



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:24 AM UTC

PDB ID : 1Y4Z / pdb_00001y4z
Title : The crystal structure of Nitrate Reductase A, NarGHI, in complex with the Q-site inhibitor pentachlorophenol
Authors : Bertero, M.G.; Rothery, R.A.; Boroumand, N.; Palak, M.; Blasco, F.; Ginet, N.; Weiner, J.H.; Strynadka, N.C.J.
Deposited on : 2004-12-01
Resolution : 2.00 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

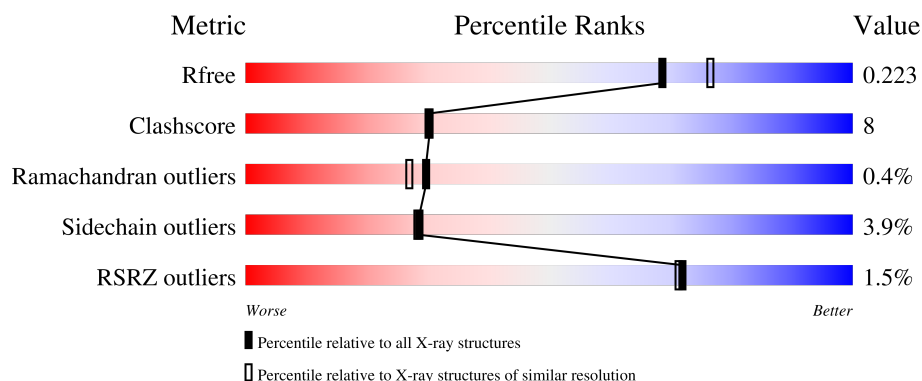
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	1246	
2	B	512	
3	C	225	

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
10	PCI	C	1808	-	X	-	-
8	F3S	B	1803	-	-	X	-

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 16919 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 Respiratory nitrate reductase 1 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1244	Total	C	N	O	S	0	0	0
			9871	6236	1731	1856	48			

- Molecule 2 is a protein called Respiratory nitrate reductase 1 beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	509	Total	C	N	O	S	0	0	0
			4049	2562	701	755	31			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	26	ALA	CYS	engineered mutation	UNP P11349

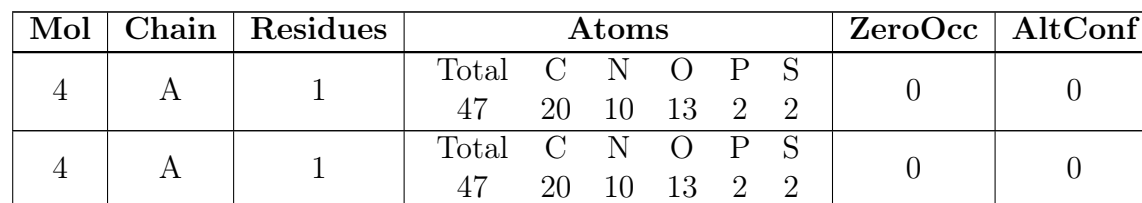
- Molecule 3 is a protein called Respiratory nitrate reductase 1 gamma chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	217	Total	C	N	O	S	0	0	0
			1723	1141	291	278	13			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	1	FME	MET	modified residue	UNP P11350

- Molecule 4 is PHOSPHORIC ACID 4-(2-AMINO-4-OXO-3,4,5,6,-TETRAHYDRO-PTE RIDIN-6-YL)-2-HYDROXY-3,4-DIMERCAPTO-BUT-3-EN-YL ESTER GUANYLATE ESTER (CCD ID: MD1) (formula: C₂₀H₂₆N₁₀O₁₃P₂S₂).

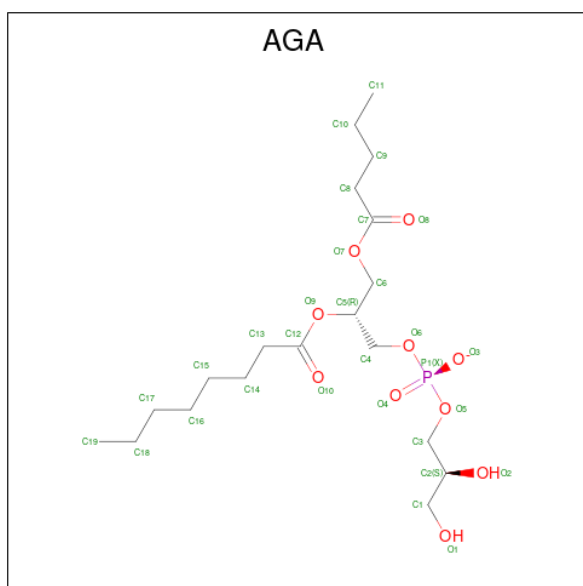


- | Mol | Chain | Residues | Atoms | ZeroOcc | AltConf |
|-----|-------|----------|-----------------|---------|---------|
| 5 | A | 1 | Total Mo
1 1 | 0 | 0 |

-

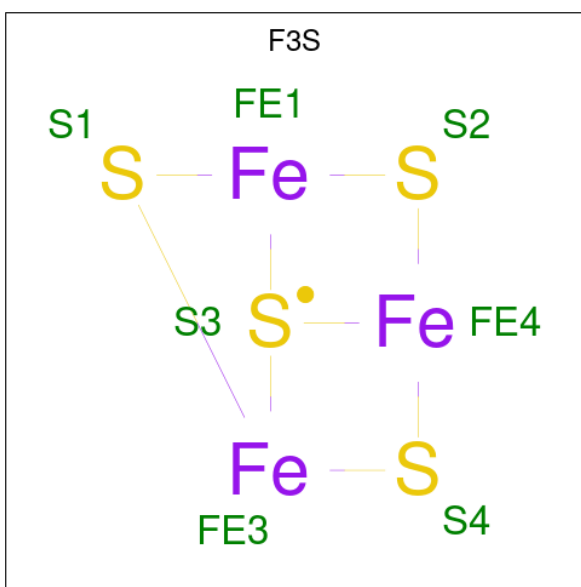
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		
6	B	1	Total	Fe	S	0	0
			8	4	4		

- Molecule 7 is (1S)-2-{{{[(2S)-2,3-DIHYDROXYPROPYL]OXY}(HYDROXY)PHOSPHORYL]OXY}-1-[(PENTANOYLOXY)METHYL]ETHYL OCTANOATE (CCD ID: AGA) (formula: C₁₉H₃₆O₁₀P).



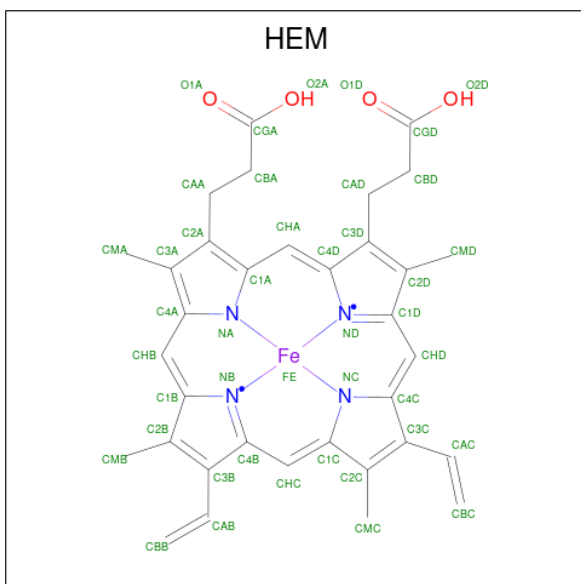
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	O	P	0	0
			25	16	8	1		

- Molecule 8 is FE3-S4 CLUSTER (CCD ID: F3S) (formula: Fe₃S₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
8	B	1	Total	Fe	S		0	0
			7	3	4			
8	B	1	Total	Fe	S		0	0
			7	3	4			

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



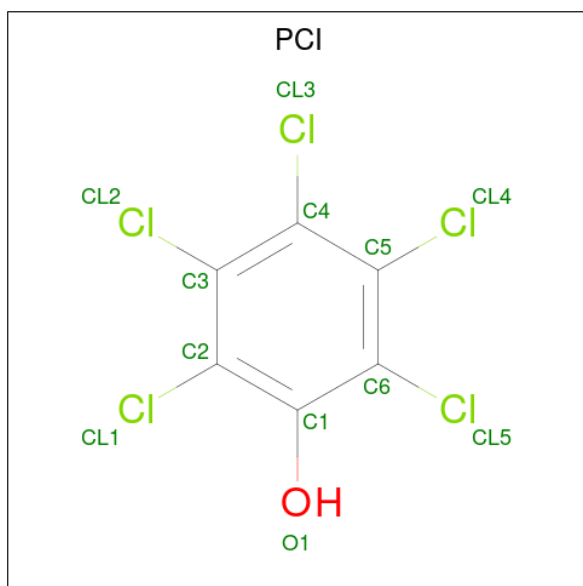
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

- Molecule 10 is PENTACHLOROPHENOL (CCD ID: PCI) (formula: C_6HCl_5O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
10	C	1	Total	C	Cl	O	0	0
			12	6	5	1		

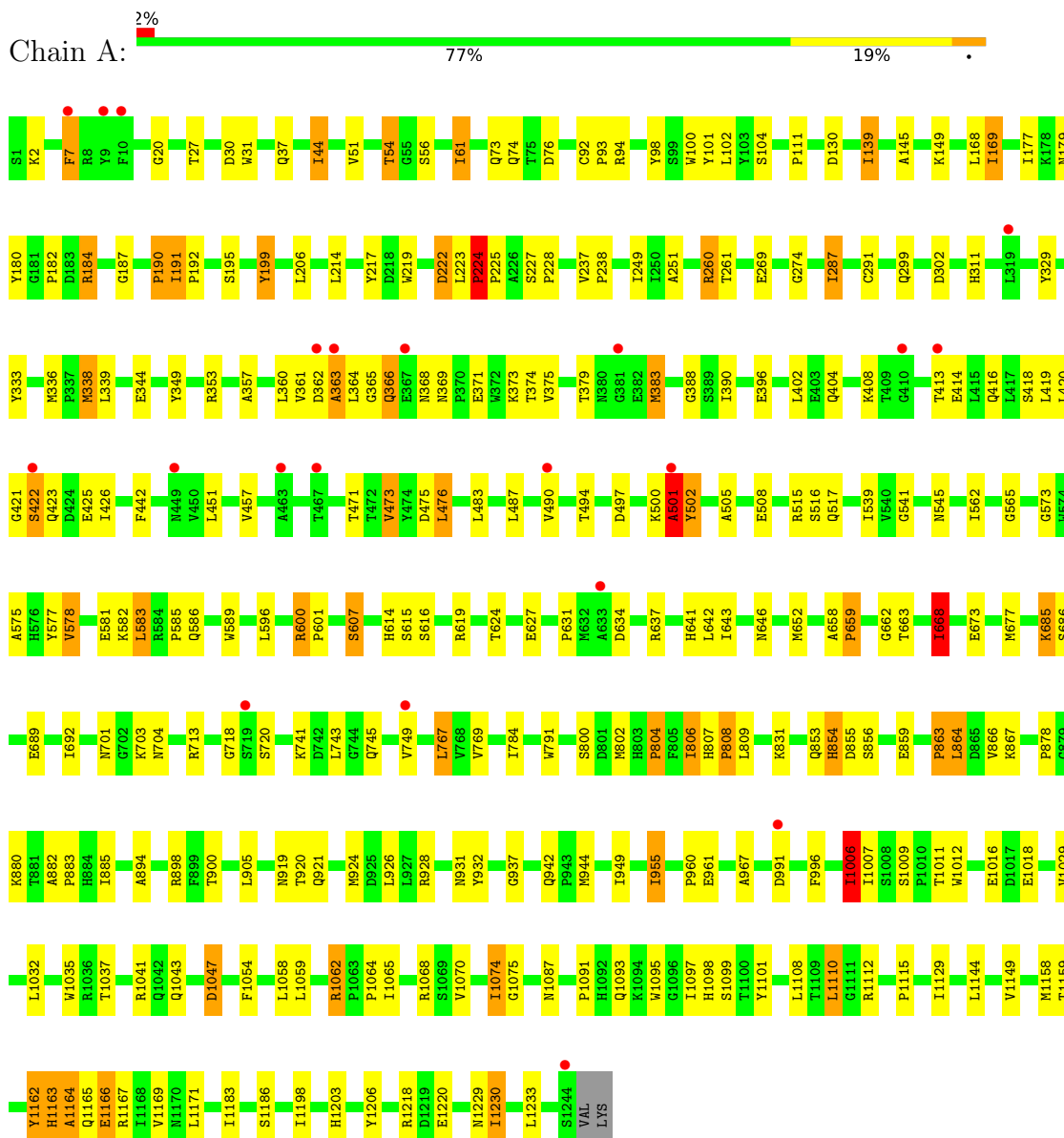
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	595	Total	O	0	0
			595	595		
11	B	368	Total	O	0	0
			368	368		
11	C	57	Total	O	0	0
			57	57		

3 Residue-property plots

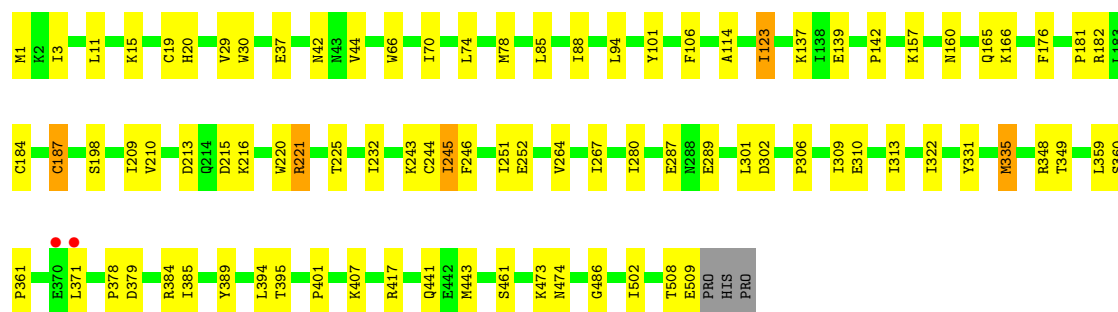
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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



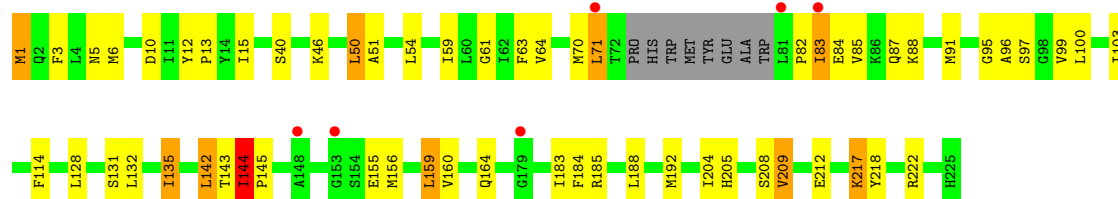
- Molecule 2: Respiratory nitrate reductase 1 beta chain

Chain B:  82% 16% ..



• Molecule 3: Respiratory nitrate reductase 1 gamma chain

Chain C:  3% 70% 22% . .



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	154.46Å 241.34Å 140.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.75 – 2.00 29.75 – 2.00	Depositor EDS
% Data completeness (in resolution range)	91.9 (29.75-2.00) 92.0 (29.75-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 2.00Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.188 , 0.233 0.181 , 0.223	Depositor DCC
R_{free} test set	9703 reflections (6.01%)	wwPDB-VP
Wilson B-factor (Å ²)	20.9	Xtriage
Anisotropy	0.842	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	16919	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.77% 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: MD1, PCI, HEM, F3S, SF4, FME, 6MO, AGA

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	0.88	6/10131 (0.1%)	1.20	78/13753 (0.6%)
2	B	0.91	0/4145	1.14	23/5608 (0.4%)
3	C	0.83	0/1758	1.10	13/2374 (0.5%)
All	All	0.88	6/16034 (0.0%)	1.17	114/21735 (0.5%)

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	1	5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1006	ILE	CA-CB	6.62	1.63	1.54
1	A	338	MET	SD-CE	-6.11	1.64	1.79
1	A	1163	HIS	C-N	-5.89	1.25	1.33
1	A	191	ILE	CA-CB	5.23	1.60	1.54
1	A	501	ALA	C-N	-5.20	1.26	1.33
1	A	54	THR	CA-CB	5.05	1.60	1.54

All (114) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1163	HIS	CA-C-N	21.13	151.66	121.24
1	A	1163	HIS	C-N-CA	21.13	151.66	121.24
1	A	501	ALA	CA-C-N	13.91	148.10	121.54
1	A	501	ALA	C-N-CA	13.91	148.10	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	1163	HIS	CA-C-O	-9.61	110.48	120.96
1	A	607	SER	N-CA-C	9.43	122.56	111.71
1	A	1164	ALA	N-CA-C	9.16	123.06	109.59
1	A	1167	ARG	N-CA-C	9.12	123.72	112.59
1	A	1070	VAL	N-CA-C	8.90	119.11	111.90
1	A	1093	GLN	N-CA-C	8.45	121.69	110.53
1	A	809	LEU	N-CA-C	-8.30	96.15	109.76
2	B	30	TRP	N-CA-C	7.87	123.01	113.41
2	B	287	GLU	N-CA-C	7.77	119.38	111.07
1	A	102	LEU	N-CA-C	7.72	120.38	111.11
1	A	179	ASN	N-CA-C	7.71	122.79	113.23
1	A	937	GLY	CA-C-N	7.57	127.95	119.32
1	A	937	GLY	C-N-CA	7.57	127.95	119.32
1	A	501	ALA	N-CA-CB	7.49	123.14	110.49
1	A	1163	HIS	CA-CB-CG	7.41	121.21	113.80
1	A	1097	ILE	N-CA-C	-7.30	95.68	107.28
1	A	573	GLY	N-CA-C	7.30	121.08	111.52
2	B	88	ILE	N-CA-C	7.24	120.10	111.05
2	B	166	LYS	N-CA-C	7.20	122.06	113.28
1	A	863	PRO	N-CA-C	6.99	123.25	113.53
2	B	187	CYS	N-CA-C	6.97	119.56	110.43
1	A	586	GLN	N-CA-C	6.94	119.44	111.11
1	A	375	VAL	N-CA-C	6.83	118.31	108.48
1	A	224	PRO	N-CA-C	-6.74	102.47	110.70
3	C	144	ILE	CB-CA-C	-6.70	107.33	113.70
1	A	1169	VAL	N-CA-C	6.65	117.42	108.11
1	A	333	TYR	N-CA-C	6.60	121.39	112.88
2	B	94	LEU	N-CA-C	6.58	117.66	109.57
1	A	582	LYS	N-CA-C	6.57	120.34	107.98
2	B	280	ILE	N-CA-C	6.57	116.72	110.42
1	A	545	ASN	N-CA-C	6.49	120.80	113.01
2	B	216	LYS	N-CA-C	6.35	120.29	112.54
3	C	61	GLY	N-CA-C	-6.32	105.17	112.50
1	A	222	ASP	N-CA-C	-6.26	105.77	113.41
1	A	1035	TRP	N-CA-C	-6.26	101.22	110.48
1	A	1206	TYR	N-CA-C	6.25	119.31	110.50
1	A	363	ALA	N-CA-C	-6.11	104.42	112.24
1	A	720	SER	N-CA-C	6.11	119.99	112.54
1	A	808	PRO	N-CA-C	6.10	125.04	112.47
3	C	209	VAL	CA-C-N	6.01	127.35	119.84
3	C	209	VAL	C-N-CA	6.01	127.35	119.84
1	A	76	ASP	N-CA-C	5.99	119.32	112.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	583	LEU	N-CA-C	-5.99	97.45	107.99
2	B	394	LEU	N-CA-C	5.94	121.19	113.88
3	C	51	ALA	N-CA-C	5.94	117.42	111.07
1	A	900	THR	N-CA-C	5.90	119.54	112.93
2	B	359	LEU	N-CA-C	-5.86	101.28	110.36
2	B	379	ASP	N-CA-C	-5.85	100.75	110.17
1	A	955	ILE	CB-CA-C	-5.83	104.51	111.97
1	A	614	HIS	N-CA-C	5.83	118.58	111.82
2	B	371	LEU	N-CA-C	-5.78	101.72	110.28
1	A	581	GLU	N-CA-C	5.76	119.57	112.54
1	A	388	GLY	N-CA-C	5.76	122.69	115.21
1	A	1163	HIS	N-CA-CB	5.73	118.36	109.48
1	A	802	MET	N-CA-C	5.64	118.37	111.82
3	C	71	LEU	N-CA-C	5.64	120.85	113.30
1	A	668	ILE	CB-CA-C	-5.63	104.76	111.97
1	A	249	ILE	N-CA-C	5.62	116.22	108.12
1	A	199	TYR	N-CA-C	-5.57	105.12	111.14
1	A	1043	GLN	N-CA-C	5.56	117.78	107.99
1	A	631	PRO	N-CA-C	-5.54	107.22	114.03
1	A	184	ARG	N-CA-C	-5.51	106.23	113.17
1	A	1065	ILE	CB-CA-C	-5.47	105.57	111.59
1	A	1218	ARG	N-CA-C	5.47	119.22	112.54
2	B	157	LYS	N-CA-C	-5.46	106.46	113.01
2	B	221	ARG	N-CA-C	5.45	118.96	111.54
1	A	502	TYR	CB-CG-CD1	5.45	128.97	120.80
1	A	1016	GLU	N-CA-C	-5.43	97.65	107.75
1	A	539	ILE	N-CA-C	-5.43	100.60	108.36
1	A	713	ARG	N-CA-C	-5.42	105.97	112.58
1	A	302	ASP	N-CA-C	5.40	117.17	111.28
1	A	1162	TYR	CA-C-N	5.38	128.74	121.05
1	A	1162	TYR	C-N-CA	5.38	128.74	121.05
3	C	217	LYS	N-CA-C	-5.37	102.93	110.50
1	A	473	VAL	N-CA-C	-5.35	105.17	110.62
1	A	1149	VAL	N-CA-C	-5.33	99.96	107.75
1	A	74	GLN	N-CA-C	-5.33	102.99	110.50
3	C	40	SER	N-CA-C	-5.28	105.15	113.02
1	A	1029	VAL	N-CA-C	5.28	116.05	110.72
1	A	853	GLN	N-CA-C	5.27	117.83	109.24
1	A	291	CYS	N-CA-C	5.26	117.87	110.14
1	A	854	HIS	N-CA-C	-5.26	103.20	110.35
2	B	443	MET	N-CA-C	-5.25	105.55	111.28
3	C	135	ILE	CB-CA-C	-5.23	105.17	112.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	361	VAL	N-CA-C	5.23	115.67	110.23
1	A	615	SER	N-CA-C	-5.22	106.76	113.02
1	A	1166	GLU	N-CA-C	5.21	121.89	110.80
1	A	494	THR	N-CA-C	-5.17	107.02	113.38
1	A	1047	ASP	N-CA-C	5.17	119.23	113.02
1	A	339	LEU	N-CA-C	5.16	118.03	109.46
2	B	29	VAL	N-CA-C	5.16	115.38	110.53
2	B	232	ILE	N-CA-C	-5.16	100.95	108.17
3	C	64	VAL	N-CA-C	-5.16	105.47	110.42
3	C	15	ILE	CB-CA-C	-5.15	105.38	111.97
1	A	111	PRO	N-CA-C	-5.13	103.14	111.14
1	A	73	GLN	N-CA-C	5.12	117.66	110.23
2	B	378	PRO	N-CA-C	5.11	119.50	111.38
3	C	218	TYR	N-CA-C	5.10	116.52	111.07
1	A	1009	SER	CA-C-N	5.08	124.69	119.56
1	A	1009	SER	C-N-CA	5.08	124.69	119.56
1	A	1220	GLU	N-CA-C	5.06	117.56	110.23
3	C	114	PHE	N-CA-C	5.05	120.29	113.72
2	B	302	ASP	CA-C-N	5.04	124.65	119.56
2	B	302	ASP	C-N-CA	5.04	124.65	119.56
1	A	260	ARG	N-CA-C	-5.04	104.31	110.61
2	B	322	ILE	CB-CA-C	-5.04	105.52	111.97
2	B	114	ALA	CA-C-N	5.02	124.92	119.85
2	B	114	ALA	C-N-CA	5.02	124.92	119.85
1	A	94	ARG	N-CA-C	-5.01	105.70	111.07
1	A	1007	ILE	N-CA-C	5.01	116.18	108.71

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	501	ALA	CA

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1163	HIS	Mainchain,Peptide
1	A	501	ALA	Mainchain,Peptide
1	A	502	TYR	Mainchain

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	9871	0	9528	178	0
2	B	4049	0	3974	61	0
3	C	1723	0	1772	33	0
4	A	94	0	42	7	0
5	A	1	0	0	0	0
6	A	8	0	0	0	0
6	B	16	0	0	0	0
7	A	25	0	29	0	0
8	B	14	0	0	3	0
9	C	86	0	60	1	0
10	C	12	0	1	1	0
11	A	595	0	0	7	1
11	B	368	0	0	8	0
11	C	57	0	0	1	0
All	All	16919	0	15406	263	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (263) 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:641:HIS:HD2	1:A:643:ILE:H	1.14	0.93
1:A:652:MET:HE1	1:A:866:VAL:HG13	1.55	0.87
2:B:3:ILE:HD12	2:B:301:LEU:CD1	2.06	0.86
1:A:338:MET:HE2	1:A:374:THR:OG1	1.77	0.84
2:B:361:PRO:HG2	2:B:384:ARG:HD3	1.59	0.84
1:A:663:THR:HG21	1:A:692:ILE:HD12	1.60	0.81
2:B:245:ILE:HD13	8:B:1803:F3S:S2	2.22	0.80
1:A:589:TRP:HA	1:A:955:ILE:HD12	1.67	0.77
1:A:641:HIS:CD2	1:A:643:ILE:H	2.03	0.76
3:C:96:ALA:O	3:C:100:LEU:HD13	1.86	0.75
1:A:404:GLN:HE22	1:A:1041:ARG:HH12	1.33	0.75
1:A:686:SER:HB3	1:A:692:ILE:HG12	1.71	0.72
1:A:1074:ILE:HD13	1:A:1075:GLY:N	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:508:GLU:OE1	1:A:515:ARG:HD2	1.90	0.71
1:A:596:LEU:O	1:A:600:ARG:HD2	1.92	0.70
1:A:652:MET:HE1	1:A:866:VAL:CG1	2.23	0.69
2:B:165:GLN:HE21	2:B:165:GLN:HA	1.58	0.69
2:B:165:GLN:HA	2:B:165:GLN:NE2	2.07	0.68
2:B:176:PHE:CD1	2:B:385:ILE:HD12	2.28	0.68
1:A:1098:HIS:CE1	4:A:2800:MD1:S13	2.87	0.67
1:A:863:PRO:HG2	1:A:864:LEU:HD22	1.78	0.66
1:A:338:MET:HE2	1:A:374:THR:CB	2.25	0.65
1:A:652:MET:HE3	1:A:867:LYS:O	1.96	0.65
1:A:619:ARG:NH1	11:A:4214:HOH:O	2.29	0.64
1:A:360:LEU:HG	1:A:383:MET:HE3	1.79	0.64
1:A:490:VAL:O	1:A:500:LYS:HE3	1.97	0.63
1:A:27:THR:HG23	3:C:222:ARG:HD3	1.81	0.62
1:A:589:TRP:HA	1:A:955:ILE:CD1	2.30	0.62
1:A:1098:HIS:HE1	4:A:2800:MD1:S13	2.22	0.62
2:B:309:ILE:O	2:B:313:ILE:HD13	2.00	0.61
1:A:20:GLY:O	3:C:217:LYS:HD2	2.00	0.61
1:A:1171:LEU:H	2:B:123:ILE:HD12	1.64	0.61
1:A:924:MET:HE2	11:A:4109:HOH:O	2.00	0.60
3:C:160:VAL:O	3:C:164:GLN:HG3	2.01	0.60
2:B:246:PHE:CD2	2:B:251:ILE:CD1	2.85	0.60
1:A:169:ILE:HD13	1:A:169:ILE:N	2.16	0.60
1:A:749:VAL:HG12	11:A:4122:HOH:O	2.01	0.59
4:A:1800:MD1:H7	4:A:1800:MD1:C11	2.32	0.59
1:A:1074:ILE:HD13	1:A:1074:ILE:C	2.28	0.59
2:B:3:ILE:CD1	2:B:301:LEU:CD1	2.80	0.58
4:A:1800:MD1:H7	4:A:1800:MD1:O11	2.03	0.58
2:B:246:PHE:HD2	2:B:251:ILE:CD1	2.17	0.58
1:A:368:ASN:ND2	1:A:396:GLU:HG2	2.18	0.58
1:A:1006:ILE:HD12	1:A:1006:ILE:H	1.68	0.58
2:B:176:PHE:HB2	2:B:385:ILE:CD1	2.34	0.58
2:B:70:ILE:HG13	11:B:2066:HOH:O	2.03	0.57
3:C:99:VAL:O	3:C:103:ILE:HG12	2.05	0.57
2:B:361:PRO:HG2	2:B:384:ARG:CD	2.33	0.57
2:B:508:THR:O	2:B:509:GLU:HB3	2.04	0.57
1:A:426:ILE:HD12	1:A:426:ILE:N	2.20	0.57
3:C:131:SER:O	3:C:135:ILE:HG12	2.04	0.57
3:C:159:LEU:HG	9:C:807:HEM:HMA3	1.88	0.56
3:C:82:PRO:HG2	3:C:85:VAL:HG23	1.88	0.56
1:A:190:PRO:HB2	1:A:191:ILE:CD1	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:SER:HB3	1:A:228:PRO:HD3	1.89	0.55
1:A:878:PRO:HB3	1:A:885:ILE:HG12	1.89	0.55
2:B:441:GLN:HG2	11:B:1912:HOH:O	2.06	0.55
1:A:686:SER:CB	1:A:692:ILE:HG12	2.36	0.55
1:A:371:GLU:OE1	1:A:371:GLU:N	2.22	0.55
1:A:919:ASN:ND2	1:A:921:GLN:H	2.04	0.55
1:A:366:GLN:CG	1:A:373:LYS:HD2	2.38	0.55
1:A:191:ILE:H	1:A:191:ILE:HD12	1.71	0.54
2:B:198:SER:HB3	11:B:1950:HOH:O	2.07	0.54
2:B:78:MET:CG	2:B:225:THR:HG22	2.36	0.54
1:A:585:PRO:HA	1:A:961:GLU:OE1	2.07	0.54
1:A:662:GLY:HA2	1:A:704:ASN:HD21	1.73	0.54
3:C:82:PRO:HG2	3:C:85:VAL:CG2	2.38	0.54
2:B:245:ILE:HD13	2:B:245:ILE:H	1.71	0.54
1:A:169:ILE:HD11	1:A:784:ILE:HD12	1.88	0.54
1:A:360:LEU:N	1:A:360:LEU:HD22	2.24	0.53
2:B:246:PHE:O	2:B:251:ILE:HD12	2.08	0.53
1:A:191:ILE:HD12	1:A:191:ILE:N	2.24	0.53
1:A:1108:LEU:HD13	2:B:106:PHE:CE2	2.44	0.53
2:B:78:MET:HG2	2:B:225:THR:HG22	1.91	0.53
1:A:949:ILE:HD12	1:A:996:PHE:CD2	2.44	0.53
2:B:246:PHE:CD2	2:B:251:ILE:HD11	2.44	0.53
1:A:190:PRO:HB2	1:A:191:ILE:HD13	1.91	0.52
1:A:56:SER:HB2	1:A:800:SER:HB2	1.90	0.52
1:A:366:GLN:HG3	1:A:373:LYS:HD2	1.91	0.52
2:B:19:CYS:O	2:B:20:HIS:HB2	2.09	0.52
3:C:50:LEU:HD13	3:C:54:LEU:HD12	1.91	0.52
2:B:210:VAL:O	2:B:243:LYS:NZ	2.43	0.52
3:C:143:THR:HB	3:C:184:PHE:CE1	2.45	0.52
1:A:187:GLY:HA3	1:A:206:LEU:HD11	1.92	0.52
1:A:589:TRP:CA	1:A:955:ILE:HD12	2.38	0.52
1:A:1171:LEU:H	2:B:123:ILE:CD1	2.22	0.52
1:A:685:LYS:O	1:A:689:GLU:HG3	2.10	0.51
4:A:1800:MD1:O11	4:A:1800:MD1:C7	2.59	0.51
2:B:473:LYS:HE3	2:B:474:ASN:OD1	2.10	0.51
1:A:600:ARG:HD3	1:A:905:LEU:HD13	1.92	0.51
2:B:20:HIS:CE1	2:B:44:VAL:HB	2.46	0.51
1:A:251:ALA:HB3	1:A:287:ILE:HD11	1.92	0.51
1:A:1115:PRO:HA	1:A:1165:GLN:OE1	2.11	0.51
2:B:137:LYS:HA	11:B:2048:HOH:O	2.10	0.51
1:A:804:PRO:O	1:A:1006:ILE:HD12	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1098:HIS:CE1	4:A:1800:MD1:S12	3.04	0.51
3:C:156:MET:HE2	10:C:1808:PCI:CL4	2.47	0.51
2:B:245:ILE:CD1	8:B:1803:F3S:S2	2.95	0.50
3:C:142:LEU:HB3	3:C:183:ILE:HD11	1.94	0.50
1:A:100:TRP:O	1:A:104:SER:HB3	2.11	0.50
1:A:641:HIS:CD2	1:A:643:ILE:HG22	2.47	0.50
1:A:658:ALA:HA	1:A:659:PRO:C	2.36	0.50
1:A:344:GLU:HG3	1:A:349:TYR:CE1	2.47	0.50
2:B:1:MET:SD	2:B:3:ILE:HD11	2.51	0.50
1:A:237:VAL:HB	1:A:238:PRO:HD2	1.93	0.50
1:A:882:ALA:HB1	1:A:883:PRO:HD2	1.93	0.50
1:A:27:THR:CG2	3:C:222:ARG:HD3	2.42	0.49
3:C:142:LEU:HB3	3:C:183:ILE:CD1	2.42	0.49
1:A:864:LEU:HD22	1:A:864:LEU:N	2.28	0.49
1:A:191:ILE:HG22	1:A:191:ILE:O	2.12	0.49
1:A:357:ALA:O	1:A:363:ALA:HA	2.12	0.49
1:A:931:ASN:O	1:A:932:TYR:HB2	2.11	0.49
2:B:78:MET:HG2	2:B:225:THR:CG2	2.42	0.49
1:A:425:GLU:C	1:A:426:ILE:HD12	2.38	0.49
1:A:1054:PHE:O	1:A:1062:ARG:NH2	2.45	0.49
1:A:1006:ILE:H	1:A:1006:ILE:CD1	2.25	0.49
1:A:517:GLN:HA	1:A:517:GLN:NE2	2.27	0.48
1:A:517:GLN:HA	1:A:517:GLN:HE21	1.77	0.48
2:B:78:MET:HG3	11:B:1962:HOH:O	2.12	0.48
1:A:7:PHE:CD1	1:A:7:PHE:N	2.82	0.48
3:C:1:FME:O1	3:C:3:PHE:HB3	2.14	0.48
2:B:3:ILE:HD12	2:B:301:LEU:HD11	1.90	0.48
1:A:169:ILE:N	1:A:169:ILE:CD1	2.77	0.48
1:A:344:GLU:HG3	1:A:349:TYR:HE1	1.77	0.48
1:A:949:ILE:HD12	1:A:996:PHE:CE2	2.49	0.48
1:A:217:TYR:CE2	1:A:223:LEU:HA	2.48	0.47
2:B:187:CYS:HB3	2:B:349:THR:O	2.15	0.47
2:B:360:SER:HB3	2:B:385:ILE:HG12	1.96	0.47
2:B:502:ILE:HD12	11:B:2149:HOH:O	2.14	0.47
1:A:451:LEU:CD1	1:A:501:ALA:HB3	2.44	0.47
1:A:624:THR:O	1:A:627:GLU:HG2	2.15	0.47
1:A:1062:ARG:HD3	11:A:4082:HOH:O	2.15	0.47
1:A:169:ILE:HD12	1:A:767:LEU:HD11	1.97	0.46
2:B:395:THR:HG21	2:B:401:PRO:HG2	1.98	0.46
1:A:92:CYS:HB2	1:A:93:PRO:HD2	1.97	0.46
1:A:749:VAL:HG23	1:A:749:VAL:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:920:THR:O	1:A:920:THR:HG23	2.16	0.46
2:B:209:ILE:HD12	2:B:246:PHE:CB	2.45	0.46
3:C:13:PRO:HB3	3:C:192:MET:SD	2.56	0.46
1:A:421:GLY:O	1:A:422:SER:HB3	2.15	0.46
1:A:1144:LEU:HD12	1:A:1144:LEU:C	2.40	0.46
3:C:84:GLU:O	3:C:88:LYS:HG3	2.16	0.46
1:A:139:ILE:HA	1:A:139:ILE:HD12	1.76	0.45
1:A:7:PHE:N	1:A:7:PHE:HD1	2.14	0.45
1:A:471:THR:HG21	1:A:476:LEU:HD13	1.98	0.45
1:A:1062:ARG:CD	11:A:4082:HOH:O	2.65	0.45
3:C:6:MET:O	3:C:10:ASP:HB2	2.16	0.45
1:A:663:THR:CG2	1:A:692:ILE:HD12	2.40	0.45
3:C:144:ILE:N	3:C:145:PRO:HD2	2.32	0.45
1:A:338:MET:HE2	1:A:374:THR:HB	1.96	0.45
1:A:854:HIS:O	1:A:855:ASP:HB2	2.17	0.45
1:A:311:HIS:CE1	1:A:483:LEU:HD13	2.52	0.45
2:B:209:ILE:HD12	2:B:246:PHE:HB3	1.99	0.45
1:A:1006:ILE:CD1	1:A:1006:ILE:N	2.80	0.45
1:A:1091:PRO:HG2	1:A:1162:TYR:CE1	2.51	0.45
1:A:627:GLU:OE2	1:A:1068:ARG:NH1	2.46	0.45
1:A:274:GLY:HA3	2:B:417:ARG:HB2	1.99	0.44
1:A:168:LEU:HD23	1:A:168:LEU:C	2.43	0.44
1:A:214:LEU:HB3	1:A:607:SER:OG	2.17	0.44
1:A:353:ARG:HA	1:A:1047:ASP:HB2	1.98	0.44
1:A:199:TYR:CD1	1:A:199:TYR:C	2.95	0.44
3:C:204:ILE:HD12	3:C:205:HIS:N	2.32	0.44
2:B:184:CYS:HB3	2:B:244:CYS:HB3	1.99	0.44
2:B:331:TYR:CE2	2:B:335:MET:HG3	2.52	0.44
3:C:184:PHE:O	3:C:188:LEU:HG	2.18	0.44
2:B:335:MET:HE3	2:B:335:MET:HA	2.00	0.44
1:A:31:TRP:CE2	2:B:213:ASP:HA	2.53	0.44
2:B:306:PRO:O	2:B:310:GLU:HG3	2.18	0.44
1:A:616:SER:HB3	1:A:619:ARG:HD3	1.99	0.44
2:B:3:ILE:HD12	2:B:301:LEU:HD12	1.93	0.44
1:A:1087:ASN:O	1:A:1159:THR:HG22	2.18	0.43
1:A:419:LEU:HD23	1:A:419:LEU:HA	1.71	0.43
1:A:217:TYR:CD1	1:A:222:ASP:HB2	2.54	0.43
3:C:63:PHE:CD1	3:C:63:PHE:C	2.96	0.43
1:A:130:ASP:OD2	1:A:130:ASP:C	2.61	0.43
1:A:261:THR:HG22	2:B:264:VAL:HG11	2.00	0.43
1:A:497:ASP:HA	1:A:505:ALA:HB2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:ILE:HA	1:A:61:ILE:O	2.18	0.43
1:A:515:ARG:HG2	1:A:516:SER:N	2.33	0.43
1:A:575:ALA:HB1	1:A:577:TYR:CE2	2.54	0.43
1:A:767:LEU:HD13	1:A:769:VAL:HG23	1.99	0.43
3:C:5:ASN:OD1	3:C:185:ARG:NH1	2.52	0.43
1:A:30:ASP:HB2	2:B:486:GLY:HA2	2.01	0.43
1:A:336:MET:HA	1:A:473:VAL:HB	2.01	0.43
1:A:701:ASN:OD1	1:A:701:ASN:C	2.62	0.43
2:B:101:TYR:CE2	2:B:142:PRO:HD3	2.53	0.43
2:B:289:GLU:HG2	11:B:2119:HOH:O	2.19	0.43
1:A:187:GLY:HA3	1:A:206:LEU:CD1	2.49	0.43
1:A:366:GLN:HG2	1:A:373:LYS:HD2	2.01	0.43
1:A:2:LYS:NZ	2:B:215:ASP:OD1	2.51	0.43
1:A:1183:ILE:O	1:A:1186:SER:HB2	2.19	0.43
1:A:192:PRO:HB3	1:A:199:TYR:CG	2.54	0.43
2:B:11:LEU:HD22	2:B:181:PRO:HG2	2.01	0.43
1:A:145:ALA:O	1:A:149:LYS:HG3	2.19	0.42
1:A:423:GLN:HB2	1:A:457:VAL:O	2.18	0.42
1:A:856:SER:O	1:A:859:GLU:HG2	2.19	0.42
1:A:880:LYS:NZ	11:A:4316:HOH:O	2.50	0.42
1:A:338:MET:CE	1:A:374:THR:HB	2.50	0.42
1:A:928:ARG:HH11	1:A:942:GLN:NE2	2.17	0.42
1:A:1229:ASN:C	1:A:1230:ILE:HD12	2.44	0.42
1:A:541:GLY:HA3	4:A:2800:MD1:O1B	2.20	0.42
2:B:160:ASN:HB2	2:B:389:TYR:CE2	2.54	0.42
1:A:219:TRP:HB2	1:A:607:SER:HB2	2.01	0.42
1:A:1230:ILE:HD12	1:A:1230:ILE:N	2.35	0.42
1:A:419:LEU:O	1:A:420:LEU:C	2.60	0.42
1:A:1037:THR:HA	1:A:1203:HIS:HB3	2.02	0.42
2:B:246:PHE:HA	8:B:1803:F3S:S4	2.60	0.42
3:C:83:ILE:HD11	3:C:156:MET:HG2	2.01	0.42
1:A:98:TYR:CD1	1:A:791:TRP:CZ3	3.08	0.42
1:A:269:GLU:HG3	2:B:15:LYS:HE3	2.01	0.42
1:A:583:LEU:C	1:A:583:LEU:HD23	2.45	0.42
1:A:169:ILE:HD11	1:A:784:ILE:CD1	2.49	0.42
1:A:180:TYR:HB3	1:A:184:ARG:HG2	2.01	0.42
1:A:685:LYS:HD3	11:A:4360:HOH:O	2.20	0.42
1:A:225:PRO:C	1:A:228:PRO:HD2	2.45	0.41
1:A:1095:TRP:CZ3	1:A:1110:LEU:HB3	2.55	0.41
1:A:1099:SER:HA	1:A:1164:ALA:O	2.20	0.41
1:A:260:ARG:HD3	1:A:260:ARG:HA	1.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:662:GLY:HA2	1:A:704:ASN:ND2	2.35	0.41
1:A:1058:LEU:HD23	1:A:1058:LEU:HA	1.95	0.41
1:A:634:ASP:OD1	1:A:637:ARG:HG3	2.20	0.41
2:B:220:TRP:C	2:B:221:ARG:HG3	2.45	0.41
3:C:12:TYR:N	3:C:13:PRO:HD2	2.35	0.41
3:C:208:SER:O	3:C:209:VAL:C	2.62	0.41
1:A:177:ILE:HG12	1:A:182:PRO:HA	2.02	0.41
1:A:223:LEU:HD12	1:A:224:PRO:HD2	2.01	0.41
1:A:703:LYS:HB2	1:A:703:LYS:HE3	1.84	0.41
1:A:369:ASN:O	1:A:373:LYS:HG3	2.21	0.41
1:A:960:PRO:O	1:A:967:ALA:HB2	2.20	0.41
2:B:165:GLN:HB2	11:B:2062:HOH:O	2.20	0.41
3:C:95:GLY:O	3:C:99:VAL:HG23	2.21	0.41
1:A:51:VAL:HB	1:A:791:TRP:CH2	2.56	0.41
1:A:442:PHE:CE2	1:A:1064:PRO:HG2	2.55	0.41
1:A:487:LEU:N	1:A:487:LEU:CD1	2.83	0.41
3:C:128:LEU:O	3:C:132:LEU:HG	2.21	0.41
1:A:101:TYR:OH	1:A:1101:TYR:HA	2.21	0.41
1:A:299:GLN:CD	1:A:1158:MET:HE2	2.46	0.41
1:A:418:SER:OG	1:A:475:ASP:OD1	2.35	0.41
1:A:641:HIS:CD2	1:A:642:LEU:N	2.89	0.41
1:A:365:GLY:HA3	1:A:408:LYS:HG3	2.02	0.41
1:A:668:ILE:N	1:A:668:ILE:HD13	2.36	0.41
1:A:949:ILE:CD1	1:A:996:PHE:CE2	3.04	0.41
1:A:1011:THR:HG22	1:A:1012:TRP:CE2	2.56	0.41
1:A:1091:PRO:HG2	1:A:1162:TYR:CD1	2.55	0.41
1:A:1112:ARG:HH11	1:A:1112:ARG:HD2	1.75	0.41
2:B:66:TRP:HB2	2:B:348:ARG:HB2	2.02	0.41
2:B:165:GLN:HE21	2:B:165:GLN:CA	2.22	0.41
2:B:252:GLU:HA	2:B:461:SER:HB2	2.03	0.41
3:C:155:GLU:HB2	11:C:1851:HOH:O	2.20	0.41
1:A:363:ALA:O	1:A:366:GLN:HB2	2.21	0.40
1:A:426:ILE:N	1:A:426:ILE:CD1	2.83	0.40
1:A:1059:LEU:HD23	1:A:1059:LEU:O	2.21	0.40
3:C:87:GLN:O	3:C:91:MET:HG3	2.21	0.40
1:A:329:TYR:CE1	1:A:565:GLY:HA2	2.56	0.40
1:A:741:LYS:HB3	1:A:745:GLN:HB2	2.04	0.40
3:C:70:MET:O	3:C:71:LEU:HD23	2.21	0.40
1:A:390:ILE:HD12	1:A:390:ILE:HA	1.83	0.40
1:A:806:ILE:HD13	1:A:807:HIS:N	2.37	0.40
3:C:143:THR:HG22	3:C:183:ILE:HG12	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:54:THR:HG21	1:A:260:ARG:NH2	2.37	0.40
1:A:362:ASP:C	1:A:364:LEU:N	2.76	0.40
1:A:379:THR:HG21	1:A:414:GLU:CD	2.47	0.40
1:A:894:ALA:O	1:A:898:ARG:HG3	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:4064:HOH:O	11:A:4064:HOH:O[3_354]	1.00	1.20

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	1242/1246 (100%)	1174 (94%)	61 (5%)	7 (1%)	21	17
2	B	507/512 (99%)	495 (98%)	12 (2%)	0	100	100
3	C	213/225 (95%)	207 (97%)	6 (3%)	0	100	100
All	All	1962/1983 (99%)	1876 (96%)	79 (4%)	7 (0%)	30	27

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	422	SER
1	A	501	ALA
1	A	578	VAL
1	A	1166	GLU
1	A	195	SER
1	A	224	PRO
1	A	718	GLY

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	1039/1043 (100%)	995 (96%)	44 (4%)	26	25
2	B	435/438 (99%)	424 (98%)	11 (2%)	42	45
3	C	179/186 (96%)	170 (95%)	9 (5%)	22	20
All	All	1653/1667 (99%)	1589 (96%)	64 (4%)	28	28

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	PHE
1	A	37	GLN
1	A	44	ILE
1	A	61	ILE
1	A	139	ILE
1	A	169	ILE
1	A	190	PRO
1	A	287	ILE
1	A	366	GLN
1	A	383	MET
1	A	402	LEU
1	A	413	THR
1	A	416	GLN
1	A	476	LEU
1	A	562	ILE
1	A	578	VAL
1	A	600	ARG
1	A	601	PRO
1	A	646	ASN
1	A	659	PRO
1	A	668	ILE
1	A	673	GLU
1	A	677	MET
1	A	685	LYS
1	A	743	LEU
1	A	767	LEU

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Mol	Chain	Res	Type
1	A	804	PRO
1	A	806	ILE
1	A	808	PRO
1	A	831	LYS
1	A	864	LEU
1	A	926	LEU
1	A	944	MET
1	A	991	ASP
1	A	1006	ILE
1	A	1018	GLU
1	A	1032	LEU
1	A	1062	ARG
1	A	1074	ILE
1	A	1110	LEU
1	A	1129	ILE
1	A	1198	ILE
1	A	1230	ILE
1	A	1233	LEU
2	B	37	GLU
2	B	42	ASN
2	B	74	LEU
2	B	85	LEU
2	B	123	ILE
2	B	139	GLU
2	B	182	ARG
2	B	245	ILE
2	B	267	ILE
2	B	335	MET
2	B	407	LYS
3	C	46	LYS
3	C	50	LEU
3	C	59	ILE
3	C	83	ILE
3	C	97	SER
3	C	142	LEU
3	C	144	ILE
3	C	159	LEU
3	C	212	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	173	ASN
1	A	179	ASN
1	A	234	GLN
1	A	245	ASN
1	A	258	GLN
1	A	366	GLN
1	A	368	ASN
1	A	369	ASN
1	A	404	GLN
1	A	461	GLN
1	A	517	GLN
1	A	559	ASN
1	A	590	GLN
1	A	604	HIS
1	A	641	HIS
1	A	698	GLN
1	A	704	ASN
1	A	708	ASN
1	A	759	ASN
1	A	919	ASN
1	A	942	GLN
1	A	1000	GLN
1	A	1023	ASN
1	A	1076	GLN
1	A	1238	ASN
2	B	110	ASN
2	B	121	GLN
2	B	160	ASN
2	B	165	GLN
2	B	294	GLN
2	B	441	GLN
2	B	451	ASN
3	C	149	GLN
3	C	175	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	FME	C	1	3	8,9,10	1.16	1 (12%)	8,9,11	1.71	2 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	FME	C	1	3	-	5/7/9/11	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	1	FME	CB-CG	2.17	1.60	1.51

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	FME	CA-N-CN	3.59	128.34	122.82
3	C	1	FME	CB-CA-N	2.18	114.49	110.52

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	1	FME	N-CA-CB-CG
3	C	1	FME	O1-CN-N-CA
3	C	1	FME	C-CA-CB-CG
3	C	1	FME	CB-CA-N-CN
3	C	1	FME	CB-CG-SD-CE

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1	FME	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 1 is monoatomic - leaving 11 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
4	MD1	A	2800	5	47,51,51	2.79	6 (12%)	56,78,78	1.42	7 (12%)
9	HEM	C	807	3	50,50,50	1.92	16 (32%)	67,82,82	0.97	5 (7%)
4	MD1	A	1800	5	47,51,51	2.74	9 (19%)	56,78,78	1.45	8 (14%)
6	SF4	B	1802	2	0,12,12	-	-	-		
6	SF4	A	1801	1	0,12,12	-	-	-		
10	PCI	C	1808	-	12,12,12	9.44	11 (91%)	18,18,18	1.47	2 (11%)
9	HEM	C	806	3	50,50,50	1.71	10 (20%)	67,82,82	0.92	2 (2%)
6	SF4	B	1804	2	0,12,12	-	-	-		
8	F3S	B	1803	2	0,9,9	-	-	-		
7	AGA	A	1309	-	24,24,29	0.95	1 (4%)	27,29,35	1.66	2 (7%)
8	F3S	B	1805	2	0,9,9	-	-	-		

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
4	MD1	A	2800	5	-	1/22/59/59	0/5/5/5
9	HEM	C	807	3	-	6/14/54/54	-
4	MD1	A	1800	5	-	7/22/59/59	0/5/5/5
6	SF4	B	1802	2	-	-	0/6/5/5
6	SF4	A	1801	1	-	-	0/6/5/5
10	PCI	C	1808	-	-	-	0/1/1/1
6	SF4	B	1804	2	-	-	0/6/5/5
8	F3S	B	1803	2	-	-	1/3/3/3
7	AGA	A	1309	-	-	3/26/26/34	-
9	HEM	C	806	3	-	4/14/54/54	-
8	F3S	B	1805	2	-	-	1/3/3/3

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1800	MD1	C7-N8	16.01	1.48	1.28
4	A	2800	MD1	C7-N8	15.76	1.48	1.28
10	C	1808	PCI	C6-CL5	-14.30	1.42	1.72
10	C	1808	PCI	C4-CL3	-13.78	1.43	1.72
10	C	1808	PCI	C2-CL1	-13.58	1.44	1.72
10	C	1808	PCI	C3-CL2	-13.56	1.44	1.72
10	C	1808	PCI	C5-CL4	-13.30	1.44	1.72
4	A	2800	MD1	PA-O3B	-6.70	1.52	1.59
10	C	1808	PCI	C1-C6	5.49	1.48	1.39
10	C	1808	PCI	C4-C3	5.11	1.51	1.39
10	C	1808	PCI	C5-C4	4.90	1.50	1.39
9	C	807	HEM	CAB-C3B	4.70	1.59	1.47
9	C	807	HEM	FE-NC	4.55	2.10	1.95
10	C	1808	PCI	C3-C2	4.44	1.49	1.39
4	A	1800	MD1	C16-C20	4.14	1.50	1.39
10	C	1808	PCI	C6-C5	3.86	1.48	1.39
9	C	806	HEM	CAC-C3C	3.86	1.57	1.47
9	C	806	HEM	CMC-C2C	3.80	1.58	1.50
9	C	807	HEM	CAC-C3C	3.79	1.57	1.47
9	C	806	HEM	CMB-C2B	3.77	1.58	1.50
9	C	807	HEM	CMC-C2C	3.69	1.58	1.50
10	C	1808	PCI	C1-C2	3.45	1.45	1.39
9	C	806	HEM	CAB-C3B	3.34	1.56	1.47
4	A	1800	MD1	C15-N17	3.27	1.45	1.38
7	A	1309	AGA	C8-C7	3.22	1.60	1.50
9	C	806	HEM	FE-NC	3.14	2.05	1.95
4	A	1800	MD1	C12-C13	2.93	1.43	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1800	MD1	C4-N3	2.91	1.40	1.34
9	C	806	HEM	C4D-ND	-2.90	1.35	1.40
9	C	807	HEM	CMB-C2B	2.89	1.56	1.50
9	C	806	HEM	CMA-C3A	2.83	1.56	1.50
9	C	806	HEM	CMD-C2D	2.76	1.56	1.50
9	C	807	HEM	CMA-C3A	2.73	1.56	1.50
9	C	807	HEM	CAD-C3D	2.72	1.58	1.51
9	C	807	HEM	CBD-CGD	2.71	1.56	1.50
4	A	2800	MD1	C4-N3	2.64	1.40	1.34
9	C	806	HEM	CAD-C3D	2.58	1.58	1.51
9	C	807	HEM	CMD-C2D	2.53	1.56	1.50
4	A	2800	MD1	C2-N3	2.47	1.39	1.33
4	A	1800	MD1	C6-N1	2.45	1.43	1.38
9	C	807	HEM	FE-NB	2.40	2.02	1.94
9	C	807	HEM	CBD-CAD	2.35	1.60	1.51
9	C	806	HEM	CBA-CGA	2.31	1.55	1.50
4	A	2800	MD1	C16-C20	2.23	1.45	1.39
4	A	1800	MD1	C17-N17	2.22	1.43	1.37
9	C	807	HEM	C4A-C3A	2.18	1.48	1.43
9	C	807	HEM	O1D-CGD	2.14	1.29	1.22
9	C	807	HEM	C1D-C2D	2.10	1.48	1.44
9	C	807	HEM	CBA-CAA	2.07	1.59	1.51
9	C	807	HEM	FE-ND	2.04	2.01	1.94
4	A	2800	MD1	C15-N17	2.02	1.42	1.38
4	A	1800	MD1	PB-O3B	2.02	1.61	1.59
4	A	1800	MD1	PB-O2B	-2.02	1.43	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1800	MD1	C17-N18-C20	5.96	122.45	114.20
4	A	2800	MD1	C17-N18-C20	5.85	122.30	114.20
7	A	1309	AGA	C9-C8-C7	5.50	133.86	113.69
7	A	1309	AGA	C14-C13-C12	4.75	131.09	113.69
10	C	1808	PCI	C6-C1-C2	4.74	122.86	117.78
4	A	2800	MD1	C2-N3-C4	3.01	117.48	112.30
4	A	1800	MD1	O14-C15-C16	-2.97	120.11	127.26
9	C	807	HEM	CAD-C3D-C4D	-2.71	119.98	124.70
4	A	1800	MD1	O3A-C10-C11	-2.62	100.58	107.96
4	A	2800	MD1	O1B-PB-O2B	2.58	124.44	112.44
4	A	1800	MD1	N17-C17-N18	-2.54	118.67	123.32
9	C	806	HEM	CMA-C3A-C2A	2.54	131.01	125.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1800	MD1	O3B-PA-O2A	-2.35	103.62	110.70
4	A	2800	MD1	N16-C17-N17	2.34	121.71	116.76
9	C	807	HEM	O1A-CGA-CBA	-2.28	115.86	123.09
10	C	1808	PCI	C1-C2-C3	-2.28	119.24	121.16
9	C	807	HEM	CMA-C3A-C2A	2.27	130.44	125.62
4	A	2800	MD1	N1-C2-N3	-2.27	119.17	123.32
4	A	1800	MD1	C2-N3-C4	2.22	116.13	112.30
4	A	2800	MD1	N17-C17-N18	-2.22	119.25	123.32
9	C	806	HEM	O1D-CGD-CBD	-2.22	116.06	123.09
9	C	807	HEM	O1D-CGD-CBD	-2.18	116.18	123.09
9	C	807	HEM	CAD-C3D-C2D	2.14	131.88	127.87
4	A	1800	MD1	C15-C16-N15	2.12	122.04	116.27
4	A	2800	MD1	C1'-N9-C8	2.06	132.58	126.73
4	A	1800	MD1	N16-C17-N17	2.05	121.08	116.76

There are no chirality outliers.

All (21) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1800	MD1	C5'-O5'-PA-O3B
4	A	1800	MD1	C5'-O5'-PA-O2A
4	A	1800	MD1	O4'-C4'-C5'-O5'
4	A	1800	MD1	C3'-C4'-C5'-O5'
7	A	1309	AGA	C8-C7-O7-C6
7	A	1309	AGA	O8-C7-O7-C6
7	A	1309	AGA	C11-C10-C9-C8
9	C	807	HEM	C2C-C3C-CAC-CBC
4	A	1800	MD1	PA-O3B-PB-O2B
4	A	1800	MD1	C5'-O5'-PA-O1A
9	C	807	HEM	C4C-C3C-CAC-CBC
9	C	806	HEM	CAD-CBD-CGD-O1D
9	C	806	HEM	CAD-CBD-CGD-O2D
9	C	806	HEM	CAA-CBA-CGA-O2A
9	C	807	HEM	CAA-CBA-CGA-O2A
9	C	807	HEM	CAD-CBD-CGD-O2D
4	A	2800	MD1	PA-O3B-PB-O2B
9	C	807	HEM	CAA-CBA-CGA-O1A
9	C	807	HEM	CAD-CBD-CGD-O1D
9	C	806	HEM	CAA-CBA-CGA-O1A
4	A	1800	MD1	PA-O3B-PB-O1B

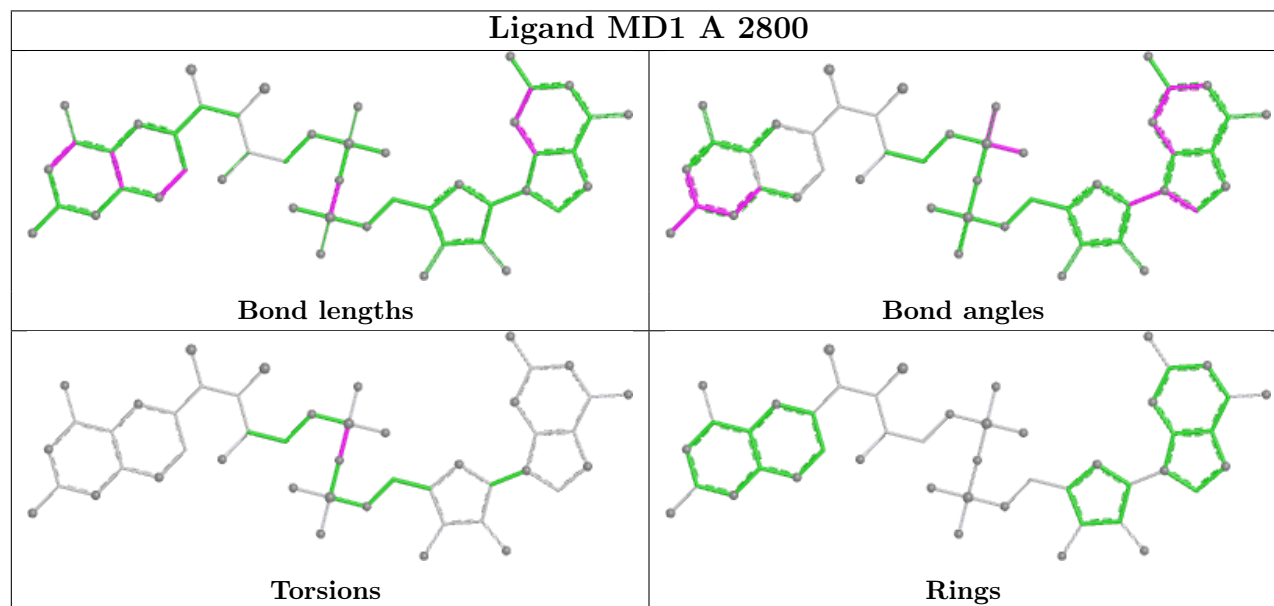
All (2) ring outliers are listed below:

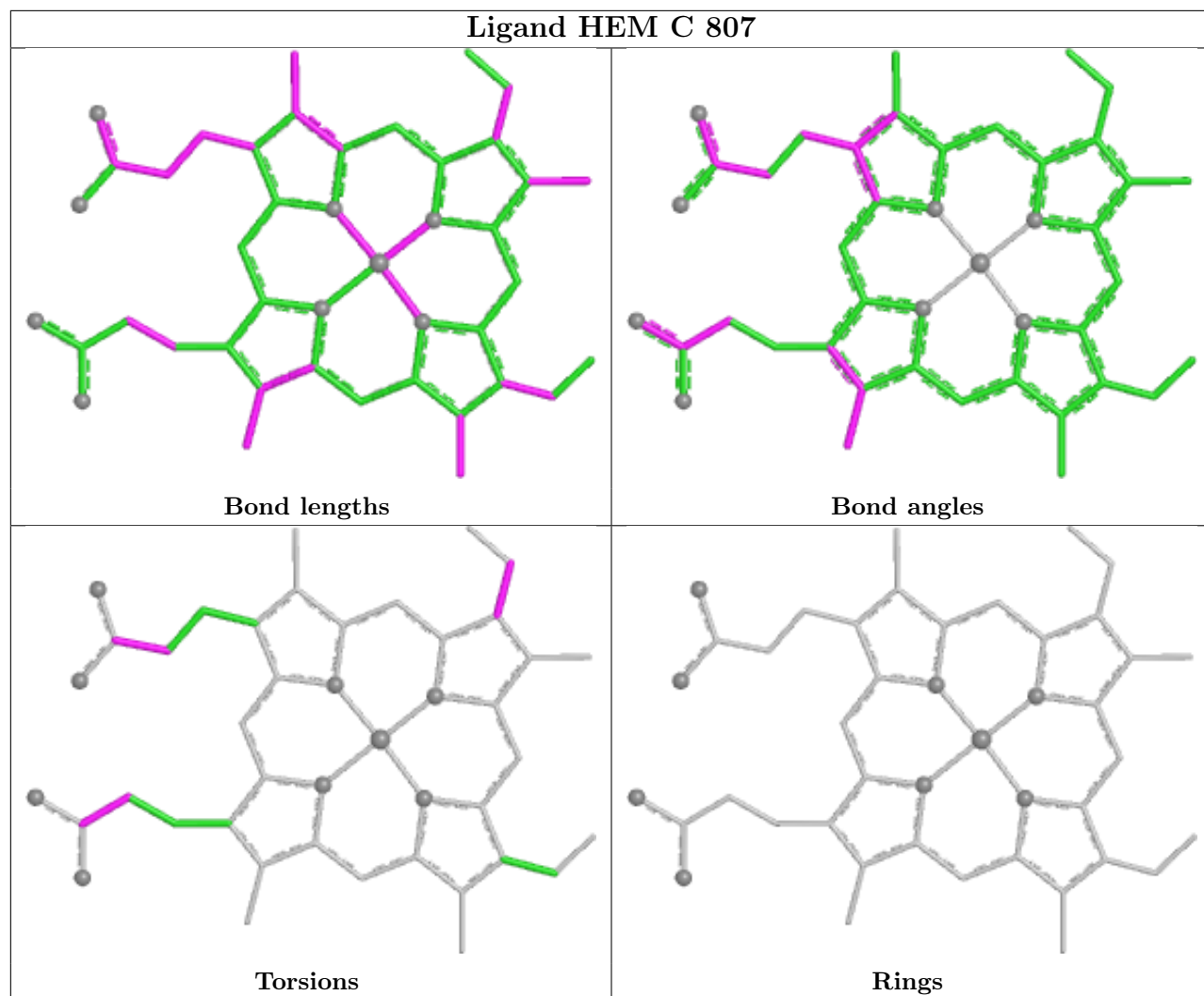
Mol	Chain	Res	Type	Atoms
8	B	1805	F3S	FE1-FE3-S1-S3
8	B	1803	F3S	FE1-FE3-S1-S3

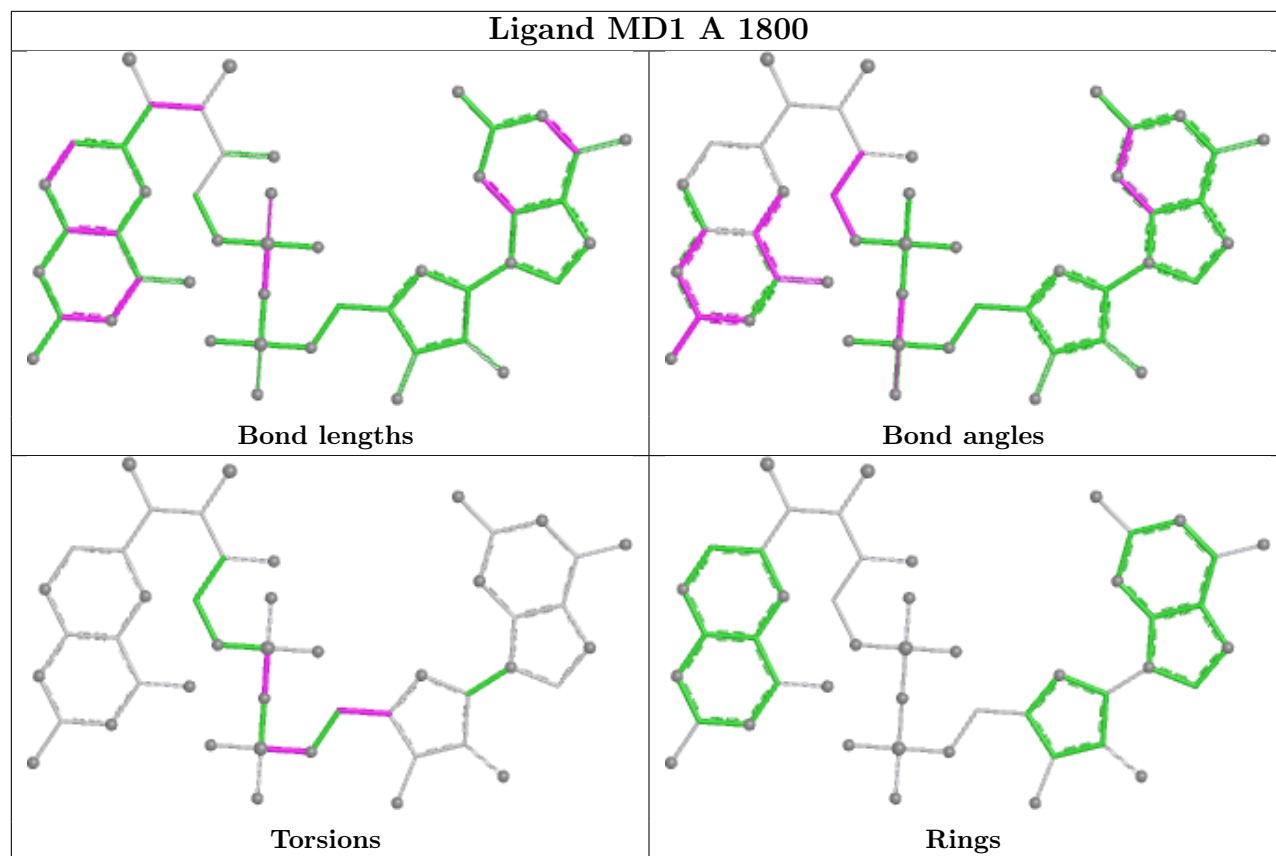
5 monomers are involved in 12 short contacts:

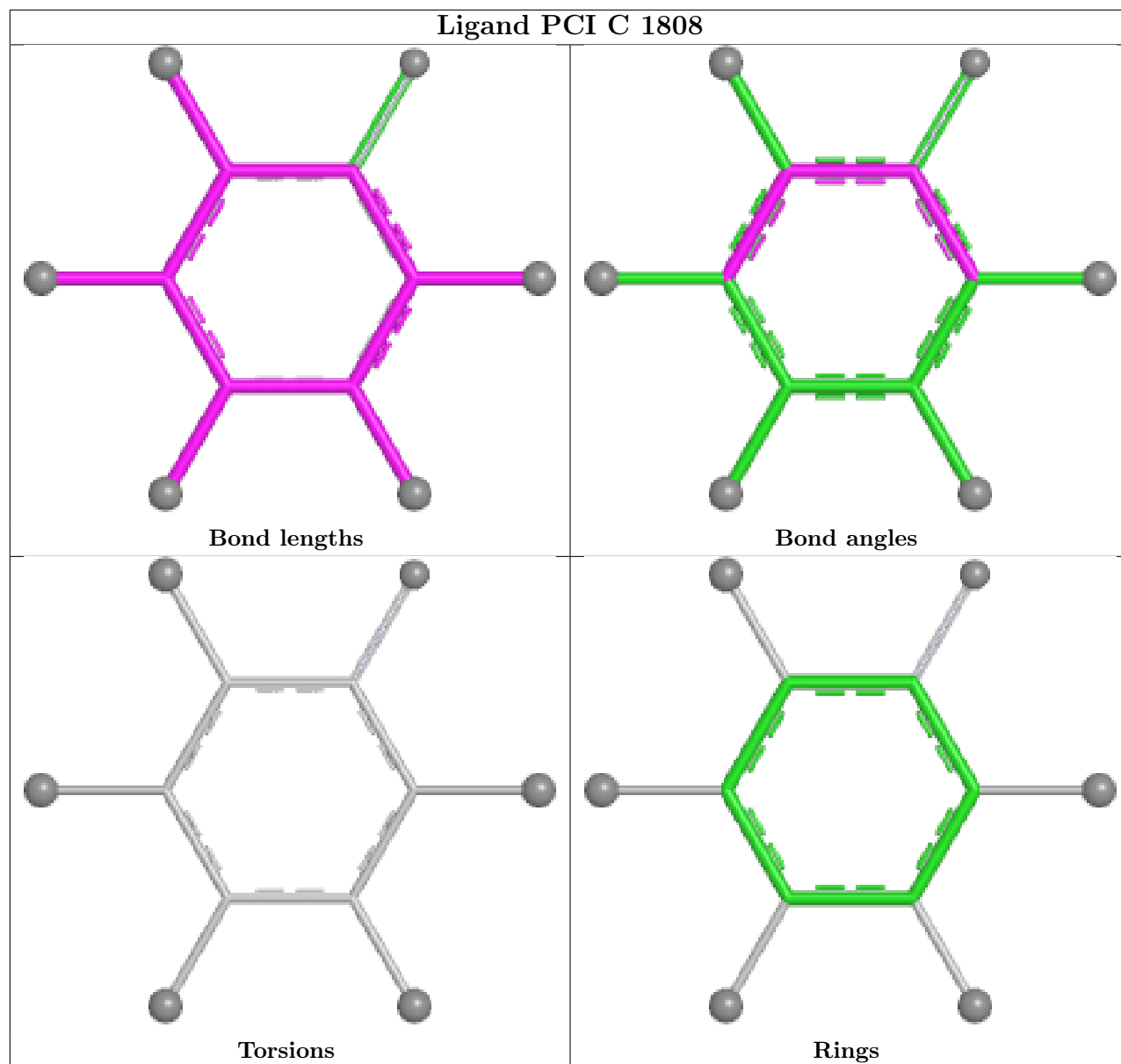
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2800	MD1	3	0
9	C	807	HEM	1	0
4	A	1800	MD1	4	0
10	C	1808	PCI	1	0
8	B	1803	F3S	3	0

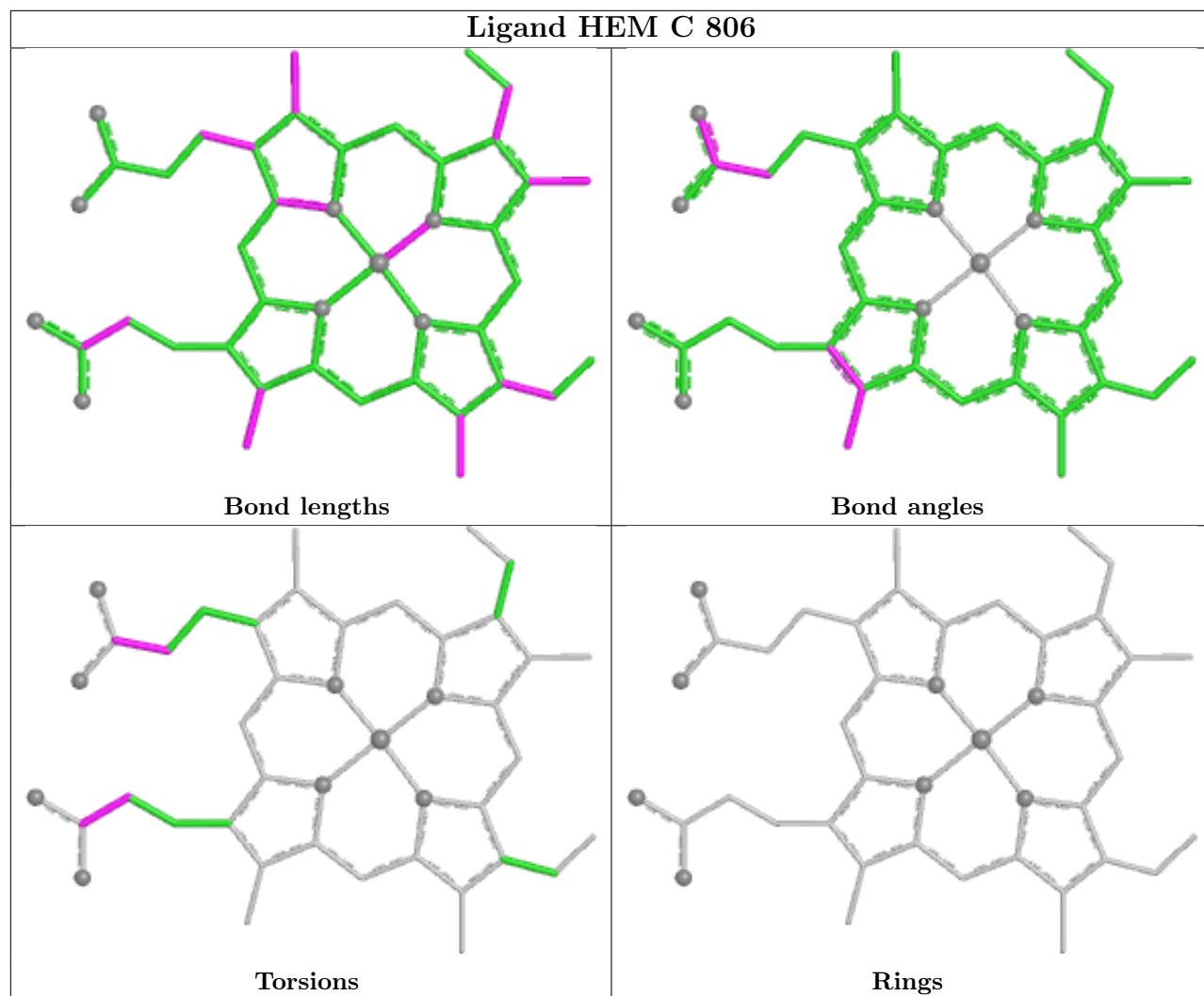
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

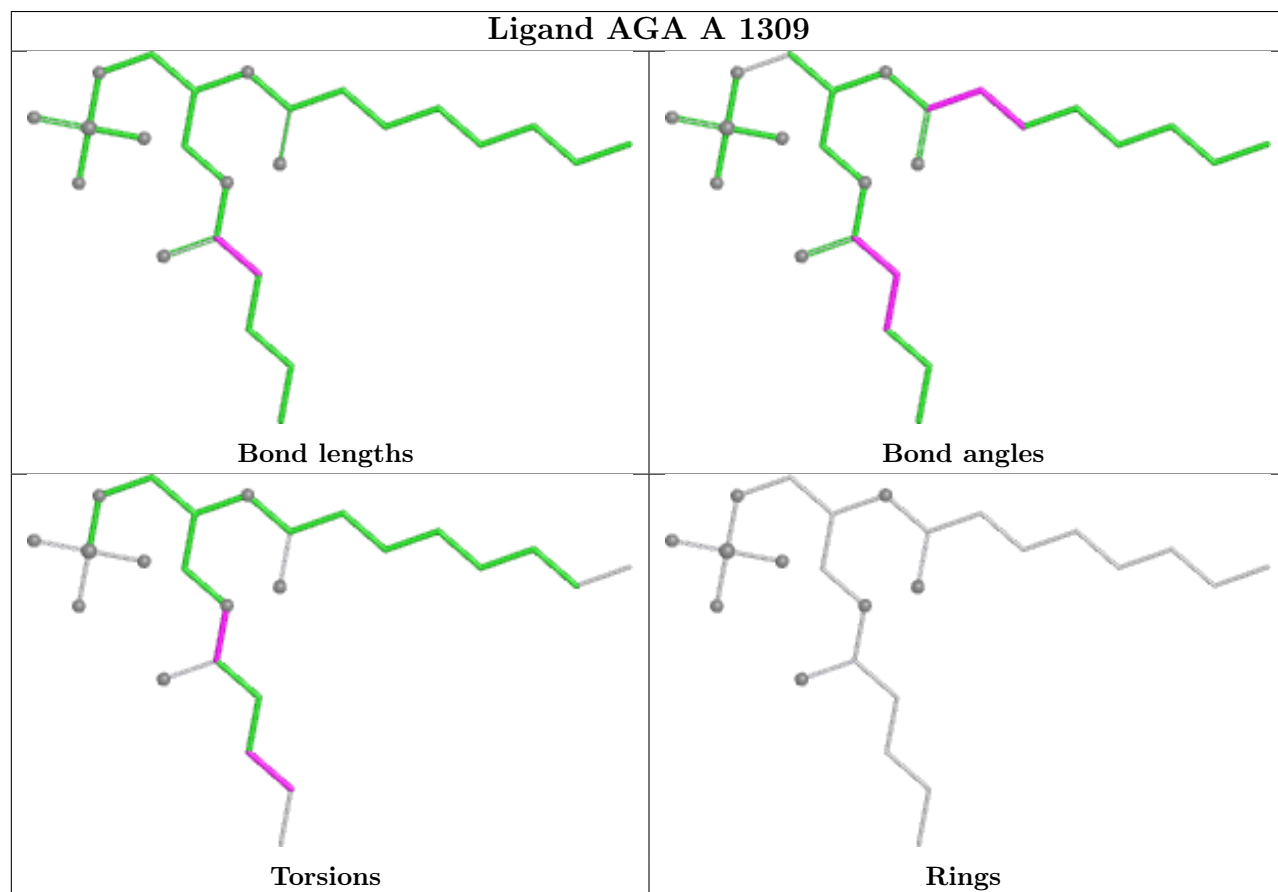
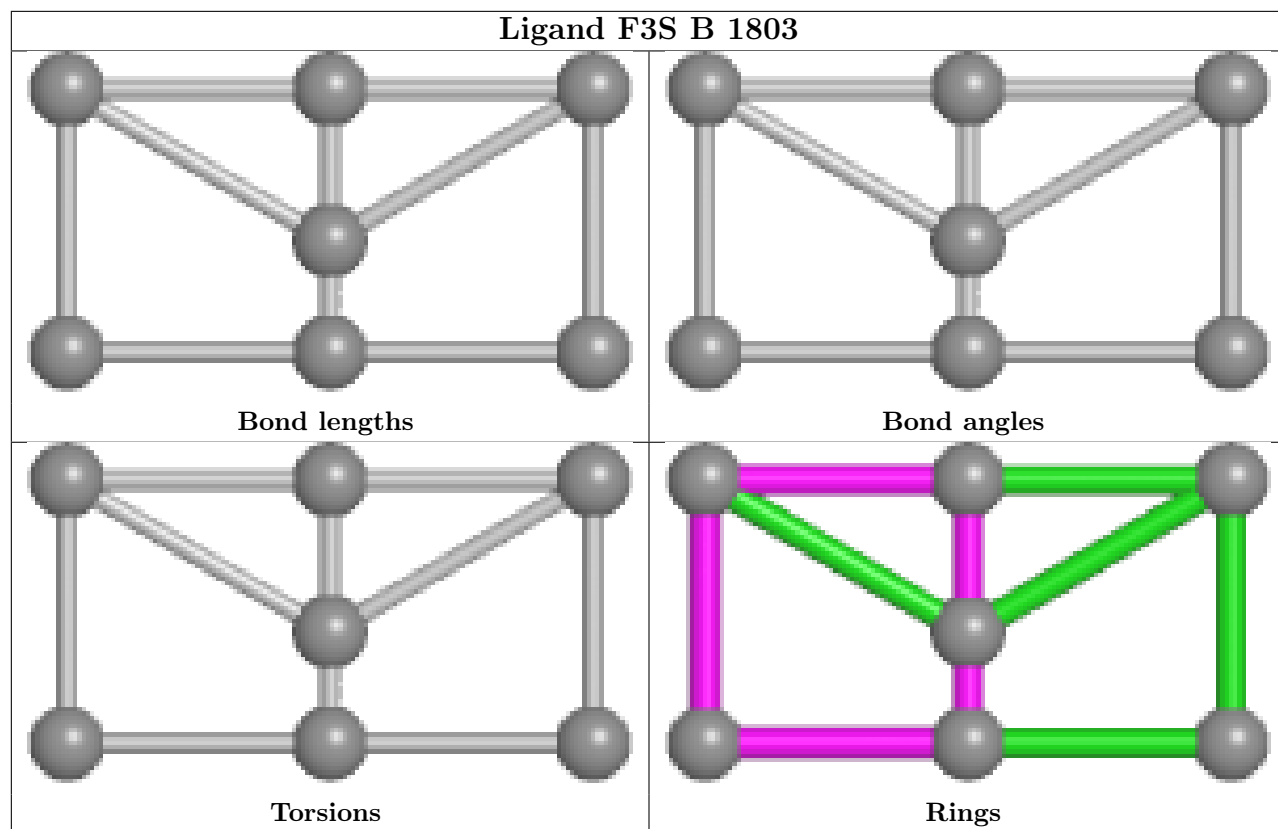


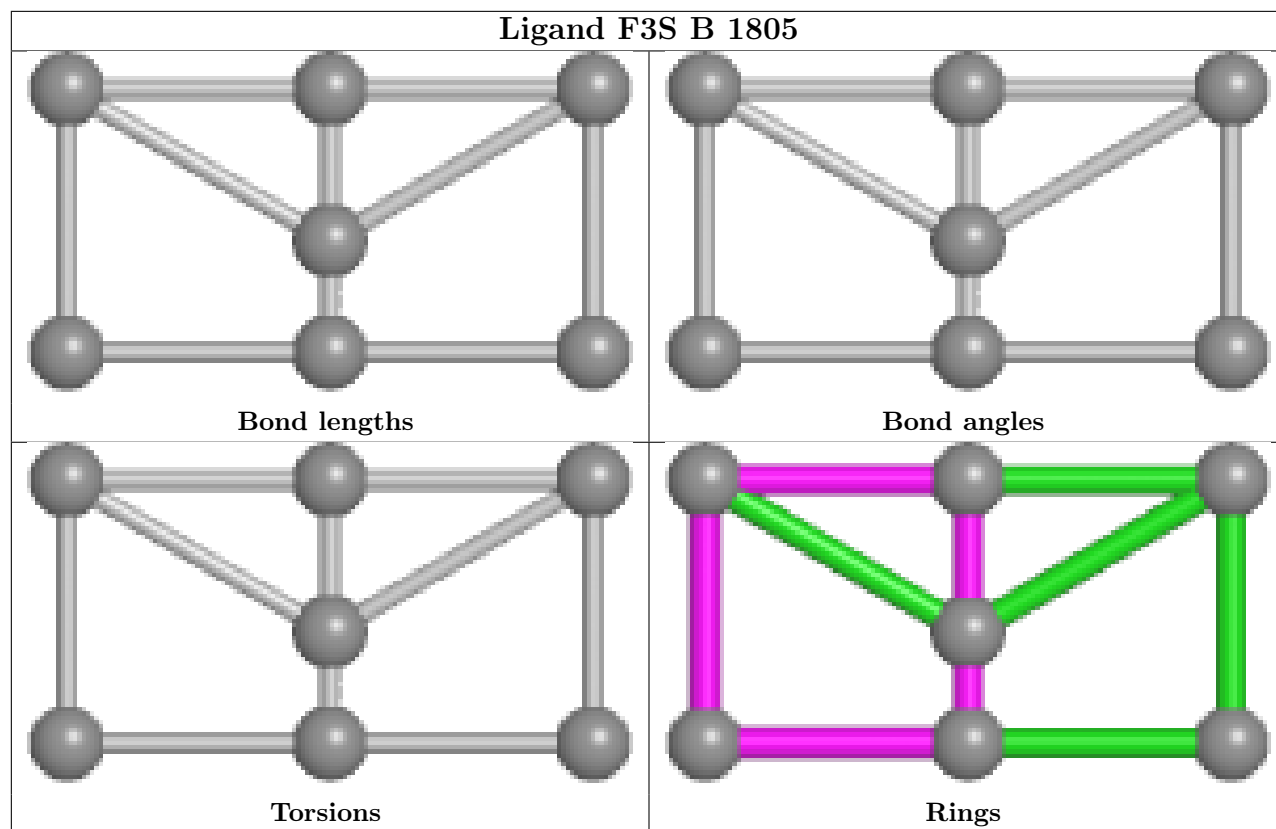












5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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	1244/1246 (99%)	-0.11	21 (1%) 69 68	14, 26, 47, 69	0
2	B	509/512 (99%)	-0.54	2 (0%) 88 88	14, 21, 33, 61	0
3	C	216/225 (96%)	0.32	6 (2%) 55 54	15, 31, 51, 57	0
All	All	1969/1983 (99%)	-0.17	29 (1%) 72 71	14, 25, 46, 69	0

All (29) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	TYR	4.8
1	A	10	PHE	4.2
1	A	501	ALA	3.4
1	A	7	PHE	3.0
1	A	362	ASP	2.8
1	A	749	VAL	2.8
1	A	422	SER	2.7
3	C	71	LEU	2.7
3	C	83	ILE	2.6
1	A	1244	SER	2.6
1	A	633	ALA	2.5
3	C	81	LEU	2.5
3	C	148	ALA	2.4
1	A	490	VAL	2.4
2	B	371	LEU	2.4
1	A	381	GLY	2.3
3	C	153	GLY	2.3
1	A	467	THR	2.3
1	A	463	ALA	2.3
1	A	413	THR	2.2
1	A	449	ASN	2.2
1	A	319	LEU	2.2
1	A	719	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	991	ASP	2.1
3	C	179	GLY	2.1
1	A	367	GLU	2.1
1	A	410	GLY	2.1
2	B	370	GLU	2.0
1	A	363	ALA	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	FME	C	1	10/11	0.85	0.13	49,56,65,65	0

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
10	PCI	C	1808	12/12	0.84	0.16	33,38,40,40	0
9	HEM	C	807	43/43	0.94	0.12	35,39,45,50	0
7	AGA	A	1309	25/30	0.94	0.10	22,27,42,44	0
5	6MO	A	3800	1/1	0.95	0.19	52,52,52,52	0
4	MD1	A	2800	47/47	0.95	0.07	19,24,33,39	0
4	MD1	A	1800	47/47	0.96	0.07	14,23,36,40	0
6	SF4	B	1804	8/8	0.97	0.05	25,29,31,33	0
6	SF4	A	1801	8/8	0.98	0.05	21,22,28,29	0
9	HEM	C	806	43/43	0.98	0.06	16,22,25,32	0
6	SF4	B	1802	8/8	0.99	0.03	21,23,24,25	0
8	F3S	B	1803	7/7	0.99	0.03	19,21,22,23	0

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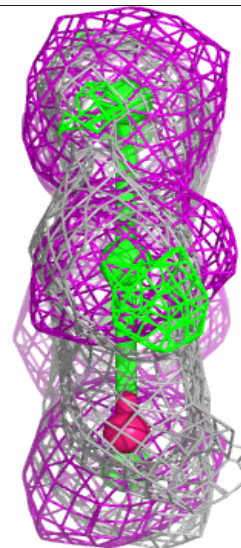
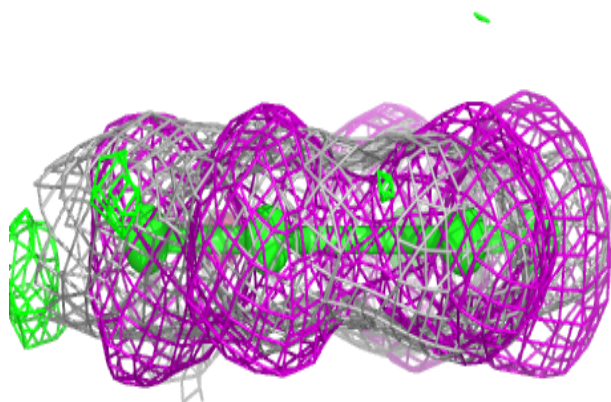
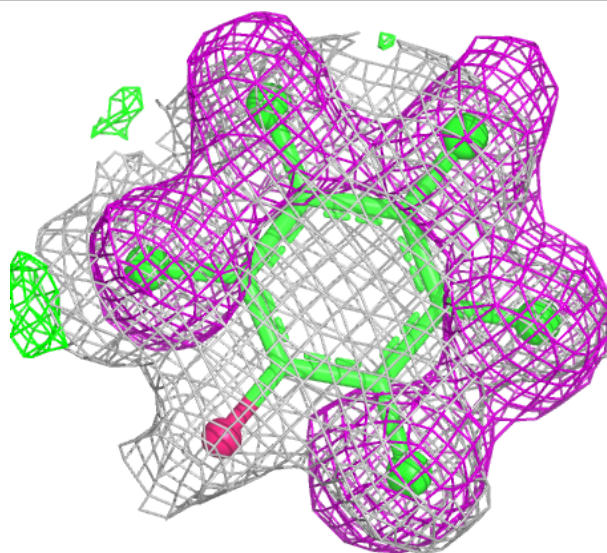
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	F3S	B	1805	7/7	0.99	0.02	18,19,20,21	0

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.

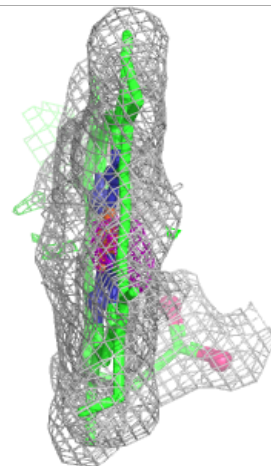
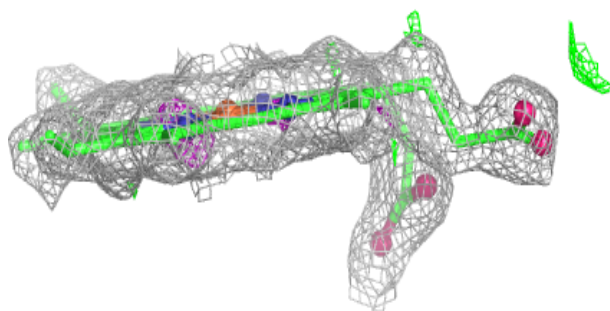
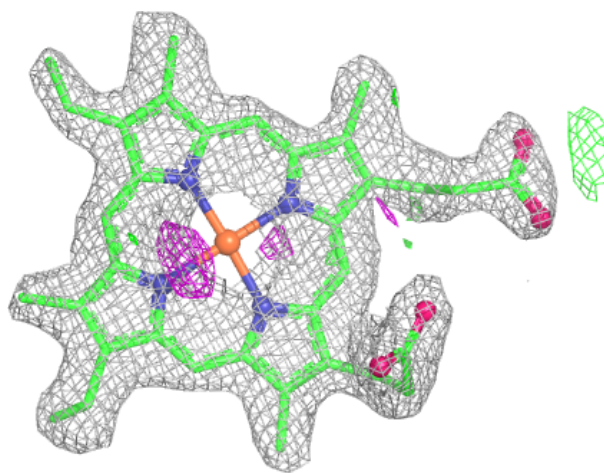
Electron density around PCI C 1808:

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



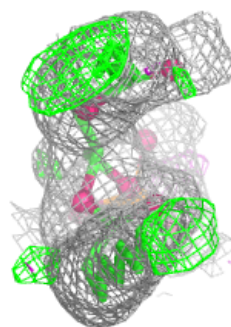
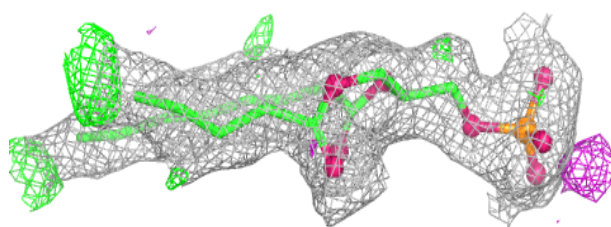
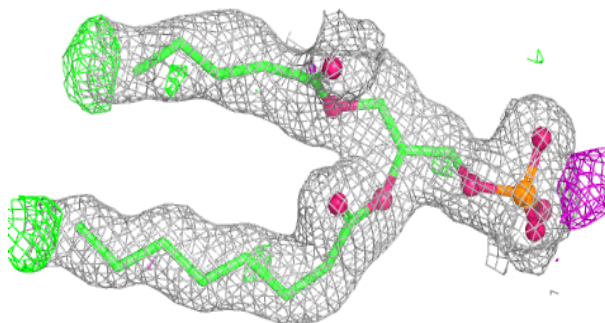
Electron density around HEM C 807:

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

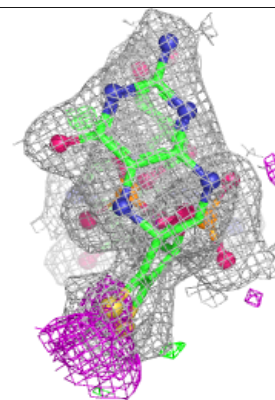
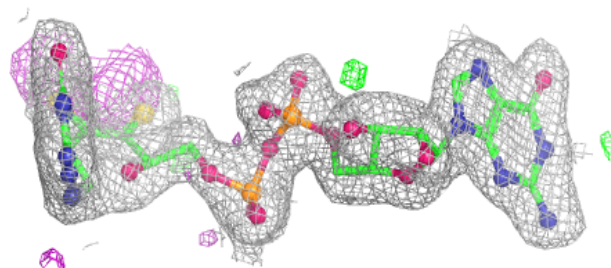
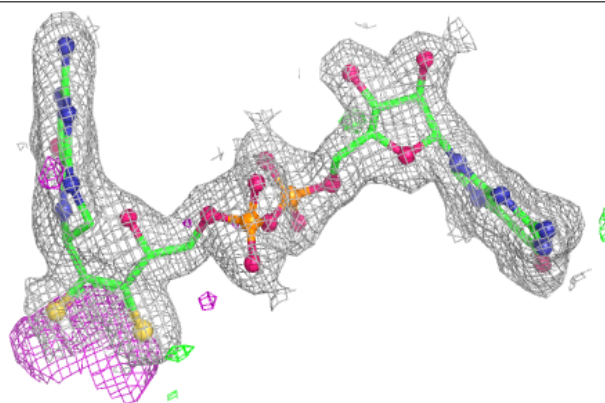


Electron density around AGA A 1309:

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

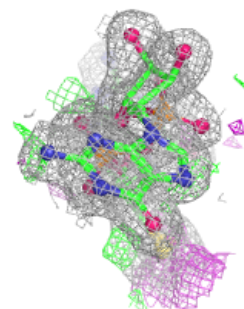
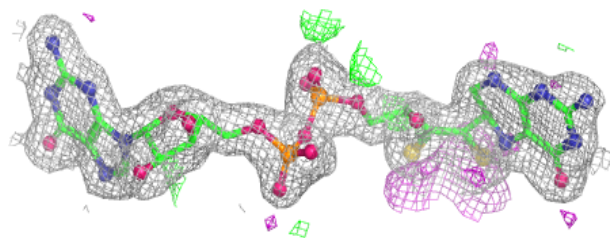
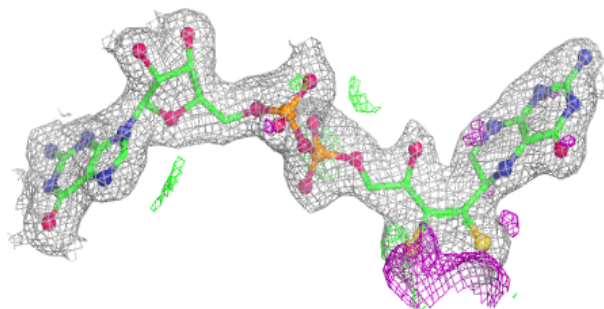
**Electron density around MD1 A 2800:**

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



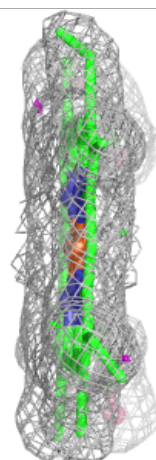
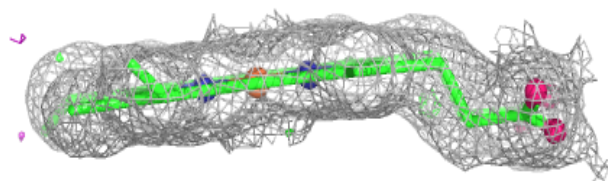
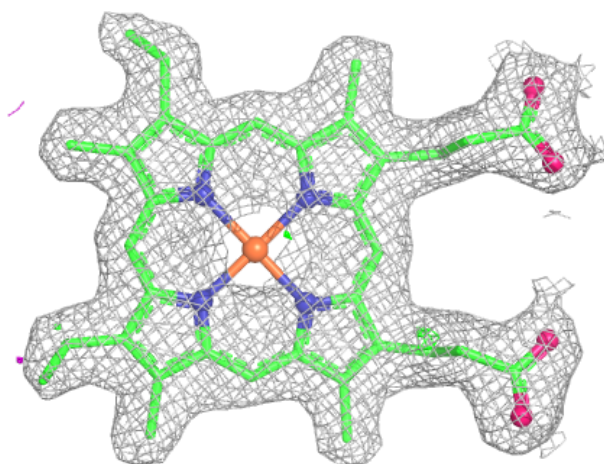
Electron density around MD1 A 1800:

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



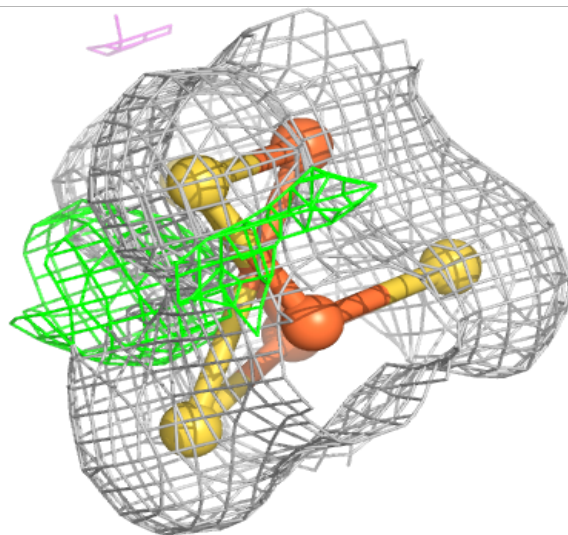
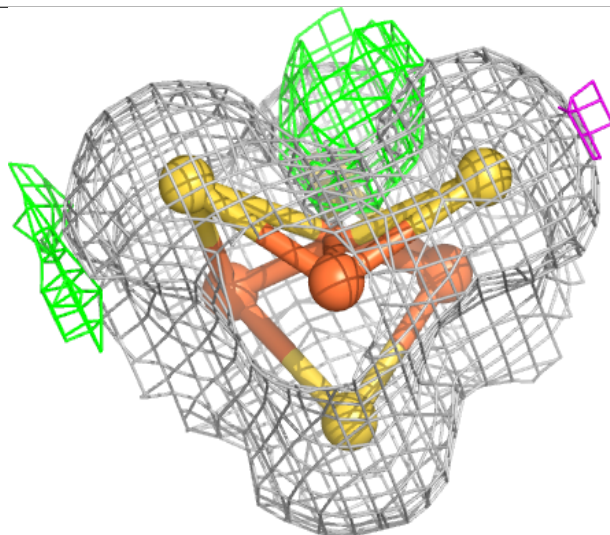
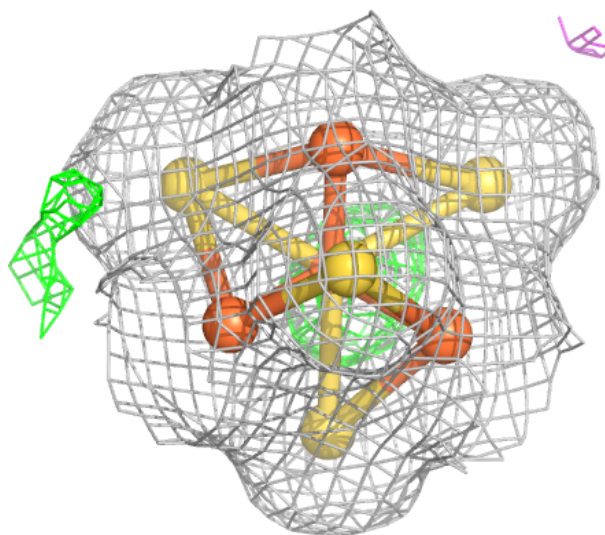
Electron density around HEM C 806:

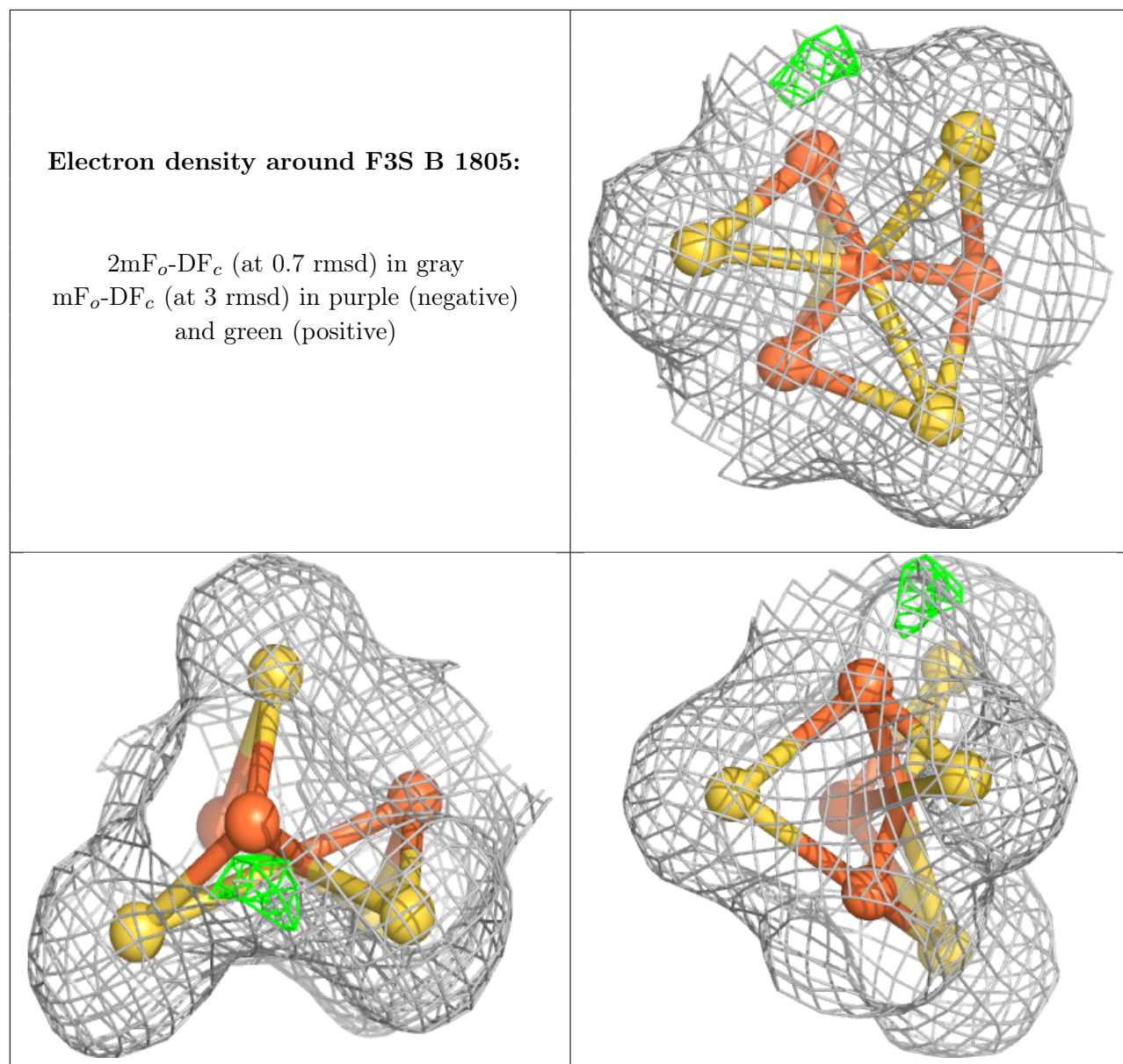
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around F3S B 1803:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.