



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 11:00 PM BST

PDB ID : 5HPW
Title : Mode of binding of antithyroid drug, propylthiouracil to lactoperoxidase: Binding studies and structure determination
Authors : Singh, R.P.; Singh, A.; Sharma, P.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2016-01-21
Resolution : 2.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.13.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.13.1

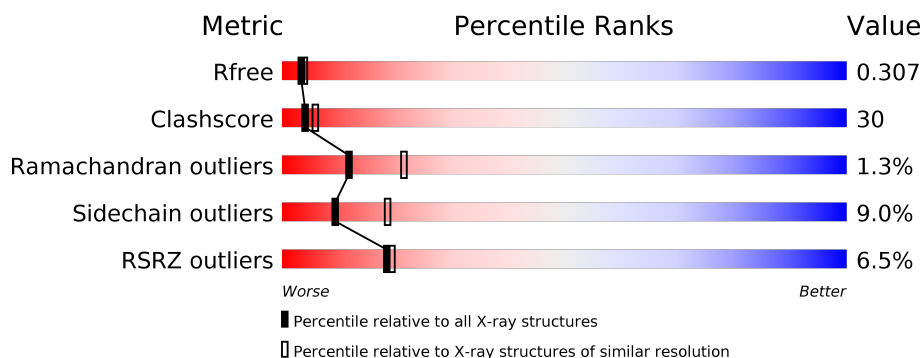
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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.



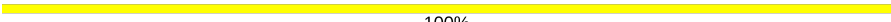

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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 on 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	595	<div> <div>5%</div> <div> <div></div> <div>50%</div> <div>45%</div> <div>• •</div> </div> </div>
1	B	595	<div> <div>6%</div> <div> <div></div> <div>55%</div> <div>42%</div> <div>•</div> </div> </div>
1	C	595	<div> <div>9%</div> <div> <div></div> <div>51%</div> <div>44%</div> <div>•</div> </div> </div>
1	D	595	<div> <div>6%</div> <div> <div></div> <div>47%</div> <div>48%</div> <div>5%</div> <div>•</div> </div> </div>
2	E	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>
2	G	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	H	2	 100%
3	F	2	 100%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	NO3	C	608	-	-	X	-
6	NO3	D	606	-	-	X	-
6	NO3	D	607	-	-	X	-
6	NO3	D	608	-	-	X	-
7	3CJ	A	609	-	X	X	-
7	3CJ	B	609	-	X	X	-
7	3CJ	C	609	-	-	X	-
7	3CJ	D	609	-	X	X	-

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 20141 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 Lactoperoxidase.

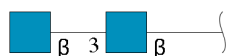
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	0	0
			4753	3021	844	862	26			
1	B	595	Total	C	N	O	S	0	0	0
			4753	3021	844	862	26			
1	C	595	Total	C	N	O	S	0	0	0
			4753	3021	844	862	26			
1	D	595	Total	C	N	O	S	0	0	0
			4753	3021	844	862	26			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



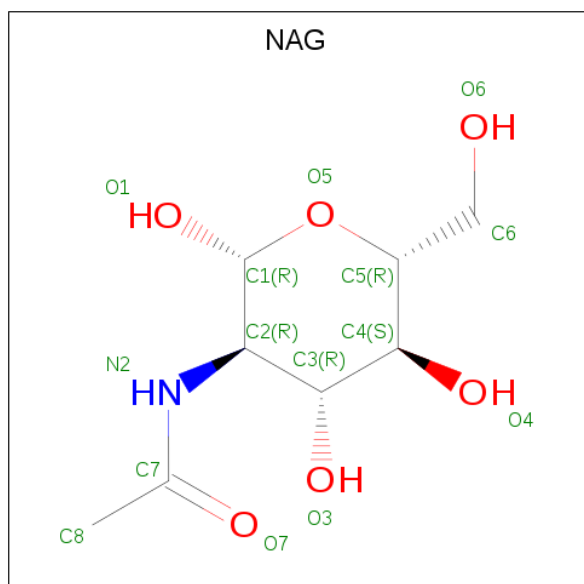
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	C	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		
4	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

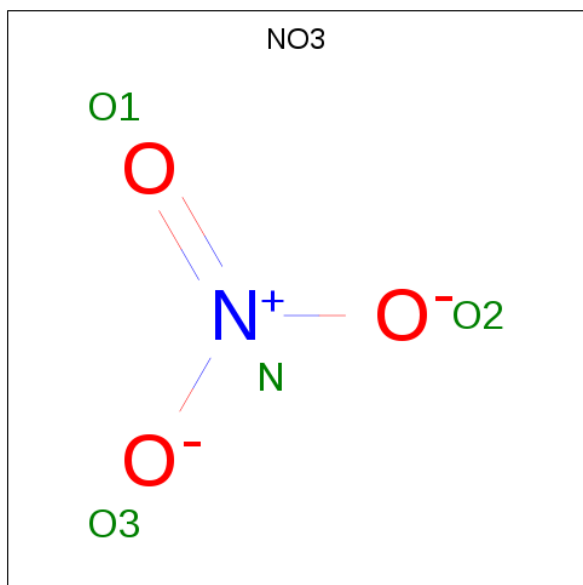
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Ca	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		
5	D	1	Total	Ca	0	0
			1	1		
5	C	1	Total	Ca	0	0
			1	1		

- Molecule 6 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



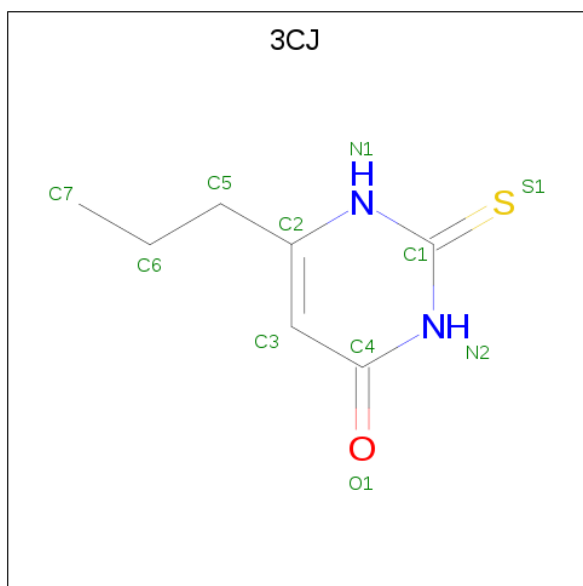
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	N	O	0	0
			4	1	3		
6	A	1	Total	N	O	0	0
			4	1	3		
6	A	1	Total	N	O	0	0
			4	1	3		
6	B	1	Total	N	O	0	0
			4	1	3		
6	B	1	Total	N	O	0	0
			4	1	3		
6	B	1	Total	N	O	0	0
			4	1	3		
6	C	1	Total	N	O	0	0
			4	1	3		
6	C	1	Total	N	O	0	0
			4	1	3		

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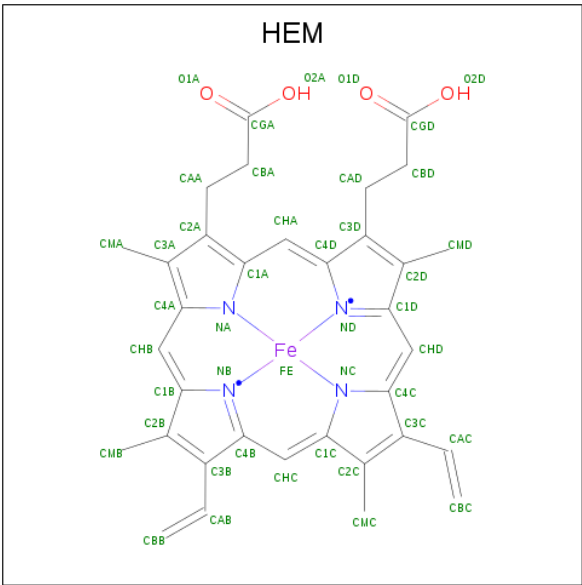
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	N	O	0	0
			4	1	3		
6	D	1	Total	N	O	0	0
			4	1	3		
6	D	1	Total	N	O	0	0
			4	1	3		
6	D	1	Total	N	O	0	0
			4	1	3		

- Molecule 7 is 6-propyl-2-thioxo-2,3-dihydropyrimidin-4(1H)-one (three-letter code: 3CJ) (formula: C₇H₁₀N₂OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	S	0	0
			11	7	2	1	1		
7	B	1	Total	C	N	O	S	0	0
			11	7	2	1	1		
7	C	1	Total	C	N	O	S	0	0
			11	7	2	1	1		
7	D	1	Total	C	N	O	S	0	0
			11	7	2	1	1		

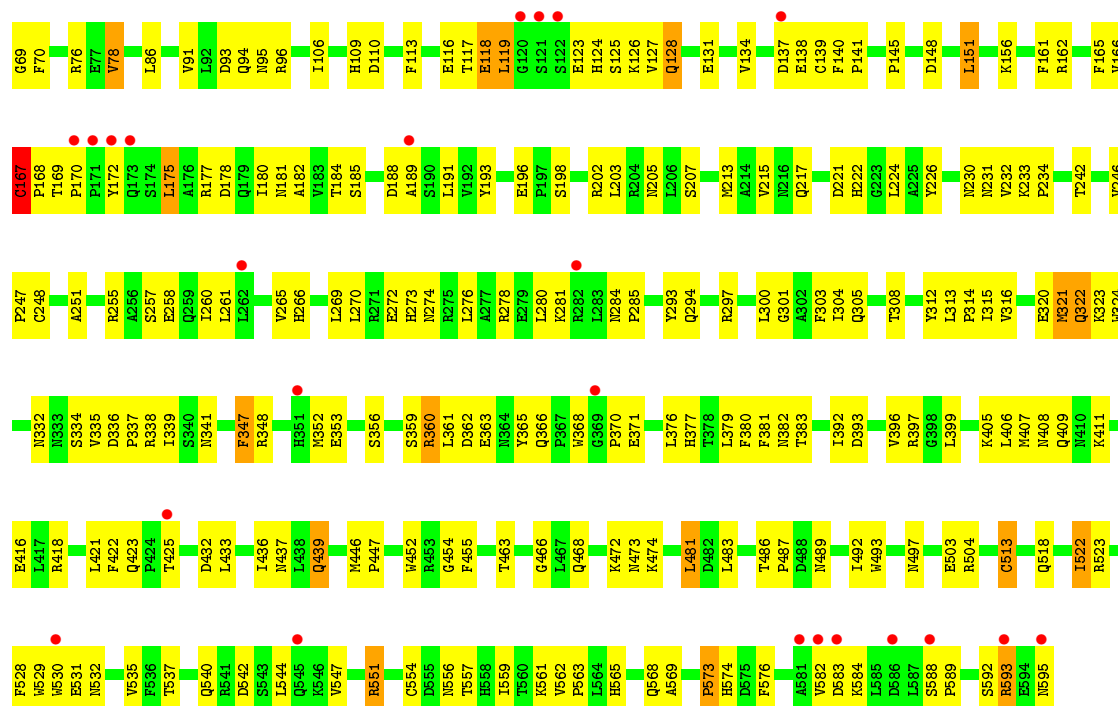
- Molecule 8 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



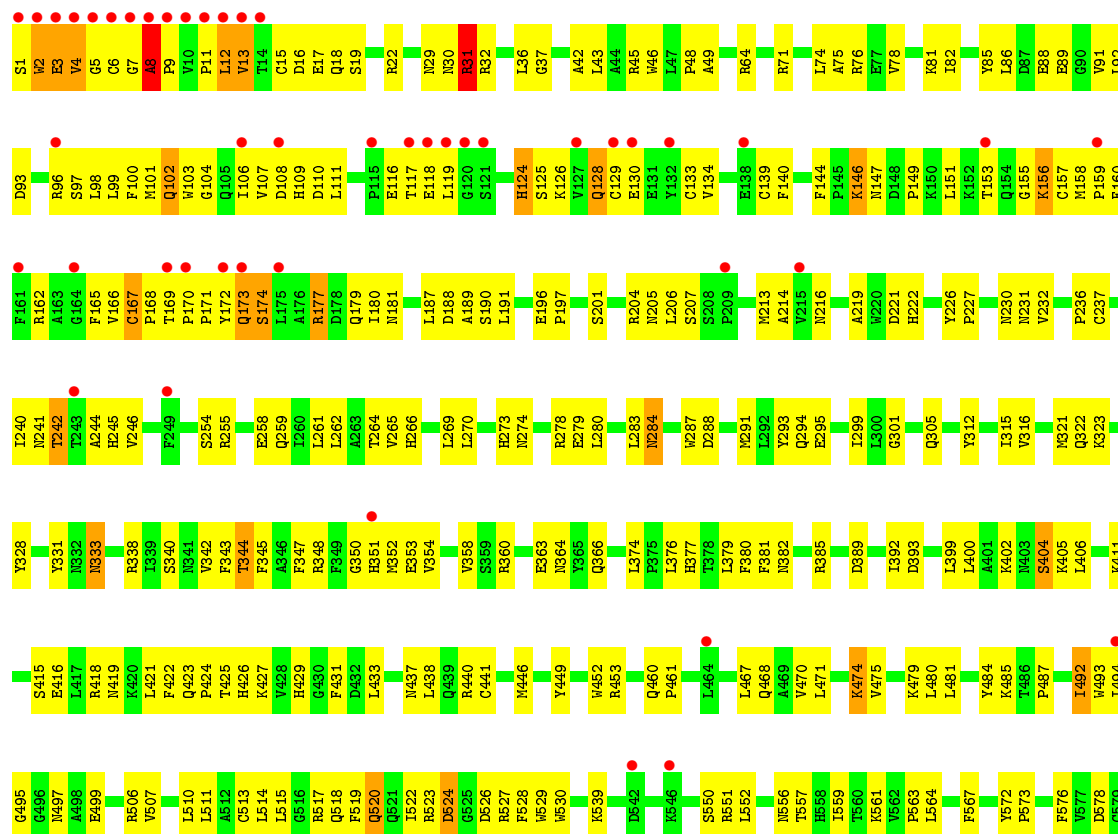
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
8	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
8	B	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
8	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
8	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

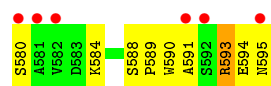
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	161	Total	O	0	0
			161	161		
9	B	155	Total	O	0	0
			155	155		
9	C	170	Total	O	0	0
			170	170		
9	D	165	Total	O	0	0
			165	165		

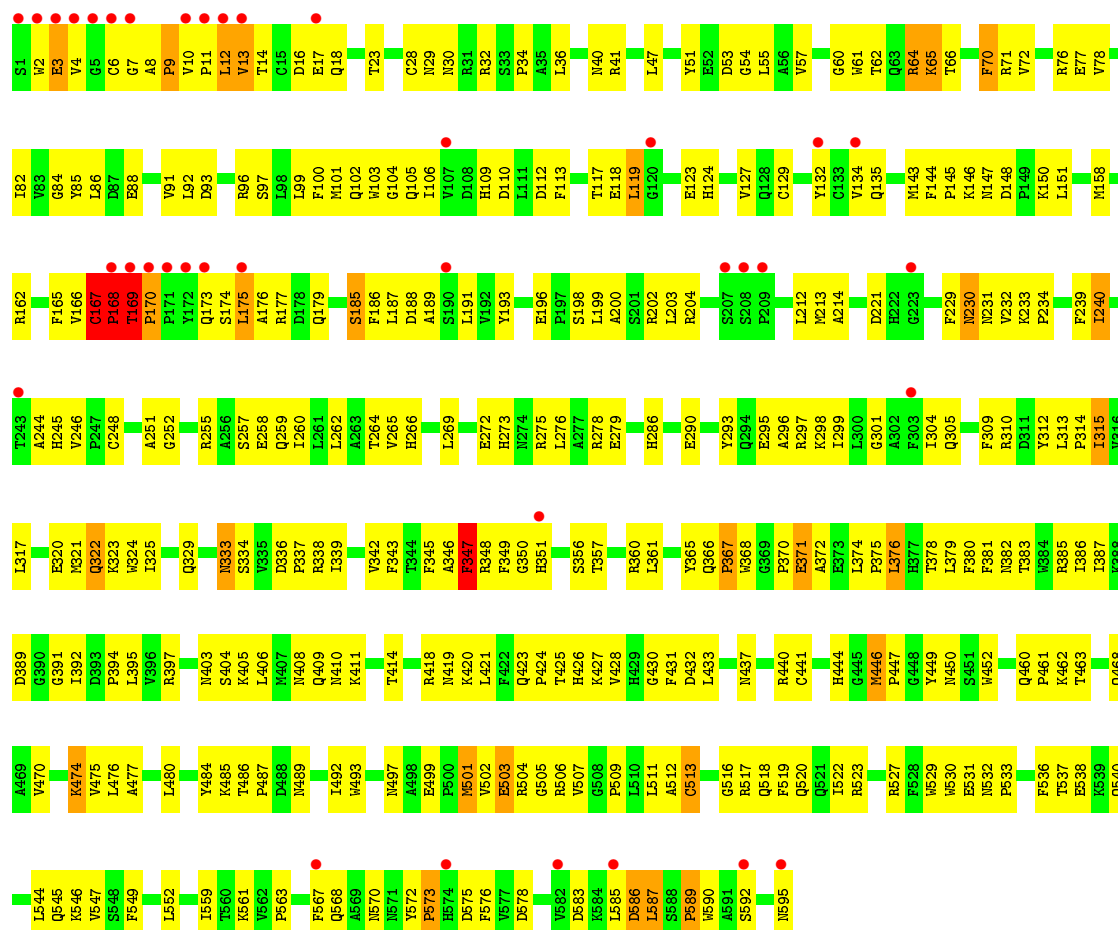


- Molecule 1: Lactoperoxidase





• Molecule 1: Lactoperoxidase



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



• Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:  100%

MAG1
MAG2

- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-3)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  100%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.22Å 82.59Å 95.08Å 80.91° 73.71° 89.96°	Depositor
Resolution (Å)	42.50 – 2.50 42.46 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.7 (42.50-2.50) 91.8 (42.46-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.260 , 0.311 0.254 , 0.307	Depositor DCC
R_{free} test set	3668 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.744	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 49.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	20141	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 40.53 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.7003e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HEM, CA, NO3, NAG, 3CJ

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	0.53	2/4882 (0.0%)	0.75	2/6632 (0.0%)
1	B	0.47	0/4882	0.76	0/6632
1	C	0.54	3/4882 (0.1%)	0.76	1/6632 (0.0%)
1	D	0.51	1/4882 (0.0%)	0.79	3/6632 (0.0%)
All	All	0.51	6/19528 (0.0%)	0.76	6/26528 (0.0%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	10	VAL	C-N	9.65	1.52	1.34
1	C	31	ARG	CA-C	-5.54	1.38	1.52
1	A	171	PRO	N-CD	5.39	1.55	1.47
1	D	168	PRO	N-CD	5.14	1.55	1.47
1	C	31	ARG	C-N	-5.10	1.22	1.34
1	C	9	PRO	N-CD	5.03	1.54	1.47

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	169	THR	C-N-CD	-7.76	103.53	120.60
1	D	167	CYS	C-N-CD	5.57	140.10	128.40
1	A	170	PRO	C-N-CD	5.51	139.97	128.40
1	A	349	PHE	N-CA-C	-5.38	96.49	111.00
1	C	8	ALA	C-N-CD	5.32	139.57	128.40
1	D	167	CYS	CA-CB-SG	5.02	123.03	114.00

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	4753	0	4646	298	0
1	B	4753	0	4646	227	0
1	C	4753	0	4649	313	0
1	D	4753	0	4647	290	0
2	E	28	0	25	1	0
2	G	28	0	25	1	0
2	H	28	0	25	0	0
3	F	28	0	25	2	0
4	A	28	0	26	0	0
4	B	14	0	13	0	0
4	C	28	0	26	0	0
4	D	28	0	26	1	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	12	0	0	1	0
6	B	12	0	0	1	0
6	C	12	0	0	4	0
6	D	12	0	0	8	0
7	A	11	0	10	11	0
7	B	11	0	10	12	0
7	C	11	0	10	9	0
7	D	11	0	10	11	0
8	A	43	0	30	12	0
8	B	43	0	30	14	0
8	C	43	0	30	17	0
8	D	43	0	30	15	0
9	A	161	0	0	15	0
9	B	155	0	0	10	0
9	C	170	0	0	20	0
9	D	165	0	0	11	0
All	All	20141	0	18939	1151	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 30.

All (1151) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:GLU:OE2	8:D:610:HEM:CMB	1.65	1.42
1:A:167:CYS:HB2	1:A:168:PRO:CD	1.55	1.32
1:D:258:GLU:OE2	8:D:610:HEM:HMB1	1.18	1.30
1:B:10:VAL:HG11	1:B:41:ARG:NH1	1.48	1.28
1:C:96:ARG:HD2	1:C:100:PHE:CD2	1.73	1.21
1:C:167:CYS:HB3	1:C:168:PRO:CD	1.68	1.17
1:C:96:ARG:HD2	1:C:100:PHE:CE2	1.79	1.16
1:A:62:THR:HG21	1:A:65:LYS:HB2	1.15	1.15
7:D:609:3CJ:H5	8:D:610:HEM:HAA1	1.25	1.13
1:C:96:ARG:NH1	1:C:100:PHE:HE2	1.45	1.12
1:D:169:THR:HB	1:D:170:PRO:HD3	1.32	1.10
1:A:62:THR:HG21	1:A:65:LYS:CB	1.83	1.08
1:C:167:CYS:HB3	1:C:168:PRO:HD2	1.29	1.08
1:B:167:CYS:HB3	1:B:168:PRO:HD2	1.11	1.07
1:A:167:CYS:HB2	1:A:168:PRO:HD3	1.24	1.07
3:F:1:NAG:O4	3:F:2:NAG:N2	1.88	1.06
1:A:167:CYS:CB	1:A:168:PRO:HD3	1.84	1.06
1:B:167:CYS:CB	1:B:168:PRO:HD2	1.87	1.04
1:C:93:ASP:OD2	1:C:96:ARG:NE	1.92	1.03
1:A:169:THR:H	1:A:170:PRO:HD2	1.20	1.02
1:C:42:ALA:HB2	1:C:166:VAL:HG11	1.41	1.02
1:B:167:CYS:HB3	1:B:168:PRO:CD	1.89	1.02
1:C:96:ARG:NH1	1:C:100:PHE:CE2	2.24	1.01
1:C:423:GLN:HG2	9:C:733:HOH:O	1.59	1.00
1:D:169:THR:CB	1:D:170:PRO:HD3	1.88	0.99
1:A:402:LYS:HD2	6:A:607:NO3:O3	1.61	0.98
1:B:42:ALA:HB2	1:B:166:VAL:HG11	1.46	0.98
1:A:167:CYS:CB	1:A:168:PRO:CD	2.38	0.98
1:A:169:THR:N	1:A:170:PRO:HD2	1.75	0.98
1:A:557:THR:OG1	1:A:559:ILE:HG12	1.65	0.97
1:C:167:CYS:CB	1:C:168:PRO:HD2	1.92	0.97
7:C:609:3CJ:H2	8:C:610:HEM:O1D	1.64	0.96
1:C:96:ARG:NH1	1:C:506:ARG:HG3	1.80	0.95
1:C:593:ARG:NH1	1:C:593:ARG:HB3	1.81	0.95
1:D:13:VAL:HG12	1:D:14:THR:H	1.29	0.95
1:B:10:VAL:HG11	1:B:41:ARG:HH12	1.12	0.93
1:B:10:VAL:CG1	1:B:41:ARG:HH12	1.81	0.93
1:A:62:THR:CG2	1:A:65:LYS:HB2	1.98	0.91
1:C:167:CYS:CB	1:C:168:PRO:CD	2.47	0.91
1:C:102:GLN:OE1	1:C:259:GLN:NE2	2.03	0.90
1:B:537:THR:OG1	1:B:540:GLN:HG3	1.71	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:GLU:OE2	8:D:610:HEM:HMB2	1.69	0.90
1:A:8:ALA:HB1	9:A:762:HOH:O	1.71	0.89
1:B:551:ARG:HD3	1:B:584:LYS:HA	1.53	0.89
1:C:96:ARG:CD	1:C:100:PHE:CE2	2.55	0.89
1:A:117:THR:HG22	1:A:162:ARG:O	1.72	0.89
1:C:312:TYR:O	1:C:315:ILE:HG12	1.73	0.89
1:A:129:CYS:O	1:A:133:CYS:HA	1.73	0.88
1:B:10:VAL:HG11	1:B:41:ARG:CZ	2.03	0.87
1:C:481:LEU:HD21	1:C:487:PRO:HG3	1.55	0.87
1:B:13:VAL:O	1:B:13:VAL:HG12	1.75	0.87
1:A:377:HIS:HB3	1:A:416:GLU:OE1	1.74	0.87
1:C:96:ARG:HH11	1:C:506:ARG:HG3	1.40	0.87
1:A:167:CYS:HB2	1:A:168:PRO:HD2	1.52	0.87
1:B:167:CYS:CB	1:B:168:PRO:CD	2.51	0.86
1:C:593:ARG:HB3	1:C:593:ARG:HH11	1.38	0.86
1:B:537:THR:HG23	1:B:540:GLN:OE1	1.75	0.86
1:D:403:ASN:HB2	6:D:607:NO3:O1	1.76	0.85
1:A:42:ALA:HB2	1:A:166:VAL:HG11	1.58	0.85
1:B:2:TRP:HH2	1:C:86:LEU:HD13	1.41	0.84
1:D:348:ARG:HH11	1:D:437:ASN:ND2	1.75	0.84
1:C:37:GLY:H	1:C:338:ARG:HG2	1.41	0.84
1:C:418:ARG:HG2	1:C:418:ARG:HH11	1.41	0.84
1:D:185:SER:HB3	1:D:339:ILE:HG12	1.58	0.84
1:D:530:TRP:CZ2	6:D:608:NO3:O2	2.30	0.84
1:C:421:LEU:HG	9:C:733:HOH:O	1.76	0.84
1:C:230:ASN:HD21	1:C:232:VAL:HG22	1.42	0.83
1:D:258:GLU:OE2	8:D:610:HEM:C2B	2.32	0.83
1:C:11:PRO:O	1:C:12:LEU:HB3	1.78	0.82
1:A:169:THR:N	1:A:170:PRO:CD	2.40	0.82
1:C:146:LYS:HG3	1:C:147:ASN:OD1	1.79	0.81
1:A:119:LEU:HD12	1:A:120:GLY:H	1.45	0.81
1:D:572:TYR:CE1	1:D:573:PRO:HB3	2.15	0.81
1:B:551:ARG:NH1	1:B:582:VAL:O	2.14	0.81
1:D:92:LEU:HD13	6:D:607:NO3:O1	1.80	0.81
1:D:310:ARG:O	1:D:314:PRO:HG2	1.81	0.81
1:B:276:LEU:O	1:B:280:LEU:HG	1.81	0.80
1:C:513:CYS:O	1:C:517:ARG:HG3	1.82	0.80
3:F:1:NAG:C4	3:F:2:NAG:HN2	1.95	0.79
1:B:332:ASN:OD1	1:B:334:SER:HB2	1.81	0.79
7:D:609:3CJ:C6	8:D:610:HEM:HAA1	2.12	0.79
1:D:333:ASN:HD22	1:D:333:ASN:H	1.29	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:423:GLN:HB3	1:C:426:HIS:HD2	1.48	0.79
1:D:230:ASN:OD1	1:D:232:VAL:HG22	1.82	0.79
1:B:10:VAL:CG1	1:B:41:ARG:NH1	2.38	0.78
1:D:13:VAL:HG12	1:D:14:THR:N	1.98	0.78
1:D:119:LEU:HD12	9:D:804:HOH:O	1.83	0.78
1:C:12:LEU:HG	1:C:13:VAL:H	1.48	0.77
1:A:322:GLN:H	1:A:322:GLN:HE21	1.30	0.77
1:C:468:GLN:HG2	1:C:474:LYS:HA	1.66	0.77
1:B:123:GLU:HB2	1:B:126:LYS:HG3	1.64	0.77
1:B:117:THR:OG1	1:B:119:LEU:HD23	1.83	0.77
7:C:609:3CJ:C6	8:C:610:HEM:HAA1	2.14	0.77
1:A:169:THR:H	1:A:170:PRO:CD	1.95	0.77
1:A:551:ARG:NH1	1:A:584:LYS:HG2	2.00	0.77
1:A:351:HIS:CE1	1:A:433:LEU:HD21	2.21	0.76
1:C:12:LEU:HG	1:C:13:VAL:N	1.99	0.76
1:D:295:GLU:O	1:D:299:ILE:HG13	1.86	0.76
1:C:125:SER:HA	1:C:128:GLN:HB3	1.67	0.76
1:C:96:ARG:NH1	1:C:506:ARG:CG	2.49	0.76
1:D:265:VAL:O	1:D:269:LEU:HG	1.86	0.75
1:B:551:ARG:HD2	1:B:583:ASP:O	1.85	0.75
1:C:146:LYS:HE3	1:C:147:ASN:HD21	1.52	0.75
1:C:348:ARG:HH11	1:C:437:ASN:ND2	1.84	0.75
1:C:452:TRP:HH2	6:C:608:NO3:O3	1.69	0.75
1:C:167:CYS:HB3	1:C:168:PRO:HD3	1.68	0.75
1:B:301:GLY:O	1:B:305:GLN:HG3	1.86	0.75
1:C:76:ARG:HH22	1:C:419:ASN:HD21	1.35	0.74
2:E:2:NAG:O3	2:E:2:NAG:H62	1.87	0.74
1:A:261:LEU:O	1:A:264:THR:HB	1.85	0.74
1:C:96:ARG:NH2	1:C:406:LEU:HD12	2.02	0.74
7:C:609:3CJ:H5	8:C:610:HEM:HAA1	1.70	0.74
1:C:159:PRO:HD2	1:C:431:PHE:HE1	1.50	0.73
1:C:348:ARG:HB2	1:C:493:TRP:CD1	2.23	0.73
1:C:96:ARG:HH21	1:C:406:LEU:HD12	1.51	0.73
1:D:113:PHE:CE1	7:D:609:3CJ:H6	2.23	0.73
1:C:519:PHE:HA	1:C:522:ILE:HG13	1.69	0.73
1:C:146:LYS:CE	1:C:147:ASN:HD21	2.02	0.73
1:C:348:ARG:HB2	1:C:493:TRP:NE1	2.02	0.73
1:A:260:ILE:HG23	1:A:261:LEU:HD23	1.70	0.73
1:A:588:SER:HB2	1:A:589:PRO:HD3	1.71	0.73
1:B:118:GLU:HG3	1:B:119:LEU:H	1.52	0.73
1:A:327:PRO:HA	9:A:719:HOH:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:170:PRO:HA	9:C:822:HOH:O	1.89	0.73
1:B:409:GLN:NE2	1:B:473:ASN:HD22	1.87	0.72
1:D:375:PRO:HG2	1:D:378:THR:HG23	1.70	0.72
1:A:421:LEU:HB3	1:A:431:PHE:HB2	1.72	0.72
8:B:608:HEM:HBB2	8:B:608:HEM:HMB1	1.72	0.72
1:C:552:LEU:HD12	1:C:556:ASN:ND2	2.05	0.72
1:C:348:ARG:CB	1:C:493:TRP:HE1	2.02	0.72
1:A:239:PHE:HZ	1:A:427:LYS:HB3	1.55	0.72
1:C:530:TRP:NE1	6:C:606:NO3:O2	2.22	0.72
1:B:2:TRP:CZ2	1:C:86:LEU:HD22	2.25	0.71
7:A:609:3CJ:H7	8:A:610:HEM:HBD2	1.73	0.71
1:C:528:PHE:HB3	9:C:840:HOH:O	1.89	0.71
1:C:452:TRP:CH2	6:C:608:NO3:O3	2.44	0.71
1:A:119:LEU:CD1	1:A:120:GLY:N	2.53	0.71
1:B:300:LEU:O	1:B:304:ILE:HD13	1.91	0.71
1:C:427:LYS:N	1:C:427:LYS:HD2	2.05	0.70
1:D:345:PHE:CD2	1:D:446:MET:SD	2.84	0.70
1:A:105:GLN:HG3	7:A:609:3CJ:S1	2.32	0.70
7:A:609:3CJ:H3	8:A:610:HEM:O1D	1.91	0.70
1:C:342:VAL:HB	1:C:452:TRP:CZ2	2.27	0.70
1:D:106:ILE:HG23	1:D:191:LEU:HD11	1.73	0.70
1:D:322:GLN:CD	1:D:322:GLN:H	1.91	0.70
1:B:213:MET:HG2	1:B:273:HIS:CD2	2.26	0.70
1:A:103:TRP:O	1:A:107:VAL:HG23	1.91	0.70
1:B:377:HIS:HA	1:B:380:PHE:CE2	2.26	0.70
1:A:230:ASN:HD21	1:A:232:VAL:HG22	1.55	0.70
1:A:340:SER:OG	1:A:343:PHE:HB2	1.92	0.70
1:B:139:CYS:SG	1:B:141:PRO:HD3	2.32	0.70
1:C:484:TYR:O	1:C:485:LYS:HB2	1.90	0.70
1:C:519:PHE:HA	1:C:522:ILE:CG1	2.21	0.70
1:A:148:ASP:O	1:A:151:LEU:HB2	1.91	0.70
1:A:119:LEU:HD12	1:A:120:GLY:N	2.06	0.70
1:B:39:ALA:HB1	1:B:182:ALA:O	1.92	0.70
1:B:257:SER:HB2	9:B:729:HOH:O	1.91	0.69
1:B:272:GLU:O	1:B:276:LEU:HG	1.93	0.69
1:C:188:ASP:OD1	1:C:190:SER:HB3	1.92	0.69
1:A:99:LEU:HD23	1:A:566:ALA:HB1	1.74	0.69
1:B:421:LEU:HD12	1:B:422:PHE:H	1.57	0.69
1:B:42:ALA:HB2	1:B:166:VAL:CG1	2.21	0.69
1:D:530:TRP:HZ2	6:D:608:NO3:O2	1.72	0.69
1:C:517:ARG:NH2	1:C:517:ARG:HB3	2.07	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:273:HIS:HD2	1:B:274:ASN:OD1	1.74	0.69
1:B:551:ARG:CD	1:B:584:LYS:HA	2.24	0.68
1:C:124:HIS:CE1	1:C:128:GLN:HB2	2.28	0.68
1:C:423:GLN:HB2	1:C:426:HIS:HB2	1.75	0.68
1:D:409:GLN:HB3	1:D:476:LEU:HD22	1.74	0.68
1:B:463:THR:HA	9:B:784:HOH:O	1.92	0.68
1:C:423:GLN:HB3	1:C:426:HIS:CD2	2.28	0.68
1:B:261:LEU:HD13	1:B:399:LEU:HD21	1.73	0.68
1:A:119:LEU:CD1	1:A:120:GLY:H	2.06	0.68
1:D:3:GLU:HG2	1:D:4:VAL:H	1.59	0.68
1:A:421:LEU:HB3	1:A:431:PHE:CB	2.24	0.68
1:D:196:GLU:HB3	9:D:781:HOH:O	1.93	0.68
1:B:3:GLU:HB3	1:B:175:LEU:HD12	1.74	0.68
1:D:570:ASN:HB3	1:D:575:ASP:HB2	1.75	0.68
1:A:367:PRO:HB2	1:D:64:ARG:NH2	2.09	0.68
1:D:30:ASN:O	1:D:34:PRO:HA	1.94	0.68
1:D:7:GLY:C	1:D:9:PRO:HD3	2.14	0.68
1:A:88:GLU:O	1:A:91:VAL:HG22	1.93	0.67
8:B:608:HEM:O1D	7:B:609:3CJ:H3	1.95	0.67
1:C:96:ARG:CZ	1:C:506:ARG:HD2	2.24	0.67
1:C:146:LYS:HE3	1:C:147:ASN:ND2	2.09	0.67
1:A:113:PHE:CE1	7:A:609:3CJ:H5	2.30	0.67
1:A:66:THR:HB	1:A:70:PHE:C	2.13	0.67
8:B:608:HEM:HH A	7:B:609:3CJ:H7	1.77	0.67
1:C:76:ARG:HH22	1:C:419:ASN:ND2	1.92	0.67
1:D:530:TRP:NE1	6:D:608:NO3:O2	2.26	0.67
1:A:464:LEU:HD12	1:A:464:LEU:O	1.94	0.67
1:A:322:GLN:H	1:A:322:GLN:NE2	1.92	0.67
1:C:418:ARG:NH1	1:C:418:ARG:HG2	2.02	0.67
1:D:350:GLY:HA3	8:D:610:HEM:CBC	2.25	0.67
1:C:316:VAL:O	1:C:507:VAL:HG22	1.95	0.66
1:C:159:PRO:HD2	1:C:431:PHE:CE1	2.29	0.66
1:D:166:VAL:O	1:D:167:CYS:CB	2.41	0.66
1:B:118:GLU:HG3	1:B:119:LEU:N	2.08	0.66
1:D:10:VAL:CG1	1:D:11:PRO:HD2	2.25	0.66
1:B:2:TRP:HZ2	1:C:86:LEU:HD22	1.59	0.66
1:D:385:ARG:O	1:D:389:ASP:HB3	1.95	0.66
1:C:204:ARG:HA	1:C:213:MET:HA	1.78	0.66
1:B:280:LEU:O	1:B:284:ASN:N	2.28	0.66
1:B:113:PHE:CE1	7:B:609:3CJ:H5	2.30	0.66
1:C:146:LYS:NZ	1:C:147:ASN:HD21	1.93	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:ARG:NH1	1:C:418:ARG:HH12	1.94	0.66
1:D:370:PRO:HG2	1:D:371:GLU:OE1	1.95	0.66
1:A:2:TRP:HD1	1:A:175:LEU:HD23	1.60	0.66
1:C:345:PHE:O	1:C:493:TRP:HD1	1.79	0.66
1:A:188:ASP:OD1	1:A:190:SER:HB3	1.95	0.66
1:D:570:ASN:HB3	1:D:575:ASP:CB	2.26	0.66
1:C:287:TRP:HA	9:C:749:HOH:O	1.95	0.66
1:D:166:VAL:O	1:D:167:CYS:HB2	1.95	0.66
1:A:17:GLU:OE2	1:A:31:ARG:HG2	1.95	0.66
1:C:204:ARG:CZ	1:C:206:LEU:HD21	2.25	0.66
1:D:10:VAL:HG12	1:D:11:PRO:HD2	1.77	0.66
1:D:530:TRP:CE2	6:D:608:NO3:O2	2.47	0.66
1:B:51:TYR:HB3	1:B:57:VAL:O	1.96	0.65
1:D:11:PRO:O	1:D:13:VAL:HG23	1.96	0.65
1:C:348:ARG:HB2	1:C:493:TRP:HE1	1.58	0.65
1:D:123:GLU:HG3	9:D:804:HOH:O	1.95	0.65
1:A:167:CYS:HB3	1:A:168:PRO:HD3	1.77	0.65
1:A:253:ASP:OD2	1:A:255:ARG:HB2	1.96	0.65
1:A:165:PHE:CD2	1:A:177:ARG:HD2	2.32	0.65
1:A:322:GLN:N	1:A:322:GLN:HE21	1.94	0.65
1:C:37:GLY:N	1:C:338:ARG:HG2	2.11	0.65
1:C:98:LEU:HA	1:C:404:SER:OG	1.97	0.65
1:A:370:PRO:O	1:D:71:ARG:NH2	2.29	0.65
1:A:99:LEU:HG	1:A:567:PHE:HE1	1.61	0.65
1:B:407:MET:SD	1:B:408:ASN:N	2.69	0.65
1:C:109:HIS:HA	1:C:255:ARG:NH2	2.11	0.65
1:C:201:SER:HA	9:C:816:HOH:O	1.95	0.65
1:A:551:ARG:NH1	1:A:584:LYS:CG	2.60	0.65
1:B:94:GLN:O	1:B:569:ALA:HB3	1.96	0.65
1:A:71:ARG:CZ	1:A:71:ARG:HB3	2.24	0.65
1:D:463:THR:HB	9:D:714:HOH:O	1.94	0.65
1:D:105:GLN:NE2	7:D:609:3CJ:S1	2.60	0.65
1:A:95:ASN:O	1:A:96:ARG:HD3	1.97	0.65
1:B:10:VAL:HG21	1:B:41:ARG:HH12	1.62	0.65
1:B:145:PRO:O	1:B:148:ASP:HB2	1.97	0.65
1:A:62:THR:HG23	1:A:64:ARG:H	1.62	0.64
1:A:148:ASP:O	1:A:151:LEU:CB	2.46	0.64
1:B:537:THR:OG1	1:B:540:GLN:CG	2.44	0.64
1:C:48:PRO:HG2	9:C:720:HOH:O	1.98	0.64
1:D:408:ASN:O	1:D:411:LYS:N	2.28	0.64
1:A:123:GLU:HB2	1:A:126:LYS:HG3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ARG:HG2	8:A:610:HEM:C2D	2.33	0.64
1:A:142:ILE:HD12	1:A:160:PHE:HB2	1.77	0.64
1:A:546:LYS:HZ1	1:A:586:ASP:H	1.46	0.64
1:C:351:HIS:CE1	1:C:433:LEU:HD21	2.32	0.64
1:A:62:THR:CG2	1:A:65:LYS:H	2.10	0.64
1:C:393:ASP:OD1	1:C:557:THR:HB	1.96	0.64
1:D:112:ASP:OD1	8:D:610:HEM:O2D	2.16	0.64
1:B:265:VAL:O	1:B:269:LEU:HG	1.98	0.63
1:C:264:THR:HG23	1:C:392:ILE:HG23	1.81	0.63
1:D:368:TRP:O	1:D:372:ALA:HB2	1.98	0.63
1:D:424:PRO:O	1:D:425:THR:HB	1.96	0.63
1:B:145:PRO:HD2	1:B:148:ASP:OD2	1.96	0.63
1:A:8:ALA:HA	9:A:813:HOH:O	1.97	0.63
1:B:230:ASN:OD1	1:B:232:VAL:HG22	1.98	0.63
1:D:8:ALA:N	1:D:9:PRO:HD3	2.13	0.63
1:B:532:ASN:O	1:B:535:VAL:HG23	1.98	0.63
8:B:608:HEM:CHA	7:B:609:3CJ:H7	2.29	0.63
1:A:123:GLU:CB	1:A:126:LYS:HG3	2.29	0.63
1:B:167:CYS:SG	1:B:168:PRO:CD	2.87	0.63
1:A:121:SER:O	1:A:123:GLU:N	2.30	0.63
1:C:110:ASP:OD1	1:C:187:LEU:HA	1.99	0.63
1:D:167:CYS:HB3	1:D:168:PRO:CD	2.28	0.63
1:C:146:LYS:HE3	1:C:147:ASN:OD1	1.98	0.62
1:B:18:GLN:HG3	9:B:745:HOH:O	1.99	0.62
1:C:140:PHE:O	1:C:160:PHE:HB3	1.99	0.62
1:D:10:VAL:HG12	1:D:11:PRO:CD	2.29	0.62
1:D:13:VAL:CG1	1:D:14:THR:H	2.08	0.62
1:D:91:VAL:O	1:D:406:LEU:N	2.28	0.62
1:B:11:PRO:O	1:B:13:VAL:HG23	1.99	0.62
1:D:16:ASP:O	1:D:18:GLN:N	2.30	0.62
1:A:2:TRP:CD1	1:A:175:LEU:HD23	2.34	0.62
1:B:353:GLU:HA	1:B:405:LYS:O	2.00	0.62
1:C:468:GLN:OE1	1:C:474:LYS:HB3	1.99	0.62
1:D:77:GLU:HG3	1:D:145:PRO:HB3	1.81	0.62
1:C:518:GLN:HE21	1:C:522:ILE:HG23	1.63	0.62
1:A:370:PRO:HG2	1:A:371:GLU:OE1	1.99	0.62
1:A:136:GLY:HA2	1:C:124:HIS:CD2	2.35	0.62
1:D:167:CYS:CB	1:D:168:PRO:CD	2.78	0.62
1:D:425:THR:HG21	9:D:812:HOH:O	2.00	0.62
1:D:446:MET:HE3	6:D:606:NO3:O1	1.99	0.62
1:D:191:LEU:H	1:D:191:LEU:HD23	1.63	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ILE:HD11	1:A:386:ILE:HG13	1.82	0.61
1:A:239:PHE:CZ	1:A:427:LYS:HB3	2.35	0.61
8:B:608:HEM:C1A	7:B:609:3CJ:N1	2.68	0.61
1:D:342:VAL:HB	1:D:446:MET:HE1	1.82	0.61
1:D:503:GLU:O	1:D:504:ARG:HB2	2.00	0.61
1:A:172:TYR:HE2	1:A:175:LEU:HB2	1.65	0.61
1:B:52:GLU:HG3	1:B:59:PHE:HA	1.81	0.61
1:C:425:THR:O	1:C:425:THR:HG22	2.01	0.61
1:D:309:PHE:HA	1:D:313:LEU:HD12	1.82	0.61
1:A:459:SER:O	1:A:461:PRO:HD3	2.01	0.61
1:A:313:LEU:HD11	1:A:519:PHE:CG	2.36	0.61
1:D:351:HIS:CD2	8:D:610:HEM:NC	2.69	0.61
1:A:174:SER:O	1:A:175:LEU:HG	2.01	0.61
1:D:240:ILE:HD13	1:D:382:ASN:HA	1.82	0.61
1:B:35:ALA:HB1	1:B:41:ARG:NE	2.16	0.61
1:D:101:MET:SD	1:D:101:MET:C	2.79	0.61
1:D:186:PHE:O	1:D:188:ASP:N	2.33	0.61
1:D:301:GLY:O	1:D:305:GLN:HG3	2.01	0.61
1:D:9:PRO:HG2	1:D:41:ARG:HH22	1.66	0.61
1:A:105:GLN:HB2	8:A:610:HEM:C2C	2.36	0.61
1:A:62:THR:HG21	1:A:65:LYS:H	1.66	0.61
1:D:325:ILE:O	1:D:325:ILE:HG22	2.01	0.61
1:D:113:PHE:HE1	7:D:609:3CJ:H6	1.66	0.61
1:A:165:PHE:CZ	1:A:169:THR:O	2.53	0.60
1:A:272:GLU:O	1:A:276:LEU:HG	2.01	0.60
1:C:168:PRO:HG3	1:C:172:TYR:HD2	1.67	0.60
1:C:539:LYS:HE2	1:C:589:PRO:HG3	1.81	0.60
1:C:151:LEU:HD11	1:C:156:LYS:HD2	1.82	0.60
1:C:169:THR:N	1:C:170:PRO:CD	2.64	0.60
1:D:144:PHE:CE1	1:D:158:MET:HG3	2.37	0.60
1:A:62:THR:HG21	1:A:65:LYS:N	2.16	0.60
1:B:13:VAL:CG1	1:B:13:VAL:O	2.49	0.60
1:B:110:ASP:OD2	1:B:189:ALA:HA	2.02	0.60
1:D:200:ALA:O	1:D:204:ARG:HG3	2.01	0.60
1:D:315:ILE:O	1:D:505:GLY:HA2	2.00	0.60
1:C:351:HIS:ND1	1:C:433:LEU:HD21	2.17	0.60
7:C:609:3CJ:H4	8:C:610:HEM:HAA1	1.82	0.60
1:D:586:ASP:O	1:D:589:PRO:HD2	2.02	0.60
7:D:609:3CJ:H2	8:D:610:HEM:O1D	2.02	0.60
1:A:81:LYS:HB2	1:A:483:LEU:HD11	1.84	0.60
1:D:7:GLY:HA2	1:D:166:VAL:HB	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:8:ALA:N	1:D:9:PRO:CD	2.65	0.60
1:A:325:ILE:O	1:A:325:ILE:HG22	2.02	0.60
1:D:492:ILE:HG23	1:D:493:TRP:N	2.17	0.60
1:B:258:GLU:O	1:B:380:PHE:HA	2.01	0.59
1:C:191:LEU:HD23	1:C:191:LEU:H	1.67	0.59
1:D:348:ARG:NH1	1:D:437:ASN:ND2	2.47	0.59
1:A:396:VAL:HA	1:A:399:LEU:HD12	1.84	0.59
1:A:342:VAL:HG11	1:A:452:TRP:CH2	2.37	0.59
1:C:12:LEU:O	1:C:13:VAL:HB	2.01	0.59
1:C:165:PHE:CG	1:C:177:ARG:HD2	2.37	0.59
8:D:610:HEM:HMC1	8:D:610:HEM:HBC2	1.84	0.59
1:B:409:GLN:HE22	1:B:473:ASN:HB2	1.66	0.59
1:C:169:THR:N	1:C:170:PRO:HD3	2.18	0.59
1:A:165:PHE:CG	1:A:177:ARG:HD2	2.37	0.59
1:A:392:ILE:O	1:A:396:VAL:HG23	2.01	0.59
1:C:165:PHE:CZ	1:C:169:THR:O	2.56	0.59
1:D:425:THR:O	1:D:425:THR:HG22	2.02	0.59
1:A:229:PHE:CD1	1:A:247:PRO:HG2	2.38	0.59
1:D:168:PRO:HB2	1:D:170:PRO:HD2	1.84	0.59
1:A:156:LYS:HG3	9:A:742:HOH:O	2.02	0.59
1:C:522:ILE:O	1:C:526:ASP:HB2	2.03	0.59
8:A:610:HEM:HMC2	8:A:610:HEM:HBC2	1.85	0.59
1:A:99:LEU:HG	1:A:567:PHE:CE1	2.38	0.59
1:C:557:THR:OG1	1:C:559:ILE:HG12	2.02	0.59
1:D:419:ASN:O	1:D:430:GLY:HA2	2.03	0.58
1:A:8:ALA:N	1:A:9:PRO:CD	2.66	0.58
1:D:106:ILE:HG23	1:D:191:LEU:CD1	2.33	0.58
1:D:96:ARG:HG3	1:D:506:ARG:HE	1.68	0.58
1:A:9:PRO:HB2	1:A:41:ARG:NH2	2.18	0.58
1:C:99:LEU:HA	1:C:399:LEU:HD22	1.85	0.58
1:D:117:THR:HG22	1:D:162:ARG:O	2.04	0.58
1:D:9:PRO:HG2	1:D:41:ARG:NH2	2.19	0.58
1:A:146:LYS:O	1:A:147:ASN:HB2	2.04	0.58
1:A:348:ARG:HG2	8:A:610:HEM:C3D	2.39	0.58
1:D:486:THR:HG23	1:D:489:ASN:H	1.69	0.58
1:D:501:MET:HA	1:D:507:VAL:O	2.03	0.58
1:A:504:ARG:HD3	9:A:831:HOH:O	2.02	0.58
1:A:66:THR:HB	1:A:70:PHE:O	2.03	0.58
1:D:199:LEU:HD12	1:D:199:LEU:O	2.04	0.58
1:B:348:ARG:HH11	1:B:437:ASN:ND2	2.02	0.58
1:B:62:THR:HB	1:B:65:LYS:HB2	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:HIS:HE1	1:C:128:GLN:HB2	1.68	0.58
1:C:301:GLY:O	1:C:305:GLN:HG3	2.03	0.58
1:A:9:PRO:HB2	1:A:41:ARG:CZ	2.34	0.58
1:B:148:ASP:HB3	1:B:151:LEU:HD22	1.85	0.58
1:B:418:ARG:HG2	1:B:432:ASP:OD2	2.03	0.57
1:D:10:VAL:HG12	1:D:11:PRO:N	2.19	0.57
1:A:222:HIS:HB3	9:A:840:HOH:O	2.04	0.57
1:A:421:LEU:HG	1:A:422:PHE:N	2.18	0.57
1:D:10:VAL:CG1	1:D:11:PRO:CD	2.82	0.57
1:D:342:VAL:HB	1:D:446:MET:CE	2.33	0.57
1:C:196:GLU:HB3	9:C:707:HOH:O	2.03	0.57
1:C:2:TRP:N	1:C:2:TRP:CE3	2.73	0.57
1:D:361:LEU:HD13	1:D:365:TYR:O	2.05	0.57
1:A:233:LYS:NZ	1:B:322:GLN:HB2	2.20	0.57
1:C:197:PRO:HD2	9:C:707:HOH:O	2.03	0.57
1:D:234:PRO:HB2	9:D:821:HOH:O	2.04	0.57
1:B:66:THR:HB	1:B:70:PHE:O	2.05	0.57
1:C:258:GLU:O	1:C:380:PHE:HA	2.04	0.57
1:C:440:ARG:NH2	8:C:610:HEM:O1A	2.38	0.57
1:D:421:LEU:HD22	1:D:433:LEU:HB2	1.86	0.57
1:D:231:ASN:O	1:D:233:LYS:HE2	2.04	0.57
1:B:168:PRO:CG	1:B:172:TYR:HB3	2.35	0.57
1:B:392:ILE:O	1:B:396:VAL:HG23	2.05	0.57
1:B:425:THR:O	1:B:425:THR:HG22	2.05	0.57
1:C:167:CYS:HB2	1:C:168:PRO:HD2	1.85	0.57
1:C:299:ILE:HD11	1:C:590:TRP:NE1	2.20	0.57
1:A:71:ARG:HB3	1:A:71:ARG:NH1	2.20	0.57
1:D:119:LEU:HD22	1:D:169:THR:HG21	1.86	0.57
1:B:406:LEU:HG	1:B:407:MET:N	2.19	0.56
1:A:117:THR:O	1:A:161:PHE:HB3	2.05	0.56
7:A:609:3CJ:C5	8:A:610:HEM:HBD2	2.35	0.56
1:C:475:VAL:HG12	1:C:479:LYS:HE2	1.88	0.56
1:D:572:TYR:CD1	1:D:573:PRO:HB3	2.38	0.56
1:C:168:PRO:HB2	1:C:170:PRO:HD2	1.87	0.56
1:B:10:VAL:CG2	1:B:41:ARG:HH12	2.16	0.56
1:C:81:LYS:HB3	9:C:821:HOH:O	2.03	0.56
1:D:492:ILE:HG23	1:D:493:TRP:H	1.68	0.56
1:C:173:GLN:O	1:C:174:SER:HB2	2.04	0.56
1:D:109:HIS:HA	1:D:255:ARG:NH2	2.20	0.56
1:A:275:ARG:HD2	1:A:555:ASP:HB3	1.88	0.56
1:A:281:LYS:HD2	1:A:285:PRO:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:THR:CG2	1:A:65:LYS:N	2.69	0.56
1:A:189:ALA:HB2	1:A:304:ILE:HD12	1.87	0.56
1:C:204:ARG:CZ	1:C:206:LEU:CD2	2.84	0.56
1:C:517:ARG:HB3	1:C:517:ARG:HH21	1.70	0.56
1:A:144:PHE:CE2	1:A:157:CYS:N	2.74	0.56
1:A:367:PRO:HB2	1:D:64:ARG:CZ	2.35	0.56
1:A:465:LYS:HA	1:A:468:GLN:HE21	1.71	0.56
1:C:133:CYS:HB2	9:C:748:HOH:O	2.06	0.56
1:B:193:TYR:CE2	1:B:297:ARG:HG3	2.41	0.55
1:C:1:SER:C	1:C:2:TRP:CE3	2.80	0.55
1:D:29:ASN:HD21	1:D:527:ARG:H	1.53	0.55
1:D:96:ARG:HD2	1:D:100:PHE:CD2	2.40	0.55
1:A:393:ASP:OD2	1:A:558:HIS:HB2	2.06	0.55
1:A:169:THR:OG1	1:A:170:PRO:HD3	2.07	0.55
1:A:213:MET:CB	1:A:270:LEU:HD11	2.36	0.55
1:B:167:CYS:SG	1:B:168:PRO:HD2	2.46	0.55
1:B:193:TYR:CD2	1:B:297:ARG:HG3	2.41	0.55
1:D:529:TRP:CD1	1:D:531:GLU:HB2	2.40	0.55
1:A:109:HIS:NE2	7:A:609:3CJ:C1	2.70	0.55
1:A:13:VAL:HG12	1:A:14:THR:N	2.22	0.55
1:A:20:PRO:O	1:A:21:TYR:CD1	2.60	0.55
1:D:113:PHE:CD1	7:D:609:3CJ:H6	2.41	0.55
1:D:199:LEU:O	1:D:203:LEU:HG	2.06	0.55
1:D:146:LYS:O	1:D:147:ASN:HB2	2.06	0.55
1:B:113:PHE:HE1	7:B:609:3CJ:H5	1.71	0.55
1:C:125:SER:CA	1:C:128:GLN:HB3	2.36	0.55
1:A:87:ASP:OD1	1:A:89:GLU:HB2	2.07	0.55
1:B:118:GLU:HG3	9:B:716:HOH:O	2.07	0.55
1:C:134:VAL:HA	9:C:716:HOH:O	2.07	0.55
7:D:609:3CJ:H7	8:D:610:HEM:HBD2	1.89	0.55
1:A:43:LEU:HD13	1:A:341:ASN:HA	1.88	0.55
1:A:499:GLU:OE1	1:A:509:PRO:HG2	2.07	0.55
1:B:123:GLU:CB	1:B:126:LYS:HG3	2.34	0.55
1:C:381:PHE:CZ	1:C:424:PRO:HG3	2.43	0.54
8:C:610:HEM:HMB1	8:C:610:HEM:HBB2	1.88	0.54
1:D:167:CYS:CB	1:D:168:PRO:HD2	2.37	0.54
1:A:367:PRO:HB2	1:D:64:ARG:HH21	1.70	0.54
1:B:377:HIS:ND1	1:B:416:GLU:OE1	2.40	0.54
1:C:97:SER:O	1:C:98:LEU:C	2.46	0.54
1:D:333:ASN:HD22	1:D:333:ASN:N	2.03	0.54
1:A:284:ASN:OD1	1:A:592:SER:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:VAL:O	1:C:111:LEU:HG	2.07	0.54
1:D:272:GLU:O	1:D:276:LEU:HG	2.07	0.54
1:B:409:GLN:HE21	1:B:473:ASN:HD22	1.55	0.54
1:C:342:VAL:HG21	1:C:452:TRP:CE2	2.42	0.54
1:C:96:ARG:CZ	1:C:506:ARG:CD	2.85	0.54
1:D:544:LEU:O	1:D:547:VAL:HG22	2.07	0.54
1:D:97:SER:O	1:D:404:SER:OG	2.26	0.54
1:B:138:GLU:OE1	1:B:162:ARG:HB2	2.06	0.54
1:C:348:ARG:NH1	1:C:437:ASN:ND2	2.54	0.54
1:A:203:LEU:HD13	1:A:213:MET:HE1	1.89	0.54
1:B:593:ARG:HG3	1:B:595:ASN:H	1.72	0.54
1:B:341:ASN:HB3	1:B:446:MET:HE1	1.89	0.54
8:B:608:HEM:HMC2	8:B:608:HEM:HBC2	1.89	0.54
1:C:7:GLY:O	1:C:8:ALA:HB3	2.07	0.54
1:A:62:THR:O	1:A:63:GLN:HB3	2.07	0.54
1:C:280:LEU:O	1:C:284:ASN:ND2	2.41	0.54
1:D:96:ARG:NH2	1:D:315:ILE:HB	2.23	0.54
1:C:1:SER:C	1:C:2:TRP:HE3	2.10	0.54
1:D:9:PRO:CG	1:D:41:ARG:NH2	2.71	0.54
1:A:408:ASN:C	1:A:408:ASN:OD1	2.46	0.53
1:C:213:MET:HG2	1:C:273:HIS:NE2	2.24	0.53
1:C:259:GLN:OE1	1:C:261:LEU:HB2	2.08	0.53
1:D:193:TYR:OH	1:D:297:ARG:HA	2.07	0.53
1:D:96:ARG:CZ	1:D:315:ILE:HB	2.38	0.53
1:C:82:ILE:HD12	1:C:480:LEU:HD23	1.91	0.53
1:D:103:TRP:O	1:D:106:ILE:N	2.36	0.53
1:D:9:PRO:HG3	1:D:41:ARG:CZ	2.39	0.53
1:A:367:PRO:HB2	1:D:64:ARG:NE	2.24	0.53
1:B:117:THR:HG22	1:B:161:PHE:HB3	1.89	0.53
1:B:30:ASN:O	1:B:34:PRO:HA	2.07	0.53
1:C:551:ARG:O	1:C:552:LEU:C	2.45	0.53
1:D:589:PRO:HB2	1:D:590:TRP:CE3	2.43	0.53
1:D:214:ALA:HA	4:D:602:NAG:O7	2.08	0.53
1:D:446:MET:CE	6:D:606:NO3:O1	2.56	0.53
1:A:15:CYS:HB3	9:A:747:HOH:O	2.09	0.53
1:A:99:LEU:CD2	1:A:566:ALA:HB1	2.39	0.53
1:A:62:THR:HG21	1:A:65:LYS:CA	2.37	0.53
1:B:117:THR:CG2	1:B:161:PHE:HB3	2.39	0.53
8:B:608:HEM:CHA	7:B:609:3CJ:N1	2.71	0.53
1:C:452:TRP:CD1	1:C:492:ILE:HG12	2.43	0.53
1:D:563:PRO:HD3	1:D:576:PHE:CE2	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ILE:CD1	1:A:160:PHE:HB2	2.38	0.53
1:B:128:GLN:HG3	1:B:134:VAL:HG21	1.91	0.53
1:B:165:PHE:CZ	1:B:169:THR:O	2.62	0.53
1:B:522:ILE:HG13	1:B:523:ARG:N	2.22	0.53
1:C:205:ASN:HB2	1:C:214:ALA:HA	1.90	0.53
1:A:16:ASP:O	1:A:18:GLN:N	2.37	0.53
1:A:233:LYS:HZ2	1:B:322:GLN:HB2	1.73	0.53
1:C:237:CYS:HA	1:C:381:PHE:O	2.09	0.53
1:C:385:ARG:NH1	1:C:389:ASP:OD2	2.42	0.53
1:D:376:LEU:HD21	1:D:380:PHE:HE1	1.74	0.53
1:C:523:ARG:HG3	1:C:529:TRP:CE2	2.43	0.52
1:D:119:LEU:CD2	1:D:169:THR:HG21	2.39	0.52
1:C:11:PRO:O	1:C:12:LEU:CB	2.51	0.52
1:C:204:ARG:HB2	1:C:206:LEU:HG	1.91	0.52
1:D:6:CYS:O	1:D:167:CYS:SG	2.67	0.52
1:A:241:ASN:ND2	1:A:244:ALA:HB2	2.24	0.52
1:B:167:CYS:SG	1:B:168:PRO:HD3	2.49	0.52
1:C:144:PHE:HE1	1:C:158:MET:HG3	1.74	0.52
1:C:437:ASN:O	1:C:440:ARG:N	2.40	0.52
1:B:2:TRP:CH2	1:C:86:LEU:HD13	2.31	0.52
1:C:97:SER:O	1:C:99:LEU:N	2.42	0.52
1:A:13:VAL:HG12	1:A:14:THR:H	1.74	0.52
1:A:492:ILE:HD11	1:A:510:LEU:HD21	1.90	0.52
1:B:93:ASP:OD2	1:B:406:LEU:HD12	2.09	0.52
1:C:125:SER:O	1:C:128:GLN:HB3	2.08	0.52
1:D:397:ARG:HG3	1:D:559:ILE:HD12	1.91	0.52
1:D:424:PRO:O	1:D:425:THR:CB	2.58	0.52
1:D:513:CYS:O	1:D:517:ARG:HG2	2.09	0.52
1:C:96:ARG:CZ	1:C:100:PHE:CE2	2.92	0.52
1:C:400:LEU:HD13	1:C:563:PRO:HD2	1.91	0.52
1:D:348:ARG:HH22	1:D:440:ARG:HG2	1.73	0.52
1:A:168:PRO:HB2	1:A:170:PRO:O	2.10	0.52
1:C:117:THR:HG22	1:C:162:ARG:O	2.09	0.52
1:C:29:ASN:HD21	1:C:527:ARG:H	1.57	0.52
1:C:552:LEU:HD12	1:C:556:ASN:HD22	1.74	0.52
1:A:52:GLU:OE2	1:A:62:THR:HG22	2.09	0.52
1:B:352:MET:O	1:B:405:LYS:HD3	2.10	0.52
1:C:64:ARG:HA	1:C:71:ARG:NH2	2.25	0.52
1:A:128:GLN:HA	1:A:132:TYR:HD1	1.75	0.52
1:C:221:ASP:HB2	1:C:226:TYR:CZ	2.44	0.52
1:D:143:MET:HG2	9:D:725:HOH:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:418:ARG:HH11	1:B:418:ARG:HG2	1.75	0.52
1:D:244:ALA:O	1:D:245:HIS:HB2	2.10	0.52
1:A:113:PHE:HE1	7:A:609:3CJ:H5	1.75	0.52
1:B:42:ALA:CB	1:B:166:VAL:HG11	2.30	0.52
1:B:551:ARG:CD	1:B:583:ASP:O	2.57	0.52
8:B:608:HEM:HAA1	7:B:609:3CJ:H4	1.92	0.52
1:C:29:ASN:HD21	1:C:527:ARG:N	2.08	0.52
1:D:16:ASP:O	1:D:17:GLU:HB3	2.10	0.52
1:C:288:ASP:OD1	1:C:291:MET:HB3	2.10	0.51
1:D:102:GLN:OE1	1:D:259:GLN:NE2	2.35	0.51
1:A:258:GLU:O	1:A:380:PHE:HA	2.09	0.51
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.46	0.51
1:B:10:VAL:CB	1:B:41:ARG:HH12	2.23	0.51
1:B:169:THR:N	1:B:170:PRO:HD2	2.26	0.51
1:D:257:SER:O	1:D:381:PHE:HA	2.11	0.51
1:A:340:SER:HG	1:A:343:PHE:HB2	1.75	0.51
1:A:551:ARG:HD2	1:A:584:LYS:HA	1.91	0.51
1:B:397:ARG:NH2	1:B:559:ILE:HD13	2.25	0.51
1:C:561:LYS:HD3	1:C:576:PHE:HB3	1.92	0.51
1:D:379:LEU:HA	1:D:382:ASN:HB2	1.91	0.51
1:A:8:ALA:N	1:A:9:PRO:HD2	2.26	0.51
1:C:146:LYS:HE3	1:C:147:ASN:CG	2.30	0.51
1:C:287:TRP:CZ3	1:C:295:GLU:HG3	2.45	0.51
1:C:75:ALA:HB1	1:C:438:LEU:HB2	1.92	0.51
1:B:25:THR:O	1:B:184:THR:HG22	2.10	0.51
1:B:37:GLY:H	1:B:338:ARG:HG2	1.76	0.51
1:C:348:ARG:CB	1:C:493:TRP:NE1	2.68	0.51
1:A:593:ARG:HD2	1:A:595:ASN:H	1.75	0.51
1:A:7:GLY:O	1:A:8:ALA:HB3	2.10	0.51
1:B:180:ILE:HG22	1:B:181:ASN:N	2.25	0.51
1:C:76:ARG:NH1	1:C:418:ARG:NH1	2.59	0.51
1:A:315:ILE:O	1:A:505:GLY:HA2	2.11	0.51
1:C:441:CYS:O	1:C:446:MET:HB2	2.10	0.51
1:D:349:PHE:CD1	1:D:349:PHE:C	2.84	0.51
1:D:499:GLU:OE1	1:D:509:PRO:HG2	2.11	0.51
1:C:116:GLU:O	1:C:117:THR:HB	2.10	0.51
1:D:349:PHE:CD1	1:D:350:GLY:N	2.78	0.51
1:B:447:PRO:HG2	1:B:452:TRP:NE1	2.25	0.51
1:B:503:GLU:O	1:B:504:ARG:HB2	2.10	0.51
1:B:530:TRP:CG	1:B:531:GLU:N	2.79	0.51
1:B:556:ASN:O	1:B:557:THR:HG23	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:ALA:O	1:B:162:ARG:NH1	2.40	0.51
1:B:321:MET:C	1:B:323:LYS:H	2.13	0.50
1:D:169:THR:HB	1:D:170:PRO:CD	2.22	0.50
1:D:474:LYS:HB3	1:D:474:LYS:NZ	2.26	0.50
1:A:245:HIS:CG	1:A:245:HIS:O	2.65	0.50
1:A:63:GLN:O	1:A:63:GLN:HG3	2.11	0.50
1:B:409:GLN:NE2	1:B:473:ASN:ND2	2.59	0.50
1:B:78:VAL:HA	1:B:483:LEU:HD13	1.93	0.50
1:C:358:VAL:HB	1:C:379:LEU:CD1	2.41	0.50
1:C:415:SER:HB2	9:C:800:HOH:O	2.11	0.50
1:D:167:CYS:HB2	1:D:168:PRO:HD2	1.91	0.50
1:A:312:TYR:O	1:A:315:ILE:HG12	2.12	0.50
1:D:221:ASP:OD1	1:D:221:ASP:C	2.50	0.50
1:D:312:TYR:N	1:D:567:PHE:HE2	2.09	0.50
1:C:125:SER:HA	1:C:128:GLN:CB	2.40	0.50
1:D:255:ARG:HH11	7:D:609:3CJ:H7	1.77	0.50
1:B:166:VAL:HG22	1:B:178:ASP:O	2.11	0.50
1:C:124:HIS:HD1	1:C:125:SER:N	2.09	0.50
1:C:259:GLN:HG3	1:C:262:LEU:HB3	1.94	0.50
1:D:204:ARG:HH22	1:D:290:GLU:HA	1.77	0.50
1:D:298:LYS:HG2	1:D:536:PHE:CZ	2.47	0.50
1:D:376:LEU:O	1:D:379:LEU:N	2.39	0.50
1:C:342:VAL:HB	1:C:452:TRP:HZ2	1.75	0.50
1:D:248:CYS:HA	1:D:383:THR:HG21	1.94	0.50
1:A:234:PRO:HB2	9:A:776:HOH:O	2.12	0.49
1:B:294:GLN:OE1	1:B:294:GLN:HA	2.12	0.49
1:B:341:ASN:HB3	6:B:605:NO3:O1	2.12	0.49
1:C:227:PRO:HG3	1:C:270:LEU:HD22	1.93	0.49
1:C:481:LEU:O	1:C:485:LYS:N	2.36	0.49
7:C:609:3CJ:S1	8:C:610:HEM:ND	2.85	0.49
1:C:98:LEU:CD1	1:C:101:MET:HE2	2.42	0.49
1:D:84:GLY:HA2	9:D:775:HOH:O	2.11	0.49
1:A:139:CYS:SG	1:A:141:PRO:HD3	2.52	0.49
1:B:205:ASN:OD1	1:B:207:SER:OG	2.30	0.49
1:B:274:ASN:O	1:B:278:ARG:HG3	2.12	0.49
1:C:527:ARG:HH11	1:C:527:ARG:HG2	1.77	0.49
1:A:313:LEU:HD11	1:A:519:PHE:CD2	2.48	0.49
1:A:442:ARG:O	1:A:445:GLY:N	2.45	0.49
1:C:331:TYR:CE2	1:C:333:ASN:HB3	2.47	0.49
1:D:346:ALA:O	1:D:348:ARG:N	2.44	0.49
1:D:502:VAL:O	1:D:502:VAL:HG23	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ARG:NH2	1:A:527:ARG:NH1	2.61	0.49
1:C:74:LEU:O	1:C:78:VAL:CG1	2.60	0.49
1:D:240:ILE:CD1	1:D:382:ASN:HA	2.42	0.49
1:D:346:ALA:C	1:D:348:ARG:H	2.16	0.49
1:D:449:TYR:OH	1:D:470:VAL:HG11	2.12	0.49
1:A:229:PHE:CG	1:A:247:PRO:HG2	2.47	0.49
1:C:342:VAL:CB	1:C:452:TRP:CZ2	2.94	0.49
1:D:502:VAL:O	1:D:503:GLU:C	2.50	0.49
1:A:347:PHE:CE1	8:A:610:HEM:HBC1	2.48	0.49
1:D:343:PHE:CD1	1:D:518:GLN:HG2	2.47	0.49
1:D:450:ASN:HD21	1:D:487:PRO:HB2	1.78	0.49
1:A:168:PRO:HB3	1:A:170:PRO:HG2	1.95	0.49
1:A:284:ASN:HD21	1:A:591:ALA:HA	1.77	0.49
1:C:363:GLU:CD	1:C:363:GLU:H	2.15	0.49
1:D:246:VAL:HG11	1:D:387:ILE:HD12	1.95	0.49
1:D:317:LEU:HD12	1:D:321:MET:HA	1.95	0.49
1:D:62:THR:HB	1:D:65:LYS:HB2	1.95	0.49
1:A:551:ARG:CZ	1:A:584:LYS:HG2	2.41	0.49
1:C:1:SER:H2	1:C:2:TRP:HZ3	1.49	0.49
1:D:314:PRO:HD3	1:D:321:MET:HE1	1.94	0.49
1:D:110:ASP:OD2	1:D:189:ALA:N	2.45	0.49
1:A:42:ALA:HB2	1:A:166:VAL:CG1	2.37	0.48
1:A:347:PHE:O	1:A:347:PHE:HD1	1.95	0.48
1:A:62:THR:O	1:A:63:GLN:CB	2.61	0.48
1:B:554:CYS:SG	1:B:562:VAL:HG21	2.52	0.48
1:C:30:ASN:HD21	1:C:333:ASN:HB2	1.78	0.48
1:A:144:PHE:HD2	1:A:156:LYS:C	2.17	0.48
1:A:503:GLU:O	1:A:504:ARG:HB2	2.13	0.48
1:A:76:ARG:NH1	1:A:432:ASP:OD2	2.46	0.48
1:B:113:PHE:CD1	7:B:609:3CJ:H5	2.48	0.48
1:B:312:TYR:CE2	1:B:316:VAL:HG21	2.48	0.48
1:C:125:SER:O	1:C:126:LYS:C	2.51	0.48
1:C:151:LEU:HA	1:C:155:GLY:O	2.13	0.48
1:C:347:PHE:HB3	8:C:610:HEM:HMD3	1.95	0.48
1:C:43:LEU:HD12	1:C:179:GLN:HB2	1.95	0.48
1:D:119:LEU:CD2	1:D:169:THR:CG2	2.91	0.48
1:A:464:LEU:O	1:A:468:GLN:HG3	2.12	0.48
1:A:51:TYR:HB3	1:A:57:VAL:O	2.13	0.48
1:B:10:VAL:HG11	1:B:41:ARG:NH2	2.28	0.48
1:B:8:ALA:HB1	1:B:9:PRO:HD2	1.96	0.48
1:C:180:ILE:HG22	1:C:181:ASN:N	2.29	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:22:ARG:CZ	1:C:528:PHE:HB2	2.43	0.48
1:C:593:ARG:HB3	1:C:593:ARG:CZ	2.43	0.48
1:D:144:PHE:HE1	1:D:158:MET:HG3	1.75	0.48
1:D:380:PHE:HE2	1:D:420:LYS:O	1.96	0.48
1:A:244:ALA:O	1:A:245:HIS:HB3	2.14	0.48
1:A:275:ARG:CD	1:A:555:ASP:HB3	2.43	0.48
1:C:377:HIS:ND1	1:C:416:GLU:OE1	2.43	0.48
1:A:58:PRO:HG3	1:A:162:ARG:CZ	2.43	0.48
1:B:213:MET:HB3	1:B:270:LEU:HD11	1.94	0.48
1:B:140:PHE:CE2	1:B:439:GLN:HG3	2.48	0.48
1:C:102:GLN:HB2	1:C:399:LEU:HD21	1.96	0.48
1:D:150:LYS:HE2	1:D:419:ASN:HD22	1.78	0.48
1:A:317:LEU:HD12	1:A:321:MET:SD	2.53	0.48
1:A:481:LEU:HA	1:A:484:TYR:O	2.14	0.48
8:A:610:HEM:CMC	8:A:610:HEM:HBC2	2.43	0.48
1:B:137:ASP:CG	1:B:138:GLU:H	2.17	0.48
1:D:187:LEU:HD21	1:D:304:ILE:HG22	1.95	0.48
1:A:91:VAL:HA	9:A:777:HOH:O	2.12	0.48
7:C:609:3CJ:S1	8:C:610:HEM:C1D	3.07	0.48
1:D:193:TYR:CZ	1:D:297:ARG:HA	2.49	0.48
1:D:93:ASP:OD2	1:D:96:ARG:HG3	2.13	0.48
1:A:146:LYS:HB3	9:A:823:HOH:O	2.12	0.48
1:C:17:GLU:HB3	1:C:18:GLN:OE1	2.14	0.48
1:C:204:ARG:NE	1:C:206:LEU:HD21	2.29	0.48
1:D:275:ARG:O	1:D:279:GLU:HG2	2.14	0.48
1:D:408:ASN:HB3	1:D:411:LYS:HB2	1.95	0.48
1:A:165:PHE:CZ	1:A:169:THR:C	2.87	0.47
1:B:113:PHE:HB2	1:B:255:ARG:NH2	2.29	0.47
1:B:91:VAL:CG1	1:B:411:LYS:HD3	2.44	0.47
1:B:418:ARG:O	1:B:432:ASP:CB	2.62	0.47
1:D:357:THR:HB	1:D:374:LEU:O	2.14	0.47
1:A:130:GLU:HG3	1:A:159:PRO:HD3	1.95	0.47
1:A:109:HIS:NE2	7:A:609:3CJ:S1	2.87	0.47
1:B:124:HIS:O	1:B:127:VAL:HB	2.14	0.47
1:A:367:PRO:CB	1:D:64:ARG:NE	2.77	0.47
1:C:17:GLU:O	1:C:18:GLN:NE2	2.46	0.47
1:C:36:LEU:HD23	1:C:338:ARG:HD3	1.96	0.47
1:A:67:ARG:N	1:A:70:PHE:O	2.45	0.47
1:A:84:GLY:CA	1:A:418:ARG:NE	2.78	0.47
1:D:213:MET:HG2	1:D:273:HIS:CD2	2.49	0.47
1:D:212:LEU:HD21	1:D:278:ARG:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:571:ASN:O	1:A:575:ASP:HB2	2.15	0.47
1:A:52:GLU:HG3	1:A:59:PHE:CD1	2.49	0.47
1:D:259:GLN:O	1:D:262:LEU:HB3	2.14	0.47
1:D:370:PRO:HG2	1:D:371:GLU:H	1.79	0.47
1:B:168:PRO:HG2	1:B:172:TYR:HB3	1.97	0.47
1:B:96:ARG:NH2	1:B:315:ILE:O	2.46	0.47
1:C:169:THR:HG22	9:C:736:HOH:O	2.13	0.47
1:C:322:GLN:HG3	9:C:810:HOH:O	2.13	0.47
1:C:22:ARG:NH1	1:C:528:PHE:HB2	2.29	0.47
1:D:264:THR:HG23	1:D:392:ILE:HG23	1.96	0.47
1:A:351:HIS:NE2	1:A:433:LEU:HD21	2.30	0.47
1:B:12:LEU:HD12	1:B:12:LEU:HA	1.79	0.47
1:C:230:ASN:ND2	1:C:232:VAL:HG22	2.22	0.47
1:C:423:GLN:CB	1:C:426:HIS:CD2	2.97	0.47
1:A:414:THR:HG22	9:A:721:HOH:O	2.15	0.47
1:A:76:ARG:HH22	1:A:419:ASN:ND2	2.13	0.47
1:B:30:ASN:ND2	1:B:36:LEU:HD12	2.29	0.47
1:B:544:LEU:O	1:B:547:VAL:HG22	2.14	0.47
1:C:221:ASP:O	1:C:222:HIS:C	2.53	0.47
1:C:511:LEU:O	1:C:515:LEU:HG	2.14	0.47
1:D:468:GLN:HG2	1:D:474:LYS:HA	1.96	0.47
1:A:224:LEU:HB2	1:A:271:ARG:NH2	2.30	0.47
1:A:363:GLU:HG2	9:A:816:HOH:O	2.15	0.47
1:B:466:GLY:HA3	9:B:749:HOH:O	2.14	0.47
1:C:96:ARG:CD	1:C:100:PHE:CD2	2.68	0.47
1:A:302:ALA:O	1:A:306:ILE:HG13	2.14	0.47
1:B:433:LEU:HD12	1:B:433:LEU:O	2.15	0.47
1:C:453:ARG:HD2	1:C:510:LEU:HD13	1.96	0.47
1:D:530:TRP:CE2	1:D:531:GLU:HG3	2.49	0.47
1:B:138:GLU:O	1:B:162:ARG:HG3	2.14	0.47
1:B:361:LEU:HB3	1:B:365:TYR:HA	1.96	0.47
1:B:376:LEU:HA	1:B:379:LEU:HD12	1.97	0.47
1:C:146:LYS:NZ	1:C:147:ASN:ND2	2.60	0.47
1:A:343:PHE:CG	1:A:518:GLN:HG2	2.49	0.46
1:A:284:ASN:ND2	1:A:591:ALA:HA	2.30	0.46
7:A:609:3CJ:H7	8:A:610:HEM:CBD	2.41	0.46
1:B:273:HIS:CD2	1:B:274:ASN:OD1	2.61	0.46
1:A:233:LYS:HA	1:A:234:PRO:C	2.34	0.46
1:A:265:VAL:O	1:A:269:LEU:HG	2.15	0.46
1:A:400:LEU:HD21	1:A:553:ILE:CD1	2.46	0.46
1:A:436:ILE:O	1:A:440:ARG:HB2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:VAL:HG12	1:B:336:ASP:N	2.30	0.46
1:B:561:LYS:O	1:B:562:VAL:HG13	2.16	0.46
1:C:563:PRO:HD3	1:C:576:PHE:CE2	2.51	0.46
1:D:346:ALA:C	1:D:348:ARG:N	2.68	0.46
1:D:343:PHE:CG	1:D:518:GLN:HG2	2.50	0.46
7:D:609:3CJ:C1	8:D:610:HEM:NA	2.78	0.46
1:B:185:SER:HB3	1:B:339:ILE:HG12	1.97	0.46
1:B:363:GLU:N	1:B:363:GLU:CD	2.67	0.46
8:B:608:HEM:HBB2	8:B:608:HEM:CMB	2.44	0.46
1:B:66:THR:HB	1:B:70:PHE:C	2.36	0.46
1:C:144:PHE:CE1	1:C:158:MET:HG3	2.50	0.46
1:C:30:ASN:ND2	1:C:333:ASN:HB2	2.30	0.46
1:C:572:TYR:HA	1:C:573:PRO:HA	1.62	0.46
1:D:113:PHE:CD1	1:D:255:ARG:HD3	2.50	0.46
1:D:313:LEU:HB2	1:D:314:PRO:HD3	1.97	0.46
1:A:113:PHE:CD1	7:A:609:3CJ:H5	2.50	0.46
1:A:62:THR:HG21	1:A:65:LYS:CG	2.43	0.46
1:B:303:PHE:HD2	1:B:304:ILE:HD12	1.80	0.46
1:B:557:THR:OG1	1:B:559:ILE:HG12	2.15	0.46
1:B:347:PHE:CE1	8:B:608:HEM:HBC1	2.51	0.46
1:C:236:PRO:CB	1:C:424:PRO:HB3	2.45	0.46
1:D:255:ARG:HD2	7:D:609:3CJ:C2	2.45	0.46
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.14	0.46
1:A:71:ARG:CB	1:A:71:ARG:NH1	2.79	0.46
1:C:171:PRO:HD3	9:C:822:HOH:O	2.15	0.46
1:D:54:GLY:HA2	9:D:853:HOH:O	2.15	0.46
1:D:99:LEU:HD21	1:D:549:PHE:CD2	2.50	0.46
1:A:112:ASP:HA	1:A:183:VAL:CG2	2.46	0.46
1:A:522:ILE:O	1:A:526:ASP:HB2	2.16	0.46
1:D:213:MET:HG2	1:D:273:HIS:NE2	2.31	0.46
1:A:113:PHE:HB2	1:A:255:ARG:CZ	2.46	0.46
1:A:9:PRO:O	1:A:10:VAL:C	2.52	0.46
1:D:148:ASP:O	1:D:151:LEU:CB	2.64	0.46
1:D:313:LEU:O	1:D:314:PRO:C	2.54	0.46
1:C:129:CYS:O	1:C:133:CYS:HA	2.15	0.46
1:C:213:MET:HG2	1:C:273:HIS:CD2	2.51	0.46
1:C:344:THR:HB	8:C:610:HEM:O2D	2.15	0.46
1:D:336:ASP:OD2	1:D:338:ARG:NH2	2.48	0.46
1:A:166:VAL:C	1:A:167:CYS:SG	2.94	0.46
1:A:213:MET:HB2	1:A:270:LEU:HD11	1.98	0.46
1:B:17:GLU:OE2	1:B:31:ARG:HG2	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:LEU:HD22	1:B:433:LEU:HB2	1.97	0.46
1:B:93:ASP:CG	1:B:96:ARG:HB2	2.36	0.46
1:C:108:ASP:HB2	1:C:347:PHE:CE2	2.50	0.46
1:C:294:GLN:OE1	1:C:294:GLN:HA	2.15	0.46
1:D:351:HIS:HD2	8:D:610:HEM:C1C	2.34	0.46
1:D:570:ASN:HB3	1:D:575:ASP:HB3	1.98	0.46
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.51	0.46
1:C:423:GLN:HG3	1:C:431:PHE:CD2	2.51	0.46
1:C:449:TYR:OH	1:C:470:VAL:HG11	2.16	0.46
7:C:609:3CJ:H5	8:C:610:HEM:CAA	2.42	0.46
1:D:418:ARG:HG2	1:D:432:ASP:OD2	2.15	0.46
1:D:545:GLN:OE1	1:D:545:GLN:HA	2.16	0.46
1:A:260:ILE:HG23	1:A:261:LEU:N	2.31	0.45
1:B:324:TRP:CZ2	1:B:513:CYS:HB2	2.51	0.45
1:B:433:LEU:HA	1:B:436:ILE:HD12	1.97	0.45
1:D:561:LYS:HE3	1:D:578:ASP:HA	1.98	0.45
9:C:807:HOH:O	2:G:1:NAG:H82	2.16	0.45
1:A:144:PHE:HE2	1:A:157:CYS:N	2.14	0.45
1:A:377:HIS:CB	1:A:416:GLU:OE1	2.57	0.45
1:A:419:ASN:O	1:A:430:GLY:HA2	2.17	0.45
1:A:47:LEU:HD21	1:A:455:PHE:HD2	1.81	0.45
1:A:82:ILE:HD13	1:A:480:LEU:HD23	1.98	0.45
1:A:86:LEU:HD23	1:D:55:LEU:HD23	1.98	0.45
1:B:257:SER:O	1:B:381:PHE:HA	2.16	0.45
1:B:418:ARG:NH1	1:B:418:ARG:HG2	2.31	0.45
1:C:244:ALA:HB1	1:C:246:VAL:HG23	1.97	0.45
1:C:31:ARG:H	1:C:31:ARG:HG2	1.59	0.45
1:C:350:GLY:HA3	8:C:610:HEM:CBC	2.47	0.45
1:D:239:PHE:CZ	1:D:427:LYS:CG	2.99	0.45
1:B:360:ARG:O	1:B:368:TRP:HB3	2.17	0.45
1:D:519:PHE:HA	1:D:522:ILE:HG12	1.97	0.45
1:A:418:ARG:HG2	1:A:418:ARG:HH11	1.81	0.45
1:C:15:CYS:HB3	1:C:17:GLU:OE2	2.15	0.45
1:C:523:ARG:HG3	1:C:529:TRP:CD2	2.51	0.45
1:C:100:PHE:HA	1:C:567:PHE:CD1	2.52	0.45
1:C:99:LEU:HA	1:C:399:LEU:CD2	2.45	0.45
1:D:421:LEU:O	1:D:431:PHE:HB2	2.16	0.45
1:D:97:SER:O	1:D:100:PHE:HB3	2.15	0.45
1:D:474:LYS:O	1:D:477:ALA:HB3	2.16	0.45
1:A:353:GLU:HA	1:A:405:LYS:O	2.17	0.45
1:A:95:ASN:HA	1:A:569:ALA:HB3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:ARG:NH1	1:B:437:ASN:ND2	2.64	0.45
1:B:454:GLY:O	1:B:455:PHE:C	2.55	0.45
1:B:528:PHE:HZ	9:B:748:HOH:O	1.99	0.45
1:C:344:THR:O	8:C:610:HEM:HAD2	2.16	0.45
1:D:246:VAL:CG1	1:D:387:ILE:HD12	2.46	0.45
1:D:484:TYR:O	1:D:485:LYS:HB2	2.17	0.45
1:D:561:LYS:CE	1:D:578:ASP:HA	2.47	0.45
1:A:392:ILE:HG22	1:A:396:VAL:CG2	2.47	0.45
1:B:35:ALA:HB1	1:B:41:ARG:HE	1.80	0.45
1:B:551:ARG:HD3	1:B:584:LYS:CA	2.37	0.45
1:C:130:GLU:HB2	1:C:159:PRO:HB3	1.99	0.45
1:C:552:LEU:O	1:C:556:ASN:ND2	2.46	0.45
1:D:590:TRP:HE3	1:D:590:TRP:H	1.65	0.45
1:A:135:GLN:HB3	1:A:135:GLN:HE21	1.49	0.45
1:A:173:GLN:O	1:A:174:SER:HB3	2.17	0.45
1:A:418:ARG:HG2	1:A:418:ARG:NH1	2.32	0.45
1:A:442:ARG:O	1:A:443:ASP:C	2.53	0.45
1:B:180:ILE:CG2	1:B:181:ASN:N	2.79	0.45
1:B:221:ASP:HB2	1:B:226:TYR:CZ	2.52	0.45
9:A:772:HOH:O	1:D:173:GLN:HB2	2.17	0.45
1:D:229:PHE:CZ	1:D:387:ILE:HD13	2.52	0.45
1:D:345:PHE:CE1	1:D:441:CYS:HA	2.52	0.45
1:D:546:LYS:NZ	1:D:546:LYS:HB2	2.31	0.45
1:A:59:PHE:CG	1:A:67:ARG:HD2	2.52	0.45
1:A:82:ILE:HD13	1:A:480:LEU:CD2	2.46	0.45
1:B:117:THR:HG21	1:B:138:GLU:OE1	2.17	0.45
1:C:527:ARG:NH1	1:C:527:ARG:HG2	2.31	0.45
1:D:12:LEU:C	1:D:13:VAL:HG23	2.37	0.45
1:D:144:PHE:HB2	1:D:151:LEU:HD13	1.98	0.45
1:D:175:LEU:HD23	1:D:176:ALA:H	1.82	0.45
1:A:400:LEU:HD21	1:A:553:ILE:HD13	1.99	0.45
1:C:168:PRO:HG3	1:C:172:TYR:CD2	2.49	0.45
1:C:29:ASN:ND2	1:C:527:ARG:H	2.14	0.45
1:D:10:VAL:HG13	1:D:11:PRO:HD2	1.98	0.45
1:A:449:TYR:HB3	1:A:487:PRO:O	2.18	0.44
1:B:563:PRO:HD3	1:B:576:PHE:CE2	2.51	0.44
1:C:551:ARG:HD3	1:C:584:LYS:HA	1.99	0.44
1:D:9:PRO:HG3	1:D:41:ARG:NH1	2.32	0.44
1:A:165:PHE:CE2	1:A:170:PRO:O	2.70	0.44
1:A:424:PRO:O	1:A:425:THR:HB	2.17	0.44
1:A:553:ILE:O	1:A:557:THR:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:ASP:N	1:B:188:ASP:OD1	2.48	0.44
1:B:260:ILE:HG13	1:B:382:ASN:O	2.17	0.44
1:C:517:ARG:CB	1:C:517:ARG:HH21	2.30	0.44
1:D:315:ILE:HD11	1:D:567:PHE:CD2	2.52	0.44
1:A:213:MET:HB3	1:A:270:LEU:HD11	1.98	0.44
1:B:393:ASP:OD1	1:B:557:THR:HB	2.18	0.44
1:B:76:ARG:NH2	9:B:702:HOH:O	2.50	0.44
1:C:124:HIS:O	1:C:125:SER:C	2.54	0.44
1:C:188:ASP:OD1	1:C:190:SER:CB	2.64	0.44
1:D:260:ILE:HD13	1:D:395:LEU:HD21	2.00	0.44
1:D:9:PRO:HG2	1:D:10:VAL:H	1.81	0.44
1:B:408:ASN:HB3	1:B:411:LYS:O	2.17	0.44
1:B:588:SER:HB2	1:B:589:PRO:HD3	2.00	0.44
1:B:91:VAL:HG11	1:B:411:LYS:HD3	1.99	0.44
1:C:188:ASP:CG	1:C:190:SER:HB3	2.37	0.44
1:C:2:TRP:CD2	1:C:2:TRP:N	2.84	0.44
1:C:468:GLN:CG	1:C:474:LYS:HA	2.40	0.44
1:C:29:ASN:O	1:C:527:ARG:HD3	2.18	0.44
1:C:88:GLU:O	1:C:91:VAL:HG22	2.17	0.44
1:A:123:GLU:HB3	1:A:126:LYS:HG3	1.99	0.44
1:A:145:PRO:O	1:A:148:ASP:HB2	2.17	0.44
1:A:313:LEU:HD11	1:A:519:PHE:CD1	2.53	0.44
1:A:559:ILE:HD13	1:A:559:ILE:N	2.33	0.44
1:C:421:LEU:HD22	1:C:433:LEU:HB2	1.98	0.44
1:A:328:TYR:CD2	1:A:531:GLU:HB3	2.52	0.44
1:A:462:LYS:HA	1:A:462:LYS:HE2	1.98	0.44
1:C:168:PRO:HD2	1:C:172:TYR:HE2	1.83	0.44
1:C:242:THR:O	1:C:245:HIS:CE1	2.71	0.44
1:C:279:GLU:O	1:C:283:LEU:HG	2.17	0.44
1:D:196:GLU:HG3	9:D:785:HOH:O	2.18	0.44
1:A:144:PHE:CD2	1:A:156:LYS:C	2.91	0.44
1:C:124:HIS:C	1:C:124:HIS:ND1	2.70	0.44
1:C:265:VAL:O	1:C:269:LEU:HG	2.18	0.44
1:C:402:LYS:HD3	6:C:607:NO3:O1	2.17	0.44
1:D:549:PHE:O	1:D:552:LEU:HB3	2.17	0.44
1:D:88:GLU:O	1:D:91:VAL:HG22	2.17	0.44
1:A:117:THR:O	1:A:117:THR:HG23	2.16	0.44
1:A:172:TYR:CE2	1:A:175:LEU:HB2	2.48	0.44
1:A:568:GLN:HG2	1:A:568:GLN:O	2.17	0.44
1:B:421:LEU:HD12	1:B:422:PHE:N	2.30	0.44
1:C:231:ASN:HB2	9:C:775:HOH:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:ILE:HG13	1:D:386:ILE:HD11	1.99	0.44
1:D:187:LEU:HD23	1:D:305:GLN:HA	2.00	0.44
1:D:60:GLY:CA	1:D:72:VAL:HG21	2.48	0.44
1:D:76:ARG:NH1	1:D:432:ASP:OD2	2.51	0.44
1:A:203:LEU:HD22	9:A:775:HOH:O	2.17	0.44
1:A:363:GLU:CG	9:A:816:HOH:O	2.65	0.44
7:C:609:3CJ:C3	8:C:610:HEM:C2A	3.01	0.44
1:B:10:VAL:HG21	1:B:41:ARG:NH1	2.32	0.43
1:C:299:ILE:HD11	1:C:590:TRP:CD1	2.52	0.43
1:B:109:HIS:NE2	7:B:609:3CJ:S1	2.91	0.43
1:C:45:ARG:CZ	1:C:49:ALA:HB2	2.48	0.43
1:D:85:TYR:CE2	1:D:91:VAL:HG11	2.53	0.43
1:A:113:PHE:HB2	1:A:255:ARG:NH2	2.33	0.43
1:A:305:GLN:NE2	1:A:529:TRP:CE3	2.86	0.43
1:B:221:ASP:O	1:B:224:LEU:HB2	2.17	0.43
1:B:94:GLN:O	1:B:569:ALA:CB	2.66	0.43
1:C:342:VAL:HG13	1:C:343:PHE:N	2.33	0.43
1:C:74:LEU:O	1:C:78:VAL:HG13	2.18	0.43
1:C:91:VAL:HG23	1:C:92:LEU:HD23	2.01	0.43
1:D:28:CYS:O	1:D:29:ASN:C	2.57	0.43
1:A:55:LEU:HD13	1:A:173:GLN:HA	2.00	0.43
1:A:382:ASN:ND2	1:A:385:ARG:HG3	2.34	0.43
8:A:610:HEM:HBB2	8:A:610:HEM:HMB2	2.00	0.43
1:C:385:ARG:HA	1:C:385:ARG:HD3	1.86	0.43
1:C:520:GLN:O	1:C:524:ASP:HB2	2.19	0.43
1:D:497:ASN:OD1	1:D:511:LEU:HD11	2.18	0.43
1:D:82:ILE:HD13	1:D:480:LEU:CD2	2.49	0.43
1:B:518:GLN:O	1:B:522:ILE:HG23	2.19	0.43
1:C:328:TYR:CZ	1:C:529:TRP:CD1	3.07	0.43
1:D:187:LEU:HG	1:D:187:LEU:O	2.17	0.43
1:D:441:CYS:SG	1:D:492:ILE:CG2	3.07	0.43
1:D:320:GLU:HG3	1:D:512:ALA:HB1	2.00	0.43
1:B:222:HIS:HA	9:B:794:HOH:O	2.19	0.43
1:B:447:PRO:HG2	1:B:452:TRP:CE2	2.54	0.43
1:B:68:ASN:ND2	1:B:489:ASN:OD1	2.44	0.43
1:C:353:GLU:HA	1:C:405:LYS:O	2.18	0.43
1:C:366:GLN:HA	1:C:366:GLN:OE1	2.18	0.43
1:C:528:PHE:O	1:C:529:TRP:C	2.57	0.43
1:D:204:ARG:HG2	1:D:293:TYR:CE1	2.53	0.43
1:D:312:TYR:O	1:D:315:ILE:HG12	2.17	0.43
1:A:398:GLY:O	1:A:402:LYS:HB2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:408:ASN:O	1:D:410:ASN:N	2.51	0.43
1:D:585:LEU:O	1:D:587:LEU:N	2.52	0.43
1:A:255:ARG:HH11	7:A:609:3CJ:H6	1.83	0.43
1:A:279:GLU:HA	1:A:279:GLU:OE2	2.19	0.43
1:A:519:PHE:HA	1:A:522:ILE:HG12	2.00	0.43
1:B:172:TYR:OH	1:B:177:ARG:HA	2.17	0.43
1:C:441:CYS:HB3	9:C:713:HOH:O	2.18	0.43
1:C:81:LYS:HE2	9:C:821:HOH:O	2.19	0.43
1:A:343:PHE:CE1	1:A:515:LEU:HD23	2.53	0.43
1:C:37:GLY:H	1:C:338:ARG:CG	2.20	0.43
1:D:119:LEU:HB3	9:D:773:HOH:O	2.19	0.43
1:D:312:TYR:O	1:D:315:ILE:CG1	2.67	0.43
1:D:391:GLY:O	1:D:394:PRO:HD2	2.19	0.43
1:A:239:PHE:CZ	1:A:427:LYS:CB	3.02	0.43
1:A:519:PHE:O	1:A:522:ILE:HG12	2.18	0.43
1:B:565:HIS:HB2	1:B:568:GLN:HG2	2.00	0.43
1:C:3:GLU:O	1:C:5:GLY:N	2.52	0.43
1:D:167:CYS:HB3	1:D:168:PRO:HD2	2.00	0.43
1:D:18:GLN:NE2	1:D:18:GLN:HA	2.33	0.43
1:A:112:ASP:HA	1:A:183:VAL:HG22	2.01	0.42
1:A:93:ASP:CG	1:A:96:ARG:HB2	2.39	0.42
1:C:110:ASP:OD2	1:C:189:ALA:N	2.49	0.42
1:C:227:PRO:HG3	1:C:270:LEU:CD2	2.48	0.42
1:C:467:LEU:HA	1:C:467:LEU:HD12	1.89	0.42
1:A:258:GLU:OE1	1:A:259:GLN:CG	2.66	0.42
1:A:84:GLY:HA2	1:A:418:ARG:NE	2.34	0.42
1:C:109:HIS:HA	1:C:255:ARG:HH22	1.81	0.42
1:C:16:ASP:O	1:C:18:GLN:HG2	2.19	0.42
1:A:165:PHE:CE1	1:A:177:ARG:CZ	3.01	0.42
1:A:543:SER:OG	1:A:589:PRO:HG2	2.19	0.42
1:B:116:GLU:HB3	9:B:746:HOH:O	2.18	0.42
1:B:191:LEU:H	1:B:191:LEU:HD23	1.85	0.42
1:C:108:ASP:HB2	1:C:347:PHE:CD2	2.54	0.42
1:C:283:LEU:HD13	1:C:591:ALA:HB2	2.00	0.42
7:C:609:3CJ:C4	8:C:610:HEM:C3A	3.02	0.42
1:D:146:LYS:O	1:D:147:ASN:CB	2.65	0.42
1:D:148:ASP:O	1:D:151:LEU:HB2	2.19	0.42
1:B:232:VAL:O	1:B:232:VAL:HG23	2.20	0.42
1:B:260:ILE:CG2	1:B:261:LEU:N	2.83	0.42
1:D:12:LEU:O	1:D:13:VAL:HB	2.20	0.42
1:D:474:LYS:HZ1	1:D:474:LYS:HB3	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:335:VAL:CG1	1:B:336:ASP:N	2.82	0.42
1:C:168:PRO:CG	1:C:172:TYR:CD2	3.03	0.42
1:C:348:ARG:NH2	8:C:610:HEM:HAD1	2.34	0.42
1:D:99:LEU:O	1:D:100:PHE:C	2.57	0.42
1:D:53:ASP:CG	1:D:57:VAL:HG23	2.40	0.42
1:A:281:LYS:HD3	1:A:292:LEU:HD11	2.02	0.42
1:A:65:LYS:HE3	1:A:65:LYS:HB3	1.61	0.42
1:A:77:GLU:O	1:A:81:LYS:HG3	2.19	0.42
1:B:246:VAL:HA	1:B:247:PRO:HD3	1.80	0.42
1:B:64:ARG:NH2	9:B:704:HOH:O	2.53	0.42
1:C:321:MET:HB3	1:C:322:GLN:OE1	2.19	0.42
1:D:376:LEU:HD21	1:D:380:PHE:CE1	2.53	0.42
1:A:363:GLU:OE2	1:A:397:ARG:NH1	2.52	0.42
1:A:572:TYR:CG	1:A:573:PRO:HA	2.55	0.42
1:A:57:VAL:HA	1:A:58:PRO:HD3	1.92	0.42
1:B:248:CYS:HB3	1:B:257:SER:OG	2.19	0.42
1:B:293:TYR:OH	1:B:297:ARG:HD2	2.18	0.42
1:B:313:LEU:N	1:B:314:PRO:CD	2.83	0.42
1:C:322:GLN:CD	1:C:322:GLN:H	2.23	0.42
1:C:36:LEU:CD2	1:C:338:ARG:HD3	2.50	0.42
1:D:272:GLU:O	1:D:276:LEU:CG	2.68	0.42
1:D:348:ARG:HH11	1:D:437:ASN:HD21	1.60	0.42
1:D:460:GLN:HA	1:D:461:PRO:HD2	1.91	0.42
1:A:124:HIS:O	1:A:127:VAL:HB	2.20	0.42
1:B:233:LYS:HB3	1:B:234:PRO:HA	2.01	0.42
1:C:180:ILE:CG2	1:C:181:ASN:N	2.83	0.42
1:C:101:MET:SD	1:C:354:VAL:HG22	2.60	0.42
1:C:529:TRP:O	1:C:530:TRP:C	2.58	0.42
1:C:550:SER:OG	1:C:563:PRO:O	2.26	0.42
1:D:446:MET:HA	1:D:447:PRO:HD3	1.93	0.42
1:A:464:LEU:HD12	1:A:464:LEU:C	2.40	0.42
8:B:608:HEM:O1D	7:B:609:3CJ:H6	2.19	0.42
1:C:106:ILE:HG13	1:C:265:VAL:HG11	2.02	0.42
1:C:348:ARG:HB3	1:C:493:TRP:HE1	1.80	0.42
1:A:24:ILE:HD13	1:A:24:ILE:HA	1.93	0.42
1:B:14:THR:HG22	1:B:15:CYS:N	2.35	0.42
1:B:166:VAL:CG2	1:B:178:ASP:HB2	2.50	0.42
1:B:215:VAL:O	1:B:217:GLN:NE2	2.53	0.42
1:B:281:LYS:HD2	1:B:285:PRO:HA	2.01	0.42
1:A:217:GLN:HA	1:A:217:GLN:OE1	2.20	0.41
1:A:237:CYS:O	1:A:240:ILE:HG13	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:113:PHE:O	1:B:181:ASN:HA	2.20	0.41
1:B:45:ARG:NH1	1:B:49:ALA:HA	2.35	0.41
1:C:240:ILE:O	1:C:241:ASN:HB2	2.20	0.41
1:C:348:ARG:NH1	1:C:437:ASN:HD22	2.18	0.41
1:A:354:VAL:HG21	8:A:610:HEM:CAB	2.50	0.41
1:A:345:PHE:CE1	1:A:440:ARG:HG3	2.54	0.41
1:C:1:SER:N	1:C:2:TRP:CE3	2.82	0.41
1:D:103:TRP:O	1:D:104:GLY:C	2.58	0.41
1:D:60:GLY:HA2	1:D:72:VAL:CG2	2.50	0.41
1:B:31:ARG:O	1:B:32:ARG:C	2.59	0.41
1:C:333:ASN:HD22	1:C:333:ASN:H	1.67	0.41
1:C:494:ILE:HG23	1:C:495:GLY:N	2.36	0.41
1:D:132:TYR:HB3	1:D:134:VAL:HG23	2.02	0.41
1:D:532:ASN:HA	1:D:533:PRO:HD3	1.89	0.41
1:A:146:LYS:HE3	1:A:147:ASN:OD1	2.20	0.41
1:A:321:MET:C	1:A:323:LYS:H	2.22	0.41
1:A:522:ILE:HG13	1:A:523:ARG:N	2.36	0.41
1:B:117:THR:HG23	1:B:161:PHE:HD2	1.85	0.41
1:B:23:THR:O	1:B:297:ARG:NH2	2.44	0.41
1:B:203:LEU:HD11	1:B:251:ALA:O	2.20	0.41
1:B:588:SER:N	1:B:589:PRO:CD	2.83	0.41
1:C:101:MET:HB3	1:C:101:MET:HE2	1.52	0.41
1:A:140:PHE:N	1:A:141:PRO:HD3	2.34	0.41
1:A:335:VAL:O	1:A:337:PRO:HD3	2.20	0.41
1:A:423:GLN:HA	1:A:424:PRO:HD3	1.92	0.41
1:B:481:LEU:HD21	1:B:487:PRO:HG3	2.01	0.41
1:C:146:LYS:CE	1:C:147:ASN:ND2	2.73	0.41
1:C:17:GLU:O	1:C:31:ARG:NH2	2.54	0.41
1:C:216:ASN:OD1	1:C:219:ALA:N	2.31	0.41
1:D:336:ASP:OD1	1:D:338:ARG:HB2	2.21	0.41
1:D:3:GLU:CG	1:D:4:VAL:H	2.31	0.41
1:D:91:VAL:HG12	1:D:411:LYS:HD3	2.02	0.41
1:A:471:LEU:O	1:A:472:LYS:HB2	2.21	0.41
1:B:362:ASP:O	1:B:397:ARG:NE	2.53	0.41
1:B:529:TRP:CD1	1:B:531:GLU:HB3	2.55	0.41
1:C:82:ILE:HD12	1:C:480:LEU:CD2	2.51	0.41
1:D:96:ARG:HD2	1:D:100:PHE:CG	2.55	0.41
1:D:251:ALA:O	1:D:252:GLY:C	2.58	0.41
1:D:347:PHE:HA	1:D:347:PHE:HD1	1.73	0.41
1:D:47:LEU:HD12	1:D:452:TRP:CZ3	2.56	0.41
1:D:91:VAL:HB	1:D:405:LYS:HG3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:PRO:O	1:D:10:VAL:CG2	2.69	0.41
1:A:572:TYR:HD2	1:A:576:PHE:CG	2.37	0.41
1:B:537:THR:HG23	1:B:540:GLN:CD	2.39	0.41
1:B:69:GLY:HA2	1:C:374:LEU:HD22	2.02	0.41
1:D:213:MET:CG	1:D:273:HIS:CD2	3.04	0.41
1:D:351:HIS:CD2	8:D:610:HEM:C1C	3.09	0.41
1:D:589:PRO:HB2	1:D:590:TRP:CZ3	2.56	0.41
1:A:165:PHE:HE2	1:A:170:PRO:O	2.03	0.41
1:A:501:MET:SD	1:A:506:ARG:HA	2.61	0.41
1:B:106:ILE:HD11	1:B:265:VAL:HB	2.03	0.41
1:B:127:VAL:O	1:B:131:GLU:HB3	2.20	0.41
1:B:213:MET:HG2	1:B:273:HIS:NE2	2.35	0.41
1:B:493:TRP:O	1:B:497:ASN:ND2	2.53	0.41
1:C:100:PHE:HA	1:C:567:PHE:HD1	1.85	0.41
1:C:149:PRO:C	1:C:151:LEU:N	2.73	0.41
1:C:46:TRP:CE2	1:C:340:SER:HB3	2.56	0.41
1:C:3:GLU:C	1:C:5:GLY:H	2.24	0.41
1:C:421:LEU:HD12	1:C:422:PHE:H	1.85	0.41
1:C:481:LEU:CD2	1:C:487:PRO:HG3	2.39	0.41
1:D:179:GLN:HG2	1:D:444:HIS:CD2	2.56	0.41
1:A:35:ALA:HB1	1:A:41:ARG:CD	2.50	0.41
1:A:424:PRO:O	1:A:425:THR:CB	2.69	0.41
1:A:418:ARG:O	1:A:432:ASP:HA	2.21	0.41
1:A:477:ALA:O	1:A:478:LYS:C	2.59	0.41
1:B:347:PHE:HB3	8:B:608:HEM:CMD	2.51	0.41
1:B:399:LEU:HA	1:B:399:LEU:HD23	1.92	0.41
1:C:506:ARG:HA	1:C:506:ARG:HD3	1.89	0.41
1:C:588:SER:N	1:C:589:PRO:CD	2.84	0.41
1:D:272:GLU:OE2	1:D:276:LEU:HG	2.20	0.41
1:D:28:CYS:HA	1:D:34:PRO:CB	2.51	0.41
1:D:423:GLN:O	1:D:426:HIS:HB2	2.20	0.41
1:D:51:TYR:HB3	1:D:57:VAL:O	2.20	0.41
1:D:523:ARG:HG3	1:D:529:TRP:CE2	2.56	0.41
1:A:121:SER:C	1:A:123:GLU:N	2.75	0.41
1:A:288:ASP:OD2	1:A:290:GLU:HB3	2.20	0.41
1:A:407:MET:SD	1:A:408:ASN:N	2.94	0.41
8:B:608:HEM:CHA	7:B:609:3CJ:H9	2.34	0.41
1:C:1:SER:N	1:C:2:TRP:CZ3	2.68	0.41
1:C:419:ASN:HD22	1:C:419:ASN:HA	1.70	0.41
8:C:610:HEM:HBC2	8:C:610:HEM:HMC2	2.02	0.41
1:D:366:GLN:HB3	1:D:367:PRO:CD	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:362:ASP:OD1	1:B:366:GLN:HB2	2.22	0.40
1:C:124:HIS:HD1	1:C:125:SER:CA	2.34	0.40
1:C:424:PRO:O	1:C:425:THR:CB	2.69	0.40
1:C:460:GLN:HA	1:C:461:PRO:HD2	1.90	0.40
1:C:85:TYR:CD2	1:C:411:LYS:HA	2.57	0.40
1:D:165:PHE:CD1	1:D:165:PHE:N	2.89	0.40
1:A:221:ASP:HB3	1:A:224:LEU:HB2	2.03	0.40
1:A:517:ARG:NH2	1:A:521:GLN:OE1	2.54	0.40
1:B:24:ILE:HD13	1:B:24:ILE:HA	1.93	0.40
1:B:332:ASN:OD1	1:B:334:SER:N	2.45	0.40
1:B:468:GLN:HG2	1:B:474:LYS:HA	2.03	0.40
1:C:103:TRP:O	1:C:104:GLY:C	2.58	0.40
1:C:274:ASN:O	1:C:278:ARG:HG3	2.21	0.40
1:C:363:GLU:CD	1:C:363:GLU:N	2.75	0.40
1:C:382:ASN:OD1	1:C:385:ARG:HB2	2.21	0.40
1:C:497:ASN:HA	1:C:511:LEU:HD11	2.03	0.40
1:D:70:PHE:CD1	1:D:70:PHE:N	2.89	0.40
1:A:309:PHE:CZ	1:A:522:ILE:HD11	2.55	0.40
1:A:549:PHE:O	1:A:552:LEU:HB3	2.21	0.40
1:B:308:THR:HA	1:B:312:TYR:HB3	2.03	0.40
8:B:608:HEM:HBA2	8:B:608:HEM:HHA	2.02	0.40
1:C:471:LEU:HD23	1:C:499:GLU:HA	2.02	0.40
1:D:61:TRP:CE2	1:D:135:GLN:NE2	2.89	0.40
1:D:324:TRP:O	1:D:520:GLN:HB2	2.21	0.40
1:D:537:THR:OG1	1:D:540:GLN:HG3	2.21	0.40
1:D:572:TYR:HA	1:D:573:PRO:HA	1.75	0.40
1:A:367:PRO:HB2	1:D:64:ARG:HE	1.86	0.40
1:A:233:LYS:NZ	1:B:322:GLN:HE21	2.19	0.40
1:A:260:ILE:CG2	1:A:261:LEU:N	2.84	0.40
1:A:588:SER:N	1:A:589:PRO:CD	2.84	0.40
1:B:45:ARG:NH2	1:B:177:ARG:O	2.53	0.40
1:C:514:LEU:O	1:C:515:LEU:C	2.60	0.40
1:C:93:ASP:HB2	1:C:406:LEU:HB2	2.03	0.40
1:D:78:VAL:O	1:D:82:ILE:HB	2.21	0.40
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.86	0.40
1:A:518:GLN:O	1:A:522:ILE:HG23	2.21	0.40
1:A:568:GLN:O	1:A:570:ASN:ND2	2.54	0.40
1:A:77:GLU:CG	1:A:81:LYS:HD2	2.51	0.40
1:B:213:MET:CB	1:B:270:LEU:HD11	2.52	0.40
1:B:320:GLU:O	1:B:323:LYS:HB3	2.21	0.40
1:B:418:ARG:O	1:B:432:ASP:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:HIS:O	1:C:126:LYS:N	2.54	0.40
1:D:2:TRP:CD1	1:D:175:LEU:CD2	3.04	0.40
1:D:296:ALA:HA	1:D:299:ILE:HD12	2.03	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	593/595 (100%)	520 (88%)	68 (12%)	5 (1%)	19	35
1	B	593/595 (100%)	524 (88%)	63 (11%)	6 (1%)	15	28
1	C	593/595 (100%)	523 (88%)	61 (10%)	9 (2%)	10	18
1	D	593/595 (100%)	515 (87%)	67 (11%)	11 (2%)	8	13
All	All	2372/2380 (100%)	2082 (88%)	259 (11%)	31 (1%)	12	21

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA
1	A	167	CYS
1	B	167	CYS
1	C	8	ALA
1	C	12	LEU
1	C	167	CYS
1	C	174	SER
1	D	13	VAL
1	D	167	CYS
1	D	174	SER
1	D	3	GLU
1	A	327	PRO

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Mol	Chain	Res	Type
1	B	27	ASP
1	C	128	GLN
1	C	352	MET
1	D	9	PRO
1	D	347	PHE
1	D	587	LEU
1	B	14	THR
1	B	370	PRO
1	C	13	VAL
1	D	367	PRO
1	D	589	PRO
1	C	4	VAL
1	C	492	ILE
1	A	9	PRO
1	A	285	PRO
1	B	492	ILE
1	D	170	PRO
1	D	516	GLY
1	B	573	PRO

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	517/517 (100%)	471 (91%)	46 (9%)	9	19
1	B	517/517 (100%)	472 (91%)	45 (9%)	10	20
1	C	517/517 (100%)	475 (92%)	42 (8%)	11	23
1	D	517/517 (100%)	463 (90%)	54 (10%)	7	13
All	All	2068/2068 (100%)	1881 (91%)	187 (9%)	9	19

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	CYS
1	A	9	PRO

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Mol	Chain	Res	Type
1	A	12	LEU
1	A	23	THR
1	A	24	ILE
1	A	32	ARG
1	A	40	ASN
1	A	64	ARG
1	A	65	LYS
1	A	71	ARG
1	A	78	VAL
1	A	116	GLU
1	A	118	GLU
1	A	119	LEU
1	A	139	CYS
1	A	154	GLN
1	A	157	CYS
1	A	167	CYS
1	A	177	ARG
1	A	201	SER
1	A	202	ARG
1	A	218	GLU
1	A	232	VAL
1	A	240	ILE
1	A	257	SER
1	A	258	GLU
1	A	266	HIS
1	A	311	ASP
1	A	322	GLN
1	A	327	PRO
1	A	344	THR
1	A	347	PHE
1	A	348	ARG
1	A	364	ASN
1	A	366	GLN
1	A	408	ASN
1	A	464	LEU
1	A	481	LEU
1	A	517	ARG
1	A	538	GLU
1	A	542	ASP
1	A	551	ARG
1	A	564	LEU
1	A	568	GLN

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Mol	Chain	Res	Type
1	A	580	SER
1	A	593	ARG
1	B	3	GLU
1	B	6	CYS
1	B	22	ARG
1	B	53	ASP
1	B	63	GLN
1	B	66	THR
1	B	78	VAL
1	B	86	LEU
1	B	95	ASN
1	B	118	GLU
1	B	119	LEU
1	B	125	SER
1	B	128	GLN
1	B	151	LEU
1	B	156	LYS
1	B	167	CYS
1	B	175	LEU
1	B	196	GLU
1	B	198	SER
1	B	202	ARG
1	B	231	ASN
1	B	242	THR
1	B	266	HIS
1	B	321	MET
1	B	322	GLN
1	B	337	PRO
1	B	347	PHE
1	B	356	SER
1	B	359	SER
1	B	360	ARG
1	B	371	GLU
1	B	383	THR
1	B	423	GLN
1	B	439	GLN
1	B	472	LYS
1	B	481	LEU
1	B	486	THR
1	B	513	CYS
1	B	522	ILE
1	B	542	ASP

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Mol	Chain	Res	Type
1	B	551	ARG
1	B	573	PRO
1	B	574	HIS
1	B	592	SER
1	B	593	ARG
1	C	2	TRP
1	C	3	GLU
1	C	4	VAL
1	C	6	CYS
1	C	19	SER
1	C	31	ARG
1	C	32	ARG
1	C	89	GLU
1	C	102	GLN
1	C	118	GLU
1	C	119	LEU
1	C	124	HIS
1	C	139	CYS
1	C	146	LYS
1	C	153	THR
1	C	156	LYS
1	C	157	CYS
1	C	173	GLN
1	C	177	ARG
1	C	207	SER
1	C	242	THR
1	C	254	SER
1	C	266	HIS
1	C	284	ASN
1	C	293	TYR
1	C	323	LYS
1	C	333	ASN
1	C	344	THR
1	C	360	ARG
1	C	364	ASN
1	C	376	LEU
1	C	404	SER
1	C	429	HIS
1	C	474	LYS
1	C	520	GLN
1	C	524	ASP
1	C	564	LEU

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Mol	Chain	Res	Type
1	C	578	ASP
1	C	580	SER
1	C	593	ARG
1	C	594	GLU
1	C	595	ASN
1	D	12	LEU
1	D	23	THR
1	D	32	ARG
1	D	36	LEU
1	D	40	ASN
1	D	64	ARG
1	D	65	LYS
1	D	66	THR
1	D	70	PHE
1	D	86	LEU
1	D	118	GLU
1	D	119	LEU
1	D	124	HIS
1	D	127	VAL
1	D	129	CYS
1	D	168	PRO
1	D	169	THR
1	D	175	LEU
1	D	177	ARG
1	D	185	SER
1	D	198	SER
1	D	202	ARG
1	D	230	ASN
1	D	240	ILE
1	D	266	HIS
1	D	286	HIS
1	D	315	ILE
1	D	322	GLN
1	D	323	LYS
1	D	329	GLN
1	D	333	ASN
1	D	334	SER
1	D	337	PRO
1	D	347	PHE
1	D	356	SER
1	D	360	ARG
1	D	371	GLU

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Mol	Chain	Res	Type
1	D	376	LEU
1	D	414	THR
1	D	428	VAL
1	D	446	MET
1	D	462	LYS
1	D	474	LYS
1	D	475	VAL
1	D	501	MET
1	D	503	GLU
1	D	513	CYS
1	D	538	GLU
1	D	568	GLN
1	D	573	PRO
1	D	583	ASP
1	D	586	ASP
1	D	592	SER
1	D	595	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (52) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	135	GLN
1	A	230	ASN
1	A	250	GLN
1	A	322	GLN
1	A	366	GLN
1	A	419	ASN
1	A	437	ASN
1	A	468	GLN
1	A	565	HIS
1	B	217	GLN
1	B	231	ASN
1	B	273	HIS
1	B	305	GLN
1	B	322	GLN
1	B	409	GLN
1	B	410	ASN
1	B	429	HIS
1	B	437	ASN
1	B	468	GLN
1	B	545	GLN

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Mol	Chain	Res	Type
1	B	574	HIS
1	C	18	GLN
1	C	94	GLN
1	C	135	GLN
1	C	147	ASN
1	C	154	GLN
1	C	217	GLN
1	C	222	HIS
1	C	230	ASN
1	C	250	GLN
1	C	286	HIS
1	C	333	ASN
1	C	403	ASN
1	C	419	ASN
1	C	426	HIS
1	C	437	ASN
1	C	521	GLN
1	C	558	HIS
1	C	595	ASN
1	D	18	GLN
1	D	29	ASN
1	D	40	ASN
1	D	128	GLN
1	D	135	GLN
1	D	154	GLN
1	D	245	HIS
1	D	322	GLN
1	D	329	GLN
1	D	333	ASN
1	D	403	ASN
1	D	437	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

8 monosaccharides 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	NAG	E	1	1,2	14,14,15	1.33	3 (21%)	17,19,21	1.45	1 (5%)
2	NAG	E	2	2	14,14,15	0.92	1 (7%)	17,19,21	2.78	6 (35%)
3	NAG	F	1	1,3	14,14,15	1.44	2 (14%)	17,19,21	2.31	6 (35%)
3	NAG	F	2	3	14,14,15	0.99	0	17,19,21	1.99	4 (23%)
2	NAG	G	1	1,2	14,14,15	0.27	0	17,19,21	0.60	0
2	NAG	G	2	2	14,14,15	0.29	0	17,19,21	0.61	0
2	NAG	H	1	1,2	14,14,15	0.84	0	17,19,21	1.49	3 (17%)
2	NAG	H	2	2	14,14,15	0.72	0	17,19,21	1.99	5 (29%)

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	NAG	E	1	1,2	-	5/6/23/26	0/1/1/1
2	NAG	E	2	2	-	4/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	6/6/23/26	0/1/1/1
2	NAG	G	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	G	2	2	-	0/6/23/26	0/1/1/1
2	NAG	H	1	1,2	-	6/6/23/26	0/1/1/1
2	NAG	H	2	2	-	4/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	F	1	NAG	C1-C2	2.83	1.56	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	C2-N2	-2.81	1.41	1.46
2	E	1	NAG	O5-C1	-2.70	1.39	1.43
2	E	2	NAG	C2-N2	-2.50	1.42	1.46
3	F	1	NAG	O5-C1	-2.07	1.40	1.43
2	E	1	NAG	O7-C7	-2.03	1.18	1.23

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	NAG	C1-O5-C5	8.57	123.80	112.19
3	F	1	NAG	O5-C5-C6	4.93	114.93	107.20
3	F	2	NAG	C4-C3-C2	-4.75	104.06	111.02
3	F	1	NAG	O3-C3-C2	4.74	119.27	109.47
2	E	1	NAG	C2-N2-C7	-4.35	116.70	122.90
2	H	2	NAG	O5-C5-C6	4.33	113.99	107.20
2	E	2	NAG	C4-C3-C2	4.17	117.14	111.02
3	F	2	NAG	O3-C3-C2	4.08	117.90	109.47
2	H	2	NAG	C3-C4-C5	-4.07	102.98	110.24
2	E	2	NAG	O4-C4-C3	-3.60	102.04	110.35
2	H	1	NAG	C2-N2-C7	-3.40	118.07	122.90
2	H	1	NAG	O5-C1-C2	-3.24	106.17	111.29
3	F	1	NAG	O4-C4-C3	-3.17	103.02	110.35
3	F	1	NAG	C3-C4-C5	3.08	115.72	110.24
3	F	2	NAG	C1-O5-C5	3.03	116.29	112.19
3	F	1	NAG	C6-C5-C4	-2.74	106.58	113.00
2	E	2	NAG	O5-C1-C2	-2.73	106.98	111.29
2	H	2	NAG	C1-O5-C5	2.64	115.77	112.19
2	H	1	NAG	C6-C5-C4	-2.57	106.99	113.00
2	E	2	NAG	O3-C3-C4	-2.51	104.53	110.35
3	F	1	NAG	O4-C4-C5	-2.50	103.09	109.30
2	H	2	NAG	O5-C5-C4	-2.37	105.07	110.83
2	E	2	NAG	C2-N2-C7	-2.21	119.75	122.90
3	F	2	NAG	C2-N2-C7	2.11	125.91	122.90
2	H	2	NAG	O5-C1-C2	-2.06	108.04	111.29

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
3	F	1	NAG	C3-C2-N2-C7

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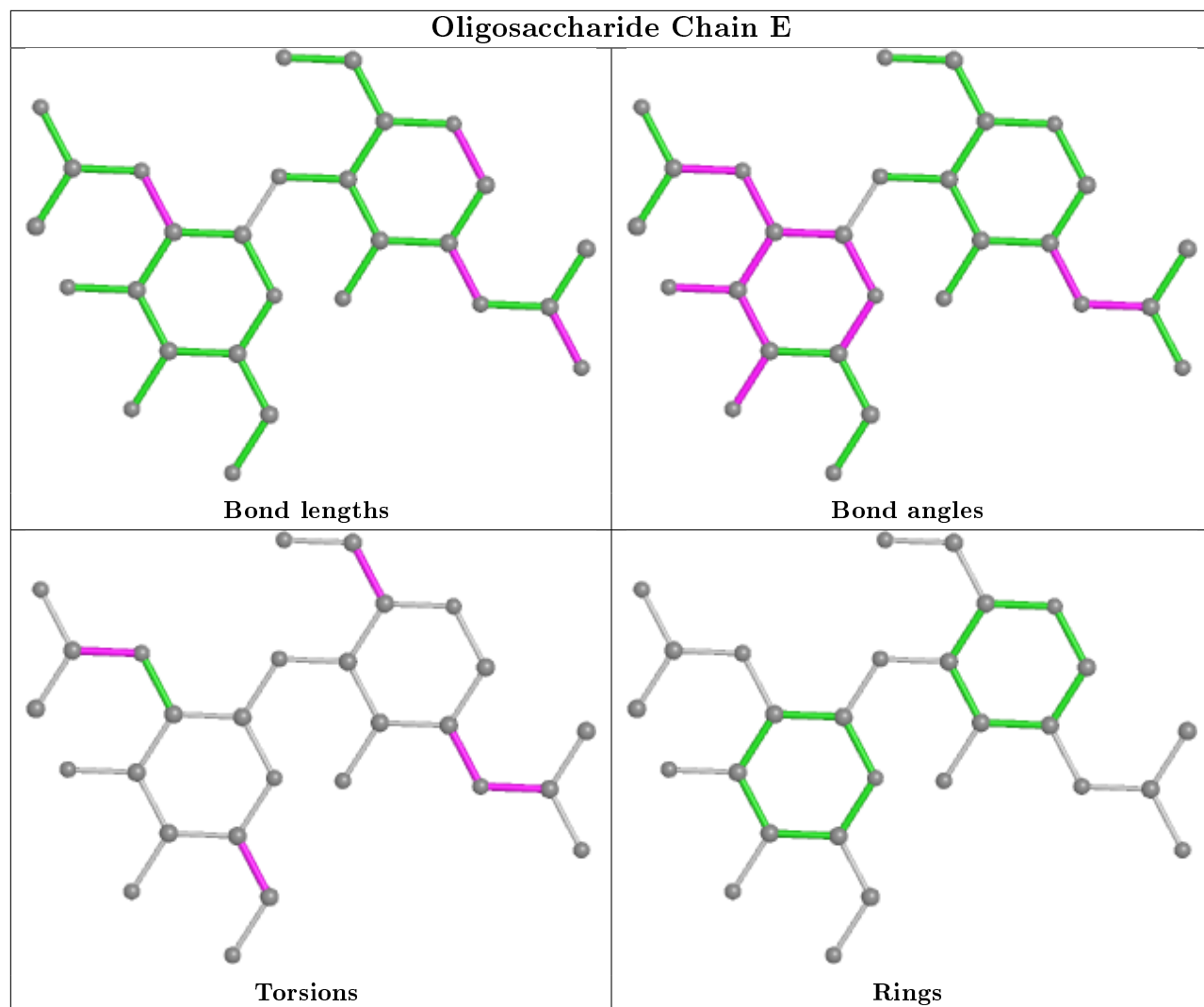
Mol	Chain	Res	Type	Atoms
2	E	1	NAG	C3-C2-N2-C7
2	E	1	NAG	O7-C7-N2-C2
2	H	1	NAG	C3-C2-N2-C7
3	F	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C8-C7-N2-C2
2	H	1	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
2	H	1	NAG	C8-C7-N2-C2
2	H	2	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	H	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C1-C2-N2-C7
2	E	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
3	F	2	NAG	C3-C2-N2-C7
2	E	2	NAG	O7-C7-N2-C2
3	F	1	NAG	C1-C2-N2-C7
2	H	1	NAG	C1-C2-N2-C7

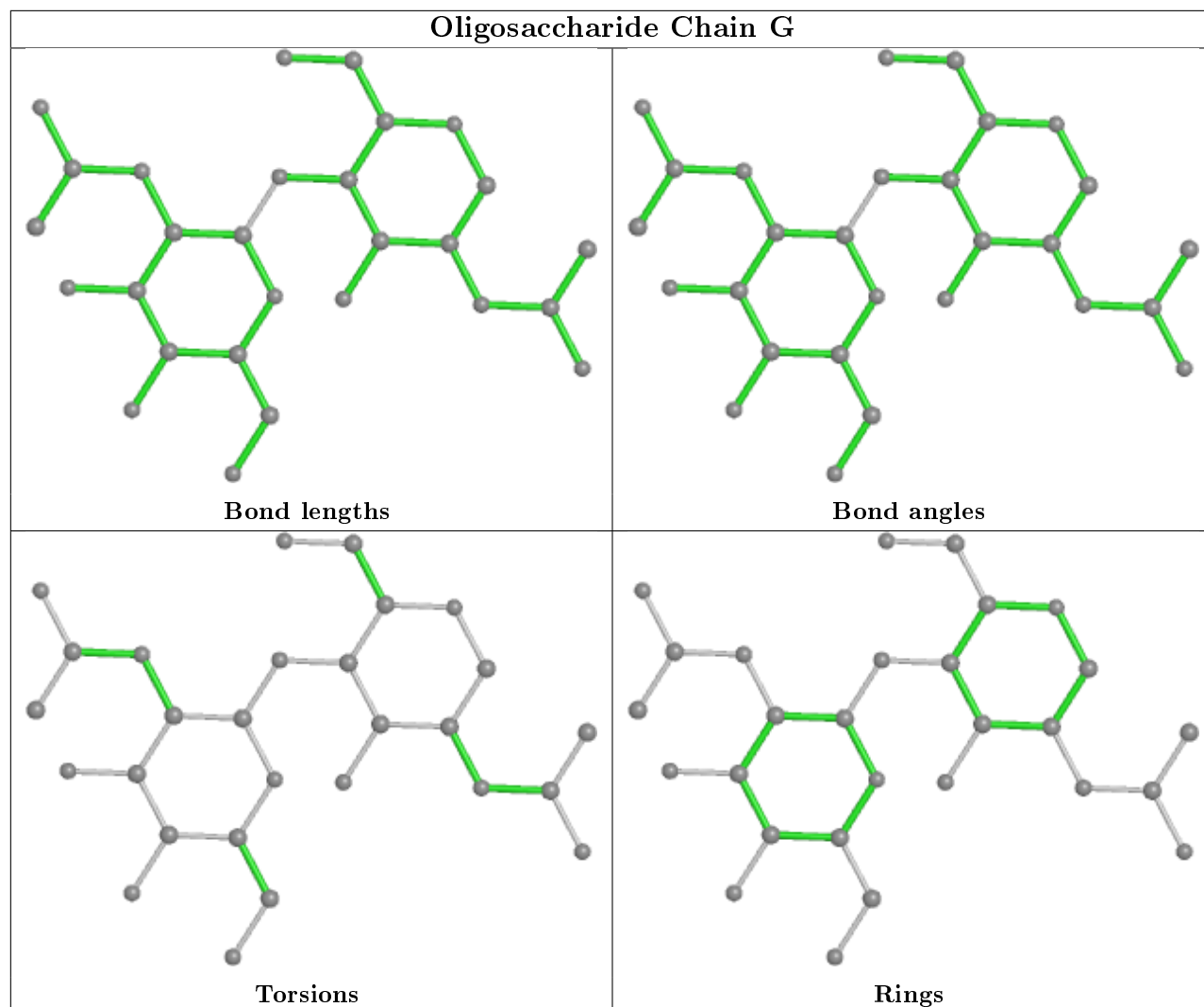
There are no ring outliers.

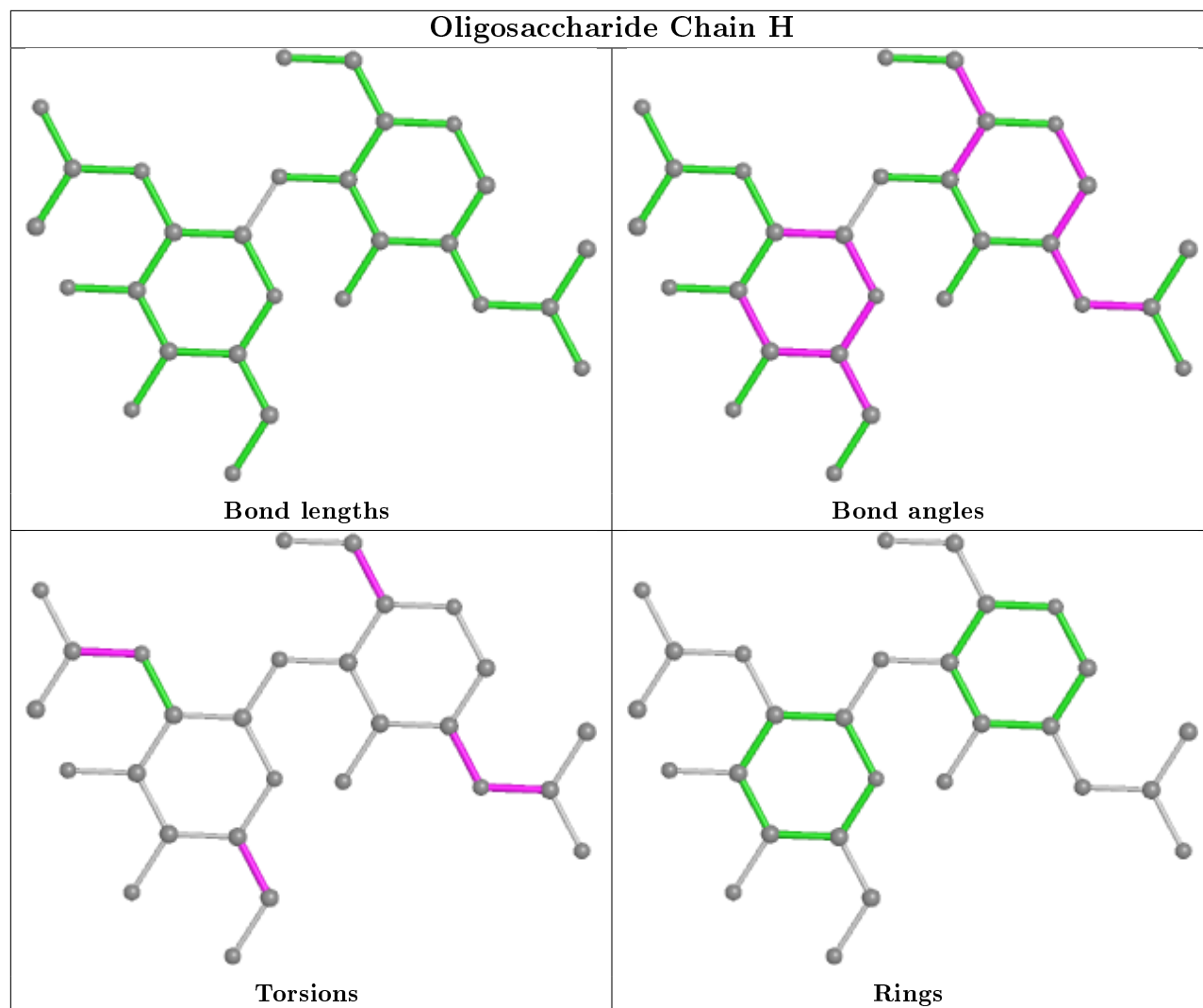
4 monomers are involved in 4 short contacts:

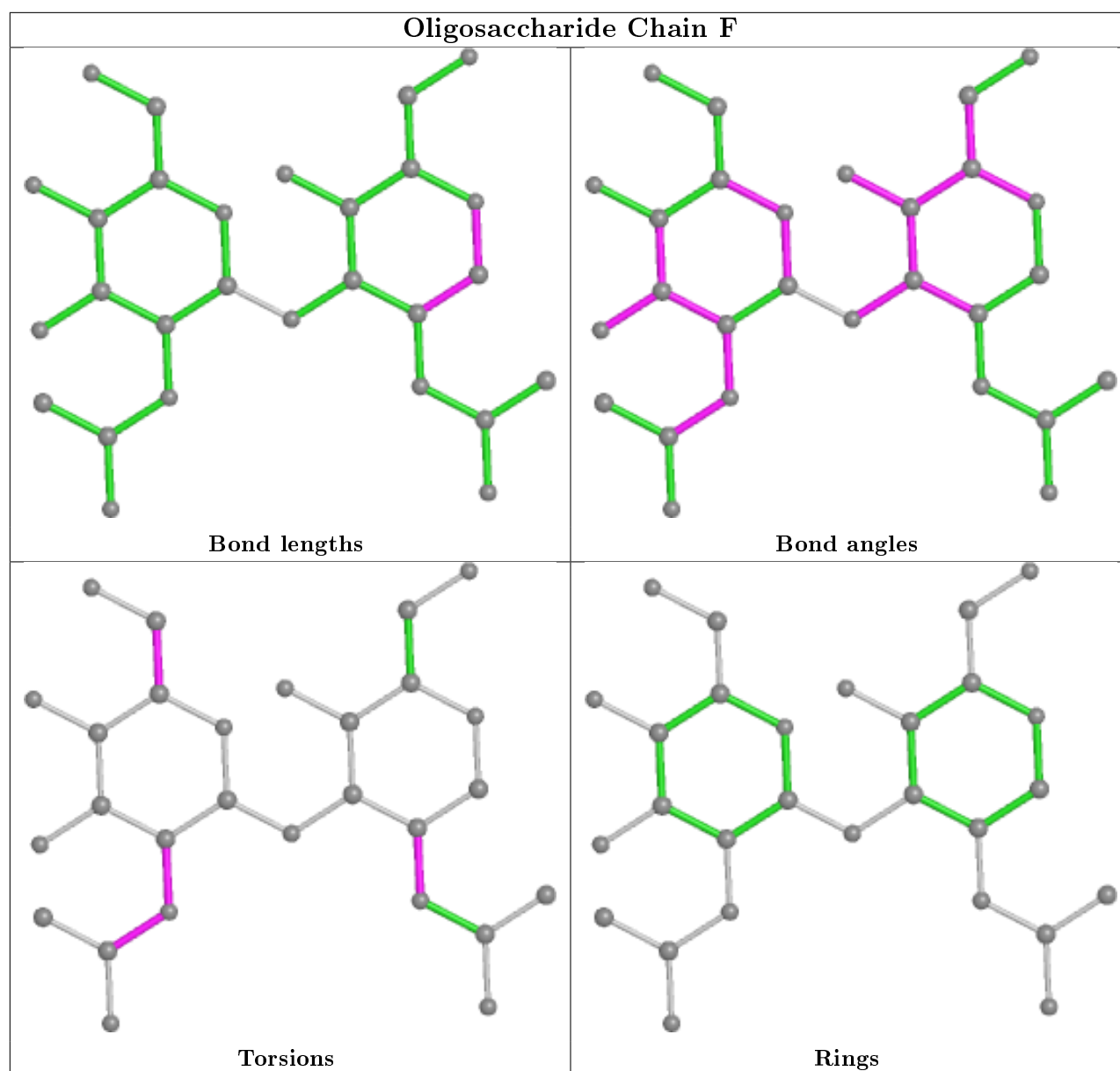
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0
3	F	2	NAG	2	0
2	G	1	NAG	1	0
3	F	1	NAG	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.









5.6 Ligand geometry [i](#)

Of 31 ligands modelled in this entry, 4 are monoatomic - leaving 27 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	HEM	D	610	1	27,50,50	1.33	3 (11%)	17,82,82	2.17	5 (29%)
7	3CJ	D	609	-	8,11,11	2.94	4 (50%)	10,14,14	6.25	7 (70%)
6	NO3	C	607	-	1,3,3	3.46	1 (100%)	0,3,3	0.00	-
7	3CJ	A	609	8	8,11,11	1.95	2 (25%)	10,14,14	4.17	7 (70%)
4	NAG	C	601	1	14,14,15	0.30	0	17,19,21	0.62	0
4	NAG	D	602	1	14,14,15	0.28	0	17,19,21	0.63	0
7	3CJ	B	609	-	8,11,11	2.52	3 (37%)	10,14,14	5.12	6 (60%)
6	NO3	B	606	-	1,3,3	3.57	1 (100%)	0,3,3	0.00	-
6	NO3	B	605	-	1,3,3	0.35	0	0,3,3	0.00	-
7	3CJ	C	609	-	8,11,11	2.19	2 (25%)	10,14,14	4.09	6 (60%)
6	NO3	A	608	-	1,3,3	0.34	0	0,3,3	0.00	-
4	NAG	B	601	1	14,14,15	1.18	1 (7%)	17,19,21	1.81	7 (41%)
4	NAG	A	601	1	14,14,15	1.01	0	17,19,21	2.38	8 (47%)
8	HEM	C	610	1	27,50,50	0.91	1 (3%)	17,82,82	2.06	7 (41%)
6	NO3	B	607	-	1,3,3	0.46	0	0,3,3	0.00	-
8	HEM	B	608	1	27,50,50	1.16	2 (7%)	17,82,82	1.84	6 (35%)
6	NO3	A	606	-	1,3,3	1.27	0	0,3,3	0.00	-
6	NO3	D	606	-	1,3,3	0.34	0	0,3,3	0.00	-
8	HEM	A	610	1,7	27,50,50	1.11	2 (7%)	17,82,82	2.29	5 (29%)
4	NAG	C	604	1	14,14,15	0.29	0	17,19,21	0.62	0
6	NO3	C	608	-	1,3,3	0.32	0	0,3,3	0.00	-
4	NAG	D	601	1	14,14,15	0.81	0	17,19,21	1.94	5 (29%)
6	NO3	D	608	-	1,3,3	0.35	0	0,3,3	0.00	-
6	NO3	D	607	-	1,3,3	3.56	1 (100%)	0,3,3	0.00	-
4	NAG	A	602	1	14,14,15	0.29	0	17,19,21	0.61	0
6	NO3	C	606	-	1,3,3	0.34	0	0,3,3	0.00	-
6	NO3	A	607	-	1,3,3	3.55	1 (100%)	0,3,3	0.00	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	604	1	-	2/6/23/26	0/1/1/1
7	3CJ	C	609	-	-	0/3/3/3	0/1/1/1
7	3CJ	A	609	8	-	3/3/3/3	0/1/1/1
4	NAG	D	601	1	-	4/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	C	601	1	-	4/6/23/26	0/1/1/1
8	HEM	D	610	1	-	0/6/54/54	-
4	NAG	D	602	1	-	0/6/23/26	0/1/1/1
4	NAG	B	601	1	-	2/6/23/26	0/1/1/1
4	NAG	A	601	1	-	5/6/23/26	0/1/1/1
8	HEM	C	610	1	-	0/6/54/54	-
7	3CJ	D	609	-	-	1/3/3/3	0/1/1/1
7	3CJ	B	609	-	-	3/3/3/3	0/1/1/1
8	HEM	B	608	1	-	2/6/54/54	-
4	NAG	A	602	1	-	0/6/23/26	0/1/1/1
8	HEM	A	610	1,7	-	0/6/54/54	-

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	609	3CJ	O1-C4	5.23	1.37	1.24
7	D	609	3CJ	O1-C4	5.21	1.37	1.24
7	B	609	3CJ	O1-C4	5.02	1.37	1.24
7	D	609	3CJ	C1-S1	4.68	1.76	1.66
7	A	609	3CJ	O1-C4	4.53	1.35	1.24
7	D	609	3CJ	C2-N1	3.65	1.40	1.34
7	B	609	3CJ	C1-S1	3.59	1.74	1.66
6	B	606	NO3	O1-N	3.57	1.40	1.24
6	D	607	NO3	O1-N	3.56	1.40	1.24
6	A	607	NO3	O1-N	3.55	1.40	1.24
6	C	607	NO3	O1-N	3.46	1.40	1.24
8	B	608	HEM	C4D-C3D	2.84	1.49	1.42
7	B	609	3CJ	C4-N2	2.78	1.37	1.33
8	D	610	HEM	C4D-C3D	2.77	1.48	1.42
8	D	610	HEM	C3B-C2B	-2.71	1.36	1.40
8	A	610	HEM	C4D-C3D	2.70	1.48	1.42
8	B	608	HEM	C3B-C2B	-2.61	1.36	1.40
7	C	609	3CJ	C1-S1	2.59	1.72	1.66
8	A	610	HEM	C1A-CHA	-2.50	1.34	1.41
8	D	610	HEM	CAA-C2A	-2.39	1.48	1.52
4	B	601	NAG	C4-C5	-2.31	1.48	1.53
7	A	609	3CJ	C1-S1	2.18	1.71	1.66
7	D	609	3CJ	C4-N2	2.14	1.36	1.33
8	C	610	HEM	C4D-C3D	2.03	1.47	1.42

All (69) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	609	3CJ	N2-C1-N1	-14.43	117.19	130.43
7	B	609	3CJ	N2-C1-N1	-12.67	118.80	130.43
7	A	609	3CJ	N2-C1-N1	-10.02	121.23	130.43
7	C	609	3CJ	N2-C1-N1	-9.32	121.88	130.43
7	D	609	3CJ	C4-N2-C1	8.78	123.11	114.74
7	D	609	3CJ	C5-C2-N1	6.71	125.94	115.95
7	B	609	3CJ	C3-C2-N1	-6.24	116.28	122.90
8	A	610	HEM	CBD-CAD-C3D	-6.04	101.34	112.48
8	D	610	HEM	CBD-CAD-C3D	-5.45	102.43	112.48
7	C	609	3CJ	C4-N2-C1	5.11	119.62	114.74
7	B	609	3CJ	C4-N2-C1	5.03	119.54	114.74
8	A	610	HEM	C1D-C2D-C3D	-4.97	103.54	107.00
7	A	609	3CJ	C3-C2-N1	-4.75	117.86	122.90
4	D	601	NAG	O5-C1-C2	-4.68	103.90	111.29
7	D	609	3CJ	C3-C2-N1	-4.67	117.94	122.90
7	A	609	3CJ	C4-N2-C1	4.40	118.94	114.74
8	B	608	HEM	CBD-CAD-C3D	-4.36	104.44	112.48
8	D	610	HEM	CMC-C2C-C3C	4.34	132.79	124.68
4	A	601	NAG	C4-C3-C2	-4.26	104.78	111.02
7	C	609	3CJ	C3-C2-N1	-4.17	118.47	122.90
7	B	609	3CJ	C1-N1-C2	3.99	124.67	115.02
7	D	609	3CJ	C5-C2-C3	-3.95	115.99	121.22
7	C	609	3CJ	C3-C4-N2	-3.92	119.50	124.08
7	C	609	3CJ	C5-C2-N1	3.80	121.60	115.95
8	C	610	HEM	CMB-C2B-C3B	3.75	131.69	124.68
4	D	601	NAG	C2-N2-C7	-3.61	117.76	122.90
8	C	610	HEM	CAD-CBD-CGD	3.61	118.72	112.67
8	C	610	HEM	CBD-CAD-C3D	-3.52	105.99	112.48
4	A	601	NAG	C1-O5-C5	3.47	116.89	112.19
7	A	609	3CJ	C5-C2-C3	3.46	125.80	121.22
7	B	609	3CJ	C5-C2-N1	3.45	121.09	115.95
4	A	601	NAG	O4-C4-C5	3.40	117.75	109.30
4	A	601	NAG	C1-C2-N2	3.38	116.26	110.49
4	A	601	NAG	O5-C5-C6	3.33	112.43	107.20
4	A	601	NAG	C2-N2-C7	-3.32	118.18	122.90
7	D	609	3CJ	C1-N1-C2	3.21	122.78	115.02
4	B	601	NAG	O5-C1-C2	-3.16	106.30	111.29
4	A	601	NAG	C3-C4-C5	-3.09	104.73	110.24
8	A	610	HEM	CMD-C2D-C3D	3.06	130.71	124.94
4	B	601	NAG	C1-O5-C5	3.05	116.32	112.19
7	D	609	3CJ	C3-C4-N2	-2.93	120.66	124.08
7	A	609	3CJ	C1-N1-C2	2.92	122.08	115.02
4	B	601	NAG	C2-N2-C7	-2.79	118.94	122.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	608	HEM	C1D-C2D-C3D	-2.78	105.06	107.00
8	D	610	HEM	CBA-CAA-C2A	-2.70	107.50	112.49
8	D	610	HEM	CMB-C2B-C3B	2.61	129.56	124.68
4	B	601	NAG	O6-C6-C5	-2.59	102.42	111.29
8	C	610	HEM	CMC-C2C-C3C	2.58	129.50	124.68
8	C	610	HEM	C1D-C2D-C3D	-2.48	105.27	107.00
8	D	610	HEM	C4C-C3C-C2C	-2.46	105.18	106.90
7	A	609	3CJ	C3-C4-N2	-2.44	121.23	124.08
8	B	608	HEM	C4C-C3C-C2C	-2.43	105.20	106.90
4	D	601	NAG	C8-C7-N2	-2.42	112.00	116.10
8	A	610	HEM	C4C-C3C-C2C	-2.38	105.24	106.90
4	B	601	NAG	C6-C5-C4	-2.37	107.45	113.00
7	B	609	3CJ	C3-C4-N2	-2.34	121.35	124.08
8	C	610	HEM	CAA-CBA-CGA	-2.31	108.79	112.67
8	B	608	HEM	CAA-C2A-C3A	-2.29	120.66	127.25
8	B	608	HEM	CMB-C2B-C3B	2.28	128.95	124.68
4	B	601	NAG	O3-C3-C4	-2.24	105.17	110.35
7	C	609	3CJ	C1-N1-C2	2.23	120.41	115.02
4	D	601	NAG	O3-C3-C4	-2.18	105.32	110.35
8	A	610	HEM	CMB-C2B-C3B	2.12	128.64	124.68
7	A	609	3CJ	C6-C5-C2	2.10	122.94	115.25
8	C	610	HEM	C3B-C4B-NB	-2.06	106.55	109.21
4	D	601	NAG	C4-C3-C2	2.05	114.03	111.02
8	B	608	HEM	CMD-C2D-C3D	2.04	128.78	124.94
4	A	601	NAG	O4-C4-C3	-2.04	105.64	110.35
4	B	601	NAG	O5-C5-C4	-2.04	105.88	110.83

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	A	609	3CJ	C2-C5-C6-C7
4	C	601	NAG	C8-C7-N2-C2
4	C	601	NAG	O7-C7-N2-C2
4	A	601	NAG	C3-C2-N2-C7
8	B	608	HEM	C1A-C2A-CAA-CBA
8	B	608	HEM	C3A-C2A-CAA-CBA
4	D	601	NAG	O5-C5-C6-O6
4	A	601	NAG	O5-C5-C6-O6
4	D	601	NAG	C8-C7-N2-C2
4	D	601	NAG	C4-C5-C6-O6
4	C	604	NAG	O5-C5-C6-O6

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Mol	Chain	Res	Type	Atoms
4	D	601	NAG	O7-C7-N2-C2
4	C	601	NAG	O5-C5-C6-O6
7	A	609	3CJ	N1-C2-C5-C6
7	B	609	3CJ	N1-C2-C5-C6
4	C	604	NAG	C4-C5-C6-O6
4	A	601	NAG	C4-C5-C6-O6
4	C	601	NAG	C4-C5-C6-O6
7	A	609	3CJ	C3-C2-C5-C6
4	B	601	NAG	C8-C7-N2-C2
7	B	609	3CJ	C3-C2-C5-C6
7	B	609	3CJ	C2-C5-C6-C7
4	A	601	NAG	C8-C7-N2-C2
4	B	601	NAG	O7-C7-N2-C2
4	A	601	NAG	O7-C7-N2-C2
7	D	609	3CJ	C2-C5-C6-C7

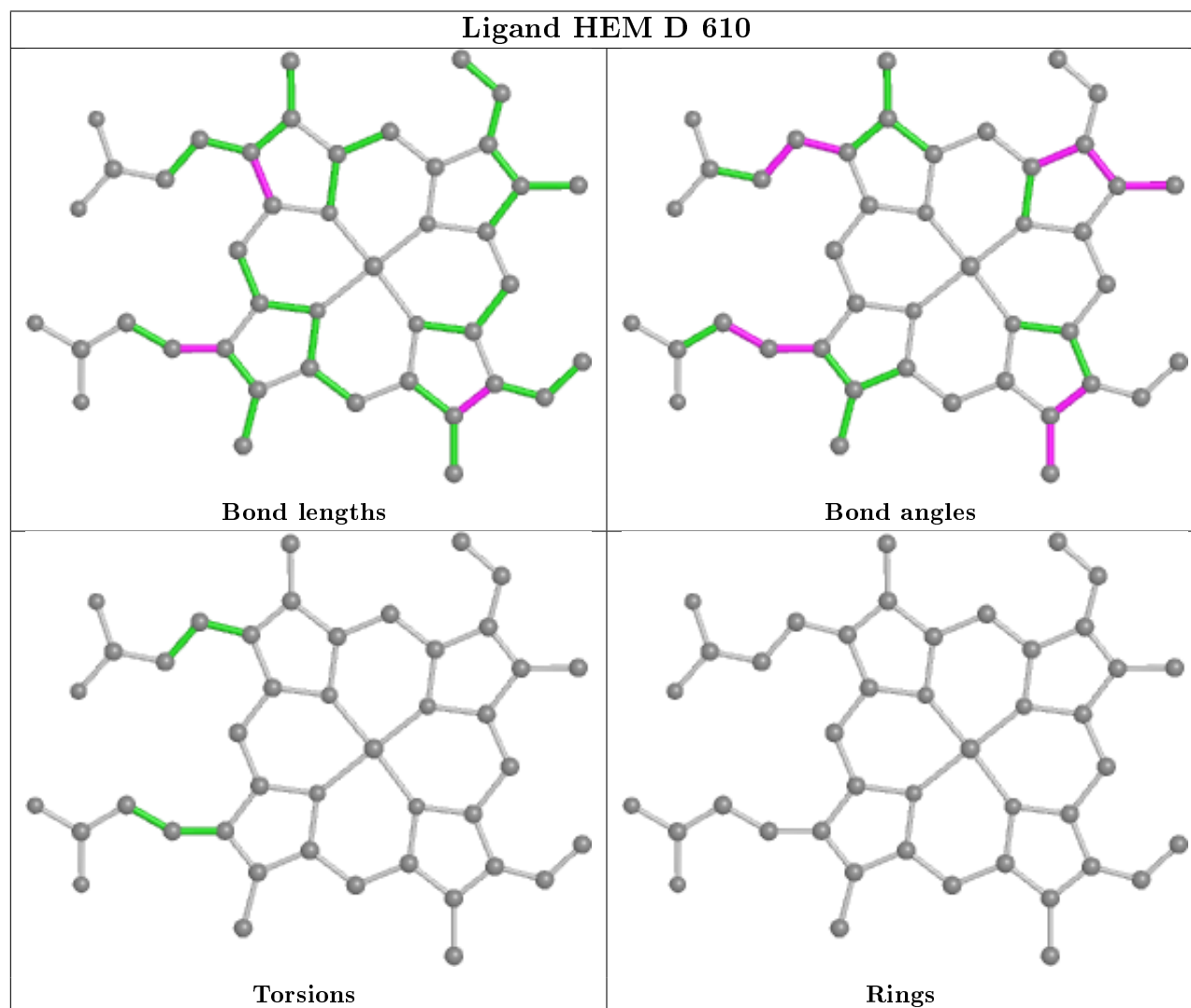
There are no ring outliers.

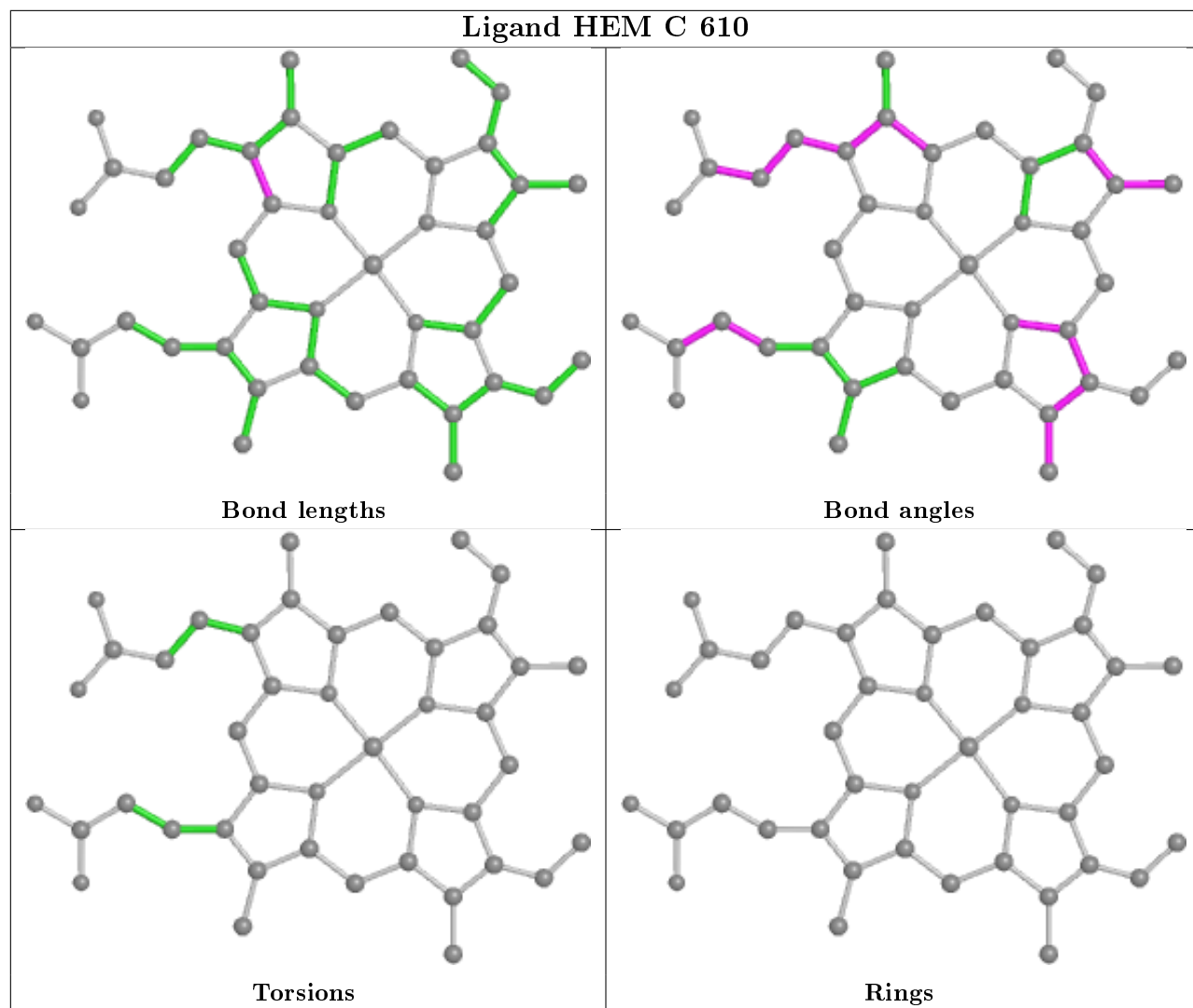
17 monomers are involved in 90 short contacts:

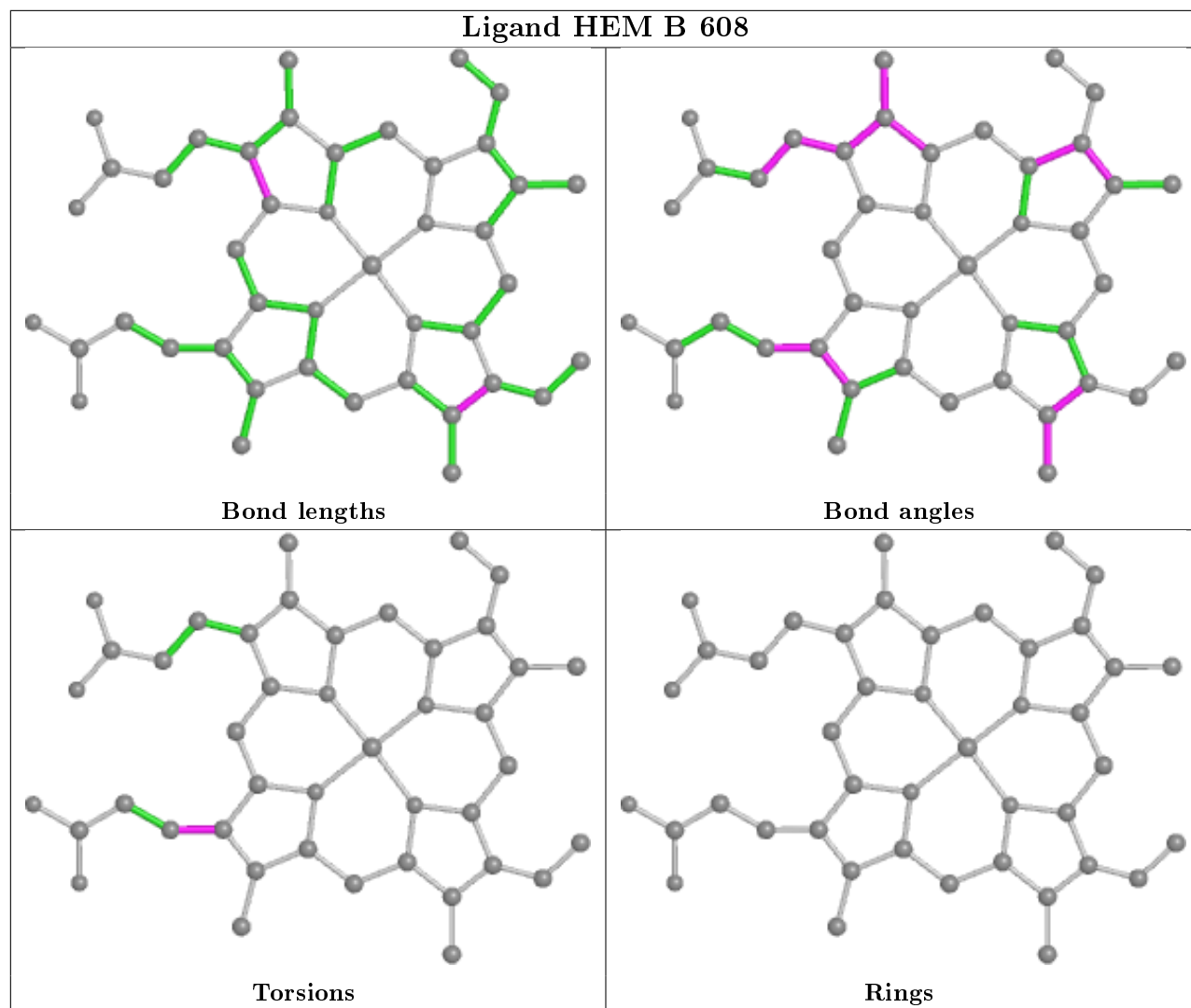
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	610	HEM	15	0
7	D	609	3CJ	11	0
6	C	607	NO3	1	0
7	A	609	3CJ	11	0
4	D	602	NAG	1	0
7	B	609	3CJ	12	0
6	B	605	NO3	1	0
7	C	609	3CJ	9	0
8	C	610	HEM	17	0
8	B	608	HEM	14	0
6	D	606	NO3	2	0
8	A	610	HEM	12	0
6	C	608	NO3	2	0
6	D	608	NO3	4	0
6	D	607	NO3	2	0
6	C	606	NO3	1	0
6	A	607	NO3	1	0

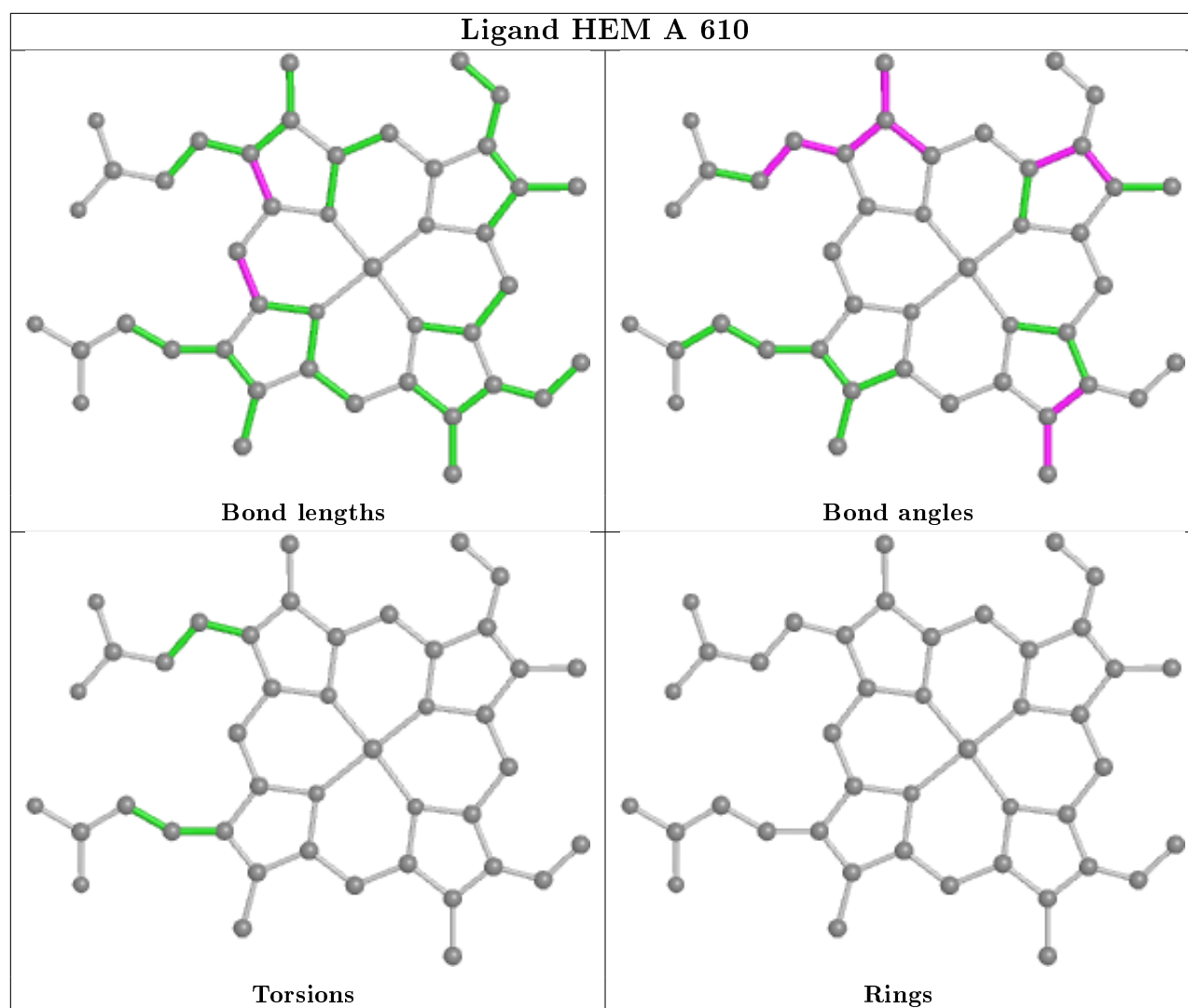
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	595/595 (100%)	0.24	31 (5%)	27 29	16, 42, 78, 117	0
1	B	595/595 (100%)	0.26	34 (5%)	23 25	20, 43, 76, 100	0
1	C	595/595 (100%)	0.43	52 (8%)	10 10	20, 43, 83, 100	0
1	D	595/595 (100%)	0.34	37 (6%)	20 21	14, 41, 79, 100	0
All	All	2380/2380 (100%)	0.32	154 (6%)	18 19	14, 42, 79, 117	0

All (154) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4	VAL	19.5
1	C	6	CYS	13.8
1	D	2	TRP	12.4
1	A	171	PRO	11.3
1	D	7	GLY	11.2
1	D	13	VAL	10.2
1	B	121	SER	9.9
1	B	1	SER	9.8
1	D	1	SER	9.6
1	A	5	GLY	9.3
1	A	2	TRP	9.2
1	D	3	GLU	9.1
1	B	2	TRP	9.1
1	C	5	GLY	8.8
1	A	1	SER	8.6
1	A	4	VAL	8.6
1	B	6	CYS	8.4
1	C	9	PRO	7.9
1	C	4	VAL	7.9
1	A	172	TYR	7.1
1	C	7	GLY	7.0

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Mol	Chain	Res	Type	RSRZ
1	B	4	VAL	6.8
1	B	5	GLY	6.5
1	C	1	SER	6.5
1	C	8	ALA	6.5
1	B	122	SER	6.5
1	C	121	SER	6.3
1	D	11	PRO	6.2
1	A	170	PRO	6.0
1	C	2	TRP	5.9
1	C	129	CYS	5.9
1	A	119	LEU	5.7
1	C	3	GLU	5.6
1	A	12	LEU	5.3
1	D	170	PRO	5.3
1	A	3	GLU	5.2
1	C	96	ARG	5.2
1	A	6	CYS	5.1
1	D	592	SER	5.1
1	C	132	TYR	5.0
1	B	3	GLU	5.0
1	A	121	SER	4.9
1	C	172	TYR	4.8
1	B	582	VAL	4.8
1	A	585	LEU	4.7
1	A	13	VAL	4.7
1	D	120	GLY	4.7
1	D	5	GLY	4.6
1	C	119	LEU	4.6
1	D	12	LEU	4.6
1	B	170	PRO	4.6
1	B	120	GLY	4.4
1	A	173	GLN	4.4
1	D	595	ASN	4.4
1	C	13	VAL	4.3
1	B	189	ALA	4.3
1	C	591	ALA	4.3
1	D	172	TYR	4.1
1	B	595	ASN	4.1
1	D	169	THR	4.1
1	D	207	SER	4.1
1	B	11	PRO	4.0
1	B	171	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	8	ALA	3.9
1	D	10	VAL	3.9
1	A	169	THR	3.8
1	A	9	PRO	3.8
1	B	8	ALA	3.7
1	C	161	PHE	3.6
1	A	122	SER	3.6
1	D	6	CYS	3.6
1	C	249	PHE	3.6
1	B	173	GLN	3.6
1	A	7	GLY	3.5
1	C	11	PRO	3.5
1	A	223	GLY	3.5
1	C	10	VAL	3.4
1	C	580	SER	3.4
1	C	595	ASN	3.3
1	B	581	ALA	3.3
1	C	138	GLU	3.3
1	C	117	THR	3.3
1	B	172	TYR	3.3
1	A	136	GLY	3.2
1	B	530	TRP	3.1
1	B	369	GLY	3.1
1	B	137	ASP	3.1
1	B	262	LEU	3.1
1	C	153	THR	3.0
1	D	209	PRO	3.0
1	B	9	PRO	3.0
1	C	209	PRO	3.0
1	C	106	ILE	3.0
1	B	583	ASP	2.9
1	D	190	SER	2.9
1	D	132	TYR	2.9
1	B	7	GLY	2.9
1	B	282	ARG	2.9
1	B	425	THR	2.8
1	C	215	VAL	2.8
1	C	169	THR	2.8
1	D	173	GLN	2.8
1	A	174	SER	2.8
1	B	545	GLN	2.8
1	A	582	VAL	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	120	GLY	2.7
1	C	127	VAL	2.7
1	C	351	HIS	2.6
1	D	574	HIS	2.6
1	C	173	GLN	2.6
1	D	171	PRO	2.6
1	D	175	LEU	2.5
1	D	351	HIS	2.5
1	A	56	ALA	2.5
1	A	137	ASP	2.5
1	C	464	LEU	2.5
1	C	542	ASP	2.5
1	D	134	VAL	2.5
1	D	243	THR	2.5
1	B	593	ARG	2.4
1	C	175	LEU	2.4
1	D	107	VAL	2.4
1	D	585	LEU	2.4
1	C	118	GLU	2.4
1	C	14	THR	2.4
1	C	130	GLU	2.4
1	C	12	LEU	2.3
1	A	425	THR	2.3
1	C	592	SER	2.3
1	D	17	GLU	2.3
1	A	10	VAL	2.2
1	C	243	THR	2.2
1	D	303	PHE	2.2
1	A	485	LYS	2.2
1	D	567	PHE	2.2
1	B	586	ASP	2.1
1	C	582	VAL	2.1
1	D	582	VAL	2.1
1	C	581	ALA	2.1
1	C	170	PRO	2.1
1	B	351	HIS	2.1
1	D	208	SER	2.1
1	A	11	PRO	2.1
1	B	10	VAL	2.1
1	C	494	ILE	2.1
1	C	108	ASP	2.1
1	B	588	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	168	PRO	2.0
1	A	21	TYR	2.0
1	C	546	LYS	2.0
1	C	115	PRO	2.0
1	C	164	GLY	2.0
1	D	223	GLY	2.0
1	C	159	PRO	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](#)

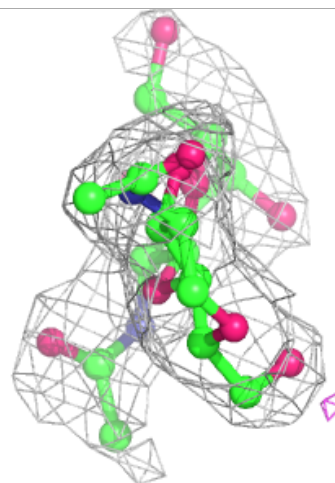
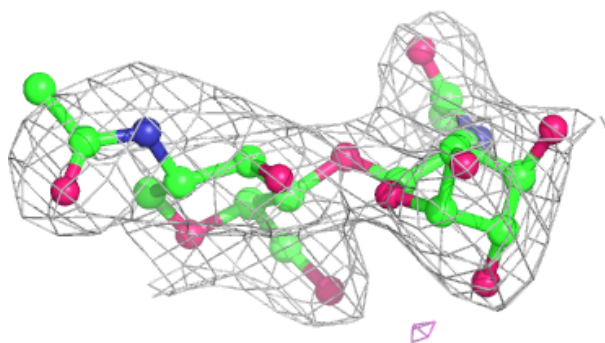
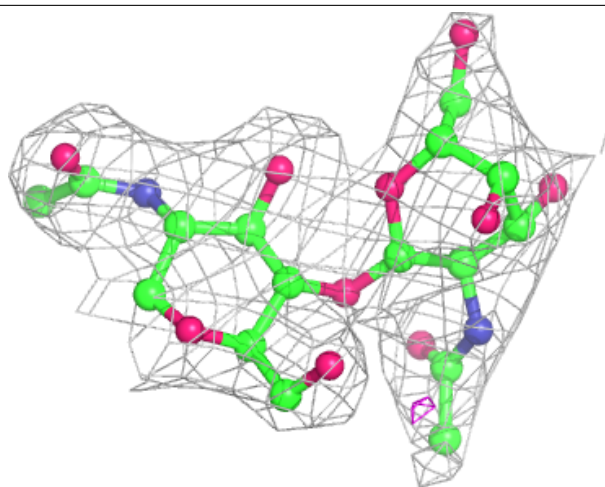
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	F	2	14/15	0.81	0.27	45,53,55,58	14
2	NAG	H	2	14/15	0.84	0.21	61,67,70,70	14
2	NAG	G	2	14/15	0.84	0.20	49,56,63,63	14
3	NAG	F	1	14/15	0.85	0.19	36,50,59,66	0
2	NAG	G	1	14/15	0.87	0.24	20,20,20,20	0
2	NAG	E	2	14/15	0.88	0.20	43,50,51,52	14
2	NAG	E	1	14/15	0.93	0.14	33,41,52,54	0
2	NAG	H	1	14/15	0.94	0.11	70,79,82,85	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

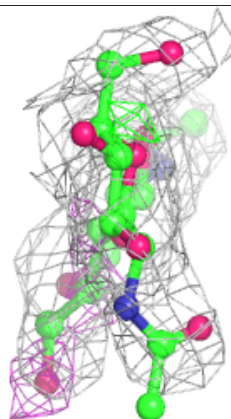
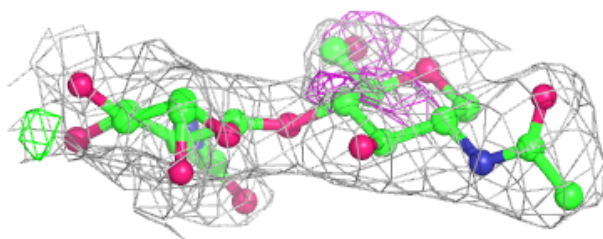
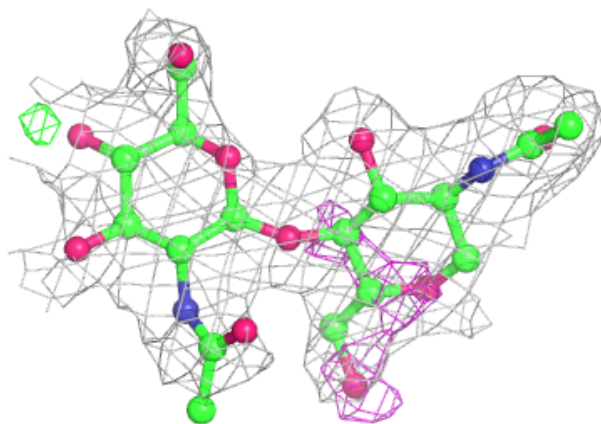
Electron density around Chain E:

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



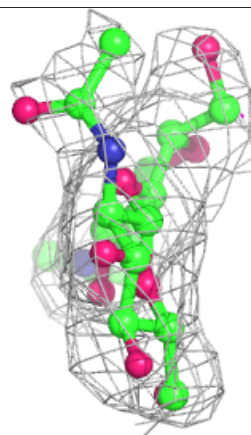
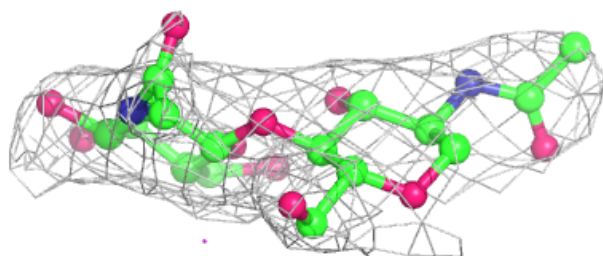
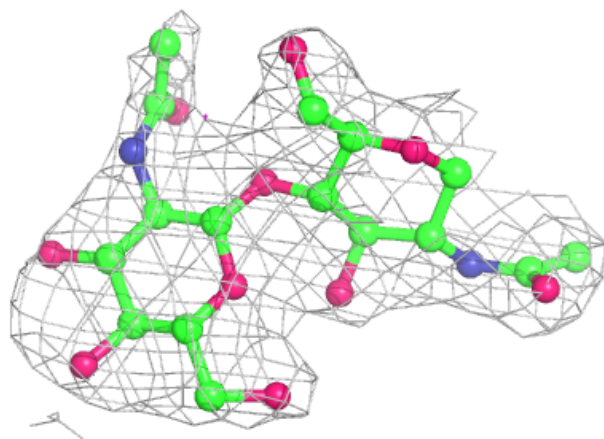
Electron density around Chain G:

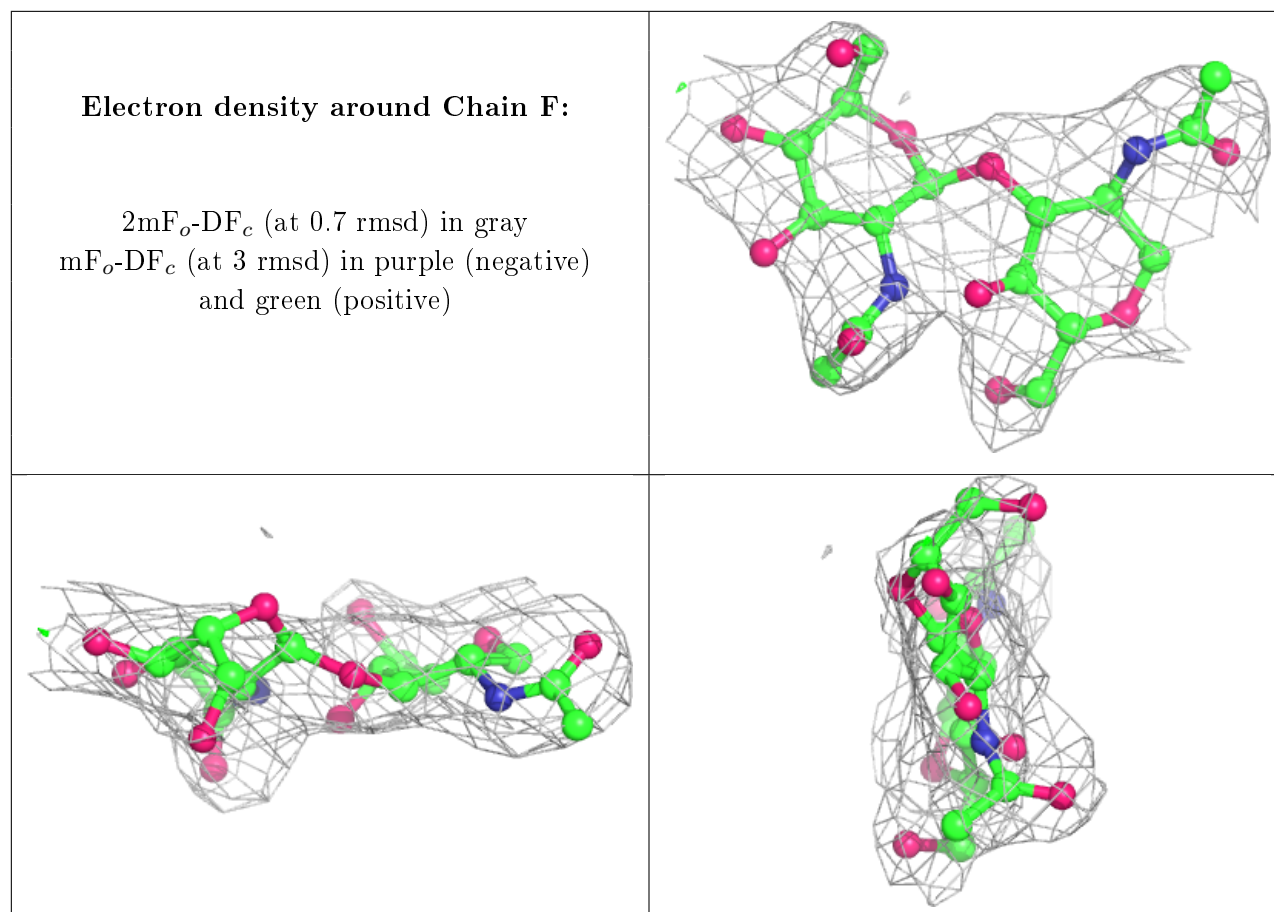
$2mF_o - DF_c$ (at 0.7 rmsd) in gray
 $mF_o - DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain H:

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





6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	C	601	14/15	0.64	0.39	78,86,89,90	0
7	3CJ	C	609	11/11	0.72	0.37	69,79,84,85	0
4	NAG	A	601	14/15	0.73	0.20	64,79,81,81	0
4	NAG	D	602	14/15	0.82	0.17	46,54,59,60	0
7	3CJ	D	609	11/11	0.83	0.41	39,48,58,58	0
7	3CJ	B	609	11/11	0.84	0.24	48,52,58,61	0
4	NAG	D	601	14/15	0.84	0.20	52,60,65,66	0
6	NO3	C	607	4/4	0.86	0.43	24,24,27,31	0
6	NO3	C	608	4/4	0.87	0.26	24,28,29,30	0
6	NO3	B	605	4/4	0.89	0.20	22,25,27,28	0
4	NAG	C	604	14/15	0.89	0.20	48,55,60,61	0
6	NO3	D	607	4/4	0.89	0.39	25,26,27,28	0

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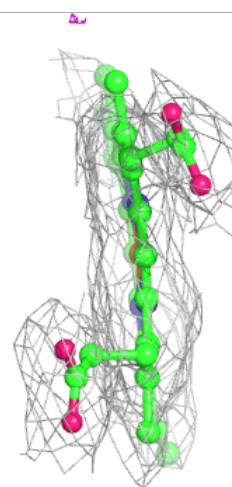
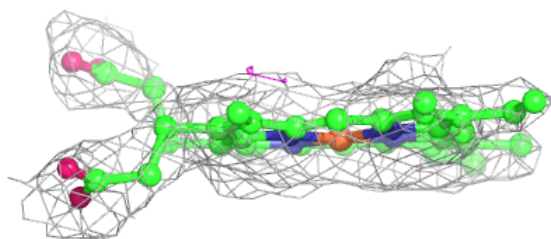
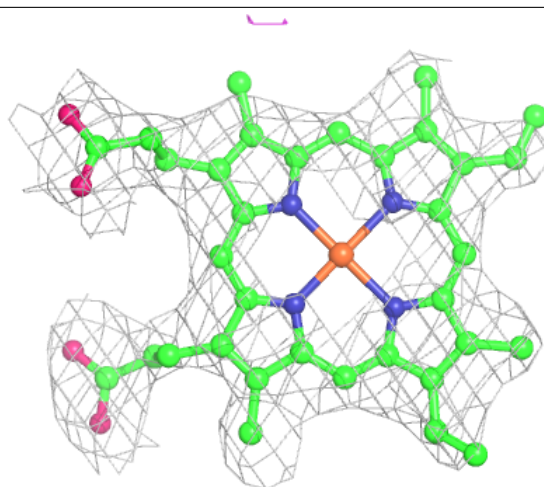
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
6	NO3	B	606	4/4	0.90	0.41	26,26,27,29	0
4	NAG	B	601	14/15	0.91	0.15	55,63,73,75	0
6	NO3	B	607	4/4	0.91	0.64	24,24,24,28	0
6	NO3	C	606	4/4	0.91	0.59	24,27,29,31	0
5	CA	A	605	1/1	0.91	0.18	43,43,43,43	0
5	CA	C	605	1/1	0.93	0.23	46,46,46,46	0
5	CA	B	604	1/1	0.93	0.13	44,44,44,44	0
7	3CJ	A	609	11/11	0.93	0.19	47,50,55,56	0
8	HEM	C	610	43/43	0.94	0.19	35,45,51,53	0
4	NAG	A	602	14/15	0.94	0.12	38,46,51,54	0
8	HEM	B	608	43/43	0.94	0.23	33,42,54,62	0
6	NO3	D	608	4/4	0.94	0.45	23,23,26,30	0
8	HEM	D	610	43/43	0.95	0.18	19,25,39,45	0
6	NO3	D	606	4/4	0.95	0.23	21,24,24,26	0
8	HEM	A	610	43/43	0.95	0.23	31,39,44,49	0
6	NO3	A	606	4/4	0.96	0.31	23,23,24,26	0
6	NO3	A	608	4/4	0.96	0.42	23,24,26,27	0
5	CA	D	605	1/1	0.97	0.23	36,36,36,36	0
6	NO3	A	607	4/4	0.97	0.17	24,26,28,32	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.

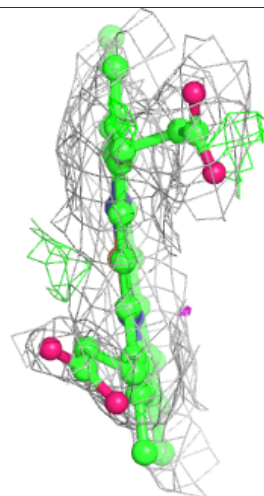
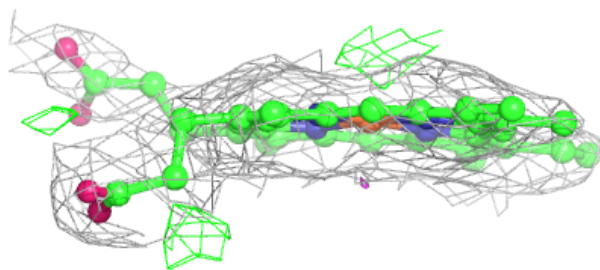
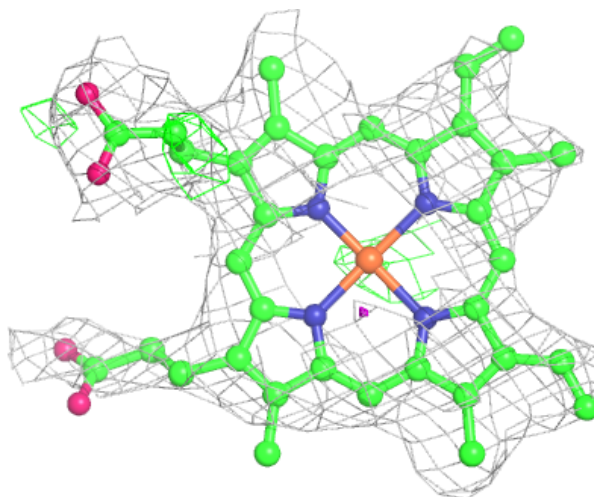
Electron density around HEM C 610:

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



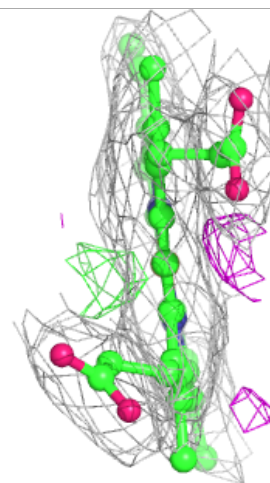
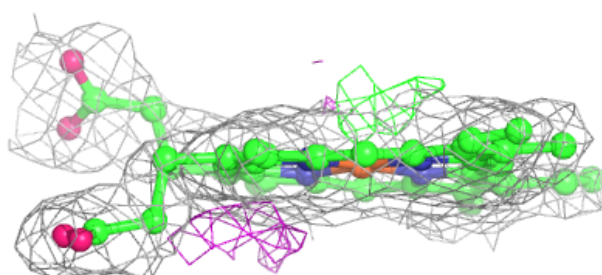
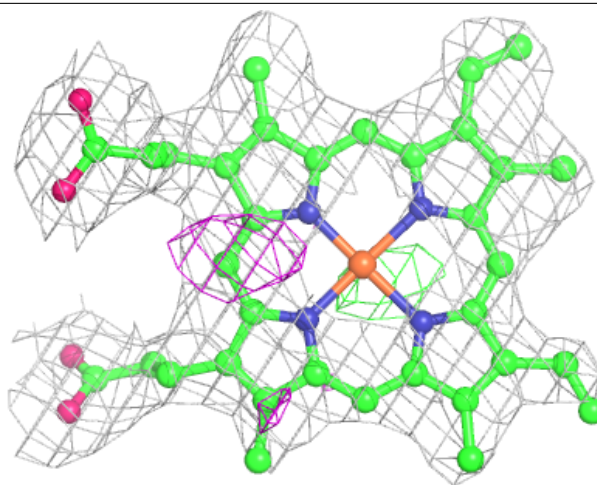
Electron density around HEM B 608:

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



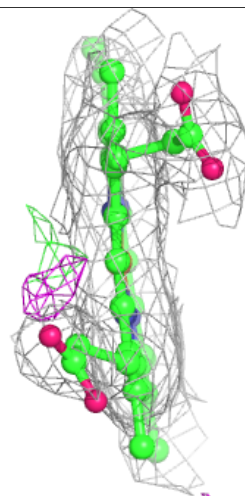
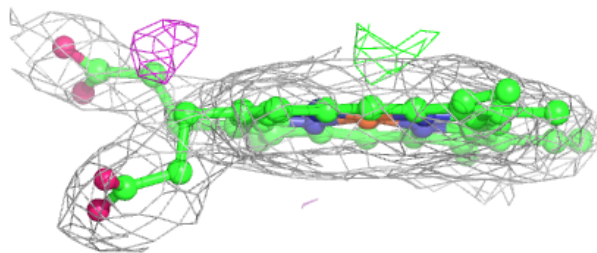
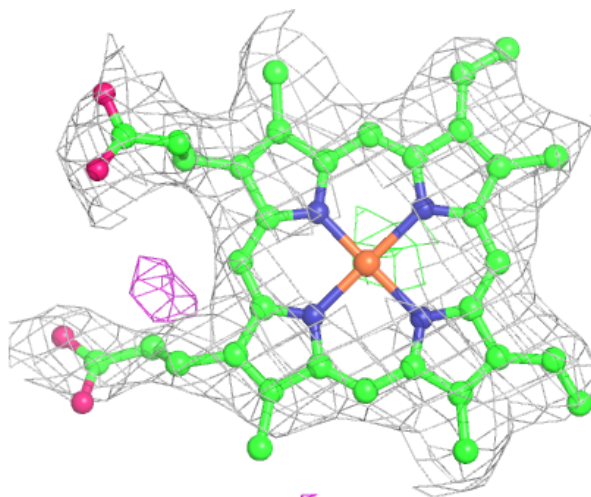
Electron density around HEM D 610:

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



Electron density around HEM A 610:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.