	1.57	1.50
6	A	801	HAS	C4A-C3A	3.03	1.51	1.45
6	A	801	HAS	C4B-C3B	-3.02	1.39	1.44
6	A	801	HAS	CHD-C4C	2.93	1.46	1.39
6	A	801	HAS	C1B-NB	-2.65	1.33	1.38
5	A	800	HEM	C2A-C3A	-2.63	1.32	1.38
5	A	800	HEM	C4B-NB	2.62	1.44	1.38
6	A	801	HAS	C3C-C4C	2.51	1.50	1.42
6	A	801	HAS	C4C-NC	-2.47	1.35	1.39
5	A	800	HEM	CHB-C4A	-2.46	1.33	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	801	HAS	C3B-C2B	2.40	1.40	1.34
5	A	800	HEM	O1A-CGA	2.31	1.29	1.22
5	A	800	HEM	CMD-C2D	2.30	1.55	1.50
5	A	800	HEM	C1C-NC	2.24	1.43	1.39
5	A	800	HEM	CBB-CAB	2.20	1.40	1.30
5	A	800	HEM	C1B-NB	-2.02	1.36	1.40

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	801	HAS	CBC-CAC-C3C	9.26	173.81	127.53
6	A	801	HAS	C2D-C3D-C4D	-7.96	100.67	106.43
5	A	800	HEM	CAC-C3C-C4C	6.80	141.05	124.82
5	A	800	HEM	CHC-C1C-NC	6.55	131.58	124.45
8	C	804	BNG	O1-C1-C2	6.10	117.54	108.27
6	A	801	HAS	CMC-C2C-C1C	5.89	134.39	125.42
8	C	804	BNG	C1-O5-C5	5.72	124.90	113.72
6	A	801	HAS	C3D-C4D-ND	5.44	115.61	110.35
5	A	800	HEM	C3C-C2C-C1C	4.99	111.77	107.05
6	A	801	HAS	C3C-C2C-C1C	-4.92	101.37	107.17
6	A	801	HAS	C2A-C1A-NA	4.81	114.97	110.32
6	A	801	HAS	C24-C23-C22	4.78	131.90	121.17
6	A	801	HAS	C21-C22-C23	-4.73	116.80	127.62
6	A	801	HAS	C3B-C4B-NB	4.72	115.26	109.84
5	A	800	HEM	CAD-C3D-C4D	4.61	132.74	124.70
5	A	800	HEM	CMD-C2D-C1D	4.59	132.21	125.03
6	A	801	HAS	CAD-C3D-C4D	4.49	132.52	124.70
8	C	804	BNG	O5-C5-C4	4.41	117.64	109.70
5	A	800	HEM	CAC-C3C-C2C	-4.33	114.35	128.43
6	A	801	HAS	C2C-C1C-NC	3.97	116.51	110.14
6	A	801	HAS	CHA-C1A-C2A	-3.94	118.64	124.86
6	A	801	HAS	CAA-CBA-CGA	-3.80	103.58	113.67
6	A	801	HAS	CAD-CBD-CGD	-3.80	103.59	113.67
6	A	801	HAS	C2B-C1B-NB	3.67	114.14	109.90
6	A	801	HAS	C25-C23-C22	-3.49	114.65	123.63
6	A	801	HAS	C4A-C3A-C2A	-3.46	101.84	106.97
5	A	800	HEM	CHB-C1B-NB	3.44	128.62	124.37
6	A	801	HAS	CMA-C3A-C4A	3.44	130.78	124.73
5	A	800	HEM	CHD-C4C-NC	-3.27	120.89	124.45
6	A	801	HAS	C3A-C4A-NA	3.17	115.50	109.64
5	A	800	HEM	CHA-C4D-ND	3.17	128.28	124.37
5	A	800	HEM	CHD-C1D-ND	3.14	127.80	124.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	800	HEM	CHC-C4B-NB	3.07	127.73	124.42
6	A	801	HAS	O11-C11-C3B	-3.03	105.70	111.26
8	C	804	BNG	O2-C2-C1	3.03	117.29	110.08
5	A	800	HEM	CAD-C3D-C2D	-3.01	122.22	127.87
6	A	801	HAS	C4B-NB-C1B	-3.00	101.65	105.21
5	A	800	HEM	CAD-CBD-CGD	-2.93	105.89	113.67
6	A	801	HAS	C27-C19-C18	-2.84	116.33	123.63
6	A	801	HAS	CHA-C4D-C3D	-2.83	120.65	124.77
5	A	800	HEM	CMC-C2C-C3C	-2.80	121.66	128.43
5	A	800	HEM	O1A-CGA-CBA	-2.70	114.54	123.09
5	A	800	HEM	C1C-CHC-C4B	-2.62	120.46	126.02
5	A	800	HEM	C4D-ND-C1D	2.61	108.29	105.21
6	A	801	HAS	CHC-C4B-NB	-2.57	121.19	124.37
6	A	801	HAS	C27-C19-C20	2.56	119.67	115.23
8	C	804	BNG	C1'-O1-C1	2.56	118.05	113.68
5	A	800	HEM	C4C-C3C-C2C	-2.55	104.60	106.81
6	A	801	HAS	C4B-C3B-C2B	-2.55	103.16	107.44
5	A	800	HEM	C4C-CHD-C1D	-2.46	120.80	126.02
6	A	801	HAS	CHD-C4A-NA	-2.46	121.78	124.45
8	C	804	BNG	C3-C4-C5	2.38	114.55	110.23
5	A	800	HEM	CHA-C4D-C3D	-2.37	120.85	125.23
6	A	801	HAS	CHB-C1B-NB	-2.22	122.04	124.42
6	A	801	HAS	C1A-C2A-C3A	-2.20	104.20	107.11
6	A	801	HAS	CHC-C1C-C2C	-2.13	121.23	127.43
5	A	800	HEM	CMB-C2B-C1B	-2.07	121.80	125.03
6	A	801	HAS	C1A-CHA-C4D	-2.06	121.63	126.02
5	A	800	HEM	CHC-C1C-C2C	-2.05	121.22	125.49
8	C	804	BNG	O5-C1-C2	-2.02	106.23	110.37

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	A	801	HAS	NA

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	C	804	BNG	O5-C5-C6-O6
8	C	804	BNG	C4-C5-C6-O6
8	C	804	BNG	O1-C1'-C2'-C3'
8	C	804	BNG	C2-C1-O1-C1'
8	C	804	BNG	O5-C1-O1-C1'

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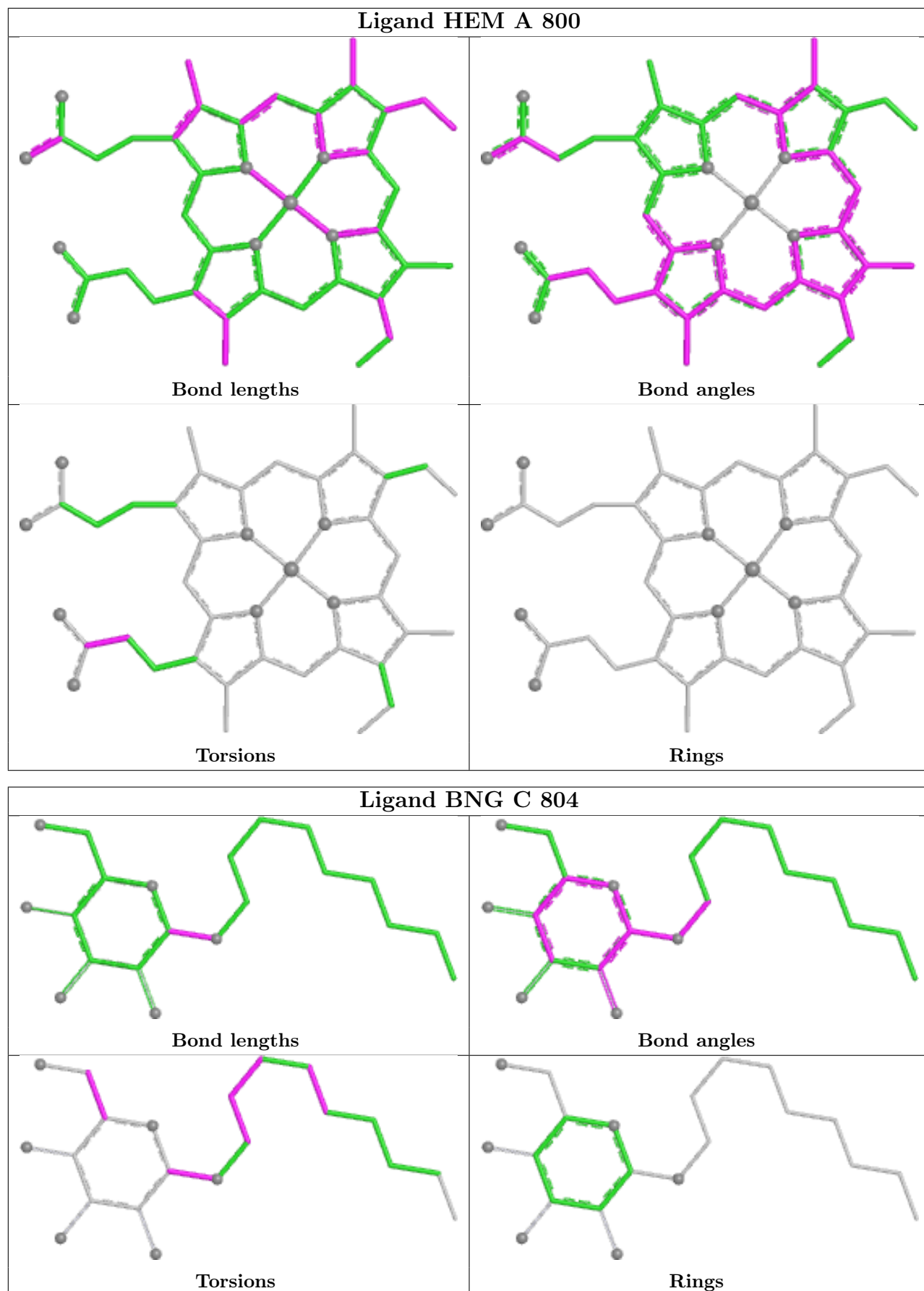
Mol	Chain	Res	Type	Atoms
6	A	801	HAS	C22-C23-C24-C28
8	C	804	BNG	C3'-C4'-C5'-C6'
6	A	801	HAS	C25-C23-C24-C28
6	A	801	HAS	CAA-CBA-CGA-O1A
6	A	801	HAS	CAD-CBD-CGD-O1D
5	A	800	HEM	CAD-CBD-CGD-O1D
8	C	804	BNG	C1'-C2'-C3'-C4'
6	A	801	HAS	CAD-CBD-CGD-O2D
5	A	800	HEM	CAD-CBD-CGD-O2D
6	A	801	HAS	CAA-CBA-CGA-O2A

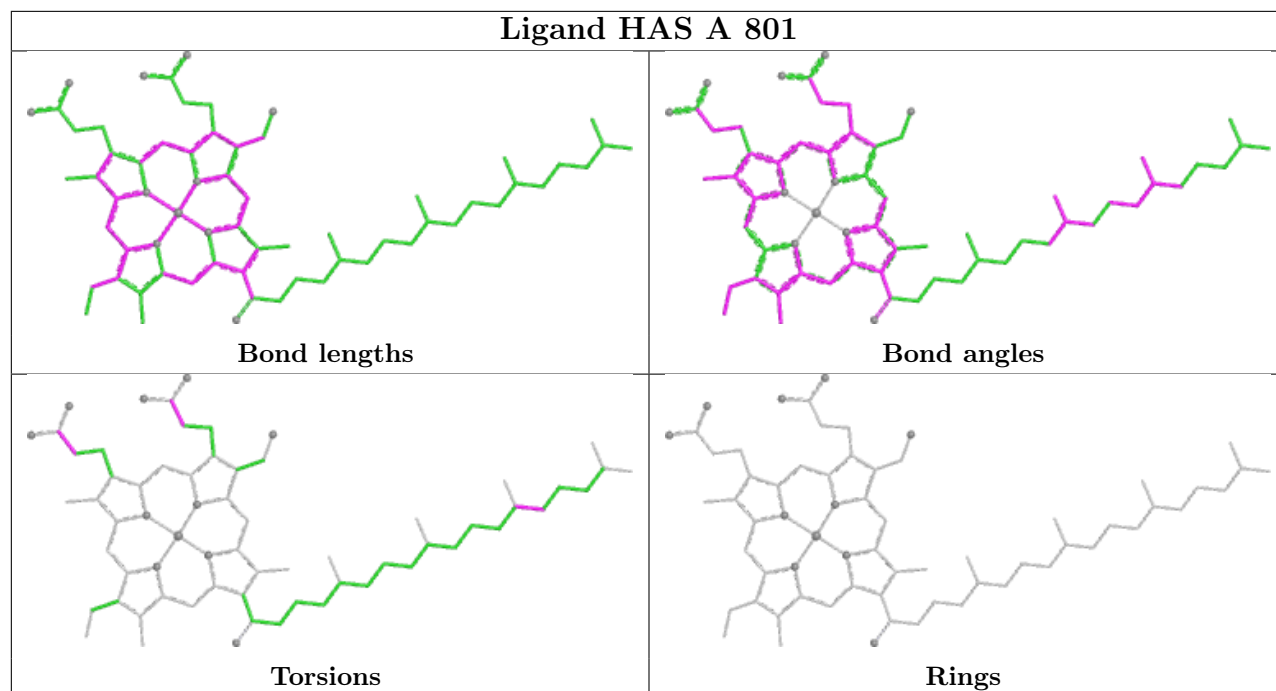
There are no ring outliers.

3 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	800	HEM	8	0
8	C	804	BNG	1	0
6	A	801	HAS	7	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, 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	557/618 (90%)	1.07	67 (12%) 9 7	79, 103, 134, 183	0
2	B	166/166 (100%)	0.88	14 (8%) 17 14	84, 101, 137, 184	0
3	C	33/33 (100%)	0.87	1 (3%) 52 43	84, 91, 130, 158	0
All	All	756/817 (92%)	1.02	82 (10%) 11 9	79, 103, 135, 184	0

All (82) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	543	GLY	4.0
1	A	196	ALA	3.9
1	A	158	VAL	3.9
2	B	10	ALA	3.9
1	A	493	LEU	3.7
2	B	7	ALA	3.7
2	B	11	ILE	3.5
1	A	227	LEU	3.5
1	A	487	GLY	3.4
1	A	126	ALA	3.3
1	A	461	PRO	3.2
3	C	25	GLY	3.1
1	A	178	VAL	3.0
1	A	223	VAL	3.0
1	A	390	ALA	3.0
1	A	460	TYR	2.9
1	A	470	ASN	2.9
1	A	6	SER	2.9
1	A	109	SER	2.9
1	A	479	VAL	2.9
1	A	206	LEU	2.9
1	A	402	TYR	2.9
1	A	159	SER	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	335	TRP	2.8
1	A	381	VAL	2.8
2	B	143	GLY	2.8
2	B	154	GLY	2.8
1	A	279	VAL	2.8
1	A	464	ALA	2.8
1	A	555	PRO	2.8
1	A	472	LEU	2.7
1	A	115	ILE	2.7
1	A	328	GLY	2.7
1	A	172	ALA	2.7
2	B	82	TYR	2.7
1	A	324	GLY	2.6
1	A	7	GLU	2.6
1	A	104	GLY	2.5
1	A	421	GLY	2.5
1	A	549	LEU	2.4
1	A	428	TRP	2.4
2	B	47	ALA	2.4
1	A	453	ILE	2.4
1	A	101	PRO	2.4
2	B	3	ASP	2.3
1	A	46	TYR	2.3
2	B	15	GLU	2.3
1	A	133	TYR	2.3
1	A	284	GLN	2.3
1	A	541	ALA	2.2
1	A	327	ARG	2.2
2	B	74	THR	2.2
1	A	12	TYR	2.2
1	A	255	ALA	2.2
1	A	483	LEU	2.2
1	A	424	VAL	2.2
1	A	141	GLY	2.2
2	B	76	PRO	2.2
1	A	330	ARG	2.1
1	A	475	ILE	2.1
1	A	76	ASN	2.1
1	A	488	LEU	2.1
1	A	539	VAL	2.1
1	A	542	TYR	2.1
2	B	8	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	41	PHE	2.1
2	B	55	PRO	2.1
1	A	497	ARG	2.1
1	A	451	ALA	2.1
1	A	473	ALA	2.1
1	A	221	PRO	2.0
2	B	155	LEU	2.0
1	A	43	ALA	2.0
1	A	49	VAL	2.0
1	A	198	LEU	2.0
1	A	215	LEU	2.0
1	A	422	LEU	2.0
1	A	474	GLY	2.0
1	A	527	ILE	2.0
1	A	441	TRP	2.0
1	A	187	VAL	2.0
1	A	468	VAL	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](#)

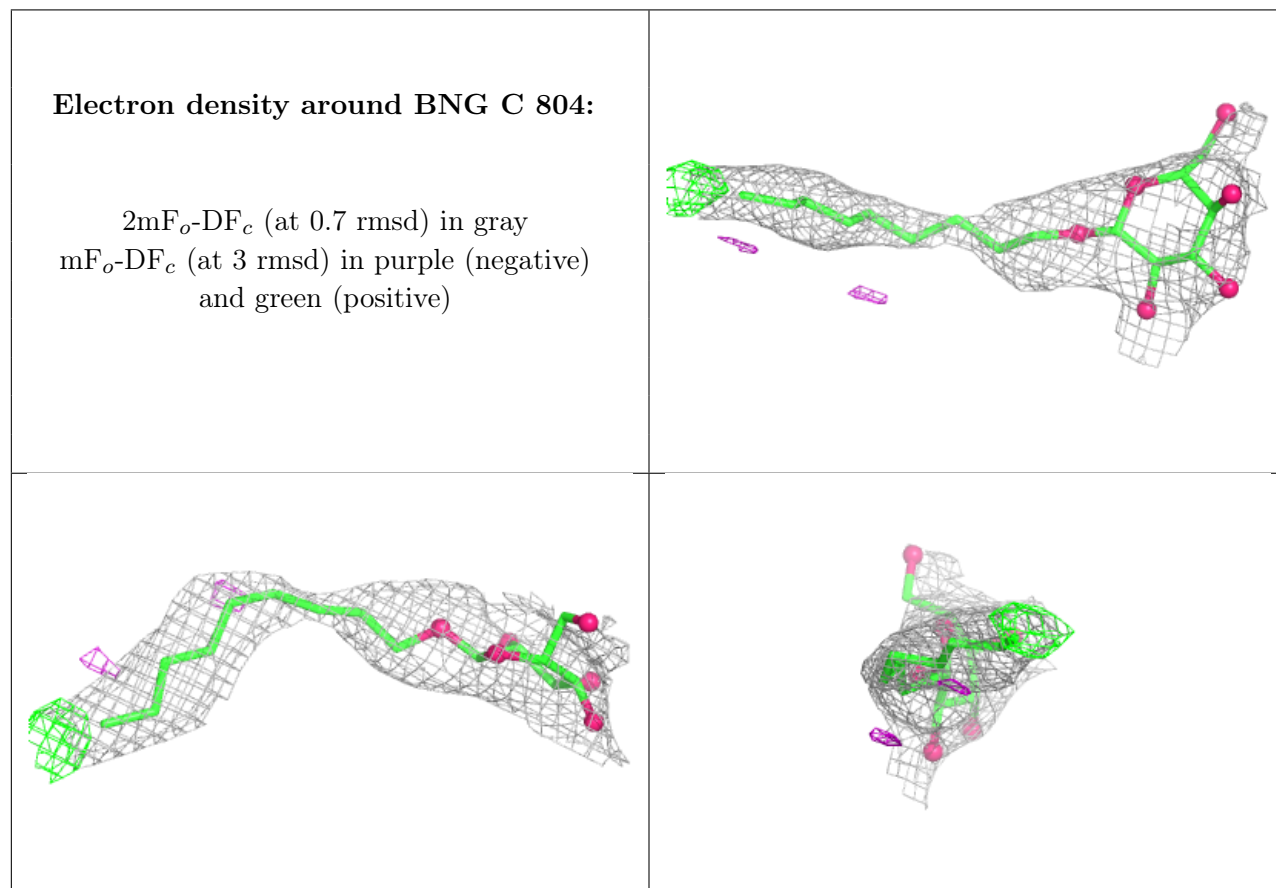
There are no oligosaccharides in this entry.

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.

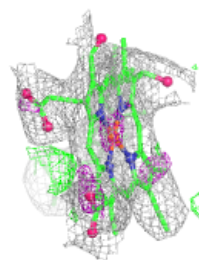
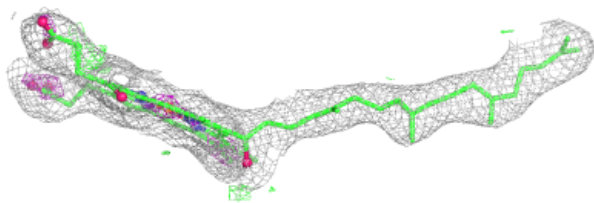
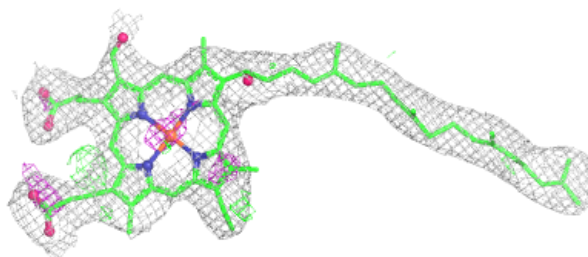
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
8	BNG	C	804	21/21	0.70	0.16	103,136,151,152	0
6	HAS	A	801	65/65	0.94	0.12	83,92,97,101	0
5	HEM	A	800	43/43	0.95	0.12	78,87,100,103	0
7	CUA	B	802	2/2	0.97	0.12	111,111,111,114	0
4	CU1	A	803	1/1	1.00	0.10	98,98,98,98	0

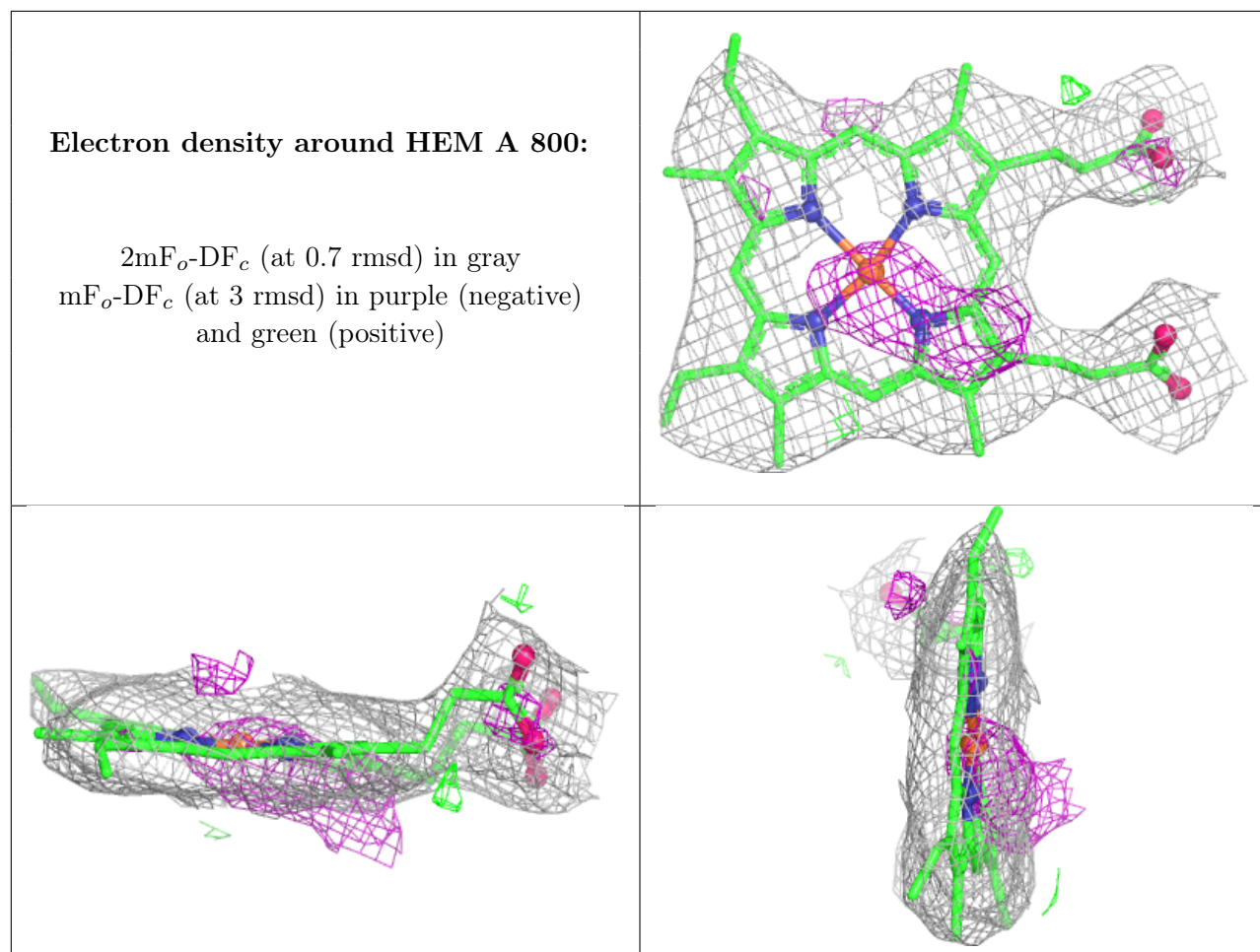
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around HAS A 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 ⓘ

There are no such residues in this entry.