



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:21 PM UTC

PDB ID : 1F4J / pdb_00001f4j
Title : STRUCTURE OF TETRAGONAL CRYSTALS OF HUMAN ERYTHROCYTE CATALASE
Authors : Safo, M.K.; Musayev, F.N.; Wu, S.H.; Abraham, D.J.; Ko, T.P.
Deposited on : 2000-06-07
Resolution : 2.40 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

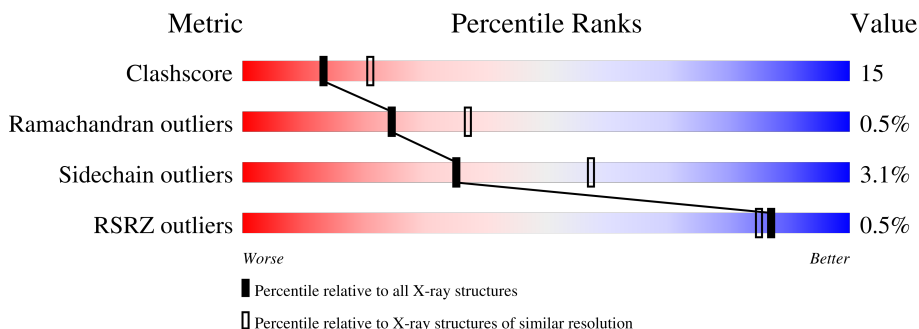
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 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))
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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	527	
1	B	527	
1	C	527	
1	D	527	

2 Entry composition [i](#)

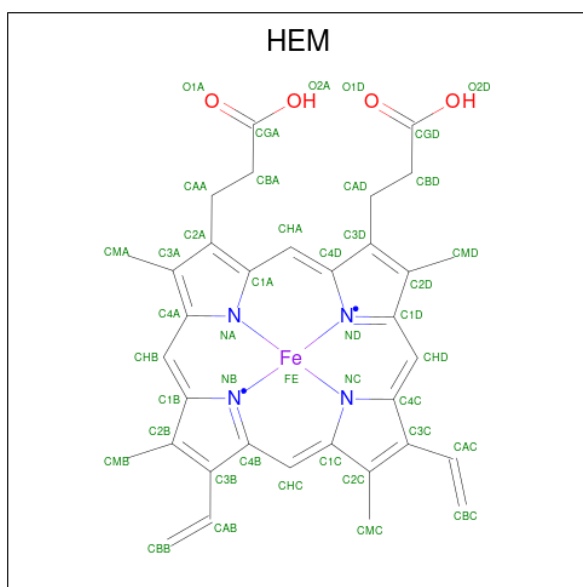
There are 3 unique types of molecules in this entry. The entry contains 16813 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	479	Total	C	N	O	S	0	0	0
			3845	2450	677	706	12			
1	B	479	Total	C	N	O	S	0	0	0
			3849	2452	677	708	12			
1	C	481	Total	C	N	O	S	0	0	0
			3863	2461	680	710	12			
1	D	479	Total	C	N	O	S	0	0	0
			3845	2450	677	706	12			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: 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		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
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		

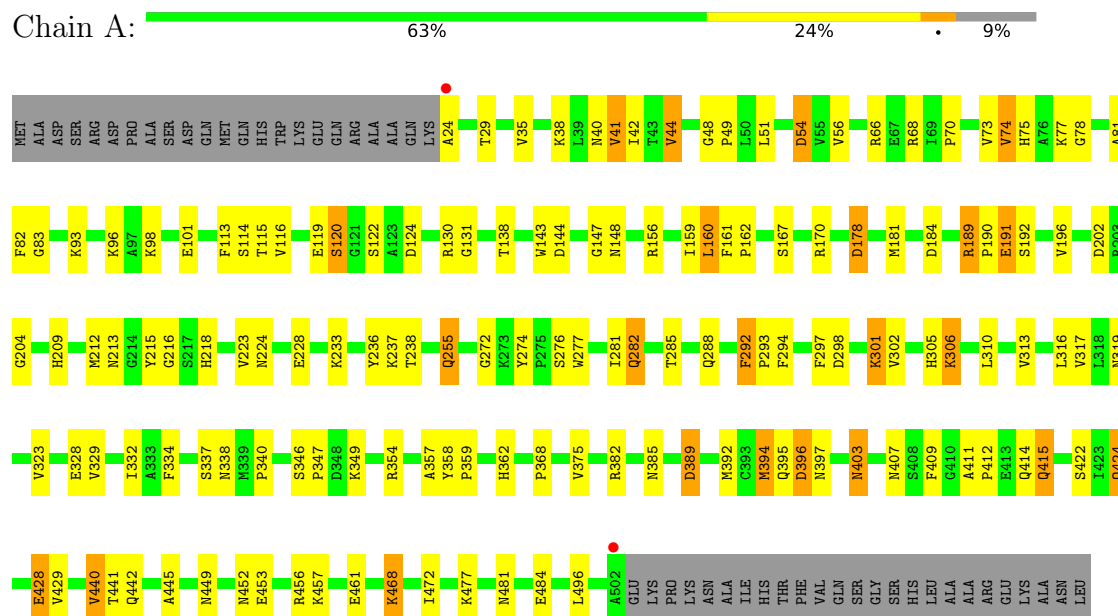
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	318	Total	O	0	0
			318	318		
3	B	312	Total	O	0	0
			312	312		
3	C	295	Total	O	0	0
			295	295		
3	D	314	Total	O	0	0
			314	314		

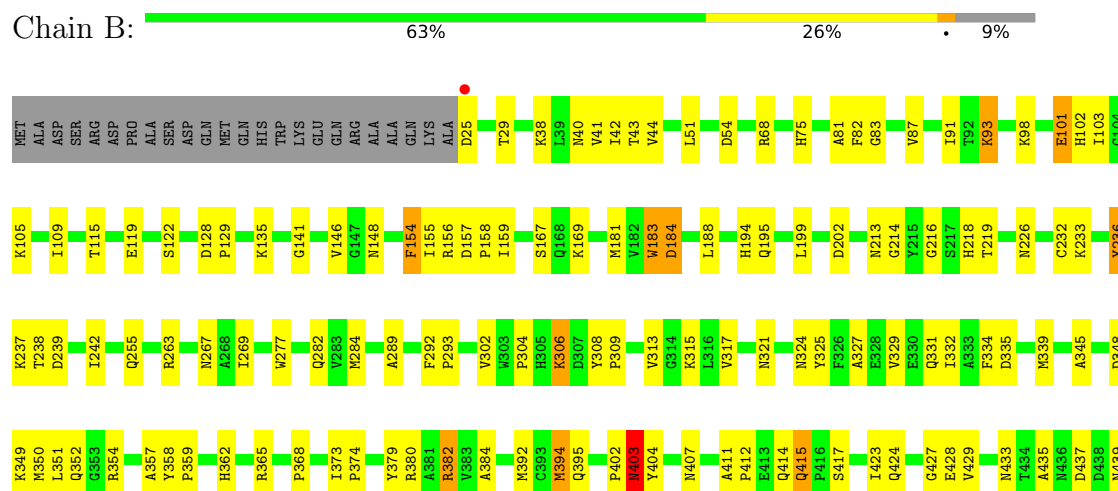
3 Residue-property plots

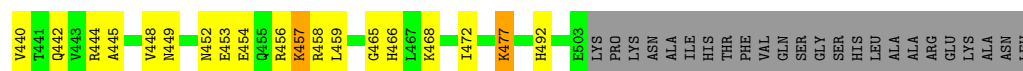
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

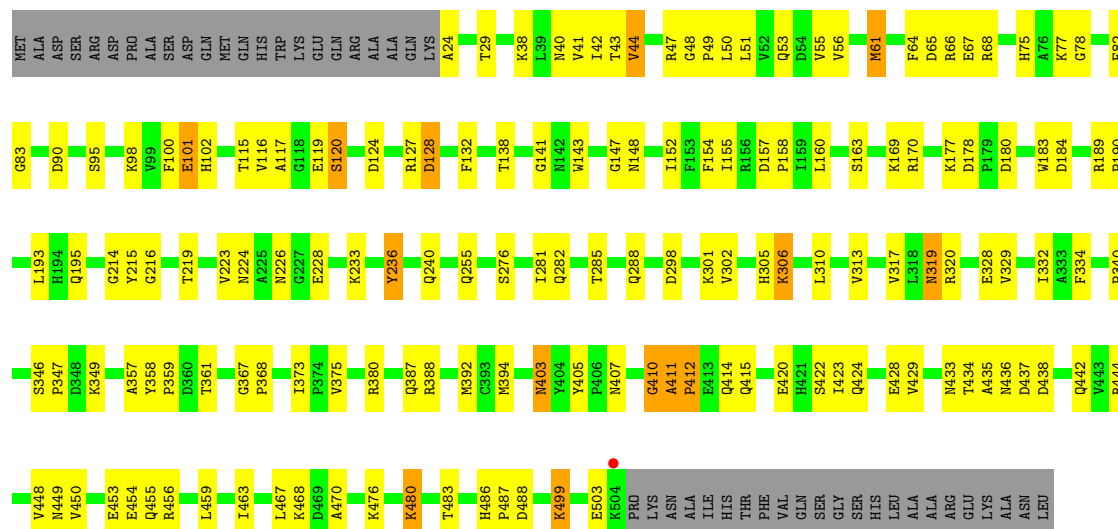


• Molecule 1: CATALASE

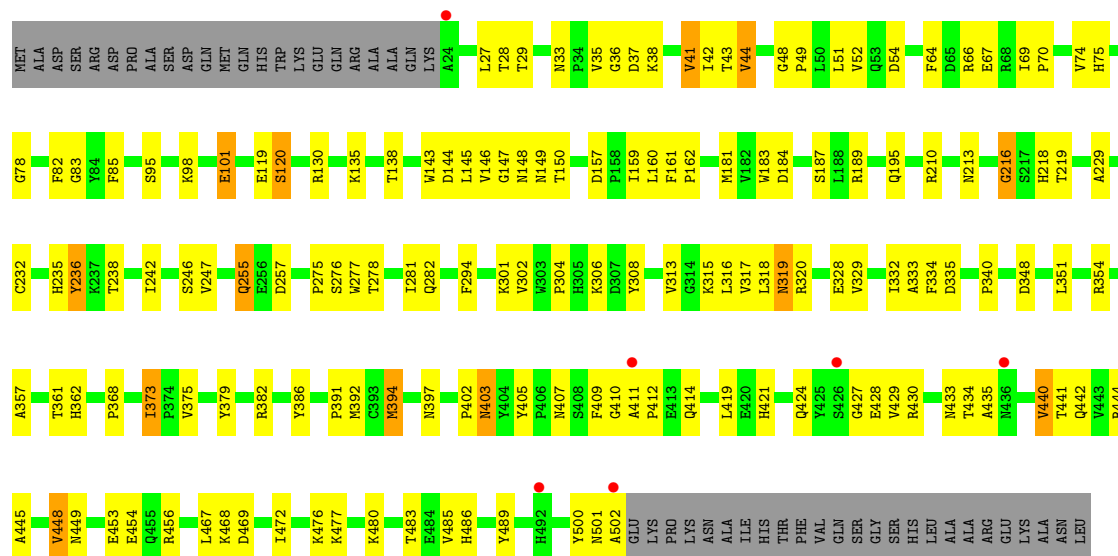




• Molecule 1: CATALASE



• Molecule 1: CATALASE



4 Data and refinement statistics

Property	Value	Source
Space group	I 41	Depositor
Cell constants a, b, c, α , β , γ	203.60Å 203.60Å 144.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	204.00 – 2.40 143.97 – 2.40	Depositor EDS
% Data completeness (in resolution range)	93.8 (204.00-2.40) 93.8 (143.97-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.55 (at 2.40Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.196 , 0.244 0.196 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	33.3	Xtriage
Anisotropy	0.338	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 58.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.017 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	16813	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% 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: 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	0.49	0/3960	1.05	28/5384 (0.5%)
1	B	0.50	0/3964	1.01	20/5389 (0.4%)
1	C	0.49	1/3978 (0.0%)	1.01	19/5407 (0.4%)
1	D	0.51	0/3960	1.03	23/5384 (0.4%)
All	All	0.50	1/15862 (0.0%)	1.03	90/21564 (0.4%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	61	MET	SD-CE	-5.80	1.65	1.79

All (90) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	216	GLY	N-CA-C	-8.45	104.18	114.66
1	B	216	GLY	N-CA-C	-8.44	104.19	114.66
1	A	216	GLY	N-CA-C	-8.12	104.59	114.66
1	C	450	VAL	N-CA-C	8.02	118.78	110.36
1	A	440	VAL	N-CA-C	8.00	117.94	111.62
1	D	308	TYR	CA-C-N	7.94	127.99	119.89
1	D	308	TYR	C-N-CA	7.94	127.99	119.89
1	C	116	VAL	N-CA-C	7.38	118.42	111.48
1	A	29	THR	N-CA-C	-7.38	98.93	110.36
1	B	379	TYR	N-CA-C	7.34	120.34	111.82
1	C	78	GLY	N-CA-C	7.34	121.82	111.10
1	A	292	PHE	CA-C-N	7.32	127.33	119.28
1	A	292	PHE	C-N-CA	7.32	127.33	119.28
1	D	448	VAL	N-CA-C	7.27	118.92	111.00
1	C	189	ARG	CA-C-N	7.21	126.91	119.56
1	C	189	ARG	C-N-CA	7.21	126.91	119.56

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	216	GLY	N-CA-C	-6.98	104.77	115.66
1	B	437	ASP	N-CA-C	-6.83	102.01	110.41
1	D	184	ASP	N-CA-C	-6.77	103.52	111.03
1	A	472	ILE	N-CA-C	6.70	117.45	110.62
1	A	357	ALA	N-CA-C	6.64	119.36	111.33
1	D	394	MET	N-CA-C	6.62	121.58	112.90
1	D	189	ARG	CA-C-N	6.56	126.25	119.56
1	D	189	ARG	C-N-CA	6.56	126.25	119.56
1	B	440	VAL	N-CA-C	6.36	119.75	113.71
1	C	152	ILE	N-CA-C	6.22	116.41	108.82
1	C	117	ALA	N-CA-C	6.20	117.83	111.14
1	C	56	VAL	N-CA-C	-6.19	104.48	110.42
1	A	389	ASP	CB-CA-C	-6.17	108.45	115.79
1	A	396	ASP	N-CA-C	-6.16	105.63	113.02
1	A	78	GLY	N-CA-C	6.14	120.07	111.10
1	B	357	ALA	N-CA-C	6.14	118.48	111.11
1	B	128	ASP	CA-C-N	-6.11	114.47	120.52
1	B	128	ASP	C-N-CA	-6.11	114.47	120.52
1	A	346	SER	N-CA-C	-6.08	103.01	110.31
1	D	257	ASP	CA-C-N	5.98	125.66	119.56
1	D	257	ASP	C-N-CA	5.98	125.66	119.56
1	B	184	ASP	N-CA-C	-5.93	104.73	111.07
1	A	68	ARG	N-CA-C	5.88	119.84	109.96
1	D	357	ALA	N-CA-C	5.86	118.14	111.11
1	D	379	TYR	N-CA-C	5.85	120.03	113.01
1	B	415	GLN	CA-C-N	5.85	127.15	119.84
1	B	415	GLN	C-N-CA	5.85	127.15	119.84
1	B	183	TRP	N-CA-C	5.84	118.60	111.82
1	C	410	GLY	N-CA-C	5.83	122.83	115.42
1	C	170	ARG	N-CA-C	5.81	118.69	110.50
1	D	440	VAL	N-CA-C	5.76	121.32	109.34
1	B	472	ILE	N-CA-C	5.71	116.44	110.62
1	A	178	ASP	CA-C-N	5.71	125.56	119.28
1	A	178	ASP	C-N-CA	5.71	125.56	119.28
1	A	170	ARG	N-CA-C	5.69	118.53	110.50
1	D	78	GLY	N-CA-C	5.66	119.55	111.12
1	A	191	GLU	N-CA-C	-5.64	106.10	112.87
1	C	437	ASP	N-CA-C	-5.63	103.49	110.41
1	A	415	GLN	CA-C-N	5.63	126.87	119.84
1	A	415	GLN	C-N-CA	5.63	126.87	119.84
1	C	178	ASP	CA-C-N	5.61	125.28	119.05
1	C	178	ASP	C-N-CA	5.61	125.28	119.05

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	422	SER	N-CA-C	5.58	118.34	109.24
1	D	69	ILE	CA-C-N	-5.58	113.97	119.99
1	D	69	ILE	C-N-CA	-5.58	113.97	119.99
1	A	394	MET	N-CA-C	5.56	120.07	113.28
1	B	403	ASN	N-CA-C	5.52	119.71	112.92
1	B	129	PRO	N-CA-C	-5.50	102.93	111.13
1	C	120	SER	N-CA-C	5.45	122.41	110.80
1	D	472	ILE	N-CA-C	5.45	117.86	111.05
1	B	29	THR	N-CA-C	-5.33	102.86	110.59
1	C	357	ALA	N-CA-C	5.33	117.50	111.11
1	A	282	GLN	N-CA-C	-5.26	101.12	109.59
1	B	122	SER	N-CA-C	5.21	116.81	110.41
1	D	219	THR	N-CA-C	-5.18	100.86	109.46
1	A	189	ARG	CA-C-N	5.17	124.89	119.82
1	A	189	ARG	C-N-CA	5.17	124.89	119.82
1	A	120	SER	N-CA-C	5.14	121.74	110.80
1	A	184	ASP	N-CA-C	-5.12	105.78	111.36
1	A	409	PHE	N-CA-C	5.12	117.43	110.88
1	A	54	ASP	N-CA-C	-5.10	101.97	109.62
1	B	440	VAL	CB-CA-C	-5.10	105.83	110.63
1	D	95	SER	N-CA-C	5.09	117.36	108.76
1	D	246	SER	N-CA-C	-5.09	103.32	110.50
1	B	325	TYR	N-CA-C	5.09	116.51	111.07
1	B	154	PHE	N-CA-C	5.08	117.72	111.82
1	C	184	ASP	N-CA-C	-5.06	105.65	111.07
1	D	29	THR	N-CA-C	-5.06	103.25	110.59
1	D	373	ILE	N-CA-C	-5.06	103.44	108.96
1	D	120	SER	N-CA-C	5.06	121.57	110.80
1	A	301	LYS	N-CA-C	5.05	117.47	109.50
1	C	436	ASN	N-CA-C	5.03	118.73	112.59
1	B	219	THR	N-CA-C	-5.02	101.13	109.46
1	C	29	THR	N-CA-C	-5.00	103.44	110.35

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	3845	0	3687	114	0
1	B	3849	0	3688	116	0
1	C	3863	0	3706	153	0
1	D	3845	0	3687	123	0
2	A	43	0	30	1	0
2	B	43	0	30	0	0
2	C	43	0	30	3	0
2	D	43	0	30	6	0
3	A	318	0	0	9	0
3	B	312	0	0	8	0
3	C	295	0	0	8	0
3	D	314	0	0	3	0
All	All	16813	0	14888	452	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 15.

All (452) 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:306:LYS:H	1:A:306:LYS:HD2	1.25	1.01
1:B:306:LYS:H	1:B:306:LYS:HD2	1.22	1.00
1:A:414:GLN:NE2	1:C:38:LYS:H	1.63	0.97
1:D:306:LYS:H	1:D:306:LYS:HD2	1.27	0.97
1:A:302:VAL:H	1:A:442:GLN:HE22	1.22	0.86
1:A:51:LEU:HD13	1:D:429:VAL:HG13	1.60	0.84
1:A:178:ASP:HB3	1:A:181:MET:HE2	1.58	0.84
1:B:407:ASN:HD21	1:B:411:ALA:HB3	1.42	0.83
1:B:402:PRO:HG2	1:B:411:ALA:HB2	1.61	0.83
1:A:306:LYS:H	1:A:306:LYS:CD	1.91	0.82
1:C:453:GLU:HA	1:C:456:ARG:NH1	1.94	0.81
1:A:407:ASN:HD21	1:A:411:ALA:HB3	1.47	0.80
1:A:428:GLU:HG3	3:A:867:HOH:O	1.82	0.79
1:B:382:ARG:HH11	1:B:382:ARG:HB2	1.48	0.79
1:B:255:GLN:HB2	1:C:255:GLN:HB2	1.65	0.79
1:C:380:ARG:HG3	1:C:380:ARG:HH11	1.48	0.78
1:A:392:MET:HB3	1:A:394:MET:HE3	1.65	0.78
1:B:302:VAL:H	1:B:442:GLN:HE22	1.32	0.77
1:C:444:ARG:O	1:C:448:VAL:HG12	1.84	0.76
1:A:394:MET:HG3	1:C:394:MET:SD	2.26	0.75
1:C:302:VAL:H	1:C:442:GLN:HE22	1.34	0.75
1:A:66:ARG:HD3	1:C:368:PRO:HG3	1.69	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:177:LYS:HE2	3:C:691:HOH:O	1.87	0.74
1:B:306:LYS:HD2	1:B:306:LYS:N	1.99	0.74
1:C:50:LEU:HD12	1:C:51:LEU:N	2.01	0.74
1:C:41:VAL:CG1	1:C:50:LEU:HD13	2.18	0.74
1:C:61:MET:HE1	1:C:64:PHE:HD2	1.53	0.72
1:C:392:MET:HE3	1:C:394:MET:CE	2.20	0.72
1:D:444:ARG:O	1:D:448:VAL:HG12	1.90	0.72
1:C:67:GLU:HG3	1:C:68:ARG:NH1	2.06	0.71
1:B:156:ARG:NH2	1:B:439:ASN:OD1	2.23	0.70
1:C:433:ASN:ND2	1:C:435:ALA:H	1.88	0.70
1:B:306:LYS:H	1:B:306:LYS:CD	1.95	0.70
1:B:395:GLN:HB2	3:B:619:HOH:O	1.90	0.70
1:A:368:PRO:HG3	1:C:66:ARG:HD3	1.72	0.70
1:C:306:LYS:CD	1:C:306:LYS:H	2.04	0.69
1:A:394:MET:SD	1:C:394:MET:HG3	2.31	0.69
1:C:306:LYS:H	1:C:306:LYS:HD2	1.57	0.69
1:A:414:GLN:HE22	1:C:38:LYS:H	1.41	0.69
1:A:457:LYS:O	1:A:461:GLU:HG3	1.92	0.69
1:A:389:ASP:HB2	1:C:67:GLU:HB2	1.74	0.68
1:B:394:MET:HG2	1:D:394:MET:HG3	1.74	0.68
1:C:61:MET:HE1	1:C:64:PHE:CD2	2.28	0.68
1:C:75:HIS:HA	1:C:115:THR:O	1.94	0.68
1:C:329:VAL:O	1:C:332:ILE:HG22	1.94	0.68
1:C:42:ILE:HG22	1:C:51:LEU:HD13	1.76	0.68
1:C:41:VAL:HG11	1:C:50:LEU:HD13	1.76	0.68
1:B:38:LYS:H	1:D:414:GLN:NE2	1.92	0.67
1:D:306:LYS:HD2	1:D:306:LYS:N	2.07	0.67
1:D:147:GLY:HA2	2:D:600:HEM:HBC1	1.77	0.67
1:A:73:VAL:HG13	1:A:74:VAL:HG22	1.77	0.67
2:A:600:HEM:HMC2	2:A:600:HEM:HBC2	1.77	0.66
1:D:411:ALA:HB1	1:D:412:PRO:CD	2.25	0.66
1:C:392:MET:HE3	1:C:394:MET:HE3	1.76	0.66
1:A:403:ASN:HD21	1:B:181:MET:HE3	1.60	0.66
1:A:329:VAL:O	1:A:332:ILE:HG22	1.96	0.65
1:C:98:LYS:O	1:C:101:GLU:HB2	1.97	0.65
1:D:407:ASN:HD21	1:D:411:ALA:HB3	1.61	0.65
1:C:424:GLN:HG3	1:D:427:GLY:O	1.98	0.64
1:B:202:ASP:OD2	1:B:458:ARG:NH2	2.30	0.64
1:B:218:HIS:CD2	1:B:351:LEU:HD13	2.33	0.64
1:D:392:MET:HE3	1:D:394:MET:CE	2.27	0.64
1:D:302:VAL:H	1:D:442:GLN:HE22	1.44	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ARG:O	1:A:148:ASN:HB2	1.97	0.64
1:B:183:TRP:HE1	1:B:466:HIS:CD2	2.15	0.63
1:C:50:LEU:HD12	1:C:51:LEU:H	1.63	0.63
1:B:154:PHE:HZ	1:B:199:LEU:HD22	1.63	0.63
1:D:410:GLY:HA2	3:D:837:HOH:O	1.98	0.62
1:C:305:HIS:HB2	1:C:306:LYS:HZ1	1.63	0.62
1:D:147:GLY:HA2	2:D:600:HEM:CBC	2.30	0.62
1:A:392:MET:HE3	1:A:394:MET:HE3	1.82	0.61
1:B:453:GLU:HA	1:B:456:ARG:NH1	2.15	0.61
1:C:433:ASN:HD22	1:C:434:THR:H	1.48	0.61
1:C:224:ASN:HD21	1:C:228:GLU:HB2	1.65	0.61
1:B:202:ASP:CG	1:B:458:ARG:HH21	2.08	0.61
1:B:184:ASP:O	1:B:188:LEU:HG	2.01	0.60
1:B:402:PRO:HA	3:B:645:HOH:O	2.02	0.60
1:C:405:TYR:OH	1:C:414:GLN:HG2	2.01	0.60
1:D:44:VAL:CG1	1:D:49:PRO:HD2	2.30	0.60
1:A:281:ILE:HG23	1:A:313:VAL:HG21	1.83	0.60
1:C:499:LYS:O	1:C:503:GLU:HG3	2.01	0.59
1:A:161:PHE:HB3	1:A:162:PRO:HD3	1.84	0.59
1:D:428:GLU:OE2	1:D:430:ARG:HD3	2.03	0.59
1:D:328:GLU:HA	1:D:375:VAL:HG11	1.84	0.58
1:D:382:ARG:HG2	1:D:382:ARG:HH11	1.68	0.58
1:C:433:ASN:HD22	1:C:434:THR:N	2.01	0.57
1:B:403:ASN:C	1:B:403:ASN:HD22	2.12	0.57
1:C:127:ARG:O	1:C:128:ASP:HB2	2.03	0.57
1:A:42:ILE:HD12	1:A:54:ASP:HA	1.86	0.57
1:A:51:LEU:HD13	1:D:429:VAL:CG1	2.35	0.57
1:B:433:ASN:ND2	1:B:435:ALA:H	2.02	0.57
1:A:83:GLY:HA3	1:A:317:VAL:O	2.05	0.57
1:B:477:LYS:HB2	1:B:477:LYS:NZ	2.20	0.57
1:C:61:MET:CE	1:C:64:PHE:HD2	2.17	0.56
1:A:98:LYS:O	1:A:101:GLU:HB2	2.04	0.56
1:A:358:TYR:HB2	1:A:359:PRO:HD3	1.86	0.56
1:A:75:HIS:HA	1:A:115:THR:O	2.06	0.56
1:C:282:GLN:CG	1:C:310:LEU:HD23	2.36	0.56
1:C:180:ASP:OD1	1:C:470:ALA:HA	2.06	0.56
1:C:403:ASN:C	1:C:403:ASN:HD22	2.14	0.56
1:C:420:GLU:CD	1:C:420:GLU:H	2.14	0.55
1:D:281:ILE:HG23	1:D:313:VAL:HG21	1.89	0.55
1:C:305:HIS:HB2	1:C:306:LYS:HE3	1.87	0.55
1:C:44:VAL:O	1:C:48:GLY:HA3	2.05	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:392:MET:HB3	1:C:394:MET:HE3	1.88	0.55
1:D:161:PHE:HB3	1:D:162:PRO:HD3	1.89	0.55
1:D:333:ALA:HB1	1:D:362:HIS:CE1	2.41	0.55
1:B:75:HIS:HA	1:B:115:THR:O	2.07	0.55
1:D:143:TRP:HB2	1:D:340:PRO:HD3	1.88	0.54
1:A:453:GLU:HA	1:A:456:ARG:HH11	1.72	0.54
1:B:492:HIS:HB2	3:B:885:HOH:O	2.05	0.54
3:B:749:HOH:O	1:C:49:PRO:HB2	2.07	0.54
1:C:224:ASN:ND2	1:C:228:GLU:HB2	2.23	0.54
1:D:304:PRO:HB3	1:D:306:LYS:HD3	1.88	0.54
1:D:392:MET:HE3	1:D:394:MET:HE3	1.89	0.54
1:B:41:VAL:HG13	1:C:157:ASP:OD1	2.07	0.54
1:D:148:ASN:ND2	2:D:600:HEM:HAC	2.23	0.54
1:C:298:ASP:OD2	1:C:301:LYS:HD3	2.08	0.54
1:A:93:LYS:HG2	3:A:738:HOH:O	2.06	0.54
1:A:297:PHE:CD2	1:A:347:PRO:HG2	2.43	0.54
1:C:302:VAL:HG22	1:C:442:GLN:HE22	1.72	0.54
1:D:453:GLU:N	1:D:456:ARG:NH1	2.56	0.54
1:B:445:ALA:O	1:B:449:ASN:HB2	2.08	0.54
1:D:448:VAL:HG13	1:D:449:ASN:ND2	2.23	0.54
1:C:306:LYS:HE3	1:C:306:LYS:N	2.23	0.53
1:C:388:ARG:NH1	3:C:886:HOH:O	2.41	0.53
1:C:392:MET:HE3	1:C:394:MET:HE1	1.90	0.53
1:B:41:VAL:HG11	1:C:158:PRO:HG2	1.89	0.53
1:D:229:ALA:HB3	1:D:421:HIS:CE1	2.43	0.53
1:A:395:GLN:HB2	3:A:656:HOH:O	2.06	0.53
1:C:44:VAL:HG13	1:C:49:PRO:HD2	1.90	0.53
1:B:91:ILE:HG12	3:B:862:HOH:O	2.08	0.53
1:B:324:ASN:ND2	1:D:397:ASN:HB3	2.24	0.53
1:C:380:ARG:HG3	1:C:380:ARG:NH1	2.23	0.53
1:D:403:ASN:C	1:D:403:ASN:HD22	2.15	0.53
1:D:42:ILE:HD12	1:D:54:ASP:HA	1.90	0.53
1:A:35:VAL:HG11	1:A:38:LYS:HB2	1.90	0.52
1:C:53:GLN:HG2	3:C:684:HOH:O	2.09	0.52
1:C:143:TRP:HB2	1:C:340:PRO:HD3	1.90	0.52
1:D:411:ALA:HB1	1:D:412:PRO:HD2	1.91	0.52
1:A:294:PHE:CG	1:A:301:LYS:HD3	2.45	0.52
1:D:294:PHE:HZ	1:D:441:THR:HG21	1.74	0.52
1:D:382:ARG:HG2	1:D:382:ARG:NH1	2.25	0.52
1:D:130:ARG:O	1:D:148:ASN:HB2	2.10	0.51
1:A:41:VAL:HG22	1:A:54:ASP:OD2	2.11	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:302:VAL:N	1:B:442:GLN:HE22	2.05	0.51
1:D:453:GLU:N	1:D:456:ARG:HH12	2.09	0.51
1:A:44:VAL:HG22	1:A:44:VAL:O	2.09	0.51
1:D:486:HIS:HB3	1:D:489:TYR:HB2	1.92	0.51
1:C:459:LEU:O	1:C:463:ILE:HG13	2.10	0.51
1:A:156:ARG:HD3	1:A:298:ASP:OD1	2.10	0.51
1:A:334:PHE:O	1:A:362:HIS:HE1	1.94	0.51
1:D:98:LYS:O	1:D:101:GLU:HB2	2.10	0.51
1:C:214:GLY:HA3	1:C:236:TYR:CD2	2.46	0.51
1:C:302:VAL:N	1:C:442:GLN:HE22	2.05	0.51
1:C:380:ARG:HH11	1:C:380:ARG:CG	2.21	0.51
1:C:392:MET:C	1:C:394:MET:HE2	2.35	0.51
1:B:414:GLN:OE1	1:D:37:ASP:HA	2.11	0.51
1:C:387:GLN:O	1:C:388:ARG:HD3	2.11	0.51
1:C:407:ASN:HD21	1:C:411:ALA:HB3	1.75	0.51
1:B:51:LEU:HD22	1:C:429:VAL:HG11	1.92	0.50
1:C:358:TYR:HB2	1:C:359:PRO:HD3	1.93	0.50
1:D:64:PHE:HA	1:D:67:GLU:HG3	1.93	0.50
1:C:183:TRP:CD2	1:C:467:LEU:HD13	2.46	0.50
1:A:407:ASN:ND2	1:A:411:ALA:HB3	2.23	0.50
1:A:453:GLU:HA	1:A:456:ARG:NH1	2.26	0.50
1:B:329:VAL:O	1:B:332:ILE:HG22	2.12	0.50
1:D:468:LYS:HG3	1:D:469:ASP:N	2.27	0.50
1:A:113:PHE:HA	1:A:131:GLY:O	2.10	0.50
1:A:337:SER:HB2	1:C:55:VAL:HG11	1.94	0.50
1:B:102:HIS:CE1	1:B:105:LYS:HB2	2.46	0.50
1:C:448:VAL:HG13	1:C:449:ASN:N	2.27	0.50
1:D:146:VAL:HG22	1:D:334:PHE:HB3	1.92	0.50
1:C:486:HIS:CE1	1:C:488:ASP:CG	2.89	0.50
1:B:154:PHE:CE1	1:B:195:GLN:HG3	2.47	0.50
1:C:320:ARG:HD2	3:C:736:HOH:O	2.11	0.50
1:D:35:VAL:HG11	1:D:38:LYS:HB2	1.92	0.50
1:D:500:TYR:C	1:D:502:ALA:H	2.19	0.50
1:D:213:ASN:ND2	1:D:242:ILE:HD11	2.26	0.50
1:C:47:ARG:HH11	1:C:47:ARG:HG3	1.77	0.50
1:C:415:GLN:O	1:C:415:GLN:HG3	2.11	0.50
1:A:51:LEU:CD1	1:D:429:VAL:HG13	2.39	0.49
1:A:255:GLN:HB2	1:D:255:GLN:HB2	1.94	0.49
1:A:415:GLN:O	1:A:415:GLN:HG3	2.12	0.49
1:C:411:ALA:HB1	1:C:412:PRO:HD2	1.93	0.49
1:B:349:LYS:HE2	1:C:43:THR:HG21	1.93	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:PHE:HZ	1:C:328:GLU:HB3	1.77	0.49
1:C:301:LYS:NZ	1:C:438:ASP:O	2.42	0.49
1:A:282:GLN:HG3	1:A:310:LEU:HD23	1.93	0.49
1:B:465:GLY:O	1:B:468:LYS:HE3	2.12	0.49
1:D:329:VAL:O	1:D:332:ILE:HG22	2.13	0.49
1:D:183:TRP:CD2	1:D:467:LEU:HD13	2.48	0.49
1:B:93:LYS:HZ2	1:B:93:LYS:HB3	1.78	0.49
1:D:130:ARG:O	1:D:148:ASN:CB	2.61	0.49
1:A:218:HIS:CD2	1:A:354:ARG:HH11	2.30	0.49
1:A:392:MET:C	1:A:394:MET:HE2	2.37	0.49
1:B:214:GLY:HA3	1:B:236:TYR:CE2	2.48	0.49
1:D:468:LYS:HD3	1:D:500:TYR:CD1	2.47	0.49
1:A:397:ASN:HA	3:A:656:HOH:O	2.13	0.48
1:B:146:VAL:HG22	1:B:334:PHE:HB3	1.95	0.48
1:B:415:GLN:HG3	1:B:415:GLN:O	2.12	0.48
1:C:302:VAL:HG22	1:C:442:GLN:NE2	2.28	0.48
1:C:305:HIS:HB2	1:C:306:LYS:CE	2.43	0.48
1:A:392:MET:HE3	1:A:394:MET:CE	2.43	0.48
1:B:87:VAL:HG12	1:B:103:ILE:HA	1.95	0.48
1:A:224:ASN:HD21	1:A:228:GLU:HB2	1.78	0.48
1:B:40:ASN:CG	1:C:433:ASN:HA	2.37	0.48
1:D:433:ASN:HD22	1:D:434:THR:N	2.12	0.48
1:B:42:ILE:HG22	1:B:51:LEU:HD13	1.95	0.48
1:C:42:ILE:O	1:C:51:LEU:HD12	2.13	0.48
1:C:423:ILE:HG22	1:C:424:GLN:H	1.79	0.48
1:C:95:SER:HA	1:C:223:VAL:O	2.14	0.48
1:D:348:ASP:OD1	1:D:348:ASP:C	2.57	0.48
1:B:68:ARG:HH21	1:C:169:LYS:HE3	1.79	0.48
1:D:159:ILE:HG22	1:D:160:LEU:HD12	1.95	0.48
1:B:238:THR:HA	1:B:277:TRP:CD1	2.48	0.48
1:D:440:VAL:HG12	1:D:485:VAL:HG22	1.95	0.48
1:A:394:MET:HE1	1:C:373:ILE:HG12	1.96	0.47
1:C:306:LYS:CD	1:C:306:LYS:N	2.75	0.47
1:D:236:TYR:HA	1:D:278:THR:O	2.14	0.47
1:A:44:VAL:O	1:A:48:GLY:HA3	2.13	0.47
1:B:327:ALA:HA	1:B:331:GLN:HE21	1.79	0.47
1:B:457:LYS:NZ	1:B:457:LYS:HB3	2.28	0.47
1:A:440:VAL:HG23	1:A:441:THR:N	2.29	0.47
1:A:481:ASN:O	1:A:484:GLU:HB2	2.14	0.47
1:C:305:HIS:HB2	1:C:306:LYS:NZ	2.29	0.47
1:C:380:ARG:HD3	3:C:833:HOH:O	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:THR:HG21	1:C:349:LYS:HE2	1.96	0.47
1:C:346:SER:HB2	1:C:347:PRO:HD2	1.97	0.47
1:A:96:LYS:HG2	1:A:223:VAL:O	2.15	0.47
1:A:306:LYS:HD2	1:A:306:LYS:N	2.08	0.47
1:A:424:GLN:HG3	1:B:427:GLY:O	2.15	0.47
1:B:382:ARG:HB2	1:B:382:ARG:NH1	2.24	0.47
1:A:77:LYS:NZ	1:A:124:ASP:OD1	2.42	0.47
1:B:109:ILE:HA	1:B:135:LYS:O	2.14	0.47
1:B:368:PRO:HG3	1:D:66:ARG:HD3	1.97	0.47
1:D:148:ASN:ND2	2:D:600:HEM:CAC	2.78	0.47
1:D:476:LYS:O	1:D:480:LYS:HG3	2.15	0.47
1:A:382:ARG:HH11	1:A:382:ARG:HG2	1.80	0.47
1:D:306:LYS:H	1:D:306:LYS:CD	2.02	0.47
1:A:213:ASN:OD1	1:A:237:LYS:HA	2.14	0.47
1:C:334:PHE:HD1	2:C:600:HEM:CGD	2.28	0.47
1:B:444:ARG:O	1:B:448:VAL:HG12	2.15	0.47
1:C:282:GLN:HG3	1:C:310:LEU:HD23	1.96	0.47
1:D:319:ASN:C	1:D:319:ASN:HD22	2.23	0.47
1:C:448:VAL:HG13	1:C:449:ASN:H	1.79	0.46
1:A:272:GLY:O	1:A:274:TYR:N	2.46	0.46
1:A:276:SER:HA	1:A:316:LEU:O	2.15	0.46
1:C:499:LYS:HB2	1:C:499:LYS:NZ	2.30	0.46
1:D:500:TYR:O	1:D:502:ALA:N	2.48	0.46
1:A:148:ASN:ND2	3:A:677:HOH:O	2.46	0.46
1:A:452:ASN:C	1:A:452:ASN:OD1	2.58	0.46
3:A:622:HOH:O	1:B:51:LEU:HB3	2.15	0.46
1:B:380:ARG:HH11	1:B:380:ARG:HG3	1.80	0.46
1:B:83:GLY:HA3	1:B:317:VAL:O	2.16	0.46
1:B:348:ASP:OD1	1:B:348:ASP:C	2.58	0.46
1:C:302:VAL:H	1:C:442:GLN:NE2	2.08	0.46
1:A:349:LYS:HE2	1:D:43:THR:HG21	1.97	0.46
1:B:407:ASN:ND2	1:B:411:ALA:HB3	2.22	0.46
1:D:27:LEU:HD12	1:D:28:THR:N	2.30	0.46
1:A:130:ARG:O	1:A:148:ASN:CB	2.63	0.46
1:B:91:ILE:HG21	1:B:313:VAL:HG22	1.98	0.46
1:B:415:GLN:O	1:D:36:GLY:HA2	2.15	0.46
1:B:458:ARG:O	1:B:459:LEU:C	2.59	0.46
1:D:183:TRP:CG	1:D:467:LEU:HD13	2.50	0.46
1:D:187:SER:HB2	1:D:477:LYS:HB3	1.98	0.46
1:A:424:GLN:HA	1:B:428:GLU:HA	1.98	0.46
1:C:453:GLU:HA	1:C:456:ARG:HH11	1.77	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:GLU:HA	1:B:456:ARG:HH11	1.77	0.46
1:C:428:GLU:HG2	3:C:646:HOH:O	2.16	0.45
1:A:159:ILE:HG22	1:A:160:LEU:HD23	1.97	0.45
1:B:411:ALA:HB1	1:B:412:PRO:CD	2.46	0.45
1:A:233:LYS:HB2	1:A:282:GLN:HB2	1.97	0.45
1:B:141:GLY:HA3	1:D:33:ASN:HD22	1.82	0.45
1:C:132:PHE:N	1:C:147:GLY:O	2.49	0.45
1:C:147:GLY:HA3	1:C:215:TYR:O	2.15	0.45
1:C:214:GLY:HA3	1:C:236:TYR:CE2	2.51	0.45
1:B:158:PRO:HG2	1:C:41:VAL:HG21	1.97	0.45
1:B:403:ASN:C	1:B:403:ASN:ND2	2.72	0.45
1:C:50:LEU:HG	1:D:52:VAL:HG21	1.99	0.45
1:C:380:ARG:NH1	1:C:380:ARG:CG	2.79	0.45
1:D:403:ASN:C	1:D:403:ASN:ND2	2.74	0.45
1:D:433:ASN:ND2	1:D:435:ALA:H	2.15	0.45
1:D:218:HIS:CD2	1:D:354:ARG:HH11	2.35	0.45
1:A:178:ASP:CB	1:A:181:MET:HE2	2.40	0.45
1:B:239:ASP:OD2	1:B:315:LYS:HE3	2.17	0.45
1:A:190:PRO:C	1:A:192:SER:N	2.71	0.45
1:C:403:ASN:HD21	1:D:181:MET:CE	2.30	0.45
1:C:423:ILE:HG22	1:C:424:GLN:N	2.32	0.45
1:D:235:HIS:NE2	1:D:282:GLN:OE1	2.50	0.45
1:C:433:ASN:ND2	1:C:434:THR:N	2.65	0.44
1:B:98:LYS:HA	1:B:101:GLU:HB2	1.99	0.44
1:A:189:ARG:HB3	1:A:191:GLU:OE1	2.17	0.44
1:C:476:LYS:HE3	3:C:866:HOH:O	2.17	0.44
1:A:77:LYS:HE3	1:A:122:SER:O	2.18	0.44
1:D:216:GLY:O	1:D:218:HIS:N	2.48	0.44
1:D:238:THR:HA	1:D:277:TRP:CD1	2.52	0.44
1:B:155:ILE:HG13	1:B:350:MET:CE	2.48	0.44
1:B:352:GLN:HB3	1:C:50:LEU:HB3	1.99	0.44
1:B:157:ASP:OD1	1:B:159:ILE:HG22	2.18	0.44
1:B:452:ASN:OD1	1:B:452:ASN:C	2.60	0.44
1:C:138:THR:OG1	1:C:141:GLY:O	2.26	0.44
1:D:232:CYS:HA	1:D:282:GLN:O	2.17	0.44
1:A:114:SER:O	1:A:130:ARG:HA	2.17	0.44
1:A:302:VAL:HG22	1:A:442:GLN:NE2	2.32	0.44
1:B:335:ASP:OD1	1:B:362:HIS:ND1	2.49	0.44
1:D:83:GLY:HA3	1:D:317:VAL:O	2.18	0.44
1:A:42:ILE:HB	1:A:54:ASP:HB2	2.00	0.44
1:A:75:HIS:CE1	1:A:116:VAL:HG22	2.53	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:385:ASN:HB2	3:A:663:HOH:O	2.17	0.44
1:A:452:ASN:O	1:A:456:ARG:HG3	2.18	0.44
1:D:74:VAL:O	1:D:75:HIS:HB2	2.18	0.44
1:D:453:GLU:O	1:D:454:GLU:C	2.61	0.44
1:A:24:ALA:N	3:A:603:HOH:O	2.51	0.43
1:A:429:VAL:HG11	1:D:51:LEU:HD22	2.00	0.43
1:B:404:TYR:CD1	1:B:404:TYR:N	2.86	0.43
1:C:154:PHE:CE1	1:C:195:GLN:HG3	2.53	0.43
1:C:454:GLU:OE1	1:C:454:GLU:HA	2.18	0.43
1:D:368:PRO:HG2	1:D:391:PRO:CG	2.48	0.43
1:D:424:GLN:HE21	1:D:424:GLN:HB2	1.57	0.43
1:D:500:TYR:C	1:D:502:ALA:N	2.74	0.43
1:B:81:ALA:C	1:B:82:PHE:CD1	2.96	0.43
1:B:373:ILE:O	1:B:374:PRO:C	2.61	0.43
1:D:159:ILE:CG2	1:D:160:LEU:HD12	2.48	0.43
1:B:304:PRO:HB3	1:B:306:LYS:HD3	2.00	0.43
1:C:358:TYR:O	1:C:359:PRO:C	2.61	0.43
1:D:82:PHE:N	1:D:82:PHE:CD1	2.86	0.43
1:D:335:ASP:OD1	1:D:362:HIS:ND1	2.51	0.43
1:B:42:ILE:HD12	1:B:54:ASP:HA	2.00	0.43
1:B:308:TYR:N	1:B:308:TYR:CD2	2.85	0.43
1:C:224:ASN:OD1	1:C:226:ASN:HB2	2.18	0.43
1:C:468:LYS:HD2	1:C:468:LYS:C	2.43	0.43
1:B:213:ASN:ND2	1:B:242:ILE:HD11	2.33	0.43
1:C:319:ASN:H	1:C:319:ASN:ND2	2.17	0.43
1:A:190:PRO:C	1:A:192:SER:H	2.27	0.43
1:A:274:TYR:CD1	1:A:319:ASN:HA	2.53	0.43
1:B:433:ASN:HA	1:C:40:ASN:CG	2.43	0.43
1:C:51:LEU:HD23	1:D:49:PRO:HB2	1.99	0.43
1:D:218:HIS:CD2	1:D:351:LEU:HD13	2.53	0.43
1:A:167:SER:HB2	1:A:181:MET:O	2.18	0.43
1:A:468:LYS:HD2	1:A:468:LYS:C	2.44	0.43
1:A:56:VAL:HG23	3:D:601:HOH:O	2.19	0.43
1:C:24:ALA:N	3:C:681:HOH:O	2.52	0.43
1:D:135:LYS:HG3	1:D:144:ASP:OD2	2.19	0.43
1:D:386:TYR:OH	1:D:411:ALA:HB3	2.19	0.43
1:B:82:PHE:CD1	1:B:82:PHE:N	2.87	0.43
1:D:210:ARG:HB2	3:D:774:HOH:O	2.18	0.43
1:A:461:GLU:HA	1:A:496:LEU:HD13	2.01	0.42
1:B:423:ILE:CG2	1:B:424:GLN:N	2.81	0.42
1:C:319:ASN:C	1:C:319:ASN:HD22	2.27	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:499:LYS:HG2	1:C:503:GLU:OE2	2.20	0.42
1:D:275:PRO:HD2	1:D:318:LEU:O	2.18	0.42
1:D:453:GLU:HA	1:D:456:ARG:HH11	1.83	0.42
1:B:263:ARG:HG2	1:B:267:ASN:ND2	2.34	0.42
1:B:423:ILE:HG22	1:B:424:GLN:N	2.34	0.42
1:C:47:ARG:HG3	1:C:47:ARG:NH1	2.34	0.42
1:C:155:ILE:HD12	1:C:160:LEU:HB2	2.00	0.42
1:A:192:SER:O	1:A:196:VAL:HG23	2.20	0.42
1:A:424:GLN:HG3	1:B:427:GLY:C	2.44	0.42
1:B:269:ILE:HB	1:B:321:ASN:HD21	1.84	0.42
1:B:309:PRO:HA	3:B:729:HOH:O	2.18	0.42
1:C:236:TYR:CD1	1:C:236:TYR:N	2.87	0.42
1:D:44:VAL:HG13	1:D:49:PRO:HD2	2.01	0.42
1:D:361:THR:HG21	2:D:600:HEM:HAA2	2.01	0.42
1:A:414:GLN:HE21	1:C:38:LYS:H	1.60	0.42
1:C:100:PHE:O	1:C:102:HIS:N	2.52	0.42
1:D:319:ASN:HD22	1:D:319:ASN:H	1.66	0.42
1:C:190:PRO:O	1:C:193:LEU:HG	2.20	0.42
1:D:301:LYS:HA	1:D:442:GLN:HE22	1.84	0.42
1:B:51:LEU:HD22	1:C:429:VAL:CG1	2.49	0.42
1:B:226:ASN:HD22	1:B:226:ASN:HA	1.62	0.42
1:C:361:THR:HG21	2:C:600:HEM:HAA2	2.01	0.42
1:C:422:SER:HB3	1:D:430:ARG:HB3	2.00	0.42
1:B:284:MET:SD	1:B:289:ALA:HA	2.59	0.42
1:B:350:MET:O	1:B:354:ARG:HG3	2.20	0.42
1:D:442:GLN:O	1:D:445:ALA:HB3	2.19	0.42
1:A:305:HIS:HB2	1:A:306:LYS:HE3	2.01	0.42
1:A:403:ASN:N	1:A:403:ASN:HD22	2.16	0.42
1:B:232:CYS:HA	1:B:282:GLN:O	2.20	0.42
1:C:480:LYS:O	1:C:483:THR:HB	2.19	0.42
1:C:90:ASP:OD1	1:C:90:ASP:C	2.63	0.42
1:C:219:THR:OG1	1:C:233:LYS:HE2	2.20	0.42
1:C:306:LYS:H	1:C:306:LYS:CE	2.31	0.42
1:C:403:ASN:HD21	1:D:181:MET:HE3	1.85	0.42
1:D:44:VAL:O	1:D:48:GLY:HA3	2.20	0.42
1:D:319:ASN:HD22	1:D:320:ARG:N	2.18	0.42
1:A:147:GLY:HA3	1:A:215:TYR:O	2.20	0.41
1:A:445:ALA:O	1:A:449:ASN:HB2	2.20	0.41
1:B:365:ARG:HD2	3:B:634:HOH:O	2.19	0.41
1:D:82:PHE:HZ	1:D:328:GLU:HB3	1.85	0.41
1:D:294:PHE:CB	1:D:301:LYS:HD3	2.50	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:PHE:HA	1:A:293:PRO:HD3	1.77	0.41
1:B:68:ARG:NH2	1:C:169:LYS:HE3	2.36	0.41
1:B:429:VAL:HG13	1:C:51:LEU:HD13	2.03	0.41
1:B:452:ASN:OD1	1:B:454:GLU:N	2.53	0.41
1:C:480:LYS:HE3	1:C:480:LYS:HB2	1.94	0.41
1:D:402:PRO:HG2	1:D:409:PHE:HB2	2.02	0.41
1:A:277:TRP:HB2	1:A:316:LEU:HB2	2.02	0.41
1:A:328:GLU:HA	1:A:375:VAL:HG11	2.03	0.41
1:A:456:ARG:NH2	3:A:824:HOH:O	2.48	0.41
1:C:281:ILE:HG23	1:C:313:VAL:HG21	2.02	0.41
1:D:145:LEU:HD12	1:D:145:LEU:HA	1.89	0.41
1:A:403:ASN:HD22	1:A:403:ASN:H	1.69	0.41
1:C:77:LYS:NZ	1:C:124:ASP:OD1	2.47	0.41
1:C:82:PHE:CD1	1:C:82:PHE:N	2.88	0.41
1:C:410:GLY:O	1:C:411:ALA:C	2.63	0.41
1:A:209:HIS:O	1:A:212:MET:HG2	2.21	0.41
1:B:141:GLY:HA3	1:D:33:ASN:ND2	2.36	0.41
1:B:392:MET:HG3	1:D:392:MET:HG3	2.02	0.41
1:C:82:PHE:CZ	1:C:328:GLU:HB3	2.55	0.41
1:A:306:LYS:CD	1:A:306:LYS:N	2.70	0.41
1:A:440:VAL:O	1:A:441:THR:C	2.63	0.41
1:B:194:HIS:CE1	1:B:442:GLN:HE21	2.39	0.41
1:B:384:ALA:HB1	1:B:412:PRO:HG2	2.03	0.41
1:C:147:GLY:HA2	2:C:600:HEM:HBC1	2.02	0.41
1:C:285:THR:OG1	1:C:288:GLN:HG3	2.21	0.41
1:D:419:LEU:HD12	1:D:419:LEU:HA	1.94	0.41
1:A:40:ASN:HA	1:D:157:ASP:OD2	2.19	0.41
1:A:44:VAL:CG1	1:A:49:PRO:HG2	2.51	0.41
1:A:70:PRO:HG3	1:D:70:PRO:HD3	2.03	0.41
1:A:81:ALA:C	1:A:82:PHE:CD1	2.99	0.41
1:A:202:ASP:C	1:A:204:GLY:H	2.29	0.41
1:A:411:ALA:HB1	1:A:412:PRO:HD2	2.03	0.41
1:B:157:ASP:OD1	1:C:41:VAL:HG23	2.20	0.41
1:B:167:SER:HA	1:B:181:MET:HE2	2.03	0.41
1:B:339:MET:HE1	1:B:345:ALA:HB2	2.03	0.41
1:C:83:GLY:HA3	1:C:317:VAL:O	2.20	0.41
1:C:367:GLY:O	1:C:368:PRO:C	2.63	0.41
1:D:41:VAL:HG22	1:D:54:ASP:OD2	2.20	0.41
1:D:149:ASN:HA	1:D:213:ASN:O	2.21	0.41
1:D:276:SER:HB2	1:D:316:LEU:O	2.20	0.41
1:A:144:ASP:HB2	1:A:338:ASN:HB2	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:395:GLN:HB3	1:A:396:ASP:H	1.62	0.40
1:B:358:TYR:HB2	1:B:359:PRO:HD3	2.03	0.40
1:D:85:PHE:HA	1:D:315:LYS:O	2.20	0.40
1:B:87:VAL:CG1	1:B:103:ILE:HA	2.51	0.40
1:B:233:LYS:HB2	1:B:282:GLN:HB2	2.04	0.40
1:B:394:MET:HE3	1:D:373:ILE:HA	2.03	0.40
1:B:411:ALA:HB1	1:B:412:PRO:HD2	2.02	0.40
1:C:61:MET:HE2	1:C:65:ASP:OD1	2.22	0.40
1:A:285:THR:OG1	1:A:288:GLN:HG3	2.20	0.40
1:B:213:ASN:OD1	1:B:237:LYS:HA	2.22	0.40
1:B:292:PHE:HA	1:B:293:PRO:HD3	1.94	0.40
1:C:163:SER:HG	1:D:405:TYR:H	1.69	0.40
1:C:424:GLN:HB2	1:D:428:GLU:HB3	2.02	0.40
1:D:440:VAL:HG12	1:D:485:VAL:CG2	2.51	0.40
1:B:169:LYS:HB2	3:B:789:HOH:O	2.21	0.40
1:C:240:GLN:CD	1:C:276:SER:H	2.29	0.40
1:C:328:GLU:HA	1:C:375:VAL:HG11	2.03	0.40
1:D:362:HIS:NE2	2:D:600:HEM:O1A	2.50	0.40
1:A:143:TRP:HB2	1:A:340:PRO:HD3	2.03	0.40
1:D:218:HIS:NE2	1:D:354:ARG:NH1	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	477/527 (90%)	448 (94%)	28 (6%)	1 (0%)	43	58
1	B	477/527 (90%)	451 (94%)	25 (5%)	1 (0%)	43	58
1	C	479/527 (91%)	446 (93%)	28 (6%)	5 (1%)	12	20
1	D	477/527 (90%)	441 (92%)	33 (7%)	3 (1%)	21	32
All	All	1910/2108 (91%)	1786 (94%)	114 (6%)	10 (0%)	24	37

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	101	GLU
1	B	101	GLU
1	D	101	GLU
1	D	120	SER
1	A	120	SER
1	C	120	SER
1	D	501	ASN
1	C	412	PRO
1	C	411	ALA
1	C	128	ASP

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	412/451 (91%)	396 (96%)	16 (4%)	28	48
1	B	413/451 (92%)	400 (97%)	13 (3%)	35	57
1	C	414/451 (92%)	403 (97%)	11 (3%)	39	62
1	D	412/451 (91%)	400 (97%)	12 (3%)	37	60
All	All	1651/1804 (92%)	1599 (97%)	52 (3%)	35	57

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	41	VAL
1	A	44	VAL
1	A	74	VAL
1	A	119	GLU
1	A	138	THR
1	A	160	LEU
1	A	236	TYR
1	A	238	THR
1	A	255	GLN
1	A	306	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	323	VAL
1	A	403	ASN
1	A	424	GLN
1	A	428	GLU
1	A	468	LYS
1	A	477	LYS
1	B	25	ASP
1	B	44	VAL
1	B	93	LYS
1	B	119	GLU
1	B	148	ASN
1	B	236	TYR
1	B	306	LYS
1	B	382	ARG
1	B	394	MET
1	B	403	ASN
1	B	417	SER
1	B	457	LYS
1	B	477	LYS
1	C	44	VAL
1	C	119	GLU
1	C	148	ASN
1	C	236	TYR
1	C	306	LYS
1	C	319	ASN
1	C	403	ASN
1	C	455	GLN
1	C	480	LYS
1	C	487	PRO
1	C	499	LYS
1	D	41	VAL
1	D	44	VAL
1	D	119	GLU
1	D	138	THR
1	D	150	THR
1	D	195	GLN
1	D	236	TYR
1	D	247	VAL
1	D	255	GLN
1	D	319	ASN
1	D	403	ASN
1	D	483	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	ASN
1	A	173	GLN
1	A	211	HIS
1	A	226	ASN
1	A	255	GLN
1	A	321	ASN
1	A	372	HIS
1	A	387	GLN
1	A	395	GLN
1	A	403	ASN
1	A	414	GLN
1	A	415	GLN
1	A	424	GLN
1	A	442	GLN
1	A	449	ASN
1	A	492	HIS
1	B	148	ASN
1	B	226	ASN
1	B	321	ASN
1	B	331	GLN
1	B	372	HIS
1	B	403	ASN
1	B	424	GLN
1	B	433	ASN
1	B	436	ASN
1	B	442	GLN
1	B	449	ASN
1	B	466	HIS
1	B	471	GLN
1	B	492	HIS
1	C	209	HIS
1	C	226	ASN
1	C	235	HIS
1	C	287	ASN
1	C	319	ASN
1	C	321	ASN
1	C	387	GLN
1	C	403	ASN
1	C	421	HIS
1	C	424	GLN
1	C	433	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	442	GLN
1	C	449	ASN
1	C	471	GLN
1	D	33	ASN
1	D	148	ASN
1	D	226	ASN
1	D	255	GLN
1	D	267	ASN
1	D	319	ASN
1	D	321	ASN
1	D	387	GLN
1	D	403	ASN
1	D	414	GLN
1	D	415	GLN
1	D	424	GLN
1	D	433	ASN
1	D	442	GLN
1	D	449	ASN
1	D	462	ASN
1	D	492	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides 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	D	600	1	50,50,50	1.30	5 (10%)	67,82,82	1.09	4 (5%)
2	HEM	C	600	1	50,50,50	1.36	7 (14%)	67,82,82	1.32	5 (7%)
2	HEM	A	600	1	50,50,50	1.36	6 (12%)	67,82,82	1.08	4 (5%)
2	HEM	B	600	1	50,50,50	1.27	5 (10%)	67,82,82	1.47	6 (8%)

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	D	600	1	-	4/14/54/54	-
2	HEM	C	600	1	-	2/14/54/54	-
2	HEM	A	600	1	-	5/14/54/54	-
2	HEM	B	600	1	-	2/14/54/54	-

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	HEM	CBC-CAC	3.98	1.49	1.30
2	D	600	HEM	CAB-C3B	-3.77	1.37	1.47
2	B	600	HEM	CBC-CAC	3.65	1.47	1.30
2	A	600	HEM	CAB-C3B	-3.60	1.37	1.47
2	C	600	HEM	CBC-CAC	3.52	1.47	1.30
2	D	600	HEM	CBC-CAC	3.15	1.45	1.30
2	C	600	HEM	C4D-C3D	3.14	1.50	1.45
2	B	600	HEM	CBB-CAB	3.04	1.45	1.30
2	B	600	HEM	C4D-C3D	2.91	1.50	1.45
2	D	600	HEM	CBB-CAB	2.87	1.44	1.30
2	B	600	HEM	CAC-C3C	-2.85	1.39	1.47
2	C	600	HEM	CBB-CAB	2.80	1.43	1.30
2	C	600	HEM	CAB-C3B	-2.70	1.40	1.47
2	C	600	HEM	CAC-C3C	-2.67	1.40	1.47
2	A	600	HEM	CAC-C3C	-2.66	1.40	1.47
2	A	600	HEM	CBB-CAB	2.55	1.42	1.30
2	C	600	HEM	FE-NB	2.25	2.01	1.94
2	D	600	HEM	C1C-C2C	2.22	1.49	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	600	HEM	CAC-C3C	-2.18	1.41	1.47
2	C	600	HEM	FE-ND	2.16	2.01	1.94
2	A	600	HEM	C1C-C2C	2.12	1.49	1.45
2	A	600	HEM	FE-ND	2.11	2.01	1.94
2	B	600	HEM	CAB-C3B	-2.01	1.42	1.47

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	HEM	C3B-C4B-NB	6.50	114.13	109.47
2	C	600	HEM	CAD-C3D-C4D	4.67	132.84	124.70
2	B	600	HEM	C4B-C3B-C2B	-4.35	103.28	107.28
2	C	600	HEM	CAD-C3D-C2D	-3.31	121.67	127.87
2	A	600	HEM	CBD-CAD-C3D	-3.18	103.73	112.53
2	B	600	HEM	CAD-C3D-C4D	3.13	130.15	124.70
2	C	600	HEM	CMA-C3A-C4A	3.07	130.10	125.42
2	D	600	HEM	CAD-C3D-C4D	3.05	130.01	124.70
2	B	600	HEM	CHC-C1C-C2C	-2.94	119.37	125.49
2	C	600	HEM	C3B-C4B-NB	2.87	111.53	109.47
2	D	600	HEM	CBD-CAD-C3D	-2.80	104.79	112.53
2	D	600	HEM	CAD-C3D-C2D	-2.54	123.10	127.87
2	A	600	HEM	CAD-C3D-C2D	-2.52	123.14	127.87
2	A	600	HEM	C3B-C4B-NB	2.40	111.19	109.47
2	B	600	HEM	C3B-C2B-C1B	2.37	108.19	106.41
2	A	600	HEM	CAD-C3D-C4D	2.35	128.80	124.70
2	C	600	HEM	C2D-C1D-ND	2.18	112.42	109.90
2	B	600	HEM	CAD-C3D-C2D	-2.07	123.98	127.87
2	D	600	HEM	CAA-C2A-C1A	2.01	128.87	124.94

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	HEM	C1A-C2A-CAA-CBA
2	B	600	HEM	C1A-C2A-CAA-CBA
2	B	600	HEM	C4D-C3D-CAD-CBD
2	C	600	HEM	C4D-C3D-CAD-CBD
2	D	600	HEM	C1A-C2A-CAA-CBA
2	A	600	HEM	C2B-C3B-CAB-CBB
2	D	600	HEM	C4D-C3D-CAD-CBD
2	A	600	HEM	C4B-C3B-CAB-CBB
2	D	600	HEM	C4C-C3C-CAC-CBC

Continued on next page...

Continued from previous page...

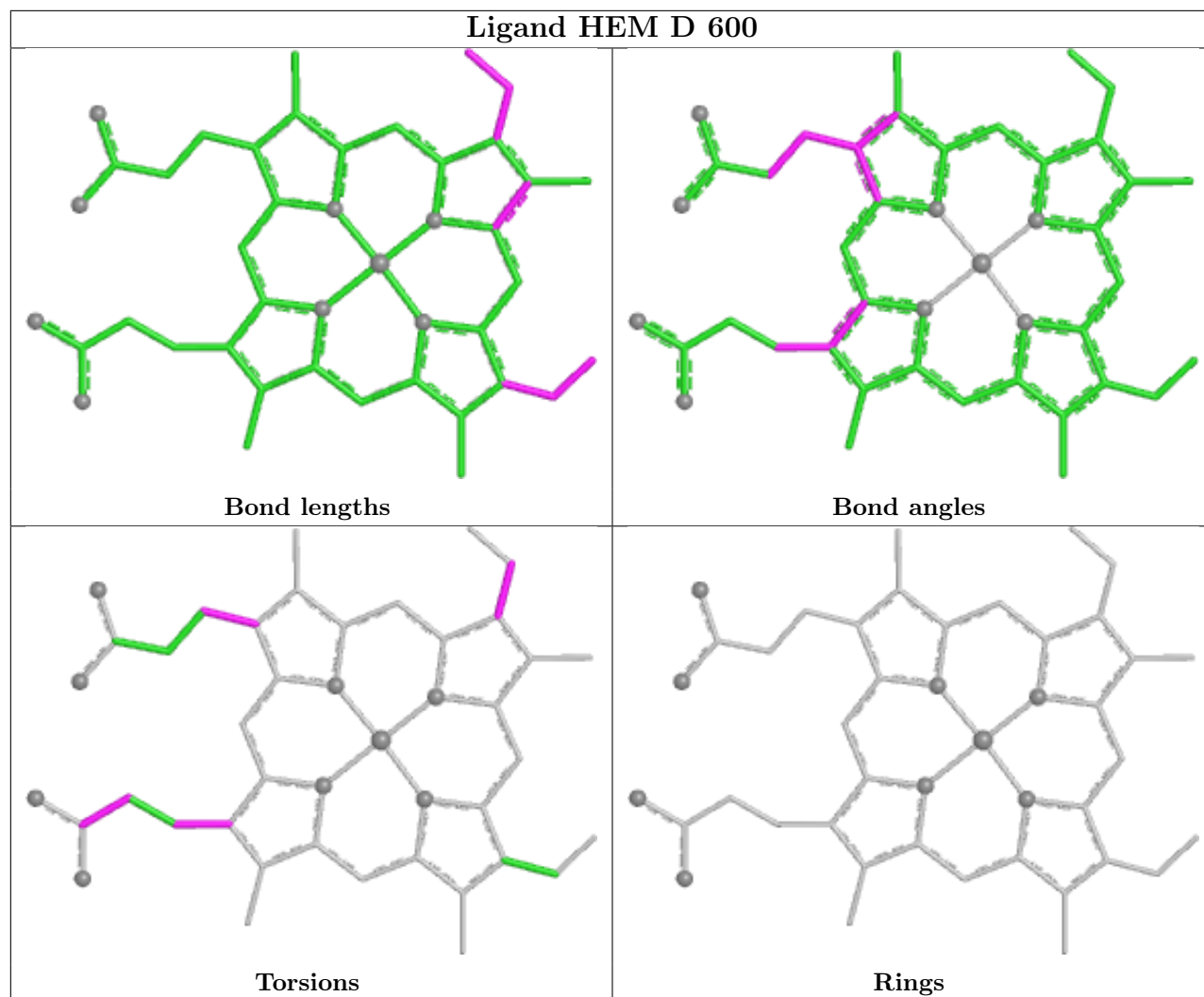
Mol	Chain	Res	Type	Atoms
2	A	600	HEM	C3A-C2A-CAA-CBA
2	C	600	HEM	C1A-C2A-CAA-CBA
2	A	600	HEM	CAD-CBD-CGD-O2D
2	D	600	HEM	CAA-CBA-CGA-O2A

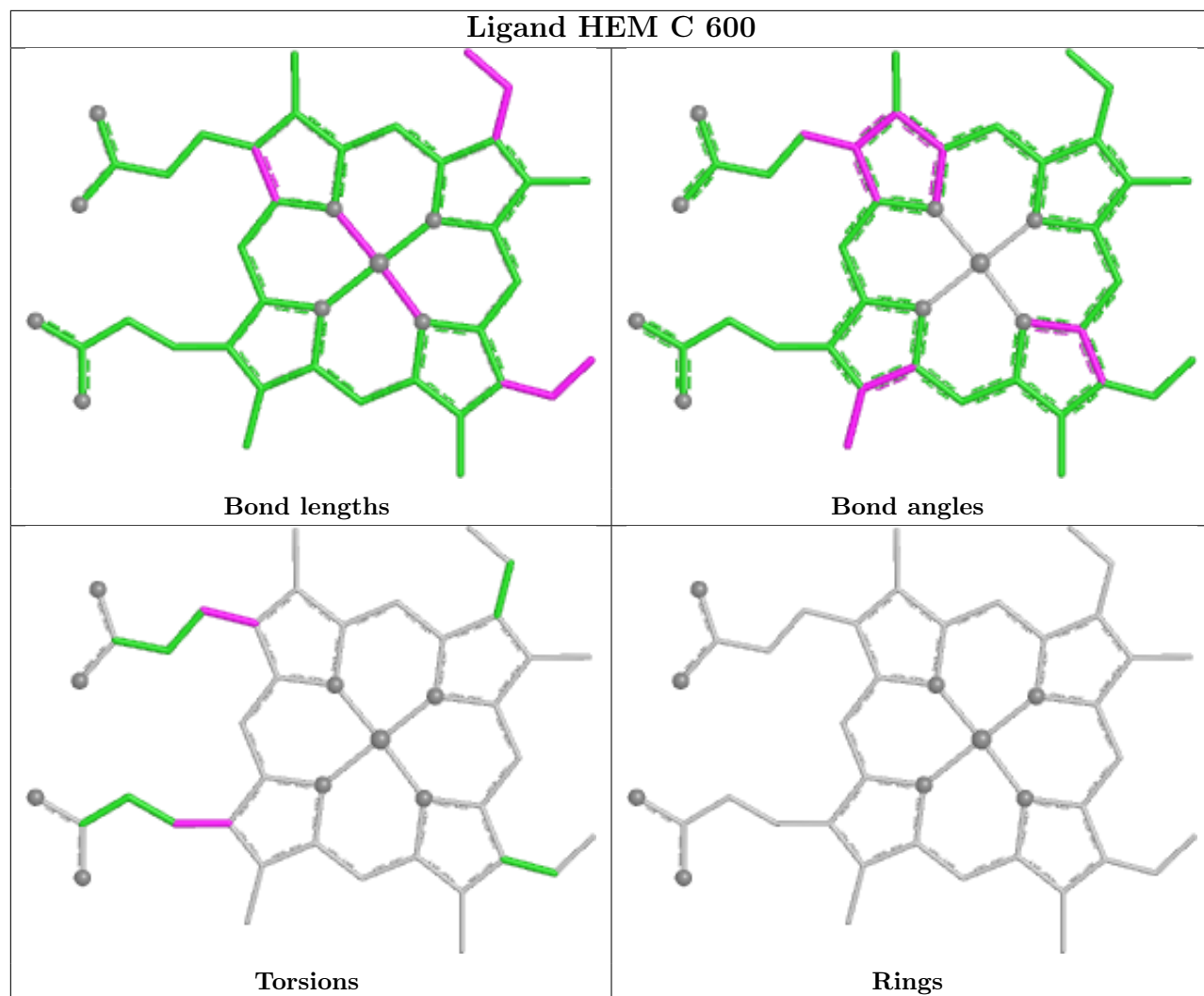
There are no ring outliers.

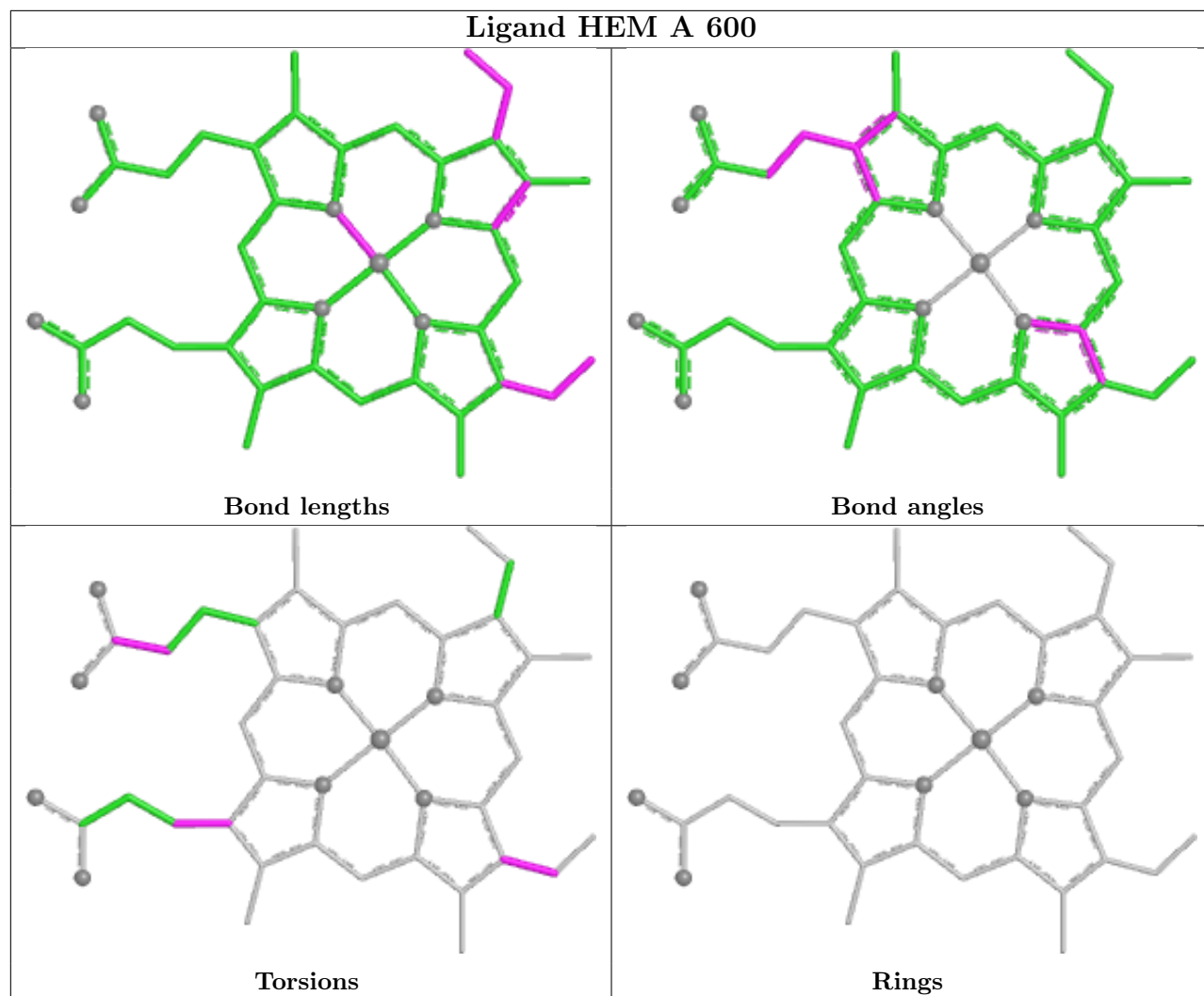
3 monomers are involved in 10 short contacts:

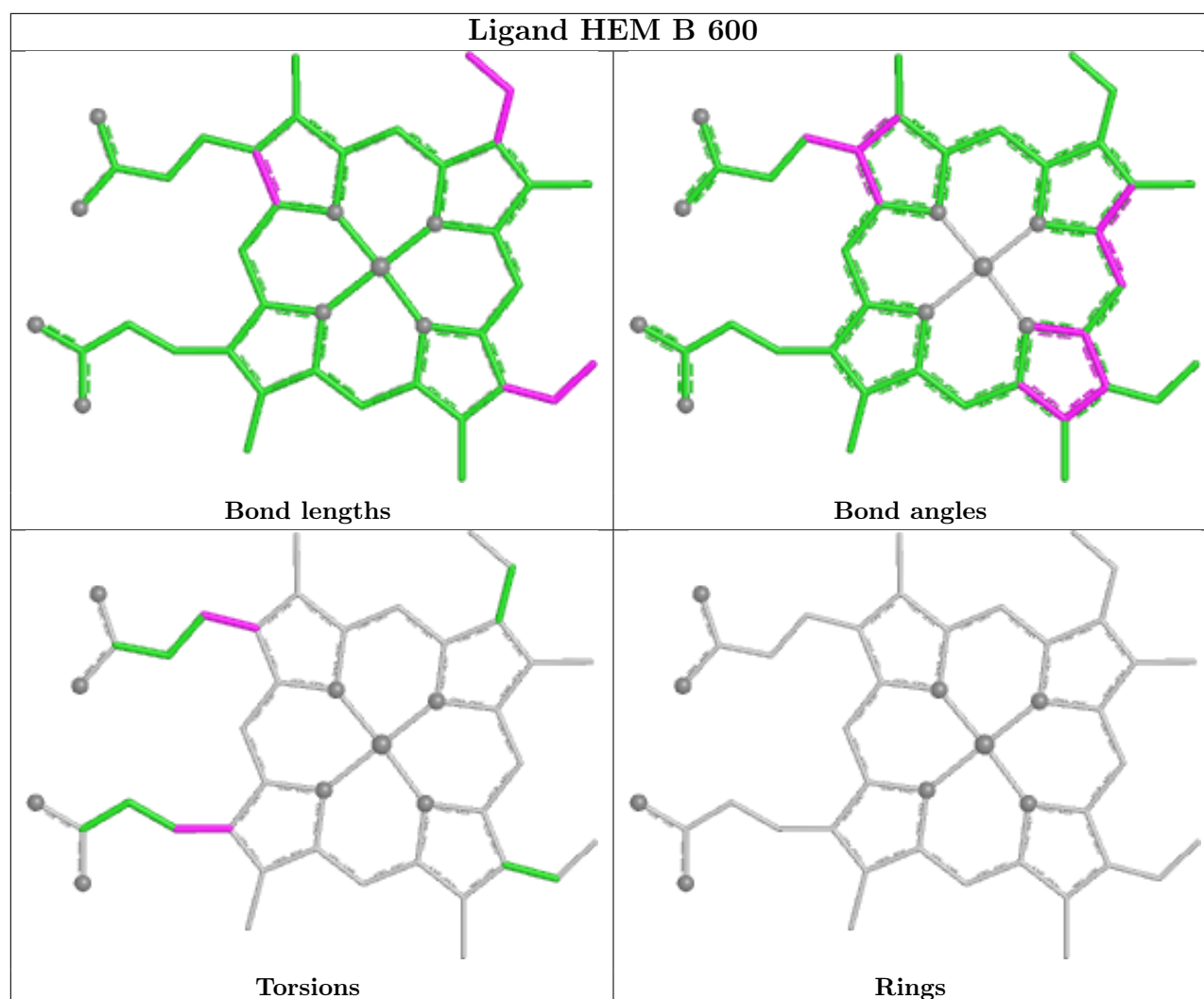
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	600	HEM	6	0
2	C	600	HEM	3	0
2	A	600	HEM	1	0

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 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	479/527 (90%)	-0.17	2 (0%) 88 86	23, 36, 53, 62	0
1	B	479/527 (90%)	-0.20	1 (0%) 91 89	24, 35, 49, 67	0
1	C	481/527 (91%)	-0.05	1 (0%) 91 89	24, 39, 55, 72	0
1	D	479/527 (90%)	-0.14	6 (1%) 75 71	26, 36, 52, 62	0
All	All	1918/2108 (90%)	-0.14	10 (0%) 87 85	23, 36, 53, 72	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	502	ALA	3.7
1	C	504	LYS	3.0
1	A	24	ALA	2.6
1	D	24	ALA	2.5
1	D	492	HIS	2.4
1	D	411	ALA	2.3
1	A	502	ALA	2.2
1	B	25	ASP	2.2
1	D	426	SER	2.1
1	D	436	ASN	2.0

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

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

6.3 Carbohydrates [i](#)

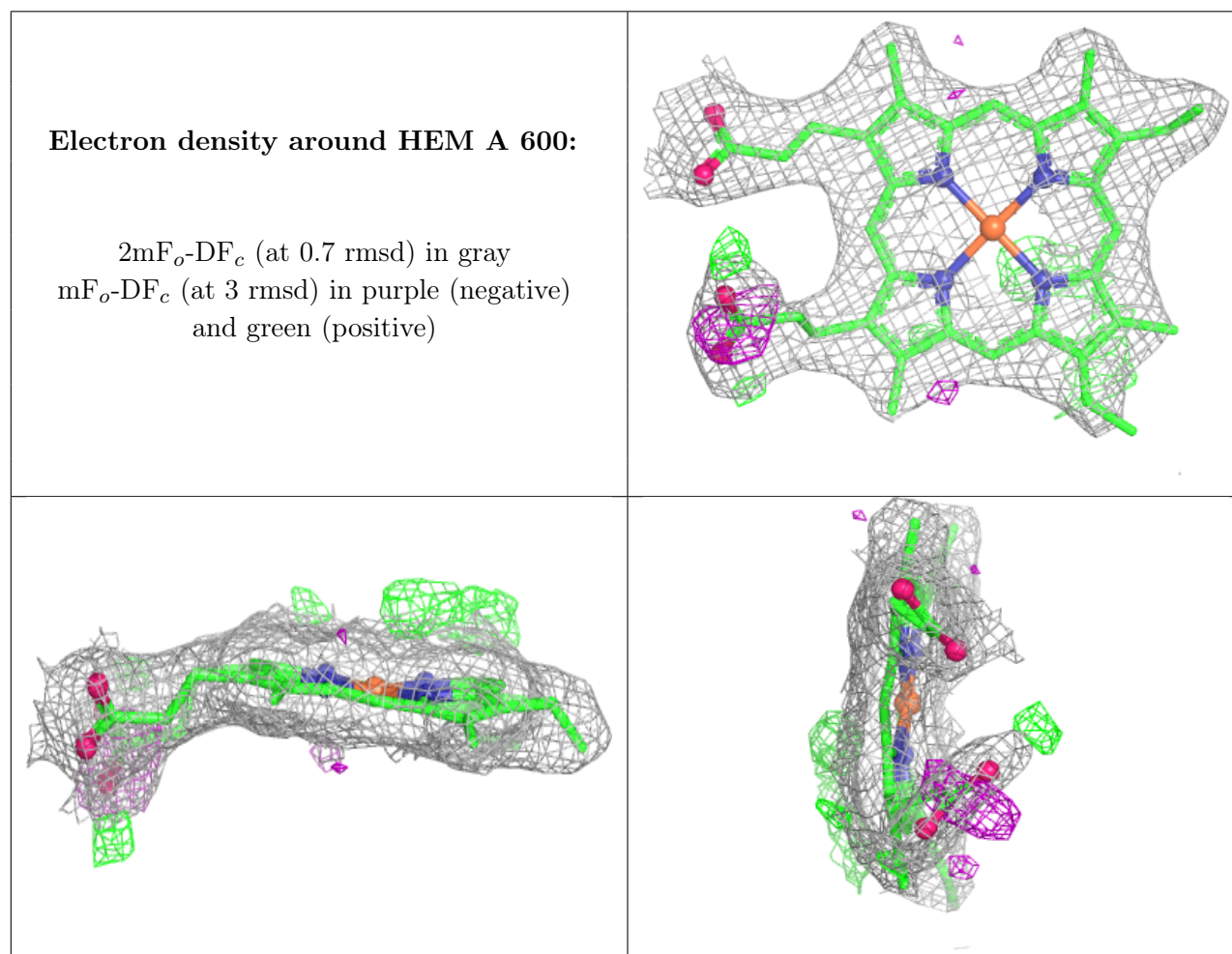
There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

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.

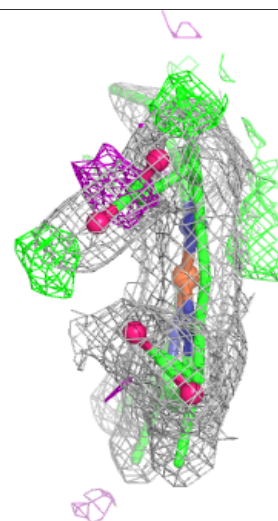
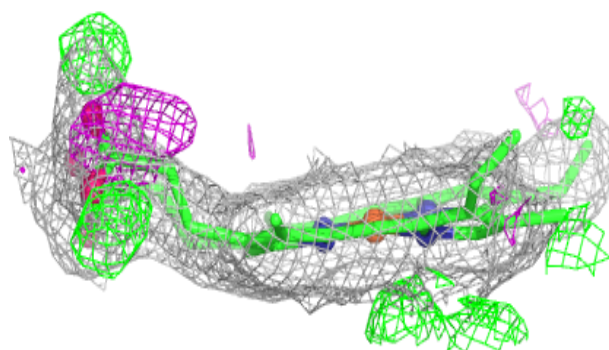
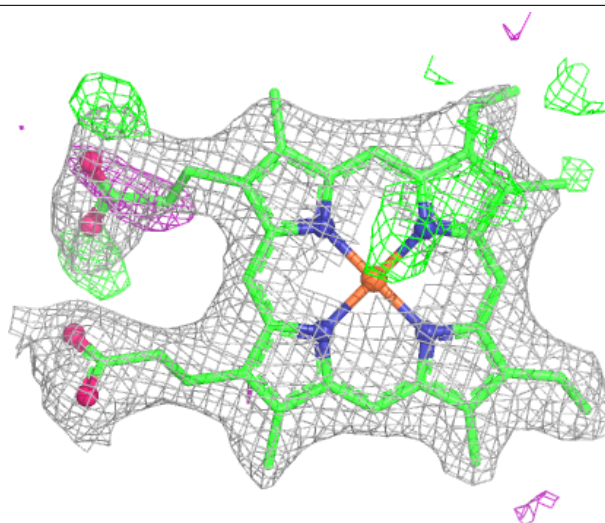
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	HEM	A	600	43/43	0.96	0.10	32,37,44,47	0
2	HEM	B	600	43/43	0.96	0.09	29,36,41,44	0
2	HEM	D	600	43/43	0.96	0.09	25,36,43,44	0
2	HEM	C	600	43/43	0.97	0.09	31,36,40,42	0

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.



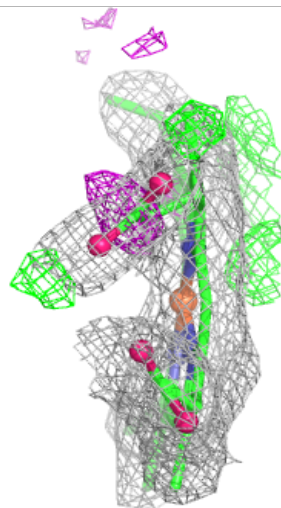
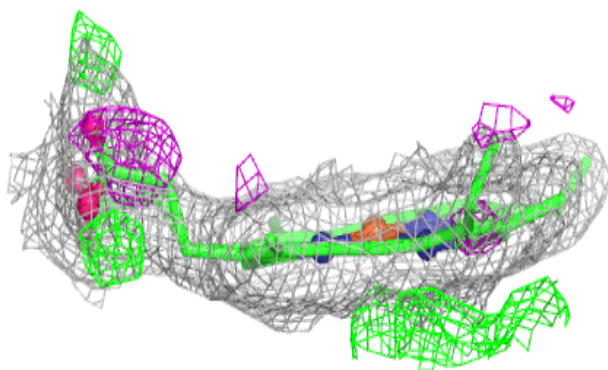
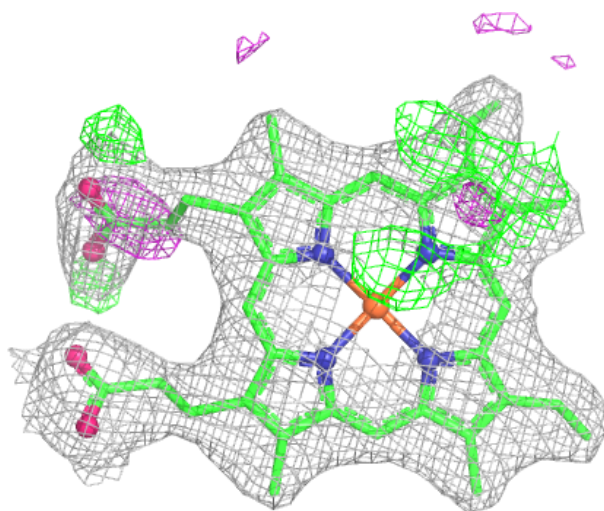
Electron density around HEM B 600:

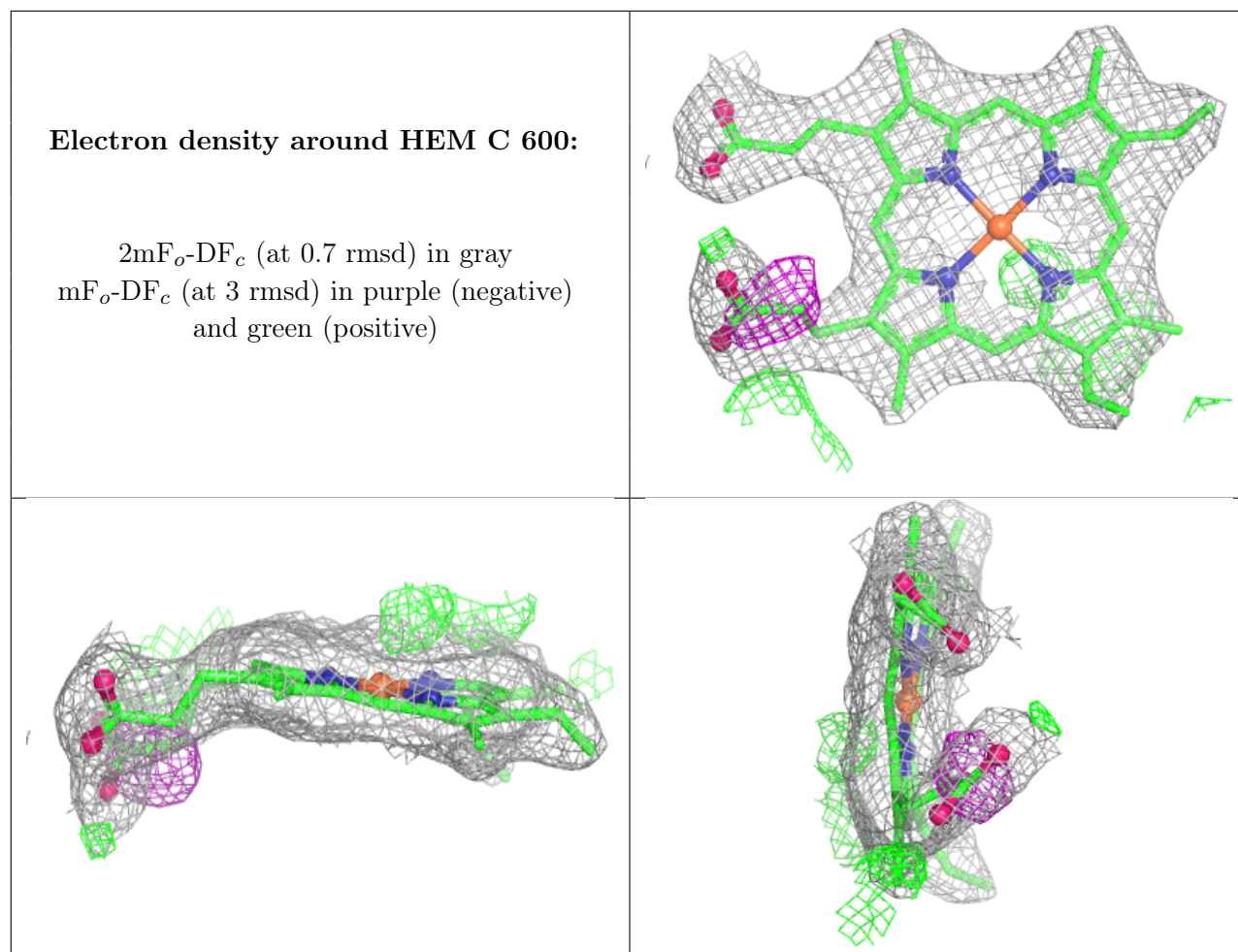
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM D 600:

$2mF_o-DF_c$ (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.