Full wwPDB X-ray Structure Validation Report ⓘ

Aug 23, 2023 – 03:52 AM EDT

PDB ID : 3EH4
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
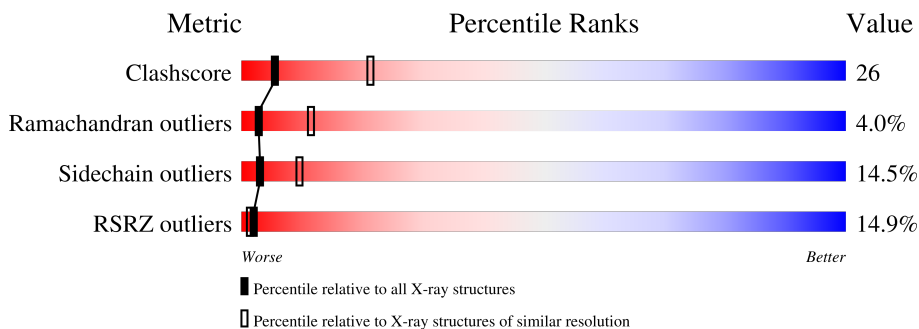http://www.wwpdb.org/validation/2017/FAQs#types.

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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	Percentile Ranks	Value
Clashscore		26
Ramachandran outliers		4.0%
Sidechain outliers		14.5%
RSRZ outliers		14.9%

Worse   *Better*

■ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (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 <=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	14% — 44% / 36% / 8% · 10%
2	B	166	14% — 56% / 37% / 7% ·
3	C	33	6% — 67% / 24% / 6% ·

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
			Total	C	N	O	S			
2	B	166	1298	844	217	233	4	0	0	0

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 259	C 179	N 39	O 41	0	0	0

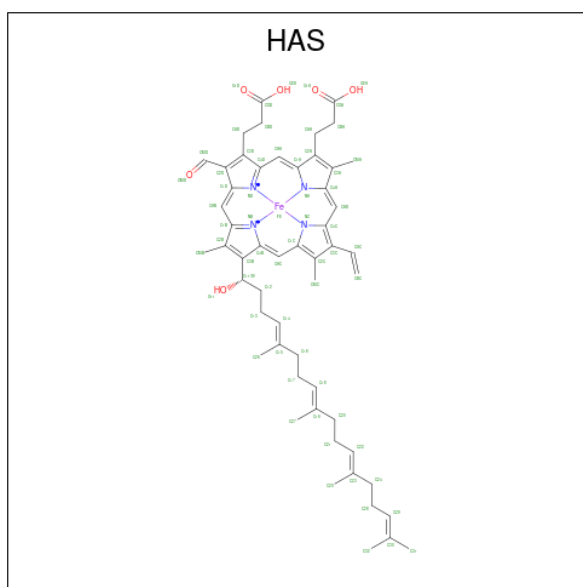- Molecule 4 is COPPER (I) ION (three-letter code: CU1) (formula: Cu).

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

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
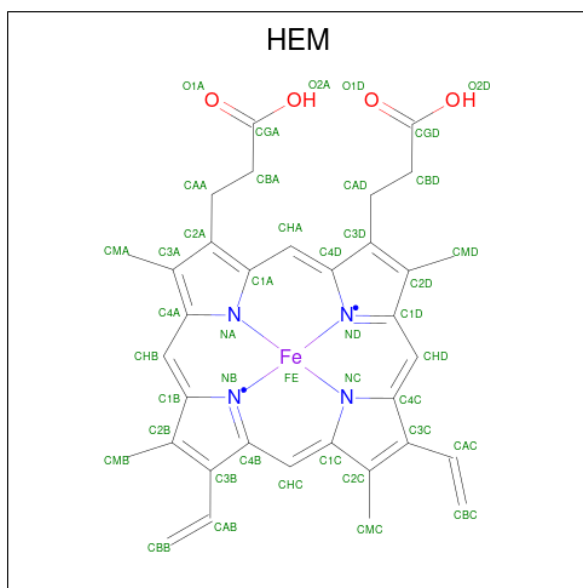
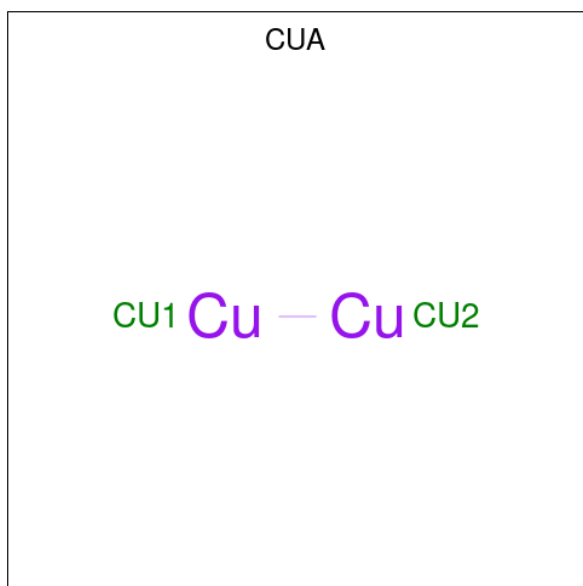| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

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

HAS

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

- Molecule 7 is DINUCLEAR COPPER ION (three-letter code: CUA) (formula: Cu_2).

CUA

CU1 **Cu** — **Cu** CU2

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

- Molecule 8 is nonyl beta-D-glucopyranoside (three-letter code: BNG) (formula: $C_{15}H_{30}O_6$).

BNG

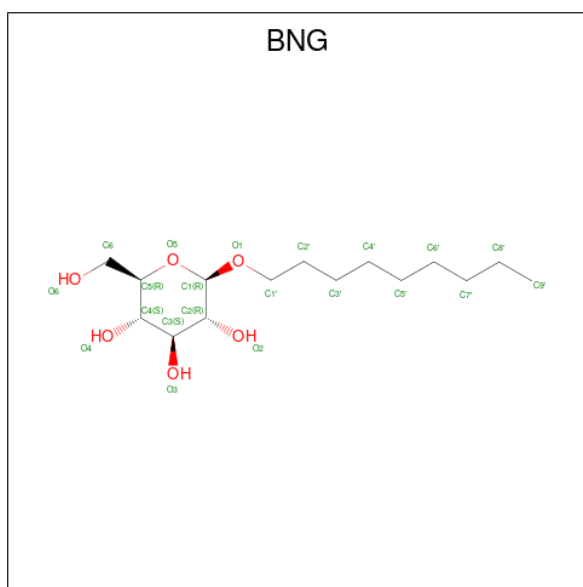

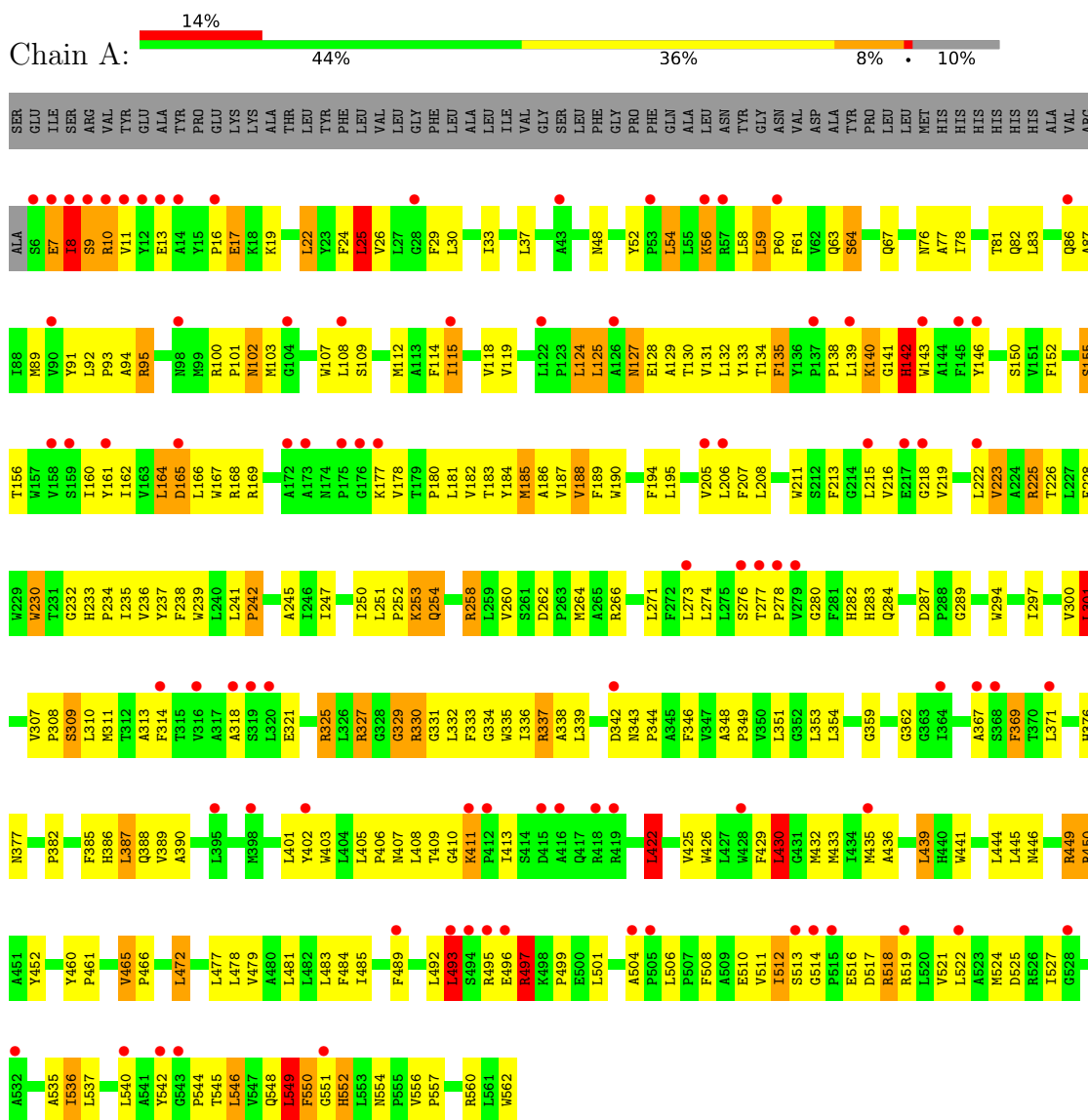| Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	C	1	Total 21	C 15	O 6	0	0

- Molecule 9 is water.

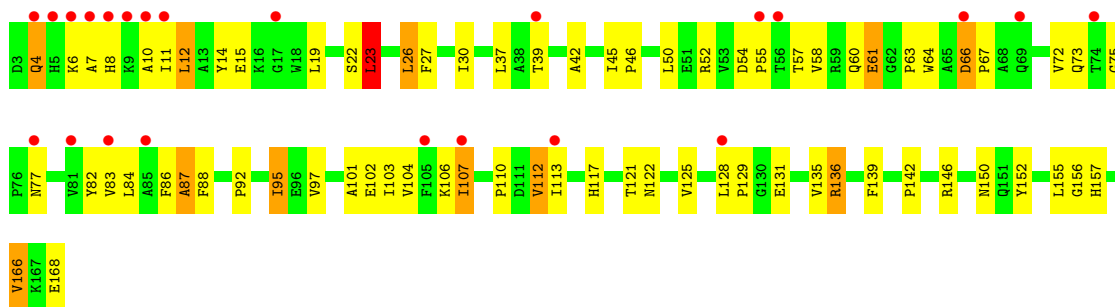| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	34	Total 34	O 34	0	0
9	B	10	Total 10	O 10	0	0
9	C	1	Total 1	O 1	0	0

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

D3 Q4 H5 K6 A7 H8 K9 A10 I11 L12 A13 Y14 E15 K16 G17 W18 L19 S22 L23 L26 F27 I30 L37 A38 T39 A42 I45 P46 L50 E51 R52 V53 D54 P55 T56 T57 V58 R59 Q60 E61 G62 P63 W64 A65 D66 P67 A68 Q69 V72 Q73 T74 G75

P76 N77 V81 Y82 V83 L84 A85 F86 A87 F88 P92 I95 E96 V97 A101 E102 I103 V104 F105 K106 I107 P110 D111 V112 I113 H117 T121 N122 V125 L128 P129 G130 E131 V135 R136 F139 P142 R146 N150 Q151 Y152 L155 G156 H157

V166 K167 E168

• Molecule 3: Cytochrome c oxidase polypeptide 2A

Chain C:

6%

67%   24%   6%   ·

E2 E3 K4 P5 K6 L9 L13 F22 W23 L24 A28 V29 R33 G34

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 – 2.60	Depositor EDS
% Data completeness (in resolution range)	99.5 (19.96-2.90) 97.6 (19.96-2.60)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.34 (at 2.59Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.198 , 0.268 0.213 , (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)	0.36 , 137.6	EDS
L-test for twinning[2]	$< |L| > = 0.50, < L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	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.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: BNG, CUA, CU1, HEM, HAS

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	1.02	3/4566 (0.1%)	1.06	16/6266 (0.3%)
2	B	1.06	0/1335	1.07	6/1822 (0.3%)
3	C	1.17	1/265 (0.4%)	0.99	0/359
All	All	1.04	4/6166 (0.1%)	1.06	22/8447 (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	A	0	3
2	B	0	1
All	All	0	4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	314	PHE	CB-CG	-5.53	1.42	1.51
1	A	337	ARG	CG-CD	5.30	1.65	1.51
3	C	22	PHE	CE2-CZ	5.21	1.47	1.37
1	A	230	TRP	CB-CG	5.10	1.59	1.50

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	493	LEU	CA-CB-CG	11.33	141.36	115.30
2	B	146	ARG	NE-CZ-NH1	-9.46	115.57	120.30
1	A	422	LEU	CA-CB-CG	7.57	132.71	115.30
1	A	301	LEU	CA-CB-CG	7.36	132.23	115.30

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WORLDWIDE

wwPDB

PROTEIN DATA BANK

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	492	LEU	CA-CB-CG	7.15	131.75	115.30
1	A	25	LEU	CA-CB-CG	7.06	131.53	115.30
1	A	164	LEU	CA-CB-CG	6.49	130.22	115.30
2	B	23	LEU	CA-CB-CG	-6.23	100.97	115.30
1	A	549	LEU	CA-CB-CG	6.22	129.62	115.30
2	B	136	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	A	472	LEU	CB-CG-CD2	-5.62	101.45	111.00
1	A	493	LEU	CB-CG-CD2	5.50	120.35	111.00
1	A	37	LEU	CA-CB-CG	5.34	127.58	115.30
2	B	146	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	A	430	LEU	CA-CB-CG	5.29	127.47	115.30
1	A	387	LEU	CA-CB-CG	-5.21	103.31	115.30
1	A	8	ILE	N-CA-C	5.20	125.05	111.00
1	A	206	LEU	CA-CB-CG	5.20	127.27	115.30
2	B	146	ARG	CB-CG-CD	-5.19	98.11	111.60
1	A	124	LEU	CA-CB-CG	5.16	127.17	115.30
1	A	478	LEU	CA-CB-CG	5.15	127.14	115.30
2	B	95	ILE	N-CA-C	-5.04	97.38	111.00

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 ⓘ

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	270	0
2	B	1298	0	1282	60	0
3	C	259	0	279	10	0
4	A	1	0	0	0	0
5	A	43	0	30	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	65	0	61	8	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	318	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 26.

All (318) 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:24:PHE:HZ	1:A:109:SER:HG	1.02	1.01
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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:511:VAL:O	1:A:511:VAL:HG12	1.94	0.66
1:A:24:PHE:CZ	1:A:109:SER:OG	2.45	0.66
1:A:211:TRP:HE1	1:A:218:GLY:HA2	1.60	0.66
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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:134:THR:O	1:A:135:PHE:C	2.38	0.62
1:A:330:ARG:HG3	1:A:330:ARG:NH2	2.13	0.62
1:A:16:PRO:O	1:A:103:MET:HE1	2.00	0.62
1:A:207:PHE:CZ	1:A:550:PHE:HE2	2.14	0.62
1:A:103:MET:HE3	1:A:107:TRP:NE1	2.14	0.62
1:A:108:LEU:O	1:A:112:MET:CB	2.41	0.61
1:A:103:MET:CE	1:A:107:TRP:HE1	2.12	0.61
1:A:344:PRO:CA	1:A:422:LEU:HD23	2.30	0.61
1:A:386:HIS:CD2	1:A:435:MET:HE1	2.36	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: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
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:103:MET:CE	1:A:107:TRP:NE1	2.67	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:103:MET:HE2	1:A:107:TRP:HE1	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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: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
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: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
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:138:PRO:HG2	2:B:129:PRO:HG2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:140:LYS:NZ	9:A:579:HOH:O	2.29	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:128:GLU:CD	1:A:560:ARG:HH22	2.15	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:511:VAL:O	1:A:512:ILE:C	2.50	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
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
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
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:101:PRO:O	1:A:102:ASN:C	2.50	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:390:ALA:HB1	1:A:432:MET:HE1	1.96	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
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
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
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: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:385:PHE:CG	6:A:801:HAS:HMA2	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:C:28:ALA:O	3:C:29:VAL:C	2.54	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: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:140:LYS:NZ	1:A:211:TRP:CE2	2.76	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:63:GLN:HB2	1:A:127:ASN:ND2	2.32	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: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
1:A:132:LEU:HG	2:B:152:TYR:CD2	2.53	0.43
1:A:233:HIS:CD2	1:A:233:HIS:C	2.90	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
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:390:ALA:HB1	1:A:432:MET:HE3	2.01	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
2:B:103:ILE:HD13	2:B:139:PHE:CD1	2.55	0.42
1:A:76:ASN:HB3	5:A:800:HEM:CAC	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:45:ILE:O	2:B:46:PRO:C	2.56	0.41
1:A:518:ARG:HG3	1:A:518:ARG:NH2	2.29	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: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
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
1:A:510:GLU:C	1:A:511:VAL:HG23	2.41	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
3:C:3:GLU:CD	3:C:4:LYS:H	2.24	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:521:VAL:HA	1:A:524:MET:HE2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 ⓘ

5.3.1 Protein backbone ⓘ

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	9
2	B	164/166 (99%)	147 (90%)	14 (8%)	3 (2%)	8	29
3	C	31/33 (94%)	25 (81%)	4 (13%)	2 (6%)	1	3
All	All	750/817 (92%)	616 (82%)	104 (14%)	30 (4%)	3	11

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

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Mol	Chain	Res	Type
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%)	387 (85%)	66 (15%)	3	9
2	B	136/136 (100%)	118 (87%)	18 (13%)	4	12
3	C	26/26 (100%)	21 (81%)	5 (19%)	1	4
All	All	615/665 (92%)	526 (86%)	89 (14%)	3	9

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ARG
1	A	17	GLU
1	A	22	LEU
1	A	25	LEU
1	A	30	LEU

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Mol	Chain	Res	Type
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	133	TYR
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	215	LEU
1	A	216	VAL
1	A	223	VAL
1	A	225	ARG
1	A	242	PRO
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	369	PHE

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Mol	Chain	Res	Type
1	A	422	LEU
1	A	430	LEU
1	A	439	LEU
1	A	449	ARG
1	A	450	ARG
1	A	452	TYR
1	A	465	VAL
1	A	472	LEU
1	A	493	LEU
1	A	497	ARG
1	A	501	LEU
1	A	513	SER
1	A	516	GLU
1	A	518	ARG
1	A	519	ARG
1	A	536	ILE
1	A	548	GLN
1	A	549	LEU
1	A	550	PHE
2	B	4	GLN
2	B	6	LYS
2	B	12	LEU
2	B	19	LEU
2	B	23	LEU
2	B	26	LEU
2	B	39	THR
2	B	58	VAL
2	B	66	ASP
2	B	72	VAL
2	B	77	ASN
2	B	102	GLU
2	B	106	LYS
2	B	107	ILE
2	B	112	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	23	TRP
3	C	24	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) 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
2	B	5	HIS
2	B	69	GLN
2	B	77	ASN
2	B	78	GLN
2	B	122	ASN
2	B	159	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
8	BNG	C	804	-	21,21,21	1.12	1 (4%)	26,26,26	2.18	6 (23%)
6	HAS	A	801	1	57,72,72	2.87	18 (31%)	48,109,109	2.13	13 (27%)
7	CUA	B	802	2	0,1,1	-	-		-	
5	HEM	A	800	1	41,50,50	2.21	14 (34%)	45,82,82	2.01	13 (28%)

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
6	HAS	A	801	1	-	7/40/122/122	-
8	BNG	C	804	-	-	7/12/32/32	0/1/1/1
5	HEM	A	800	1	-	2/12/54/54	-

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	801	HAS	C2D-C3D	11.20	1.47	1.36
5	A	800	HEM	C3D-C2D	7.44	1.52	1.36
6	A	801	HAS	CHA-C4D	7.40	1.50	1.37
6	A	801	HAS	C3C-CAC	-7.35	1.32	1.47
6	A	801	HAS	CHB-C1D	4.89	1.48	1.39
6	A	801	HAS	CHC-C4B	4.73	1.45	1.37
5	A	800	HEM	C3C-C2C	-4.73	1.33	1.40
6	A	801	HAS	CMD-C2D	4.47	1.52	1.44
5	A	800	HEM	C3C-CAC	3.96	1.55	1.47
6	A	801	HAS	CHC-C1C	3.93	1.48	1.40
6	A	801	HAS	CHD-C4A	3.90	1.46	1.39
6	A	801	HAS	C3C-C4C	3.81	1.50	1.40
6	A	801	HAS	CHD-C4C	3.67	1.46	1.39
6	A	801	HAS	CHB-C1B	3.59	1.46	1.39
5	A	800	HEM	CAB-C3B	3.54	1.57	1.47
6	A	801	HAS	CHA-C1A	3.47	1.47	1.40
5	A	800	HEM	CMB-C2B	3.39	1.58	1.50
8	C	804	BNG	O1-C1	3.24	1.45	1.40
6	A	801	HAS	C3C-C2C	3.23	1.44	1.40
6	A	801	HAS	C2A-C3A	3.18	1.47	1.37
6	A	801	HAS	C1D-C2D	-2.83	1.41	1.45
5	A	800	HEM	C2C-C1C	2.66	1.48	1.42
5	A	800	HEM	CMA-C3A	2.58	1.57	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	800	HEM	C4A-CHB	-2.55	1.33	1.41
5	A	800	HEM	C4B-NB	2.51	1.44	1.38
6	A	801	HAS	CAA-C2A	-2.46	1.47	1.52
6	A	801	HAS	C3B-C2B	2.42	1.40	1.34
5	A	800	HEM	C1A-NA	2.35	1.41	1.36
5	A	800	HEM	O1A-CGA	2.26	1.29	1.22
5	A	800	HEM	CMD-C2D	2.21	1.55	1.50
5	A	800	HEM	CBB-CAB	2.15	1.40	1.30
6	A	801	HAS	C1D-ND	-2.10	1.32	1.36
5	A	800	HEM	C1B-NB	-2.07	1.36	1.40

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	804	BNG	O1-C1-C2	5.92	117.54	108.30
8	C	804	BNG	C1-O5-C5	5.71	124.90	113.69
6	A	801	HAS	C4B-C3B-C2B	-5.48	103.16	108.79
6	A	801	HAS	C24-C23-C22	5.33	131.90	121.12
5	A	800	HEM	CMD-C2D-C1D	4.71	132.21	125.04
6	A	801	HAS	CAD-CBD-CGD	-4.65	103.59	113.60
5	A	800	HEM	CAD-C3D-C4D	4.62	132.74	124.66
6	A	801	HAS	C21-C22-C23	-4.51	116.80	127.66
8	C	804	BNG	O5-C5-C4	4.37	117.64	109.69
6	A	801	HAS	CAA-CBA-CGA	-3.63	103.58	113.76
6	A	801	HAS	C1D-CHB-C1B	3.58	128.77	119.86
5	A	800	HEM	CAD-CBD-CGD	-3.58	105.89	113.60
6	A	801	HAS	C25-C23-C22	-3.52	114.65	123.68
5	A	800	HEM	CHB-C1B-NB	3.43	128.62	124.38
5	A	800	HEM	C2C-C3C-C4C	-3.29	104.60	106.90
5	A	800	HEM	CHA-C4D-ND	3.16	128.28	124.38
6	A	801	HAS	C4B-CHC-C1C	3.14	127.17	118.67
5	A	800	HEM	C4D-ND-C1D	3.12	108.29	105.07
5	A	800	HEM	CHD-C1D-ND	3.10	127.80	124.43
5	A	800	HEM	CAD-C3D-C2D	-3.04	122.22	127.88
5	A	800	HEM	CHC-C4B-NB	3.03	127.73	124.43
8	C	804	BNG	O2-C2-C1	2.98	117.29	110.05
6	A	801	HAS	CAD-C3D-C4D	2.86	132.52	124.62
6	A	801	HAS	C27-C19-C18	-2.86	116.33	123.68
5	A	800	HEM	O1A-CGA-CBA	-2.66	114.54	123.08
6	A	801	HAS	C27-C19-C20	2.61	119.67	115.27
8	C	804	BNG	C1'-O1-C1	2.54	118.05	113.84
8	C	804	BNG	C3-C4-C5	2.42	114.55	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	A	800	HEM	CHA-C4D-C3D	-2.38	120.85	125.33
6	A	801	HAS	CHB-C1D-C2D	-2.19	123.16	126.66
6	A	801	HAS	C20-C21-C22	2.18	119.04	111.88
5	A	800	HEM	CMB-C2B-C1B	-2.13	121.80	125.04

There are no chirality outliers.

All (16) torsion outliers are listed below:

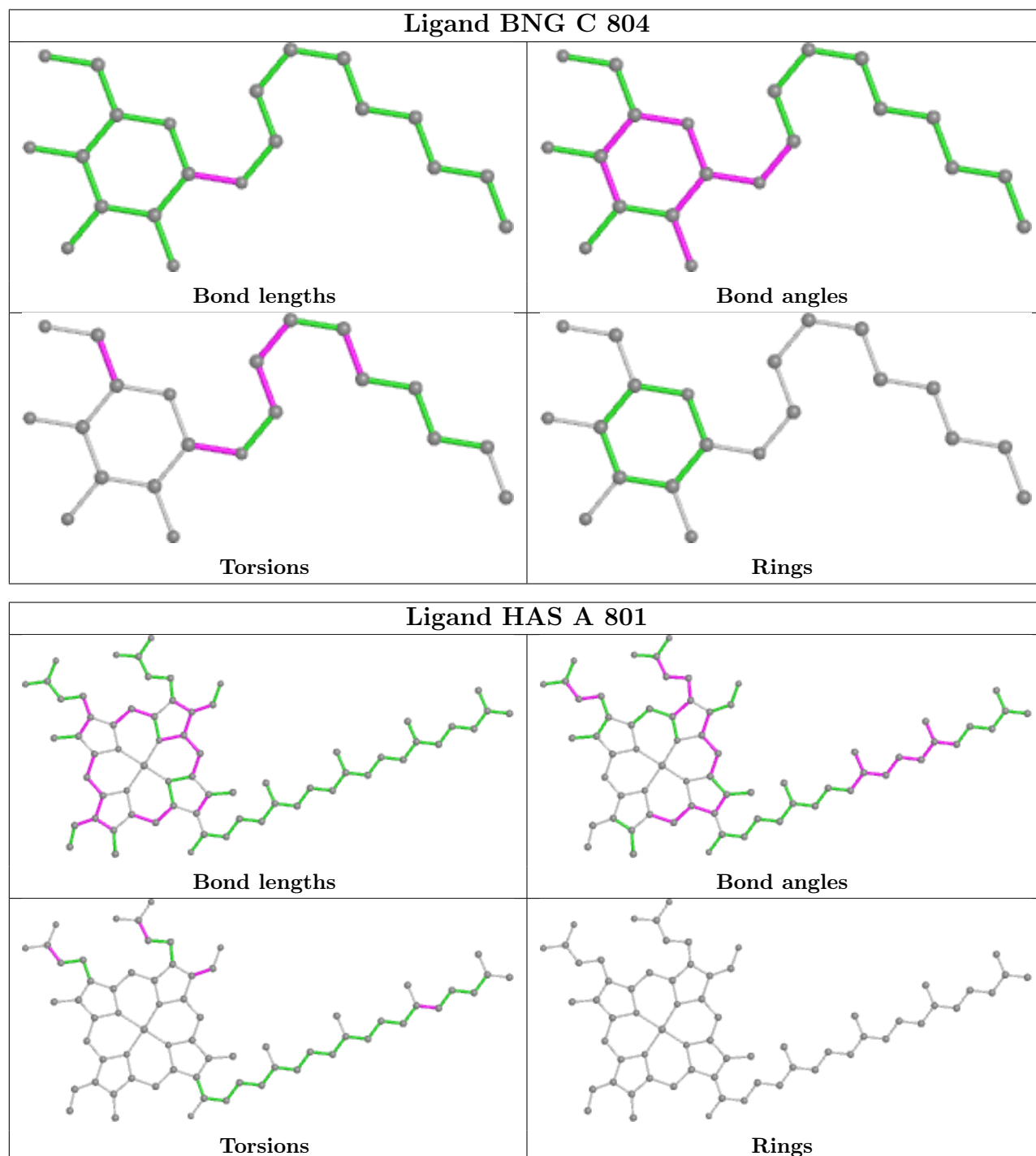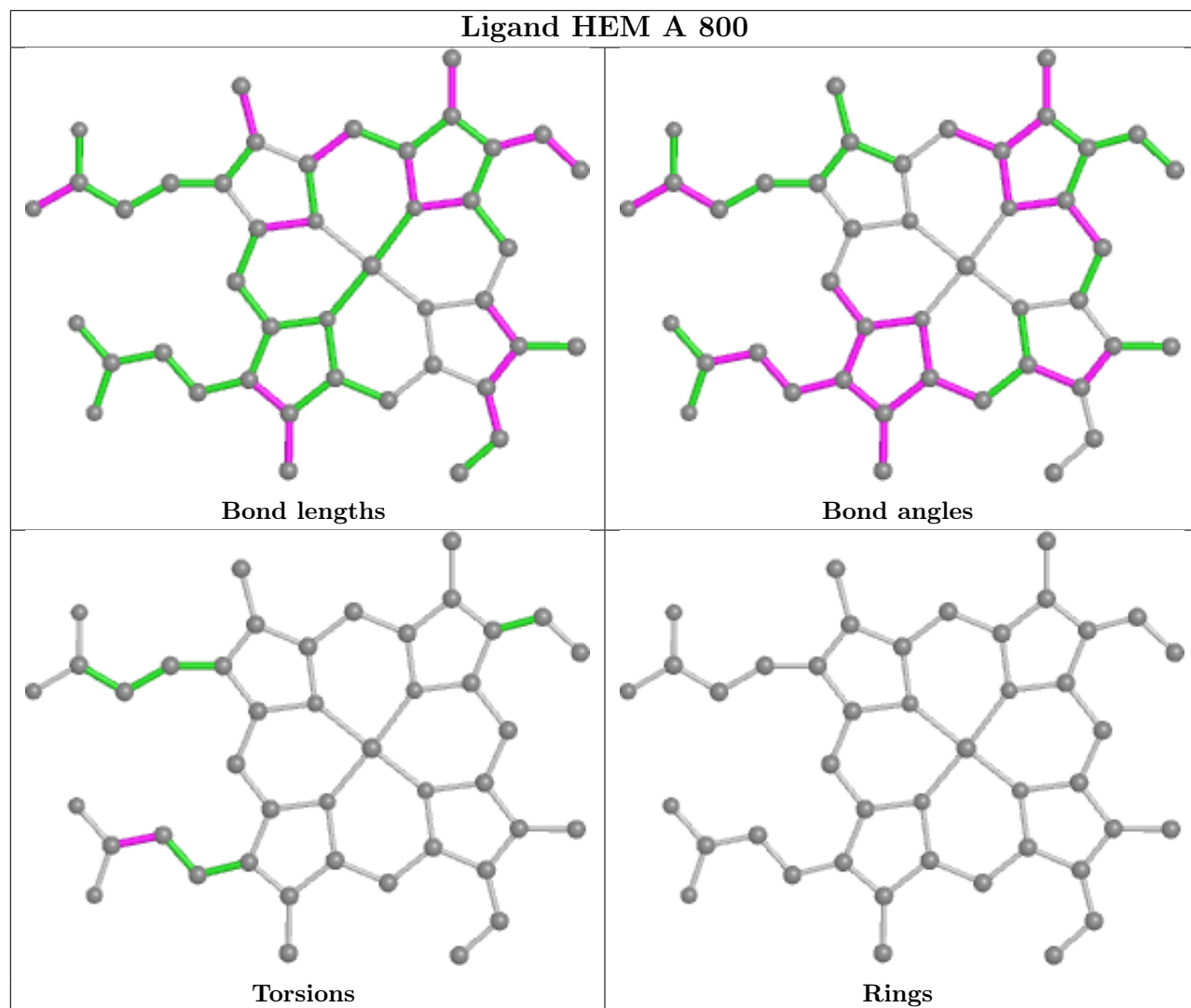| Mol	Chain	Res	Type	Atoms
8	C	804	BNG	O5-C5-C6-O6
8	C	804	BNG	C4-C5-C6-O6
8	C	804	BNG	O1-C1'-C2'-C3'
8	C	804	BNG	C2-C1-O1-C1'
8	C	804	BNG	O5-C1-O1-C1'
6	A	801	HAS	C22-C23-C24-C28
6	A	801	HAS	C25-C23-C24-C28
8	C	804	BNG	C3'-C4'-C5'-C6'
6	A	801	HAS	CAD-CBD-CGD-O1D
5	A	800	HEM	CAD-CBD-CGD-O1D
6	A	801	HAS	CAD-CBD-CGD-O2D
8	C	804	BNG	C1'-C2'-C3'-C4'
5	A	800	HEM	CAD-CBD-CGD-O2D
6	A	801	HAS	CAA-CBA-CGA-O1A
6	A	801	HAS	C1D-C2D-CMD-OMD
6	A	801	HAS	CAA-CBA-CGA-O2A

There are no ring outliers.

3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	C	804	BNG	1	0
6	A	801	HAS	8	0
5	A	800	HEM	8	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 then 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.

Ligand BNG C 804

Bond lengths

Bond angles

Torsions

Rings

Ligand HAS A 801

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 800

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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(Å²)	Q<0.9
1	A	557/618 (90%)	0.75	88 (15%)	2	1	79, 103, 134, 183	0
2	B	166/166 (100%)	0.58	23 (13%)	2	2	84, 101, 137, 184	0
3	C	33/33 (100%)	0.19	2 (6%)	21	17	84, 91, 130, 158	0
All	All	756/817 (92%)	0.69	113 (14%)	2	1	79, 103, 135, 184	0

All (113) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	493	LEU	9.3
1	A	494	SER	7.9
1	A	12	TYR	7.2
1	A	9	SER	6.7
1	A	7	GLU	6.5
1	A	8	ILE	6.5
1	A	402	TYR	6.2
1	A	143	TRP	5.7
2	B	10	ALA	5.5
1	A	10	ARG	4.9
2	B	5	HIS	4.9
1	A	172	ALA	4.9
1	A	496	GLU	4.5
1	A	173	ALA	4.4
1	A	528	GLY	4.3
1	A	543	GLY	4.3
3	C	2	GLU	4.0
1	A	11	VAL	4.0
1	A	415	ASP	3.9
1	A	215	LEU	3.9
1	A	416	ALA	3.8
1	A	277	THR	3.7
2	B	9	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	515	PRO	3.6
1	A	368	SER	3.6
1	A	28	GLY	3.6
1	A	6	SER	3.6
2	B	39	THR	3.6
1	A	320	LEU	3.5
1	A	551	GLY	3.4
1	A	56	LYS	3.4
1	A	139	LEU	3.4
1	A	16	PRO	3.4
1	A	98	ASN	3.4
2	B	7	ALA	3.4
1	A	318	ALA	3.3
1	A	217	GLU	3.3
1	A	14	ALA	3.3
2	B	11	ILE	3.3
1	A	145	PHE	3.3
1	A	398	MET	3.3
1	A	495	ARG	3.2
1	A	522	LEU	3.2
2	B	77	ASN	3.2
2	B	4	GLN	3.2
1	A	206	LEU	3.2
1	A	122	LEU	3.1
1	A	126	ALA	3.1
1	A	57	ARG	3.1
3	C	3	GLU	3.1
2	B	85	ALA	3.1
1	A	165	ASP	3.1
1	A	395	LEU	3.0
1	A	513	SER	3.0
2	B	128	LEU	3.0
1	A	542	TYR	3.0
1	A	222	LEU	2.9
1	A	428	TRP	2.9
2	B	74	THR	2.8
1	A	532	ALA	2.8
1	A	90	VAL	2.8
1	A	218	GLY	2.7
1	A	137	PRO	2.7
2	B	83	VAL	2.7
1	A	205	VAL	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	69	GLN	2.6
1	A	342	ASP	2.6
2	B	81	VAL	2.6
1	A	177	LYS	2.6
1	A	158	VAL	2.6
1	A	60	PRO	2.5
1	A	276	SER	2.5
1	A	316	VAL	2.5
1	A	489	PHE	2.5
1	A	504	ALA	2.5
1	A	53	PRO	2.5
1	A	514	GLY	2.5
1	A	505	PRO	2.4
2	B	107	ILE	2.4
1	A	104	GLY	2.4
1	A	419	ARG	2.4
1	A	278	PRO	2.4
1	A	161	TYR	2.4
2	B	105	PHE	2.4
1	A	411	LYS	2.4
2	B	113	ILE	2.4
1	A	108	LEU	2.3
1	A	364	ILE	2.3
2	B	56	THR	2.3
2	B	8	HIS	2.3
1	A	279	VAL	2.3
1	A	273	LEU	2.3
1	A	115	ILE	2.3
1	A	435	MET	2.3
1	A	367	ALA	2.2
1	A	519	ARG	2.2
1	A	86	GLN	2.2
1	A	159	SER	2.2
1	A	319	SER	2.2
2	B	66	ASP	2.2
1	A	418	ARG	2.2
1	A	146	TYR	2.2
1	A	13	GLU	2.2
1	A	314	PHE	2.1
2	B	55	PRO	2.1
1	A	412	PRO	2.1
1	A	176	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	43	ALA	2.1
2	B	17	GLY	2.1
1	A	175	PRO	2.1
1	A	371	LEU	2.0
1	A	540	LEU	2.0
2	B	6	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 monosaccharides 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.

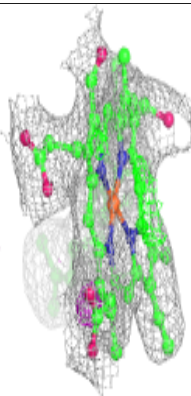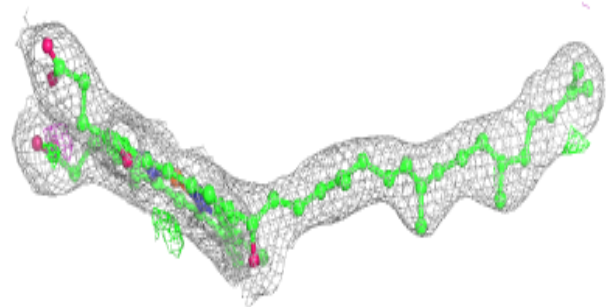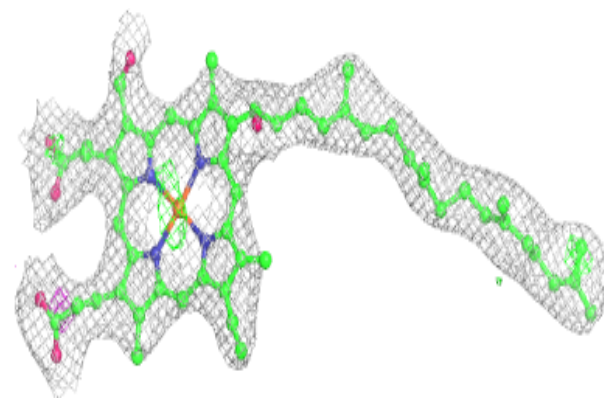| Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
8	BNG	C	804	21/21	0.63	0.34	103,136,151,152	0
6	HAS	A	801	65/65	0.95	0.21	83,92,97,101	0
5	HEM	A	800	43/43	0.95	0.16	78,87,100,103	0
7	CUA	B	802	2/2	0.98	0.06	111,111,111,114	0
4	CU1	A	803	1/1	0.98	0.11	98,98,98,98	0

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.
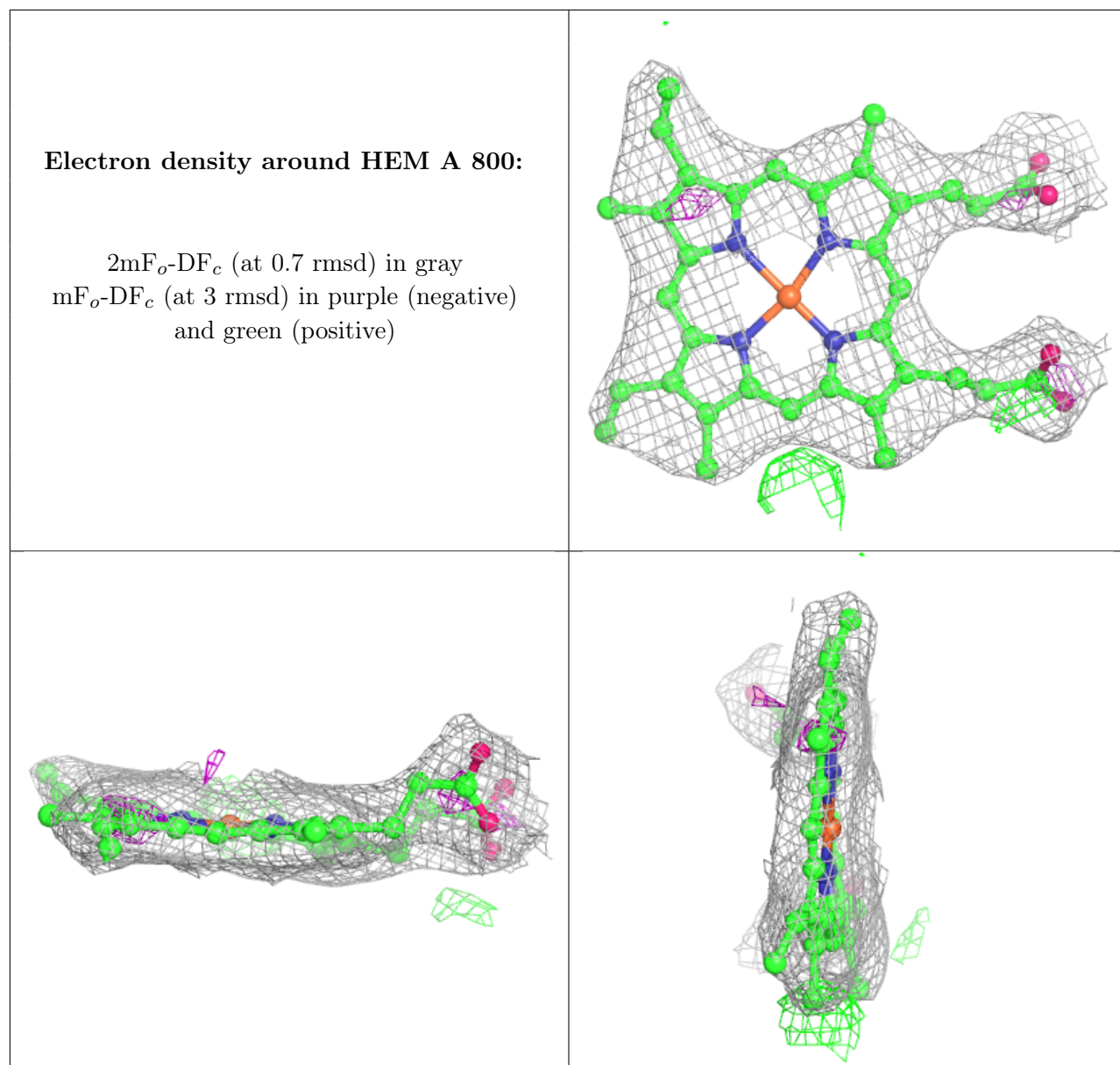
Electron density around BNG C 804:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)
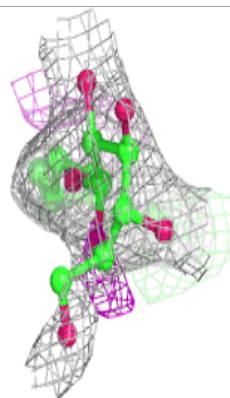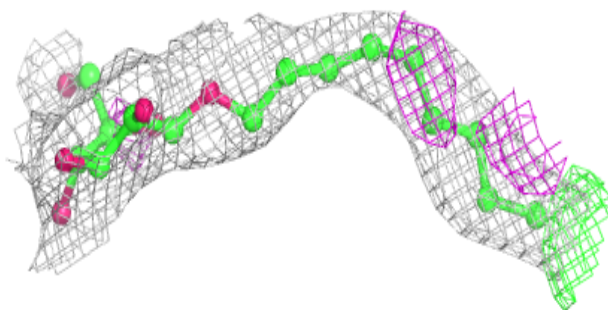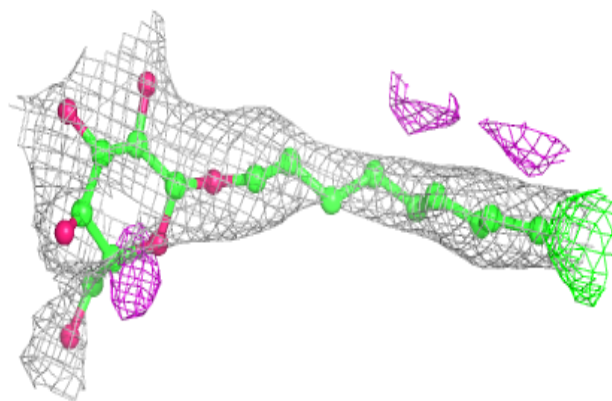
Electron density around HAS A 801:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around HEM A 800:

$2mF_o$-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.