Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2024 – 05:52 PM EST

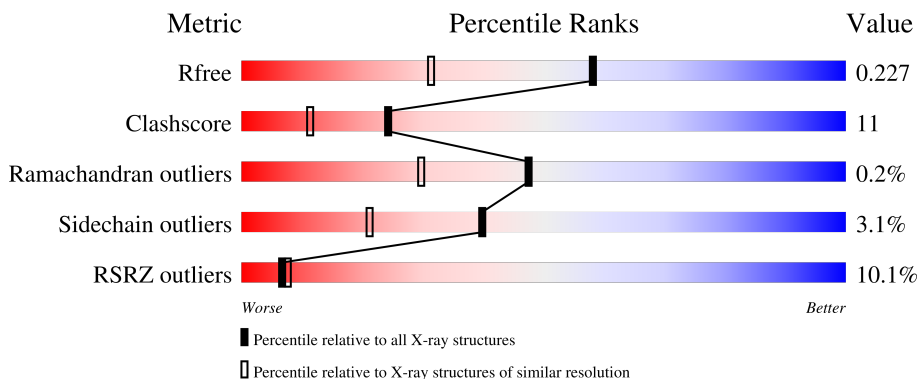|		
PDB ID	:	3VLJ
Title	:	Crystal Structure Analysis of the Cyanide Arg409Leu Variant Complexes with o-Dianisidine in KatG from HALOARCULA MARISMORTUI
Authors	:	Sato, T.; Higuchi, W.; Yoshimatsu, K.; Fujiwara, T.
Deposited on	:	2011-12-01
Resolution	:	1.70 Å(reported)

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1 Overall quality at a glance ⓘ

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

The reported resolution of this entry is 1.70 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.227
Clashscore		11
Ramachandran outliers		0.2%
Sidechain outliers		3.1%
RSRZ outliers		10.1%

Worse   *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4298 (1.70-1.70)
Clashscore	141614	4695 (1.70-1.70)
Ramachandran outliers	138981	4610 (1.70-1.70)
Sidechain outliers	138945	4610 (1.70-1.70)
RSRZ outliers	127900	4222 (1.70-1.70)

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	737	9% / 80% / 14% · ·
1	B	737	10% / 79% / 16% · ·

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
3	DDJ	A	801	-	-	-	X
3	DDJ	B	801	-	-	X	X
4	CYN	A	802	-	-	X	X

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 11994 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-peroxidase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	706	Total 5565	C 3483	N 930	O 1133	S 19	0	0	0
1	B	705	Total 5556	C 3478	N 929	O 1130	S 19	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	409	LEU	ARG	engineered mutation	UNP O59651
A	732	HIS	-	expression tag	UNP O59651
A	733	HIS	-	expression tag	UNP O59651
A	734	HIS	-	expression tag	UNP O59651
A	735	HIS	-	expression tag	UNP O59651
A	736	HIS	-	expression tag	UNP O59651
A	737	HIS	-	expression tag	UNP O59651
B	409	LEU	ARG	engineered mutation	UNP O59651
B	732	HIS	-	expression tag	UNP O59651
B	733	HIS	-	expression tag	UNP O59651
B	734	HIS	-	expression tag	UNP O59651
B	735	HIS	-	expression tag	UNP O59651
B	736	HIS	-	expression tag	UNP O59651
B	737	HIS	-	expression tag	UNP O59651

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).
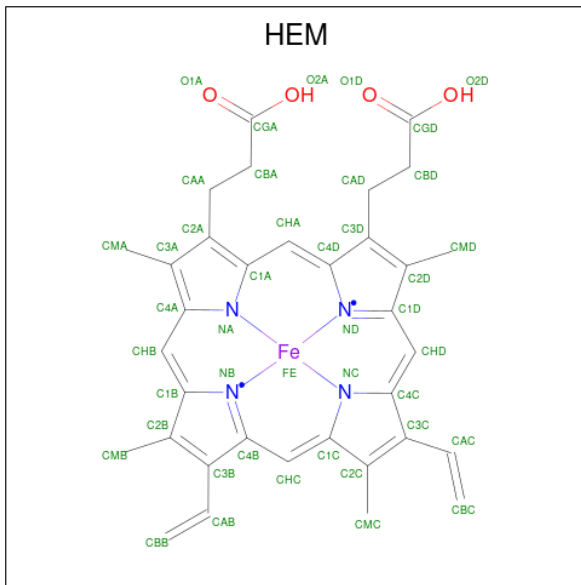
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
2	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 3 is 3,3'-dimethoxybiphenyl-4,4'-diamine (three-letter code: DDJ) (formula: $C_{14}H_{16}N_2O_2$).
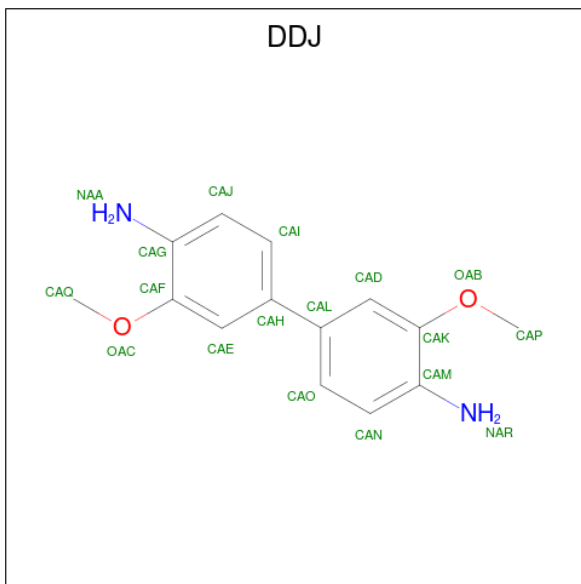
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			18	14	2	2		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total 18	C 14	N 2	O 2	0	0

- Molecule 4 is CYANIDE ION (three-letter code: CYN) (formula: CN).
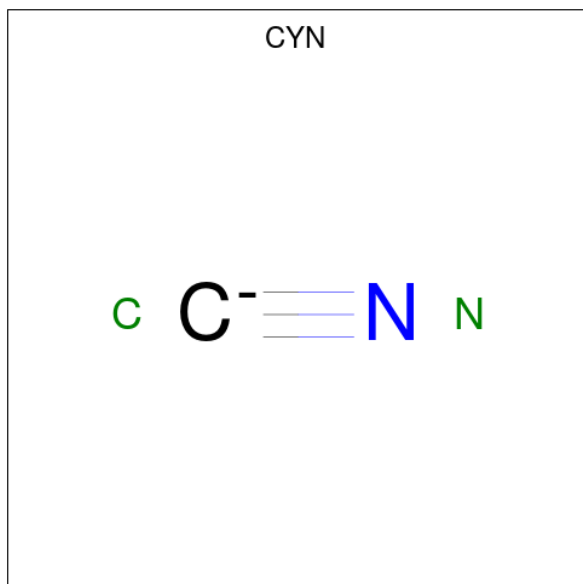
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 2	C 1	N 1	0	0
4	B	1	Total 2	C 1	N 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	454	Total 454	O 454	0	0
5	B	293	Total 293	O 293	0	0

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Catalase-peroxidase 2
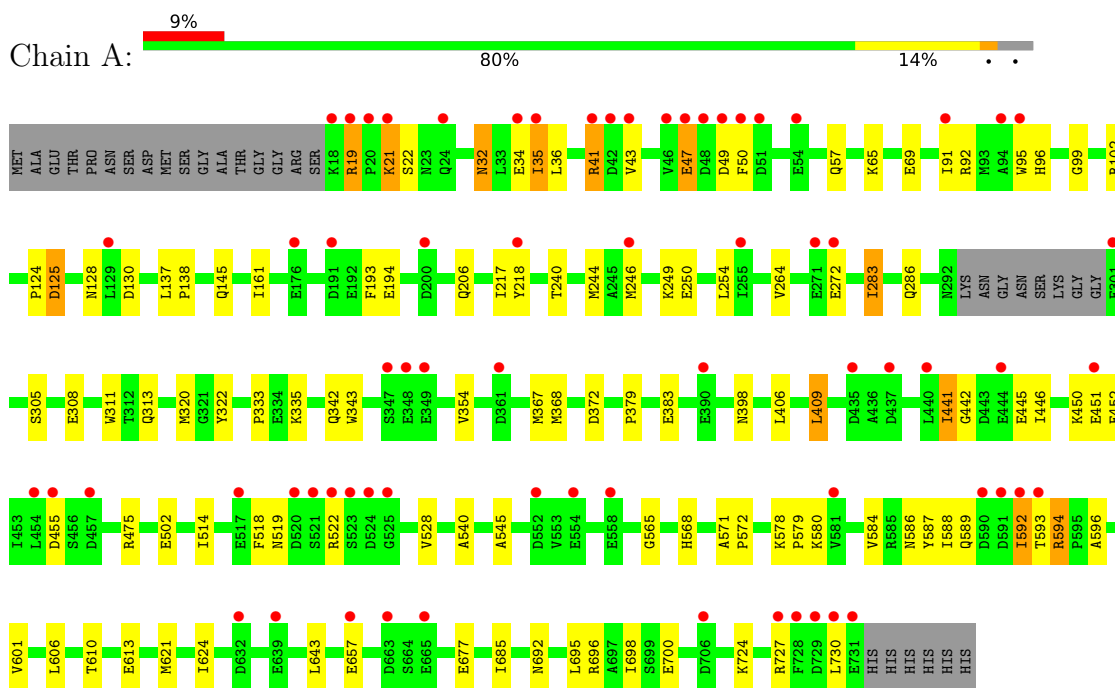
• Molecule 1: Catalase-peroxidase 2
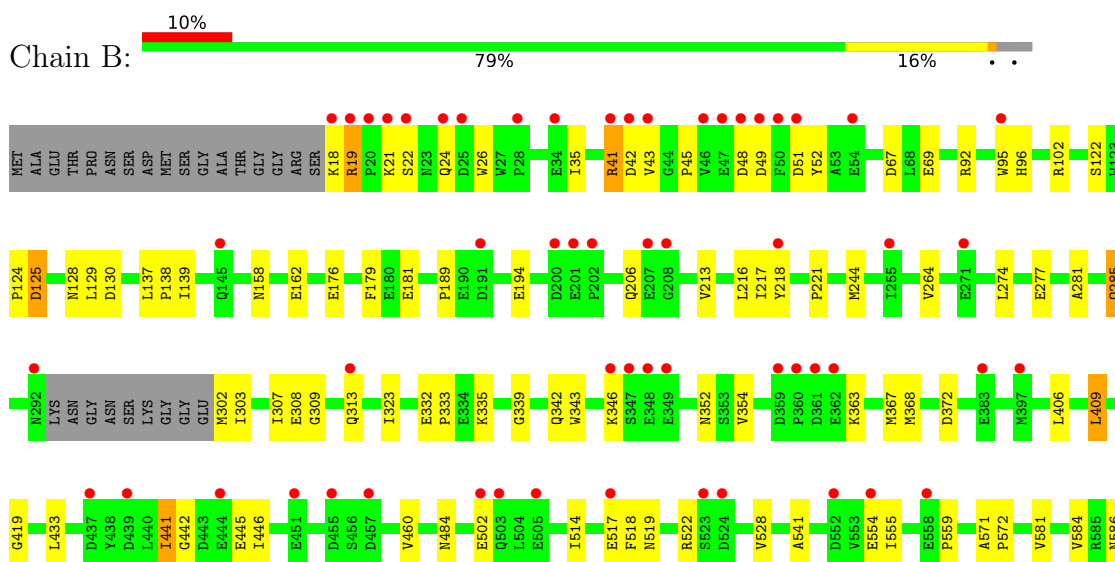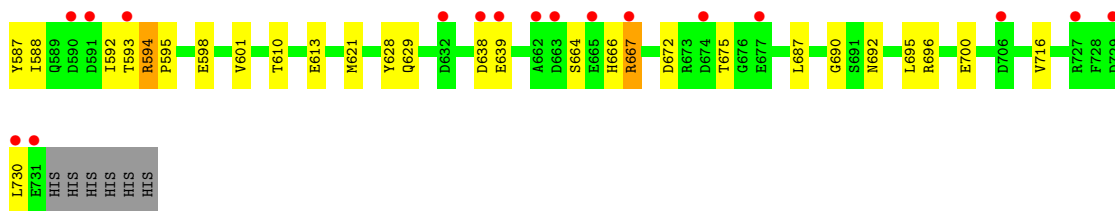
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	315.21Å 80.76Å 75.43Å 90.00° 99.50° 90.00°	Depositor
Resolution (Å)	36.74 – 1.70 36.73 – 1.70	Depositor EDS
% Data completeness (in resolution range)	99.5 (36.74-1.70) 99.7 (36.73-1.70)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.19 (at 1.70Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.216 , 0.234 0.210 , 0.227	Depositor DCC
R_{free} test set	10041 reflections (4.93%)	wwPDB-VP
Wilson B-factor (Å^2)	19.6	Xtriage
Anisotropy	0.426	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.40 , 56.4	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11994	wwPDB-VP
Average B, all atoms (Å^2)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: DDJ, CYN, 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	0.31	0/5700	0.56	0/7747
1	B	0.28	0/5691	0.53	0/7735
All	All	0.29	0/11391	0.55	0/15482

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5565	0	5210	141	0
1	B	5556	0	5204	105	0
2	A	43	0	30	1	0
2	B	43	0	30	2	0
3	A	18	0	16	5	0
3	B	18	0	16	9	0
4	A	2	0	0	3	0
4	B	2	0	0	0	0
5	A	454	0	0	3	0
5	B	293	0	0	4	0
All	All	11994	0	10506	239	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (239) 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:246:MET:HE1	1:A:254:LEU:HD12	1.23	1.11
1:B:35:ILE:HD11	1:B:601:VAL:HG12	1.34	1.07
1:B:92:ARG:HE	3:B:801:DDJ:HAQ	1.25	0.99
1:A:246:MET:CE	1:A:254:LEU:HD12	1.97	0.93
1:A:32:ASN:O	1:A:35:ILE:HD12	1.68	0.93
1:A:698:ILE:HD12	1:B:45:PRO:HD3	1.53	0.90
1:A:35:ILE:HD13	1:A:36:LEU:H	1.38	0.89
1:A:368:MET:HG3	1:A:372:ASP:HB2	1.55	0.89
1:A:565:GLY:H	1:A:568:HIS:HD2	1.17	0.88
1:A:217:ILE:HG22	1:A:218:TYR:CD1	2.08	0.88
1:A:580:LYS:HA	1:A:589:GLN:HE21	1.40	0.86
1:A:218:TYR:CZ	1:A:244:MET:SD	2.69	0.86
1:A:727:ARG:HA	1:A:727:ARG:HH11	1.39	0.86
1:A:593:THR:H	1:A:594:ARG:HH21	1.24	0.86
1:A:217:ILE:HG22	1:A:218:TYR:CE1	2.14	0.82
1:A:594:ARG:H	1:A:594:ARG:HE	1.28	0.81
1:B:19:ARG:HD3	1:B:19:ARG:H	1.43	0.81
1:B:218:TYR:CZ	1:B:244:MET:SD	2.75	0.80
1:A:91:ILE:HD11	1:A:161:ILE:HG13	1.63	0.79
1:B:217:ILE:HG22	1:B:218:TYR:CD1	2.17	0.79
1:A:311:TRP:HD1	1:A:368:MET:HE1	1.47	0.79
1:A:588:ILE:HD11	1:A:685:ILE:HD13	1.65	0.79
1:A:35:ILE:HD13	1:A:36:LEU:N	1.97	0.78
1:B:692:ASN:HD22	1:B:695:LEU:H	1.27	0.77
1:A:692:ASN:HD22	1:A:695:LEU:H	1.33	0.77
1:B:217:ILE:HG22	1:B:218:TYR:CE1	2.21	0.76
1:A:311:TRP:CD1	1:A:368:MET:HE1	2.21	0.76
1:A:95:TRP:CH2	1:A:218:TYR:CE1	2.75	0.75
1:A:592:ILE:HD13	1:A:592:ILE:H	1.50	0.75
1:B:584:VAL:HG13	1:B:621:MET:HG2	1.69	0.74
1:A:311:TRP:HD1	1:A:368:MET:CE	2.01	0.73
1:B:92:ARG:NE	3:B:801:DDJ:HAQ	2.03	0.72
1:A:519:ASN:HD21	1:A:528:VAL:H	1.38	0.71
1:B:441:ILE:HD13	1:B:441:ILE:H	1.55	0.71
1:A:19:ARG:HH12	1:A:21:LYS:HZ1	1.38	0.70
1:A:125:ASP:OD2	3:A:801:DDJ:HAQB	1.91	0.70
1:A:580:LYS:HA	1:A:589:GLN:NE2	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:368:MET:HG3	1:B:372:ASP:HB2	1.75	0.69
1:A:19:ARG:HH12	1:A:21:LYS:NZ	1.91	0.68
1:A:91:ILE:CD1	1:A:161:ILE:HG13	2.23	0.68
1:A:217:ILE:HG22	1:A:218:TYR:HD1	1.58	0.68
1:B:519:ASN:HD21	1:B:528:VAL:H	1.41	0.68
1:B:555:ILE:HD12	1:B:716:VAL:HG13	1.75	0.68
1:B:502:GLU:H	1:B:502:GLU:CD	1.97	0.68
1:B:95:TRP:CH2	1:B:218:TYR:CE1	2.82	0.68
1:A:125:ASP:HA	3:A:801:DDJ:HAQB	1.75	0.67
1:A:589:GLN:O	1:A:592:ILE:HD12	1.94	0.67
1:A:596:ALA:HB1	1:A:685:ILE:HD11	1.76	0.67
1:A:35:ILE:HD11	1:A:601:VAL:CG1	2.25	0.67
1:B:666:HIS:H	1:B:667:ARG:HH21	1.41	0.66
1:B:19:ARG:HD3	1:B:19:ARG:N	2.11	0.66
1:B:41:ARG:N	1:B:41:ARG:HD3	2.10	0.66
1:B:194:GLU:OE2	3:B:801:DDJ:HAPB	1.95	0.66
1:A:283:ILE:HD13	1:A:283:ILE:O	1.96	0.66
1:B:571:ALA:HB3	1:B:572:PRO:HD3	1.79	0.65
1:B:22:SER:HB2	1:B:24:GLN:OE1	1.97	0.65
1:B:323:ILE:HD12	1:B:323:ILE:H	1.62	0.65
1:A:502:GLU:CD	1:A:502:GLU:H	1.96	0.65
1:A:584:VAL:HG13	1:A:621:MET:HG2	1.78	0.64
1:A:311:TRP:CD1	1:A:368:MET:CE	2.80	0.64
1:B:514:ILE:O	1:B:517:GLU:HG2	1.96	0.64
1:A:124:PRO:HG3	1:A:194:GLU:HG3	1.81	0.63
1:B:313:GLN:HA	1:B:354:VAL:HG22	1.79	0.63
1:A:95:TRP:CH2	1:A:218:TYR:CZ	2.87	0.63
1:A:95:TRP:HH2	1:A:218:TYR:CZ	2.16	0.63
1:A:21:LYS:NZ	1:A:21:LYS:HB2	2.14	0.63
1:A:125:ASP:HA	3:A:801:DDJ:CAQ	2.29	0.63
1:A:305:SER:HA	3:A:801:DDJ:CAE	2.29	0.63
1:A:368:MET:HE2	1:A:372:ASP:HB3	1.80	0.63
1:A:727:ARG:NH2	1:A:730:LEU:HG	2.13	0.62
1:A:305:SER:HA	3:A:801:DDJ:HAE	1.82	0.62
1:A:95:TRP:HD1	4:A:802:CYN:N	1.98	0.61
1:B:217:ILE:HG22	1:B:218:TYR:HD1	1.66	0.61
1:B:514:ILE:HA	1:B:517:GLU:OE1	2.00	0.60
1:A:698:ILE:CD1	1:B:45:PRO:HD3	2.29	0.60
1:A:368:MET:HG3	1:A:372:ASP:CB	2.31	0.60
1:A:594:ARG:H	1:A:594:ARG:NE	2.00	0.59
1:A:308:GLU:H	1:A:342:GLN:HE22	1.49	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:323:ILE:HD12	1:B:323:ILE:N	2.16	0.59
1:A:47:GLU:HG3	1:A:49:ASP:OD1	2.03	0.59
1:A:95:TRP:CD1	4:A:802:CYN:N	2.70	0.59
1:A:518:PHE:O	1:A:522:ARG:HG2	2.04	0.58
1:A:588:ILE:HD11	1:A:685:ILE:CD1	2.32	0.58
1:B:95:TRP:HH2	1:B:218:TYR:CZ	2.21	0.58
1:B:441:ILE:HD13	1:B:441:ILE:N	2.19	0.57
1:B:95:TRP:CH2	1:B:218:TYR:CZ	2.92	0.57
1:B:139:ILE:HG12	5:B:945:HOH:O	2.04	0.57
1:A:41:ARG:HD2	1:B:41:ARG:HE	1.70	0.57
1:B:666:HIS:N	1:B:667:ARG:HH21	2.01	0.57
1:A:724:LYS:HB2	1:A:724:LYS:NZ	2.19	0.57
1:A:685:ILE:N	1:A:685:ILE:HD12	2.20	0.56
1:B:221:PRO:HD3	3:B:801:DDJ:HAJ	1.86	0.56
1:A:41:ARG:NH1	1:A:43:VAL:HG13	2.21	0.56
1:A:95:TRP:HH2	1:A:218:TYR:CE1	2.24	0.56
1:A:571:ALA:HB3	1:A:572:PRO:HD3	1.88	0.56
1:A:41:ARG:H	1:A:41:ARG:HD3	1.71	0.56
1:A:21:LYS:HB2	1:A:21:LYS:HZ3	1.69	0.56
1:A:545:ALA:HB1	1:A:624:ILE:HD12	1.87	0.56
1:B:594:ARG:H	1:B:594:ARG:HE	1.54	0.55
1:B:125:ASP:OD2	1:B:216:LEU:HD22	2.06	0.55
1:A:65:LYS:O	1:A:69:GLU:HG3	2.07	0.54
1:A:441:ILE:HB	1:A:445:GLU:HB2	1.89	0.54
1:A:441:ILE:HD13	1:A:441:ILE:H	1.73	0.54
1:B:441:ILE:H	1:B:441:ILE:CD1	2.21	0.54
1:A:35:ILE:HD11	1:A:36:LEU:HG	1.89	0.53
1:B:308:GLU:H	1:B:342:GLN:HE22	1.54	0.53
1:A:249:LYS:HE2	5:A:1184:HOH:O	2.08	0.53
1:A:452:GLU:CG	1:A:514:ILE:HD12	2.38	0.53
1:A:35:ILE:HD11	1:A:601:VAL:HG13	1.89	0.52
1:A:283:ILE:HD12	1:B:687:LEU:HB3	1.91	0.52
1:A:565:GLY:H	1:A:568:HIS:CD2	2.09	0.52
1:A:727:ARG:HA	1:A:727:ARG:NH1	2.16	0.52
1:A:47:GLU:H	1:A:47:GLU:CD	2.12	0.51
1:B:158:ASN:O	1:B:162:GLU:HG3	2.10	0.51
1:A:322:TYR:CE1	1:A:368:MET:CE	2.93	0.51
1:B:581:VAL:HG13	1:B:588:ILE:HD13	1.92	0.51
1:B:125:ASP:HA	3:B:801:DDJ:CAE	2.41	0.51
1:A:593:THR:H	1:A:594:ARG:NH2	2.01	0.51
1:B:555:ILE:CD1	1:B:716:VAL:HG13	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:LEU:HD21	5:B:1082:HOH:O	2.11	0.51
1:A:368:MET:HE2	1:A:372:ASP:CB	2.40	0.50
1:A:442:GLY:O	1:A:446:ILE:HG12	2.10	0.50
1:B:696:ARG:O	1:B:700:GLU:HG3	2.11	0.50
1:B:581:VAL:HG13	1:B:588:ILE:CD1	2.41	0.50
1:B:213:VAL:HB	1:B:216:LEU:HD12	1.94	0.50
1:A:441:ILE:HD13	1:A:441:ILE:N	2.26	0.50
1:B:442:GLY:O	1:B:446:ILE:HG13	2.12	0.50
1:B:18:LYS:NZ	1:B:18:LYS:HB3	2.28	0.49
1:B:323:ILE:H	1:B:323:ILE:CD1	2.26	0.49
1:A:322:TYR:CE1	1:A:368:MET:HE2	2.47	0.49
1:B:610:THR:OG1	1:B:613:GLU:HG3	2.13	0.49
1:A:379:PRO:O	1:A:383:GLU:HG3	2.13	0.49
1:B:441:ILE:HB	1:B:445:GLU:HB2	1.95	0.48
1:B:124:PRO:HG3	1:B:194:GLU:HG3	1.96	0.48
1:B:666:HIS:H	1:B:667:ARG:NH2	2.09	0.48
1:A:333:PRO:HD3	1:A:343:TRP:CZ3	2.49	0.48
1:A:624:ILE:HD11	1:A:643:LEU:HB2	1.95	0.47
1:B:128:ASN:HA	1:B:130:ASP:OD2	2.15	0.47
1:A:246:MET:SD	1:A:254:LEU:HD12	2.54	0.47
1:B:281:ALA:HB1	1:B:285:GLN:HG3	1.96	0.47
1:A:452:GLU:HG3	1:A:514:ILE:HD12	1.94	0.47
1:A:592:ILE:H	1:A:592:ILE:CD1	2.21	0.47
1:A:320:MET:HG2	5:A:1352:HOH:O	2.15	0.47
1:A:41:ARG:HD3	1:A:41:ARG:N	2.29	0.47
1:A:545:ALA:CB	1:A:624:ILE:HD12	2.44	0.47
1:A:406:LEU:O	1:A:409:LEU:HD22	2.14	0.47
1:B:333:PRO:HD3	1:B:343:TRP:CZ3	2.50	0.47
1:A:217:ILE:C	1:A:218:TYR:HD1	2.18	0.47
1:A:545:ALA:HB1	1:A:624:ILE:CD1	2.45	0.47
1:B:595:PRO:HD2	1:B:598:GLU:CD	2.35	0.46
2:B:800:HEM:HBA1	3:B:801:DDJ:HAQB	1.97	0.46
1:A:21:LYS:HG3	1:A:22:SER:N	2.30	0.46
1:A:441:ILE:H	1:A:441:ILE:CD1	2.28	0.46
1:B:302:MET:N	5:B:926:HOH:O	2.49	0.46
1:A:246:MET:SD	1:A:254:LEU:CD1	3.04	0.46
1:A:610:THR:OG1	1:A:613:GLU:HG3	2.16	0.45
1:A:145:GLN:HG2	5:A:1269:HOH:O	2.16	0.45
1:A:451:GLU:HG2	1:A:455:ASP:OD2	2.15	0.45
1:B:332:GLU:OE2	1:B:346:LYS:HE3	2.17	0.45
1:A:193:PHE:O	1:A:194:GLU:HB2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:TRP:CD1	1:A:96:HIS:HD2	2.34	0.45
1:A:99:GLY:O	1:A:218:TYR:CE1	2.69	0.45
1:B:52:TYR:HB3	1:B:176:GLU:HG3	1.97	0.45
1:A:137:LEU:HB3	1:A:138:PRO:HD3	1.98	0.45
1:A:217:ILE:HG22	1:A:218:TYR:HE1	1.73	0.45
1:B:460:VAL:HG13	1:B:541:ALA:HB1	1.98	0.45
1:A:727:ARG:HH11	1:A:727:ARG:CA	2.21	0.44
1:B:307:ILE:CG2	1:B:367:MET:HE1	2.46	0.44
1:A:450:LYS:HG3	1:A:540:ALA:HB2	1.99	0.44
1:B:514:ILE:HA	1:B:517:GLU:CD	2.37	0.44
1:B:518:PHE:O	1:B:522:ARG:HG2	2.17	0.44
1:A:92:ARG:HG3	4:A:802:CYN:N	2.33	0.44
1:A:322:TYR:CE1	1:A:368:MET:HE1	2.53	0.44
1:A:313:GLN:HA	1:A:354:VAL:HG22	2.00	0.44
1:B:217:ILE:C	1:B:218:TYR:HD1	2.21	0.44
1:B:67:ASP:HB3	1:B:139:ILE:CD1	2.48	0.44
1:A:218:TYR:CE2	1:A:244:MET:SD	3.09	0.44
1:A:246:MET:CE	1:A:254:LEU:CD1	2.85	0.43
1:B:628:TYR:CE1	1:B:629:GLN:HG3	2.52	0.43
1:A:368:MET:HE3	1:A:372:ASP:OD2	2.18	0.43
1:B:217:ILE:HG22	1:B:218:TYR:HE1	1.76	0.43
1:B:368:MET:HG3	1:B:372:ASP:CB	2.47	0.43
1:B:593:THR:H	1:B:594:ARG:HH21	1.66	0.43
1:A:41:ARG:HD2	1:B:41:ARG:NE	2.33	0.43
1:A:128:ASN:HA	1:A:130:ASP:OD2	2.17	0.43
1:A:246:MET:HE3	1:A:250:GLU:HB3	2.01	0.43
1:B:352:ASN:HB3	1:B:363:LYS:HB2	2.01	0.43
1:A:594:ARG:HE	1:A:594:ARG:N	2.06	0.43
1:A:19:ARG:HD3	1:A:19:ARG:N	2.33	0.43
1:A:21:LYS:NZ	1:A:21:LYS:CB	2.82	0.43
1:B:122:SER:HB3	1:B:277:GLU:HG3	2.01	0.43
1:A:32:ASN:HD21	1:A:34:GLU:HB2	1.84	0.42
1:A:283:ILE:HD12	1:B:687:LEU:CB	2.48	0.42
1:B:221:PRO:HG3	3:B:801:DDJ:CAI	2.49	0.42
1:A:35:ILE:CD1	1:A:36:LEU:HG	2.48	0.42
1:A:696:ARG:O	1:A:700:GLU:HG3	2.19	0.42
1:B:43:VAL:HG23	1:B:179:PHE:HB2	2.02	0.42
1:A:578:LYS:HA	1:A:579:PRO:HD3	1.85	0.42
1:B:189:PRO:HG3	1:B:206:GLN:HE22	1.85	0.42
1:A:286:GLN:NE2	1:B:690:GLY:HA3	2.35	0.42
1:B:42:ASP:HB2	1:B:48:ASP:OD1	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:LEU:HD13	1:B:484:ASN:ND2	2.35	0.42
3:B:801:DDJ:HAI	3:B:801:DDJ:HAD	1.81	0.42
1:B:264:VAL:HG22	1:B:309:GLY:O	2.20	0.42
1:B:587:TYR:O	1:B:588:ILE:HD13	2.20	0.42
1:A:587:TYR:OH	1:A:589:GLN:HG2	2.20	0.41
1:B:95:TRP:CD1	1:B:96:HIS:HD2	2.38	0.41
1:B:335:LYS:HE3	1:B:339:GLY:O	2.19	0.41
1:B:667:ARG:HE	1:B:667:ARG:N	2.18	0.41
1:B:137:LEU:HB3	1:B:138:PRO:HD3	2.01	0.41
1:A:264:VAL:HG12	2:A:800:HEM:CAA	2.50	0.41
1:A:475:ARG:HB2	1:A:606:LEU:HD22	2.00	0.41
1:B:274:LEU:HD21	1:B:303:ILE:HB	2.02	0.41
1:A:368:MET:CE	1:A:372:ASP:CB	2.98	0.41
1:B:96:HIS:HE1	3:B:801:DDJ:OAC	2.03	0.41
1:B:218:TYR:CE1	1:B:244:MET:SD	3.13	0.41
1:B:124:PRO:HG3	1:B:194:GLU:CG	2.50	0.41
1:A:283:ILE:HD11	1:B:687:LEU:C	2.40	0.41
1:B:21:LYS:HD3	1:B:26:TRP:CE2	2.54	0.41
1:A:218:TYR:CE1	1:A:244:MET:SD	3.12	0.41
1:A:308:GLU:H	1:A:342:GLN:NE2	2.17	0.41
1:B:129:LEU:HD23	1:B:129:LEU:HA	1.89	0.41
1:B:419:GLY:HA3	5:B:920:HOH:O	2.20	0.41
1:A:249:LYS:HG2	1:A:398:ASN:OD1	2.21	0.41
1:A:286:GLN:HE22	1:B:690:GLY:HA3	1.86	0.41
1:B:638:ASP:OD2	1:B:639:GLU:HG3	2.21	0.41
1:A:685:ILE:CD1	1:A:685:ILE:N	2.84	0.41
1:A:217:ILE:C	1:A:218:TYR:CD1	2.94	0.40
1:A:249:LYS:CB	1:A:249:LYS:NZ	2.85	0.40
1:A:35:ILE:CD1	1:A:36:LEU:N	2.77	0.40
1:A:368:MET:CE	1:A:372:ASP:CG	2.90	0.40
1:A:311:TRP:CD1	1:A:368:MET:HE3	2.54	0.40
1:B:264:VAL:HG12	2:B:800:HEM:CAA	2.52	0.40
1:B:323:ILE:N	1:B:323:ILE:CD1	2.84	0.40
1:B:406:LEU:O	1:B:409:LEU:HD22	2.20	0.40
1:B:441:ILE:HD11	1:B:559:PRO:HB3	2.03	0.40
1:B:664:SER:OG	1:B:667:ARG:HB2	2.22	0.40
1:A:240:THR:O	1:A:244:MET:HG3	2.21	0.40
1:B:672:ASP:HB3	1:B:675:THR:OG1	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	702/737 (95%)	688 (98%)	13 (2%)	1 (0%)	51	33
1	B	701/737 (95%)	683 (97%)	16 (2%)	2 (0%)	41	24
All	All	1403/1474 (95%)	1371 (98%)	29 (2%)	3 (0%)	47	30

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	49	ASP
1	A	47	GLU
1	B	592	ILE

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	585/608 (96%)	564 (96%)	21 (4%)	35	16
1	B	584/608 (96%)	569 (97%)	15 (3%)	46	28
All	All	1169/1216 (96%)	1133 (97%)	36 (3%)	40	21

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	19	ARG
1	A	21	LYS
1	A	32	ASN

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Mol	Chain	Res	Type
1	A	35	ILE
1	A	41	ARG
1	A	50	PHE
1	A	57	GLN
1	A	102	ARG
1	A	125	ASP
1	A	206	GLN
1	A	272	GLU
1	A	283	ILE
1	A	335	LYS
1	A	367	MET
1	A	409	LEU
1	A	441	ILE
1	A	586	ASN
1	A	592	ILE
1	A	594	ARG
1	A	657	GLU
1	A	677	GLU
1	B	19	ARG
1	B	41	ARG
1	B	51	ASP
1	B	69	GLU
1	B	102	ARG
1	B	125	ASP
1	B	181	GLU
1	B	285	GLN
1	B	409	LEU
1	B	441	ILE
1	B	554	GLU
1	B	586	ASN
1	B	594	ARG
1	B	667	ARG
1	B	730	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	GLN
1	A	32	ASN
1	A	206	GLN
1	A	286	GLN
1	A	342	GLN

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Mol	Chain	Res	Type
1	A	513	ASN
1	A	515	GLN
1	A	519	ASN
1	A	568	HIS
1	A	586	ASN
1	A	589	GLN
1	A	608	ASN
1	A	666	HIS
1	A	692	ASN
1	B	38	GLN
1	B	206	GLN
1	B	286	GLN
1	B	342	GLN
1	B	352	ASN
1	B	358	HIS
1	B	513	ASN
1	B	515	GLN
1	B	519	ASN
1	B	544	GLN
1	B	586	ASN
1	B	692	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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	#$|Z| > 2$
3	DDJ	A	801	-	19,19,19	1.07	1 (5%)	26,26,26	3.09	7 (26%)
4	CYN	B	802	2	0,1,1	-	-	-		
4	CYN	A	802	-	0,1,1	-	-	-		
2	HEM	B	800	1,4	41,50,50	1.95	12 (29%)	45,82,82	5.90	27 (60%)
2	HEM	A	800	1	41,50,50	1.83	10 (24%)	45,82,82	3.37	19 (42%)
3	DDJ	B	801	-	19,19,19	1.08	1 (5%)	26,26,26	3.03	6 (23%)

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	DDJ	B	801	-	-	4/8/8/8	0/2/2/2
2	HEM	B	800	1,4	-	4/12/54/54	-
2	HEM	A	800	1	-	3/12/54/54	-
3	DDJ	A	801	-	-	4/8/8/8	0/2/2/2

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	HEM	CBB-CAB	5.00	1.55	1.30
2	A	800	HEM	CBB-CAB	4.99	1.55	1.30
2	B	800	HEM	C3C-C2C	-4.45	1.34	1.40
2	A	800	HEM	C3C-C2C	-4.22	1.34	1.40
2	B	800	HEM	CBA-CGA	-4.19	1.40	1.50
2	B	800	HEM	CBD-CGD	-4.05	1.41	1.50
2	B	800	HEM	CBC-CAC	4.03	1.56	1.29
3	A	801	DDJ	CAL-CAH	-3.84	1.39	1.49
3	B	801	DDJ	CAL-CAH	-3.84	1.39	1.49
2	A	800	HEM	CBC-CAC	3.83	1.54	1.29
2	A	800	HEM	CBA-CGA	-3.71	1.42	1.50
2	A	800	HEM	CBD-CGD	-3.47	1.42	1.50
2	B	800	HEM	FE-ND	2.80	2.10	1.96
2	B	800	HEM	C3C-CAC	2.67	1.53	1.47
2	A	800	HEM	C3C-CAC	2.64	1.53	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	800	HEM	CBD-CAD	2.35	1.59	1.52
2	A	800	HEM	O1A-CGA	2.34	1.29	1.22
2	A	800	HEM	CBD-CAD	2.32	1.59	1.52
2	B	800	HEM	C4D-ND	-2.32	1.36	1.40
2	A	800	HEM	C4D-ND	-2.24	1.36	1.40
2	B	800	HEM	O1A-CGA	2.21	1.29	1.22
2	B	800	HEM	FE-NB	2.07	2.07	1.96
2	A	800	HEM	CHA-C4D	2.04	1.40	1.35
2	B	800	HEM	CHA-C4D	2.04	1.40	1.35

All (59) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	800	HEM	C4C-CHD-C1D	16.11	143.82	122.56
2	B	800	HEM	C4B-CHC-C1C	14.80	142.10	122.56
2	B	800	HEM	CHD-C1D-ND	-11.45	111.99	124.43
2	A	800	HEM	C4B-CHC-C1C	10.86	136.89	122.56
2	B	800	HEM	C4A-C3A-C2A	-10.49	99.70	107.00
2	B	800	HEM	C1D-C2D-C3D	-10.14	96.30	106.96
2	B	800	HEM	CHC-C4B-NB	-9.69	113.91	124.43
3	A	801	DDJ	OAC-CAF-CAG	9.10	120.07	114.05
3	A	801	DDJ	OAB-CAK-CAM	9.06	120.03	114.05
3	B	801	DDJ	OAB-CAK-CAM	9.00	119.99	114.05
2	B	800	HEM	CHB-C1B-NB	-8.60	113.75	124.38
3	B	801	DDJ	OAC-CAF-CAG	8.59	119.73	114.05
2	A	800	HEM	C4A-C3A-C2A	-8.45	101.12	107.00
2	B	800	HEM	C2D-C1D-ND	8.17	119.67	109.88
2	B	800	HEM	CHA-C4D-ND	-8.16	114.30	124.38
2	A	800	HEM	CHB-C1B-NB	-7.09	115.62	124.38
2	B	800	HEM	C2C-C3C-C4C	6.81	111.66	106.90
2	A	800	HEM	CHC-C4B-NB	-6.32	117.56	124.43
2	B	800	HEM	CHA-C4D-C3D	6.18	136.92	125.33
2	B	800	HEM	CMC-C2C-C3C	6.14	136.17	124.68
2	A	800	HEM	C2C-C3C-C4C	5.85	110.98	106.90
2	B	800	HEM	CHC-C4B-C3B	5.49	132.98	124.57
2	B	800	HEM	C2B-C1B-NB	5.34	116.16	109.84
3	B	801	DDJ	CAQ-OAC-CAF	-5.26	109.58	117.53
2	B	800	HEM	CBA-CAA-C2A	5.24	121.56	112.62
2	B	800	HEM	C4D-C3D-C2D	5.17	114.43	106.90
2	B	800	HEM	CAD-C3D-C4D	-5.16	115.64	124.66
3	A	801	DDJ	CAP-OAB-CAK	-5.13	109.79	117.53
3	B	801	DDJ	CAP-OAB-CAK	-5.07	109.88	117.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	800	HEM	C3B-C2B-C1B	-5.02	102.76	106.49
2	B	800	HEM	CMD-C2D-C1D	4.89	132.49	125.04
2	A	800	HEM	C2B-C1B-NB	4.86	115.60	109.84
3	A	801	DDJ	CAQ-OAC-CAF	-4.76	110.34	117.53
2	A	800	HEM	C3B-C2B-C1B	-4.65	103.03	106.49
2	B	800	HEM	O2D-CGD-O1D	-4.52	112.03	123.30
2	B	800	HEM	O2D-CGD-CBD	4.50	128.50	114.03
2	B	800	HEM	C1B-NB-C4B	-4.27	100.67	105.07
2	A	800	HEM	CBA-CAA-C2A	4.21	119.81	112.62
2	B	800	HEM	CMA-C3A-C4A	4.02	134.65	128.46
2	A	800	HEM	CAA-CBA-CGA	-3.93	102.74	113.76
2	A	800	HEM	CMA-C3A-C2A	3.80	132.11	124.94
2	B	800	HEM	C4D-ND-C1D	-3.80	101.15	105.07
2	A	800	HEM	C1B-NB-C4B	-3.78	101.17	105.07
2	A	800	HEM	CMC-C2C-C3C	3.77	131.74	124.68
2	A	800	HEM	C4C-CHD-C1D	3.62	127.33	122.56
2	A	800	HEM	CHC-C4B-C3B	3.48	129.90	124.57
2	A	800	HEM	O2D-CGD-CBD	3.01	123.70	114.03
2	A	800	HEM	O2A-CGA-O1A	-2.89	116.11	123.30
2	B	800	HEM	C3C-C4C-NC	-2.87	105.53	110.94
2	B	800	HEM	CAA-CBA-CGA	-2.85	105.76	113.76
2	A	800	HEM	C3C-C4C-NC	-2.52	106.19	110.94
3	A	801	DDJ	OAC-CAF-CAE	-2.47	119.88	124.12
3	A	801	DDJ	OAB-CAK-CAD	-2.38	120.03	124.12
3	B	801	DDJ	OAB-CAK-CAD	-2.37	120.03	124.12
3	B	801	DDJ	OAC-CAF-CAE	-2.28	120.19	124.12
2	A	800	HEM	O1D-CGD-CBD	-2.06	116.47	123.08
2	A	800	HEM	CMB-C2B-C3B	2.04	133.30	128.30
2	B	800	HEM	CHD-C1D-C2D	2.03	128.15	124.98
3	A	801	DDJ	CAN-CAM-CAK	2.01	119.99	118.25

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	801	DDJ	CAM-CAK-OAB-CAP
3	B	801	DDJ	CAM-CAK-OAB-CAP
3	B	801	DDJ	CAG-CAF-OAC-CAQ
3	A	801	DDJ	CAE-CAF-OAC-CAQ
3	B	801	DDJ	CAD-CAK-OAB-CAP
3	A	801	DDJ	CAD-CAK-OAB-CAP
3	A	801	DDJ	CAG-CAF-OAC-CAQ

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Mol	Chain	Res	Type	Atoms
3	B	801	DDJ	CAE-CAF-OAC-CAQ
2	A	800	HEM	C2B-C3B-CAB-CBB
2	B	800	HEM	CAA-CBA-CGA-O1A
2	B	800	HEM	CAA-CBA-CGA-O2A
2	A	800	HEM	CAA-CBA-CGA-O1A
2	A	800	HEM	CAA-CBA-CGA-O2A
2	B	800	HEM	CAD-CBD-CGD-O2D
2	B	800	HEM	CAD-CBD-CGD-O1D

There are no ring outliers.

5 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	801	DDJ	5	0
4	A	802	CYN	3	0
2	B	800	HEM	2	0
2	A	800	HEM	1	0
3	B	801	DDJ	9	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 800

Bond lengths

Bond angles

Torsions

Rings

Ligand HEM A 800

Bond lengths

Bond angles

Torsions

Rings
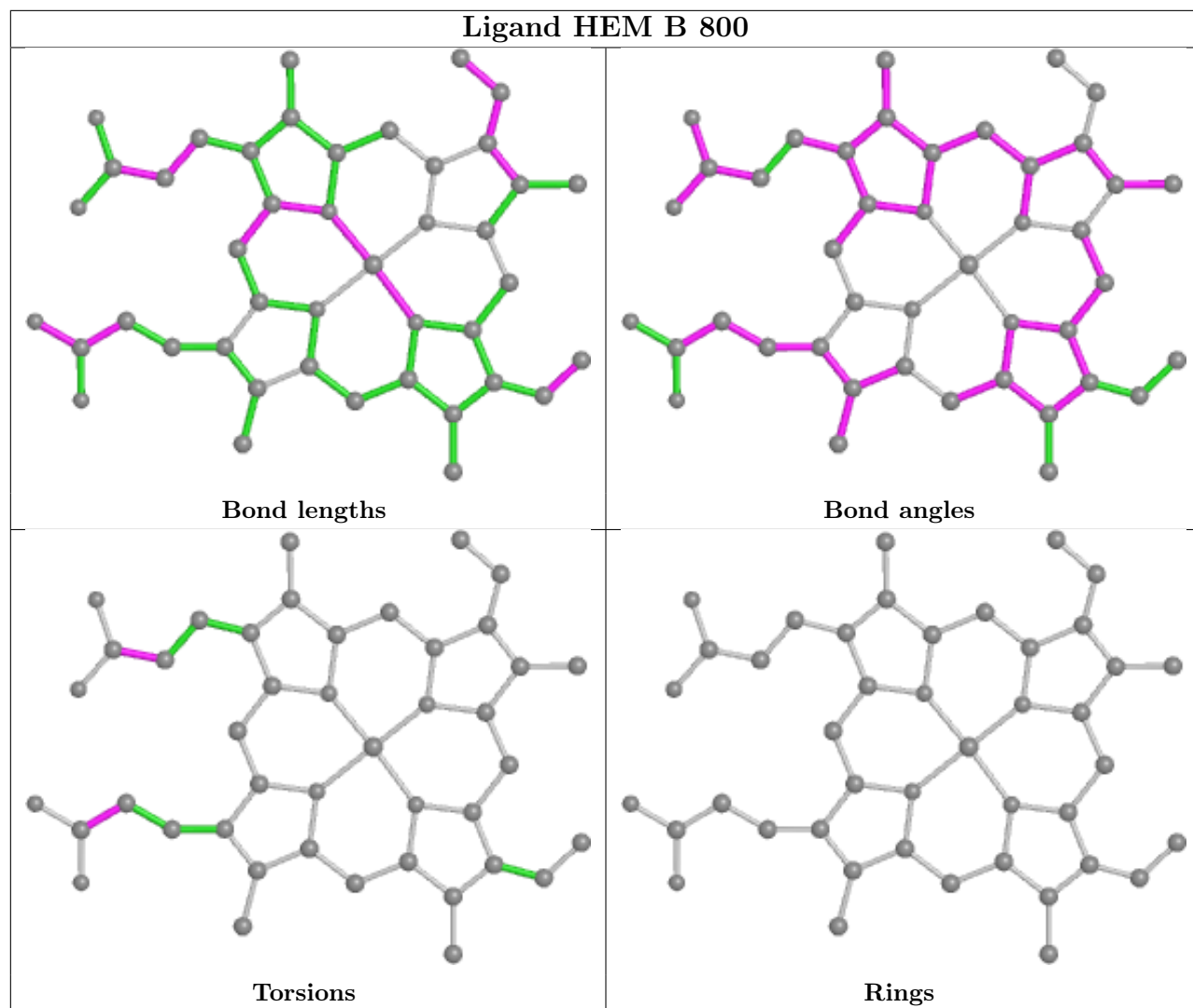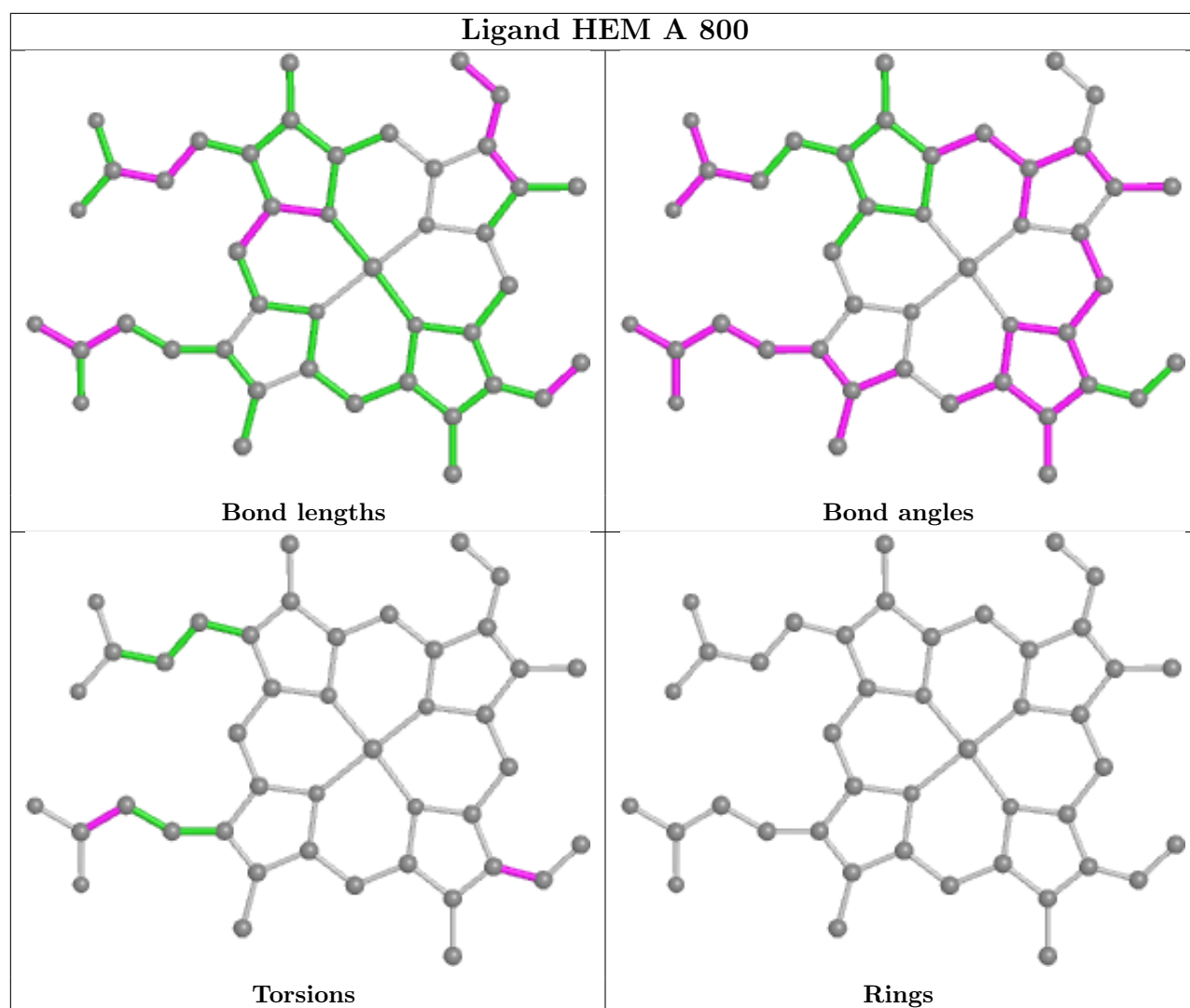
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	706/737 (95%)	0.56	69 (9%)	7	8	11, 19, 40, 62	0
1	B	705/737 (95%)	0.70	74 (10%)	6	7	15, 25, 42, 64	0
All	All	1411/1474 (95%)	0.63	143 (10%)	7	8	11, 22, 41, 64	0

All (143) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	50	PHE	15.8
1	A	50	PHE	14.9
1	B	730	LEU	14.6
1	A	730	LEU	13.3
1	B	18	LYS	10.9
1	A	19	ARG	10.5
1	A	49	ASP	9.6
1	A	731	GLU	9.4
1	B	20	PRO	9.0
1	A	20	PRO	8.4
1	A	523	SER	8.2
1	A	48	ASP	7.6
1	B	19	ARG	7.4
1	A	591	ASP	7.3
1	A	18	LYS	7.3
1	B	729	ASP	7.2
1	B	48	ASP	7.1
1	B	523	SER	6.8
1	B	43	VAL	6.6
1	B	361	ASP	6.5
1	B	49	ASP	6.5
1	B	591	ASP	6.4
1	A	729	ASP	6.4
1	B	437	ASP	6.4

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Mol	Chain	Res	Type	RSRZ
1	B	663	ASP	5.8
1	A	437	ASP	5.5
1	B	349	GLU	5.2
1	A	524	ASP	5.2
1	B	200	ASP	5.2
1	A	21	LYS	5.0
1	B	638	ASP	4.8
1	A	663	ASP	4.8
1	B	731	GLU	4.7
1	B	457	ASP	4.6
1	B	292	ASN	4.5
1	B	42	ASP	4.4
1	A	218	TYR	4.3
1	B	21	LYS	4.3
1	B	360	PRO	4.3
1	B	47	GLU	4.2
1	A	525	GLY	4.2
1	A	590	ASP	4.0
1	B	348	GLU	4.0
1	A	348	GLU	4.0
1	B	218	TYR	3.9
1	A	349	GLU	3.8
1	A	191	ASP	3.8
1	B	677	GLU	3.8
1	A	593	THR	3.7
1	B	662	ALA	3.7
1	A	522	ARG	3.7
1	B	191	ASP	3.6
1	A	347	SER	3.6
1	B	22	SER	3.6
1	A	665	GLU	3.6
1	B	347	SER	3.5
1	B	524	ASP	3.5
1	A	41	ARG	3.5
1	A	517	GLU	3.4
1	A	24	GLN	3.4
1	A	552	ASP	3.4
1	A	706	ASP	3.3
1	A	42	ASP	3.3
1	A	727	ARG	3.3
1	B	590	ASP	3.3
1	A	454	LEU	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	457	ASP	3.2
1	A	51	ASP	3.2
1	A	271	GLU	3.1
1	B	54	GLU	3.1
1	A	520	ASP	3.1
1	B	727	ARG	3.0
1	B	552	ASP	3.0
1	B	632	ASP	3.0
1	B	24	GLN	3.0
1	A	272	GLU	3.0
1	B	517	GLU	2.9
1	B	455	ASP	2.9
1	B	706	ASP	2.9
1	A	558	GLU	2.9
1	B	346	LYS	2.8
1	A	444	GLU	2.8
1	B	639	GLU	2.8
1	A	95	TRP	2.8
1	B	201	GLU	2.7
1	B	362	GLU	2.7
1	B	674	ASP	2.7
1	B	25	ASP	2.7
1	B	665	GLU	2.7
1	A	592	ILE	2.7
1	A	440	LEU	2.7
1	A	54	GLU	2.7
1	B	359	ASP	2.7
1	B	28	PRO	2.7
1	B	207	GLU	2.6
1	B	383	GLU	2.6
1	B	593	THR	2.6
1	B	208	GLY	2.5
1	A	47	GLU	2.5
1	A	361	ASP	2.5
1	B	558	GLU	2.5
1	A	246	MET	2.5
1	A	455	ASP	2.5
1	B	451	GLU	2.5
1	A	521	SER	2.5
1	A	91	ILE	2.5
1	B	255	ILE	2.5
1	A	632	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	439	ASP	2.4
1	B	271	GLU	2.4
1	B	444	GLU	2.4
1	B	95	TRP	2.4
1	B	397	MET	2.4
1	B	34	GLU	2.4
1	B	202	PRO	2.3
1	A	581	VAL	2.3
1	B	554	GLU	2.3
1	A	129	LEU	2.3
1	B	41	ARG	2.2
1	B	503	GLN	2.2
1	A	46	VAL	2.2
1	A	451	GLU	2.2
1	A	35	ILE	2.2
1	A	94	ALA	2.2
1	A	657	GLU	2.2
1	B	313	GLN	2.1
1	A	301	GLU	2.1
1	A	639	GLU	2.1
1	B	505	GLU	2.1
1	B	46	VAL	2.1
1	A	34	GLU	2.1
1	A	554	GLU	2.1
1	B	145	GLN	2.1
1	A	435	ASP	2.1
1	A	255	ILE	2.1
1	B	667	ARG	2.0
1	B	51	ASP	2.0
1	A	43	VAL	2.0
1	A	728	PHE	2.0
1	A	176	GLU	2.0
1	B	502	GLU	2.0
1	A	200	ASP	2.0
1	A	390	GLU	2.0

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

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

6.3 Carbohydrates (i)

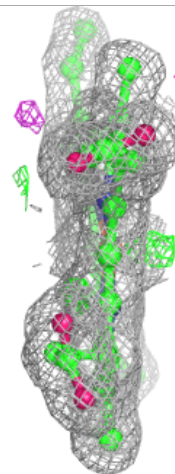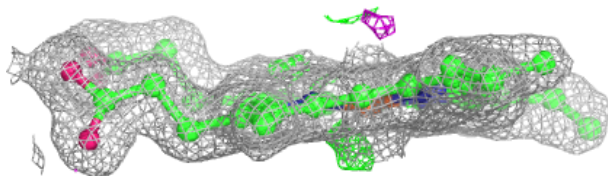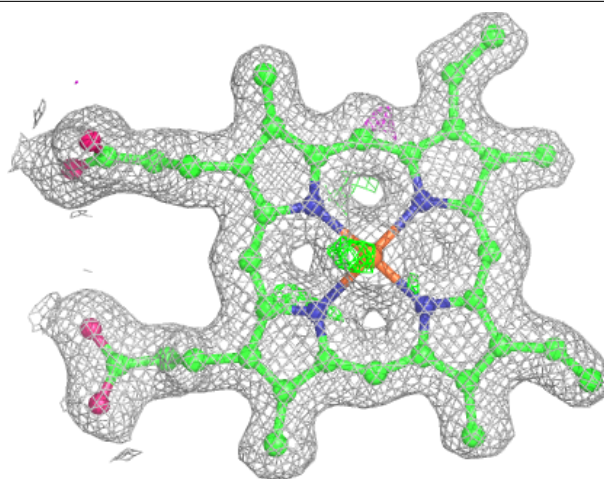There are no monosaccharides in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.
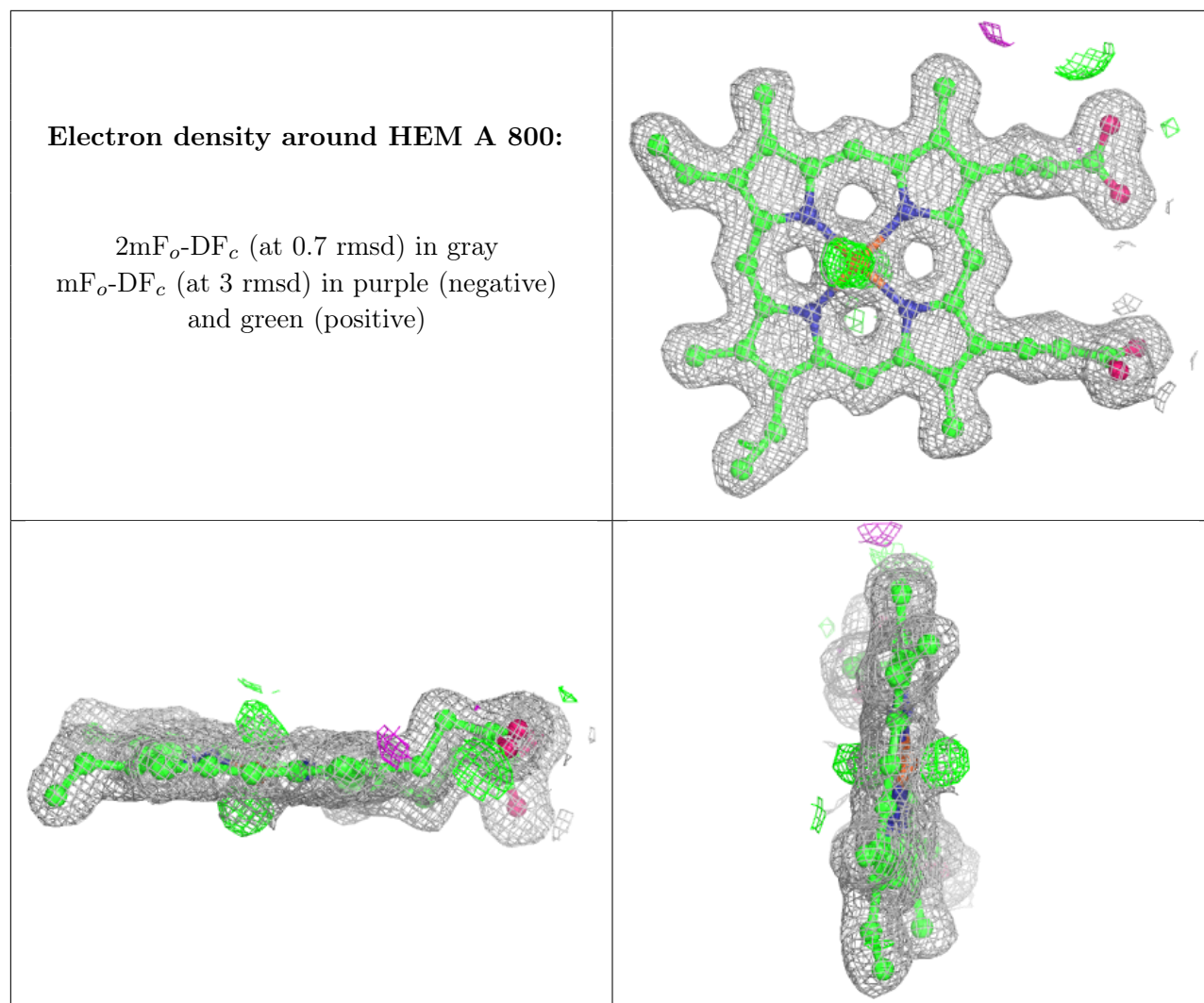
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	DDJ	B	801	18/18	-0.05	0.97	58,58,58,59	18
3	DDJ	A	801	18/18	0.21	0.84	57,58,58,58	18
4	CYN	A	802	2/2	0.43	0.46	34,34,34,36	0
4	CYN	B	802	2/2	0.85	0.19	34,34,34,36	0
2	HEM	B	800	43/43	0.98	0.14	16,18,20,23	0
2	HEM	A	800	43/43	0.99	0.13	8,11,13,16	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 B 800:

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

Electron density around HEM A 800:

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

6.5　Other polymers ⓘ

There are no such residues in this entry.