Full wwPDB X-ray Structure Validation Report ⓘ

Sep 4, 2023 – 08:10 PM EDT

PDB ID	:	3TTX
Title	:	Structure of the F413K variant of E. coli KatE
Authors	:	Loewen, P.C.; Jha, V.
Deposited on	:	2011-09-15
Resolution	:	1.74 Å(reported)

The following versions of software and data (see references ⓘ) were used in the production of this report:

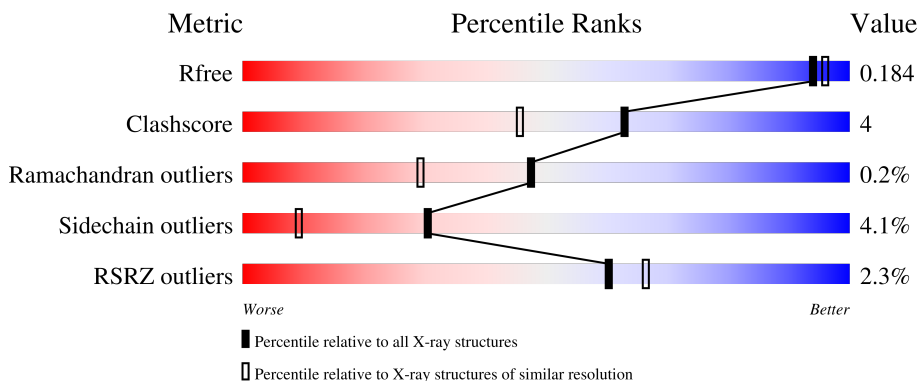|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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.

| | 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))
R_{free}	130704	3764 (1.76-1.72)
Clashscore	141614	3923 (1.76-1.72)
Ramachandran outliers	138981	3878 (1.76-1.72)
Sidechain outliers	138945	3878 (1.76-1.72)
RSRZ outliers	127900	3705 (1.76-1.72)

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	753	% 86% 9% · ·
1	B	753	3% 85% 9% · ·
1	C	753	3% 82% 11% · ·
1	D	753	.% 85% 10% · ·

2 Entity composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 26010 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Catalase HPII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	726	Total	C	N	O	S	0	1	0
			5745	3644	1007	1082	12			
1	B	726	Total	C	N	O	S	0	1	0
			5746	3645	1007	1082	12			
1	C	726	Total	C	N	O	S	0	1	0
			5745	3644	1007	1082	12			
1	D	726	Total	C	N	O	S	0	1	0
			5746	3645	1007	1082	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	413	LYS	PHE	engineered mutation	UNP P21179
B	413	LYS	PHE	engineered mutation	UNP P21179
C	413	LYS	PHE	engineered mutation	UNP P21179
D	413	LYS	PHE	engineered mutation	UNP P21179

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

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

- Molecule 3 is water.

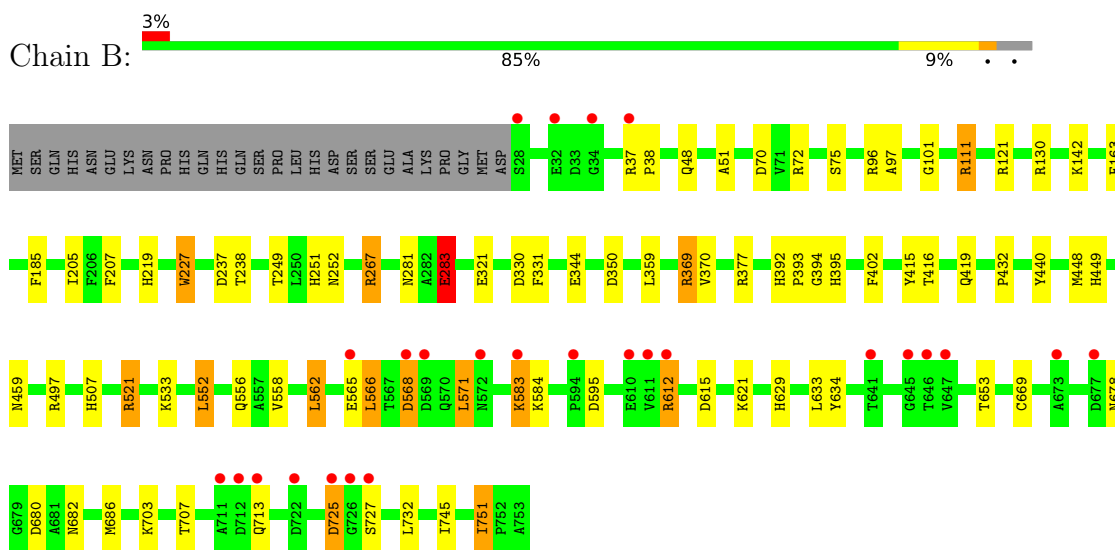| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	771	Total	O	0	0
			771	771		
3	B	650	Total	O	0	0
			650	650		
3	C	690	Total	O	0	0
			690	690		
3	D	745	Total	O	0	0
			745	745		

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.
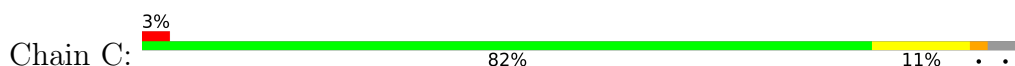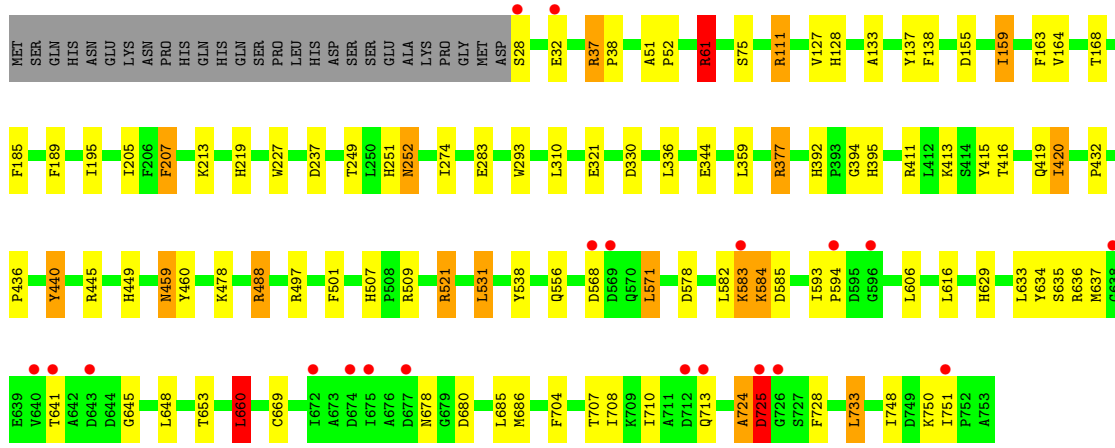
- Molecule 1: Catalase HPII
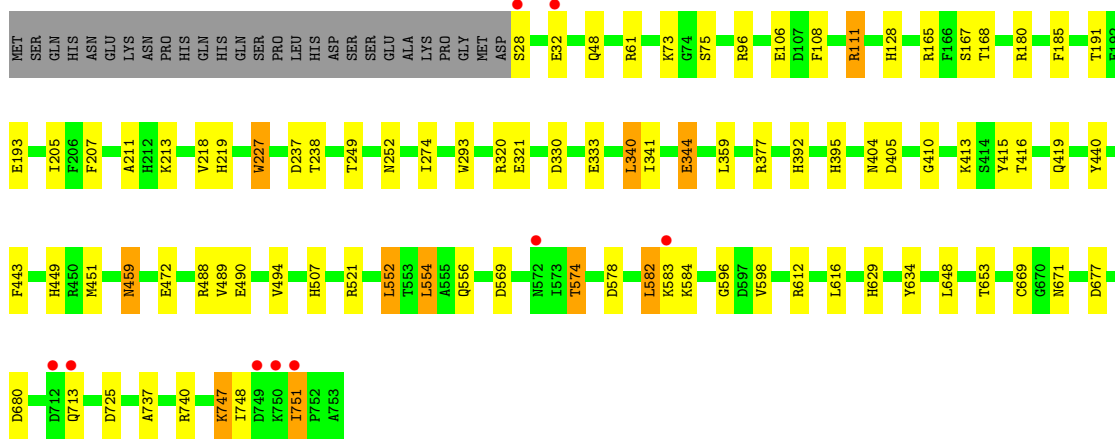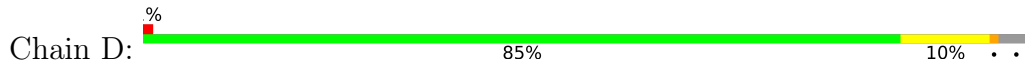
Chain A:

- Molecule 1: Catalase HPII

Chain B:

- Molecule 1: Catalase HPII

Chain C:

MET SER GLN HIS ASN GLU LYS ASN PRO HIS GLN HIS GLN SER PRO LEU HIS ASP SER SER GLU ALA LYS PRO GLY MET ASP S28 E32 R37 P38 A51 P52 R61 S75 R111 V127 H128 A133 Y137 F138 D155 I159 F163 V164 T168

F185 F189 I195 I205 F206 F207 K213 H219 W227 D237 T249 L250 H251 N252 I274 E283 W293 L310 E321 D330 L336 E344 L359 R377 H392 P393 G394 H395 R411 L412 K413 S414 Y415 T416 Q419 I420 P432

P436 Y440 R445 H449 N459 Y460 K478 R488 R497 F501 H507 P508 R509 R521 L531 Y538 Q556 D568 D569 Q570 L571 D578 L582 K583 K584 D585 I593 P594 D595 G596 L606 L616 H629 L633 Y634 S635 R636 M637 G638

E639 V640 T641 A642 D643 D644 G645 L648 T653 L660 C669 I672 A673 D674 I675 A676 D677 N678 G679 D680 L685 M686 F704 T707 I708 K709 I710 A711 D712 Q713 A724 D725 G726 S727 F728 L733 I748 D749 K750 I751 P752 A753

• Molecule 1: Catalase HPII

Chain D:

%

85% 10%

MET SER GLN HIS ASN GLU LYS ASN PRO HIS GLN HIS GLN SER PRO LEU HIS ASP SER SER GLU ALA LYS PRO GLY MET ASP S28 E32 Q48 R61 K73 G74 S75 R96 E106 D107 F108 R111 H128 R165 F166 S167 T168 R180 F185 T191 E192

E193 I205 F206 F207 A211 H212 K213 V218 H219 W227 D237 T238 T249 N252 I274 W293 R320 E321 D330 E333 L340 I341 E344 L359 R377 H392 H395 N404 D405 G410 K413 S414 Y415 T416 Q419 Y440

F443 H449 R450 M451 N459 E472 R488 V489 E490 V494 H507 R521 L552 T553 L554 A555 Q556 D569 N572 I573 T574 D578 L582 K583 K584 G596 D597 V598 R612 L616 H629 Y634 L648 T653 C669 G670 N671 D677

D680 D712 Q713 D725 A737 R740 K747 I748 D749 K750 I751 P752 A753

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	93.50Å 132.96Å 122.03Å 90.00° 109.69° 90.00°	Depositor
Resolution (Å)	35.18 – 1.74 35.18 – 1.74	Depositor EDS
% Data completeness (in resolution range)	97.0 (35.18-1.74) 97.1 (35.18-1.74)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$< I/\sigma(I) >$ [1]	2.54 (at 1.74Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.146 , 0.185 0.146 , 0.184	Depositor DCC
R_{free} test set	14075 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	12.3	Xtriage
Anisotropy	0.022	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 44.6	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	26010	wwPDB-VP
Average B, all atoms (Å^2)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.52% 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 (i)

5.1   Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: OCS, HEM

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	1.27	19/5895 (0.3%)	1.03	15/8012 (0.2%)
1	B	1.22	9/5895 (0.2%)	1.04	16/8012 (0.2%)
1	C	1.23	13/5895 (0.2%)	1.03	17/8012 (0.2%)
1	D	1.25	12/5895 (0.2%)	1.04	19/8012 (0.2%)
All	All	1.24	53/23580 (0.2%)	1.04	67/32048 (0.2%)

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	C	0	2

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	189	PHE	CE2-CZ	7.83	1.52	1.37
1	B	321	GLU	CB-CG	7.71	1.66	1.52
1	D	333	GLU	CD-OE2	-7.57	1.17	1.25
1	A	321	GLU	CD-OE1	7.52	1.33	1.25
1	C	321	GLU	CD-OE1	7.48	1.33	1.25
1	A	383	PHE	CE1-CZ	7.40	1.51	1.37
1	A	440	TYR	CE1-CZ	7.35	1.48	1.38
1	A	684	TYR	CD2-CE2	6.93	1.49	1.39
1	B	283	GLU	CG-CD	6.89	1.62	1.51
1	B	568	ASP	CB-CG	6.85	1.66	1.51
1	A	41	GLU	CG-CD	6.71	1.62	1.51
1	B	497	ARG	CZ-NH2	6.51	1.41	1.33
1	D	320	ARG	CZ-NH1	6.12	1.41	1.33
1	A	334	TYR	CD1-CE1	6.11	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	344	GLU	CD-OE1	6.10	1.32	1.25
1	C	419	GLN	CB-CG	6.01	1.68	1.52
1	C	207	PHE	CE1-CZ	6.00	1.48	1.37
1	A	489	VAL	CB-CG1	5.97	1.65	1.52
1	D	167	SER	CB-OG	5.87	1.49	1.42
1	A	440	TYR	CD1-CE1	5.77	1.48	1.39
1	D	494	VAL	CB-CG1	5.76	1.65	1.52
1	D	443	PHE	CG-CD2	5.72	1.47	1.38
1	A	411	ARG	CZ-NH1	5.71	1.40	1.33
1	C	497	ARG	CZ-NH2	5.70	1.40	1.33
1	B	163	PHE	CE1-CZ	5.68	1.48	1.37
1	C	127	VAL	CB-CG2	5.61	1.64	1.52
1	D	293	TRP	CE3-CZ3	5.57	1.48	1.38
1	C	501	PHE	CE1-CZ	5.55	1.48	1.37
1	B	331	PHE	CE2-CZ	5.55	1.47	1.37
1	D	489	VAL	CB-CG1	5.51	1.64	1.52
1	A	338	PHE	CE1-CZ	5.50	1.47	1.37
1	A	242	TYR	CD1-CE1	5.47	1.47	1.39
1	A	213	LYS	CD-CE	5.46	1.64	1.51
1	D	108	PHE	CE2-CZ	5.46	1.47	1.37
1	A	603	VAL	CB-CG1	-5.45	1.41	1.52
1	C	538	TYR	CD2-CE2	5.40	1.47	1.39
1	A	239	PHE	CE1-CZ	5.38	1.47	1.37
1	D	193	GLU	CG-CD	5.35	1.59	1.51
1	D	472	GLU	CD-OE2	5.32	1.31	1.25
1	A	190	TYR	CE1-CZ	5.32	1.45	1.38
1	B	521	ARG	CG-CD	5.31	1.65	1.51
1	A	289	VAL	CB-CG1	5.31	1.64	1.52
1	A	111	ARG	CG-CD	5.30	1.65	1.51
1	C	111	ARG	CG-CD	5.18	1.64	1.51
1	B	402	PHE	CD2-CE2	5.17	1.49	1.39
1	C	138	PHE	CE2-CZ	5.15	1.47	1.37
1	C	440	TYR	CE1-CZ	5.14	1.45	1.38
1	D	218	VAL	CB-CG2	5.09	1.63	1.52
1	C	163	PHE	CD1-CE1	5.08	1.49	1.39
1	A	303	VAL	CB-CG1	5.06	1.63	1.52
1	A	428	PHE	CE2-CZ	5.06	1.47	1.37
1	B	227	TRP	CZ3-CH2	5.05	1.48	1.40
1	D	106	GLU	CD-OE2	5.02	1.31	1.25

All (67) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	111	ARG	NE-CZ-NH2	-13.18	113.71	120.30
1	B	111	ARG	NE-CZ-NH1	-11.18	114.71	120.30
1	C	111	ARG	NE-CZ-NH1	-10.96	114.82	120.30
1	B	521	ARG	NE-CZ-NH2	10.90	125.75	120.30
1	D	320	ARG	NE-CZ-NH2	-8.93	115.84	120.30
1	D	61	ARG	NE-CZ-NH2	7.87	124.24	120.30
1	D	554	LEU	CB-CG-CD2	7.64	123.98	111.00
1	A	111	ARG	NE-CZ-NH1	7.41	124.00	120.30
1	C	37	ARG	NE-CZ-NH1	7.36	123.98	120.30
1	B	130	ARG	NE-CZ-NH2	-7.11	116.75	120.30
1	B	350	ASP	CB-CG-OD1	-7.09	111.92	118.30
1	B	96	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	D	111	ARG	NE-CZ-NH1	-7.07	116.77	120.30
1	B	70	ASP	CB-CG-OD1	7.03	124.63	118.30
1	B	111	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	A	377	ARG	NE-CZ-NH2	-6.81	116.90	120.30
1	D	340	LEU	CB-CG-CD1	6.71	122.40	111.00
1	D	165	ARG	NE-CZ-NH2	-6.66	116.97	120.30
1	C	420	ILE	CG1-CB-CG2	-6.46	97.18	111.40
1	B	377	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	C	660	LEU	CB-CG-CD1	6.43	121.93	111.00
1	D	680	ASP	CB-CG-OD2	6.42	124.08	118.30
1	C	509	ARG	NE-CZ-NH2	6.40	123.50	120.30
1	D	377	ARG	NE-CZ-NH2	-6.39	117.11	120.30
1	C	37	ARG	NE-CZ-NH2	-6.31	117.14	120.30
1	B	521	ARG	NE-CZ-NH1	-6.28	117.16	120.30
1	B	130	ARG	NE-CZ-NH1	6.27	123.44	120.30
1	B	72	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	C	377	ARG	NE-CZ-NH1	-6.25	117.17	120.30
1	A	552	LEU	CB-CG-CD1	6.23	121.59	111.00
1	B	121	ARG	NE-CZ-NH2	-6.15	117.23	120.30
1	A	542	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	C	61	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	C	155	ASP	CB-CG-OD1	-6.03	112.88	118.30
1	A	740	ARG	NE-CZ-NH1	5.96	123.28	120.30
1	C	445	ARG	NE-CZ-NH1	5.93	123.27	120.30
1	D	340	LEU	CB-CG-CD2	5.86	120.96	111.00
1	C	571	LEU	CA-CB-CG	5.85	128.76	115.30
1	A	710	ILE	N-CA-C	5.80	126.66	111.00
1	B	419	GLN	CB-CA-C	5.71	121.82	110.40
1	C	213	LYS	CD-CE-NZ	-5.68	98.64	111.70
1	D	582	LEU	CB-CG-CD1	5.55	120.43	111.00
1	A	350	ASP	CB-CG-OD1	-5.54	113.32	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	377	ARG	CG-CD-NE	-5.51	100.23	111.80
1	A	420	ILE	CG1-CB-CG2	-5.50	99.31	111.40
1	B	615	ASP	CB-CG-OD2	5.46	123.21	118.30
1	D	569	ASP	CB-CG-OD1	5.45	123.21	118.30
1	D	96	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	C	733	LEU	CB-CG-CD1	5.42	120.21	111.00
1	C	531	LEU	CB-CG-CD1	5.41	120.20	111.00
1	A	419	GLN	CB-CA-C	5.40	121.19	110.40
1	D	180	ARG	NE-CZ-NH2	-5.35	117.62	120.30
1	D	344	GLU	CA-CB-CG	5.35	125.17	113.40
1	B	267	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	D	598	VAL	CG1-CB-CG2	5.27	119.33	110.90
1	B	521	ARG	CD-NE-CZ	5.26	130.96	123.60
1	D	740	ARG	NE-CZ-NH2	-5.26	117.67	120.30
1	A	260	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	C	725	ASP	N-CA-C	5.20	125.03	111.00
1	D	61	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	A	121	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	C	419	GLN	CB-CA-C	5.17	120.75	110.40
1	C	585	ASP	CB-CG-OD2	5.16	122.95	118.30
1	A	213	LYS	CD-CE-NZ	-5.15	99.85	111.70
1	D	419	GLN	CB-CA-C	5.13	120.66	110.40
1	D	725	ASP	CB-CG-OD1	5.04	122.84	118.30
1	A	241	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	724	ALA	Peptide
1	C	725	ASP	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	5745	0	5579	40	1

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	5746	0	5584	51	1
1	C	5745	0	5580	61	0
1	D	5746	0	5584	50	0
2	A	43	0	30	2	0
2	B	43	0	30	4	0
2	C	43	0	30	4	0
2	D	43	0	30	1	0
3	A	771	0	0	14	0
3	B	650	0	0	12	0
3	C	690	0	0	18	1
3	D	745	0	0	13	1
All	All	26010	0	22447	196	2

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

All (196) 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:D:392:HIS:ND1	1:D:415:TYR:CB	1.69	1.52
1:B:392:HIS:ND1	1:B:415:TYR:CB	1.71	1.49
1:C:392:HIS:ND1	1:C:415:TYR:CB	1.84	1.40
1:D:449[B]:HIS:CE1	3:D:3262:HOH:O	1.71	1.32
1:D:392:HIS:CE1	1:D:415:TYR:HB2	1.64	1.29
1:C:449[A]:HIS:CE1	3:C:3266:HOH:O	1.65	1.26
1:B:392:HIS:CE1	1:B:415:TYR:HB2	1.71	1.24
1:C:392:HIS:ND1	1:C:415:TYR:HB2	0.91	1.23
1:A:713:GLN:HG2	3:A:2153:HOH:O	1.40	1.19
1:B:392:HIS:ND1	1:B:415:TYR:HB2	0.80	1.12
1:D:392:HIS:ND1	1:D:415:TYR:HB2	0.80	1.11
1:D:451:MET:SD	3:D:3264:HOH:O	2.07	1.10
1:C:392:HIS:CE1	1:C:415:TYR:HB2	1.88	1.07
1:A:710:ILE:HG12	1:A:715:GLU:OE1	1.55	1.05
1:B:267:ARG:HG3	3:B:3310:HOH:O	1.64	0.97
1:A:111:ARG:HB2	3:A:3292:HOH:O	1.68	0.92
1:D:521:ARG:HD3	3:D:3252:HOH:O	1.78	0.82
1:A:28:SER:OG	1:A:28:SER:O	1.98	0.80
1:C:416:THR:HG21	3:C:3270:HOH:O	1.81	0.79
1:B:521:ARG:HD3	3:B:3047:HOH:O	1.81	0.79
3:B:2705:HOH:O	1:D:73:LYS:CD	2.30	0.79
3:B:2705:HOH:O	1:D:73:LYS:HE3	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2705:HOH:O	1:D:73:LYS:CE	2.34	0.74
1:D:552:LEU:HD23	1:D:552:LEU:O	1.87	0.74
3:B:2705:HOH:O	1:D:73:LYS:HD3	1.89	0.72
1:C:704:PHE:O	1:C:707:THR:HG22	1.90	0.72
1:D:629:HIS:HD2	3:D:1554:HOH:O	1.74	0.71
1:D:321:GLU:HG3	3:D:2151:HOH:O	1.92	0.70
1:C:283:GLU:OE1	3:C:2292:HOH:O	2.09	0.69
1:B:533:LYS:HE2	3:B:3100:HOH:O	1.94	0.68
1:D:392:HIS:ND1	1:D:415:TYR:HB3	1.99	0.68
1:A:479:ARG:NH2	3:A:2607:HOH:O	2.08	0.67
1:C:416:THR:CG2	3:C:3270:HOH:O	2.40	0.66
1:B:583:LYS:H	1:B:583:LYS:NZ	1.95	0.65
1:D:677:ASP:HB2	3:D:3247:HOH:O	1.95	0.65
1:A:29:LEU:HB2	3:C:2405:HOH:O	1.98	0.63
1:B:392:HIS:ND1	1:B:415:TYR:CG	2.63	0.63
1:B:552:LEU:HD21	1:B:571:LEU:HD12	1.80	0.63
1:B:281:ASN:OD1	1:B:283:GLU:HG3	1.99	0.63
1:A:751:ILE:O	1:A:751:ILE:HD12	1.97	0.62
1:B:330:ASP:OD1	1:B:629:HIS:HE1	1.82	0.62
1:C:488:ARG:HD2	3:C:2379:HOH:O	1.98	0.62
1:A:111:ARG:HD3	3:A:3287:HOH:O	1.99	0.62
1:B:111:ARG:HB2	3:B:3290:HOH:O	1.99	0.61
1:B:449[A]:HIS:CG	1:D:449[A]:HIS:CG	2.44	0.61
1:C:330:ASP:OD1	1:C:629:HIS:HE1	1.83	0.60
1:A:395:HIS:HE1	3:A:3308:HOH:O	1.84	0.60
1:B:392:HIS:ND1	1:B:415:TYR:HB3	2.04	0.60
1:D:416:THR:HG21	3:D:3280:HOH:O	2.00	0.60
1:D:552:LEU:CD2	1:D:556:GLN:NE2	2.65	0.59
1:B:583:LYS:O	1:B:584:LYS:HB3	2.02	0.59
1:C:449[A]:HIS:ND1	3:C:3267:HOH:O	0.76	0.59
1:D:392:HIS:ND1	1:D:415:TYR:CG	2.64	0.59
1:A:29:LEU:HD22	3:C:2405:HOH:O	2.02	0.58
1:A:274:ILE:HD12	2:A:760:HEM:HMB1	1.87	0.57
1:B:612:ARG:HB2	1:B:612:ARG:NH1	2.20	0.57
1:B:359:LEU:H	1:B:507:HIS:HD2	1.52	0.57
1:C:583:LYS:O	1:C:584:LYS:HB3	2.04	0.57
1:D:111:ARG:HD3	3:D:3305:HOH:O	2.05	0.57
1:C:556:GLN:NE2	3:C:2533:HOH:O	2.37	0.56
1:A:416:THR:HG21	3:A:3307:HOH:O	2.05	0.56
1:D:330:ASP:OD1	1:D:629:HIS:HE1	1.87	0.56
2:B:760:HEM:CMC	2:B:760:HEM:HBC2	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:533:LYS:NZ	3:A:2232:HOH:O	2.38	0.55
1:B:416:THR:HG21	3:B:3285:HOH:O	2.05	0.55
1:B:678:ASN:OD1	1:B:680:ASP:HB2	2.06	0.55
1:C:678:ASN:OD1	1:C:680:ASP:HB2	2.06	0.55
1:D:274:ILE:HD12	2:D:760:HEM:HMB1	1.87	0.55
1:A:36:HIS:HE1	3:A:1872:HOH:O	1.89	0.55
1:A:690:LYS:HG3	1:A:751:ILE:HD11	1.89	0.55
1:B:629:HIS:HD2	3:B:1055:HOH:O	1.88	0.55
1:B:682:ASN:HB3	1:B:707:THR:HG21	1.89	0.55
1:C:488:ARG:CD	3:C:2379:HOH:O	2.52	0.54
1:B:612:ARG:O	1:B:612:ARG:HG3	2.06	0.54
1:B:634:TYR:O	1:B:653:THR:HA	2.07	0.54
1:A:459:ASN:ND2	1:B:219:HIS:HB3	2.23	0.54
1:B:395:HIS:HE1	3:B:3300:HOH:O	1.91	0.54
2:C:760:HEM:CMB	2:C:760:HEM:HBB2	2.38	0.54
1:B:38:PRO:HG2	1:B:51:ALA:HB2	1.91	0.53
1:C:578:ASP:HB2	1:C:582:LEU:O	2.07	0.53
1:D:747:LYS:H	1:D:747:LYS:HD2	1.74	0.53
1:C:137:TYR:HB2	1:C:159:ILE:CD1	2.39	0.52
1:D:341:ILE:HG13	3:D:3022:HOH:O	2.09	0.52
1:A:682:ASN:HB3	1:A:707:THR:HG21	1.92	0.52
1:A:111:ARG:NH2	3:A:3292:HOH:O	2.43	0.52
1:C:359:LEU:H	1:C:507:HIS:HD2	1.58	0.52
1:B:448:MET:HG3	1:B:449[A]:HIS:CD2	2.45	0.51
1:B:725:ASP:OD2	1:B:727:SER:HB3	2.11	0.51
1:A:111:ARG:CD	3:A:3287:HOH:O	2.58	0.51
1:B:449[B]:HIS:CD2	1:D:449[B]:HIS:CD2	2.99	0.50
1:C:724:ALA:O	1:C:725:ASP:HB2	2.11	0.50
1:C:629:HIS:HD2	3:C:1129:HOH:O	1.95	0.50
1:C:748:ILE:O	1:C:751:ILE:HG22	2.12	0.50
1:B:686:MET:HB3	1:B:751:ILE:HD11	1.93	0.50
1:D:449[B]:HIS:NE2	3:D:3262:HOH:O	2.03	0.50
1:B:37:ARG:HD3	3:B:2886:HOH:O	2.12	0.49
1:D:211:ALA:CB	1:D:410:GLY:HA3	2.43	0.49
2:B:760:HEM:HMB1	2:B:760:HEM:HBB2	1.94	0.49
1:C:274:ILE:HD12	2:C:760:HEM:HMB1	1.95	0.49
1:D:552:LEU:HD22	1:D:556:GLN:NE2	2.27	0.49
1:B:556:GLN:HG2	1:B:566:LEU:HD23	1.94	0.49
2:B:760:HEM:HBB2	2:B:760:HEM:CMB	2.43	0.49
2:C:760:HEM:HBB2	2:C:760:HEM:HMB1	1.94	0.48
1:D:634:TYR:O	1:D:653:THR:HA	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:111:ARG:HD3	3:C:3296:HOH:O	2.13	0.48
1:C:686:MET:HB3	1:C:751:ILE:HD11	1.94	0.48
1:D:578:ASP:CG	1:D:583:LYS:HG2	2.33	0.48
1:A:469:TRP:CE3	1:A:471:ARG:HG3	2.48	0.48
1:D:552:LEU:HD23	1:D:552:LEU:C	2.33	0.48
1:B:392:HIS:CG	1:B:415:TYR:CB	2.83	0.48
1:A:111:ARG:CZ	3:A:3292:HOH:O	2.62	0.48
1:D:671:ASN:ND2	3:D:2248:HOH:O	2.41	0.47
2:B:760:HEM:HBC2	2:B:760:HEM:HMC1	1.95	0.47
1:D:574:THR:HG23	3:D:1614:HOH:O	2.14	0.47
1:B:583:LYS:H	1:B:583:LYS:HZ3	1.63	0.46
1:A:128:HIS:CE1	1:A:169:VAL:HG22	2.51	0.46
1:B:207:PHE:O	1:B:249:THR:HA	2.16	0.46
1:C:395:HIS:HE1	3:C:3269:HOH:O	1.99	0.46
1:D:128:HIS:HA	1:D:168:THR:O	2.15	0.46
1:D:395:HIS:HE1	3:D:3303:HOH:O	1.98	0.46
1:D:488:ARG:NH1	1:D:490:GLU:OE1	2.46	0.46
1:A:449[A]:HIS:CD2	1:C:449[A]:HIS:CD2	3.03	0.46
1:C:111:ARG:CD	3:C:3296:HOH:O	2.64	0.46
1:C:195:ILE:HD11	1:C:436:PRO:HA	1.98	0.46
1:A:36:HIS:CD2	1:A:36:HIS:H	2.35	0.45
1:B:562:LEU:HA	1:C:637:MET:HB2	1.99	0.45
1:C:359:LEU:H	1:C:507:HIS:CD2	2.35	0.45
1:B:251:HIS:CE1	1:B:507:HIS:HB3	2.52	0.45
1:B:392:HIS:CD2	1:B:394:GLY:H	2.34	0.44
1:C:634:TYR:O	1:C:653:THR:HA	2.17	0.44
1:D:552:LEU:HD21	1:D:556:GLN:NE2	2.32	0.44
3:A:3250:HOH:O	1:C:111:ARG:HD3	2.16	0.44
1:C:708:ILE:HG13	1:C:710:ILE:HG12	1.99	0.44
1:C:51:ALA:HB1	1:C:52:PRO:HD2	2.00	0.44
1:A:278:ARG:HH12	1:A:487:GLU:CD	2.21	0.44
1:B:393:PRO:HD2	1:B:415:TYR:CG	2.52	0.44
1:A:607:LEU:HD11	1:A:632:LEU:HB3	1.99	0.44
1:C:28:SER:N	3:C:2523:HOH:O	2.50	0.44
1:A:449[B]:HIS:CG	1:C:449[B]:HIS:CG	2.54	0.44
1:B:344:GLU:H	1:B:344:GLU:CD	2.21	0.44
1:B:359:LEU:H	1:B:507:HIS:CD2	2.35	0.44
1:B:612:ARG:HB2	1:B:612:ARG:HH11	1.82	0.44
1:C:459:ASN:H	1:C:459:ASN:HD22	1.66	0.44
1:D:359:LEU:H	1:D:507:HIS:HD2	1.66	0.44
1:C:411:ARG:HG2	2:C:760:HEM:C2C	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:252:ASN:HD22	1:A:252:ASN:HA	1.70	0.43
1:A:448:MET:O	1:A:449[B]:HIS:HB2	2.18	0.43
1:C:310:LEU:HD13	1:C:660:LEU:HB3	1.99	0.43
1:A:144:LEU:HD11	1:A:370:VAL:HG13	1.99	0.43
1:C:252:ASN:HD22	1:C:252:ASN:HA	1.65	0.43
1:A:38:PRO:HG2	1:A:51:ALA:HB2	2.00	0.43
1:A:319:ARG:HD3	1:D:227:TRP:O	2.18	0.43
1:A:696:ALA:HB1	1:A:728:PHE:CZ	2.54	0.43
1:B:725:ASP:OD2	1:B:727:SER:N	2.49	0.43
1:C:459:ASN:ND2	1:D:219:HIS:HB3	2.33	0.43
1:B:97:ALA:O	1:B:101:GLY:HA3	2.18	0.43
1:C:207:PHE:O	1:C:249:THR:HA	2.18	0.43
1:A:416:THR:HB	3:A:3250:HOH:O	2.18	0.43
1:B:583:LYS:H	1:B:583:LYS:HZ2	1.63	0.43
1:C:724:ALA:O	1:C:725:ASP:CB	2.67	0.43
1:C:634:TYR:CG	1:C:635:SER:N	2.87	0.43
1:D:552:LEU:CD2	1:D:552:LEU:C	2.86	0.43
1:C:219:HIS:HB3	1:D:459:ASN:ND2	2.34	0.42
1:A:92:GLN:HA	1:D:213:LYS:HD3	2.00	0.42
1:D:748:ILE:HA	1:D:751:ILE:HG23	2.01	0.42
1:C:460:TYR:CE2	1:D:238:THR:HB	2.54	0.42
1:A:411:ARG:HG2	2:A:760:HEM:C2C	2.54	0.42
1:A:460:TYR:CE2	1:B:238:THR:HB	2.54	0.42
1:B:558:VAL:HG12	1:B:562:LEU:HD22	2.01	0.42
1:C:392:HIS:CD2	1:C:394:GLY:H	2.37	0.42
1:C:449[A]:HIS:CE1	3:C:3267:HOH:O	1.64	0.42
1:B:38:PRO:HA	1:B:48:GLN:OE1	2.20	0.42
1:C:251:HIS:CE1	1:C:507:HIS:HB3	2.55	0.42
1:C:521:ARG:HH11	1:C:521:ARG:HB2	1.85	0.42
1:C:583:LYS:HE2	1:C:583:LYS:HB2	1.76	0.42
1:C:593:ILE:HA	1:C:594:PRO:HD2	1.92	0.41
1:D:48:GLN:HE21	1:D:48:GLN:HB3	1.74	0.41
1:B:732:LEU:C	1:B:732:LEU:HD13	2.41	0.41
1:C:293:TRP:CZ3	1:C:336:LEU:HB2	2.56	0.41
1:D:207:PHE:O	1:D:249:THR:HA	2.20	0.41
1:D:552:LEU:HD21	1:D:556:GLN:CD	2.41	0.41
1:A:128:HIS:HA	1:A:168:THR:O	2.21	0.41
1:C:725:ASP:HA	1:C:728:PHE:HB3	2.03	0.41
1:D:596:GLY:HA3	1:D:737:ALA:O	2.21	0.41
3:A:938:HOH:O	1:C:52:PRO:HG3	2.20	0.41
1:A:104:LEU:HB3	3:C:775:HOH:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:393:PRO:HD2	1:A:415:TYR:CG	2.56	0.40
1:B:369:ARG:HE	1:B:369:ARG:HB2	1.23	0.40
1:C:38:PRO:HG2	1:C:51:ALA:HB2	2.03	0.40
1:C:748:ILE:O	1:C:751:ILE:CG2	2.69	0.40
1:D:404:ASN:O	1:D:405:ASP:C	2.59	0.40
1:C:128:HIS:HA	1:C:168:THR:O	2.20	0.40
1:C:61:ARG:HG3	3:C:2648:HOH:O	2.20	0.40
1:B:521:ARG:HD2	1:B:745:ILE:HG21	2.03	0.40
1:C:133:ALA:HA	1:C:164:VAL:O	2.22	0.40
1:C:641:THR:CG2	1:C:645:GLY:HA2	2.51	0.40

All (2) 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)
1:A:59:ASP:OD1	1:B:369:ARG:NH1[2_545]	2.10	0.10
3:C:2040:HOH:O	3:D:2980:HOH:O[2_545]	2.13	0.07

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	724/753 (96%)	703 (97%)	19 (3%)	2 (0%)	41	23
1	B	724/753 (96%)	703 (97%)	19 (3%)	2 (0%)	41	23
1	C	724/753 (96%)	701 (97%)	21 (3%)	2 (0%)	41	23
1	D	724/753 (96%)	708 (98%)	15 (2%)	1 (0%)	51	33
All	All	2896/3012 (96%)	2815 (97%)	74 (3%)	7 (0%)	47	29

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	711	ALA
1	B	725	ASP
1	A	75	SER
1	C	75	SER
1	B	75	SER
1	C	725	ASP
1	D	75	SER

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	611/635 (96%)	596 (98%)	15 (2%)	47	24
1	B	611/635 (96%)	585 (96%)	26 (4%)	29	8
1	C	611/635 (96%)	577 (94%)	34 (6%)	21	4
1	D	611/635 (96%)	587 (96%)	24 (4%)	32	10
All	All	2444/2540 (96%)	2345 (96%)	99 (4%)	30	9

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

Mol	Chain	Res	Type
1	A	29	LEU
1	A	73	LYS
1	A	185	PHE
1	A	191	THR
1	A	205	ILE
1	A	227	TRP
1	A	252	ASN
1	A	369	ARG
1	A	420	ILE
1	A	432	PRO
1	A	440	TYR
1	A	459	ASN
1	A	552	LEU
1	A	732	LEU
1	A	750	LYS

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Mol	Chain	Res	Type
1	B	142	LYS
1	B	185	PHE
1	B	205	ILE
1	B	227	TRP
1	B	237	ASP
1	B	252	ASN
1	B	283	GLU
1	B	369	ARG
1	B	370	VAL
1	B	432	PRO
1	B	440	TYR
1	B	459	ASN
1	B	552	LEU
1	B	562	LEU
1	B	565	GLU
1	B	566	LEU
1	B	568	ASP
1	B	571	LEU
1	B	583	LYS
1	B	595	ASP
1	B	612	ARG
1	B	621	LYS
1	B	633	LEU
1	B	703	LYS
1	B	713	GLN
1	B	751	ILE
1	C	32	GLU
1	C	37	ARG
1	C	61	ARG
1	C	159	ILE
1	C	185	PHE
1	C	205	ILE
1	C	227	TRP
1	C	237	ASP
1	C	252	ASN
1	C	377	ARG
1	C	413	LYS
1	C	420	ILE
1	C	432	PRO
1	C	440	TYR
1	C	459	ASN
1	C	478	LYS

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Mol	Chain	Res	Type
1	C	488	ARG
1	C	521	ARG
1	C	531	LEU
1	C	568	ASP
1	C	571	LEU
1	C	583	LYS
1	C	584	LYS
1	C	606	LEU
1	C	616	LEU
1	C	633	LEU
1	C	636	ARG
1	C	648	LEU
1	C	660	LEU
1	C	685	LEU
1	C	713	GLN
1	C	725	ASP
1	C	733	LEU
1	C	750	LYS
1	D	28	SER
1	D	32	GLU
1	D	185	PHE
1	D	191	THR
1	D	205	ILE
1	D	227	TRP
1	D	237	ASP
1	D	252	ASN
1	D	340	LEU
1	D	344	GLU
1	D	413	LYS
1	D	440	TYR
1	D	459	ASN
1	D	552	LEU
1	D	554	LEU
1	D	574	THR
1	D	582	LEU
1	D	584	LYS
1	D	612	ARG
1	D	616	LEU
1	D	648	LEU
1	D	713	GLN
1	D	747	LYS
1	D	751	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	HIS
1	A	252	ASN
1	A	459	ASN
1	A	515	GLN
1	A	556	GLN
1	A	713	GLN
1	B	252	ASN
1	B	459	ASN
1	B	507	HIS
1	B	629	HIS
1	C	252	ASN
1	C	368	GLN
1	C	459	ASN
1	C	507	HIS
1	C	556	GLN
1	C	629	HIS
1	C	671	ASN
1	D	48	GLN
1	D	252	ASN
1	D	459	ASN
1	D	507	HIS
1	D	546	GLN
1	D	556	GLN
1	D	629	HIS
1	D	671	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

4 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	OCS	A	669	1	7,8,9	0.87	0	6,11,13	0.89	0
1	OCS	C	669	1	7,8,9	1.42	0	6,11,13	1.41	1 (16%)
1	OCS	D	669	1	7,8,9	1.22	0	6,11,13	1.93	2 (33%)
1	OCS	B	669	1	7,8,9	1.54	1 (14%)	6,11,13	2.54	3 (50%)

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
1	OCS	A	669	1	-	2/4/7/9	-
1	OCS	C	669	1	-	1/4/7/9	-
1	OCS	D	669	1	-	1/4/7/9	-
1	OCS	B	669	1	-	1/4/7/9	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	669	OCS	CB-CA	-3.63	1.50	1.53

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	669	OCS	OD1-SG-CB	4.89	112.75	106.94
1	D	669	OCS	OD1-SG-CB	3.91	111.59	106.94
1	B	669	OCS	OD3-SG-CB	-2.59	103.87	106.94
1	D	669	OCS	OD3-SG-CB	-2.35	104.15	106.94
1	B	669	OCS	OD2-SG-CB	-2.30	102.07	105.74
1	C	669	OCS	OD3-SG-CB	2.15	109.50	106.94

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	669	OCS	N-CA-CB-SG
1	B	669	OCS	N-CA-CB-SG
1	C	669	OCS	N-CA-CB-SG
1	D	669	OCS	N-CA-CB-SG
1	A	669	OCS	CA-CB-SG-OD1

There are no ring outliers.

No monomer is involved in short contacts.

5.5   Carbohydrates (i)

There are no monosaccharides in this entry.

5.6   Ligand geometry (i)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	HEM	B	760	3,1	41,50,50	2.00	12 (29%)	45,82,82	3.02	21 (46%)
2	HEM	A	760	3,1	41,50,50	2.24	9 (21%)	45,82,82	2.68	20 (44%)
2	HEM	C	760	3,1	41,50,50	1.93	13 (31%)	45,82,82	2.60	16 (35%)
2	HEM	D	760	3,1	41,50,50	1.66	8 (19%)	45,82,82	2.56	16 (35%)

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
2	HEM	B	760	3,1	-	4/12/54/54	-
2	HEM	A	760	3,1	-	2/12/54/54	-
2	HEM	C	760	3,1	-	3/12/54/54	-
2	HEM	D	760	3,1	-	3/12/54/54	-

All (42) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760	HEM	C3C-C2C	-7.56	1.29	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	760	HEM	C3D-C2D	6.51	1.50	1.36
2	B	760	HEM	C3D-C2D	6.29	1.50	1.36
2	D	760	HEM	C3D-C2D	6.14	1.49	1.36
2	C	760	HEM	C3D-C2D	5.79	1.49	1.36
2	A	760	HEM	CMC-C2C	3.98	1.61	1.51
2	A	760	HEM	C4A-NA	3.82	1.44	1.36
2	B	760	HEM	C1B-NB	-3.60	1.34	1.40
2	C	760	HEM	CAA-C2A	3.59	1.57	1.52
2	B	760	HEM	C3C-C2C	-3.56	1.35	1.40
2	B	760	HEM	FE-NB	3.21	2.12	1.96
2	C	760	HEM	CAB-C3B	3.17	1.56	1.47
2	C	760	HEM	FE-ND	3.05	2.12	1.96
2	D	760	HEM	C3C-CAC	3.02	1.54	1.47
2	B	760	HEM	O1A-CGA	2.96	1.31	1.22
2	A	760	HEM	CMB-C2B	2.95	1.57	1.50
2	C	760	HEM	CMB-C2B	2.86	1.56	1.50
2	A	760	HEM	C3C-CAC	2.77	1.53	1.47
2	C	760	HEM	C3C-C2C	-2.75	1.36	1.40
2	D	760	HEM	CAB-C3B	2.75	1.54	1.47
2	B	760	HEM	CMA-C3A	2.74	1.57	1.51
2	C	760	HEM	C4D-ND	-2.71	1.35	1.40
2	B	760	HEM	CHA-C4D	2.65	1.41	1.35
2	D	760	HEM	C3C-C2C	-2.64	1.36	1.40
2	C	760	HEM	CMC-C2C	2.63	1.57	1.51
2	B	760	HEM	C4A-NA	2.63	1.41	1.36
2	A	760	HEM	CHB-C1B	2.62	1.41	1.35
2	B	760	HEM	FE-ND	2.46	2.09	1.96
2	C	760	HEM	C4A-NA	2.46	1.41	1.36
2	B	760	HEM	CAB-C3B	2.43	1.54	1.47
2	D	760	HEM	CBD-CAD	2.39	1.59	1.52
2	B	760	HEM	C1A-NA	2.30	1.40	1.36
2	C	760	HEM	CBD-CAD	2.23	1.59	1.52
2	D	760	HEM	CMB-C2B	2.20	1.55	1.50
2	C	760	HEM	FE-NB	2.16	2.07	1.96
2	D	760	HEM	FE-NB	2.12	2.07	1.96
2	D	760	HEM	CHB-C1B	2.08	1.40	1.35
2	C	760	HEM	CMA-C3A	2.05	1.55	1.51
2	A	760	HEM	CBD-CAD	2.04	1.58	1.52
2	B	760	HEM	CMC-C2C	2.02	1.56	1.51
2	C	760	HEM	CHA-C4D	2.02	1.40	1.35
2	A	760	HEM	CAA-C2A	2.01	1.55	1.52

All (73) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	760	HEM	CBD-CAD-C3D	-9.59	85.97	112.63
2	D	760	HEM	CBD-CAD-C3D	-9.49	86.26	112.63
2	A	760	HEM	CBD-CAD-C3D	-8.61	88.72	112.63
2	B	760	HEM	C1B-NB-C4B	7.89	113.22	105.07
2	B	760	HEM	CBD-CAD-C3D	-7.68	91.30	112.63
2	B	760	HEM	C4D-ND-C1D	6.97	112.27	105.07
2	D	760	HEM	CAD-CBD-CGD	-6.50	99.62	113.60
2	B	760	HEM	CHA-C4D-ND	6.30	132.16	124.38
2	C	760	HEM	C4D-ND-C1D	5.87	111.14	105.07
2	C	760	HEM	CAD-CBD-CGD	-5.55	101.66	113.60
2	B	760	HEM	CHC-C4B-NB	5.27	130.16	124.43
2	A	760	HEM	C1B-NB-C4B	5.12	110.36	105.07
2	A	760	HEM	O2D-CGD-O1D	-4.72	111.54	123.30
2	A	760	HEM	CAD-C3D-C4D	4.60	132.70	124.66
2	C	760	HEM	O2D-CGD-O1D	-4.36	112.44	123.30
2	A	760	HEM	CAD-CBD-CGD	-4.32	104.31	113.60
2	A	760	HEM	C4D-ND-C1D	4.20	109.42	105.07
2	D	760	HEM	CMD-C2D-C1D	4.16	131.38	125.04
2	B	760	HEM	CAD-CBD-CGD	-4.14	104.70	113.60
2	A	760	HEM	CHB-C1B-NB	4.11	129.46	124.38
2	C	760	HEM	C4B-C3B-C2B	4.04	110.32	107.11
2	D	760	HEM	CMA-C3A-C4A	-3.81	122.61	128.46
2	B	760	HEM	O2D-CGD-O1D	-3.80	113.84	123.30
2	A	760	HEM	CMA-C3A-C4A	-3.74	122.71	128.46
2	D	760	HEM	C4D-ND-C1D	3.68	108.88	105.07
2	B	760	HEM	CAA-CBA-CGA	-3.66	103.51	113.76
2	A	760	HEM	C2C-C3C-C4C	3.56	109.39	106.90
2	A	760	HEM	C4B-C3B-C2B	3.50	109.90	107.11
2	D	760	HEM	O2D-CGD-CBD	3.45	125.10	114.03
2	B	760	HEM	O2D-CGD-CBD	3.42	125.03	114.03
2	D	760	HEM	O2D-CGD-O1D	-3.41	114.81	123.30
2	B	760	HEM	C3C-C4C-NC	-3.40	104.52	110.94
2	C	760	HEM	C2C-C3C-C4C	3.39	109.27	106.90
2	A	760	HEM	CAD-C3D-C2D	-3.35	121.63	127.88
2	C	760	HEM	C1B-NB-C4B	3.30	108.48	105.07
2	C	760	HEM	CHD-C1D-ND	3.30	128.01	124.43
2	B	760	HEM	C2B-C1B-NB	-3.18	106.07	109.84
2	D	760	HEM	CAD-C3D-C4D	3.16	130.19	124.66
2	B	760	HEM	C3D-C4D-ND	-3.11	106.70	110.17
2	D	760	HEM	CAA-CBA-CGA	-3.06	105.18	113.76
2	B	760	HEM	C4B-CHC-C1C	3.00	126.52	122.56
2	B	760	HEM	C2C-C3C-C4C	2.97	108.97	106.90
2	B	760	HEM	CMD-C2D-C1D	2.94	129.52	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	760	HEM	O2D-CGD-CBD	2.89	123.32	114.03
2	C	760	HEM	CAA-CBA-CGA	-2.83	105.83	113.76
2	D	760	HEM	CHA-C4D-ND	2.79	127.83	124.38
2	B	760	HEM	C4C-CHD-C1D	2.77	126.22	122.56
2	B	760	HEM	CAD-C3D-C4D	2.71	129.40	124.66
2	C	760	HEM	CAD-C3D-C4D	2.71	129.39	124.66
2	A	760	HEM	CMD-C2D-C1D	2.66	129.09	125.04
2	C	760	HEM	CHB-C1B-NB	2.64	127.64	124.38
2	D	760	HEM	C4C-CHD-C1D	2.64	126.04	122.56
2	C	760	HEM	C3C-C4C-NC	-2.52	106.18	110.94
2	C	760	HEM	CMA-C3A-C4A	-2.44	124.71	128.46
2	C	760	HEM	CBB-CAB-C3B	-2.43	115.51	127.62
2	A	760	HEM	C3C-C4C-NC	-2.42	106.37	110.94
2	B	760	HEM	C4A-C3A-C2A	2.38	108.65	107.00
2	A	760	HEM	C4A-C3A-C2A	2.33	108.62	107.00
2	B	760	HEM	CHA-C4D-C3D	-2.32	120.97	125.33
2	A	760	HEM	CHD-C1D-ND	2.32	126.95	124.43
2	D	760	HEM	C4A-C3A-C2A	2.27	108.58	107.00
2	A	760	HEM	C2B-C1B-NB	-2.24	107.18	109.84
2	D	760	HEM	C4B-CHC-C1C	2.21	125.47	122.56
2	D	760	HEM	C1B-NB-C4B	2.21	107.35	105.07
2	D	760	HEM	C3B-C2B-C1B	2.20	108.12	106.49
2	B	760	HEM	C3B-C2B-C1B	2.20	108.12	106.49
2	C	760	HEM	CHC-C4B-NB	2.16	126.78	124.43
2	A	760	HEM	CHC-C4B-NB	2.13	126.75	124.43
2	A	760	HEM	CAA-CBA-CGA	-2.13	107.79	113.76
2	A	760	HEM	CHA-C4D-ND	2.12	127.00	124.38
2	C	760	HEM	C2B-C1B-NB	-2.10	107.36	109.84
2	B	760	HEM	CHB-C1B-NB	2.03	126.89	124.38
2	D	760	HEM	CMA-C3A-C2A	2.03	128.76	124.94

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	760	HEM	CAA-CBA-CGA-O2A
2	A	760	HEM	CAA-CBA-CGA-O1A
2	C	760	HEM	CAA-CBA-CGA-O1A
2	A	760	HEM	CAA-CBA-CGA-O2A
2	B	760	HEM	CAA-CBA-CGA-O2A
2	D	760	HEM	CAA-CBA-CGA-O1A
2	B	760	HEM	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
2	C	760	HEM	CAA-CBA-CGA-O2A
2	B	760	HEM	CAD-CBD-CGD-O2D
2	B	760	HEM	CAD-CBD-CGD-O1D
2	C	760	HEM	CAD-CBD-CGD-O2D
2	D	760	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.
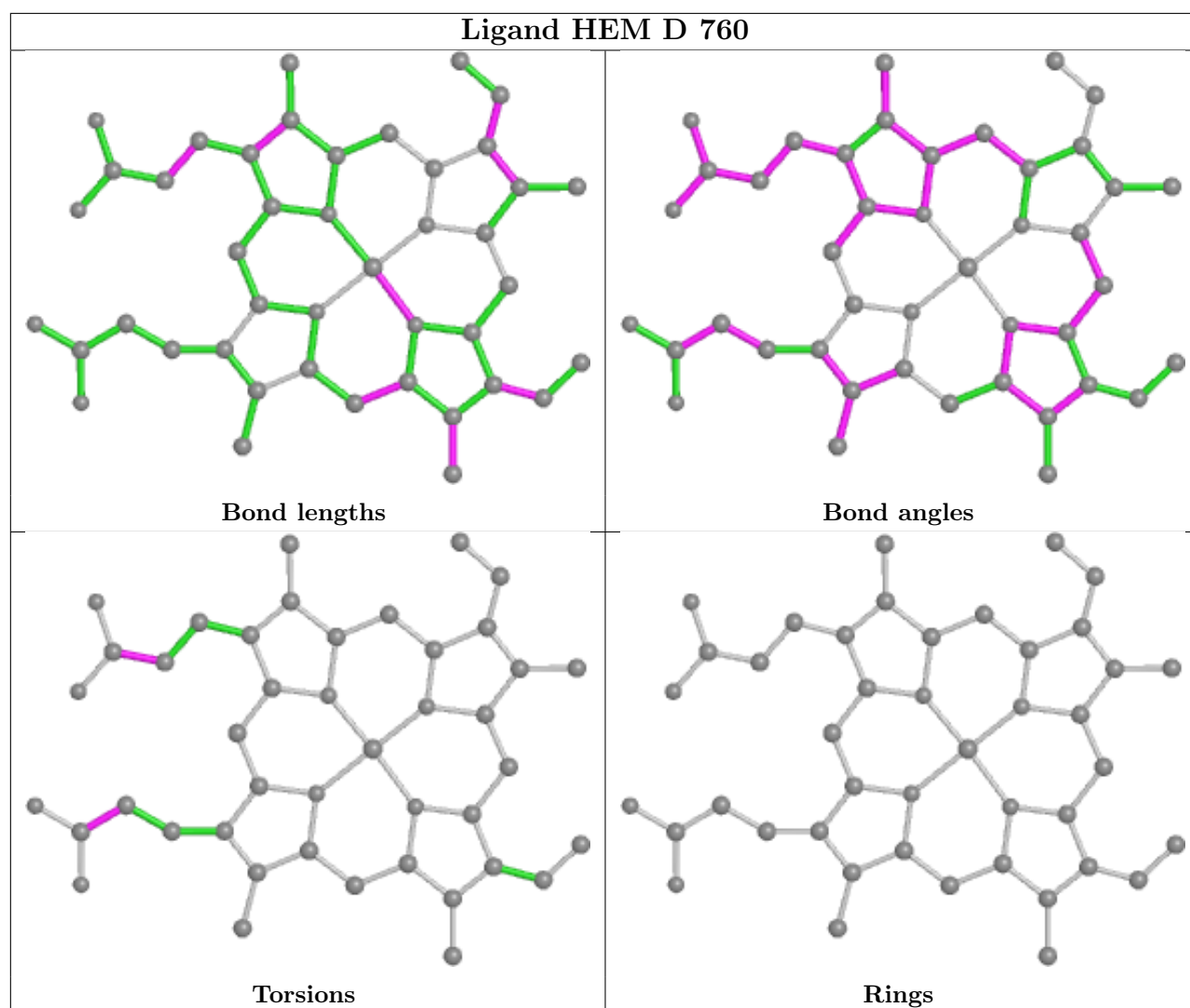
4 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	760	HEM	4	0
2	A	760	HEM	2	0
2	C	760	HEM	4	0
2	D	760	HEM	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less 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 HEM B 760

Bond lengths

Bond angles

Torsions

Rings

Full wwPDB X-ray Structure Validation Report

Ligand HEM A 760

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM C 760

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM D 760

Bond lengths

Bond angles

Torsions

Rings
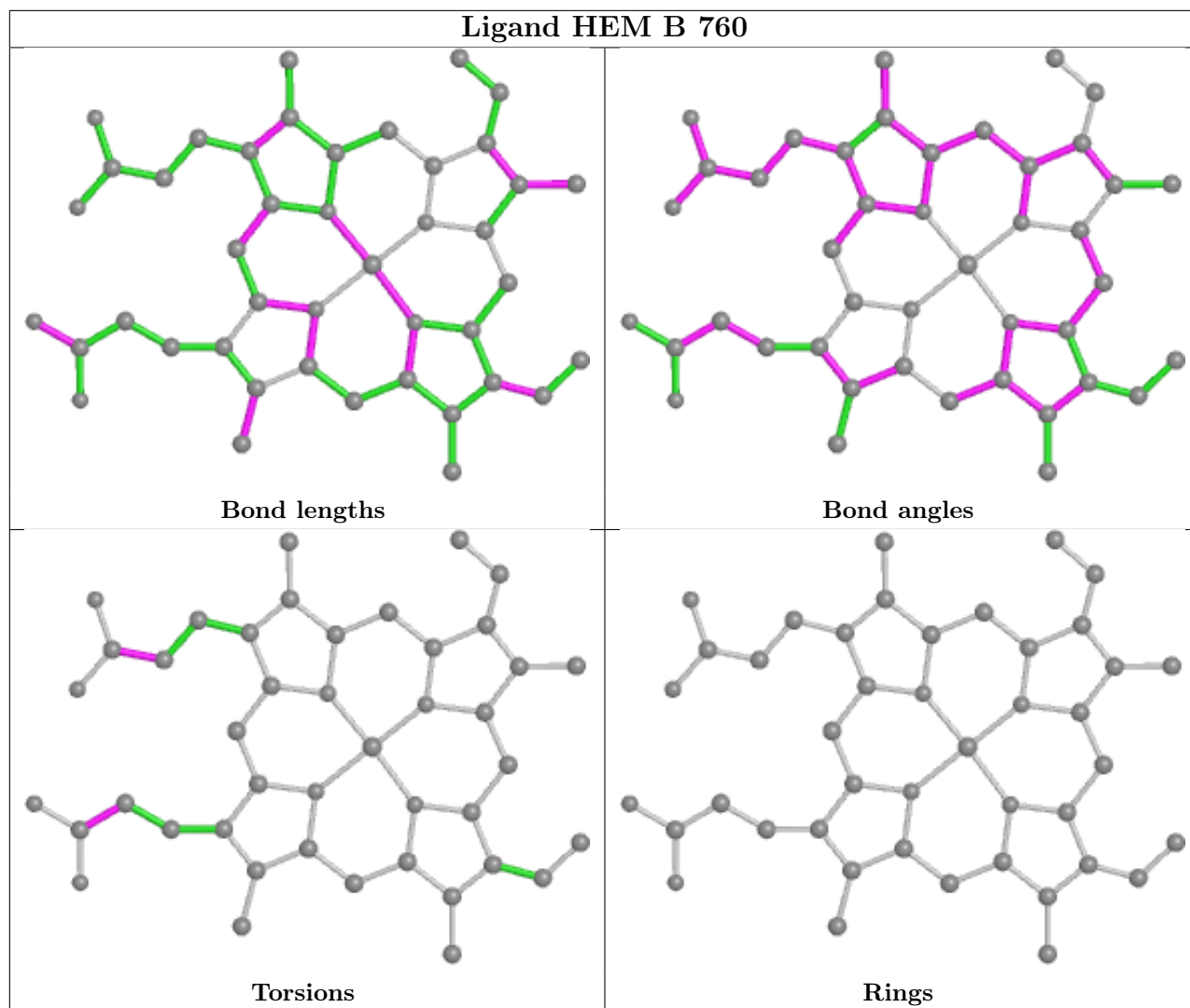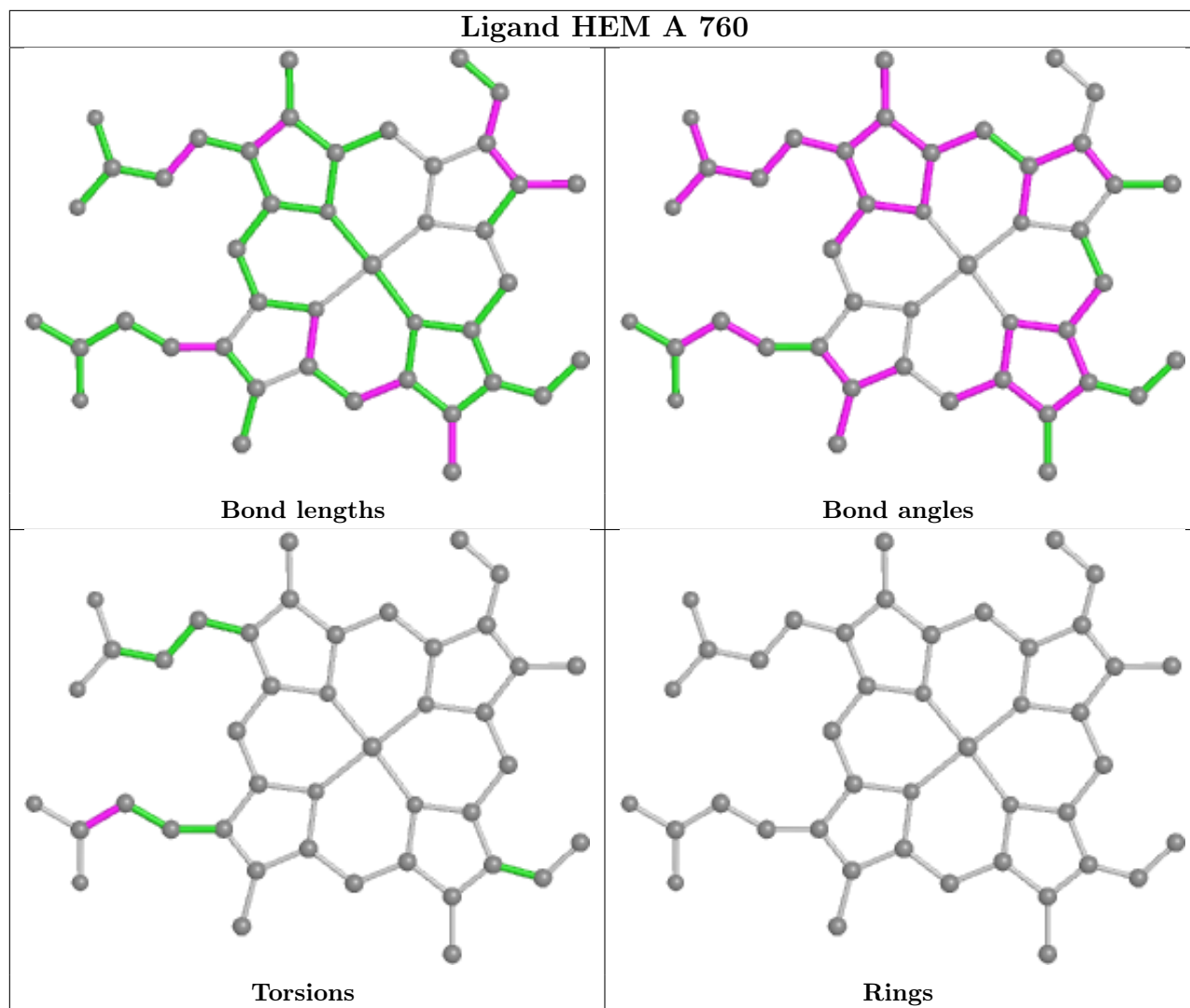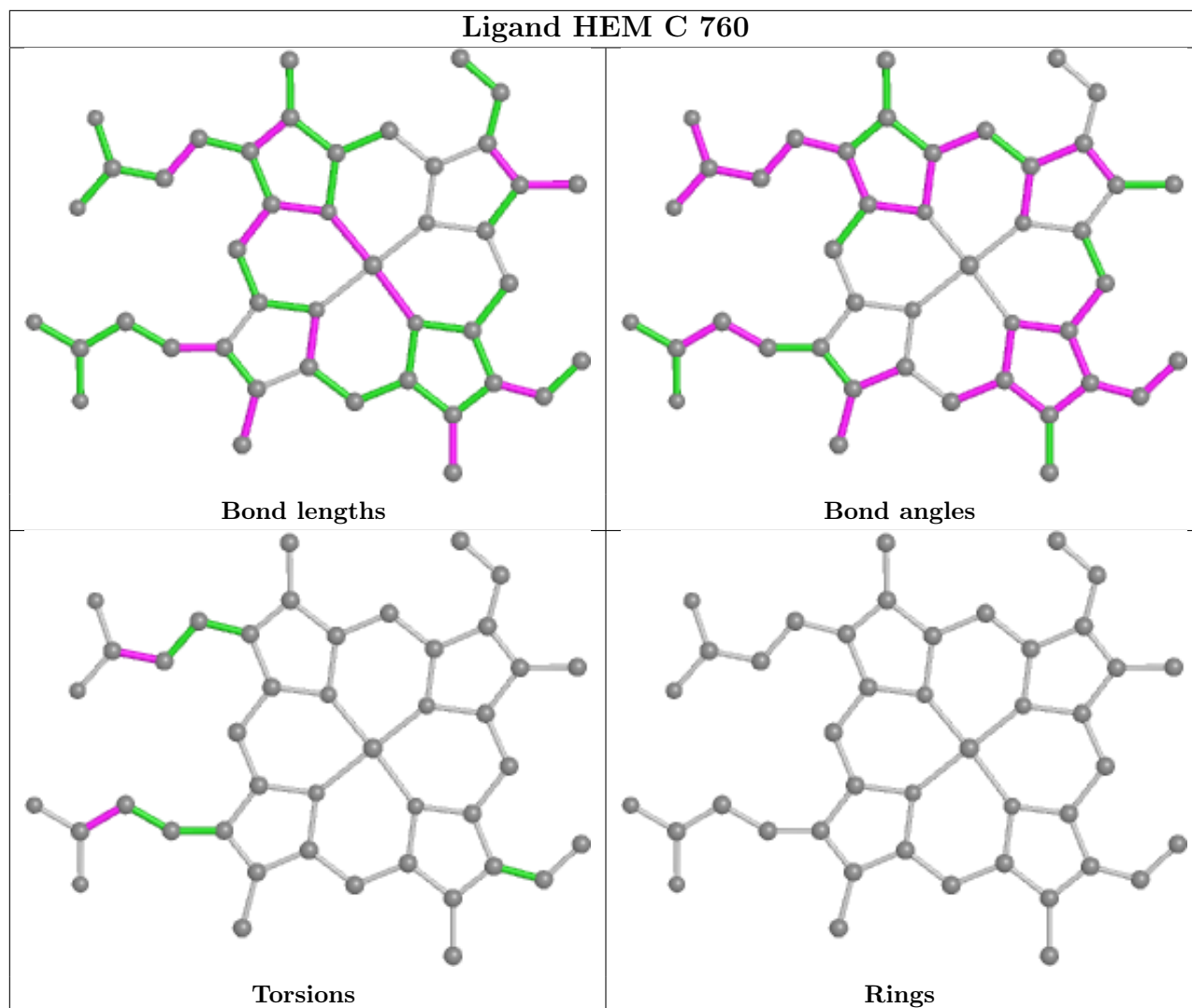
5.7 Other polymers ⓘ

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(Å^2)	Q<0.9
1	A	725/753 (96%)	-0.54	11 (1%)	73	80	4, 10, 27, 46	1 (0%)
1	B	725/753 (96%)	-0.36	26 (3%)	42	48	5, 12, 33, 48	1 (0%)
1	C	725/753 (96%)	-0.42	20 (2%)	53	58	5, 11, 32, 47	1 (0%)
1	D	725/753 (96%)	-0.58	9 (1%)	79	84	4, 10, 26, 46	1 (0%)
All	All	2900/3012 (96%)	-0.47	66 (2%)	60	66	4, 11, 31, 48	4 (0%)

All (66) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	726	GLY	7.1
1	A	710	ILE	7.0
1	B	28	SER	4.4
1	B	32	GLU	4.4
1	D	28	SER	4.3
1	A	32	GLU	4.3
1	A	713	GLN	4.2
1	B	673	ALA	4.0
1	A	711	ALA	3.7
1	A	28	SER	3.7
1	C	726	GLY	3.6
1	B	713	GLN	3.5
1	C	594	PRO	3.5
1	D	749	ASP	3.3
1	B	711	ALA	3.3
1	C	751	ILE	3.2
1	C	596	GLY	3.2
1	C	675	ILE	3.2
1	B	647	VAL	3.1
1	B	677	ASP	3.0
1	B	712	ASP	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	612	ARG	2.9
1	B	572	ASN	2.8
1	A	712	ASP	2.8
1	D	750	LYS	2.7
1	C	568	ASP	2.7
1	B	583	LYS	2.6
1	A	37	ARG	2.6
1	D	583	LYS	2.6
1	B	568	ASP	2.6
1	A	29	LEU	2.6
1	B	727	SER	2.6
1	C	641	THR	2.5
1	C	677	ASP	2.5
1	C	713	GLN	2.5
1	C	725	ASP	2.4
1	A	726	GLY	2.4
1	D	713	GLN	2.4
1	B	641	THR	2.4
1	B	725	ASP	2.4
1	A	749	ASP	2.3
1	B	34	GLY	2.3
1	A	35	SER	2.3
1	B	610	GLU	2.3
1	C	672	ILE	2.3
1	B	645	GLY	2.3
1	B	646	THR	2.2
1	D	572	ASN	2.2
1	B	565	GLU	2.2
1	C	640	VAL	2.2
1	C	28	SER	2.2
1	B	611	VAL	2.2
1	D	751	ILE	2.2
1	C	32	GLU	2.1
1	D	712	ASP	2.1
1	C	643	ASP	2.1
1	B	37	ARG	2.1
1	D	32	GLU	2.1
1	B	722	ASP	2.1
1	C	569	ASP	2.1
1	C	674	ASP	2.1
1	C	712	ASP	2.1
1	C	583	LYS	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	638	GLY	2.0
1	B	569	ASP	2.0
1	B	594	PRO	2.0

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

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
1	OCS	C	669	9/10	0.92	0.16	26,29,36,36	0
1	OCS	A	669	9/10	0.94	0.09	15,18,27,29	0
1	OCS	B	669	9/10	0.95	0.14	27,29,36,37	0
1	OCS	D	669	9/10	0.96	0.10	19,20,25,28	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

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
2	HEM	A	760	43/43	0.98	0.08	3,6,12,18	0
2	HEM	B	760	43/43	0.98	0.07	4,7,13,21	0
2	HEM	C	760	43/43	0.98	0.07	3,7,13,21	0
2	HEM	D	760	43/43	0.98	0.07	2,6,12,17	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.
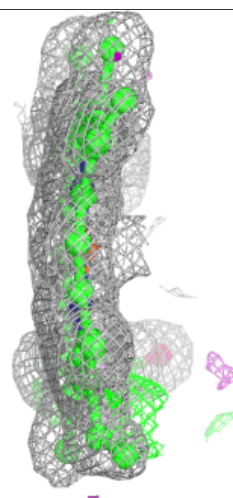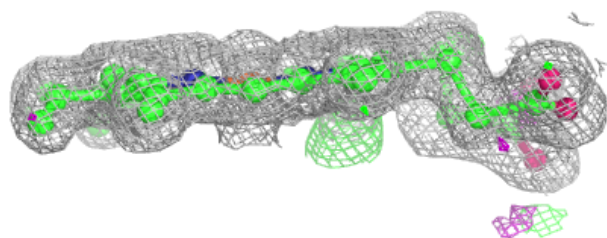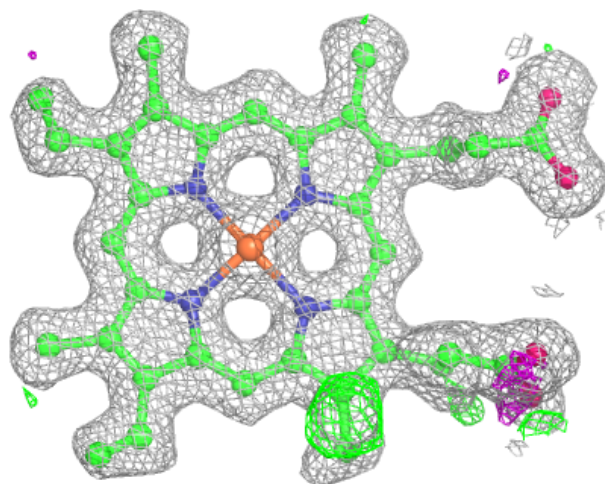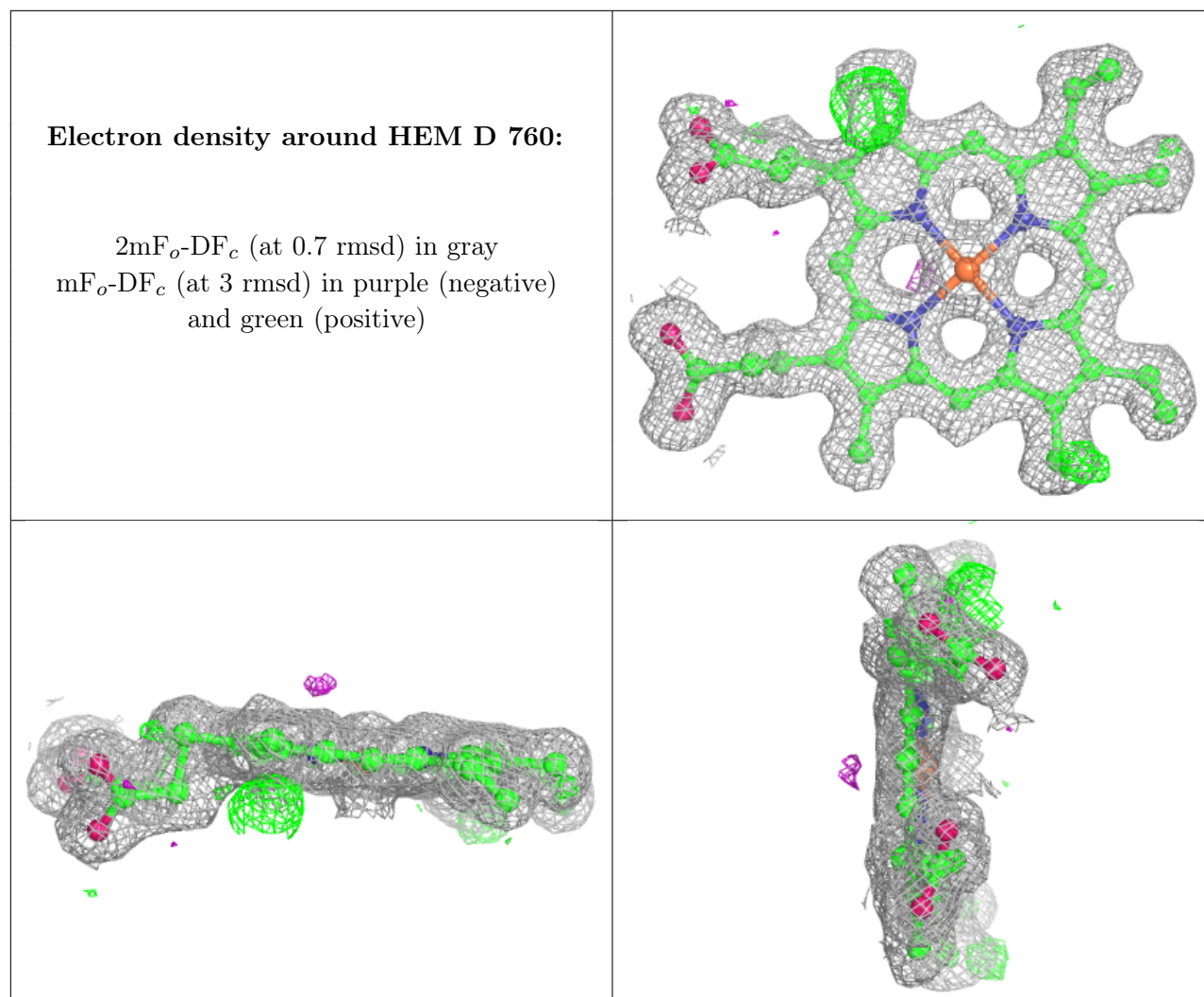
Electron density around HEM A 760:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
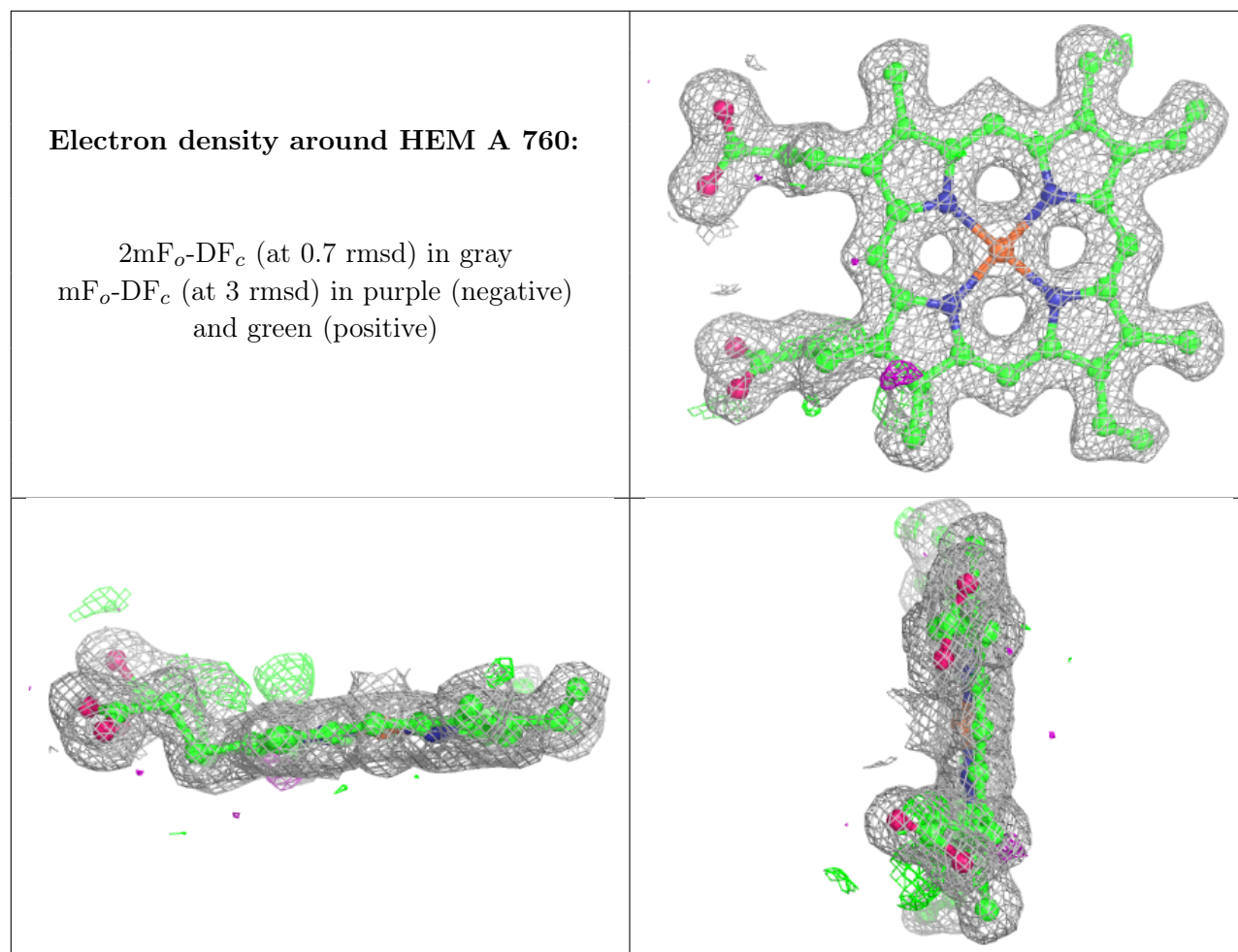
Electron density around HEM B 760:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
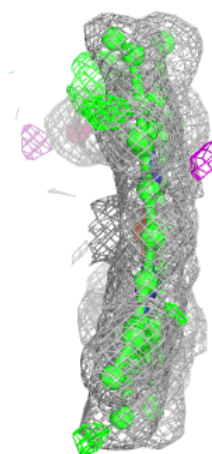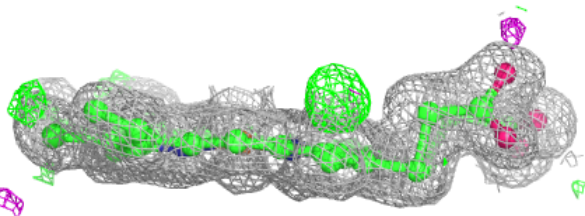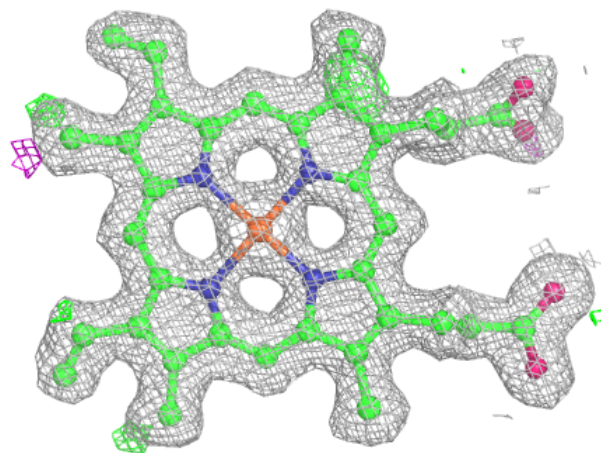
Electron density around HEM C 760:

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

Electron density around HEM D 760:

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

6.5   Other polymers   ⓘ

There are no such residues in this entry.