



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2026 – 05:35 PM EDT

PDB ID : 4L27 / pdb_00004l27
Title : Crystal structure of delta1-39 and delta516-525 human cystathionine beta-synthase D444N mutant containing C-terminal 6xHis tag
Authors : Ereno, J.; Majtan, T.; Oyenarte, I.; Kraus, J.P.; Martinez, L.A.
Deposited on : 2013-06-04
Resolution : 3.39 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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

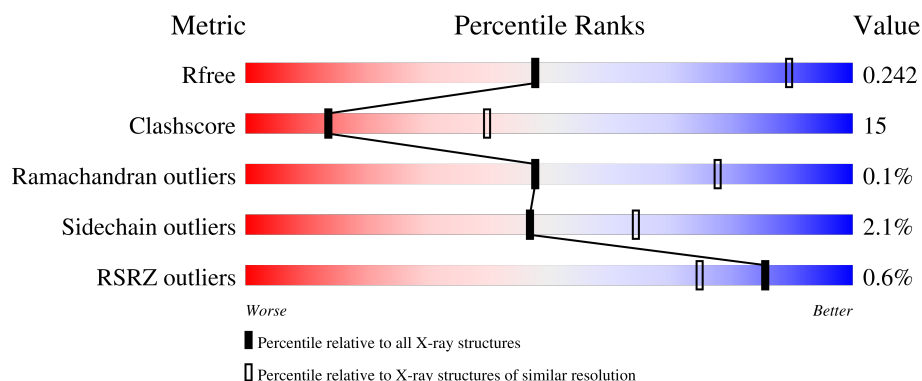
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.39 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)

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	548	64% 22% 11%
1	B	548	66% 22% 11%
1	C	548	66% 23% 10%
1	D	548	68% 21% 10%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 15361 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 Cystathionine beta-synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	490	Total	C	N	O	S	0	0	0
			3791	2402	661	706	22			
1	D	491	Total	C	N	O	S	0	0	0
			3788	2398	662	706	22			
1	A	485	Total	C	N	O	S	0	0	0
			3757	2381	656	698	22			
1	C	491	Total	C	N	O	S	0	0	0
			3793	2403	665	703	22			

There are 76 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	444	ASN	ASP	engineered mutation	UNP P35520
B	?	-	ILE	deletion	UNP P35520
B	?	-	GLN	deletion	UNP P35520
B	?	-	TYR	deletion	UNP P35520
B	?	-	HIS	deletion	UNP P35520
B	?	-	SER	deletion	UNP P35520
B	?	-	THR	deletion	UNP P35520
B	?	-	GLY	deletion	UNP P35520
B	?	-	LYS	deletion	UNP P35520
B	?	-	SER	deletion	UNP P35520
B	?	-	SER	deletion	UNP P35520
B	552	LEU	-	expression tag	UNP P35520
B	553	GLU	-	expression tag	UNP P35520
B	554	HIS	-	expression tag	UNP P35520
B	555	HIS	-	expression tag	UNP P35520
B	556	HIS	-	expression tag	UNP P35520
B	557	HIS	-	expression tag	UNP P35520
B	558	HIS	-	expression tag	UNP P35520
B	559	HIS	-	expression tag	UNP P35520
D	444	ASN	ASP	engineered mutation	UNP P35520
D	?	-	ILE	deletion	UNP P35520

Continued on next page...

Continued from previous page...

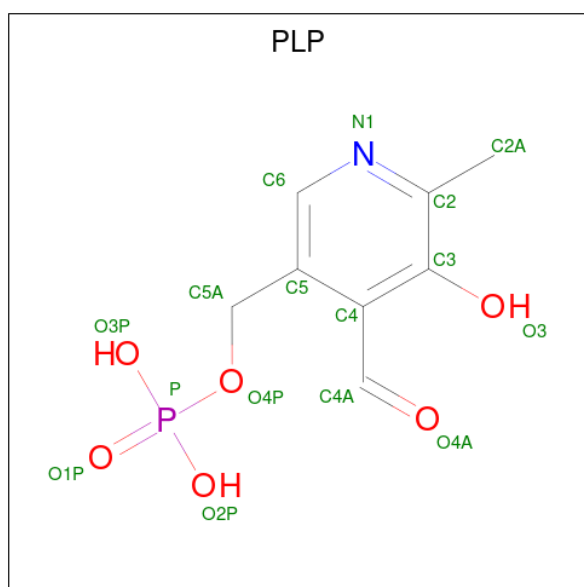
Chain	Residue	Modelled	Actual	Comment	Reference
D	?	-	GLN	deletion	UNP P35520
D	?	-	TYR	deletion	UNP P35520
D	?	-	HIS	deletion	UNP P35520
D	?	-	SER	deletion	UNP P35520
D	?	-	THR	deletion	UNP P35520
D	?	-	GLY	deletion	UNP P35520
D	?	-	LYS	deletion	UNP P35520
D	?	-	SER	deletion	UNP P35520
D	?	-	SER	deletion	UNP P35520
D	552	LEU	-	expression tag	UNP P35520
D	553	GLU	-	expression tag	UNP P35520
D	554	HIS	-	expression tag	UNP P35520
D	555	HIS	-	expression tag	UNP P35520
D	556	HIS	-	expression tag	UNP P35520
D	557	HIS	-	expression tag	UNP P35520
D	558	HIS	-	expression tag	UNP P35520
D	559	HIS	-	expression tag	UNP P35520
A	444	ASN	ASP	engineered mutation	UNP P35520
A	?	-	ILE	deletion	UNP P35520
A	?	-	GLN	deletion	UNP P35520
A	?	-	TYR	deletion	UNP P35520
A	?	-	HIS	deletion	UNP P35520
A	?	-	SER	deletion	UNP P35520
A	?	-	THR	deletion	UNP P35520
A	?	-	GLY	deletion	UNP P35520
A	?	-	LYS	deletion	UNP P35520
A	?	-	SER	deletion	UNP P35520
A	?	-	SER	deletion	UNP P35520
A	552	LEU	-	expression tag	UNP P35520
A	553	GLU	-	expression tag	UNP P35520
A	554	HIS	-	expression tag	UNP P35520
A	555	HIS	-	expression tag	UNP P35520
A	556	HIS	-	expression tag	UNP P35520
A	557	HIS	-	expression tag	UNP P35520
A	558	HIS	-	expression tag	UNP P35520
A	559	HIS	-	expression tag	UNP P35520
C	444	ASN	ASP	engineered mutation	UNP P35520
C	?	-	ILE	deletion	UNP P35520
C	?	-	GLN	deletion	UNP P35520
C	?	-	TYR	deletion	UNP P35520
C	?	-	HIS	deletion	UNP P35520
C	?	-	SER	deletion	UNP P35520

Continued on next page...

Continued from previous page...

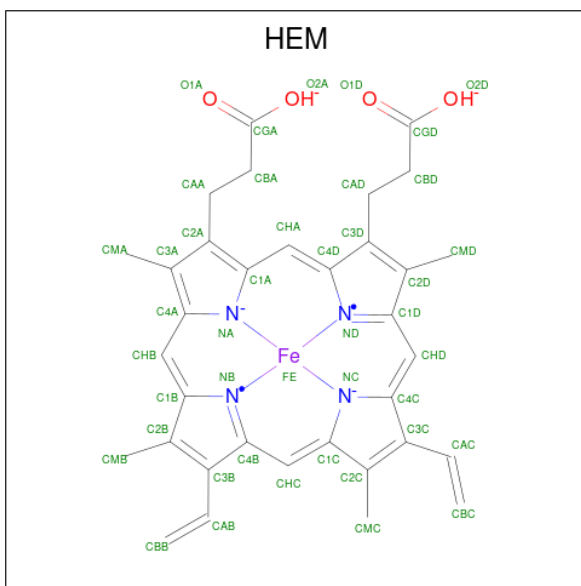
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	THR	deletion	UNP P35520
C	?	-	GLY	deletion	UNP P35520
C	?	-	LYS	deletion	UNP P35520
C	?	-	SER	deletion	UNP P35520
C	?	-	SER	deletion	UNP P35520
C	552	LEU	-	expression tag	UNP P35520
C	553	GLU	-	expression tag	UNP P35520
C	554	HIS	-	expression tag	UNP P35520
C	555	HIS	-	expression tag	UNP P35520
C	556	HIS	-	expression tag	UNP P35520
C	557	HIS	-	expression tag	UNP P35520
C	558	HIS	-	expression tag	UNP P35520
C	559	HIS	-	expression tag	UNP P35520

- Molecule 2 is PYRIDOXAL-5'-PHOSPHATE (CCD ID: PLP) (formula: $C_8H_{10}NO_6P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	D	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	A	1	Total	C	N	O	P	0	0
			15	8	1	5	1		
2	C	1	Total	C	N	O	P	0	0
			15	8	1	5	1		

- Molecule 3 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula:

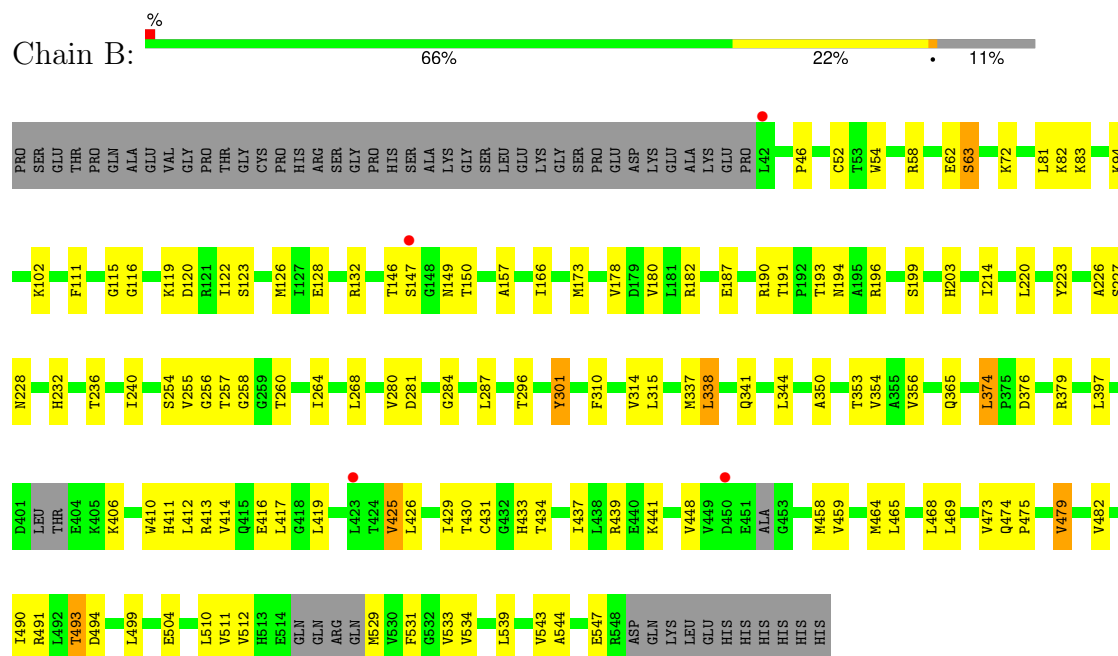
$$\text{C}_{34}\text{H}_{32}\text{FeN}_4\text{O}_4).$$


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

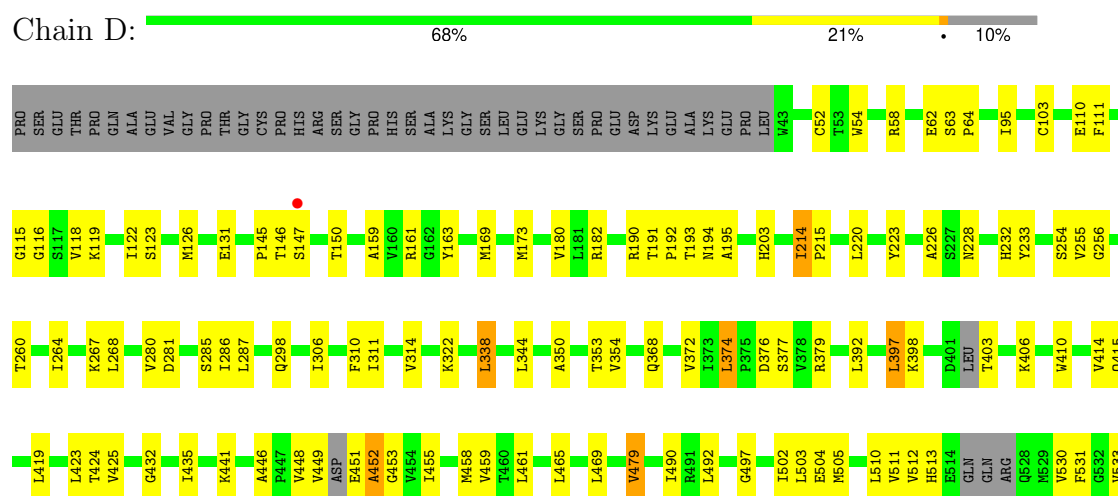
3 Residue-property plots [i](#)

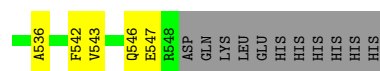
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

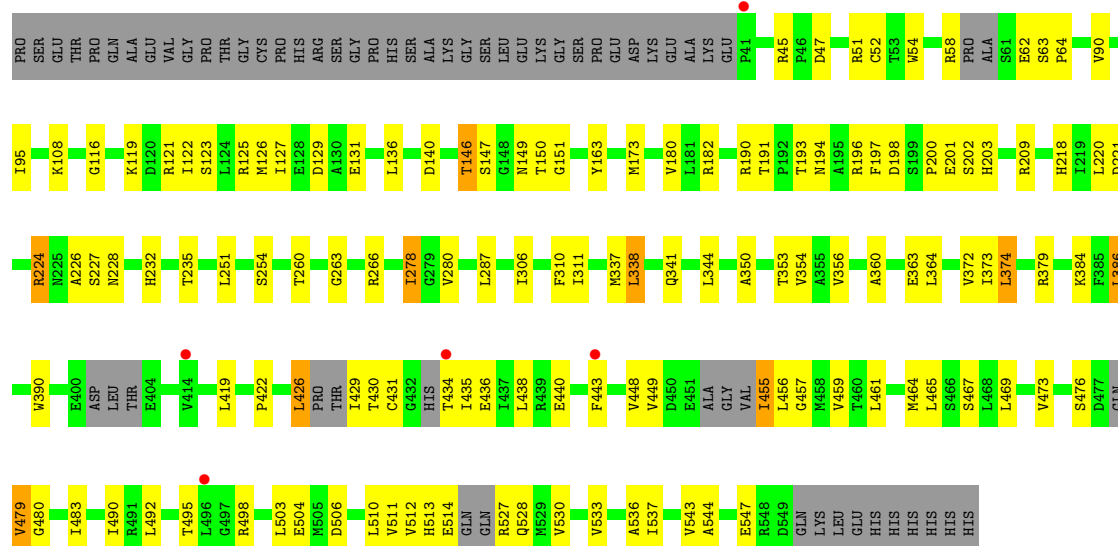


• Molecule 1: Cystathionine beta-synthase

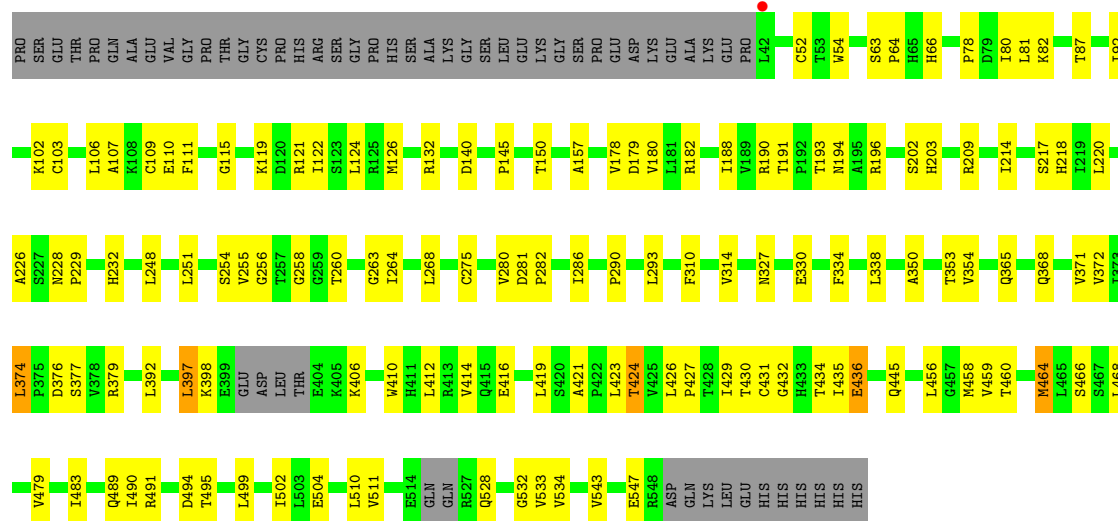




• Molecule 1: Cystathionine beta-synthase



• Molecule 1: Cystathionine beta-synthase



4 Data and refinement statistics

Property	Value	Source
Space group	P 65	Depositor
Cell constants a, b, c, α , β , γ	190.45Å 190.45Å 140.85Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	56.62 – 3.39 56.62 – 3.39	Depositor EDS
% Data completeness (in resolution range)	99.7 (56.62-3.39) 99.3 (56.62-3.39)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.85 (at 3.40Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.8.1_1168)	Depositor
R, R_{free}	0.206 , 0.244 0.207 , 0.242	Depositor DCC
R_{free} test set	2009 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	120.5	Xtriage
Anisotropy	0.195	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 62.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.25$	Xtriage
Estimated twinning fraction	0.079 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	15361	wwPDB-VP
Average B, all atoms (Å ²)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.35% 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, PLP

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	0.40	1/3820 (0.0%)	0.95	10/5157 (0.2%)
1	B	0.38	0/3861	0.88	9/5225 (0.2%)
1	C	0.40	0/3864	0.92	7/5230 (0.1%)
1	D	0.38	1/3858 (0.0%)	0.89	12/5220 (0.2%)
All	All	0.39	2/15403 (0.0%)	0.91	38/20832 (0.2%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	SER	C-N	6.89	1.42	1.33
1	D	116	GLY	C-N	-6.66	1.25	1.33

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	116	GLY	O-C-N	-12.63	108.48	122.50
1	A	123	SER	O-C-N	-10.28	110.99	122.09
1	A	116	GLY	CA-C-N	9.51	137.61	122.21
1	A	116	GLY	C-N-CA	9.51	137.61	122.21
1	C	124	LEU	O-C-N	-9.18	112.62	122.07
1	C	124	LEU	CA-C-N	8.97	132.49	120.65
1	C	124	LEU	C-N-CA	8.97	132.49	120.65
1	D	116	GLY	O-C-N	-8.96	112.56	122.50
1	B	123	SER	O-C-N	-8.10	113.34	122.09
1	C	374	LEU	CA-C-N	7.33	126.59	118.97
1	C	374	LEU	C-N-CA	7.33	126.59	118.97
1	B	374	LEU	CA-C-N	7.21	126.47	118.97
1	B	374	LEU	C-N-CA	7.21	126.47	118.97
1	D	123	SER	O-C-N	-6.67	114.89	122.09
1	D	116	GLY	CA-C-N	6.66	133.00	122.21

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	116	GLY	C-N-CA	6.66	133.00	122.21
1	B	63	SER	CA-C-N	6.56	126.26	119.64
1	B	63	SER	C-N-CA	6.56	126.26	119.64
1	D	63	SER	CA-C-N	6.48	126.11	119.56
1	D	63	SER	C-N-CA	6.48	126.11	119.56
1	D	374	LEU	CA-C-N	6.23	125.45	118.97
1	D	374	LEU	C-N-CA	6.23	125.45	118.97
1	A	374	LEU	CA-C-N	6.01	125.22	118.97
1	A	374	LEU	C-N-CA	6.01	125.22	118.97
1	C	63	SER	CA-C-N	5.93	125.55	119.56
1	C	63	SER	C-N-CA	5.93	125.55	119.56
1	A	457	GLY	N-CA-C	5.92	118.57	110.58
1	A	123	SER	CA-C-N	5.75	127.92	120.44
1	A	123	SER	C-N-CA	5.75	127.92	120.44
1	D	214	ILE	N-CA-C	5.70	114.23	107.73
1	B	255	VAL	N-CA-C	5.51	115.92	107.77
1	D	255	VAL	N-CA-C	5.43	115.81	107.77
1	D	298	GLN	N-CA-C	5.42	117.53	110.43
1	B	116	GLY	O-C-N	-5.42	116.49	122.50
1	A	146	THR	N-CA-C	5.36	116.99	108.79
1	B	214	ILE	N-CA-C	5.22	113.58	107.89
1	D	146	THR	N-CA-C	5.04	116.50	108.79
1	B	146	THR	N-CA-C	5.03	116.49	108.79

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	3757	0	3811	143	1
1	B	3791	0	3845	101	0
1	C	3793	0	3849	112	1
1	D	3788	0	3832	96	0
2	A	15	0	7	3	0
2	B	15	0	7	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	15	0	7	2	0
2	D	15	0	7	1	0
3	A	43	0	30	15	0
3	B	43	0	30	12	0
3	C	43	0	30	14	0
3	D	43	0	30	9	0
All	All	15361	0	15485	451	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (451) 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:431:CYS:SG	1:A:464:MET:HE1	1.47	1.53
1:B:178:VAL:CG2	1:B:190:ARG:HH21	1.36	1.39
1:B:178:VAL:HG21	1:B:190:ARG:NH2	1.29	1.38
1:B:178:VAL:CG2	1:B:190:ARG:NH2	1.94	1.24
1:A:431:CYS:SG	1:A:464:MET:CE	2.32	1.18
1:A:480:GLY:HA2	1:A:483:ILE:CD1	1.73	1.17
1:B:439:ARG:NH2	1:B:465:LEU:HD21	1.61	1.16
1:A:492:LEU:HD23	1:A:511:VAL:HG21	1.15	1.08
1:A:479:VAL:O	1:A:483:ILE:HG13	1.54	1.07
1:A:58:ARG:NE	1:A:62:GLU:OE2	1.86	1.07
1:A:480:GLY:HA2	1:A:483:ILE:HD12	1.01	1.01
1:B:178:VAL:HG22	1:B:190:ARG:HH21	1.26	0.98
1:A:480:GLY:CA	1:A:483:ILE:HD12	1.93	0.98
1:D:264:ILE:O	1:D:268:LEU:HD13	1.63	0.96
1:B:439:ARG:HH21	1:B:465:LEU:HD21	1.20	0.95
1:D:451:GLU:O	1:D:453:GLY:N	2.00	0.95
3:A:602:HEM:HBD1	3:A:602:HEM:HH A	1.45	0.95
1:B:178:VAL:HG21	1:B:190:ARG:HH22	1.23	0.94
1:C:264:ILE:O	1:C:268:LEU:HD13	1.66	0.93
1:A:232:HIS:HD2	1:A:260:THR:HA	1.32	0.92
1:A:429:ILE:HD11	1:A:434:THR:CG2	2.01	0.90
1:D:419:LEU:HD12	1:D:511:VAL:HG11	1.53	0.90
1:C:431:CYS:SG	1:C:435:ILE:HD11	2.12	0.90
1:A:465:LEU:O	1:A:469:LEU:HD13	1.71	0.89
1:A:492:LEU:HD23	1:A:511:VAL:CG2	2.02	0.89
1:B:264:ILE:O	1:B:268:LEU:HD13	1.74	0.88
1:B:54:TRP:HD1	3:B:602:HEM:CBB	1.87	0.88

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:467:SER:C	1:A:473:VAL:HG12	1.99	0.87
1:A:492:LEU:CD2	1:A:511:VAL:HG21	2.01	0.87
1:C:431:CYS:O	1:C:435:ILE:HG13	1.74	0.86
1:B:63:SER:HB2	3:B:602:HEM:HAB	1.59	0.84
1:D:419:LEU:CD1	1:D:511:VAL:HG11	2.07	0.84
3:A:602:HEM:HHA	3:A:602:HEM:CBD	2.06	0.83
1:C:397:LEU:HD13	1:C:397:LEU:C	2.04	0.82
1:A:260:THR:OG1	2:A:601:PLP:O1P	1.98	0.82
1:A:429:ILE:CD1	1:A:434:THR:CG2	2.57	0.82
1:A:429:ILE:HD11	1:A:434:THR:HG22	1.61	0.80
1:A:232:HIS:CD2	1:A:260:THR:HA	2.16	0.80
1:D:392:LEU:CD2	1:D:397:LEU:HD12	2.12	0.79
1:C:334:PHE:O	1:C:338:LEU:HD23	1.82	0.79
3:B:602:HEM:HBD1	3:B:602:HEM:HHA	1.65	0.79
1:B:54:TRP:CD1	3:B:602:HEM:HBB2	2.17	0.78
1:D:397:LEU:C	1:D:397:LEU:HD13	2.09	0.78
1:B:193:THR:O	1:B:194:ASN:OD1	2.02	0.77
1:D:392:LEU:HD21	1:D:397:LEU:HD12	1.66	0.77
1:A:449:VAL:HG22	1:A:455:ILE:HG12	1.64	0.77
1:C:334:PHE:O	1:C:338:LEU:CD2	2.33	0.77
1:A:126:MET:HE2	1:A:220:LEU:HB3	1.67	0.76
1:A:58:ARG:HH11	1:A:62:GLU:CD	1.93	0.75
1:A:350:ALA:HB1	1:A:374:LEU:HD22	1.69	0.74
1:A:426:LEU:HD13	1:A:426:LEU:C	2.13	0.74
1:C:397:LEU:HD13	1:C:398:LYS:O	1.88	0.73
1:D:490:ILE:HD12	1:D:502:ILE:HD12	1.71	0.72
1:C:126:MET:HE2	1:C:220:LEU:HB3	1.71	0.72
1:C:464:MET:O	1:C:468:LEU:HD13	1.89	0.72
3:B:602:HEM:HHA	3:B:602:HEM:CBD	2.21	0.71
1:A:429:ILE:CD1	1:A:434:THR:HG22	2.18	0.70
1:C:256:GLY:HA3	2:C:601:PLP:H5A1	1.74	0.70
1:B:54:TRP:CD1	3:B:602:HEM:CBB	2.72	0.70
1:B:193:THR:O	1:B:194:ASN:CG	2.35	0.70
1:A:430:THR:OG1	1:A:476:SER:O	2.10	0.69
1:A:467:SER:HB3	1:A:473:VAL:CG1	2.22	0.69
1:B:58:ARG:NE	1:B:62:GLU:OE1	2.25	0.69
1:B:126:MET:HE2	1:B:220:LEU:HB3	1.75	0.68
1:A:147:SER:HA	1:A:173:MET:HE3	1.75	0.68
1:A:512:VAL:HG12	1:A:513:HIS:N	2.06	0.68
1:C:232:HIS:CD2	1:C:260:THR:HA	2.29	0.68
1:D:122:ILE:O	1:D:126:MET:HG3	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:543:VAL:O	1:C:547:GLU:HG3	1.93	0.68
1:C:397:LEU:HD13	1:C:398:LYS:C	2.19	0.68
1:A:419:LEU:CD1	1:A:511:VAL:HG11	2.23	0.67
1:A:431:CYS:HG	1:A:464:MET:CE	2.08	0.67
1:C:423:LEU:HD12	1:C:424:THR:H	1.59	0.67
1:A:430:THR:HG1	1:A:476:SER:C	2.03	0.67
1:D:350:ALA:HB1	1:D:374:LEU:HD22	1.76	0.67
1:A:434:THR:HG21	1:A:479:VAL:HG21	1.77	0.67
1:C:412:LEU:HB3	1:C:416:GLU:OE1	1.95	0.67
1:C:431:CYS:O	1:C:435:ILE:CG1	2.42	0.66
1:D:191:THR:HG21	1:D:203:HIS:HA	1.78	0.66
3:D:602:HEM:HMB1	3:D:602:HEM:HBB2	1.77	0.66
1:D:451:GLU:N	1:D:451:GLU:OE2	2.30	0.65
1:B:232:HIS:CD2	1:B:260:THR:HA	2.31	0.65
1:D:119:LYS:HD2	1:D:150:THR:OG1	1.96	0.65
1:A:182:ARG:NH1	1:C:504:GLU:OE1	2.30	0.64
1:A:479:VAL:C	1:A:483:ILE:HG13	2.22	0.64
1:D:126:MET:HE2	1:D:220:LEU:HB3	1.80	0.64
1:A:459:VAL:HG11	1:A:479:VAL:HG13	1.78	0.64
1:C:81:LEU:HD21	1:C:157:ALA:HA	1.80	0.64
1:C:263:GLY:HA2	3:C:602:HEM:HBC1	1.79	0.64
1:A:480:GLY:CA	1:A:483:ILE:CD1	2.62	0.64
1:A:191:THR:HG21	1:A:203:HIS:HA	1.80	0.64
1:D:58:ARG:NE	1:D:62:GLU:OE1	2.31	0.63
1:A:180:VAL:HG21	1:A:379:ARG:NH1	2.13	0.63
1:A:363:GLU:CG	1:A:364:LEU:N	2.62	0.63
1:D:232:HIS:CD2	1:D:260:THR:HA	2.33	0.63
1:A:51:ARG:C	1:A:52:CYS:CA	2.71	0.63
1:D:465:LEU:O	1:D:469:LEU:HD13	1.98	0.63
3:C:602:HEM:HBD2	3:C:602:HEM:HHHA	1.80	0.63
1:C:392:LEU:CD2	1:C:397:LEU:HD12	2.29	0.63
1:D:397:LEU:HD13	1:D:398:LYS:O	1.98	0.62
1:D:451:GLU:C	1:D:453:GLY:N	2.54	0.62
1:A:254:SER:HB3	1:A:306:ILE:HG21	1.81	0.62
1:A:429:ILE:CD1	1:A:434:THR:HG23	2.28	0.62
1:C:397:LEU:C	1:C:397:LEU:CD1	2.72	0.62
1:C:350:ALA:HB1	1:C:374:LEU:HD22	1.80	0.62
1:D:147:SER:HA	1:D:173:MET:HE3	1.81	0.62
1:B:94:LYS:NZ	1:D:159:ALA:O	2.33	0.62
1:D:264:ILE:O	1:D:268:LEU:CD1	2.43	0.62
1:D:451:GLU:C	1:D:453:GLY:H	2.08	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:LEU:HD12	1:A:344:LEU:HD12	1.82	0.62
1:B:350:ALA:HB1	1:B:374:LEU:HD22	1.80	0.61
1:C:406:LYS:HE3	1:C:410:TRP:CE2	2.35	0.61
1:A:467:SER:HB3	1:A:473:VAL:HG12	1.82	0.61
1:B:254:SER:HA	1:B:280:VAL:HB	1.82	0.61
1:D:415:GLN:HB3	1:D:492:LEU:HB3	1.82	0.61
1:A:363:GLU:HG3	1:A:364:LEU:N	2.16	0.60
1:A:512:VAL:HG12	1:A:513:HIS:H	1.66	0.60
1:C:64:PRO:HG3	3:C:602:HEM:HMA1	1.83	0.60
1:C:226:ALA:HA	3:C:602:HEM:HMD2	1.83	0.60
1:A:140:ASP:OD2	1:A:218:HIS:NE2	2.29	0.60
1:B:430:THR:OG1	1:B:475:PRO:O	2.18	0.60
3:A:602:HEM:HBA2	3:A:602:HEM:HBD2	1.83	0.60
1:A:430:THR:OG1	1:A:476:SER:C	2.45	0.60
1:C:412:LEU:HD22	1:C:416:GLU:OE1	2.01	0.60
1:C:458:MET:HE1	1:C:533:VAL:HG11	1.83	0.60
1:B:543:VAL:O	1:B:547:GLU:HG2	2.02	0.60
1:A:122:ILE:HG21	1:A:228:ASN:OD1	2.02	0.60
1:C:226:ALA:HA	3:C:602:HEM:CMD	2.31	0.60
1:D:254:SER:HA	1:D:280:VAL:HB	1.84	0.60
1:D:397:LEU:C	1:D:397:LEU:CD1	2.75	0.59
1:C:264:ILE:O	1:C:268:LEU:CD1	2.44	0.59
1:A:543:VAL:O	1:A:547:GLU:HG2	2.03	0.59
1:A:363:GLU:CG	1:A:364:LEU:HD12	2.32	0.59
1:A:480:GLY:HA2	1:A:483:ILE:CG1	2.30	0.59
1:C:122:ILE:O	1:C:126:MET:HG3	2.02	0.59
1:C:229:PRO:HB2	3:C:602:HEM:HAC	1.85	0.59
1:B:63:SER:CB	3:B:602:HEM:HAB	2.33	0.59
1:D:510:LEU:HD22	1:D:533:VAL:HG12	1.85	0.59
1:A:467:SER:CB	1:A:473:VAL:CG1	2.81	0.58
1:B:490:ILE:HG22	1:B:491:ARG:O	2.03	0.58
1:B:226:ALA:HA	3:B:602:HEM:HMD2	1.84	0.58
1:C:464:MET:O	1:C:468:LEU:CD1	2.50	0.58
1:D:397:LEU:HD13	1:D:398:LYS:C	2.29	0.58
1:C:191:THR:HG21	1:C:203:HIS:HA	1.85	0.58
1:B:510:LEU:HD22	1:B:533:VAL:HG22	1.85	0.58
1:B:431:CYS:O	1:B:434:THR:OG1	2.17	0.58
3:D:602:HEM:HBD2	3:D:602:HEM:HHA	1.86	0.58
1:A:338:LEU:HD21	1:A:354:VAL:HG21	1.84	0.57
1:B:122:ILE:O	1:B:126:MET:HG3	2.04	0.57
1:C:490:ILE:HD12	1:C:502:ILE:HD12	1.86	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LYS:HB3	1:B:150:THR:HA	1.86	0.57
1:A:193:THR:O	1:A:194:ASN:ND2	2.36	0.57
1:B:147:SER:HA	1:B:173:MET:HE3	1.86	0.57
1:C:122:ILE:HG21	1:C:228:ASN:OD1	2.04	0.57
1:B:434:THR:HG21	1:B:479:VAL:HG21	1.87	0.57
1:D:54:TRP:HD1	3:D:602:HEM:HAB	1.69	0.57
1:B:196:ARG:O	1:B:199:SER:OG	2.23	0.56
1:C:431:CYS:SG	1:C:435:ILE:CD1	2.89	0.56
1:C:119:LYS:HB3	1:C:150:THR:HA	1.87	0.56
1:C:254:SER:HA	1:C:280:VAL:HB	1.87	0.56
1:A:512:VAL:CG1	1:A:513:HIS:H	2.18	0.56
1:D:256:GLY:HA3	2:D:601:PLP:H5A1	1.88	0.56
1:D:193:THR:O	1:D:194:ASN:ND2	2.39	0.56
1:A:449:VAL:HG22	1:A:455:ILE:CG1	2.34	0.56
1:A:512:VAL:CG1	1:A:513:HIS:N	2.68	0.56
1:D:403:THR:HA	1:D:406:LYS:HD2	1.88	0.56
1:C:419:LEU:HD21	1:C:534:VAL:HG22	1.88	0.56
1:C:429:ILE:HG23	1:C:434:THR:OG1	2.06	0.56
1:A:200:PRO:HB2	1:A:209:ARG:NH1	2.21	0.55
1:C:334:PHE:O	1:C:338:LEU:HD22	2.06	0.55
1:D:423:LEU:HD22	1:D:441:LYS:HD2	1.87	0.55
1:D:338:LEU:HD21	1:D:354:VAL:HG21	1.87	0.55
1:C:54:TRP:HD1	3:C:602:HEM:CAB	2.20	0.55
1:B:431:CYS:HB3	1:B:464:MET:SD	2.46	0.55
1:A:504:GLU:OE1	1:C:182:ARG:NH1	2.40	0.55
1:B:102:LYS:HB2	1:B:365:GLN:HA	1.88	0.55
1:C:52:CYS:HA	3:C:602:HEM:C1A	2.42	0.55
1:A:467:SER:O	1:A:473:VAL:HG12	2.06	0.54
1:B:264:ILE:O	1:B:268:LEU:CD1	2.52	0.54
1:A:422:PRO:HA	1:A:443:PHE:CE2	2.42	0.54
1:A:426:LEU:C	1:A:426:LEU:CD1	2.80	0.54
1:B:264:ILE:CG2	1:B:268:LEU:HD13	2.37	0.54
1:A:467:SER:CB	1:A:473:VAL:HG12	2.38	0.54
1:A:492:LEU:CD2	1:A:511:VAL:CG2	2.74	0.54
1:A:54:TRP:HD1	3:A:602:HEM:CBB	2.20	0.54
1:C:459:VAL:HG12	1:C:483:ILE:HA	1.90	0.54
1:B:191:THR:HG21	1:B:203:HIS:HA	1.89	0.54
1:C:78:PRO:HG2	1:C:82:LYS:HD3	1.90	0.54
1:D:122:ILE:HG21	1:D:228:ASN:OD1	2.08	0.53
1:A:278:ILE:HD12	1:A:360:ALA:HB1	1.88	0.53
1:D:406:LYS:HD3	1:D:410:TRP:CE2	2.43	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:GLU:O	1:B:132:ARG:HG3	2.08	0.53
1:B:439:ARG:HH22	1:B:465:LEU:HD21	1.65	0.53
1:B:490:ILE:HG22	1:B:491:ARG:N	2.23	0.53
1:B:264:ILE:HG22	1:B:268:LEU:HD13	1.89	0.53
1:B:429:ILE:HD11	1:B:433:HIS:ND1	2.24	0.53
1:B:119:LYS:HD2	1:B:150:THR:OG1	2.08	0.53
1:A:510:LEU:HD22	1:A:533:VAL:HG22	1.91	0.53
3:A:602:HEM:HHA	3:A:602:HEM:HBA2	1.91	0.53
1:D:419:LEU:CD1	1:D:511:VAL:CG1	2.84	0.52
1:A:196:ARG:O	1:A:202:SER:HB3	2.09	0.52
1:A:436:GLU:O	1:A:440:GLU:HB2	2.10	0.52
1:D:111:PHE:HB2	1:D:377:SER:HB3	1.90	0.52
1:B:458:MET:HE1	1:B:510:LEU:HD21	1.92	0.52
3:A:602:HEM:HBD1	3:A:602:HEM:CHA	2.19	0.52
1:B:433:HIS:O	1:B:437:ILE:HG12	2.10	0.52
1:D:119:LYS:HB3	1:D:150:THR:HA	1.90	0.52
1:A:527:ARG:HG3	1:A:528:GLN:H	1.73	0.52
1:D:353:THR:HG22	1:D:372:VAL:HG13	1.92	0.51
1:D:543:VAL:O	1:D:547:GLU:HG3	2.10	0.51
1:B:256:GLY:HA3	2:B:601:PLP:H5A1	1.91	0.51
1:B:490:ILE:CG2	1:B:491:ARG:N	2.72	0.51
1:B:284:GLY:HA2	1:B:296:THR:HG21	1.93	0.51
1:A:514:GLU:C	1:A:527:ARG:HH21	2.18	0.51
1:A:465:LEU:O	1:A:469:LEU:CD1	2.51	0.51
1:C:193:THR:HG22	1:C:194:ASN:N	2.25	0.51
1:B:182:ARG:NH1	1:D:504:GLU:OE1	2.43	0.51
1:A:226:ALA:HA	3:A:602:HEM:HMD2	1.93	0.51
1:A:449:VAL:HG22	1:A:455:ILE:HA	1.92	0.51
1:B:226:ALA:HA	3:B:602:HEM:CMD	2.41	0.51
1:A:119:LYS:HG3	1:A:149:ASN:CB	2.41	0.51
1:B:414:VAL:HG23	1:B:417:LEU:HD12	1.92	0.51
1:A:119:LYS:HB3	1:A:150:THR:HA	1.91	0.51
1:C:132:ARG:HG2	1:C:132:ARG:HH11	1.75	0.51
1:A:490:ILE:O	1:A:511:VAL:HA	2.11	0.51
1:A:122:ILE:O	1:A:126:MET:HG3	2.10	0.51
1:C:193:THR:O	1:C:194:ASN:ND2	2.43	0.51
1:A:126:MET:HG2	1:A:227:SER:HB2	1.93	0.50
1:A:149:ASN:ND2	2:A:601:PLP:H2A1	2.27	0.50
3:C:602:HEM:HMC2	3:C:602:HEM:HBC2	1.93	0.50
1:B:411:HIS:O	1:B:412:LEU:HG	2.11	0.50
1:D:338:LEU:HD12	1:D:344:LEU:HD12	1.92	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:397:LEU:CD1	1:C:398:LYS:O	2.59	0.50
1:B:459:VAL:HG11	1:B:479:VAL:HG13	1.93	0.50
1:D:131:GLU:OE2	1:D:161:ARG:NH1	2.44	0.50
1:D:264:ILE:HG23	1:D:268:LEU:CD1	2.41	0.50
1:A:58:ARG:CZ	1:A:62:GLU:OE2	2.56	0.50
1:C:338:LEU:HD11	1:C:354:VAL:HG21	1.93	0.50
1:B:236:THR:HB	1:B:264:ILE:HD11	1.93	0.50
1:B:180:VAL:HG21	1:B:379:ARG:NH1	2.26	0.50
1:B:115:GLY:N	1:B:120:ASP:OD2	2.44	0.50
1:C:214:ILE:HG22	1:C:217:SER:HB3	1.94	0.50
1:A:419:LEU:HD13	1:A:511:VAL:HG11	1.93	0.50
1:A:435:ILE:HG13	1:A:464:MET:HE2	1.93	0.50
1:B:126:MET:HG2	1:B:227:SER:HB2	1.94	0.49
1:C:102:LYS:HB2	1:C:365:GLN:HA	1.93	0.49
1:A:119:LYS:CG	1:A:149:ASN:HB3	2.42	0.49
1:D:451:GLU:O	1:D:452:ALA:C	2.53	0.49
1:D:223:TYR:O	1:D:314:VAL:HG13	2.13	0.49
1:B:425:VAL:HG13	1:B:448:VAL:HG22	1.95	0.49
1:D:115:GLY:O	1:D:379:ARG:NH2	2.45	0.49
1:A:467:SER:CB	1:A:473:VAL:HG11	2.43	0.49
1:B:52:CYS:HA	3:B:602:HEM:C1A	2.48	0.49
1:A:455:ILE:HD11	1:A:530:VAL:CG2	2.43	0.49
1:C:115:GLY:O	1:C:379:ARG:NH2	2.46	0.49
1:C:491:ARG:HB2	1:C:494:ASP:CG	2.37	0.49
1:A:527:ARG:HG3	1:A:528:GLN:N	2.28	0.49
1:D:322:LYS:NZ	1:C:66:HIS:HB2	2.26	0.49
1:C:427:PRO:HG3	1:C:456:LEU:HD12	1.95	0.49
1:B:190:ARG:HG3	1:D:505:MET:C	2.38	0.48
1:B:414:VAL:CG2	1:B:417:LEU:HD12	2.43	0.48
1:D:111:PHE:HB3	1:D:376:ASP:C	2.38	0.48
1:D:461:LEU:O	1:D:465:LEU:HG	2.13	0.48
1:D:513:HIS:HB2	1:D:531:PHE:HE2	1.78	0.48
1:C:353:THR:HG22	1:C:372:VAL:HG13	1.95	0.48
1:D:287:LEU:HD23	1:D:311:ILE:HD13	1.94	0.48
1:A:438:LEU:HD22	1:A:461:LEU:HD13	1.94	0.48
1:A:45:ARG:NH2	1:A:47:ASP:OD2	2.47	0.48
1:A:131:GLU:OE1	1:A:163:TYR:OH	2.27	0.48
1:C:459:VAL:HG11	1:C:479:VAL:CG1	2.43	0.48
1:B:412:LEU:HD13	1:B:416:GLU:OE1	2.14	0.48
1:A:479:VAL:HG12	1:A:483:ILE:HD11	1.96	0.48
1:A:121:ARG:NH1	1:A:235:THR:OG1	2.47	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:54:TRP:HB2	3:B:602:HEM:C4B	2.48	0.47
1:D:122:ILE:O	1:D:126:MET:CG	2.62	0.47
1:A:200:PRO:HB2	1:A:209:ARG:HH11	1.79	0.47
1:C:293:LEU:HD12	1:C:293:LEU:N	2.28	0.47
1:B:81:LEU:HD21	1:B:157:ALA:HA	1.96	0.47
1:D:410:TRP:CE2	1:D:497:GLY:HA3	2.50	0.47
1:B:193:THR:HG22	1:B:194:ASN:N	2.29	0.47
1:D:448:VAL:CG2	1:D:459:VAL:HG13	2.45	0.47
1:C:87:THR:HB	1:C:109:CYS:O	2.14	0.47
1:B:419:LEU:HD21	1:B:534:VAL:HG22	1.96	0.47
1:D:54:TRP:HB2	3:D:602:HEM:C4B	2.50	0.47
1:D:264:ILE:C	1:D:268:LEU:HD13	2.35	0.47
1:D:459:VAL:HG11	1:D:479:VAL:HG13	1.97	0.47
1:A:544:ALA:HA	1:A:547:GLU:HG3	1.96	0.47
1:B:314:VAL:HG12	3:B:602:HEM:CMD	2.45	0.47
1:A:119:LYS:HG3	1:A:149:ASN:HB3	1.97	0.47
1:C:406:LYS:HE3	1:C:410:TRP:CD1	2.49	0.47
1:C:406:LYS:HE3	1:C:410:TRP:CD2	2.49	0.47
1:A:266:ARG:HD2	3:A:602:HEM:HBC2	1.97	0.46
1:C:419:LEU:HD11	1:C:511:VAL:HG21	1.96	0.46
1:D:449:VAL:HA	1:D:455:ILE:HA	1.97	0.46
1:C:510:LEU:HD22	1:C:533:VAL:HG12	1.97	0.46
1:D:103:CYS:HB2	1:D:368:GLN:O	2.14	0.46
1:A:119:LYS:HD2	1:A:150:THR:OG1	2.16	0.46
1:A:386:LEU:HD23	1:C:179:ASP:HB3	1.98	0.46
1:C:432:GLY:O	1:C:436:GLU:HG2	2.16	0.46
1:A:197:PHE:CE2	1:A:310:PHE:HB3	2.51	0.46
1:C:314:VAL:HG12	3:C:602:HEM:CMD	2.45	0.46
1:A:287:LEU:HD23	1:A:311:ILE:HD13	1.97	0.46
1:D:226:ALA:HA	3:D:602:HEM:HMD2	1.97	0.46
1:D:264:ILE:CG2	1:D:268:LEU:HD13	2.46	0.46
1:A:537:ILE:HD12	1:C:209:ARG:CZ	2.46	0.46
1:A:90:VAL:HG21	1:C:80:ILE:HD13	1.98	0.46
1:A:353:THR:HG22	1:A:372:VAL:HG13	1.98	0.46
1:B:149:ASN:ND2	2:B:601:PLP:H2A1	2.30	0.46
1:A:434:THR:O	1:A:438:LEU:HB3	2.16	0.46
1:B:280:VAL:HG13	1:B:356:VAL:HG21	1.97	0.45
1:B:499:LEU:HD23	1:B:539:LEU:HD22	1.98	0.45
1:D:286:ILE:HD11	1:D:310:PHE:HA	1.98	0.45
1:A:125:ARG:NE	1:A:129:ASP:OD1	2.50	0.45
1:A:495:THR:HG23	1:A:498:ARG:H	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:ASP:OD2	1:C:282:PRO:HD2	2.16	0.45
1:C:392:LEU:HD21	1:C:397:LEU:HD12	1.97	0.45
1:C:419:LEU:HD13	1:C:532:GLY:HA3	1.97	0.45
1:B:166:ILE:HG12	1:B:187:GLU:HB2	1.97	0.45
1:A:95:ILE:HD12	1:A:338:LEU:HD13	1.98	0.45
1:A:384:LYS:O	1:A:390:TRP:HB3	2.17	0.45
1:A:449:VAL:HG11	1:A:528:GLN:HG3	1.98	0.45
1:C:106:LEU:HB2	1:C:371:VAL:HG22	1.98	0.45
1:C:178:VAL:HG13	1:C:188:ILE:HD13	1.99	0.45
1:B:544:ALA:HA	1:B:547:GLU:HG3	1.98	0.45
1:A:455:ILE:HG22	1:A:455:ILE:O	2.15	0.45
1:B:490:ILE:HG23	1:B:494:ASP:HB2	1.97	0.45
1:D:192:PRO:HG2	1:D:195:ALA:HB2	1.99	0.45
1:D:264:ILE:HG23	1:D:268:LEU:HD13	1.99	0.45
1:A:434:THR:CG2	1:A:479:VAL:HG21	2.46	0.44
1:C:290:PRO:HD2	1:C:293:LEU:CD1	2.47	0.44
1:B:46:PRO:HB2	1:B:310:PHE:CE1	2.52	0.44
1:B:264:ILE:C	1:B:268:LEU:HD13	2.41	0.44
1:B:504:GLU:OE1	1:D:182:ARG:NH1	2.51	0.44
1:D:64:PRO:HG3	3:D:602:HEM:CHB	2.48	0.44
1:B:406:LYS:HD3	1:B:410:TRP:CE2	2.53	0.44
1:D:226:ALA:HA	3:D:602:HEM:CMD	2.47	0.44
1:A:198:ASP:HB2	1:C:466:SER:OG	2.17	0.44
1:C:52:CYS:HA	3:C:602:HEM:NA	2.33	0.44
1:C:92:ILE:HD11	1:C:107:ALA:HB2	2.00	0.44
1:B:223:TYR:CE1	1:B:257:THR:HG22	2.52	0.44
1:D:542:PHE:O	1:D:546:GLN:HG2	2.18	0.44
1:C:111:PHE:HB3	1:C:376:ASP:C	2.43	0.44
1:B:468:LEU:HD23	1:B:473:VAL:O	2.18	0.44
1:D:458:MET:HE1	1:D:533:VAL:HG11	2.00	0.44
1:A:131:GLU:HG3	1:A:136:LEU:HD23	2.00	0.44
1:A:363:GLU:HG3	1:A:364:LEU:HD12	2.00	0.44
1:D:95:ILE:HD12	1:D:338:LEU:HD13	1.99	0.44
1:A:461:LEU:O	1:A:464:MET:HB2	2.17	0.44
1:C:392:LEU:HD23	1:C:397:LEU:HD12	2.00	0.44
1:C:432:GLY:HA2	1:C:435:ILE:HD12	2.00	0.44
1:D:54:TRP:HD1	3:D:602:HEM:CAB	2.29	0.43
1:B:413:ARG:HD2	1:B:493:THR:HA	1.99	0.43
1:B:240:ILE:HD12	1:B:264:ILE:HD12	1.99	0.43
1:D:503:LEU:HD13	1:D:536:ALA:HA	2.00	0.43
1:A:63:SER:HB3	3:A:602:HEM:CAB	2.48	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:ASP:OD2	1:C:218:HIS:CE1	2.71	0.43
1:A:146:THR:HG21	1:A:151:GLY:HA3	2.00	0.43
1:A:503:LEU:HA	1:A:506:ASP:O	2.19	0.43
1:C:423:LEU:HD12	1:C:424:THR:N	2.30	0.43
1:B:111:PHE:HB3	1:B:376:ASP:C	2.44	0.43
1:D:220:LEU:HD23	1:D:220:LEU:HA	1.84	0.43
1:C:286:ILE:HD11	1:C:310:PHE:HA	2.00	0.43
1:D:169:MET:O	1:D:190:ARG:HA	2.18	0.43
1:C:110:GLU:OE2	1:C:121:ARG:NH2	2.50	0.43
1:C:145:PRO:HB2	1:C:203:HIS:CD2	2.53	0.43
1:A:337:MET:HG2	1:A:341:GLN:HG3	2.01	0.43
1:C:248:LEU:HG	1:C:275:CYS:SG	2.58	0.43
1:B:119:LYS:HG3	1:B:149:ASN:CB	2.49	0.43
1:D:254:SER:HB2	1:D:306:ILE:HG21	2.01	0.43
1:B:102:LYS:HD2	1:B:365:GLN:HA	2.01	0.43
1:A:54:TRP:CD1	3:A:602:HEM:CBB	3.02	0.43
1:D:392:LEU:HD23	1:D:397:LEU:HD12	1.94	0.43
1:D:512:VAL:HG12	1:D:530:VAL:HG22	2.00	0.43
1:C:293:LEU:CD1	1:C:293:LEU:H	2.32	0.43
1:C:489:GLN:NE2	1:C:528:GLN:OE1	2.50	0.43
1:B:397:LEU:HD23	1:B:397:LEU:HA	1.92	0.42
1:B:429:ILE:HG13	1:B:430:THR:N	2.33	0.42
1:D:448:VAL:HG21	1:D:459:VAL:HG13	2.01	0.42
1:A:479:VAL:HG12	1:A:483:ILE:CG1	2.49	0.42
1:A:503:LEU:HD13	1:A:536:ALA:HA	2.01	0.42
1:C:111:PHE:HB2	1:C:377:SER:HB3	2.01	0.42
1:B:529:MET:HG2	1:B:531:PHE:CE1	2.54	0.42
1:C:445:GLN:HB3	1:C:460:THR:HG22	2.01	0.42
1:D:52:CYS:HA	3:D:602:HEM:C1A	2.54	0.42
1:A:280:VAL:HG13	1:A:356:VAL:HG21	2.01	0.42
1:A:464:MET:HE3	1:A:464:MET:HB3	1.89	0.42
1:B:281:ASP:OD2	1:B:287:LEU:HD12	2.19	0.42
1:A:467:SER:HB2	1:A:473:VAL:HG11	2.01	0.42
1:C:54:TRP:HB2	3:C:602:HEM:C4B	2.55	0.42
1:B:469:LEU:HD23	1:B:469:LEU:O	2.19	0.42
1:A:419:LEU:HD12	1:A:511:VAL:HG11	1.99	0.42
1:D:110:GLU:HG2	1:D:118:VAL:HB	2.02	0.42
1:A:51:ARG:HB3	3:A:602:HEM:O1A	2.19	0.42
1:A:108:LYS:HB3	1:A:373:ILE:HD13	2.00	0.42
1:C:406:LYS:HE3	1:C:410:TRP:NE1	2.35	0.42
1:C:196:ARG:O	1:C:202:SER:HB3	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:293:LEU:N	1:C:293:LEU:CD1	2.82	0.42
1:C:397:LEU:CD1	1:C:397:LEU:O	2.68	0.42
1:C:499:LEU:HD21	1:C:534:VAL:HG11	2.02	0.42
1:B:264:ILE:HG23	1:B:268:LEU:CD1	2.49	0.42
1:D:446:ALA:O	1:D:459:VAL:HG22	2.20	0.42
1:D:281:ASP:OD1	1:D:285:SER:HB3	2.20	0.42
1:C:412:LEU:O	1:C:495:THR:HA	2.20	0.42
1:B:338:LEU:HD12	1:B:344:LEU:HD12	2.02	0.41
1:D:353:THR:CG2	1:D:372:VAL:HG13	2.50	0.41
1:A:221:ASP:OD1	1:A:224:ARG:NH1	2.52	0.41
1:A:426:LEU:HB3	1:A:429:ILE:HG23	2.01	0.41
1:A:448:VAL:O	1:A:456:LEU:N	2.52	0.41
1:B:301:TYR:CD2	1:B:301:TYR:N	2.88	0.41
3:C:602:HEM:HBC2	3:C:602:HEM:CMC	2.50	0.41
1:D:432:GLY:HA2	1:D:435:ILE:HD12	2.01	0.41
1:B:122:ILE:HG21	1:B:228:ASN:OD1	2.19	0.41
1:D:190:ARG:HA	1:D:190:ARG:HD2	1.89	0.41
1:C:327:ASN:OD1	1:C:330:GLU:HB2	2.20	0.41
1:C:426:LEU:O	1:C:429:ILE:HG22	2.20	0.41
1:C:190:ARG:HD2	1:C:190:ARG:HA	1.83	0.41
1:C:229:PRO:HB2	3:C:602:HEM:CAC	2.48	0.41
1:D:233:TYR:O	1:D:267:LYS:HD2	2.20	0.41
1:A:136:LEU:HG	1:A:163:TYR:HE2	1.85	0.41
1:D:180:VAL:HG21	1:D:379:ARG:NH1	2.36	0.41
1:D:406:LYS:HD3	1:D:410:TRP:NE1	2.35	0.41
1:B:83:LYS:HA	1:B:83:LYS:HD2	1.82	0.41
1:A:435:ILE:HD11	1:A:464:MET:HB3	2.02	0.41
1:C:110:GLU:OE2	1:C:121:ARG:NE	2.49	0.41
1:D:214:ILE:HA	1:D:215:PRO:HD3	1.91	0.41
1:A:51:ARG:CB	3:A:602:HEM:O1A	2.68	0.41
1:A:226:ALA:HA	3:A:602:HEM:CMD	2.51	0.41
1:A:263:GLY:HA2	3:A:602:HEM:HBC1	2.03	0.41
1:A:422:PRO:HA	1:A:443:PHE:HE2	1.86	0.41
1:B:264:ILE:CG2	1:B:268:LEU:CD1	2.99	0.41
1:D:180:VAL:HG21	1:D:379:ARG:HH11	1.86	0.41
1:B:338:LEU:HD21	1:B:354:VAL:HG21	2.03	0.40
1:D:145:PRO:HB2	1:D:203:HIS:CD2	2.56	0.40
1:A:180:VAL:HG21	1:A:379:ARG:HH11	1.83	0.40
1:A:190:ARG:NH1	1:C:504:GLU:O	2.44	0.40
1:C:103:CYS:HB2	1:C:368:GLN:O	2.21	0.40
1:C:430:THR:O	1:C:434:THR:OG1	2.38	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:82:LYS:N	1:B:82:LYS:HD2	2.36	0.40
1:D:131:GLU:OE1	1:D:163:TYR:OH	2.31	0.40
1:D:322:LYS:NZ	1:C:132:ARG:HH12	2.19	0.40
1:A:260:THR:CB	2:A:601:PLP:O1P	2.69	0.40
1:C:255:VAL:HG13	1:C:258:GLY:HA2	2.04	0.40
1:B:376:ASP:CG	2:B:601:PLP:H2A2	2.47	0.40
1:A:64:PRO:HG3	3:A:602:HEM:CMA	2.51	0.40
1:C:180:VAL:HG21	1:C:379:ARG:NH1	2.37	0.40
1:B:434:THR:OG1	1:B:464:MET:HE3	2.21	0.40
1:C:260:THR:OG1	2:C:601:PLP:O1P	2.32	0.40
1:B:258:GLY:HA3	1:B:315:LEU:HD13	2.03	0.40
1:B:337:MET:HG2	1:B:341:GLN:HG3	2.02	0.40
1:A:191:THR:HB	1:A:201:GLU:O	2.21	0.40
1:C:82:LYS:N	1:C:82:LYS:HD2	2.37	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:LEU:CD2	1:C:421:ALA:CB[5_455]	2.13	0.07

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	467/548 (85%)	455 (97%)	12 (3%)	0	100	100
1	B	482/548 (88%)	475 (98%)	7 (2%)	0	100	100
1	C	485/548 (88%)	478 (99%)	7 (1%)	0	100	100
1	D	483/548 (88%)	475 (98%)	7 (1%)	1 (0%)	43	71
All	All	1917/2192 (88%)	1883 (98%)	33 (2%)	1 (0%)	48	78

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	452	ALA

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	408/463 (88%)	399 (98%)	9 (2%)	45	63
1	B	413/463 (89%)	400 (97%)	13 (3%)	35	59
1	C	411/463 (89%)	405 (98%)	6 (2%)	57	69
1	D	411/463 (89%)	405 (98%)	6 (2%)	57	69
All	All	1643/1852 (89%)	1609 (98%)	34 (2%)	47	64

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	72	LYS
1	B	301	TYR
1	B	338	LEU
1	B	353	THR
1	B	425	VAL
1	B	426	LEU
1	B	441	LYS
1	B	474	GLN
1	B	479	VAL
1	B	482	VAL
1	B	493	THR
1	B	511	VAL
1	B	512	VAL
1	D	338	LEU
1	D	397	LEU
1	D	414	VAL
1	D	424	THR
1	D	425	VAL
1	D	479	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	127	ILE
1	A	224	ARG
1	A	251	LEU
1	A	278	ILE
1	A	338	LEU
1	A	386	LEU
1	A	426	LEU
1	A	455	ILE
1	A	479	VAL
1	C	251	LEU
1	C	397	LEU
1	C	414	VAL
1	C	424	THR
1	C	436	GLU
1	C	464	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	65	HIS
1	B	93	ASN
1	B	463	ASN
1	D	65	HIS
1	D	194	ASN
1	D	415	GLN
1	A	194	ASN
1	A	298	GLN
1	A	393	GLN
1	A	415	GLN
1	A	513	HIS
1	C	66	HIS
1	C	93	ASN
1	C	194	ASN
1	C	513	HIS

5.3.3 RNA ⓘ

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](#)

8 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	HEM	A	602	1	50,50,50	2.00	14 (28%)	67,82,82	1.93	18 (26%)
2	PLP	D	601	1	15,15,16	1.30	1 (6%)	21,22,23	1.11	2 (9%)
3	HEM	B	602	1	50,50,50	1.87	8 (16%)	67,82,82	1.37	9 (13%)
3	HEM	C	602	1	50,50,50	1.86	11 (22%)	67,82,82	1.62	12 (17%)
2	PLP	A	601	1	15,15,16	1.34	2 (13%)	21,22,23	1.16	1 (4%)
2	PLP	C	601	1	15,15,16	1.26	1 (6%)	21,22,23	1.10	2 (9%)
3	HEM	D	602	1	50,50,50	1.91	8 (16%)	67,82,82	1.24	1 (1%)
2	PLP	B	601	1	15,15,16	1.30	2 (13%)	21,22,23	1.12	1 (4%)

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	HEM	A	602	1	-	12/14/54/54	-
2	PLP	D	601	1	-	0/6/6/8	0/1/1/1
3	HEM	B	602	1	-	8/14/54/54	-
3	HEM	C	602	1	-	4/14/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	PLP	A	601	1	-	0/6/6/8	0/1/1/1
2	PLP	C	601	1	-	0/6/6/8	0/1/1/1
3	HEM	D	602	1	-	9/14/54/54	-
2	PLP	B	601	1	-	0/6/6/8	0/1/1/1

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	602	HEM	C3D-C2D	8.03	1.54	1.36
3	D	602	HEM	C3D-C2D	8.01	1.54	1.36
3	B	602	HEM	C3D-C2D	7.73	1.53	1.36
3	C	602	HEM	C3D-C2D	7.40	1.52	1.36
3	D	602	HEM	FE-ND	5.08	2.10	1.94
3	A	602	HEM	FE-NA	4.88	2.11	1.95
3	B	602	HEM	FE-ND	4.71	2.09	1.94
3	D	602	HEM	FE-NA	4.26	2.09	1.95
3	B	602	HEM	FE-NA	4.11	2.08	1.95
3	C	602	HEM	FE-NB	4.08	2.07	1.94
3	A	602	HEM	FE-ND	3.74	2.06	1.94
3	C	602	HEM	FE-NA	3.60	2.07	1.95
3	C	602	HEM	FE-ND	3.52	2.05	1.94
3	C	602	HEM	CAB-C3B	3.23	1.56	1.47
3	D	602	HEM	CAB-C3B	3.08	1.55	1.47
3	B	602	HEM	FE-NB	2.93	2.03	1.94
3	A	602	HEM	CAC-C3C	2.89	1.55	1.47
3	A	602	HEM	CAB-C3B	2.82	1.54	1.47
3	D	602	HEM	CAC-C3C	2.81	1.54	1.47
3	A	602	HEM	C1A-NA	-2.74	1.34	1.39
3	A	602	HEM	FE-NB	2.68	2.03	1.94
3	C	602	HEM	CAC-C3C	2.57	1.54	1.47
3	B	602	HEM	CAC-C3C	2.51	1.54	1.47
3	C	602	HEM	CMB-C2B	2.50	1.55	1.50
3	C	602	HEM	CMA-C3A	2.49	1.55	1.50
3	A	602	HEM	O2D-CGD	-2.47	1.22	1.30
3	B	602	HEM	FE-NC	2.42	2.03	1.95
3	D	602	HEM	FE-NB	2.41	2.02	1.94
3	A	602	HEM	C4D-ND	-2.40	1.36	1.40
3	A	602	HEM	O2A-CGA	-2.36	1.23	1.30
3	B	602	HEM	CMB-C2B	2.34	1.55	1.50
2	A	601	PLP	C2-N1	2.28	1.37	1.33
2	B	601	PLP	P-O3P	-2.28	1.46	1.54
3	B	602	HEM	CAB-C3B	2.26	1.53	1.47

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	PLP	C3-C2	-2.25	1.38	1.41
2	D	601	PLP	C3-C2	-2.23	1.38	1.41
3	D	602	HEM	CMB-C2B	2.21	1.55	1.50
3	C	602	HEM	CAA-C2A	2.20	1.57	1.51
3	D	602	HEM	FE-NC	2.13	2.02	1.95
3	C	602	HEM	CMC-C2C	2.11	1.55	1.50
3	A	602	HEM	FE-NC	2.09	2.02	1.95
3	A	602	HEM	CMB-C2B	2.08	1.55	1.50
3	A	602	HEM	C2A-C3A	-2.07	1.33	1.38
3	C	602	HEM	C1A-C2A	2.06	1.48	1.44
2	C	601	PLP	C2A-C2	2.01	1.53	1.50
3	A	602	HEM	CMC-C2C	2.01	1.54	1.50
2	B	601	PLP	C2A-C2	2.01	1.53	1.50

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	602	HEM	CAA-CBA-CGA	-6.80	95.62	113.67
3	D	602	HEM	C4D-ND-C1D	5.26	111.44	105.21
3	B	602	HEM	C4D-ND-C1D	4.59	110.65	105.21
3	A	602	HEM	CAA-C2A-C1A	4.53	133.79	124.94
3	A	602	HEM	C4D-ND-C1D	4.44	110.47	105.21
3	C	602	HEM	CMA-C3A-C4A	-4.09	119.19	125.42
3	A	602	HEM	C3B-C4B-NB	-4.01	106.59	109.47
3	C	602	HEM	C3B-C4B-NB	-3.87	106.69	109.47
3	C	602	HEM	C4D-ND-C1D	3.85	109.77	105.21
3	A	602	HEM	O1A-CGA-CBA	-3.61	111.66	123.09
3	C	602	HEM	CHC-C1C-NC	3.57	128.34	124.45
3	A	602	HEM	C1A-CHA-C4D	3.50	134.48	126.25
3	C	602	HEM	CMA-C3A-C2A	3.40	132.84	125.62
3	B	602	HEM	CAD-C3D-C4D	3.22	130.31	124.70
3	A	602	HEM	C1B-NB-C4B	3.17	108.96	105.21
3	B	602	HEM	C3B-C2B-C1B	3.12	108.75	106.41
3	B	602	HEM	C3B-C4B-NB	-3.10	107.24	109.47
3	A	602	HEM	O1D-CGD-CBD	-3.10	113.26	123.09
3	C	602	HEM	C1B-NB-C4B	3.08	108.85	105.21
3	C	602	HEM	CAA-CBA-CGA	3.00	121.64	113.67
3	A	602	HEM	O2A-CGA-CBA	2.92	123.22	114.00
3	B	602	HEM	C1B-NB-C4B	2.75	108.47	105.21
3	A	602	HEM	CAA-C2A-C3A	-2.75	120.91	127.07
3	A	602	HEM	O2D-CGD-O1D	2.72	130.33	123.33
3	C	602	HEM	C3B-C2B-C1B	2.64	108.39	106.41

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	PLP	O3P-P-O1P	2.60	120.97	110.83
3	B	602	HEM	C1A-CHA-C4D	2.60	132.35	126.25
3	A	602	HEM	CBA-CAA-C2A	2.60	119.71	112.53
3	A	602	HEM	C4D-C3D-C2D	-2.58	103.14	106.89
2	C	601	PLP	O3P-P-O1P	2.51	120.61	110.83
2	A	601	PLP	O3P-P-O1P	2.50	120.58	110.83
3	A	602	HEM	CHA-C1A-NA	-2.48	119.37	123.86
2	D	601	PLP	O3P-P-O1P	2.47	120.47	110.83
3	B	602	HEM	C4D-C3D-C2D	-2.40	103.39	106.89
3	A	602	HEM	CHC-C4B-NB	2.40	127.01	124.42
3	A	602	HEM	CAD-C3D-C4D	2.30	128.70	124.70
3	C	602	HEM	CHB-C4A-NA	2.28	128.00	123.86
3	C	602	HEM	CHA-C1A-C2A	2.21	130.13	125.30
3	B	602	HEM	CHC-C4B-NB	2.20	126.79	124.42
3	A	602	HEM	C3B-C2B-C1B	2.14	108.02	106.41
3	B	602	HEM	C2B-C1B-NB	-2.13	107.39	109.84
2	C	601	PLP	O4P-C5A-C5	2.13	113.34	109.36
3	A	602	HEM	CHA-C1A-C2A	2.12	129.95	125.30
3	C	602	HEM	CHC-C1C-C2C	-2.12	121.08	125.49
2	D	601	PLP	O4P-C5A-C5	2.01	113.13	109.36
3	C	602	HEM	C4D-C3D-C2D	-2.01	103.97	106.89

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	HEM	C2B-C3B-CAB-CBB
3	B	602	HEM	C4B-C3B-CAB-CBB
3	B	602	HEM	C2D-C3D-CAD-CBD
3	B	602	HEM	C4D-C3D-CAD-CBD
3	A	602	HEM	C2D-C3D-CAD-CBD
3	A	602	HEM	C4D-C3D-CAD-CBD
3	A	602	HEM	C1A-C2A-CAA-CBA
3	A	602	HEM	C3A-C2A-CAA-CBA
3	D	602	HEM	C1A-C2A-CAA-CBA
3	C	602	HEM	C3A-C2A-CAA-CBA
3	A	602	HEM	C2A-CAA-CBA-CGA
3	D	602	HEM	C4D-C3D-CAD-CBD
3	A	602	HEM	C2B-C3B-CAB-CBB
3	A	602	HEM	C4B-C3B-CAB-CBB
3	A	602	HEM	C3D-CAD-CBD-CGD
3	D	602	HEM	C2D-C3D-CAD-CBD

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	C	602	HEM	C4D-C3D-CAD-CBD
3	C	602	HEM	C1A-C2A-CAA-CBA
3	D	602	HEM	C3A-C2A-CAA-CBA
3	C	602	HEM	C2D-C3D-CAD-CBD
3	B	602	HEM	CAD-CBD-CGD-O1D
3	B	602	HEM	CAD-CBD-CGD-O2D
3	A	602	HEM	CAD-CBD-CGD-O1D
3	A	602	HEM	CAD-CBD-CGD-O2D
3	B	602	HEM	CAA-CBA-CGA-O2A
3	D	602	HEM	C2A-CAA-CBA-CGA
3	D	602	HEM	CAA-CBA-CGA-O2A
3	A	602	HEM	CAA-CBA-CGA-O2A
3	B	602	HEM	CAA-CBA-CGA-O1A
3	A	602	HEM	CAA-CBA-CGA-O1A
3	D	602	HEM	CAD-CBD-CGD-O2D
3	D	602	HEM	CAD-CBD-CGD-O1D
3	D	602	HEM	CAA-CBA-CGA-O1A

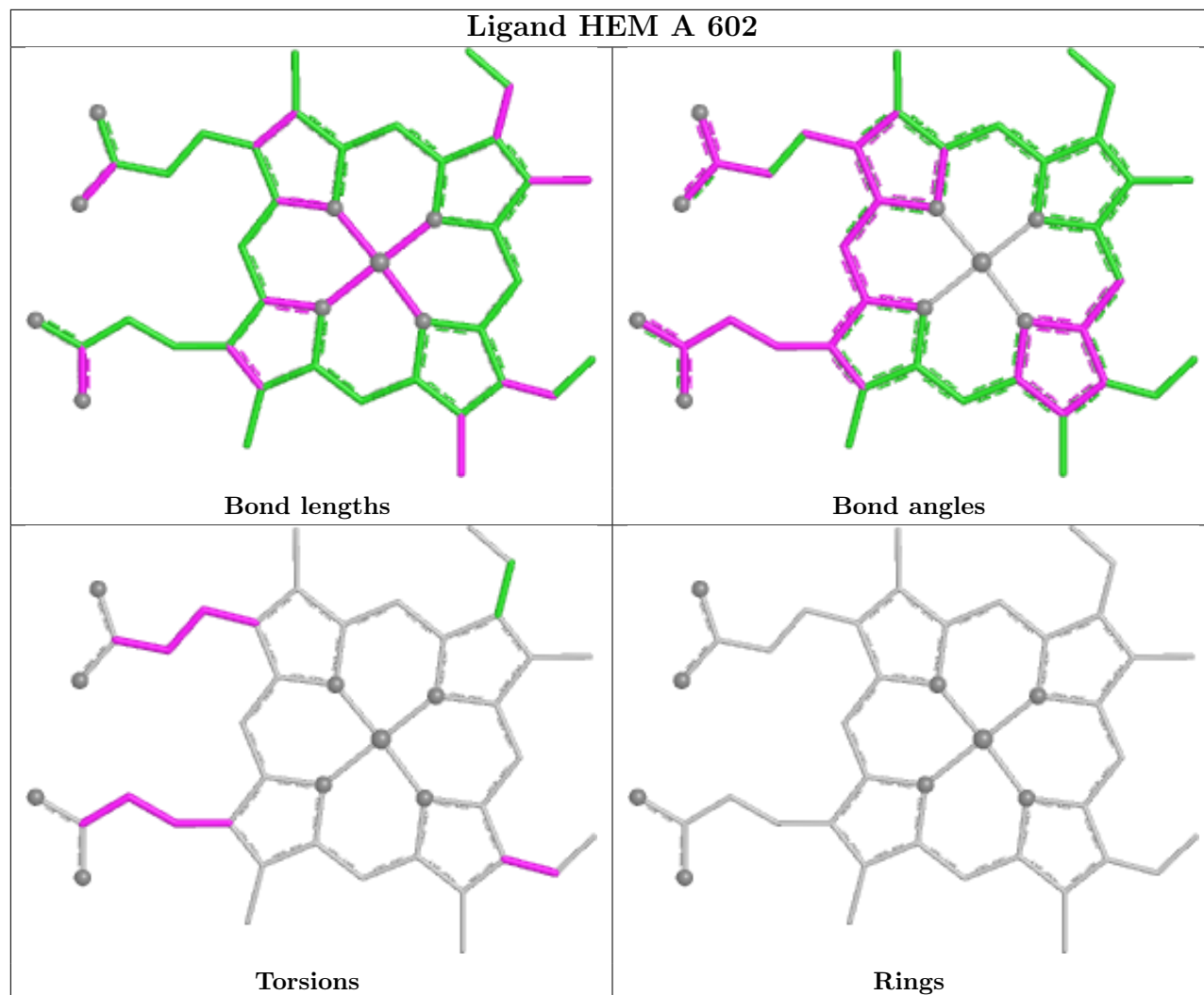
There are no ring outliers.

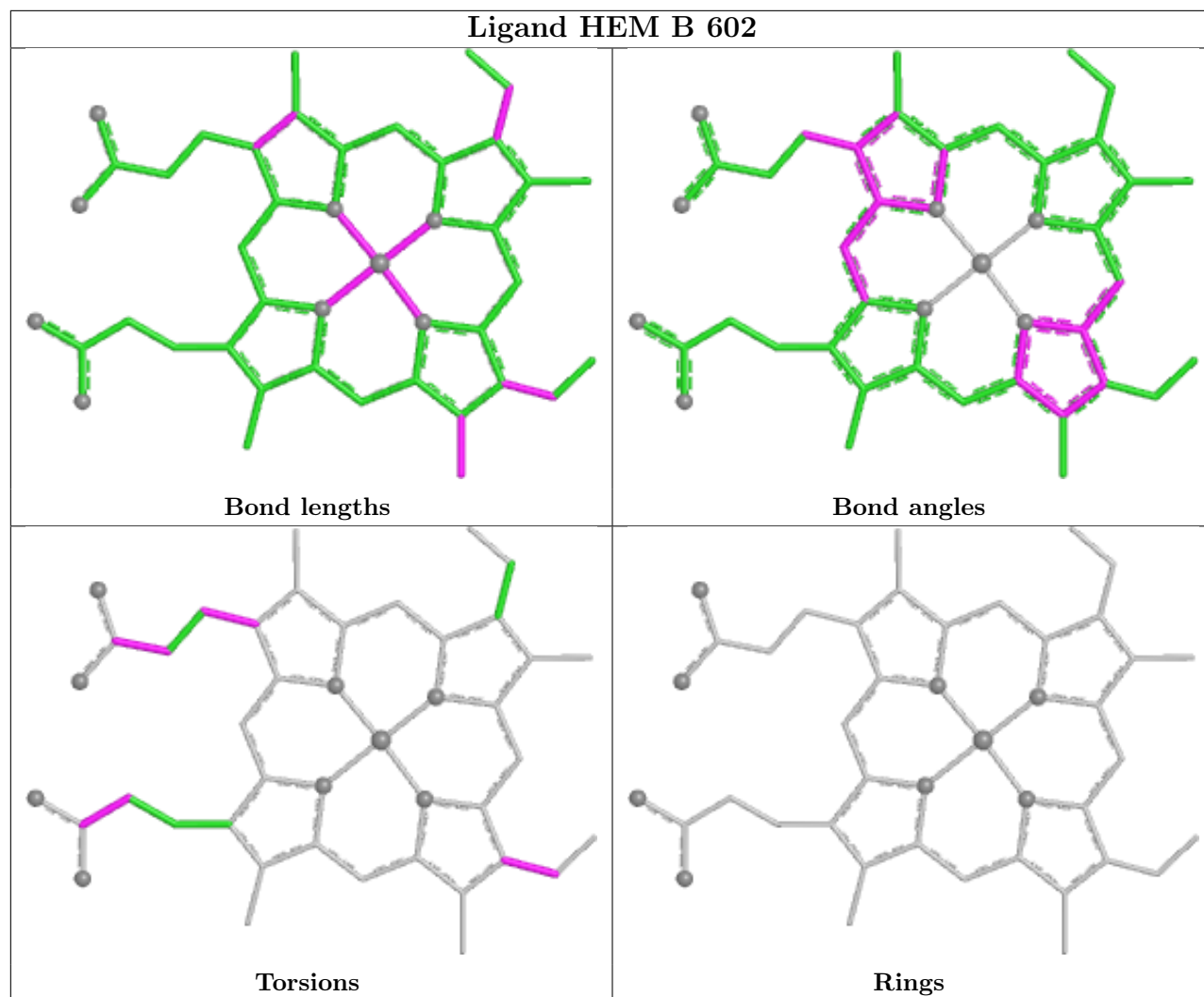
8 monomers are involved in 59 short contacts:

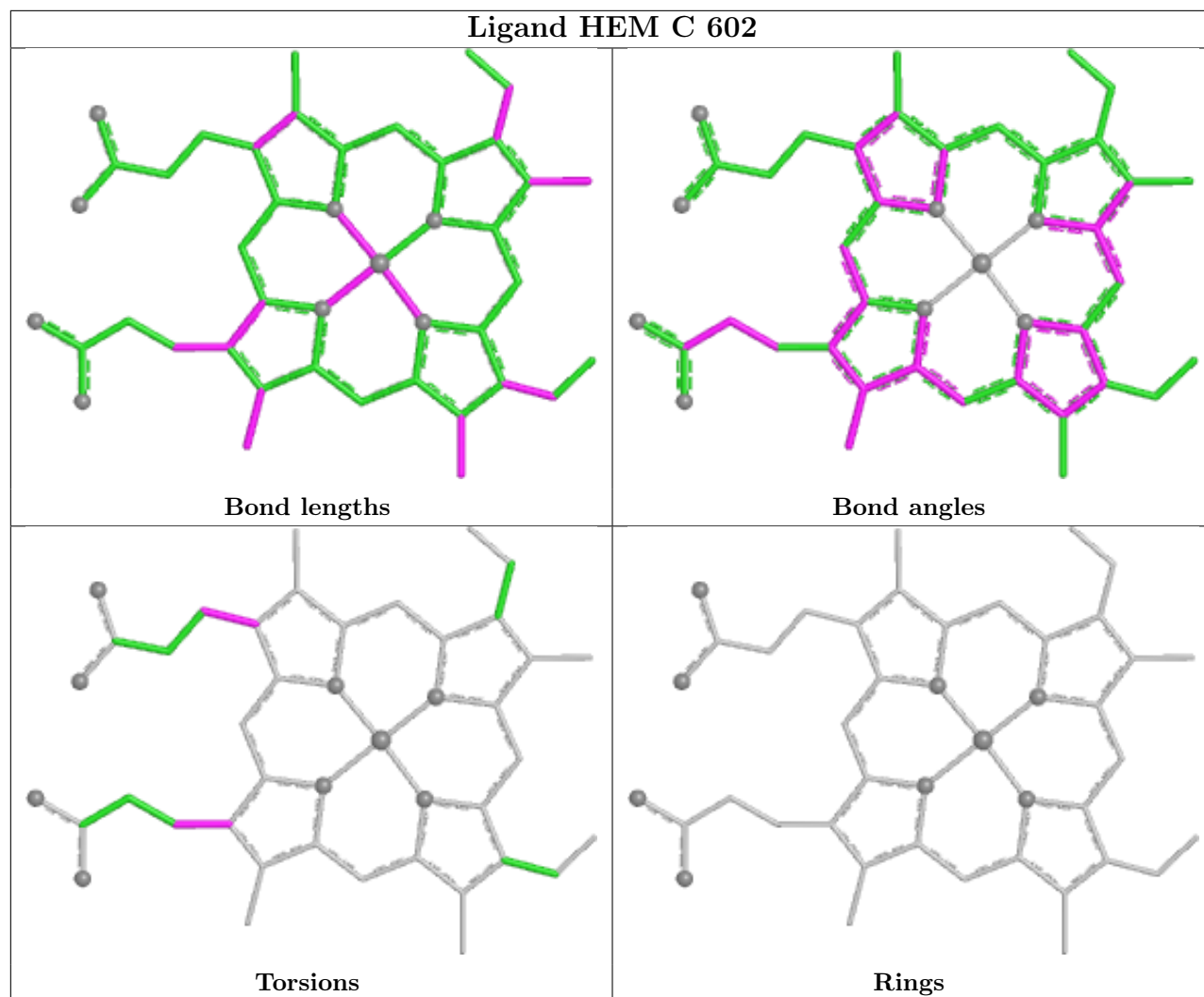
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	602	HEM	15	0
2	D	601	PLP	1	0
3	B	602	HEM	12	0
3	C	602	HEM	14	0
2	A	601	PLP	3	0
2	C	601	PLP	2	0
3	D	602	HEM	9	0
2	B	601	PLP	3	0

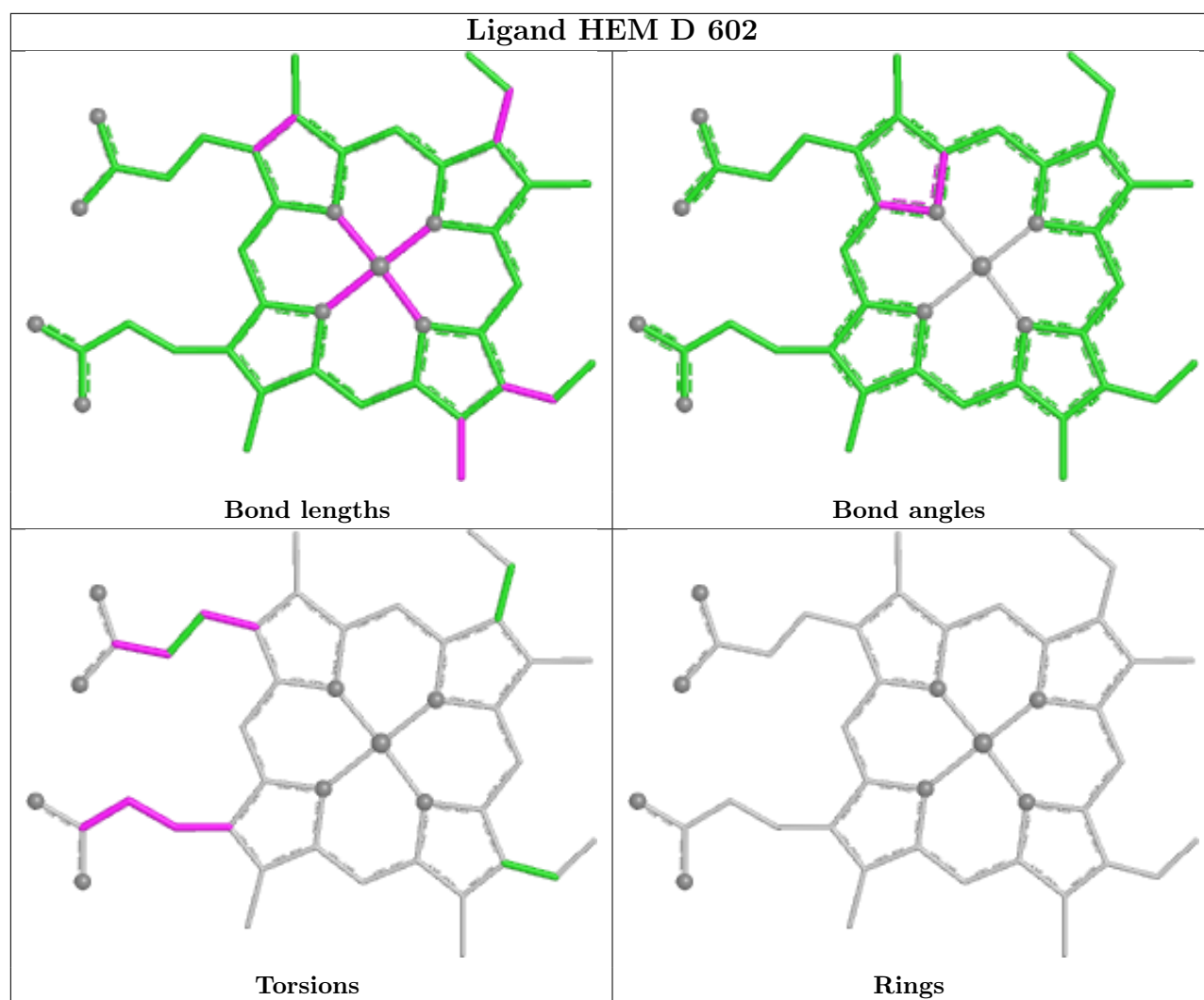
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	485/548 (88%)	-0.36	5 (1%) 79 66	43, 83, 160, 205	0
1	B	490/548 (89%)	-0.55	4 (0%) 82 71	40, 84, 141, 214	0
1	C	491/548 (89%)	-0.47	1 (0%) 91 87	39, 78, 137, 185	0
1	D	491/548 (89%)	-0.59	1 (0%) 91 87	34, 75, 159, 207	0
All	All	1957/2192 (89%)	-0.49	11 (0%) 85 75	34, 80, 154, 214	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	414	VAL	2.9
1	B	423	LEU	2.8
1	D	147	SER	2.7
1	A	434	THR	2.6
1	A	443	PHE	2.4
1	A	41	PRO	2.2
1	C	42	LEU	2.2
1	B	450	ASP	2.1
1	A	496	LEU	2.1
1	B	42	LEU	2.0
1	B	147	SER	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](#)

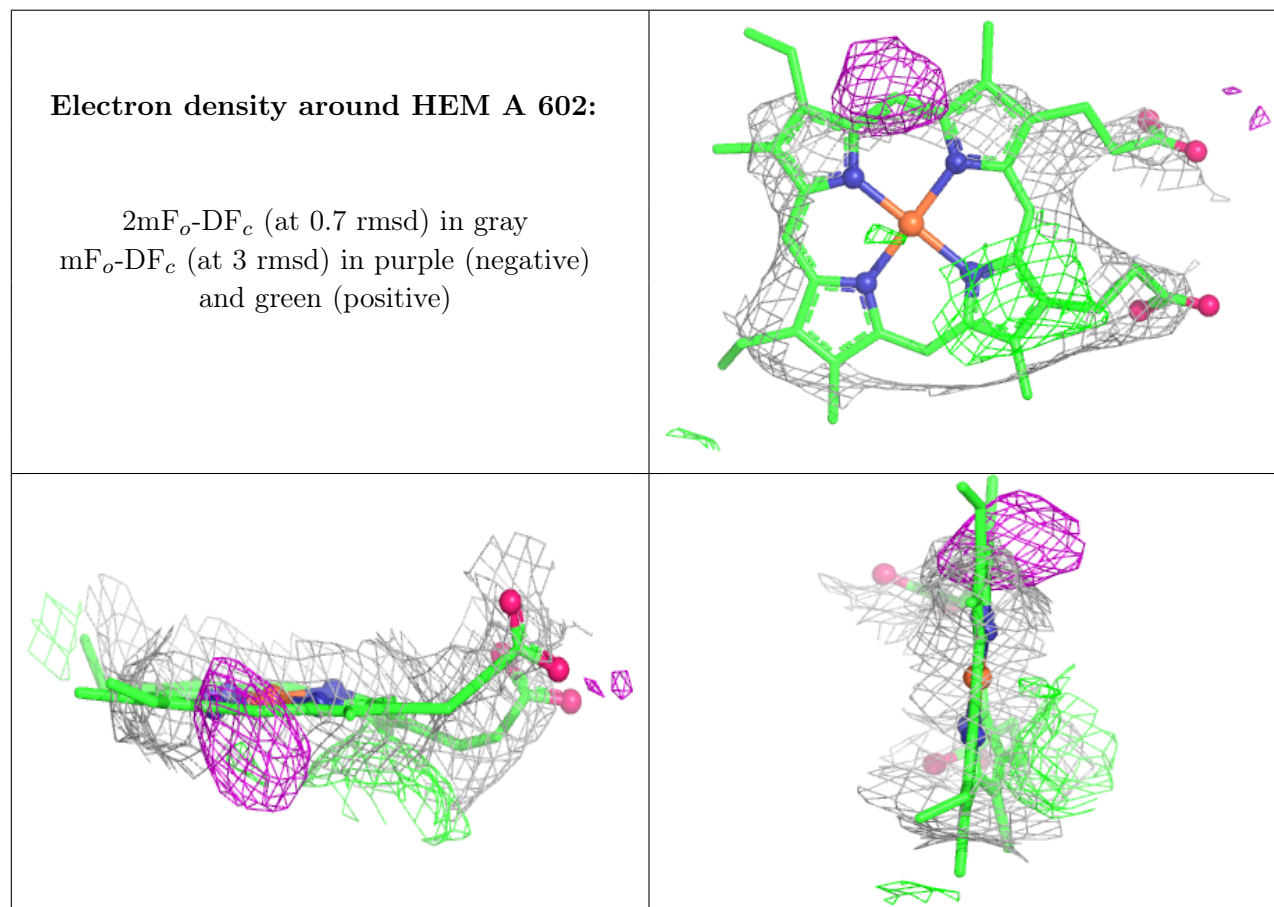
There are no oligosaccharides in this entry.

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.

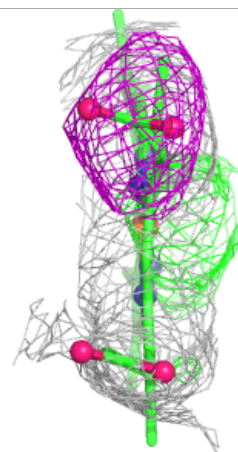
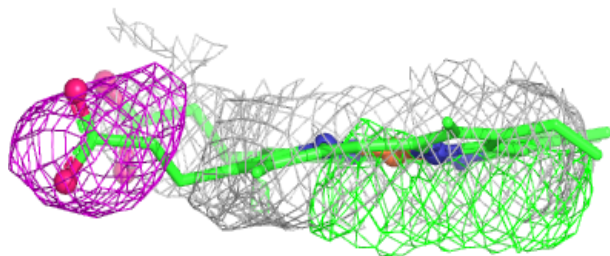
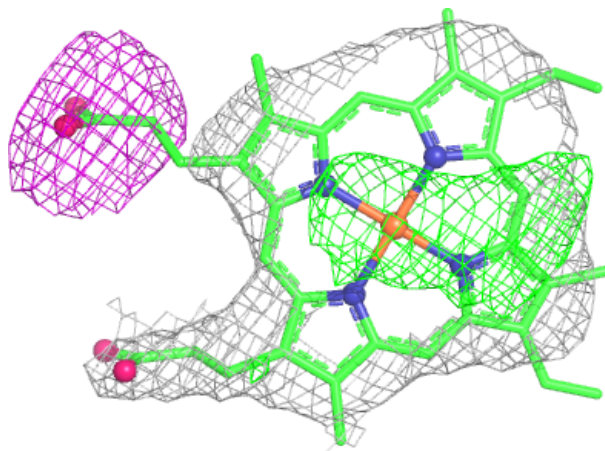
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	PLP	A	601	15/16	0.93	0.08	50,67,77,77	0
2	PLP	C	601	15/16	0.93	0.09	45,56,60,63	0
3	HEM	A	602	43/43	0.93	0.12	106,106,107,107	0
3	HEM	C	602	43/43	0.93	0.14	79,79,80,80	0
2	PLP	D	601	15/16	0.94	0.08	49,56,65,66	0
3	HEM	D	602	43/43	0.96	0.10	79,79,80,80	0
2	PLP	B	601	15/16	0.96	0.06	57,70,80,81	0
3	HEM	B	602	43/43	0.96	0.10	112,112,113,113	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.



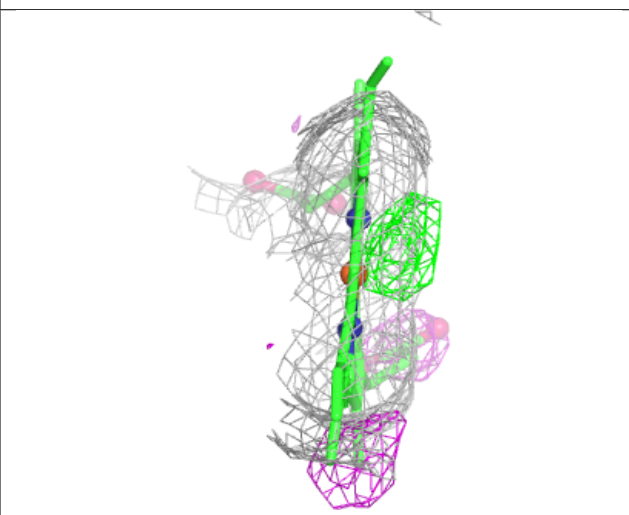
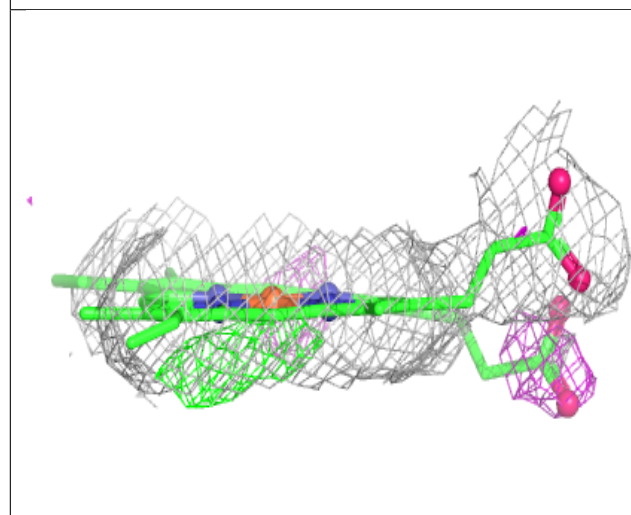
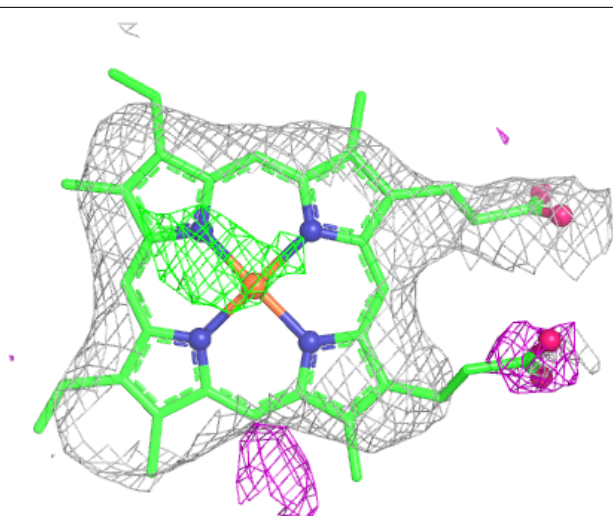
Electron density around HEM C 602:

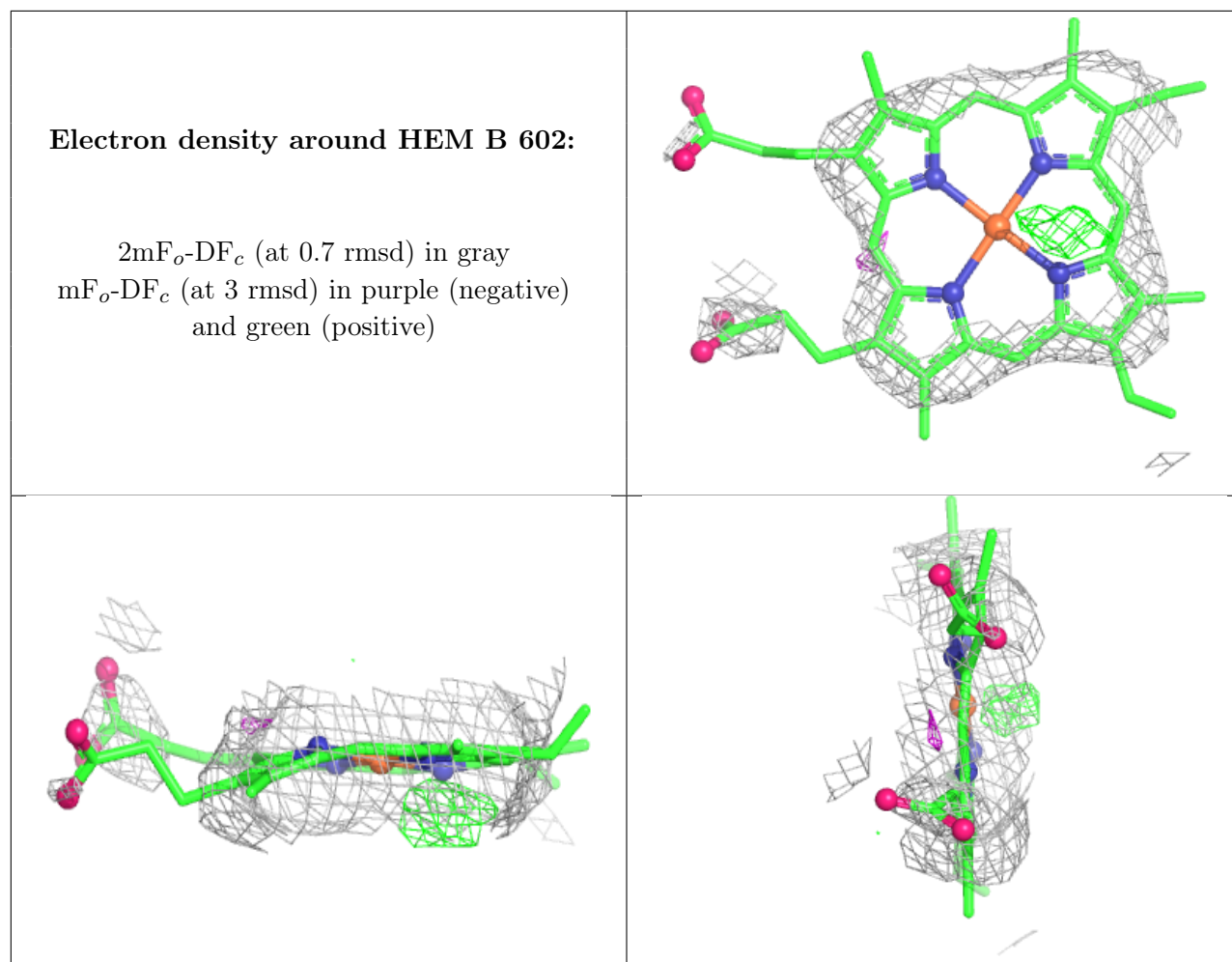
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM D 602:

$2mF_o-DF_c$ (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.