



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:03 AM UTC

PDB ID : 5GUX / pdb_00005gux
Title : Cytochrome c-dependent nitric oxide reductase (cNOR) from *Pseudomonas aeruginosa* in complex with xenon
Authors : Ishii, S.; Terasaka, E.; Sugimoto, H.; Shiro, Y.; Tosha, T.
Deposited on : 2016-08-31
Resolution : 3.30 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

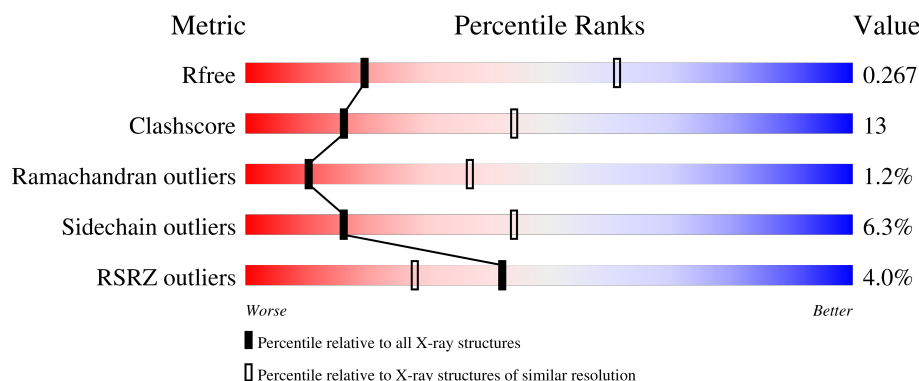
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1169 (3.32-3.28)
Clashscore	190562	1209 (3.32-3.28)
Ramachandran outliers	187476	1188 (3.32-3.28)
Sidechain outliers	187428	1187 (3.32-3.28)
RSRZ outliers	180081	1169 (3.32-3.28)

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	L	213	4% 67% 31% .
2	H	225	5% 67% 30% .
3	B	465	3% 69% 24% ..
4	C	146	3% 76% 20% ..

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
8	XE	B	808	-	-	X	-
8	XE	B	809	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 8265 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 Antibody fab fragment light chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	L	213	Total	C	N	O	S	0	0	0
			1669	1047	277	338	7			

- Molecule 2 is a protein called Antibody fab fragment heavy chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	H	225	Total	C	N	O	S	0	0	0
			1692	1065	280	338	9			

- Molecule 3 is a protein called Nitric oxide reductase subunit B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	B	449	Total	C	N	O	S	0	0	0
			3576	2416	563	572	25			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	?	-	ARG	deletion	UNP Q59647

- Molecule 4 is a protein called Nitric oxide reductase subunit C.

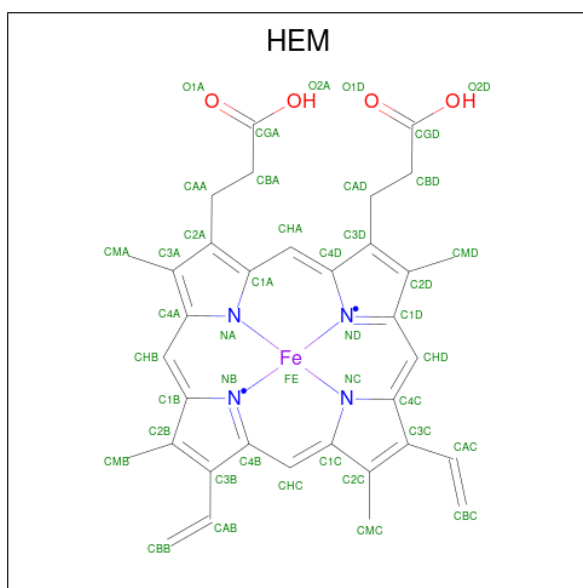
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	C	142	Total	C	N	O	S	0	0	0
			1123	720	195	202	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	100	LYS	ASN	conflict	UNP Q59646

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

- Molecule 6 is FE (III) ION (CCD ID: FE) (formula: Fe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total	Fe		
			1	1	0	0

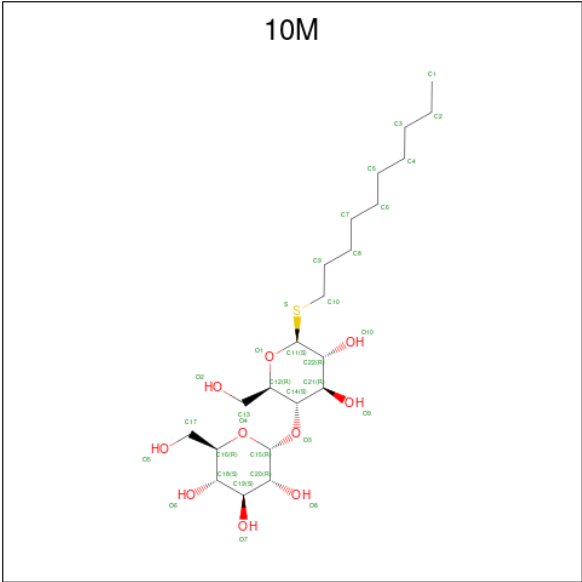
- Molecule 7 is OXYGEN ATOM (CCD ID: O) (formula: O).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	B	1	Total	O		
			1	1	0	0

- Molecule 8 is XENON (CCD ID: XE) (formula: Xe).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	7	Total	Xe		
			7	7	0	0

- Molecule 9 is decyl 4-O-alpha-D-glucopyranosyl-1-thio-beta-D-glucopyranoside (CCD ID: 10M) (formula: $C_{22}H_{42}O_{10}S$).

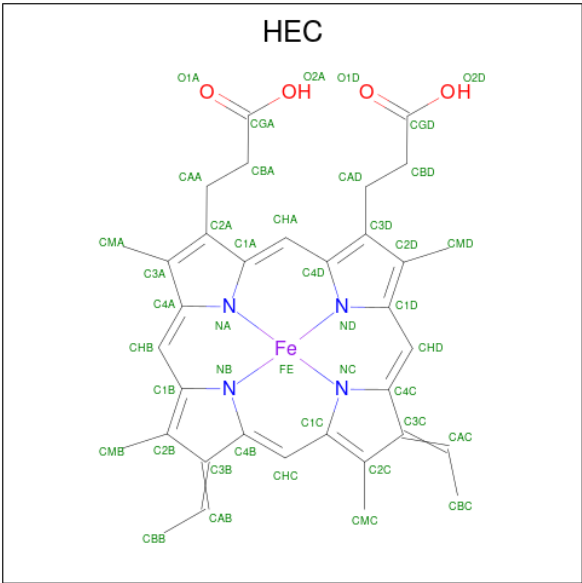


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
9	B	1	Total	C	O	S	0	0
			33	22	10	1		
9	B	1	Total	C	O	S	0	0
			33	22	10	1		

- Molecule 10 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total	Ca	0	0
			1	1		

- Molecule 11 is HEME C (CCD ID: HEC) (formula: C₃₄H₃₄FeN₄O₄).

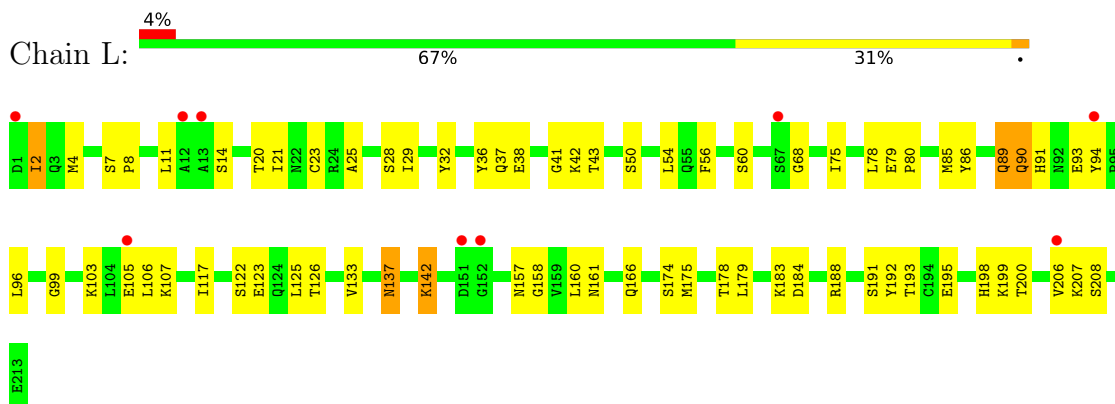


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

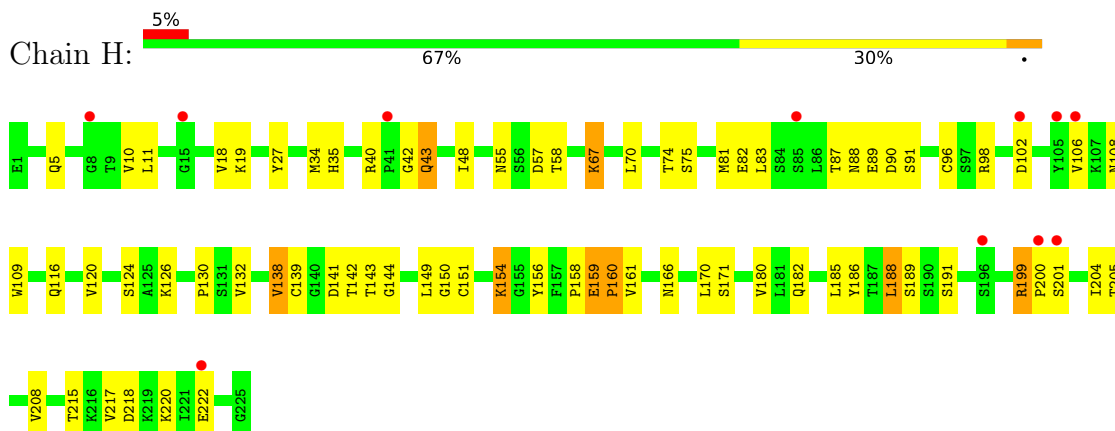
3 Residue-property plots

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.

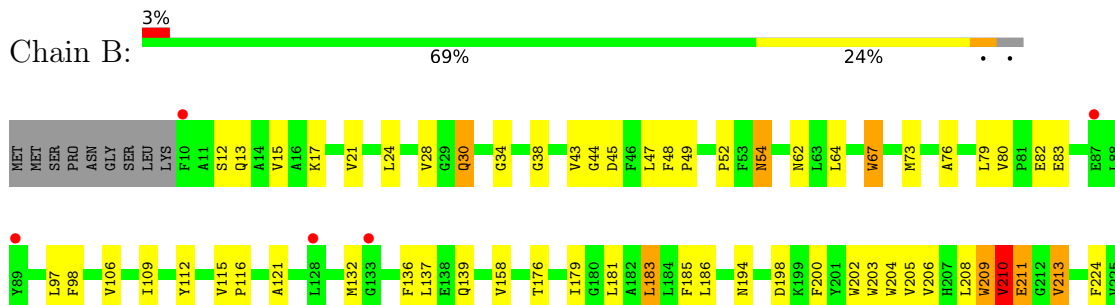
- Molecule 1: Antibody fab fragment light chain

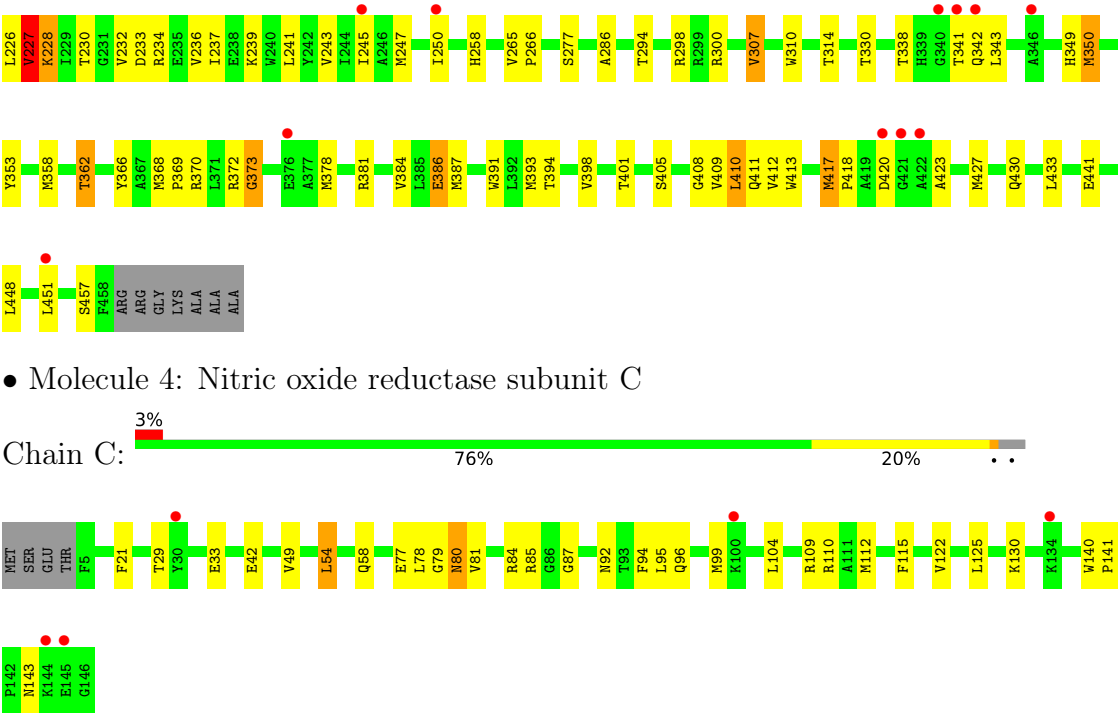


- Molecule 2: Antibody fab fragment heavy chain



- Molecule 3: Nitric oxide reductase subunit B





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	89.84Å 105.38Å 192.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.39 – 3.30 39.39 – 3.30	Depositor EDS
% Data completeness (in resolution range)	96.9 (39.39-3.30) 97.1 (39.39-3.30)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.37 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.209 , 0.268 0.208 , 0.267	Depositor DCC
R_{free} test set	1369 reflections (4.86%)	wwPDB-VP
Wilson B-factor (Å ²)	84.8	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 27.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	8265	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: XE, 10M, O, FE, HEM, HEC, CA

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	L	0.74	0/1709	1.02	3/2317 (0.1%)
2	H	0.75	0/1735	1.09	4/2367 (0.2%)
3	B	0.73	0/3693	1.09	5/5039 (0.1%)
4	C	0.73	0/1153	1.07	3/1559 (0.2%)
All	All	0.74	0/8290	1.07	15/11282 (0.1%)

There are no bond length outliers.

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	67	LYS	N-CA-C	7.58	119.54	111.28
3	B	228	LYS	N-CA-C	7.28	119.21	111.28
3	B	265	VAL	CA-C-N	6.72	128.24	119.84
3	B	265	VAL	C-N-CA	6.72	128.24	119.84
4	C	112	MET	CA-C-N	-5.92	114.66	120.52
4	C	112	MET	C-N-CA	-5.92	114.66	120.52
2	H	185	LEU	N-CA-C	5.90	119.33	109.95
2	H	150	GLY	N-CA-C	5.75	119.53	111.14
1	L	137	ASN	N-CA-C	5.66	118.13	108.90
1	L	32	TYR	N-CA-C	5.64	118.38	108.56
2	H	199	ARG	N-CA-C	5.42	117.00	108.23
4	C	85	ARG	N-CA-C	5.33	117.27	110.61
3	B	227	VAL	N-CA-C	-5.31	105.15	110.30
1	L	93	GLU	N-CA-C	5.12	116.63	108.79
3	B	210	VAL	N-CA-C	5.01	115.73	110.62

There are no chirality outliers.

There are no planarity outliers.

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	L	1669	0	1606	46	0
2	H	1692	0	1647	57	0
3	B	3576	0	3619	98	0
4	C	1123	0	1092	25	0
5	B	86	0	60	5	0
6	B	1	0	0	0	0
7	B	1	0	0	1	0
8	B	7	0	0	7	0
9	B	66	0	84	2	0
10	B	1	0	0	0	0
11	C	43	0	30	5	0
All	All	8265	0	8138	214	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 13.

All (214) 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)
2:H:199:ARG:CG	2:H:200:PRO:HA	1.80	1.10
2:H:199:ARG:HG3	2:H:200:PRO:HA	1.33	1.09
1:L:195:GLU:HG2	1:L:206:VAL:HG22	1.36	1.08
2:H:48:ILE:CD1	2:H:81:MET:HE1	1.93	0.99
3:B:73:MET:HE3	8:B:808:XE:XE	2.39	0.99
2:H:159:GLU:HG3	2:H:160:PRO:HA	1.46	0.97
3:B:73:MET:CE	8:B:808:XE:XE	2.91	0.95
3:B:230:THR:HG22	3:B:232:VAL:HG23	1.45	0.95
1:L:96:LEU:HD11	2:H:108:ASN:HB3	1.50	0.92
2:H:48:ILE:HD13	2:H:81:MET:HE1	1.52	0.86
3:B:372:ARG:HH21	3:B:378:MET:HE1	1.39	0.85
2:H:159:GLU:HG3	2:H:160:PRO:CA	2.06	0.85
2:H:199:ARG:HG2	2:H:200:PRO:HA	1.59	0.84
3:B:427:MET:HE3	11:C:201:HEC:HAD1	1.59	0.83
3:B:83:GLU:OE1	3:B:234:ARG:NH2	2.12	0.81
1:L:37:GLN:HG3	1:L:86:TYR:CE2	2.18	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:149:LEU:HD11	2:H:199:ARG:HD3	1.65	0.79
2:H:199:ARG:CG	2:H:200:PRO:CA	2.62	0.78
3:B:230:THR:CG2	3:B:232:VAL:HG23	2.12	0.78
2:H:48:ILE:HD12	2:H:81:MET:HE1	1.64	0.77
2:H:199:ARG:HG2	2:H:200:PRO:CA	2.15	0.77
3:B:341:THR:HG22	3:B:343:LEU:H	1.49	0.76
3:B:226:LEU:O	3:B:230:THR:HB	1.86	0.76
1:L:8:PRO:HG3	1:L:11:LEU:HD13	1.70	0.74
2:H:154:LYS:HE2	2:H:182:GLN:HE22	1.51	0.74
1:L:75:ILE:HG21	1:L:78:LEU:HD23	1.69	0.72
3:B:405:SER:O	3:B:409:VAL:HG23	1.92	0.69
2:H:130:PRO:HB3	2:H:156:TYR:HB3	1.74	0.69
3:B:298:ARG:HG3	3:B:300:ARG:O	1.93	0.69
3:B:338:THR:O	3:B:341:THR:HB	1.93	0.68
1:L:161:ASN:HB3	1:L:175:MET:HE3	1.75	0.68
2:H:102:ASP:O	4:C:109:ARG:NH2	2.27	0.67
3:B:121:ALA:CB	4:C:58:GLN:HG2	2.24	0.67
3:B:408:GLY:O	3:B:412:VAL:HG23	1.95	0.67
1:L:125:LEU:O	1:L:183:LYS:HD2	1.95	0.66
3:B:393:MET:HE3	3:B:451:LEU:HB2	1.76	0.66
3:B:109:ILE:O	3:B:112:TYR:HB2	1.96	0.66
3:B:342:GLN:H	3:B:411:GLN:NE2	1.94	0.65
1:L:195:GLU:CG	1:L:206:VAL:HG22	2.19	0.65
3:B:387:MET:O	3:B:391:TRP:HD1	1.79	0.65
3:B:194:ASN:HD22	4:C:42:GLU:HG3	1.61	0.65
1:L:96:LEU:CD1	2:H:108:ASN:HB3	2.26	0.64
3:B:136:PHE:CE1	8:B:809:XE:XE	3.29	0.64
3:B:17:LYS:O	3:B:21:VAL:HG23	1.99	0.63
1:L:198:HIS:HD2	1:L:200:THR:OG1	1.81	0.62
3:B:387:MET:O	3:B:391:TRP:CD1	2.53	0.61
2:H:222:GLU:HA	2:H:222:GLU:OE1	2.00	0.61
3:B:247:MET:HE1	3:B:286:ALA:HB2	1.82	0.60
2:H:27:TYR:CE2	2:H:98:ARG:HD2	2.36	0.60
3:B:413:TRP:HD1	3:B:417:MET:CE	2.14	0.60
2:H:70:LEU:CD2	2:H:81:MET:HG3	2.32	0.59
2:H:11:LEU:HD21	2:H:158:PRO:HG3	1.84	0.59
4:C:140:TRP:CG	4:C:141:PRO:HA	2.38	0.59
3:B:310:TRP:HB3	3:B:362:THR:OG1	2.02	0.58
4:C:92:ASN:OD1	4:C:130:LYS:HE2	2.04	0.58
3:B:121:ALA:HB1	4:C:58:GLN:HG2	1.86	0.58
3:B:30:GLN:NE2	3:B:67:TRP:HE1	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:384:VAL:HA	3:B:387:MET:HE2	1.84	0.57
3:B:137:LEU:HA	3:B:139:GLN:HE22	1.70	0.57
1:L:29:ILE:HG21	1:L:90:GLN:HG3	1.85	0.56
1:L:184:ASP:HB3	1:L:188:ARG:NH2	2.20	0.56
3:B:349:HIS:CD2	5:B:801:HEM:NC	2.73	0.56
1:L:193:THR:HA	1:L:208:SER:HB3	1.88	0.56
3:B:239:LYS:O	3:B:243:VAL:HG23	2.06	0.55
2:H:199:ARG:HG2	2:H:200:PRO:N	2.20	0.55
3:B:350:MET:HE3	3:B:401:THR:HG21	1.89	0.54
1:L:79:GLU:HG3	1:L:80:PRO:HD2	1.89	0.54
1:L:4:MET:HB3	1:L:99:GLY:HA2	1.88	0.54
2:H:199:ARG:HA	2:H:201:SER:N	2.22	0.54
2:H:199:ARG:HA	2:H:201:SER:H	1.73	0.54
4:C:96:GLN:HA	4:C:122:VAL:HG11	1.89	0.54
3:B:13:GLN:HE22	3:B:82:GLU:HG3	1.74	0.53
1:L:96:LEU:HD11	2:H:108:ASN:CB	2.31	0.53
2:H:87:THR:HG22	2:H:89:GLU:H	1.73	0.53
3:B:230:THR:HG21	3:B:294:THR:O	2.08	0.53
3:B:417:MET:HB2	3:B:418:PRO:HD3	1.89	0.53
2:H:132:VAL:HG21	2:H:217:VAL:HG21	1.91	0.52
3:B:372:ARG:HH21	3:B:378:MET:CE	2.18	0.52
1:L:54:LEU:HD11	1:L:60:SER:HA	1.92	0.52
3:B:49:PRO:O	3:B:52:PRO:HD3	2.10	0.52
3:B:233:ASP:O	3:B:236:VAL:HG22	2.10	0.51
1:L:43:THR:HG23	2:H:116:GLN:HG3	1.93	0.51
2:H:19:LYS:HB2	2:H:82:GLU:HG3	1.92	0.51
3:B:258:HIS:CE1	5:B:802:HEM:CHD	2.93	0.51
3:B:241:LEU:O	3:B:245:ILE:HG12	2.10	0.51
3:B:314:THR:OG1	3:B:358:MET:HB3	2.10	0.51
1:L:193:THR:OG1	1:L:208:SER:HB3	2.11	0.51
3:B:198:ASP:C	3:B:198:ASP:OD1	2.54	0.51
3:B:204:TRP:O	3:B:208:LEU:HB2	2.10	0.51
2:H:48:ILE:HG21	2:H:81:MET:CE	2.41	0.51
3:B:52:PRO:HB2	3:B:54:ASN:ND2	2.26	0.51
2:H:67:LYS:HE3	2:H:90:ASP:OD1	2.11	0.50
1:L:96:LEU:HD13	2:H:108:ASN:HD22	1.76	0.50
3:B:230:THR:CG2	3:B:294:THR:O	2.60	0.50
2:H:161:VAL:CG1	2:H:208:VAL:HG13	2.42	0.50
1:L:192:TYR:O	1:L:208:SER:HB2	2.11	0.50
2:H:70:LEU:HD23	2:H:81:MET:HG3	1.94	0.50
2:H:81:MET:HE2	2:H:83:LEU:HD21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:372:ARG:O	3:B:373:GLY:C	2.54	0.50
3:B:97:LEU:O	3:B:98:PHE:C	2.55	0.50
2:H:149:LEU:HD11	2:H:199:ARG:CD	2.40	0.50
3:B:307:VAL:HG11	3:B:366:TYR:HB2	1.94	0.50
3:B:73:MET:HE1	8:B:808:XE:XE	2.87	0.49
3:B:62:ASN:ND2	3:B:112:TYR:OH	2.44	0.49
3:B:115:VAL:HG12	3:B:116:PRO:O	2.12	0.49
3:B:202:TRP:HZ3	3:B:203:TRP:CZ2	2.30	0.49
1:L:192:TYR:O	1:L:208:SER:CB	2.60	0.49
3:B:43:VAL:O	3:B:45:ASP:N	2.45	0.49
3:B:205:VAL:O	3:B:209:TRP:HB2	2.12	0.49
1:L:2:ILE:HD11	1:L:4:MET:SD	2.53	0.49
3:B:410:LEU:HB3	3:B:433:LEU:HD21	1.95	0.49
4:C:140:TRP:CD2	4:C:141:PRO:HA	2.47	0.49
3:B:393:MET:HE1	3:B:451:LEU:HD13	1.95	0.48
3:B:413:TRP:HD1	3:B:417:MET:HE2	1.77	0.48
1:L:38:GLU:HB3	1:L:85:MET:HB3	1.95	0.48
3:B:413:TRP:HD1	3:B:417:MET:HE3	1.78	0.48
3:B:418:PRO:HG2	3:B:423:ALA:HA	1.96	0.48
3:B:82:GLU:OE1	3:B:228:LYS:HE3	2.14	0.48
3:B:353:TYR:O	3:B:358:MET:HG3	2.14	0.48
1:L:50:SER:H	1:L:91:HIS:CE1	2.31	0.48
3:B:411:GLN:HB2	3:B:433:LEU:HD11	1.96	0.48
2:H:188:LEU:HD12	2:H:188:LEU:C	2.39	0.48
2:H:220:LYS:HE3	2:H:222:GLU:OE2	2.13	0.48
4:C:95:LEU:O	4:C:99:MET:HG2	2.13	0.48
4:C:80:ASN:HD21	4:C:84:ARG:HH12	1.62	0.47
1:L:158:GLY:O	1:L:179:LEU:HA	2.14	0.47
2:H:57:ASP:OD1	2:H:58:THR:N	2.46	0.47
3:B:136:PHE:CD1	8:B:809:XE:XE	3.45	0.47
3:B:211:GLU:OE2	7:B:804:O:O	2.32	0.47
2:H:156:TYR:CE1	2:H:186:TYR:HB2	2.50	0.47
2:H:106:VAL:HG22	2:H:109:TRP:HB2	1.96	0.47
3:B:372:ARG:NH2	3:B:378:MET:HE1	2.21	0.47
4:C:122:VAL:O	4:C:125:LEU:HB2	2.15	0.47
2:H:87:THR:HG22	2:H:88:ASN:N	2.29	0.47
3:B:64:LEU:HD23	8:B:809:XE:XE	2.92	0.47
3:B:179:ILE:HG22	3:B:183:LEU:HD22	1.97	0.47
4:C:77:GLU:OE1	4:C:79:GLY:HA3	2.15	0.47
3:B:230:THR:CG2	3:B:232:VAL:CG2	2.90	0.46
1:L:106:LEU:O	1:L:166:GLN:NE2	2.38	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:34:MET:HE2	2:H:34:MET:HB2	1.75	0.46
3:B:342:GLN:H	3:B:411:GLN:HE22	1.59	0.46
3:B:369:PRO:HG3	3:B:378:MET:HE2	1.97	0.46
2:H:42:GLY:O	2:H:43:GLN:HB2	2.14	0.46
3:B:386:GLU:HG3	3:B:457:SER:OG	2.15	0.46
3:B:48:PHE:CG	3:B:49:PRO:HA	2.51	0.46
8:B:807:XE:XE	8:B:808:XE:XE	3.90	0.46
2:H:138:VAL:O	2:H:141:ASP:HB2	2.17	0.45
1:L:79:GLU:O	1:L:80:PRO:C	2.58	0.45
1:L:123:GLU:OE2	1:L:123:GLU:N	2.45	0.45
3:B:350:MET:HE3	3:B:401:THR:CG2	2.46	0.45
9:B:812:10M:H10A	9:B:812:10M:H22	1.89	0.45
4:C:115:PHE:CE2	11:C:201:HEC:HBB2	2.52	0.45
1:L:56:PHE:CE1	4:C:94:PHE:CE1	3.05	0.45
1:L:137:ASN:ND2	1:L:174:SER:HB3	2.32	0.44
3:B:200:PHE:HE2	4:C:29:THR:HG23	1.82	0.44
3:B:121:ALA:HA	3:B:132:MET:HE1	1.98	0.44
1:L:4:MET:HG3	1:L:23:CYS:SG	2.57	0.44
2:H:138:VAL:O	2:H:139:CYS:C	2.60	0.44
1:L:28:SER:HA	1:L:68:GLY:O	2.18	0.44
1:L:160:LEU:HD23	2:H:180:VAL:CG2	2.48	0.44
1:L:133:VAL:HG22	1:L:178:THR:OG1	2.17	0.44
2:H:10:VAL:HG21	2:H:18:VAL:HG21	1.99	0.44
3:B:12:SER:O	3:B:15:VAL:HG22	2.18	0.44
2:H:161:VAL:HG13	2:H:208:VAL:HG13	2.00	0.43
1:L:78:LEU:HD23	1:L:78:LEU:HA	1.76	0.43
3:B:30:GLN:HE21	3:B:67:TRP:HE1	1.66	0.43
3:B:137:LEU:HA	3:B:139:GLN:NE2	2.33	0.43
3:B:227:VAL:HG23	3:B:237:ILE:HG21	2.00	0.43
1:L:85:MET:HB2	1:L:85:MET:HE2	1.75	0.43
9:B:813:10M:H16	9:B:813:10M:H13	2.00	0.43
2:H:159:GLU:CG	2:H:160:PRO:HA	2.34	0.43
2:H:222:GLU:OE1	2:H:222:GLU:CA	2.66	0.43
3:B:430:GLN:NE2	4:C:110:ARG:HH22	2.17	0.43
4:C:78:LEU:O	4:C:81:VAL:HG12	2.19	0.43
2:H:205:THR:HG21	2:H:218:ASP:HB3	2.00	0.43
3:B:394:THR:O	3:B:398:VAL:HG23	2.18	0.43
3:B:413:TRP:HA	3:B:417:MET:HG3	2.00	0.43
3:B:181:LEU:HD23	3:B:181:LEU:C	2.44	0.42
4:C:115:PHE:CD2	11:C:201:HEC:HBB2	2.53	0.42
3:B:13:GLN:NE2	3:B:82:GLU:HG3	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:206:VAL:O	1:L:207:LYS:HG2	2.20	0.42
2:H:91:SER:HA	2:H:120:VAL:O	2.18	0.42
2:H:35:HIS:O	2:H:96:CYS:HA	2.19	0.42
3:B:420:ASP:OD1	4:C:143:ASN:HB2	2.19	0.42
3:B:183:LEU:O	3:B:186:LEU:HB2	2.19	0.42
3:B:202:TRP:CZ2	3:B:206:VAL:HG21	2.55	0.42
1:L:41:GLY:O	1:L:42:LYS:HG3	2.19	0.42
1:L:85:MET:HE2	1:L:103:LYS:HD2	2.02	0.41
3:B:76:ALA:O	3:B:80:VAL:HB	2.20	0.41
3:B:34:GLY:C	5:B:801:HEM:HMB3	2.45	0.41
3:B:38:GLY:HA3	3:B:441:GLU:OE1	2.20	0.41
2:H:130:PRO:CB	2:H:156:TYR:HB3	2.48	0.41
1:L:36:TYR:HE2	1:L:89:GLN:HE21	1.69	0.41
3:B:210:VAL:HG11	5:B:802:HEM:C2B	2.55	0.41
3:B:250:ILE:HG23	4:C:21:PHE:CE2	2.55	0.41
3:B:277:SER:HB3	3:B:330:THR:OG1	2.20	0.41
3:B:24:LEU:HD23	3:B:24:LEU:HA	1.85	0.41
3:B:28:VAL:HG22	3:B:451:LEU:HD21	2.03	0.41
1:L:105:GLU:OE1	1:L:142:LYS:HE3	2.21	0.41
2:H:55:ASN:C	2:H:55:ASN:OD1	2.64	0.41
3:B:417:MET:HB2	3:B:418:PRO:CD	2.50	0.41
1:L:94:TYR:CD1	1:L:94:TYR:C	2.98	0.41
1:L:122:SER:O	1:L:126:THR:HG23	2.21	0.41
2:H:170:LEU:HD12	2:H:171:SER:N	2.35	0.41
1:L:4:MET:HB3	1:L:99:GLY:CA	2.50	0.41
3:B:210:VAL:CG1	5:B:802:HEM:C2B	3.04	0.41
4:C:140:TRP:CD1	4:C:141:PRO:HA	2.56	0.41
2:H:166:ASN:HD21	2:H:204:ILE:HA	1.86	0.40
3:B:79:LEU:HB2	3:B:224:PHE:CE2	2.56	0.40
4:C:80:ASN:HD22	4:C:80:ASN:H	1.70	0.40
4:C:54:LEU:HD22	4:C:58:GLN:NE2	2.37	0.40
1:L:2:ILE:HD13	1:L:25:ALA:HB1	2.03	0.40
4:C:109:ARG:NH1	11:C:201:HEC:O2D	2.54	0.40
4:C:109:ARG:HH11	11:C:201:HEC:CGD	2.33	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	L	211/213 (99%)	200 (95%)	10 (5%)	1 (0%)	24	55
2	H	223/225 (99%)	202 (91%)	18 (8%)	3 (1%)	9	35
3	B	447/465 (96%)	414 (93%)	26 (6%)	7 (2%)	7	31
4	C	140/146 (96%)	130 (93%)	9 (6%)	1 (1%)	18	49
All	All	1021/1049 (97%)	946 (93%)	63 (6%)	12 (1%)	10	37

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	B	44	GLY
2	H	43	GLN
2	H	143	THR
2	H	144	GLY
3	B	209	TRP
4	C	87	GLY
1	L	199	LYS
3	B	185	PHE
3	B	266	PRO
3	B	47	LEU
3	B	213	VAL
3	B	373	GLY

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	L	189/189 (100%)	177 (94%)	12 (6%)	16	44
2	H	192/192 (100%)	176 (92%)	16 (8%)	10	34
3	B	360/371 (97%)	339 (94%)	21 (6%)	18	47
4	C	116/120 (97%)	111 (96%)	5 (4%)	26	54
All	All	857/872 (98%)	803 (94%)	54 (6%)	16	44

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	L	2	ILE
1	L	7	SER
1	L	14	SER
1	L	20	THR
1	L	21	ILE
1	L	89	GLN
1	L	90	GLN
1	L	107	LYS
1	L	117	ILE
1	L	142	LYS
1	L	157	ASN
1	L	191	SER
2	H	5	GLN
2	H	40	ARG
2	H	74	THR
2	H	75	SER
2	H	124	SER
2	H	126	LYS
2	H	138	VAL
2	H	142	THR
2	H	151	CYS
2	H	154	LYS
2	H	159	GLU
2	H	160	PRO
2	H	188	LEU
2	H	189	SER
2	H	191	SER
2	H	215	THR
3	B	30	GLN
3	B	54	ASN
3	B	67	TRP
3	B	106	VAL
3	B	158	VAL

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Mol	Chain	Res	Type
3	B	176	THR
3	B	183	LEU
3	B	210	VAL
3	B	211	GLU
3	B	213	VAL
3	B	227	VAL
3	B	307	VAL
3	B	350	MET
3	B	362	THR
3	B	368	MET
3	B	370	ARG
3	B	381	ARG
3	B	386	GLU
3	B	410	LEU
3	B	417	MET
3	B	448	LEU
4	C	33	GLU
4	C	49	VAL
4	C	54	LEU
4	C	80	ASN
4	C	104	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	L	89	GLN
1	L	91	HIS
1	L	161	ASN
1	L	198	HIS
2	H	5	GLN
2	H	108	ASN
2	H	182	GLN
3	B	30	GLN
3	B	54	ASN
3	B	62	ASN
3	B	126	ASN
3	B	139	GLN
3	B	383	GLN
3	B	411	GLN
3	B	430	GLN
4	C	31	HIS
4	C	60	ASN

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Mol	Chain	Res	Type
4	C	80	ASN
4	C	96	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 10 are monoatomic - leaving 5 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$
9	10M	B	813	-	34,34,34	0.51	0	44,45,45	0.50	0
9	10M	B	812	-	34,34,34	0.97	0	44,45,45	1.11	4 (9%)
5	HEM	B	801	3,10	50,50,50	1.94	11 (22%)	67,82,82	2.51	26 (38%)
11	HEC	C	201	4	46,50,50	1.97	7 (15%)	58,82,82	1.69	10 (17%)
5	HEM	B	802	3,10,7	50,50,50	1.79	7 (14%)	67,82,82	1.82	18 (26%)

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
9	10M	B	813	-	-	9/19/59/59	0/2/2/2
9	10M	B	812	-	-	10/19/59/59	0/2/2/2
5	HEM	B	801	3,10	-	6/14/54/54	-
11	HEC	C	201	4	-	6/14/54/54	-
5	HEM	B	802	3,10,7	-	6/14/54/54	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	801	HEM	C3D-C2D	7.77	1.53	1.36
5	B	802	HEM	C3D-C2D	7.66	1.53	1.36
11	C	201	HEC	CAB-C3B	6.68	1.56	1.35
11	C	201	HEC	CAC-C3C	6.67	1.56	1.35
5	B	801	HEM	FE-NC	5.75	2.14	1.95
5	B	802	HEM	FE-NA	5.38	2.12	1.95
11	C	201	HEC	C3D-C2D	4.98	1.51	1.38
5	B	801	HEM	CMC-C2C	3.22	1.57	1.50
5	B	801	HEM	FE-ND	3.19	2.04	1.94
5	B	802	HEM	CAB-C3B	3.18	1.55	1.47
5	B	801	HEM	FE-NA	3.01	2.05	1.95
5	B	802	HEM	CAC-C3C	2.94	1.55	1.47
5	B	801	HEM	CAB-C3B	2.93	1.55	1.47
5	B	801	HEM	CMB-C2B	2.85	1.56	1.50
11	C	201	HEC	CMB-C2B	2.79	1.56	1.50
5	B	801	HEM	CAC-C3C	2.72	1.54	1.47
5	B	802	HEM	FE-NB	2.67	2.03	1.94
5	B	801	HEM	CMD-C2D	2.58	1.56	1.50
5	B	801	HEM	FE-NB	2.51	2.02	1.94
11	C	201	HEC	CMD-C2D	2.20	1.55	1.50
11	C	201	HEC	C3C-C2C	-2.19	1.33	1.41
5	B	802	HEM	CMA-C3A	2.18	1.55	1.50
11	C	201	HEC	CMA-C3A	2.16	1.55	1.50
5	B	801	HEM	C2A-C3A	-2.05	1.33	1.38
5	B	802	HEM	CMB-C2B	2.03	1.54	1.50

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	C	201	HEC	CBB-CAB-C3B	-6.52	114.41	127.43
5	B	801	HEM	C4C-C3C-C2C	6.42	112.38	106.81
11	C	201	HEC	CBC-CAC-C3C	-5.87	115.70	127.43
5	B	801	HEM	CMC-C2C-C1C	5.26	133.99	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	801	HEM	C3C-C2C-C1C	-4.90	102.41	107.05
5	B	801	HEM	CHD-C1D-ND	4.77	129.55	124.42
5	B	801	HEM	O1D-CGD-CBD	-4.73	108.09	123.09
5	B	801	HEM	CHC-C4B-NB	4.70	129.48	124.42
5	B	801	HEM	O2D-CGD-CBD	4.66	128.73	114.00
5	B	801	HEM	C4B-C3B-C2B	4.66	111.56	107.28
5	B	802	HEM	C4D-ND-C1D	4.54	110.58	105.21
5	B	802	HEM	CHA-C4D-ND	4.52	129.96	124.37
5	B	801	HEM	CHC-C1C-NC	-4.51	119.55	124.45
5	B	802	HEM	CHD-C4C-NC	-4.20	119.89	124.45
5	B	801	HEM	C4D-ND-C1D	4.16	110.14	105.21
5	B	801	HEM	C3B-C4B-NB	-4.03	106.58	109.47
5	B	801	HEM	CAD-C3D-C4D	3.96	131.59	124.70
5	B	802	HEM	O2D-CGD-CBD	3.95	126.47	114.00
5	B	801	HEM	C3B-C2B-C1B	-3.77	103.58	106.41
5	B	802	HEM	CMD-C2D-C1D	3.66	130.75	125.03
5	B	801	HEM	CMB-C2B-C1B	3.61	130.68	125.03
5	B	801	HEM	CBD-CAD-C3D	-3.60	102.57	112.53
11	C	201	HEC	CBD-CAD-C3D	-3.39	103.17	112.53
5	B	801	HEM	CMA-C3A-C4A	-3.31	120.38	125.42
5	B	802	HEM	CHA-C1A-NA	-3.27	117.94	123.86
5	B	802	HEM	O1D-CGD-CBD	-3.17	113.04	123.09
5	B	802	HEM	C3B-C4B-NB	3.08	111.68	109.47
5	B	802	HEM	CBA-CAA-C2A	-3.05	104.11	112.53
9	B	812	10M	C11-O1-C12	3.03	118.00	112.56
11	C	201	HEC	C4D-ND-C1D	3.00	110.71	105.82
5	B	801	HEM	CMA-C3A-C2A	2.86	131.69	125.62
5	B	801	HEM	C4D-C3D-C2D	-2.86	102.73	106.89
5	B	802	HEM	CAA-C2A-C1A	2.85	130.51	124.94
5	B	802	HEM	C1D-C2D-C3D	-2.74	104.09	106.98
5	B	802	HEM	CHA-C1A-C2A	2.65	131.10	125.30
5	B	801	HEM	CAA-CBA-CGA	-2.53	106.95	113.67
5	B	802	HEM	CAD-C3D-C4D	2.53	129.10	124.70
11	C	201	HEC	C1D-C2D-C3D	-2.51	103.94	106.82
5	B	802	HEM	CAD-CBD-CGD	-2.46	107.15	113.67
5	B	801	HEM	O2A-CGA-CBA	2.45	121.73	114.00
5	B	802	HEM	C3B-C2B-C1B	2.44	108.24	106.41
5	B	801	HEM	CHB-C1B-NB	-2.39	121.41	124.37
11	C	201	HEC	CHD-C1D-ND	2.38	128.18	123.86
11	C	201	HEC	CHC-C4B-NB	2.38	127.04	124.45
5	B	801	HEM	C4A-CHB-C1B	2.34	131.75	126.25
5	B	802	HEM	CHA-C4D-C3D	-2.34	120.91	125.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	B	812	10M	C15-O3-C14	2.31	123.45	117.98
5	B	801	HEM	CHD-C1D-C2D	-2.24	121.49	125.03
5	B	802	HEM	CHD-C4C-C3C	2.24	128.98	125.21
11	C	201	HEC	CMD-C2D-C3D	2.23	130.35	125.62
5	B	802	HEM	CHC-C4B-NB	-2.23	122.03	124.42
11	C	201	HEC	CHD-C1D-C2D	-2.21	121.02	127.43
9	B	812	10M	C19-C18-C16	2.21	114.23	110.23
5	B	801	HEM	CBB-CAB-C3B	-2.14	116.83	127.53
5	B	801	HEM	CBC-CAC-C3C	-2.14	116.85	127.53
9	B	812	10M	O1-C11-C22	2.04	113.13	110.32
5	B	801	HEM	CMC-C2C-C3C	-2.01	123.55	128.43
11	C	201	HEC	CMB-C2B-C1B	-2.01	122.36	125.42

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
9	B	812	10M	C22-C11-S-C10
11	C	201	HEC	C2B-C3B-CAB-CBB
11	C	201	HEC	C4B-C3B-CAB-CBB
9	B	812	10M	C18-C16-C17-O5
9	B	812	10M	O4-C16-C17-O5
9	B	813	10M	C3-C4-C5-C6
9	B	812	10M	C7-C8-C9-C10
9	B	813	10M	C6-C7-C8-C9
5	B	802	HEM	C2C-C3C-CAC-CBC
9	B	812	10M	C4-C5-C6-C7
9	B	813	10M	C2-C3-C4-C5
9	B	812	10M	C1-C2-C3-C4
9	B	812	10M	O1-C12-C13-O2
9	B	813	10M	C1-C2-C3-C4
5	B	801	HEM	C2B-C3B-CAB-CBB
5	B	801	HEM	C2C-C3C-CAC-CBC
5	B	802	HEM	C4C-C3C-CAC-CBC
9	B	812	10M	C6-C7-C8-C9
11	C	201	HEC	C4C-C3C-CAC-CBC
11	C	201	HEC	C2C-C3C-CAC-CBC
9	B	813	10M	C7-C8-C9-C10
9	B	813	10M	O4-C16-C17-O5
5	B	802	HEM	CAA-CBA-CGA-O1A
5	B	802	HEM	CAD-CBD-CGD-O1D
11	C	201	HEC	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
11	C	201	HEC	CAD-CBD-CGD-O2D
5	B	802	HEM	CAD-CBD-CGD-O2D
9	B	812	10M	C3-C4-C5-C6
5	B	802	HEM	CAA-CBA-CGA-O2A
9	B	813	10M	C5-C6-C7-C8
9	B	812	10M	C2-C3-C4-C5
9	B	813	10M	O1-C12-C13-O2
9	B	813	10M	C14-C12-C13-O2
5	B	801	HEM	C4B-C3B-CAB-CBB
5	B	801	HEM	C4C-C3C-CAC-CBC
5	B	801	HEM	CAD-CBD-CGD-O2D
5	B	801	HEM	CAA-CBA-CGA-O2A

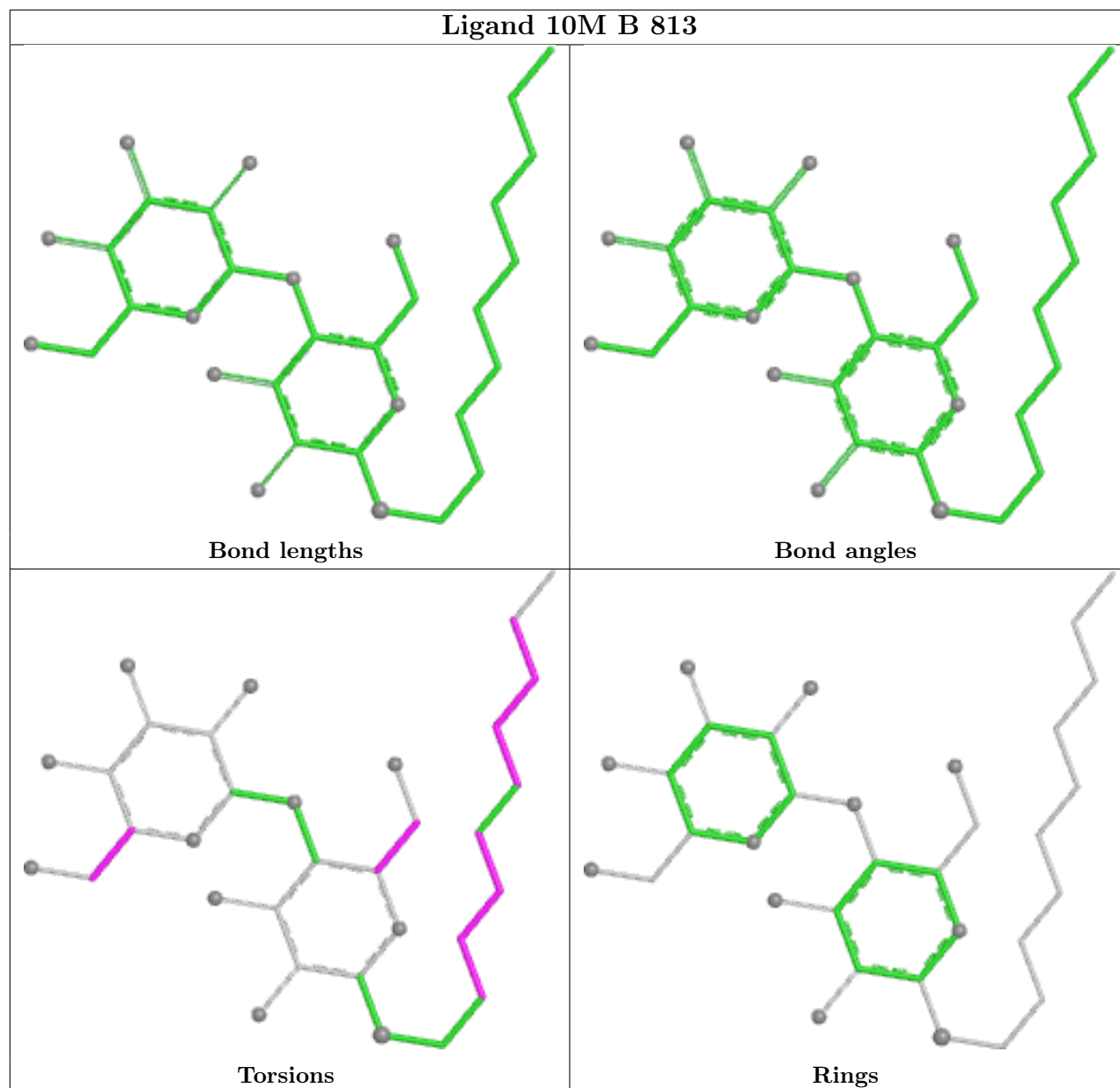
There are no ring outliers.

5 monomers are involved in 12 short contacts:

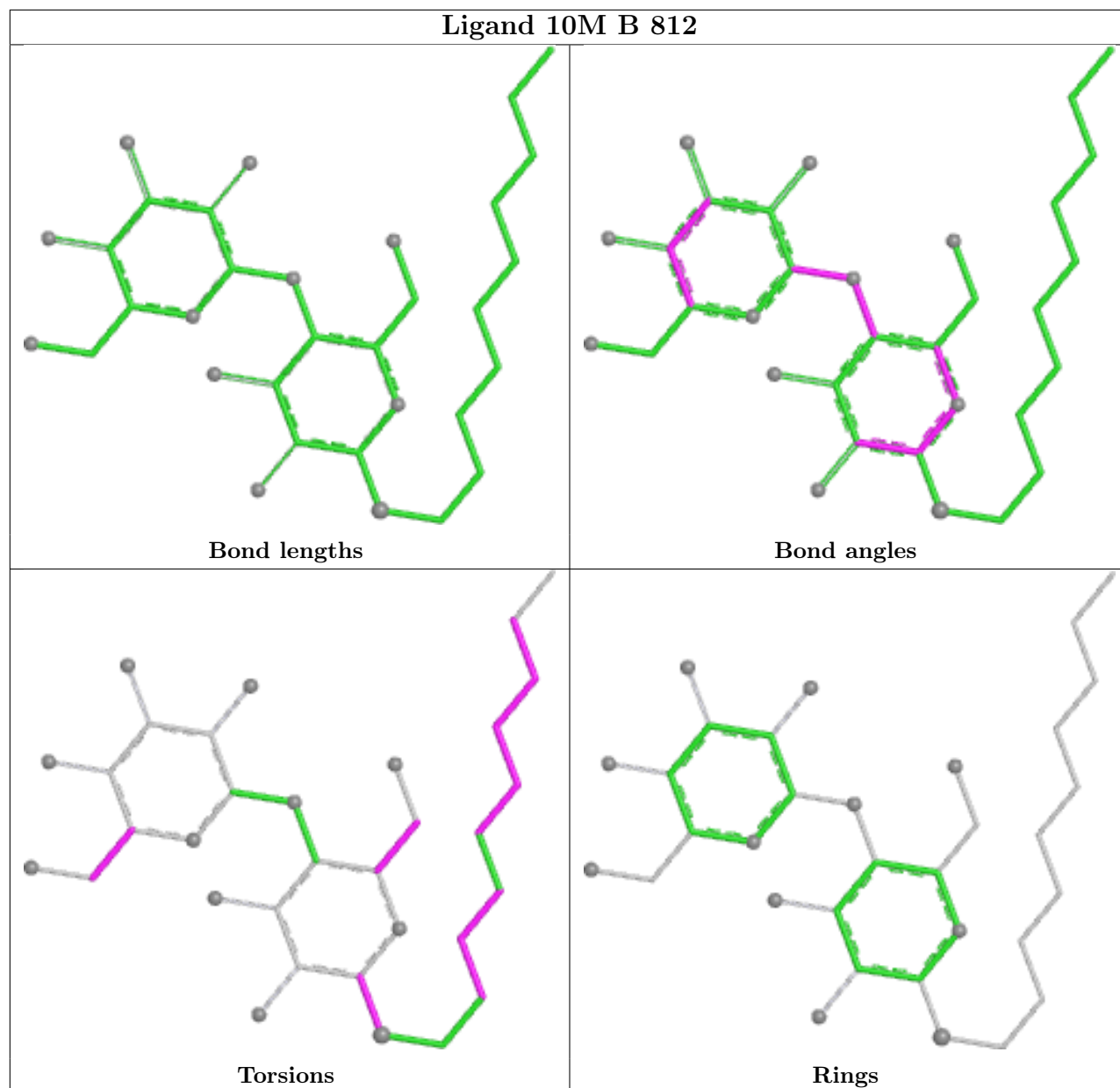
Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	B	813	10M	1	0
9	B	812	10M	1	0
5	B	801	HEM	2	0
11	C	201	HEC	5	0
5	B	802	HEM	3	0

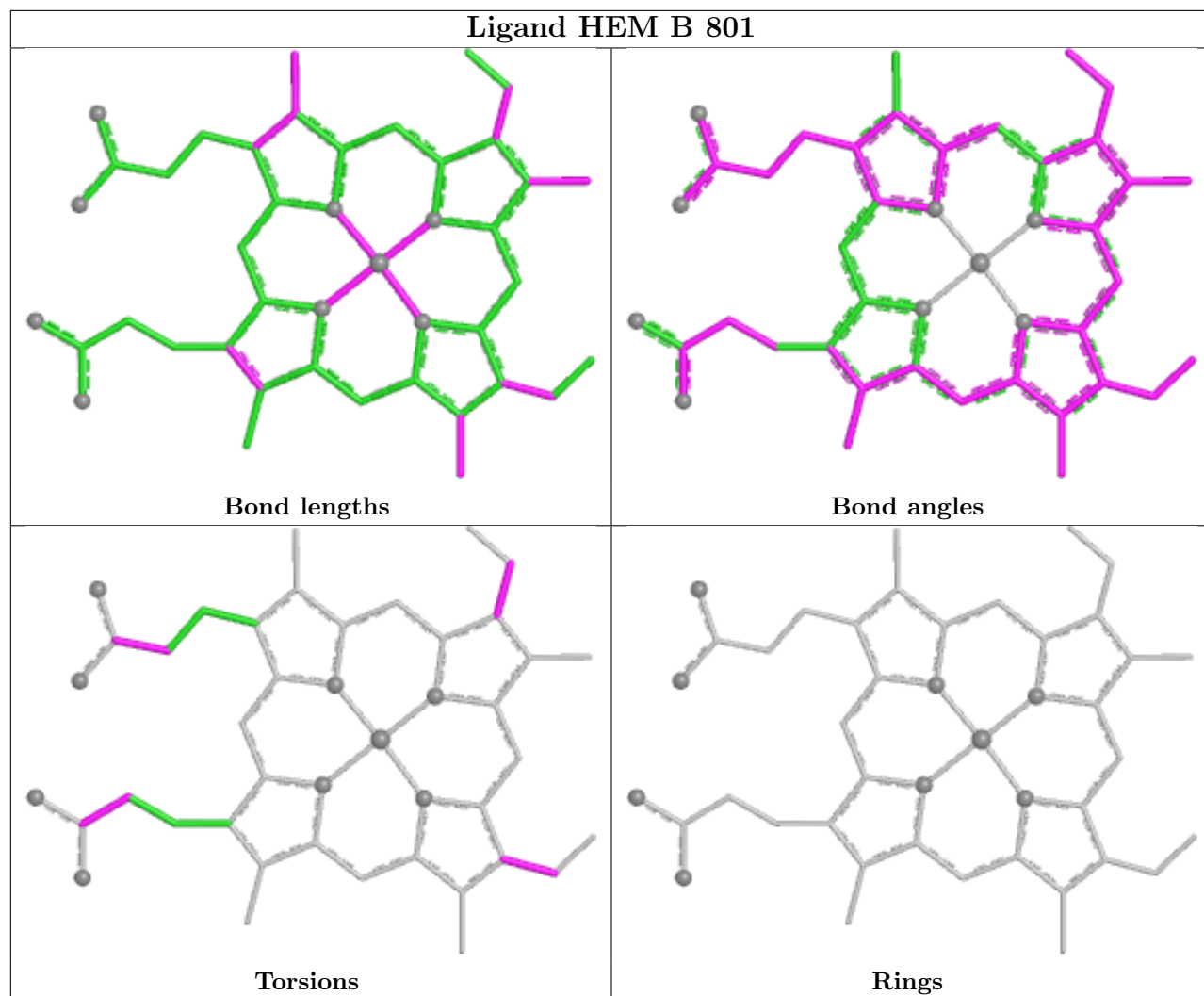
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand 10M B 813

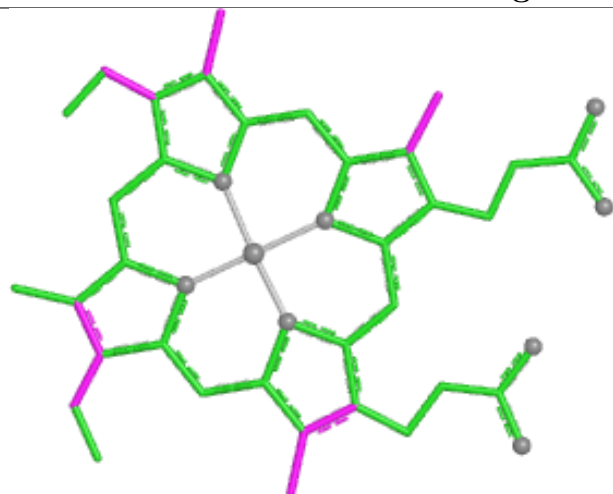


Ligand 10M B 812

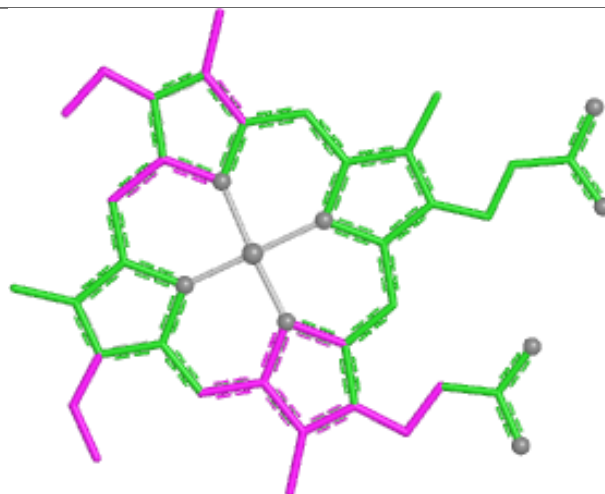




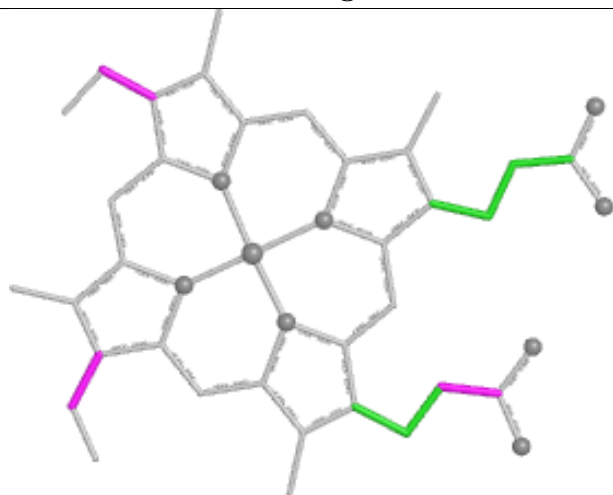
Ligand HEC C 201



Bond lengths



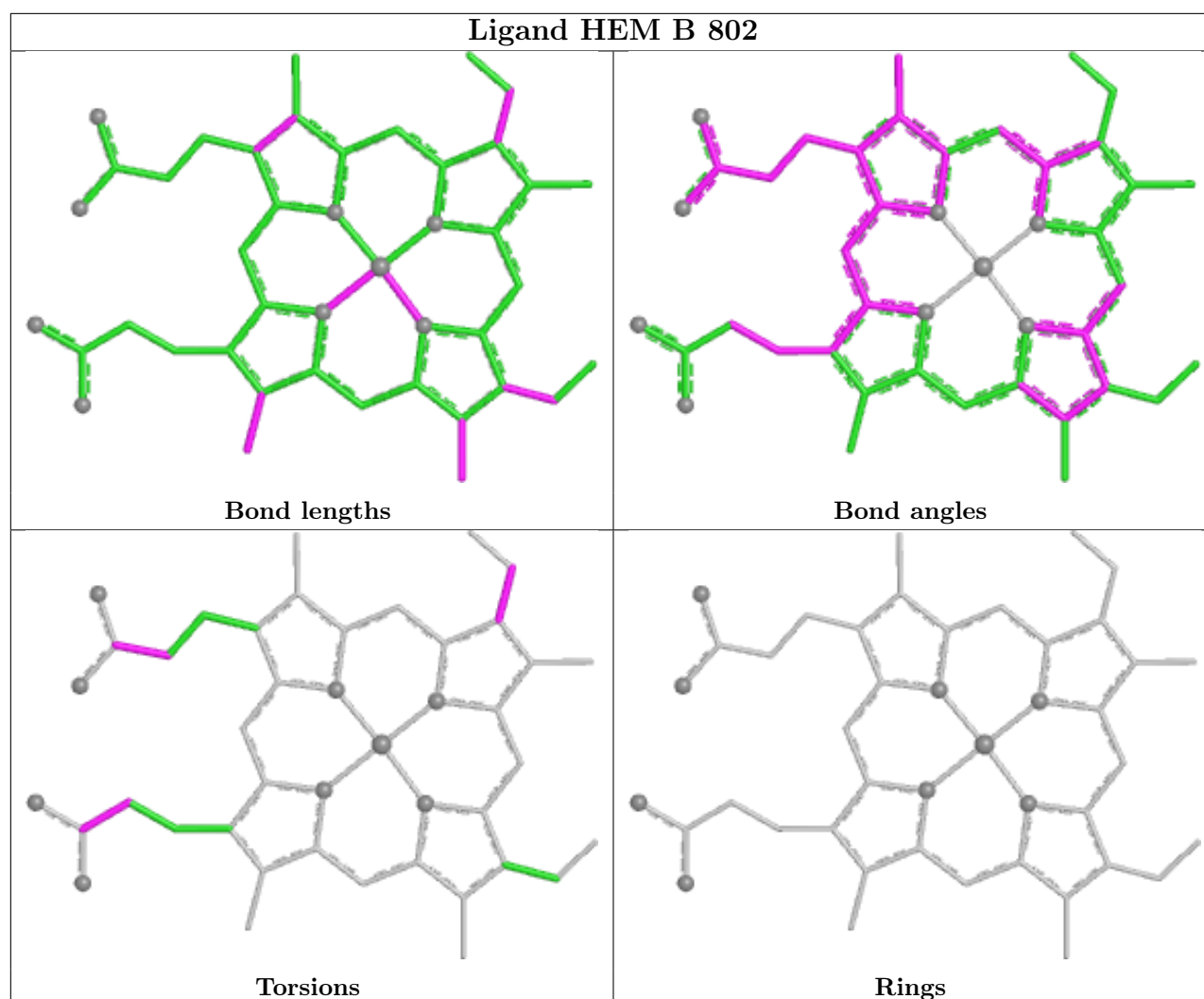
Bond angles



Torsions



Rings



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	L	213/213 (100%)	-0.05	9 (4%)	40 26	50, 77, 104, 156	0
2	H	225/225 (100%)	0.19	11 (4%)	35 23	55, 76, 124, 187	0
3	B	449/465 (96%)	0.15	16 (3%)	46 31	63, 91, 124, 161	0
4	C	142/146 (97%)	0.09	5 (3%)	47 31	61, 89, 120, 137	0
All	All	1029/1049 (98%)	0.11	41 (3%)	42 28	50, 85, 121, 187	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	B	420	ASP	8.1
1	L	152	GLY	5.0
3	B	421	GLY	4.6
3	B	128	LEU	4.4
2	H	85	SER	3.8
4	C	100	LYS	3.7
3	B	340	GLY	3.7
2	H	105	TYR	3.5
3	B	341	THR	3.4
3	B	10	PHE	3.0
3	B	422	ALA	2.9
1	L	206	VAL	2.8
1	L	105	GLU	2.8
2	H	222	GLU	2.8
4	C	144	LYS	2.7
3	B	89	TYR	2.7
1	L	13	ALA	2.6
1	L	67	SER	2.4
3	B	250	ILE	2.4
3	B	87	GLU	2.4
4	C	145	GLU	2.4

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Mol	Chain	Res	Type	RSRZ
3	B	245	ILE	2.4
4	C	134	LYS	2.4
3	B	342	GLN	2.4
2	H	196	SER	2.3
3	B	346	ALA	2.3
2	H	106	VAL	2.3
2	H	200	PRO	2.3
2	H	102	ASP	2.3
2	H	8	GLY	2.3
2	H	41	PRO	2.2
3	B	451	LEU	2.1
3	B	376	GLU	2.1
1	L	94	TYR	2.1
4	C	30	TYR	2.1
2	H	201	SER	2.1
1	L	1	ASP	2.1
1	L	151	ASP	2.1
1	L	12	ALA	2.1
2	H	15	GLY	2.0
3	B	133	GLY	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
7	O	B	804	1/1	0.83	0.13	80,80,80,80	0
9	10M	B	812	33/33	0.85	0.15	112,142,153,157	0
9	10M	B	813	33/33	0.89	0.14	85,156,182,196	0

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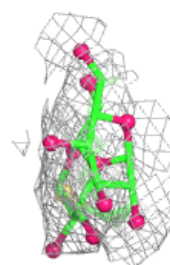
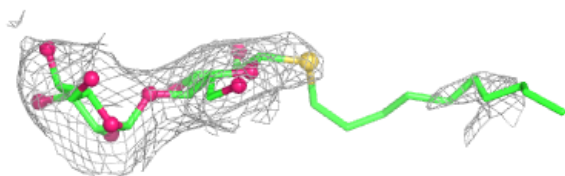
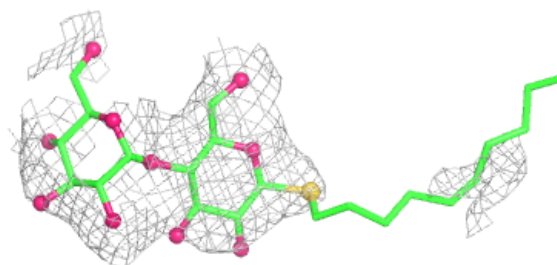
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	XE	B	810	1/1	0.96	0.08	87,87,87,87	1
8	XE	B	805	1/1	0.97	0.06	98,98,98,98	1
8	XE	B	811	1/1	0.97	0.22	89,89,89,89	1
10	CA	B	814	1/1	0.97	0.11	97,97,97,97	0
8	XE	B	808	1/1	0.98	0.04	93,93,93,93	1
5	HEM	B	801	43/43	0.98	0.10	62,71,83,96	0
11	HEC	C	201	43/43	0.98	0.09	56,63,82,87	0
8	XE	B	806	1/1	0.99	0.03	91,91,91,91	1
8	XE	B	807	1/1	0.99	0.02	94,94,94,94	1
5	HEM	B	802	43/43	0.99	0.08	71,85,93,102	0
8	XE	B	809	1/1	0.99	0.10	85,85,85,85	1
6	FE	B	803	1/1	0.99	0.05	80,80,80,80	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.

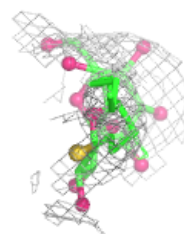
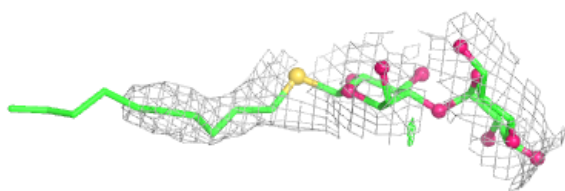
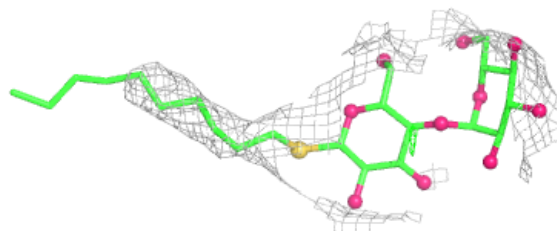
Electron density around 10M B 812:

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



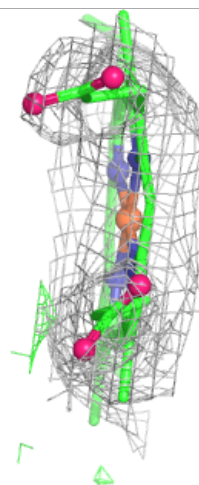
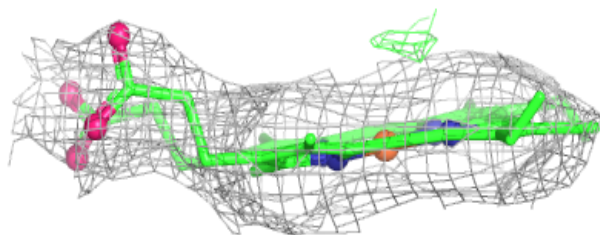
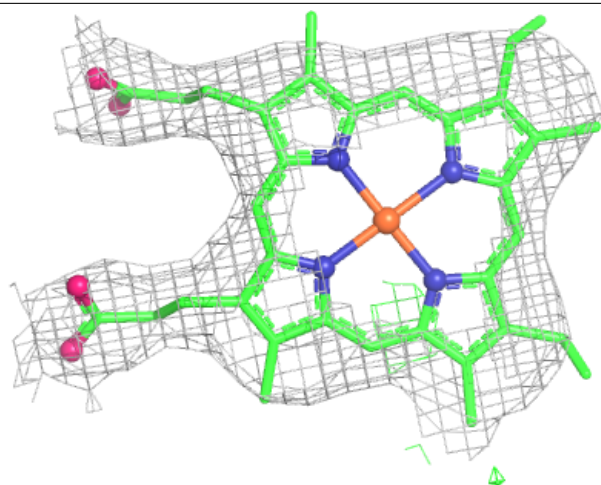
Electron density around 10M B 813:

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



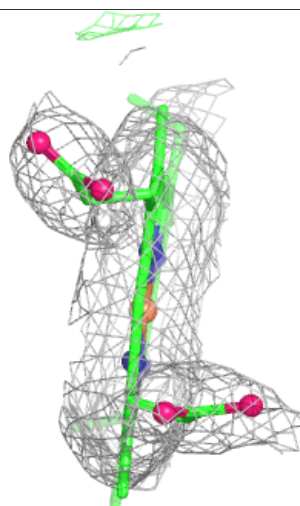
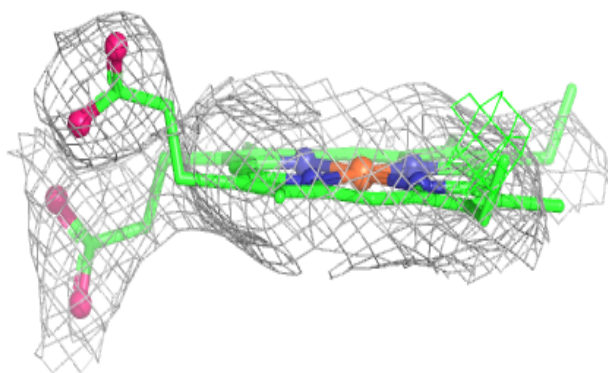
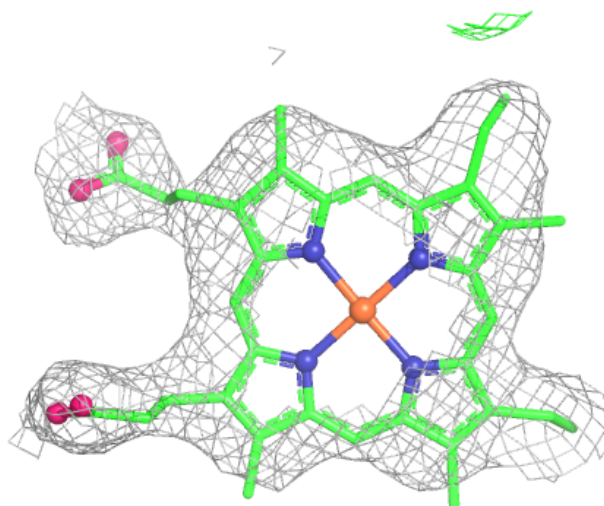
Electron density around HEM B 801:

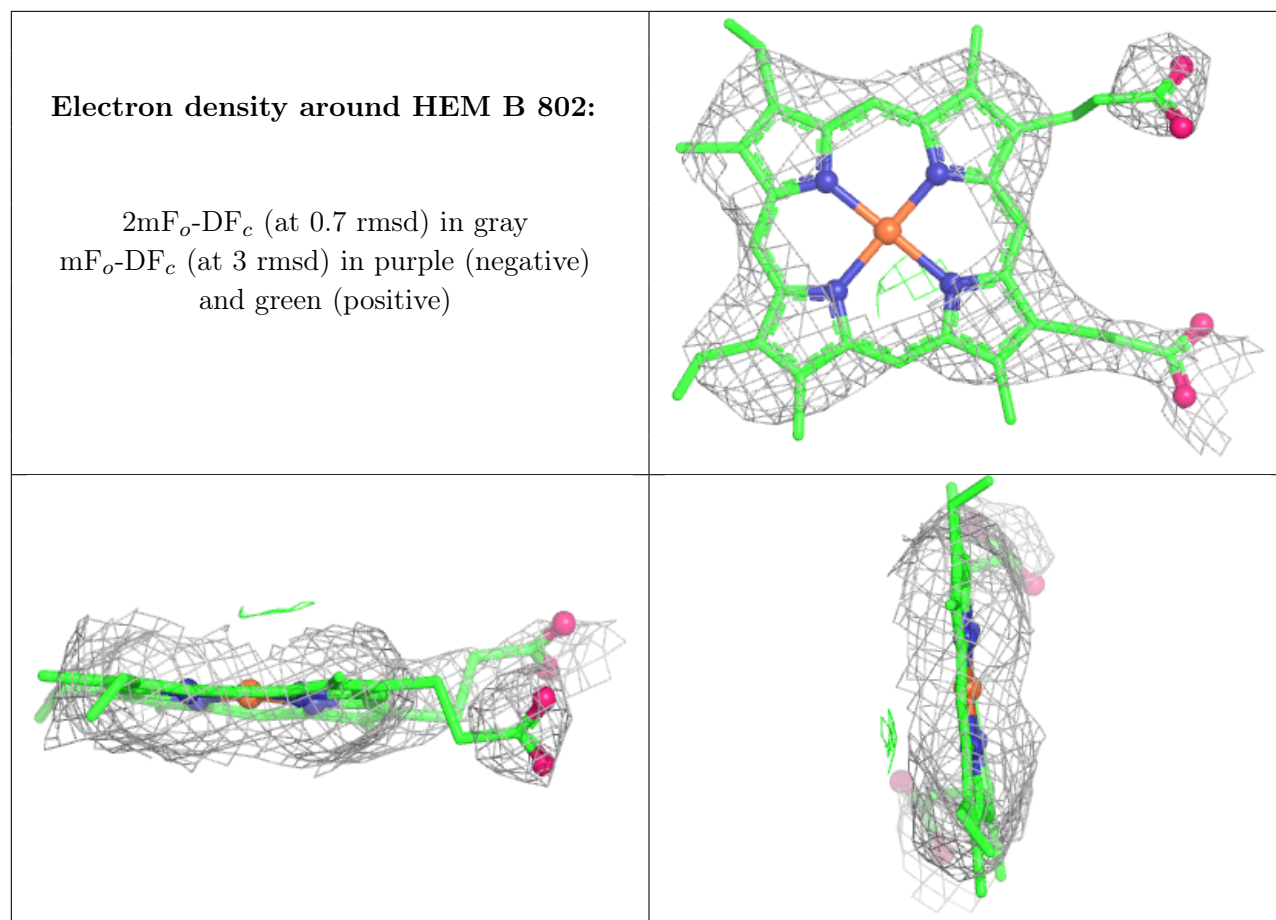
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEC C 201:

$2mF_o-DF_c$ (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.