



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 03:11 AM JST

PDB ID : 5HPW / pdb_00005hpw
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

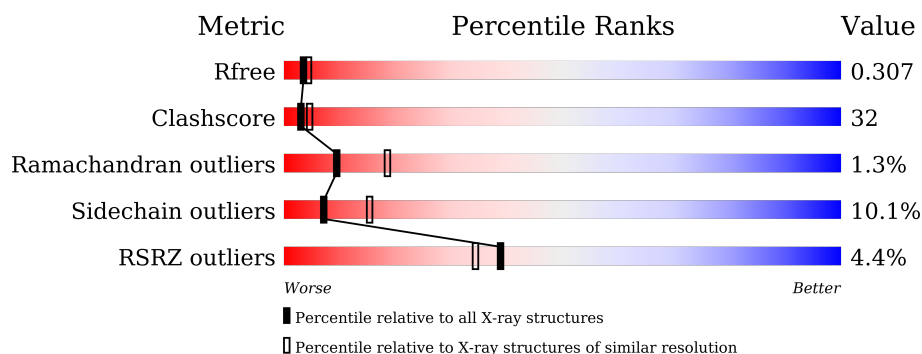
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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.



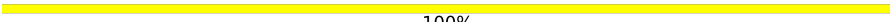
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	595	4% 44% 47% 8%
1	B	595	3% 48% 44% 7%
1	C	595	5% 47% 43% 9%
1	D	595	5% 39% 49% 11%
2	E	2	50% 50%
2	G	2	50% 50%

Continued on next page...

Continued from previous page...

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	B	603	-	-	X	-
6	NO3	C	606	-	-	X	-
6	NO3	D	604	-	-	X	-
6	NO3	D	605	-	-	X	-
6	NO3	D	606	-	-	X	-
7	3CJ	A	607	-	X	X	-
7	3CJ	B	607	-	-	X	-
7	3CJ	C	607	-	-	X	-
7	3CJ	D	607	-	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.



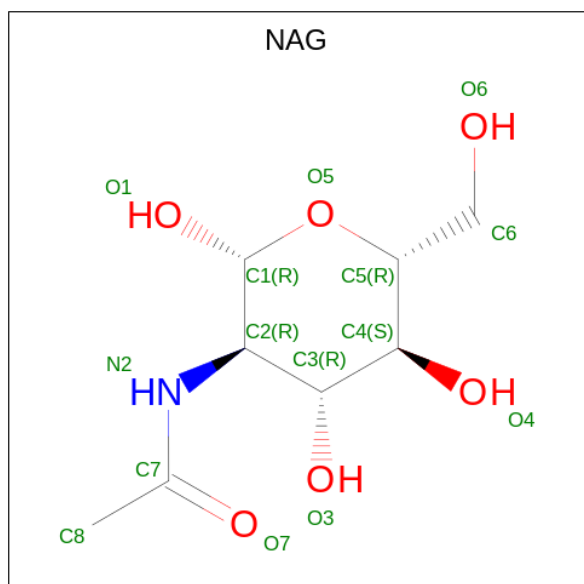
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	G	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	H	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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 (CCD ID: 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 (CCD ID: CA) (formula: Ca).

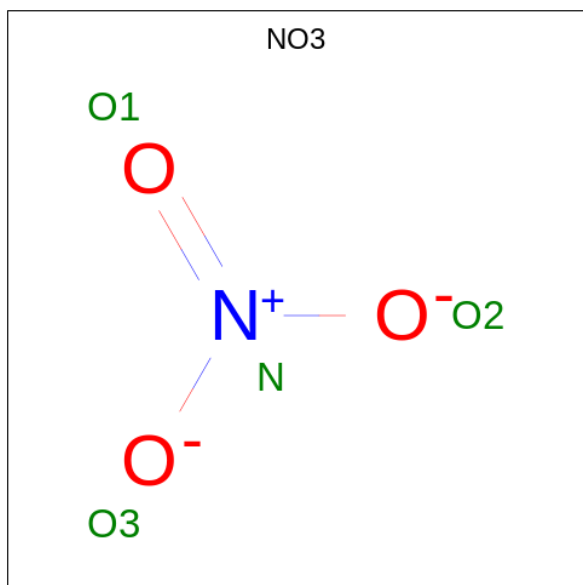
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

Continued on next page...

Continued from previous page...

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

- Molecule 6 is NITRATE ION (CCD ID: NO3) (formula: NO₃).



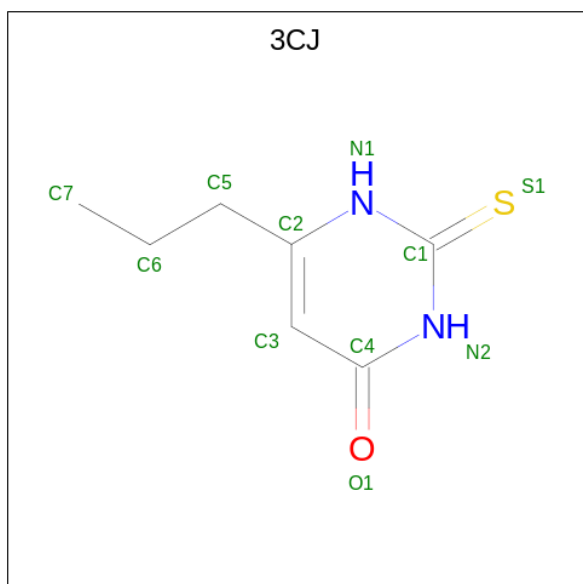
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	N	O	0	0
			4	1	3		
6	A	1	Total	N	O	0	0
			4	1	3		
6	A	1	Total	N	O	0	0
			4	1	3		
6	B	1	Total	N	O	0	0
			4	1	3		
6	B	1	Total	N	O	0	0
			4	1	3		
6	B	1	Total	N	O	0	0
			4	1	3		
6	C	1	Total	N	O	0	0
			4	1	3		
6	C	1	Total	N	O	0	0
			4	1	3		

Continued on next page...

Continued from previous page...

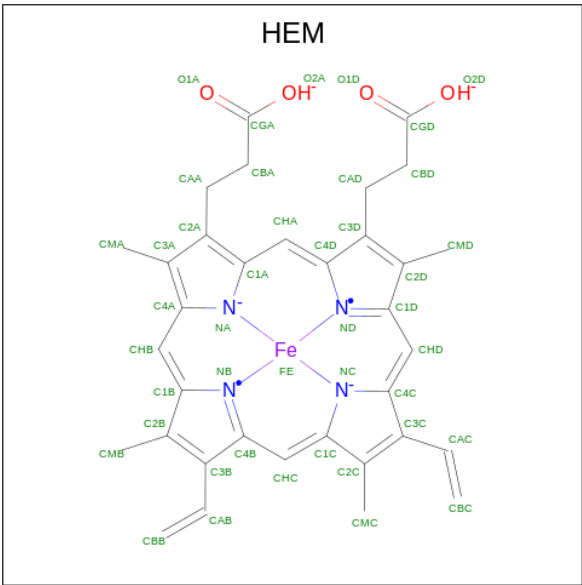
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	C	1	Total	N	O	0	0
			4	1	3		
6	D	1	Total	N	O	0	0
			4	1	3		
6	D	1	Total	N	O	0	0
			4	1	3		
6	D	1	Total	N	O	0	0
			4	1	3		

- Molecule 7 is 6-propyl-2-thioxo-2,3-dihydropyrimidin-4(1H)-one (CCD ID: 3CJ) (formula: $C_7H_{10}N_2OS$).



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 (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

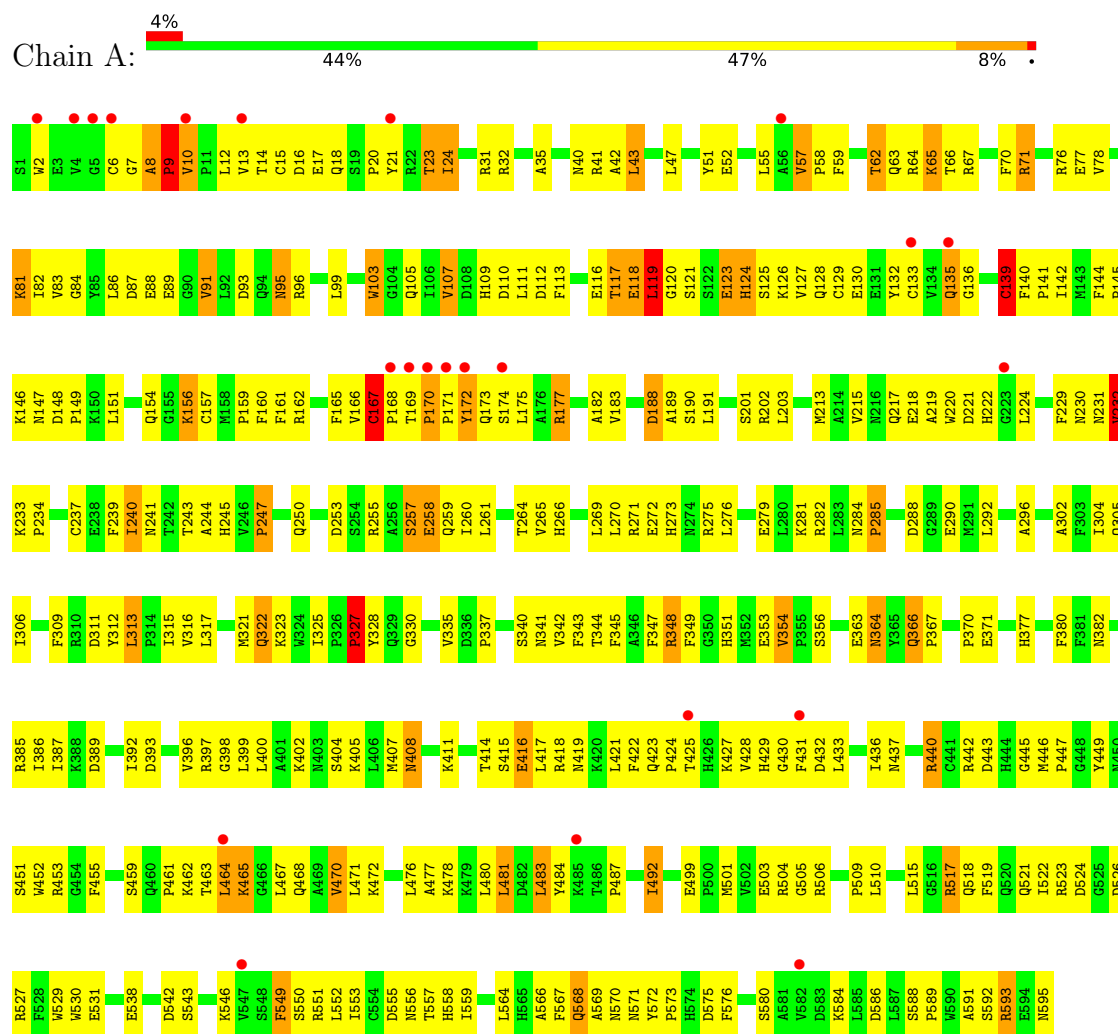
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	158	Total	O	0	0
			158	158		
9	B	157	Total	O	0	0
			157	157		
9	C	168	Total	O	0	0
			168	168		
9	D	168	Total	O	0	0
			168	168		

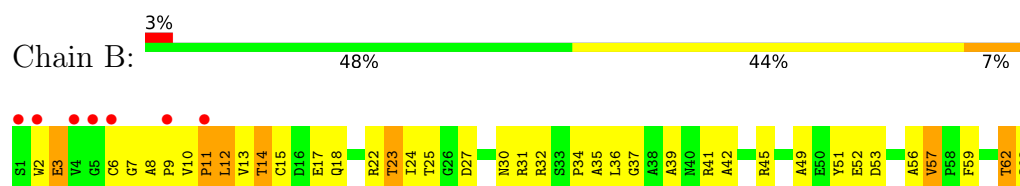
3 Residue-property plots

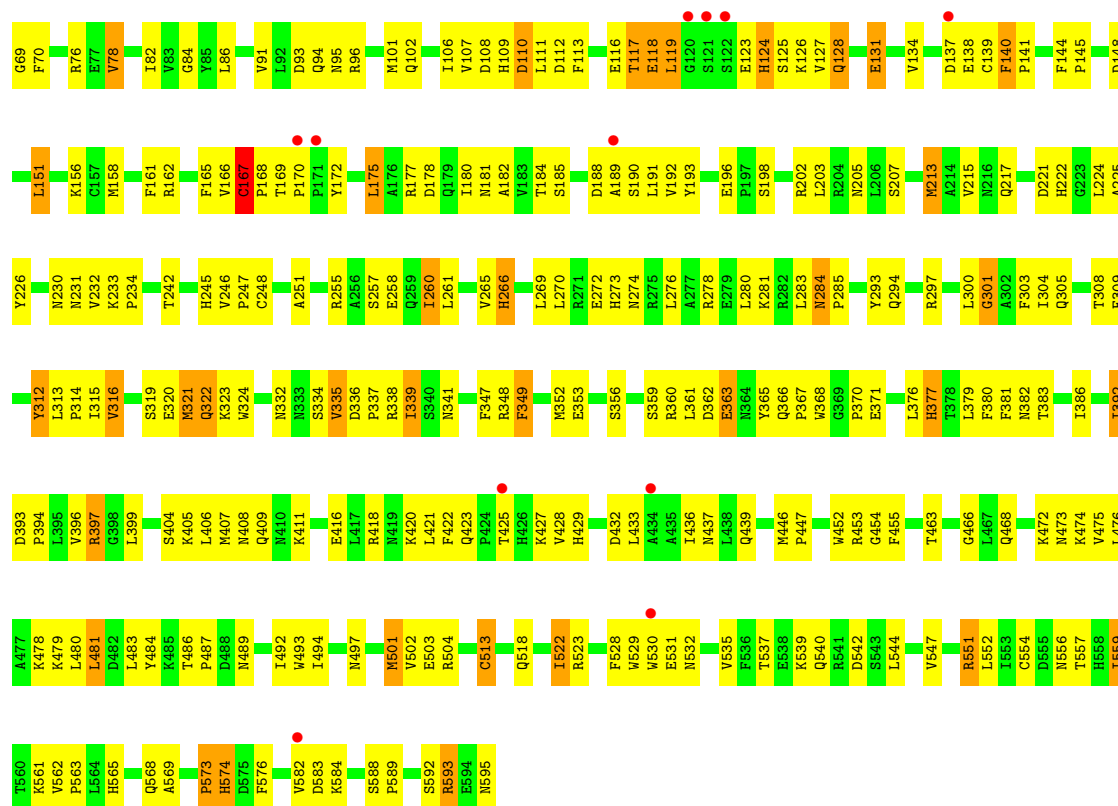
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Lactoperoxidase

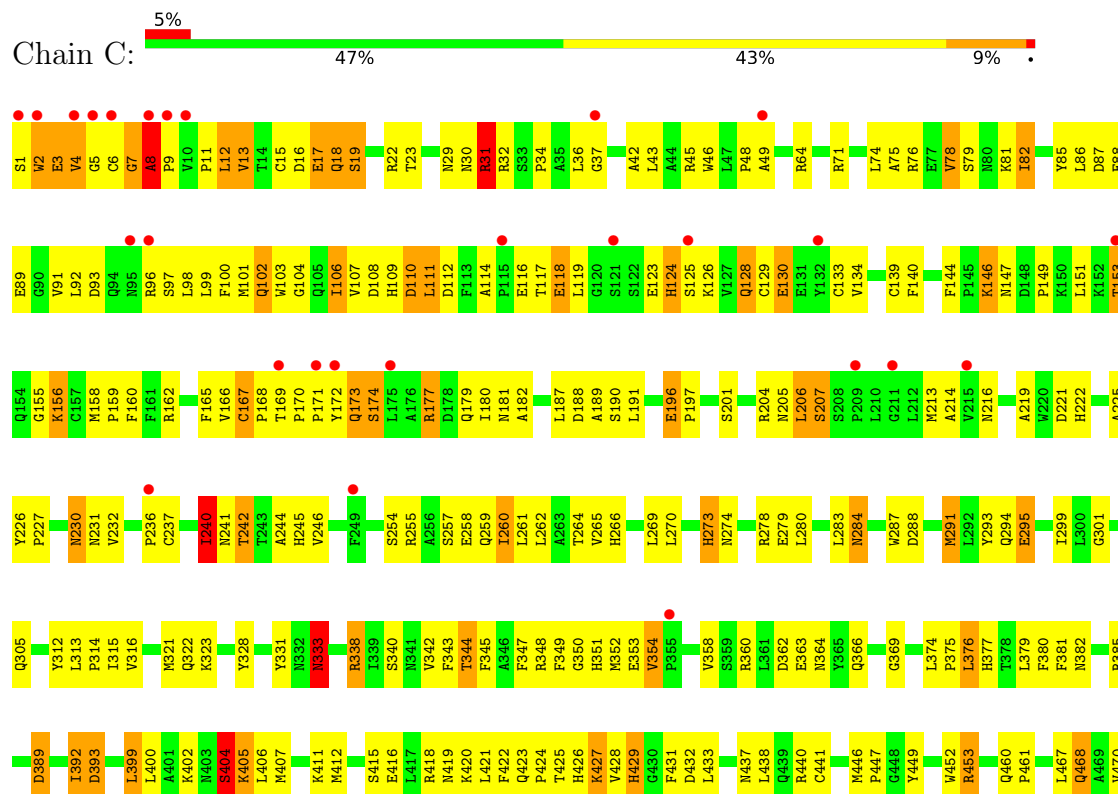


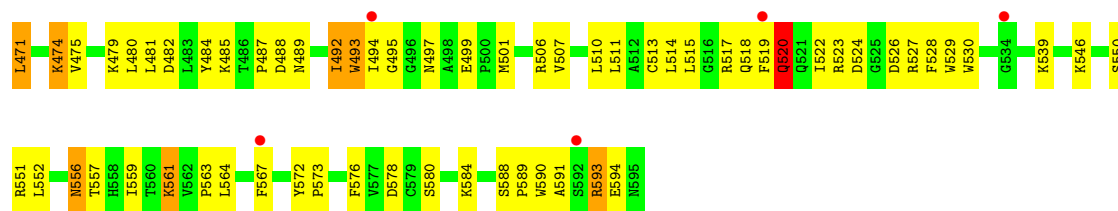
• Molecule 1: Lactoperoxidase



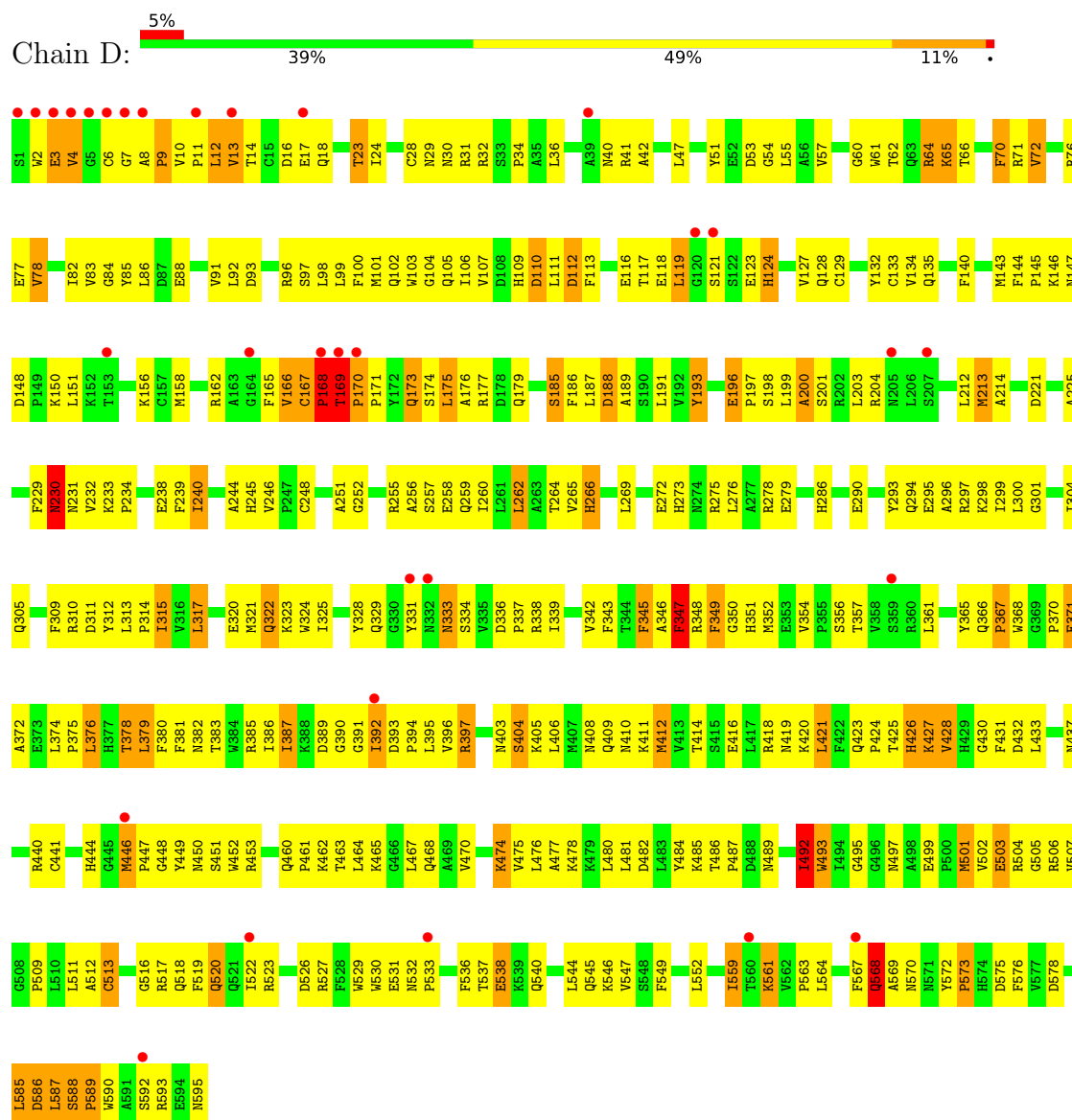


• Molecule 1: Lactoperoxidase





● 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

Chain G:  50% 50%

MAG1
MAG2

- 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 42.50 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.7 (42.50-2.50) 91.7 (42.50-2.50)	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	3683 reflections (4.63%)	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 , 43.0	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: NAG, HEM, NO3, 3CJ, CA

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	0.68	5/4882 (0.1%)	1.22	59/6632 (0.9%)
1	B	0.62	2/4882 (0.0%)	1.19	48/6632 (0.7%)
1	C	0.68	6/4882 (0.1%)	1.19	56/6632 (0.8%)
1	D	0.63	1/4882 (0.0%)	1.23	66/6632 (1.0%)
All	All	0.66	14/19528 (0.1%)	1.21	229/26528 (0.9%)

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	10	VAL	C-N	14.32	1.52	1.34
1	C	31	ARG	CA-C	-11.34	1.38	1.52
1	C	31	ARG	C-N	-8.94	1.22	1.33
1	C	240	ILE	C-N	7.17	1.43	1.33
1	B	107	VAL	C-O	-6.59	1.16	1.24
1	C	8	ALA	C-N	6.02	1.41	1.34
1	A	170	PRO	C-N	5.74	1.41	1.33
1	A	107	VAL	C-O	-5.71	1.17	1.24
1	A	440	ARG	C-O	-5.58	1.17	1.24
1	A	171	PRO	N-CD	5.46	1.55	1.47
1	D	168	PRO	N-CD	5.21	1.55	1.47
1	C	9	PRO	N-CD	5.10	1.54	1.47
1	C	405	LYS	C-O	-5.08	1.17	1.24
1	B	551	ARG	C-O	-5.00	1.18	1.24

All (229) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	349	PHE	N-CA-C	-13.77	96.49	113.28
1	D	4	VAL	N-CA-C	-10.88	102.45	111.81
1	D	111	LEU	N-CA-C	10.67	122.49	111.07

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	124	HIS	N-CA-C	-10.53	100.54	113.50
1	A	492	ILE	N-CA-C	10.44	121.32	110.36
1	C	349	PHE	N-CA-C	-10.34	100.06	112.89
1	C	392	ILE	N-CA-C	10.15	120.17	110.42
1	B	111	LEU	N-CA-C	10.11	122.06	111.14
1	C	206	LEU	N-CA-C	9.96	123.38	111.33
1	A	111	LEU	N-CA-C	9.79	122.03	111.36
1	D	349	PHE	N-CA-C	-9.62	100.80	112.54
1	D	128	GLN	N-CA-C	-9.45	101.18	112.89
1	B	427	LYS	N-CA-C	9.43	121.16	111.07
1	C	428	VAL	N-CA-C	9.35	122.45	109.45
1	A	57	VAL	N-CA-C	9.08	117.94	107.77
1	A	316	VAL	N-CA-C	-9.04	102.03	110.53
1	B	124	HIS	N-CA-C	-8.83	101.58	111.82
1	C	118	GLU	N-CA-C	-8.74	101.71	114.39
1	A	62	THR	N-CA-C	8.71	120.85	111.36
1	B	312	TYR	N-CA-C	8.50	120.33	111.14
1	D	121	SER	N-CA-C	-8.38	103.07	113.38
1	B	316	VAL	N-CA-C	-8.38	102.69	110.82
1	B	349	PHE	N-CA-C	-8.31	102.19	111.82
1	B	428	VAL	N-CA-C	8.09	121.90	109.12
1	D	225	ALA	N-CA-C	8.08	121.46	110.55
1	B	392	ILE	N-CA-C	8.05	118.14	110.42
1	C	31	ARG	O-C-N	7.92	130.65	122.09
1	B	225	ALA	N-CA-C	7.91	121.23	110.55
1	B	7	GLY	N-CA-C	7.88	122.26	111.54
1	D	23	THR	N-CA-C	-7.87	100.38	110.53
1	D	392	ILE	N-CA-C	7.83	118.63	110.72
1	D	412	MET	N-CA-C	7.66	120.74	111.40
1	D	171	PRO	N-CA-C	7.58	124.28	111.32
1	C	389	ASP	N-CA-C	7.52	120.91	108.49
1	C	111	LEU	N-CA-C	7.48	120.15	111.02
1	C	333	ASN	N-CA-C	7.47	122.24	113.20
1	D	168	PRO	CA-C-N	7.46	128.94	120.06
1	D	168	PRO	C-N-CA	7.46	128.94	120.06
1	D	196	GLU	N-CA-C	-7.45	100.03	110.31
1	C	196	GLU	CA-C-N	7.35	126.61	118.97
1	C	196	GLU	C-N-CA	7.35	126.61	118.97
1	D	588	SER	N-CA-C	7.35	122.16	112.17
1	A	231	ASN	N-CA-C	7.28	120.08	111.71
1	A	110	ASP	N-CA-C	-7.24	103.46	111.36
1	A	451	SER	N-CA-C	-7.20	103.47	111.82

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	345	PHE	N-CA-C	-7.17	104.68	113.50
1	C	7	GLY	N-CA-C	7.15	122.20	111.18
1	A	366	GLN	N-CA-C	-7.15	101.73	110.31
1	A	463	THR	N-CA-C	7.07	120.93	110.46
1	B	156	LYS	N-CA-C	7.07	120.39	111.69
1	D	379	LEU	N-CA-C	7.06	120.84	112.93
1	D	520	GLN	N-CA-C	-7.03	103.70	111.36
1	C	31	ARG	N-CA-C	7.03	118.73	111.14
1	D	256	ALA	N-CA-C	7.01	119.81	111.33
1	D	112	ASP	N-CA-C	7.00	118.82	108.60
1	C	230	ASN	N-CA-C	-6.95	100.16	110.23
1	A	465	LYS	N-CA-C	-6.93	103.49	112.23
1	A	453	ARG	N-CA-C	-6.89	103.70	111.14
1	A	440	ARG	N-CA-C	6.86	118.55	111.14
1	D	31	ARG	N-CA-C	6.84	119.74	111.40
1	A	476	LEU	N-CA-C	-6.83	103.91	111.36
1	D	390	GLY	N-CA-C	6.78	123.15	115.08
1	B	501	MET	N-CA-C	6.76	120.03	110.50
1	D	110	ASP	N-CA-C	-6.74	103.86	111.07
1	D	397	ARG	N-CA-C	-6.73	103.94	111.28
1	D	166	VAL	N-CA-C	6.70	117.78	110.21
1	D	230	ASN	N-CA-C	-6.69	99.63	110.20
1	A	188	ASP	N-CA-C	6.66	121.05	112.26
1	B	397	ARG	N-CA-C	-6.64	104.11	111.82
1	A	170	PRO	CA-C-N	-6.64	113.15	119.85
1	A	170	PRO	C-N-CA	-6.64	113.15	119.85
1	A	404	SER	N-CA-C	-6.61	100.18	110.17
1	C	354	VAL	CA-C-N	6.59	127.04	120.52
1	C	354	VAL	C-N-CA	6.59	127.04	120.52
1	C	225	ALA	N-CA-C	6.58	121.02	109.96
1	C	429	HIS	N-CA-C	-6.57	102.55	111.55
1	A	123	GLU	N-CA-C	6.56	119.59	108.90
1	B	335	VAL	N-CA-C	6.53	118.57	109.55
1	D	428	VAL	N-CA-C	6.52	118.80	108.89
1	C	34	PRO	N-CA-C	6.51	124.05	114.80
1	C	420	LYS	N-CA-C	6.48	120.50	112.59
1	B	110	ASP	N-CA-C	-6.46	103.86	111.03
1	B	475	VAL	N-CA-C	6.46	117.21	110.62
1	A	43	LEU	N-CA-C	-6.44	102.03	110.53
1	D	238	GLU	N-CA-C	-6.43	105.08	113.12
1	D	200	ALA	N-CA-C	-6.37	104.42	111.36
1	A	125	SER	N-CA-C	-6.37	104.61	112.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	339	ILE	N-CA-C	-6.37	100.55	109.21
1	C	130	GLU	N-CA-C	6.34	117.86	111.07
1	C	87	ASP	N-CA-C	6.33	118.60	108.41
1	C	182	ALA	N-CA-C	6.31	120.44	112.87
1	B	502	VAL	N-CA-C	-6.29	100.87	109.55
1	A	81	LYS	N-CA-C	6.29	119.11	111.82
1	A	191	LEU	N-CA-C	-6.28	105.26	113.17
1	A	23	THR	N-CA-C	-6.26	102.43	110.19
1	A	257	SER	N-CA-C	6.26	119.85	112.72
1	D	193	TYR	N-CA-C	6.25	119.08	111.82
1	B	301	GLY	N-CA-C	-6.23	104.95	112.49
1	C	19	SER	CA-C-N	6.22	127.17	120.83
1	C	19	SER	C-N-CA	6.22	127.17	120.83
1	B	108	ASP	N-CA-C	-6.20	104.58	111.71
1	B	429	HIS	N-CA-C	-6.19	97.80	108.56
1	D	83	VAL	N-CA-C	6.18	117.74	111.00
1	D	451	SER	N-CA-C	-6.18	104.55	111.28
1	D	378	THR	N-CA-C	-6.17	104.45	112.23
1	B	131	GLU	N-CA-C	6.16	117.66	111.07
1	B	453	ARG	N-CA-C	-6.10	104.63	111.28
1	A	447	PRO	N-CA-C	-6.08	102.29	111.41
1	A	556	ASN	N-CA-C	6.07	120.42	111.87
1	A	429	HIS	N-CA-C	-6.03	102.30	110.68
1	B	82	ILE	N-CA-C	6.02	116.38	111.62
1	D	453	ARG	N-CA-C	-6.00	104.74	111.28
1	B	319	SER	N-CA-C	5.98	119.41	111.75
1	C	257	SER	N-CA-C	5.97	120.56	113.16
1	D	173	GLN	N-CA-C	5.96	117.98	107.61
1	D	169	THR	CA-C-N	5.96	126.51	120.38
1	D	169	THR	C-N-CA	5.96	126.51	120.38
1	B	266	HIS	N-CA-C	-5.94	104.89	111.36
1	D	188	ASP	N-CA-C	5.94	119.83	112.59
1	D	404	SER	N-CA-C	-5.93	101.99	110.59
1	A	117	THR	N-CA-C	5.92	118.38	108.96
1	B	213	MET	N-CA-C	-5.91	100.86	110.20
1	D	107	VAL	N-CA-C	-5.90	104.88	110.42
1	D	294	GLN	N-CA-C	5.88	117.49	111.14
1	D	593	ARG	N-CA-C	5.83	118.46	109.07
1	B	284	ASN	CA-C-N	5.83	125.52	119.05
1	B	284	ASN	C-N-CA	5.83	125.52	119.05
1	A	83	VAL	N-CA-C	5.82	117.75	111.58
1	A	232	VAL	N-CA-C	5.80	117.52	109.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	TYR	N-CA-C	5.80	117.42	109.18
1	B	539	LYS	N-CA-C	-5.80	104.87	111.07
1	D	140	PHE	CA-C-N	5.79	127.08	119.84
1	D	140	PHE	C-N-CA	5.79	127.08	119.84
1	C	488	ASP	N-CA-C	-5.78	104.94	112.23
1	A	182	ALA	N-CA-C	5.78	119.43	112.38
1	C	313	LEU	N-CA-C	5.78	120.76	113.25
1	A	119	LEU	CB-CA-C	-5.76	109.95	116.63
1	C	468	GLN	N-CA-C	-5.76	105.14	111.82
1	B	11	PRO	N-CA-C	-5.73	103.19	111.22
1	C	79	SER	N-CA-C	-5.71	104.97	111.14
1	D	311	ASP	N-CA-C	5.71	120.30	111.56
1	C	369	GLY	CA-C-N	5.71	126.97	119.84
1	C	369	GLY	C-N-CA	5.71	126.97	119.84
1	B	309	PHE	N-CA-C	5.68	119.38	112.23
1	B	420	LYS	N-CA-C	5.67	118.98	112.57
1	C	453	ARG	N-CA-C	-5.67	105.10	111.28
1	A	247	PRO	N-CA-C	5.65	119.13	111.22
1	A	446	MET	N-CA-C	5.65	116.81	109.64
1	C	404	SER	N-CA-C	-5.63	103.26	110.53
1	C	123	GLU	N-CA-C	5.63	118.41	110.14
1	C	556	ASN	N-CA-C	5.62	120.13	112.88
1	B	57	VAL	N-CA-C	5.62	113.43	107.76
1	B	82	ILE	CB-CA-C	-5.61	106.06	111.05
1	D	72	VAL	CB-CA-C	-5.61	105.72	110.94
1	D	317	LEU	N-CA-C	5.61	117.48	111.36
1	C	427	LYS	N-CA-C	5.60	118.31	111.82
1	C	520	GLN	N-CA-C	-5.57	105.30	111.71
1	D	42	ALA	N-CA-C	5.56	118.38	110.10
1	A	330	GLY	N-CA-C	5.54	117.21	111.95
1	C	23	THR	N-CA-C	-5.53	102.57	110.59
1	C	114	ALA	CA-C-N	5.53	125.48	119.78
1	C	114	ALA	C-N-CA	5.53	125.48	119.78
1	B	404	SER	N-CA-C	-5.53	102.58	110.59
1	C	482	ASP	N-CA-C	-5.53	105.16	111.07
1	B	552	LEU	N-CA-C	-5.50	105.28	111.28
1	D	426	HIS	N-CA-C	-5.50	100.94	109.24
1	B	112	ASP	N-CA-C	5.49	117.15	108.96
1	A	470	VAL	N-CA-C	5.47	117.93	111.09
1	D	393	ASP	N-CA-C	5.47	120.37	113.25
1	A	118	GLU	N-CA-C	-5.46	106.47	114.39
1	C	110	ASP	N-CA-C	-5.45	104.37	111.02

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	484	TYR	N-CA-C	-5.45	100.23	108.67
1	A	296	ALA	N-CA-C	-5.44	105.25	111.07
1	D	266	HIS	N-CA-C	-5.43	105.44	111.36
1	A	139	CYS	N-CA-C	-5.43	101.62	110.20
1	A	282	ARG	N-CA-C	-5.43	105.00	111.03
1	A	549	PHE	N-CA-C	-5.43	105.36	111.28
1	D	559	ILE	N-CA-C	-5.43	101.73	108.89
1	A	243	THR	N-CA-C	-5.42	105.06	110.97
1	D	568	GLN	N-CA-C	5.38	118.16	110.68
1	A	156	LYS	N-CA-C	5.38	119.15	112.59
1	C	447	PRO	N-CA-C	-5.37	102.80	111.77
1	C	8	ALA	CA-C-N	-5.36	113.01	118.85
1	C	8	ALA	C-N-CA	-5.36	113.01	118.85
1	C	338	ARG	N-CA-C	5.36	117.85	110.35
1	D	124	HIS	N-CA-C	5.34	119.65	113.18
1	A	313	LEU	N-CA-C	5.33	121.60	109.81
1	D	262	LEU	N-CA-C	-5.33	104.89	111.40
1	C	493	TRP	N-CA-C	5.33	117.09	111.28
1	D	387	ILE	N-CA-C	5.32	115.53	110.42
1	A	364	ASN	N-CA-C	-5.30	105.09	112.30
1	B	377	HIS	N-CA-C	5.30	119.23	112.34
1	A	356	SER	N-CA-C	5.29	117.79	111.71
1	B	386	ILE	CB-CA-C	-5.29	105.56	111.80
1	A	95	ASN	N-CA-C	5.29	117.64	110.88
1	D	492	ILE	N-CA-C	5.28	115.72	110.23
1	A	428	VAL	N-CA-C	5.28	116.58	108.71
1	C	153	THR	N-CA-C	5.28	120.37	113.88
1	C	412	MET	N-CA-C	5.27	119.62	111.56
1	C	112	ASP	N-CA-C	5.26	117.18	109.24
1	A	389	ASP	N-CA-C	5.25	116.46	107.28
1	D	169	THR	C-N-CD	-5.24	103.53	125.00
1	C	393	ASP	N-CA-C	5.22	120.04	113.25
1	A	103	TRP	N-CA-C	-5.22	107.05	113.41
1	C	260	ILE	N-CA-C	5.19	120.14	109.34
1	D	354	VAL	N-CA-C	5.19	114.03	108.95
1	D	493	TRP	N-CA-C	5.18	117.60	111.33
1	D	421	LEU	N-CA-C	-5.17	101.28	109.76
1	D	328	TYR	N-CA-C	5.17	116.68	108.67
1	A	530	TRP	N-CA-C	5.17	118.68	112.38
1	B	476	LEU	N-CA-C	-5.14	105.56	111.07
1	D	495	GLY	N-CA-C	-5.14	106.56	112.73
1	C	471	LEU	N-CA-C	5.14	119.26	112.89

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	THR	N-CA-C	5.13	116.67	108.41
1	C	295	GLU	N-CA-C	-5.11	105.79	112.23
1	D	448	GLY	N-CA-C	5.10	120.40	112.60
1	A	354	VAL	CA-C-N	5.10	126.22	120.66
1	A	354	VAL	C-N-CA	5.10	126.22	120.66
1	B	102	GLN	N-CA-C	5.10	118.65	112.23
1	D	213	MET	N-CA-C	-5.09	101.98	110.17
1	D	427	LYS	N-CA-C	5.08	120.33	113.72
1	A	387	ILE	N-CA-C	5.07	115.22	110.30
1	B	559	ILE	CB-CA-C	-5.07	105.83	111.35
1	C	489	ASN	N-CA-C	5.06	119.17	112.89
1	A	416	GLU	N-CA-C	-5.04	105.30	111.75
1	B	84	GLY	N-CA-C	5.04	118.39	111.54
1	D	416	GLU	N-CA-C	-5.02	105.26	111.33
1	B	140	PHE	CA-C-N	5.00	125.00	119.90
1	B	140	PHE	C-N-CA	5.00	125.00	119.90

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	309	0
1	B	4753	0	4646	246	0
1	C	4753	0	4649	327	0
1	D	4753	0	4647	312	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	1	0
4	C	28	0	26	0	0
4	D	28	0	26	1	0
5	A	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	2	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	158	0	0	15	0
9	B	157	0	0	10	0
9	C	168	0	0	20	0
9	D	168	0	0	11	0
All	All	20141	0	18939	1217	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 32.

All (1217) 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:608: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:608: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:607:3CJ:H5	8:D:608: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:731:HOH:O	1.59	1.00
1:D:342:VAL:HB	1:D:446:MET:HE1	1.42	1.00
1:D:169:THR:CB	1:D:170:PRO:HD3	1.88	0.99
1:A:402:LYS:HD2	6:A:605: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:607:3CJ:H2	8:C:608: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
1:D:258:GLU:OE2	8:D:608: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:HG12	1:B:13:VAL:O	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:605: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:HH11	1:C:418:ARG:HG2	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:606:NO3:O2	2.30	0.84
1:C:421:LEU:HG	9:C:731: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:608:HEM:C2B	2.32	0.83
1:D:342:VAL:CB	1:D:446:MET:HE1	2.08	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:605: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:607:3CJ:C6	8:D:608:HEM:HAA1	2.12	0.79
1:D:333:ASN:HD22	1:D:333:ASN:H	1.29	0.79
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:803: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:607:3CJ:C6	8:C:608:HEM:HAA1	2.14	0.77
1:A:169:THR:H	1:A:170:PRO:CD	1.95	0.77

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:96:ARG:NH1	1:C:506:ARG:CG	2.49	0.76
1:C:125:SER:HA	1:C:128:GLN:HB3	1.67	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:606:NO3:O3	1.69	0.75
1:D:322:GLN:CD	1:D:322:GLN:H	1.91	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:H62	2:E:2:NAG:O3	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:607:3CJ:H5	8:C:608:HEM:HAA1	1.70	0.74
1:C:159:PRO:HD2	1:C:431:PHE:HE1	1.50	0.73
1:C:96:ARG:HH21	1:C:406:LEU:HD12	1.51	0.73
1:C:348:ARG:HB2	1:C:493:TRP:CD1	2.23	0.73
1:D:113:PHE:CE1	7:D:607:3CJ: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
1:C:170:PRO:HA	9:C:818:HOH:O	1.89	0.73
1:B:409:GLN:NE2	1:B:473:ASN:HD22	1.87	0.72
1:C:98:LEU:HD11	1:C:101:MET:HE2	1.69	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:606:HEM:HMB1	8:B:606:HEM:HBB2	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:66:THR:HB	1:A:70:PHE:C	2.13	0.72
1:A:239:PHE:HZ	1:A:427:LYS:HB3	1.55	0.72
1:C:530:TRP:NE1	6:C:604:NO3:O2	2.22	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2:TRP:CZ2	1:C:86:LEU:HD22	2.25	0.71
7:A:607:3CJ:H7	8:A:608:HEM:HBD2	1.73	0.71
1:C:528:PHE:HB3	9:C:836:HOH:O	1.89	0.71
1:C:452:TRP:CH2	6:C:606:NO3:O3	2.44	0.71
1:D:7:GLY:C	1:D:9:PRO:HD3	2.14	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:607:3CJ:S1	2.32	0.70
7:A:607:3CJ:H3	8:A:608: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: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:42:ALA:HB2	1:B:166:VAL:CG1	2.21	0.69
1:B:421:LEU:HD12	1:B:422:PHE:H	1.57	0.69
1:D:530:TRP:HZ2	6:D:606:NO3:O2	1.72	0.69
1:C:517:ARG:NH2	1:C:517:ARG:HB3	2.07	0.69
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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:D:352:MET:HE1	1:D:412:MET:HE3	1.76	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:A:88:GLU:O	1:A:91:VAL:HG22	1.93	0.67
8:B:606:HEM:O1D	7:B:607:3CJ: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:607:3CJ:H5	2.30	0.67
8:B:606:HEM:HH A	7:B:607:3CJ: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:606: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:HG2	1:C:418:ARG:NH1	2.02	0.67
1:D:350:GLY:HA3	8:D:608:HEM:CBC	2.25	0.67
1:C:159:PRO:HD2	1:C:431:PHE:CE1	2.29	0.66
1:C:316:VAL:O	1:C:507:VAL:HG22	1.95	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:113:PHE:CE1	7:B:607:3CJ:H5	2.30	0.66
1:B:280:LEU:O	1:B:284:ASN:N	2.28	0.66
1:C:76:ARG:NH1	1:C:418:ARG:HH12	1.94	0.66
1:C:146:LYS:NZ	1:C:147:ASN:HD21	1.93	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:B:446:MET:HE1	6:B:603:NO3:O1	1.96	0.66
1:C:287:TRP:HA	9:C:746: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:606: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:D:101:MET:SD	1:D:101:MET:C	2.79	0.65
1:C:348:ARG:HB2	1:C:493:TRP:HE1	1.58	0.65
1:D:123:GLU:HG3	9:D:803: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:HE21	1:A:322:GLN:N	1.94	0.65
1:A:370:PRO:O	1:D:71:ARG:NH2	2.29	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: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:812: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:HB3	1:A:71:ARG:CZ	2.24	0.65
1:D:105:GLN:NE2	7:D:607:3CJ:S1	2.60	0.65
1:D:463:THR:HB	9:D:714:HOH:O	1.94	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:719: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
1:A:348:ARG:HG2	8:A:608:HEM:C2D	2.33	0.64
1:A:142:ILE:HD12	1:A:160:PHE:HB2	1.77	0.64
1:A:203:LEU:HB3	1:A:213:MET:HE1	1.80	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:608:HEM:O2D	2.16	0.64
1:B:265:VAL:O	1:B:269:LEU:HG	1.98	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:811:HOH:O	1.97	0.63
1:A:546:LYS:HZ1	1:A:586:ASP:H	1.47	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:606:HEM:CHA	7:B:607:3CJ: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:C:314:PRO:HG3	1:C:321:MET:HE2	1.79	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:136:GLY:HA2	1:C:124:HIS:CD2	2.35	0.62
1:A:370:PRO:HG2	1:A:371:GLU:OE1	1.99	0.62
1:D:167:CYS:CB	1:D:168:PRO:CD	2.78	0.62
1:D:425:THR:HG21	9:D:811:HOH:O	2.00	0.62
1:D:191:LEU:H	1:D:191:LEU:HD23	1.63	0.61
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:606:HEM:C1A	7:B:607:3CJ:N1	2.68	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
8:A:608:HEM:HBB2	8:A:608:HEM:HMB1	1.83	0.61
1:B:52:GLU:HG3	1:B:59:PHE:HA	1.81	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:313:LEU:HD11	1:A:519:PHE:CG	2.36	0.61
1:A:459:SER:O	1:A:461:PRO:HD3	2.01	0.61
1:D:351:HIS:CD2	8:D:608:HEM:NC	2.69	0.61
1:A:174:SER:O	1:A:175:LEU:HG	2.01	0.61
1:D:203:LEU:HB3	1:D:213:MET:HE1	1.83	0.61
1:D:240:ILE:HD13	1:D:382:ASN:HA	1.82	0.61
1:D:446:MET:HE3	6:D:604:NO3:O1	2.00	0.61
1:B:35:ALA:HB1	1:B:41:ARG:NE	2.16	0.61
1:D:9:PRO:HG2	1:D:41:ARG:HH22	1.66	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:A:62:THR:HG21	1:A:65:LYS:H	1.66	0.61
1:A:105:GLN:HB2	8:A:608:HEM:C2C	2.36	0.61
1:D:113:PHE:HE1	7:D:607:3CJ:H6	1.66	0.61
1:D:314:PRO:HG3	1:D:321:MET:HE2	1.82	0.61
1:D:325:ILE:HG22	1:D:325:ILE:O	2.01	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:O	1:B:13:VAL:CG1	2.49	0.60
1:B:110:ASP:OD2	1:B:189:ALA:HA	2.02	0.60
1:C:1:SER:C	1:C:2:TRP:CE3	2.80	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:607:3CJ:H4	8:C:608:HEM:HAA1	1.82	0.60
1:D:586:ASP:O	1:D:589:PRO:HD2	2.02	0.60
7:D:607:3CJ:H2	8:D:608: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
1:D:8:ALA:N	1:D:9:PRO:CD	2.65	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:348:ARG:NH1	1:D:437:ASN:ND2	2.47	0.59
1:A:342:VAL:HG11	1:A:452:TRP:CH2	2.37	0.59
1:A:396:VAL:HA	1:A:399:LEU:HD12	1.84	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
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:HG22	1:D:425:THR:O	2.02	0.59
1:A:229:PHE:CD1	1:A:247:PRO:HG2	2.38	0.59
1:C:97:SER:O	1:C:98:LEU:C	2.46	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
1:A:99:LEU:HG	1:A:567:PHE:CE1	2.38	0.59
1:A:325:ILE:HG22	1:A:325:ILE:O	2.02	0.59
8:A:608:HEM:HBC2	8:A:608:HEM:HMC2	1.85	0.59
1:C:557:THR:OG1	1:C:559:ILE:HG12	2.02	0.59
1:D:342:VAL:CA	1:D:446:MET:HE1	2.32	0.58
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:96:ARG:HG3	1:D:506:ARG:HE	1.68	0.58
1:D:106:ILE:HG23	1:D:191:LEU:CD1	2.33	0.58
1:A:9:PRO:HB2	1:A:41:ARG:NH2	2.18	0.58
1:C:1:SER:C	1:C:2:TRP:HE3	2.10	0.58
1:C:99:LEU:HA	1:C:399:LEU:HD22	1.85	0.58
1:D:9:PRO:HG2	1:D:41:ARG:NH2	2.19	0.58
1:D:117:THR:HG22	1:D:162:ARG:O	2.04	0.58
1:A:146:LYS:O	1:A:147:ASN:HB2	2.04	0.58
1:A:408:ASN:OD1	1:A:408:ASN:C	2.46	0.58
1:A:348:ARG:HG2	8:A:608:HEM:C3D	2.39	0.58
1:C:98:LEU:CD1	1:C:101:MET:HE2	2.32	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:66:THR:HB	1:A:70:PHE:O	2.03	0.58
1:A:504:ARG:HD3	9:A:829:HOH:O	2.02	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

Continued on next page...

Continued from previous page...

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:C:551:ARG:O	1:C:552:LEU:C	2.45	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:838: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:C:2:TRP:CE3	1:C:2:TRP:N	2.73	0.57
1:C:196:GLU:HB3	9:C:707:HOH:O	2.03	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:820: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:608:HEM:O1A	2.38	0.57
1:B:144:PHE:HE1	1:B:158:MET:HE3	1.68	0.57
8:C:608:HEM:HMB2	8:C:608:HEM:HBB2	1.85	0.57
1:D:421:LEU:HD22	1:D:433:LEU:HB2	1.86	0.57
1:D:133:CYS:O	1:D:143:MET:HE1	2.04	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: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:607:3CJ:C5	8:A:608: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:B:10:VAL:CG2	1:B:41:ARG:HH12	2.16	0.56
1:C:81:LYS:HB3	9:C:817:HOH:O	2.03	0.56
1:C:168:PRO:HB2	1:C:170:PRO:HD2	1.87	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:275:ARG:HD2	1:A:555:ASP:HB3	1.88	0.56
1:A:62:THR:CG2	1:A:65:LYS:N	2.69	0.56
1:A:281:LYS:HD2	1:A:285:PRO:HA	1.87	0.56
1:A:189:ALA:HB2	1:A:304:ILE:HD12	1.87	0.56
1:C:146:LYS:HE3	1:C:147:ASN:CG	2.30	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:745:HOH:O	2.06	0.56
1:B:193:TYR:CE2	1:B:297:ARG:HG3	2.41	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:D:349:PHE:CD1	1:D:349:PHE:C	2.84	0.55
1:A:393:ASP:OD2	1:A:558:HIS:HB2	2.06	0.55
1:B:347:PHE:HB3	8:B:606:HEM:HMD2	1.86	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: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:A:109:HIS:NE2	7:A:607:3CJ:C1	2.70	0.55
1:D:113:PHE:CD1	7:D:607:3CJ:H6	2.41	0.55
1:D:199:LEU:O	1:D:203:LEU:HG	2.06	0.55
1:B:321:MET:C	1:B:323:LYS:H	2.13	0.55
1:B:341:ASN:HB3	1:B:446:MET:HE1	1.88	0.55
1:D:146:LYS:O	1:D:147:ASN:HB2	2.06	0.55
1:B:113:PHE:HE1	7:B:607:3CJ: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:715:HOH:O	2.07	0.55
1:D:221:ASP:C	1:D:221:ASP:OD1	2.50	0.55
7:D:607:3CJ:H7	8:D:608: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:425:THR:HG22	1:B:425:THR:O	2.05	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
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:96:ARG:CZ	1:C:506:ARG:CD	2.85	0.54
1:C:342:VAL:HG21	1:C:452:TRP:CE2	2.42	0.54
1:D:97:SER:O	1:D:404:SER:OG	2.26	0.54
1:D:544:LEU:O	1:D:547:VAL:HG22	2.07	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:D:346:ALA:C	1:D:348:ARG:H	2.16	0.54
1:B:593:ARG:HG3	1:B:595:ASN:H	1.72	0.54
1:D:502:VAL:O	1:D:503:GLU:C	2.50	0.54
8:B:606:HEM:HBC2	8:B:606:HEM:HMC2	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:C:363:GLU:H	1:C:363:GLU:CD	2.15	0.54
1:D:96:ARG:NH2	1:D:315:ILE:HB	2.23	0.54
1:D:9:PRO:CG	1:D:41:ARG:NH2	2.71	0.54
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:96:ARG:CZ	1:D:315:ILE:HB	2.38	0.53
1:D:193:TYR:OH	1:D:297:ARG:HA	2.07	0.53
1:C:82:ILE:HD12	1:C:480:LEU:HD23	1.91	0.53
1:D:9:PRO:HG3	1:D:41:ARG:CZ	2.39	0.53
1:D:103:TRP:O	1:D:106:ILE:N	2.36	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:A:144:PHE:HD2	1:A:156:LYS:C	2.17	0.53
1:C:125:SER:O	1:C:126:LYS:C	2.51	0.53
1:D:214:ALA:HA	4:D:602:NAG:O7	2.08	0.53
1:D:446:MET:CE	6:D:604:NO3:O1	2.56	0.53
1:D:589:PRO:HB2	1:D:590:TRP:CE3	2.43	0.53
1:A:15:CYS:HB3	9:A:747:HOH:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:THR:HG21	1:A:65:LYS:CA	2.37	0.53
1:A:99:LEU:CD2	1:A:566:ALA:HB1	2.39	0.53
1:B:117:THR:CG2	1:B:161:PHE:HB3	2.39	0.53
8:B:606:HEM:CHA	7:B:607:3CJ: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
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:B:137:ASP:CG	1:B:138:GLU:H	2.17	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:C:550:SER:OG	1:C:563:PRO:O	2.26	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:165:PHE:CZ	1:A:169:THR:C	2.87	0.52
1:A:241:ASN:ND2	1:A:244:ALA:HB2	2.24	0.52
1:B:2:TRP:CH2	1:C:86:LEU:HD13	2.31	0.52
1:B:167:CYS:SG	1:B:168:PRO:HD3	2.49	0.52
1:C:97:SER:O	1:C:99:LEU:N	2.42	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: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:29:ASN:HD21	1:C:527:ARG:H	1.57	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:117:THR:HG22	1:C:162:ARG:O	2.09	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
1:B:418:ARG:HG2	1:B:418:ARG:HH11	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:607:3CJ: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:606:HEM:HAA1	7:B:607:3CJ:H4	1.92	0.52
1:C:29:ASN:HD21	1:C:527:ARG:N	2.08	0.52
1:C:221:ASP:O	1:C:222:HIS:C	2.53	0.52
1:D:16:ASP:O	1:D:17:GLU:HB3	2.10	0.52
1:B:341:ASN:OD1	1:B:446:MET:HE3	2.09	0.51
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: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
8:D:608:HEM:HMC2	8:D:608:HEM:HBC2	1.92	0.51
1:A:8:ALA:N	1:A:9:PRO:HD2	2.26	0.51
1:A:233:LYS:HA	1:A:234:PRO:C	2.34	0.51
1:B:363:GLU:N	1:B:363:GLU:CD	2.67	0.51
1:C:75:ALA:HB1	1:C:438:LEU:HB2	1.92	0.51
1:C:287:TRP:CZ3	1:C:295:GLU:HG3	2.45	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:B:66:THR:HB	1:B:70:PHE:C	2.36	0.51
1:C:348:ARG:CB	1:C:493:TRP:NE1	2.68	0.51
1:A:7:GLY:O	1:A:8:ALA:HB3	2.10	0.51
1:A:593:ARG:HD2	1:A:595:ASN:H	1.75	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:313:LEU:O	1:D:314:PRO:C	2.54	0.51
1:D:349:PHE:CD1	1:D:350:GLY:N	2.78	0.51
1:A:9:PRO:O	1:A:10:VAL:C	2.52	0.51
1:B:56:ALA:O	1:B:162:ARG:NH1	2.40	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
1:D:474:LYS:NZ	1:D:474:LYS:HB3	2.26	0.50
1:A:166:VAL:C	1:A:167:CYS:SG	2.94	0.50
1:B:93:ASP:CG	1:B:96:ARG:HB2	2.36	0.50
1:A:245:HIS:O	1:A:245:HIS:CG	2.65	0.50
1:B:78:VAL:HA	1:B:483:LEU:HD13	1.93	0.50
1:B:409:GLN:NE2	1:B:473:ASN:ND2	2.59	0.50
1:C:358:VAL:HB	1:C:379:LEU:CD1	2.41	0.50
1:C:415:SER:HB2	9:C:797:HOH:O	2.11	0.50
1:D:167:CYS:HB2	1:D:168:PRO:HD2	1.91	0.50
1:D:346:ALA:C	1:D:348:ARG:N	2.68	0.50
1:A:312:TYR:O	1:A:315:ILE:HG12	2.12	0.50
1:D:169:THR:HB	1:D:170:PRO:CD	2.22	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:607:3CJ: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:B:454:GLY:O	1:B:455:PHE:C	2.55	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:603:NO3:O1	2.12	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:607:3CJ:S1	8:C:608:HEM:ND	2.85	0.49
1:D:84:GLY:HA2	9:D:775:HOH:O	2.11	0.49
1:A:63:GLN:O	1:A:63:GLN:HG3	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
1:A:31:ARG:NH2	1:A:527:ARG:NH1	2.61	0.49
1:A:442:ARG:O	1:A:443:ASP:C	2.53	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: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:A:347:PHE:CE1	8:A:608:HEM:HBC1	2.48	0.49
1:C:124:HIS:O	1:C:125:SER:C	2.54	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:188:ASP:CG	1:C:190:SER:HB3	2.37	0.49
1:D:62:THR:HB	1:D:65:LYS:HB2	1.95	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: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: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:C:124:HIS:ND1	1:C:124:HIS:C	2.70	0.48
1:D:12:LEU:C	1:D:13:VAL:HG23	2.37	0.48
1:A:62:THR:O	1:A:63:GLN:CB	2.61	0.48
1:A:347:PHE:O	1:A:347:PHE:HD1	1.95	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ARG:NH1	1:A:432:ASP:OD2	2.46	0.48
1:A:503:GLU:O	1:A:504:ARG:HB2	2.13	0.48
1:B:113:PHE:CD1	7:B:607:3CJ:H5	2.48	0.48
1:B:312:TYR:CE2	1:B:316:VAL:HG21	2.48	0.48
1:C:43:LEU:HD12	1:C:179:GLN:HB2	1.95	0.48
1:C:151:LEU:HA	1:C:155:GLY:O	2.13	0.48
1:C:347:PHE:HB3	8:C:608:HEM:HMD3	1.95	0.48
1:D:119:LEU:CD2	1:D:169:THR:CG2	2.91	0.48
1:A:51:TYR:HB3	1:A:57:VAL:O	2.13	0.48
1:A:464:LEU:O	1:A:468:GLN:HG3	2.12	0.48
1:B:8:ALA:HB1	1:B:9:PRO:HD2	1.96	0.48
1:B:10:VAL:HG11	1:B:41:ARG:NH2	2.28	0.48
1:C:22:ARG:CZ	1:C:528:PHE:HB2	2.43	0.48
1:C:180:ILE:HG22	1:C:181:ASN:N	2.29	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:144:PHE:CD2	1:A:156:LYS:C	2.91	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:D:28:CYS:O	1:D:29:ASN:C	2.57	0.48
1:A:58:PRO:HG3	1:A:162:ARG:CZ	2.43	0.48
1:B:140:PHE:CE2	1:B:439:GLN:HG3	2.48	0.48
1:B:213:MET:HB3	1:B:270:LEU:HD11	1.94	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:608:HEM:HBC2	8:A:608:HEM:CMC	2.43	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
1:A:203:LEU:HD13	1:A:213:MET:HE1	1.96	0.48
1:C:528:PHE:O	1:C:529:TRP:C	2.57	0.48
7:C:607:3CJ:S1	8:C:608:HEM:C1D	3.07	0.48
1:D:93:ASP:OD2	1:D:96:ARG:HG3	2.13	0.48
1:D:193:TYR:CZ	1:D:297:ARG:HA	2.49	0.48
1:A:146:LYS:HB3	9:A:821: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:408:ASN:HB3	1:D:411:LYS:HB2	1.95	0.48
1:A:321:MET:HE3	1:A:325:ILE:HB	1.96	0.47
1:B:91:VAL:CG1	1:B:411:LYS:HD3	2.44	0.47
1:B:113:PHE:HB2	1:B:255:ARG:NH2	2.29	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:109:HIS:NE2	7:A:607:3CJ:S1	2.87	0.47
1:A:130:GLU:HG3	1:A:159:PRO:HD3	1.95	0.47
1:B:124:HIS:O	1:B:127:VAL:HB	2.14	0.47
1:A:93:ASP:CG	1:A:96:ARG:HB2	2.39	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:212:LEU:HD21	1:D:278:ARG:HG3	1.95	0.47
1:D:213:MET:HG2	1:D:273:HIS:CD2	2.49	0.47
1:A:52:GLU:HG3	1:A:59:PHE:CD1	2.49	0.47
1:A:571:ASN:O	1:A:575:ASP:HB2	2.15	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:96:ARG:NH2	1:B:315:ILE:O	2.46	0.47
1:B:168:PRO:HG2	1:B:172:TYR:HB3	1.97	0.47
1:C:22:ARG:NH1	1:C:528:PHE:HB2	2.29	0.47
1:C:169:THR:HG22	9:C:734:HOH:O	2.13	0.47
1:C:322:GLN:HG3	9:C:806:HOH:O	2.13	0.47
1:D:264:THR:HG23	1:D:392:ILE:HG23	1.96	0.47
1:A:76:ARG:HH22	1:A:419:ASN:ND2	2.13	0.47
1:A:351:HIS:NE2	1:A:433:LEU:HD21	2.30	0.47
1:A:414:THR:HG22	9:A:721:HOH:O	2.15	0.47
1:B:12:LEU:HD12	1:B:12:LEU:HA	1.79	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: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:C:511:LEU:O	1:C:515:LEU:HG	2.14	0.47
1:D:53:ASP:CG	1:D:57:VAL:HG23	2.40	0.47
1:D:99:LEU:O	1:D:100:PHE:C	2.57	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:814:HOH:O	2.15	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	1:B:433:LEU:HD12	2.15	0.47
1:C:322:GLN:CD	1:C:322:GLN:H	2.23	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:C:529:TRP:O	1:C:530:TRP:C	2.58	0.47
1:A:284:ASN:ND2	1:A:591:ALA:HA	2.30	0.46
1:A:343:PHE:CG	1:A:518:GLN:HG2	2.49	0.46
1:A:464:LEU:HD12	1:A:464:LEU:C	2.40	0.46
7:A:607:3CJ:H7	8:A:608:HEM:CBD	2.41	0.46
1:B:273:HIS:CD2	1:B:274:ASN:OD1	2.61	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
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:343:PHE:CG	1:D:518:GLN:HG2	2.50	0.46
7:D:607:3CJ:C1	8:D:608:HEM:NA	2.78	0.46
1:B:185:SER:HB3	1:B:339:ILE:HG12	1.97	0.46
8:B:606:HEM:HBB2	8:B:606:HEM:CMB	2.44	0.46
1:C:30:ASN:ND2	1:C:333:ASN:HB2	2.30	0.46
1:C:144:PHE:CE1	1:C:158:MET:HG3	2.50	0.46
1:C:572:TYR:HA	1:C:573:PRO:HA	1.62	0.46
1:D:103:TRP:O	1:D:104:GLY:C	2.58	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:62:THR:HG21	1:A:65:LYS:CG	2.43	0.46
1:A:113:PHE:CD1	7:A:607:3CJ:H5	2.50	0.46
1:B:303:PHE:HD2	1:B:304:ILE:HD12	1.80	0.46
1:B:347:PHE:CE1	8:B:606:HEM:HBC1	2.51	0.46
1:B:557:THR:OG1	1:B:559:ILE:HG12	2.15	0.46
1:C:236:PRO:CB	1:C:424:PRO:HB3	2.45	0.46
1:D:255:ARG:HD2	7:D:607:3CJ:C2	2.45	0.46
1:A:71:ARG:NH1	1:A:71:ARG:CB	2.79	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.14	0.46
1:B:31:ARG:O	1:B:32:ARG:C	2.59	0.46
1:C:171:PRO:HD3	9:C:818: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:D:148:ASP:O	1:D:151:LEU:CB	2.64	0.46
1:A:321:MET:C	1:A:323:LYS:H	2.22	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:608:HEM:O2D	2.15	0.46
1:D:336:ASP:OD2	1:D:338:ARG:NH2	2.48	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
1:B:421:LEU:HD22	1:B:433:LEU:HB2	1.97	0.46
1:C:108:ASP:HB2	1:C:347:PHE:CE2	2.50	0.46
1:C:294:GLN:HA	1:C:294:GLN:OE1	2.15	0.46
1:D:251:ALA:O	1:D:252:GLY:C	2.58	0.46
1:D:351:HIS:HD2	8:D:608: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:B:537:THR:HG23	1:B:540:GLN:CD	2.39	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:607:3CJ:H5	8:C:608: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
9:C:849:HOH:O	2:G:1:NAG:H82	2.16	0.45
1:D:7:GLY:C	1:D:9:PRO:CD	2.88	0.45
1:D:561:LYS:HE3	1:D:578:ASP:HA	1.98	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:ASN:O	1:A:430:GLY:HA2	2.17	0.45
1:A:477:ALA:O	1:A:478:LYS:C	2.59	0.45
1:B:257:SER:O	1:B:381:PHE:HA	2.16	0.45
1:B:418:ARG:HG2	1:B:418:ARG:NH1	2.31	0.45
1:C:31:ARG:H	1:C:31:ARG:HG2	1.59	0.45
1:C:149:PRO:C	1:C:151:LEU:N	2.73	0.45
1:C:244:ALA:HB1	1:C:246:VAL:HG23	1.97	0.45
1:C:350:GLY:HA3	8:C:608:HEM:CBC	2.47	0.45
1:D:239:PHE:CZ	1:D:427:LYS:CG	2.99	0.45
1:A:121:SER:C	1:A:123:GLU:N	2.75	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:HH11	1:A:418:ARG:HG2	1.81	0.45
1:C:15:CYS:HB3	1:C:17:GLU:OE2	2.15	0.45
1:C:99:LEU:HA	1:C:399:LEU:CD2	2.45	0.45
1:C:100:PHE:HA	1:C:567:PHE:CD1	2.52	0.45
1:C:523:ARG:HG3	1:C:529:TRP:CD2	2.51	0.45
1:D:421:LEU:O	1:D:431:PHE:HB2	2.16	0.45
1:C:103:TRP:O	1:C:104:GLY:C	2.58	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:95:ASN:HA	1:A:569:ALA:HB3	1.97	0.45
1:A:353:GLU:HA	1:A:405:LYS:O	2.17	0.45
1:B:348:ARG:NH1	1:B:437:ASN:ND2	2.64	0.45
1:B:528:PHE:HZ	9:B:748:HOH:O	1.99	0.45
1:C:344:THR:O	8:C:608:HEM:HAD2	2.16	0.45
1:D:9:PRO:C	1:D:10:VAL:HG23	2.42	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:514:LEU:O	1:C:515:LEU:C	2.60	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:HE21	1:A:135:GLN:HB3	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
9:A:772:HOH:O	1:D:173:GLN:HB2	2.17	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HB2	1:D:546:LYS:NZ	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:HG2	1:C:527:ARG:NH1	2.31	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:A:549:PHE:O	1:A:550:SER:C	2.59	0.45
1:C:29:ASN:ND2	1:C:527:ARG:H	2.14	0.45
1:C:168:PRO:HG3	1:C:172:TYR:CD2	2.49	0.45
1:C:363:GLU:CD	1:C:363:GLU:N	2.75	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
1:B:188:ASP:OD1	1:B:188:ASP:N	2.48	0.44
1:B:260:ILE:HG13	1:B:382:ASN:O	2.17	0.44
1:C:517:ARG:HH21	1:C:517:ARG:CB	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:A:408:ASN:O	1:A:411:LYS:C	2.60	0.44
1:B:76:ARG:NH2	9:B:702:HOH:O	2.50	0.44
1:B:353:GLU:C	1:B:405:LYS:HB3	2.42	0.44
1:B:393:ASP:OD1	1:B:557:THR:HB	2.18	0.44
1:C:3:GLU:C	1:C:5:GLY:H	2.24	0.44
1:C:188:ASP:OD1	1:C:190:SER:CB	2.64	0.44
1:D:9:PRO:HG2	1:D:10:VAL:H	1.81	0.44
1:D:260:ILE:HD13	1:D:395:LEU:HD21	2.00	0.44
1:B:91:VAL:HG11	1:B:411:LYS:HD3	1.99	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:C:2:TRP:N	1:C:2:TRP:CD2	2.84	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:468:GLN:CG	1:C:474:LYS:HA	2.40	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:N	1:A:559:ILE:HD13	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:HE2	1:A:462:LYS:HA	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:B:393:ASP:O	1:B:394:PRO:C	2.59	0.44
1:B:479:LYS:O	1:B:480:LEU:C	2.60	0.44
1:C:265:VAL:O	1:C:269:LEU:HG	2.18	0.44
1:C:402:LYS:HD3	6:C:605:NO3:O1	2.17	0.44
1:D:88:GLU:O	1:D:91:VAL:HG22	2.17	0.44
1:D:549:PHE:O	1:D:552:LEU:HB3	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:O	1:A:568:GLN:HG2	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:772:HOH:O	2.17	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:D:187:LEU:HD23	1:D:305:GLN:HA	2.00	0.44
1:D:260:ILE:HG13	1:D:386:ILE:HD11	1.99	0.44
1:D:463:THR:O	1:D:464:LEU:C	2.60	0.44
1:A:203:LEU:HD22	9:A:775:HOH:O	2.17	0.44
1:A:363:GLU:CG	9:A:814:HOH:O	2.65	0.44
7:C:607:3CJ:C3	8:C:608:HEM:C2A	3.01	0.44
1:D:16:ASP:OD1	1:D:18:GLN:C	2.61	0.44
1:D:586:ASP:C	1:D:588:SER:H	2.26	0.44
1:A:219:ALA:C	1:A:220:TRP:CD1	2.96	0.43
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:D:93:ASP:CG	1:D:96:ARG:HB2	2.43	0.43
1:B:109:HIS:NE2	7:B:607:3CJ:S1	2.91	0.43
1:C:17:GLU:C	1:C:18:GLN:CD	2.85	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:94:GLN:O	1:B:569:ALA:CB	2.66	0.43
1:B:117:THR:HG1	1:B:119:LEU:HD23	1.81	0.43
1:B:221:ASP:O	1:B:224:LEU:HB2	2.17	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:C:273:HIS:CD2	1:C:273:HIS:C	2.93	0.43
1:C:342:VAL:HG13	1:C:343:PHE:N	2.33	0.43
1:C:407:MET:HE3	1:C:501:MET:HE3	1.99	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
1:C:385:ARG:HD3	1:C:385:ARG:HA	1.86	0.43
1:C:520:GLN:O	1:C:524:ASP:HB2	2.19	0.43
1:D:82:ILE:HD13	1:D:480:LEU:CD2	2.49	0.43
1:D:300:LEU:O	1:D:301:GLY:C	2.61	0.43
1:D:497:ASN:OD1	1:D:511:LEU:HD11	2.18	0.43
1:B:518:GLN:O	1:B:522:ILE:HG23	2.19	0.43
1:C:293:TYR:CD1	1:C:293:TYR:C	2.97	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:320:GLU:HG3	1:D:512:ALA:HB1	2.00	0.43
1:D:441:CYS:SG	1:D:492:ILE:CG2	3.07	0.43
1:A:415:SER:C	1:A:417:LEU:N	2.75	0.43
1:B:68:ASN:ND2	1:B:489:ASN:OD1	2.44	0.43
1:B:222:HIS:HA	9:B:792:HOH:O	2.19	0.43
1:B:447:PRO:HG2	1:B:452:TRP:CE2	2.54	0.43
1:C:353:GLU:HA	1:C:405:LYS:O	2.18	0.43
1:C:366:GLN:OE1	1:C:366:GLN:HA	2.18	0.43
1:C:407:MET:SD	1:C:407:MET:C	3.02	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
1:A:501:MET:HE3	1:A:501:MET:HB2	1.89	0.43
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:607:3CJ:H6	1.83	0.43
1:A:279:GLU:OE2	1:A:279:GLU:HA	2.19	0.43
1:A:519:PHE:HA	1:A:522:ILE:HG12	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:TYR:OH	1:B:177:ARG:HA	2.17	0.43
1:C:81:LYS:HE2	9:C:817:HOH:O	2.19	0.43
1:C:441:CYS:HB3	9:C:713:HOH:O	2.18	0.43
1:A:343:PHE:CE1	1:A:515:LEU:HD23	2.53	0.43
1:B:407:MET:HB3	1:B:501:MET:HE3	2.00	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:18:GLN:HA	1:D:18:GLN:NE2	2.33	0.43
1:D:167:CYS:HB3	1:D:168:PRO:HD2	2.00	0.43
1:D:568:GLN:O	1:D:569:ALA:C	2.61	0.43
1:A:112:ASP:HA	1:A:183:VAL:HG22	2.01	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:375:PRO:O	1:C:376:LEU:C	2.61	0.42
1:C:467:LEU:HD12	1:C:467:LEU:HA	1.89	0.42
1:A:84:GLY:HA2	1:A:418:ARG:NE	2.34	0.42
1:A:258:GLU:OE1	1:A:259:GLN:CG	2.66	0.42
1:C:16:ASP:O	1:C:18:GLN:HG2	2.19	0.42
1:C:109:HIS:HA	1:C:255:ARG:HH22	1.81	0.42
1:C:362:ASP:OD1	1:C:362:ASP:C	2.62	0.42
1:D:467:LEU:O	1:D:468:GLN:C	2.61	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:B:321:MET:C	1:B:323:LYS:N	2.76	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
1:C:437:ASN:O	1:C:438:LEU:C	2.62	0.42
7:C:607:3CJ:C4	8:C:608: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:D:230:ASN:CG	1:D:232:VAL:HG22	2.44	0.42
1:D:478:LYS:O	1:D:482:ASP:CG	2.62	0.42
1:B:205:ASN:CG	4:B:601:NAG:N2	2.77	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:608:HEM:HAD1	2.34	0.42
1:A:65:LYS:HB3	1:A:65:LYS:HE3	1.61	0.42
1:A:77:GLU:O	1:A:81:LYS:HG3	2.19	0.42
1:A:281:LYS:HD3	1:A:292:LEU:HD11	2.02	0.42
1:B:64:ARG:NH2	9:B:704:HOH:O	2.53	0.42
1:B:246:VAL:HA	1:B:247:PRO:HD3	1.80	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:57:VAL:HA	1:A:58:PRO:HD3	1.92	0.42
1:A:149:PRO:C	1:A:151:LEU:N	2.75	0.42
1:A:233:LYS:HZ1	1:B:322:GLN:HB2	1.82	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:B:232:VAL:O	1:B:232:VAL:HG23	2.20	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:36:LEU:CD2	1:C:338:ARG:HD3	2.50	0.42
1:D:197:PRO:C	1:D:199:LEU:H	2.27	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:B:349:PHE:CD1	1:B:349:PHE:C	2.97	0.42
1:C:101:MET:SD	1:C:354:VAL:HG22	2.60	0.42
1:C:180:ILE:CG2	1:C:181:ASN:N	2.83	0.42
1:D:446:MET:HA	1:D:447:PRO:HD3	1.93	0.42
8:B:606:HEM:O1D	7:B:607:3CJ:H6	2.19	0.42
1:C:106:ILE:HG13	1:C:265:VAL:HG11	2.02	0.42
1:C:206:LEU:O	1:C:207:SER:C	2.62	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:137:ASP:CG	1:B:138:GLU:N	2.78	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:574:HIS:CD2	1:B:574:HIS:C	2.98	0.42
1:A:217:GLN:OE1	1:A:217:GLN:HA	2.20	0.41
1:A:237:CYS:O	1:A:240:ILE:HG13	2.20	0.41
1:B:45:ARG:NH1	1:B:49:ALA:HA	2.35	0.41
1:B:113:PHE:O	1:B:181:ASN:HA	2.20	0.41
1:B:530:TRP:CD1	1:B:531:GLU:H	2.38	0.41
1:C:98:LEU:O	1:C:99:LEU:C	2.62	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:345:PHE:CE1	1:A:440:ARG:HG3	2.54	0.41
1:A:354:VAL:HG21	8:A:608:HEM:CAB	2.50	0.41
1:C:1:SER:N	1:C:2:TRP:CE3	2.82	0.41
1:D:60:GLY:HA2	1:D:72:VAL:CG2	2.50	0.41
1:D:396:VAL:O	1:D:397:ARG:C	2.61	0.41
1:C:333:ASN:H	1:C:333:ASN:HD22	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:522:ILE:HG13	1:A:523:ARG:N	2.36	0.41
1:B:23:THR:O	1:B:297:ARG:NH2	2.44	0.41
1:B:117:THR:HG23	1:B:161:PHE:HD2	1.85	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:D:201:SER:C	1:D:203:LEU:H	2.28	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:366:GLN:O	1:B:367:PRO:C	2.64	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: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:D:331:TYR:CD1	1:D:526:ASP:C	2.98	0.41
1:D:336:ASP:OD1	1:D:338:ARG:HB2	2.21	0.41
1:A:471:LEU:O	1:A:472:LYS:HB2	2.21	0.41
1:B:190:SER:C	1:B:192:VAL:N	2.78	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:82:ILE:HD12	1:C:480:LEU:CD2	2.51	0.41
1:D:9:PRO:O	1:D:10:VAL:CG2	2.69	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
1:D:96:ARG:HD2	1:D:100:PHE:CG	2.55	0.41
1:D:347:PHE:HD1	1:D:347:PHE:HA	1.73	0.41
1:D:375:PRO:O	1:D:376:LEU:C	2.63	0.41
1:D:537:THR:O	1:D:538:GLU:C	2.63	0.41
1:A:572:TYR:HD2	1:A:576:PHE:CG	2.37	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:608:HEM:C1C	3.09	0.41
1:D:589:PRO:HB2	1:D:590:TRP:CZ3	2.56	0.41
1:A:35:ALA:HB1	1:A:41:ARG:CD	2.50	0.41
1:A:165:PHE:HE2	1:A:170:PRO:O	2.03	0.41
1:A:418:ARG:O	1:A:432:ASP:HA	2.21	0.41
1:A:467:LEU:O	1:A:468:GLN:C	2.62	0.41
1:A:501:MET:SD	1:A:506:ARG:HA	2.61	0.41
1:A:523:ARG:O	1:A:524:ASP:C	2.64	0.41
1:B:101:MET:SD	1:B:101:MET:C	3.04	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:190:SER:C	1:B:192:VAL:H	2.28	0.41
1:B:213:MET:HG2	1:B:273:HIS:NE2	2.35	0.41
1:B:399:LEU:HD23	1:B:399:LEU:HA	1.92	0.41
1:B:493:TRP:O	1:B:497:ASN:ND2	2.53	0.41
1:B:556:ASN:C	1:B:557:THR:HG23	2.46	0.41
1:C:46:TRP:CE2	1:C:340:SER:HB3	2.56	0.41
1:C:100:PHE:HA	1:C:567:PHE:HD1	1.85	0.41
1:C:102:GLN:CD	1:C:259:GLN:NE2	2.76	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:C:506:ARG:HD3	1:C:506:ARG:HA	1.89	0.41
1:C:588:SER:N	1:C:589:PRO:CD	2.84	0.41
1:D:28:CYS:HA	1:D:34:PRO:CB	2.51	0.41
1:D:51:TYR:HB3	1:D:57:VAL:O	2.20	0.41
1:D:98:LEU:O	1:D:99:LEU:C	2.60	0.41
1:D:179:GLN:HG2	1:D:444:HIS:CD2	2.56	0.41
1:D:272:GLU:OE2	1:D:276:LEU:HG	2.20	0.41
1:D:423:GLN:O	1:D:426:HIS:HB2	2.20	0.41
1:D:523:ARG:HG3	1:D:529:TRP:CE2	2.56	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:588:SER:O	1:D:589:PRO:C	2.64	0.41
1:A:165:PHE:HZ	1:A:170:PRO:C	2.29	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
1:A:455:PHE:CD1	1:A:455:PHE:C	2.99	0.41
8:B:606:HEM:CHA	7:B:607:3CJ: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:608:HEM:HBC2	8:C:608:HEM:HMC2	2.02	0.41
1:D:366:GLN:HB3	1:D:367:PRO:CD	2.51	0.41
1:A:432:ASP:OD1	1:A:432:ASP:C	2.64	0.40
1:B:14:THR:HG22	1:B:15:CYS:N	2.35	0.40
1:B:362:ASP:OD1	1:B:366:GLN:HB2	2.22	0.40
1:C:85:TYR:CD2	1:C:411:LYS:HA	2.57	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: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:274:ASN:O	1:C:278:ARG:HG3	2.21	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:367:PRO:HB2	1:D:64:ARG:HE	1.86	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:606:HEM:HHA	8:B:606:HEM:HBA2	2.02	0.40
1:C:432:ASP:OD1	1:C:432:ASP:C	2.65	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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ARG:NH2	1:B:177:ARG:O	2.53	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:77:GLU:CG	1:A:81:LYS:HD2	2.51	0.40
1:A:203:LEU:HA	1:A:203:LEU:HD23	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: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
1:C:124:HIS:O	1:C:126:LYS:N	2.54	0.40
1:C:146:LYS:C	1:C:147:ASN:CG	2.89	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%)	16	31
1	B	593/595 (100%)	524 (88%)	63 (11%)	6 (1%)	12	24
1	C	593/595 (100%)	523 (88%)	61 (10%)	9 (2%)	8	16
1	D	593/595 (100%)	515 (87%)	67 (11%)	11 (2%)	6	11
All	All	2372/2380 (100%)	2082 (88%)	259 (11%)	31 (1%)	9	18

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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%)	469 (91%)	48 (9%)	8 18

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	517/517 (100%)	468 (90%)	49 (10%)	8	17
1	C	517/517 (100%)	467 (90%)	50 (10%)	8	17
1	D	517/517 (100%)	456 (88%)	61 (12%)	5	11
All	All	2068/2068 (100%)	1860 (90%)	208 (10%)	7	15

All (208) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	CYS
1	A	9	PRO
1	A	12	LEU
1	A	23	THR
1	A	24	ILE
1	A	32	ARG
1	A	40	ASN
1	A	65	LYS
1	A	71	ARG
1	A	78	VAL
1	A	91	VAL
1	A	116	GLU
1	A	118	GLU
1	A	119	LEU
1	A	135	GLN
1	A	139	CYS
1	A	154	GLN
1	A	167	CYS
1	A	177	ARG
1	A	201	SER
1	A	202	ARG
1	A	215	VAL
1	A	218	GLU
1	A	232	VAL
1	A	240	ILE
1	A	250	GLN
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	348	ARG
1	A	364	ASN
1	A	366	GLN
1	A	408	ASN
1	A	464	LEU
1	A	470	VAL
1	A	481	LEU
1	A	483	LEU
1	A	517	ARG
1	A	538	GLU
1	A	542	ASP
1	A	564	LEU
1	A	568	GLN
1	A	580	SER
1	A	593	ARG
1	B	3	GLU
1	B	6	CYS
1	B	12	LEU
1	B	22	ARG
1	B	23	THR
1	B	53	ASP
1	B	62	THR
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	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	245	HIS
1	B	260	ILE
1	B	266	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	283	LEU
1	B	321	MET
1	B	322	GLN
1	B	337	PRO
1	B	356	SER
1	B	359	SER
1	B	363	GLU
1	B	371	GLU
1	B	383	THR
1	B	423	GLN
1	B	472	LYS
1	B	478	LYS
1	B	481	LEU
1	B	486	THR
1	B	494	ILE
1	B	513	CYS
1	B	522	ILE
1	B	542	ASP
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	17	GLU
1	C	18	GLN
1	C	19	SER
1	C	31	ARG
1	C	32	ARG
1	C	78	VAL
1	C	82	ILE
1	C	89	GLU
1	C	102	GLN
1	C	106	ILE
1	C	118	GLU
1	C	119	LEU
1	C	124	HIS
1	C	139	CYS
1	C	146	LYS
1	C	153	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	156	LYS
1	C	173	GLN
1	C	177	ARG
1	C	207	SER
1	C	240	ILE
1	C	242	THR
1	C	254	SER
1	C	260	ILE
1	C	266	HIS
1	C	273	HIS
1	C	284	ASN
1	C	291	MET
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	399	LEU
1	C	404	SER
1	C	429	HIS
1	C	474	LYS
1	C	520	GLN
1	C	546	LYS
1	C	561	LYS
1	C	564	LEU
1	C	578	ASP
1	C	580	SER
1	C	593	ARG
1	C	594	GLU
1	D	12	LEU
1	D	23	THR
1	D	24	ILE
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	78	VAL
1	D	86	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	116	GLU
1	D	118	GLU
1	D	119	LEU
1	D	124	HIS
1	D	127	VAL
1	D	129	CYS
1	D	156	LYS
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	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	371	GLU
1	D	376	LEU
1	D	414	THR
1	D	428	VAL
1	D	446	MET
1	D	462	LYS
1	D	465	LYS
1	D	474	LYS
1	D	475	VAL
1	D	481	LEU
1	D	492	ILE
1	D	501	MET
1	D	503	GLU
1	D	513	CYS
1	D	538	GLU
1	D	561	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	564	LEU
1	D	568	GLN
1	D	573	PRO
1	D	585	LEU
1	D	586	ASP
1	D	592	SER
1	D	595	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	GLN
1	A	135	GLN
1	A	230	ASN
1	A	245	HIS
1	A	250	GLN
1	A	322	GLN
1	A	419	ASN
1	A	423	GLN
1	A	468	GLN
1	A	532	ASN
1	A	556	ASN
1	A	565	HIS
1	A	568	GLN
1	B	30	ASN
1	B	217	GLN
1	B	231	ASN
1	B	273	HIS
1	B	305	GLN
1	B	322	GLN
1	B	329	GLN
1	B	409	GLN
1	B	410	ASN
1	B	423	GLN
1	B	429	HIS
1	B	437	ASN
1	B	439	GLN
1	B	468	GLN
1	C	18	GLN
1	C	94	GLN
1	C	135	GLN
1	C	147	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	154	GLN
1	C	222	HIS
1	C	230	ASN
1	C	250	GLN
1	C	266	HIS
1	C	286	HIS
1	C	333	ASN
1	C	403	ASN
1	C	419	ASN
1	C	423	GLN
1	C	437	ASN
1	C	532	ASN
1	C	558	HIS
1	C	595	ASN
1	D	18	GLN
1	D	29	ASN
1	D	40	ASN
1	D	63	GLN
1	D	128	GLN
1	D	135	GLN
1	D	273	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
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
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	1	NAG	C3-C2-N2-C7
3	F	2	NAG	C8-C7-N2-C2
3	F	2	NAG	O7-C7-N2-C2
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	1	NAG	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

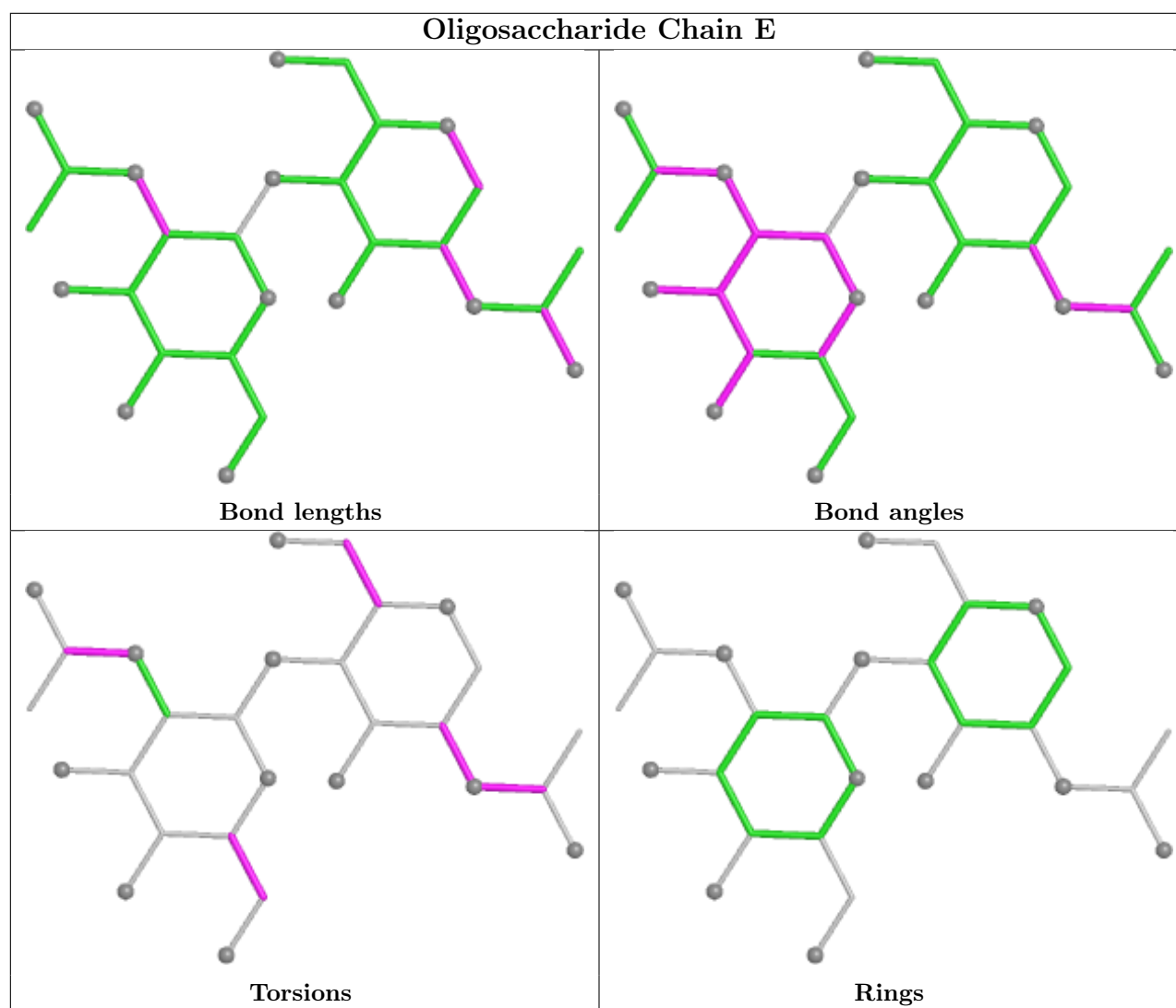
Mol	Chain	Res	Type	Atoms
2	H	2	NAG	C8-C7-N2-C2
2	H	2	NAG	O7-C7-N2-C2
2	H	2	NAG	O5-C5-C6-O6
2	H	1	NAG	C4-C5-C6-O6
2	H	2	NAG	C4-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
2	H	1	NAG	O7-C7-N2-C2
2	E	1	NAG	C4-C5-C6-O6
2	E	2	NAG	C4-C5-C6-O6
3	F	2	NAG	C1-C2-N2-C7
2	E	1	NAG	O5-C5-C6-O6
2	E	2	NAG	C8-C7-N2-C2
3	F	2	NAG	C3-C2-N2-C7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

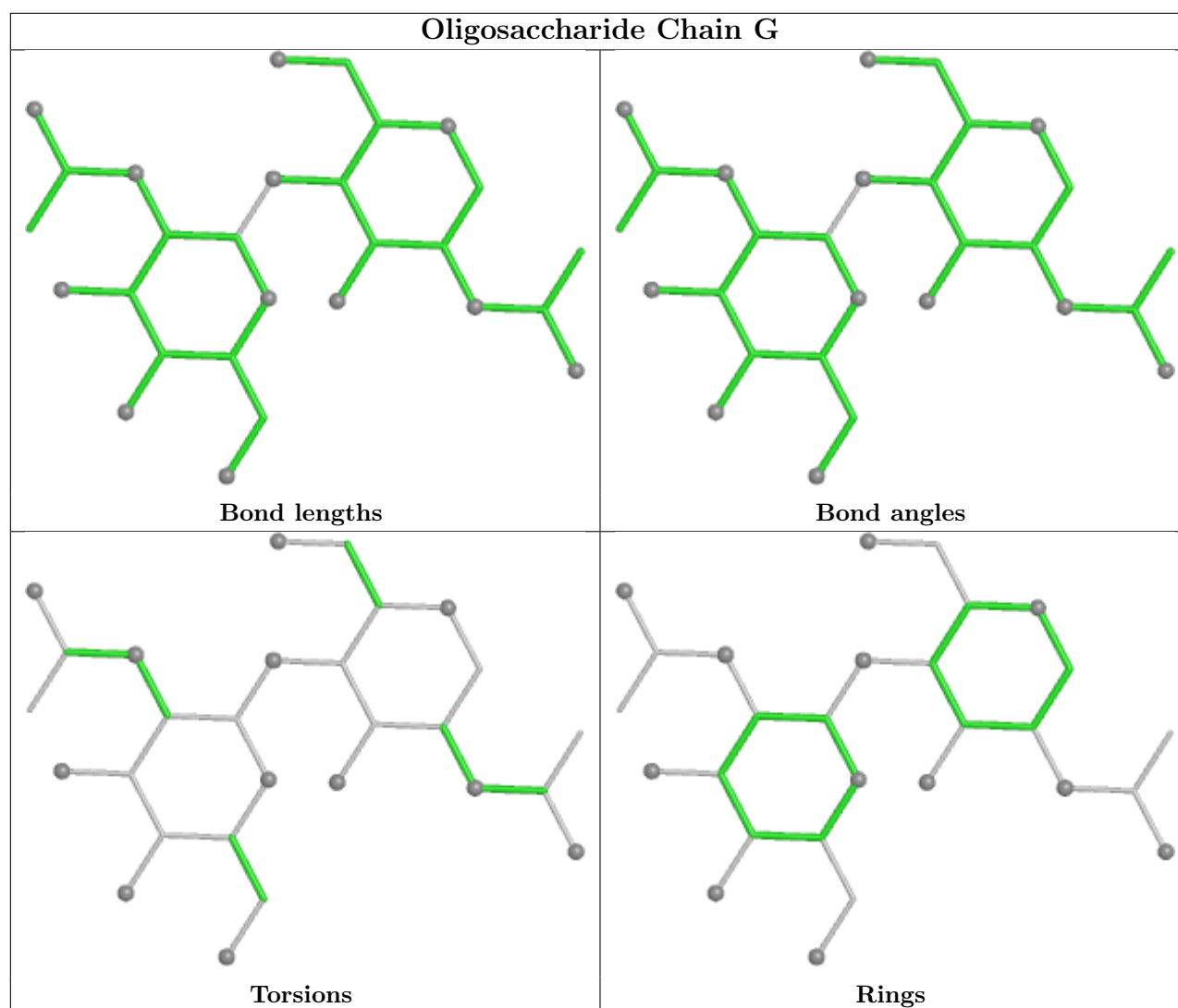
There are no ring outliers.

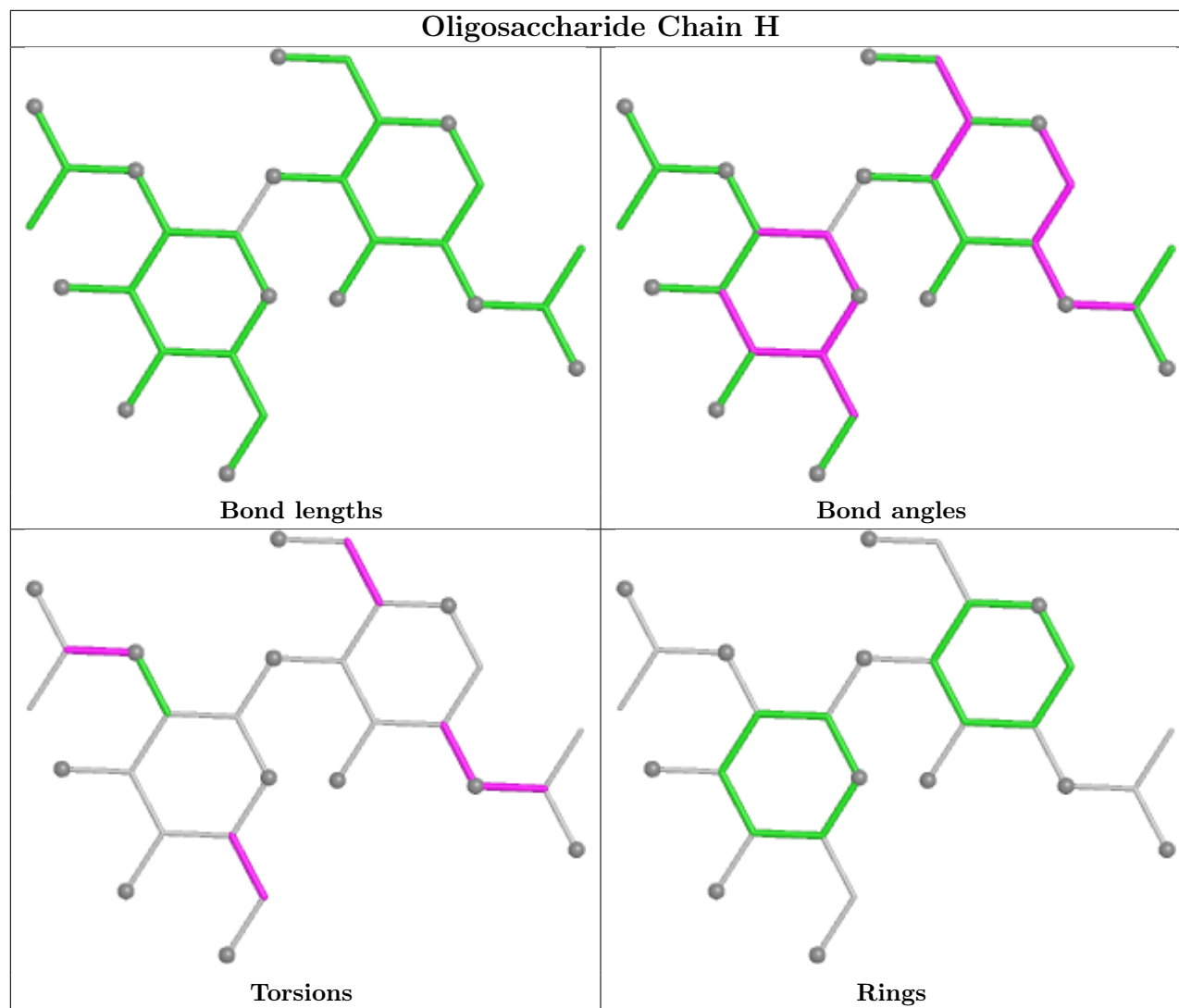
4 monomers are involved in 4 short contacts:

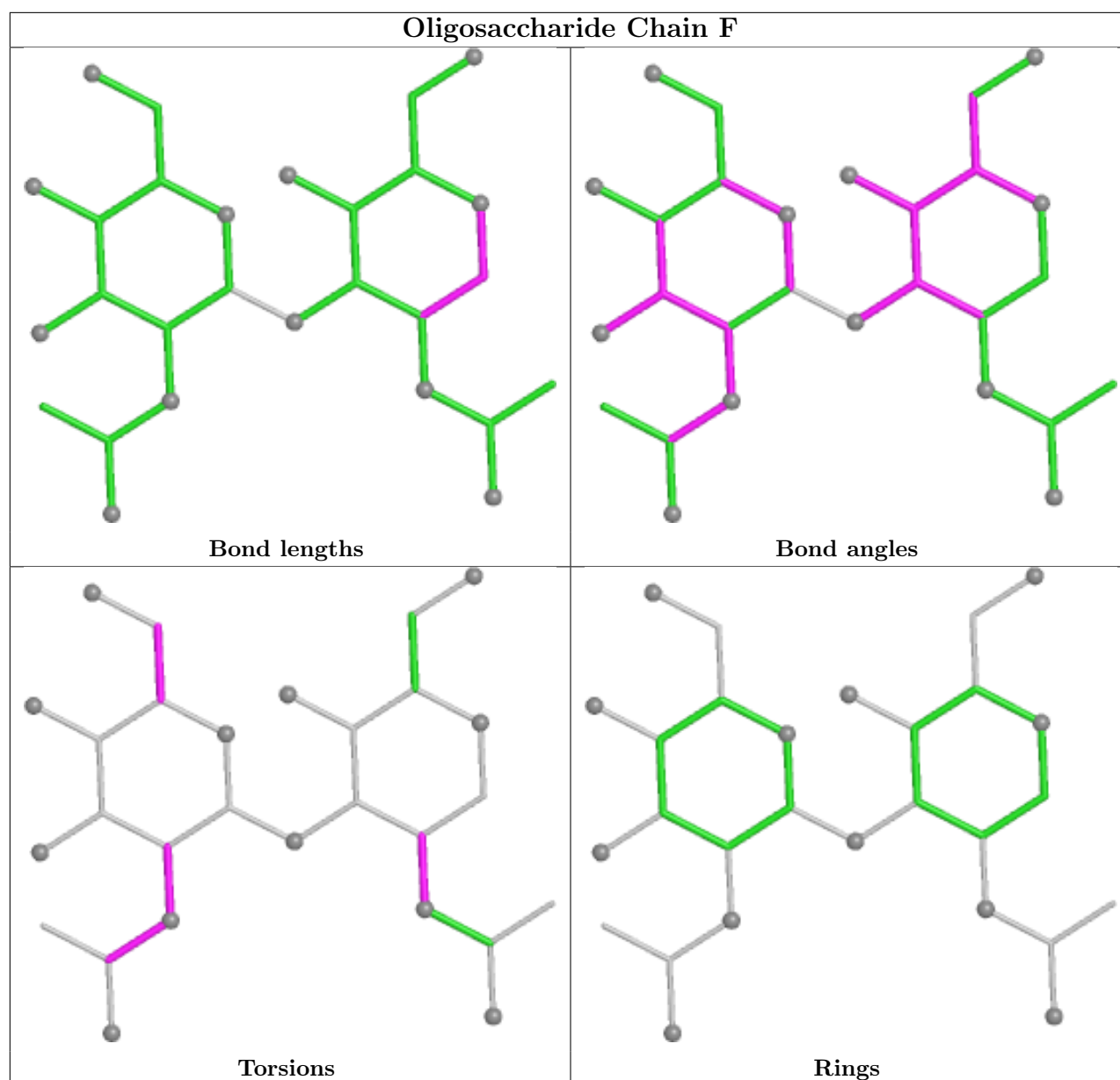
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	2	NAG	1	0
3	F	2	NAG	2	0
2	G	1	NAG	1	0
3	F	1	NAG	2	0

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
6	NO3	D	606	-	1,3,3	0.35	0	0,3,3	-	-
4	NAG	A	602	1	14,14,15	0.29	0	17,19,21	0.61	0
6	NO3	C	605	-	1,3,3	3.46	1 (100%)	0,3,3	-	-
4	NAG	C	601	1	14,14,15	0.30	0	17,19,21	0.62	0
6	NO3	C	604	-	1,3,3	0.34	0	0,3,3	-	-
4	NAG	B	601	1	14,14,15	1.18	1 (7%)	17,19,21	1.81	7 (41%)
8	HEM	B	606	1	50,50,50	1.92	15 (30%)	66,82,82	1.83	17 (25%)
8	HEM	D	608	1	50,50,50	1.82	17 (34%)	66,82,82	1.80	14 (21%)
4	NAG	A	601	1	14,14,15	1.01	0	17,19,21	2.38	8 (47%)
6	NO3	A	604	-	1,3,3	1.27	0	0,3,3	-	-
8	HEM	A	608	1,7	50,50,50	1.86	15 (30%)	66,82,82	1.88	12 (18%)
8	HEM	C	608	1	50,50,50	1.68	12 (24%)	66,82,82	1.91	19 (28%)
6	NO3	D	605	-	1,3,3	3.56	1 (100%)	0,3,3	-	-
6	NO3	B	604	-	1,3,3	3.57	1 (100%)	0,3,3	-	-
6	NO3	D	604	-	1,3,3	0.34	0	0,3,3	-	-
6	NO3	B	603	-	1,3,3	0.35	0	0,3,3	-	-
6	NO3	B	605	-	1,3,3	0.46	0	0,3,3	-	-
4	NAG	D	602	1	14,14,15	0.28	0	17,19,21	0.63	0
7	3CJ	C	607	-	11,11,11	2.32	2 (18%)	14,14,14	3.26	8 (57%)
7	3CJ	B	607	-	11,11,11	2.25	2 (18%)	14,14,14	3.15	7 (50%)
6	NO3	A	605	-	1,3,3	3.55	1 (100%)	0,3,3	-	-
6	NO3	C	606	-	1,3,3	0.32	0	0,3,3	-	-
4	NAG	C	602	1	14,14,15	0.29	0	17,19,21	0.62	0
7	3CJ	A	607	8	11,11,11	2.06	2 (18%)	14,14,14	3.22	9 (64%)
4	NAG	D	601	1	14,14,15	0.81	0	17,19,21	1.94	5 (29%)
6	NO3	A	606	-	1,3,3	0.34	0	0,3,3	-	-
7	3CJ	D	607	-	11,11,11	2.70	6 (54%)	14,14,14	3.59	10 (71%)

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	A	601	1	-	5/6/23/26	0/1/1/1
4	NAG	C	602	1	-	2/6/23/26	0/1/1/1
4	NAG	A	602	1	-	0/6/23/26	0/1/1/1
8	HEM	A	608	1,7	-	4/14/54/54	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	3CJ	D	607	-	-	3/3/3/3	0/1/1/1
7	3CJ	A	607	8	-	1/3/3/3	0/1/1/1
8	HEM	C	608	1	-	4/14/54/54	-
4	NAG	C	601	1	-	4/6/23/26	0/1/1/1
4	NAG	D	601	1	-	4/6/23/26	0/1/1/1
8	HEM	B	606	1	-	4/14/54/54	-
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
7	3CJ	C	607	-	-	1/3/3/3	0/1/1/1
7	3CJ	B	607	-	-	1/3/3/3	0/1/1/1
8	HEM	D	608	1	-	2/14/54/54	-

All (76) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	607	3CJ	O1-C4	6.80	1.37	1.24
7	D	607	3CJ	O1-C4	6.78	1.37	1.24
7	B	607	3CJ	O1-C4	6.53	1.37	1.24
7	A	607	3CJ	O1-C4	5.89	1.35	1.24
8	A	608	HEM	C4D-ND	-4.90	1.31	1.40
8	A	608	HEM	C1B-NB	-4.86	1.31	1.40
8	D	608	HEM	C1B-NB	-4.80	1.32	1.40
8	B	606	HEM	C1B-NB	-4.44	1.32	1.40
8	B	606	HEM	FE-NB	4.34	2.08	1.94
8	B	606	HEM	C3C-C4C	-4.04	1.38	1.46
8	C	608	HEM	C1B-NB	-3.99	1.33	1.40
8	B	606	HEM	C4D-ND	-3.93	1.33	1.40
8	C	608	HEM	FE-NC	3.88	2.08	1.95
8	C	608	HEM	C4D-ND	-3.79	1.33	1.40
8	C	608	HEM	FE-NB	3.78	2.06	1.94
8	D	608	HEM	FE-NB	3.78	2.06	1.94
6	B	604	NO3	O1-N	3.57	1.40	1.24
6	D	605	NO3	O1-N	3.56	1.40	1.24
6	A	605	NO3	O1-N	3.55	1.40	1.24
7	D	607	3CJ	C1-S1	3.55	1.76	1.68
8	A	608	HEM	C3C-C4C	-3.46	1.39	1.46
6	C	605	NO3	O1-N	3.46	1.40	1.24
8	B	606	HEM	FE-NC	3.38	2.06	1.95
8	A	608	HEM	FE-NB	3.37	2.05	1.94
8	A	608	HEM	FE-NC	3.27	2.06	1.95
8	D	608	HEM	C4B-NB	-3.21	1.32	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	608	HEM	C4C-NC	-3.20	1.33	1.39
8	A	608	HEM	CHD-C4C	-3.16	1.32	1.38
8	D	608	HEM	C1C-C2C	-3.15	1.39	1.45
8	B	606	HEM	CHD-C4C	-3.03	1.32	1.38
8	D	608	HEM	C4D-ND	-3.03	1.35	1.40
8	A	608	HEM	C4B-NB	-2.94	1.32	1.38
8	B	606	HEM	C1A-NA	-2.92	1.34	1.39
8	B	606	HEM	C4B-NB	-2.90	1.32	1.38
8	A	608	HEM	FE-ND	-2.85	1.85	1.94
8	D	608	HEM	C1C-NC	-2.83	1.34	1.39
8	B	606	HEM	FE-ND	-2.82	1.86	1.94
8	C	608	HEM	C4B-NB	-2.81	1.33	1.38
8	D	608	HEM	FE-ND	-2.77	1.86	1.94
8	B	606	HEM	C1C-NC	-2.68	1.34	1.39
7	B	607	3CJ	C1-S1	2.60	1.74	1.68
8	D	608	HEM	C1D-ND	-2.57	1.33	1.38
8	D	608	HEM	C1D-C2D	2.54	1.49	1.44
8	B	606	HEM	C3B-C4B	2.50	1.49	1.44
8	A	608	HEM	C1C-NC	-2.45	1.35	1.39
8	B	606	HEM	C4C-NC	-2.44	1.35	1.39
8	A	608	HEM	C1A-NA	-2.44	1.35	1.39
8	C	608	HEM	C4C-NC	-2.41	1.35	1.39
8	C	608	HEM	C4A-NA	-2.40	1.35	1.39
8	A	608	HEM	CHA-C1A	-2.39	1.34	1.39
7	C	607	3CJ	C3-C2	2.36	1.40	1.36
7	D	607	3CJ	C1-N1	2.33	1.39	1.36
8	A	608	HEM	C4A-NA	-2.32	1.35	1.39
8	D	608	HEM	O1D-CGD	2.32	1.29	1.22
4	B	601	NAG	C4-C5	-2.31	1.48	1.53
8	B	606	HEM	C4D-C3D	2.30	1.49	1.45
8	D	608	HEM	C1A-C2A	-2.26	1.40	1.44
8	C	608	HEM	C3C-C4C	-2.26	1.42	1.46
8	D	608	HEM	FE-NC	2.22	2.02	1.95
8	D	608	HEM	C4D-C3D	2.21	1.48	1.45
8	C	608	HEM	CHD-C4C	-2.17	1.34	1.38
7	A	607	3CJ	C3-C2	2.15	1.39	1.36
8	A	608	HEM	C4C-NC	-2.14	1.35	1.39
8	D	608	HEM	C1A-NA	-2.13	1.35	1.39
7	D	607	3CJ	C1-N2	-2.13	1.33	1.36
8	C	608	HEM	C1A-NA	-2.12	1.35	1.39
8	A	608	HEM	C4D-C3D	2.11	1.48	1.45
8	B	606	HEM	C1C-C2C	-2.11	1.41	1.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	B	606	HEM	C1D-ND	-2.11	1.34	1.38
7	D	607	3CJ	C2-N1	2.11	1.40	1.37
8	C	608	HEM	C2A-C3A	-2.10	1.33	1.38
8	D	608	HEM	CHD-C4C	-2.10	1.34	1.38
8	A	608	HEM	C1D-ND	-2.09	1.34	1.38
8	C	608	HEM	C1B-C2B	-2.06	1.40	1.44
8	D	608	HEM	C3B-C4B	2.06	1.49	1.44
7	D	607	3CJ	C3-C2	2.05	1.39	1.36

All (116) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	607	3CJ	C5-C2-N1	7.16	125.94	115.53
7	A	607	3CJ	C1-N2-C4	-6.31	118.94	125.29
7	B	607	3CJ	C1-N2-C4	-5.71	119.54	125.29
8	C	608	HEM	C1B-NB-C4B	5.70	110.96	105.07
7	C	607	3CJ	C1-N2-C4	-5.64	119.62	125.29
7	D	607	3CJ	C5-C2-C3	-5.62	115.99	125.02
8	A	608	HEM	CHC-C4B-NB	5.36	130.25	124.42
8	A	608	HEM	CHD-C1D-C2D	-5.34	116.63	124.98
7	C	607	3CJ	N2-C1-N1	5.30	121.88	115.19
8	A	608	HEM	C1B-NB-C4B	5.27	110.52	105.07
8	B	606	HEM	CHD-C1D-ND	5.18	130.05	124.42
7	B	607	3CJ	C3-C4-N2	5.14	121.35	115.14
7	A	607	3CJ	C3-C4-N2	5.05	121.23	115.14
8	C	608	HEM	CHD-C1D-ND	5.03	129.88	124.42
8	B	606	HEM	CHD-C1D-C2D	-5.02	117.13	124.98
7	B	607	3CJ	O1-C4-C3	-4.80	118.73	125.47
7	A	607	3CJ	N2-C1-N1	4.78	121.23	115.19
8	A	608	HEM	CHD-C1D-ND	4.71	129.53	124.42
4	D	601	NAG	O5-C1-C2	-4.68	103.90	111.29
7	D	607	3CJ	C3-C4-N2	4.58	120.66	115.14
7	D	607	3CJ	O1-C4-C3	-4.52	119.12	125.47
7	C	607	3CJ	C1-N1-C2	-4.52	120.41	123.54
4	A	601	NAG	C4-C3-C2	-4.26	104.78	111.02
7	B	607	3CJ	C3-C2-N1	-4.22	116.28	119.62
8	C	608	HEM	CHD-C1D-C2D	-4.20	118.42	124.98
8	D	608	HEM	CHD-C1D-ND	4.19	128.97	124.42
7	C	607	3CJ	C5-C2-N1	4.18	121.60	115.53
8	D	608	HEM	C4B-C3B-C2B	-4.13	103.83	107.11
8	A	608	HEM	CBD-CAD-C3D	-4.06	101.34	112.63
8	D	608	HEM	CHC-C4B-NB	4.05	128.82	124.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	606	HEM	CHC-C4B-NB	4.02	128.78	124.42
7	A	607	3CJ	C6-C5-C2	4.01	122.94	114.52
8	C	608	HEM	CHC-C4B-NB	4.00	128.76	124.42
7	A	607	3CJ	O1-C4-C3	-3.95	119.93	125.47
7	D	607	3CJ	S1-C1-N2	-3.87	116.99	122.08
7	B	607	3CJ	C5-C2-N1	3.83	121.09	115.53
8	D	608	HEM	CBD-CAD-C3D	-3.67	102.43	112.63
8	B	606	HEM	C1B-NB-C4B	3.63	108.83	105.07
7	C	607	3CJ	C3-C4-N2	3.61	119.50	115.14
4	D	601	NAG	C2-N2-C7	-3.61	117.76	122.90
8	D	608	HEM	CHD-C1D-C2D	-3.59	119.37	124.98
8	C	608	HEM	CHB-C1B-NB	3.59	128.80	124.37
4	A	601	NAG	C1-O5-C5	3.47	116.89	112.19
4	A	601	NAG	O4-C4-C5	3.40	117.75	109.30
7	C	607	3CJ	S1-C1-N2	-3.40	117.61	122.08
8	D	608	HEM	CHA-C4D-ND	3.39	128.56	124.37
8	B	606	HEM	C4C-NC-C1C	3.38	108.66	105.35
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
8	A	608	HEM	C2D-C1D-ND	3.29	113.82	109.88
7	C	607	3CJ	O1-C4-C3	-3.26	120.90	125.47
7	C	607	3CJ	C5-C2-C3	-3.25	119.80	125.02
8	A	608	HEM	C1D-C2D-C3D	-3.25	103.54	106.96
8	D	608	HEM	C1B-NB-C4B	3.25	108.42	105.07
4	B	601	NAG	O5-C1-C2	-3.16	106.30	111.29
8	A	608	HEM	O2A-CGA-CBA	3.13	124.10	114.03
8	B	606	HEM	CAA-C2A-C1A	3.10	131.00	124.89
4	A	601	NAG	C3-C4-C5	-3.09	104.73	110.24
7	D	607	3CJ	C6-C5-C2	3.08	120.98	114.52
4	B	601	NAG	C1-O5-C5	3.05	116.32	112.19
8	D	608	HEM	C1A-CHA-C4D	-2.99	119.26	126.34
8	D	608	HEM	CHA-C4D-C3D	-2.97	119.75	125.33
8	B	606	HEM	CBD-CAD-C3D	-2.95	104.44	112.63
7	D	607	3CJ	C4-C3-C2	-2.95	118.26	120.64
8	C	608	HEM	CMA-C3A-C4A	2.94	129.84	125.37
8	A	608	HEM	CHA-C4D-ND	2.89	127.94	124.37
8	C	608	HEM	C4C-NC-C1C	2.88	108.16	105.35
7	B	607	3CJ	N2-C1-N1	2.86	118.80	115.19
7	D	607	3CJ	S1-C1-N1	2.84	125.81	122.08
8	B	606	HEM	CAA-C2A-C3A	-2.80	120.66	127.07
4	B	601	NAG	C2-N2-C7	-2.79	118.94	122.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	608	HEM	O2D-CGD-CBD	2.75	122.86	114.03
8	B	606	HEM	O2D-CGD-CBD	2.73	122.82	114.03
8	B	606	HEM	CAD-C3D-C4D	2.69	129.36	124.66
8	D	608	HEM	CMD-C2D-C1D	2.64	129.06	125.04
4	B	601	NAG	O6-C6-C5	-2.59	102.42	111.29
8	D	608	HEM	CHB-C4A-NA	2.55	128.54	123.85
7	A	607	3CJ	S1-C1-N1	-2.54	118.74	122.08
8	B	606	HEM	CHB-C4A-NA	2.52	128.48	123.85
7	A	607	3CJ	C4-C3-C2	-2.51	118.62	120.64
8	A	608	HEM	O2A-CGA-O1A	-2.45	117.20	123.30
8	D	608	HEM	C4A-NA-C1A	2.42	107.72	105.35
4	D	601	NAG	C8-C7-N2	-2.42	112.00	116.10
8	C	608	HEM	O2A-CGA-CBA	2.41	121.77	114.03
8	C	608	HEM	CHA-C4D-ND	2.41	127.34	124.37
8	C	608	HEM	CAA-C2A-C1A	2.39	129.59	124.89
8	C	608	HEM	CBD-CAD-C3D	-2.39	105.99	112.63
8	C	608	HEM	CAD-CBD-CGD	2.38	118.72	113.60
4	B	601	NAG	C6-C5-C4	-2.37	107.45	113.00
8	B	606	HEM	CHA-C4D-ND	2.30	127.21	124.37
8	B	606	HEM	C2D-C1D-ND	2.29	112.63	109.88
8	B	606	HEM	O2D-CGD-O1D	-2.28	117.61	123.30
8	A	608	HEM	CHA-C4D-C3D	-2.28	121.04	125.33
4	B	601	NAG	O3-C3-C4	-2.24	105.17	110.35
8	C	608	HEM	CAA-CBA-CGA	-2.24	108.79	113.60
7	A	607	3CJ	C3-C2-N1	-2.23	117.86	119.62
8	C	608	HEM	CAA-C2A-C3A	-2.18	122.07	127.07
4	D	601	NAG	O3-C3-C4	-2.18	105.32	110.35
7	D	607	3CJ	C1-N2-C4	-2.16	123.11	125.29
8	B	606	HEM	C4C-CHD-C1D	-2.15	121.41	126.06
8	D	608	HEM	CMC-C2C-C1C	-2.15	120.93	124.71
8	D	608	HEM	CAD-C3D-C4D	2.13	128.39	124.66
7	D	607	3CJ	C3-C2-N1	-2.12	117.94	119.62
8	C	608	HEM	O2D-CGD-O1D	-2.10	118.07	123.30
7	A	607	3CJ	C1-N1-C2	-2.10	122.08	123.54
8	B	606	HEM	CAD-C3D-C2D	-2.08	124.00	127.88
8	C	608	HEM	CHA-C4D-C3D	-2.08	121.42	125.33
4	D	601	NAG	C4-C3-C2	2.05	114.03	111.02
8	C	608	HEM	CHB-C1B-C2B	-2.05	121.05	126.73
4	A	601	NAG	O4-C4-C3	-2.04	105.64	110.35
8	A	608	HEM	CAA-C2A-C1A	2.04	128.90	124.89
4	B	601	NAG	O5-C5-C4	-2.04	105.88	110.83
7	B	607	3CJ	S1-C1-N2	-2.03	119.40	122.08

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	C	608	HEM	CAD-C3D-C4D	2.01	128.17	124.66
8	B	606	HEM	CHB-C4A-C3A	-2.01	121.56	127.24

There are no chirality outliers.

All (37) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	NAG	C3-C2-N2-C7
4	C	601	NAG	C8-C7-N2-C2
4	C	601	NAG	O7-C7-N2-C2
7	A	607	3CJ	C2-C5-C6-C7
7	B	607	3CJ	C2-C5-C6-C7
7	D	607	3CJ	C2-C5-C6-C7
8	B	606	HEM	C1A-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	602	NAG	O5-C5-C6-O6
4	D	601	NAG	O7-C7-N2-C2
4	C	601	NAG	O5-C5-C6-O6
4	C	602	NAG	C4-C5-C6-O6
4	A	601	NAG	C4-C5-C6-O6
4	C	601	NAG	C4-C5-C6-O6
8	B	606	HEM	C3A-C2A-CAA-CBA
4	B	601	NAG	C8-C7-N2-C2
4	A	601	NAG	C8-C7-N2-C2
7	D	607	3CJ	N1-C2-C5-C6
4	B	601	NAG	O7-C7-N2-C2
4	A	601	NAG	O7-C7-N2-C2
8	C	608	HEM	CAD-CBD-CGD-O2D
8	A	608	HEM	C1A-C2A-CAA-CBA
8	C	608	HEM	CAD-CBD-CGD-O1D
8	C	608	HEM	CAA-CBA-CGA-O2A
8	A	608	HEM	CAD-CBD-CGD-O1D
8	A	608	HEM	CAD-CBD-CGD-O2D
8	B	606	HEM	CAD-CBD-CGD-O2D
8	C	608	HEM	CAA-CBA-CGA-O1A
8	B	606	HEM	CAD-CBD-CGD-O1D
8	D	608	HEM	CAD-CBD-CGD-O2D
7	C	607	3CJ	N1-C2-C5-C6
7	D	607	3CJ	C3-C2-C5-C6

Continued on next page...

Continued from previous page...

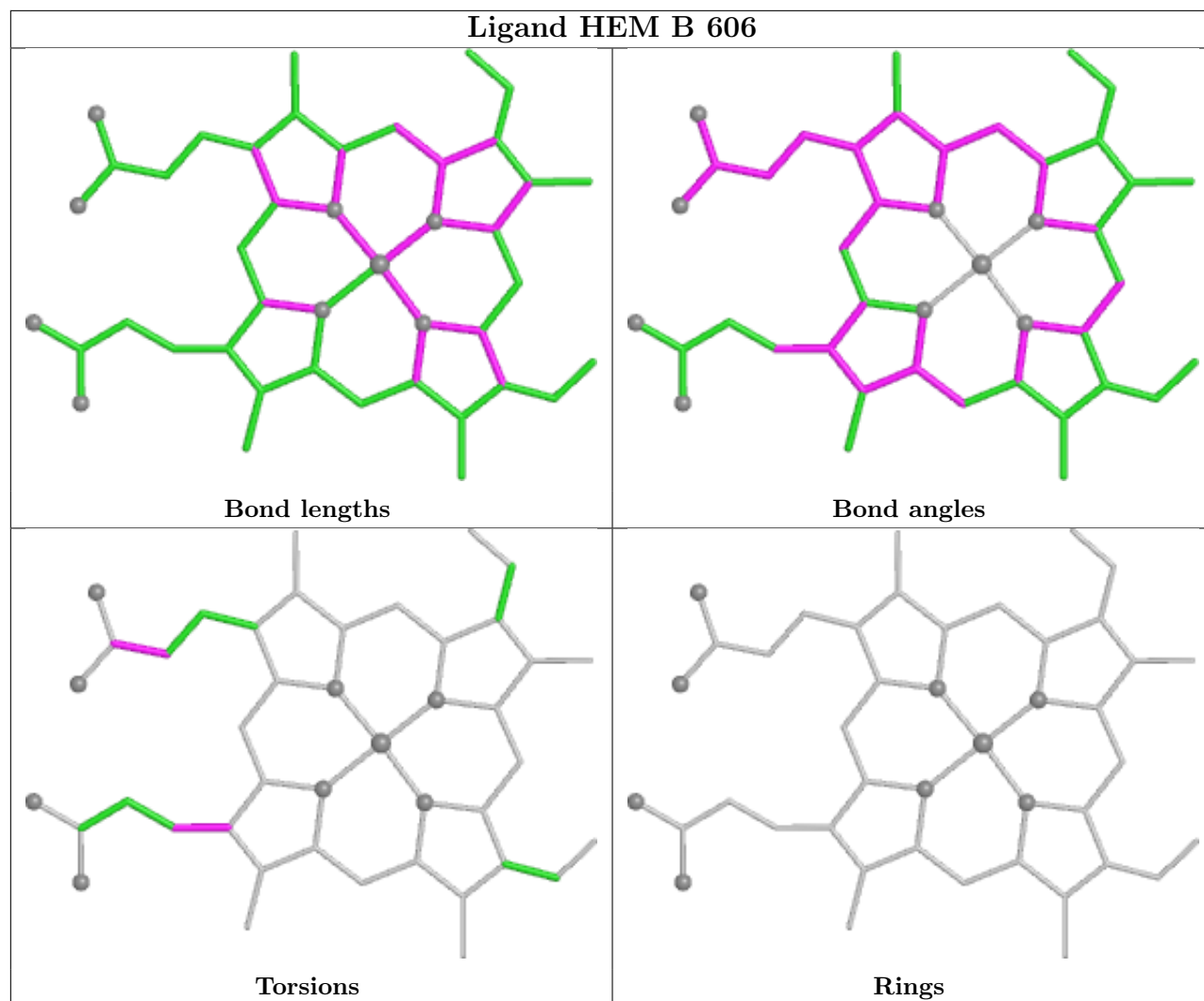
Mol	Chain	Res	Type	Atoms
8	D	608	HEM	CAD-CBD-CGD-O1D
8	A	608	HEM	C3A-C2A-CAA-CBA

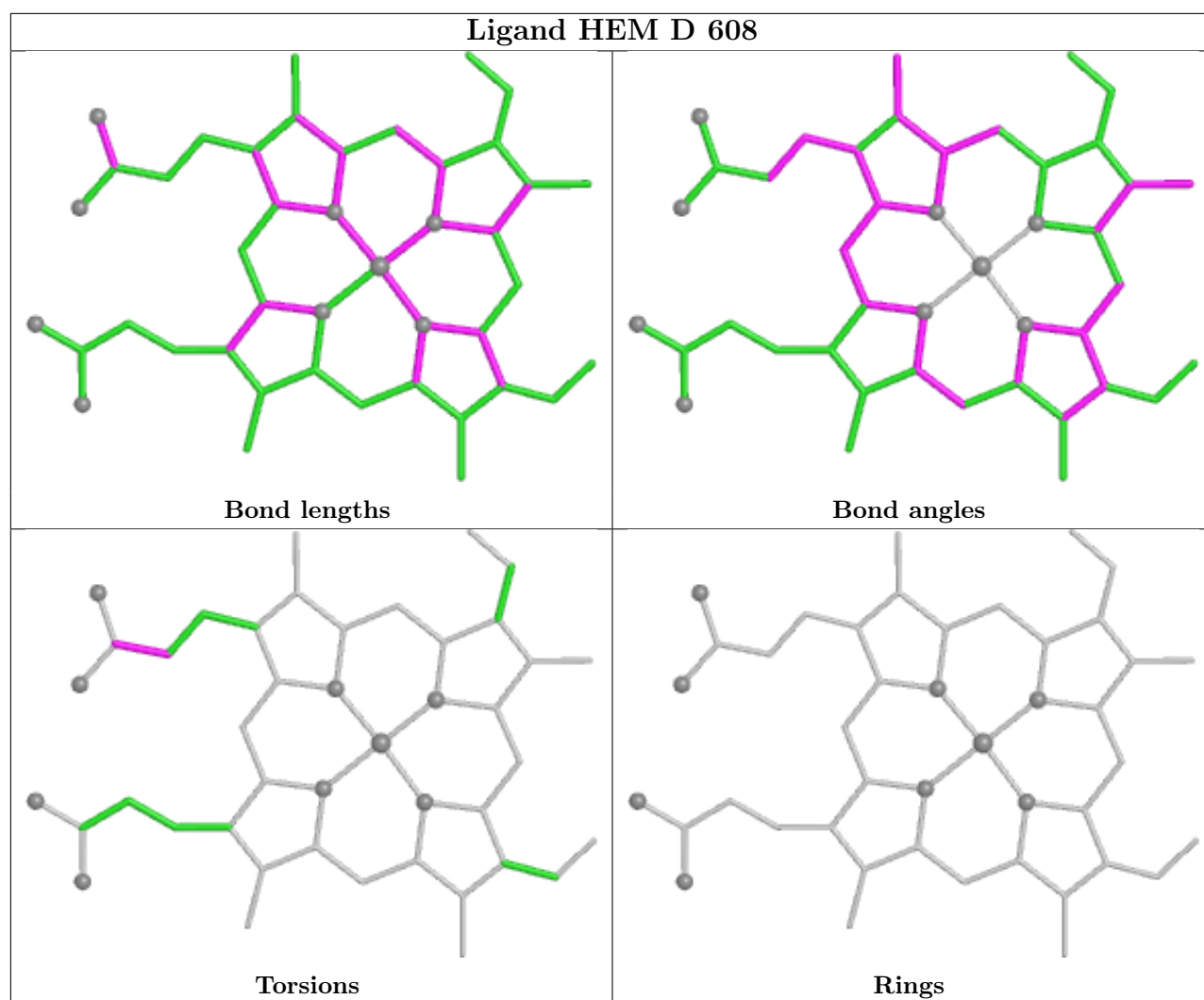
There are no ring outliers.

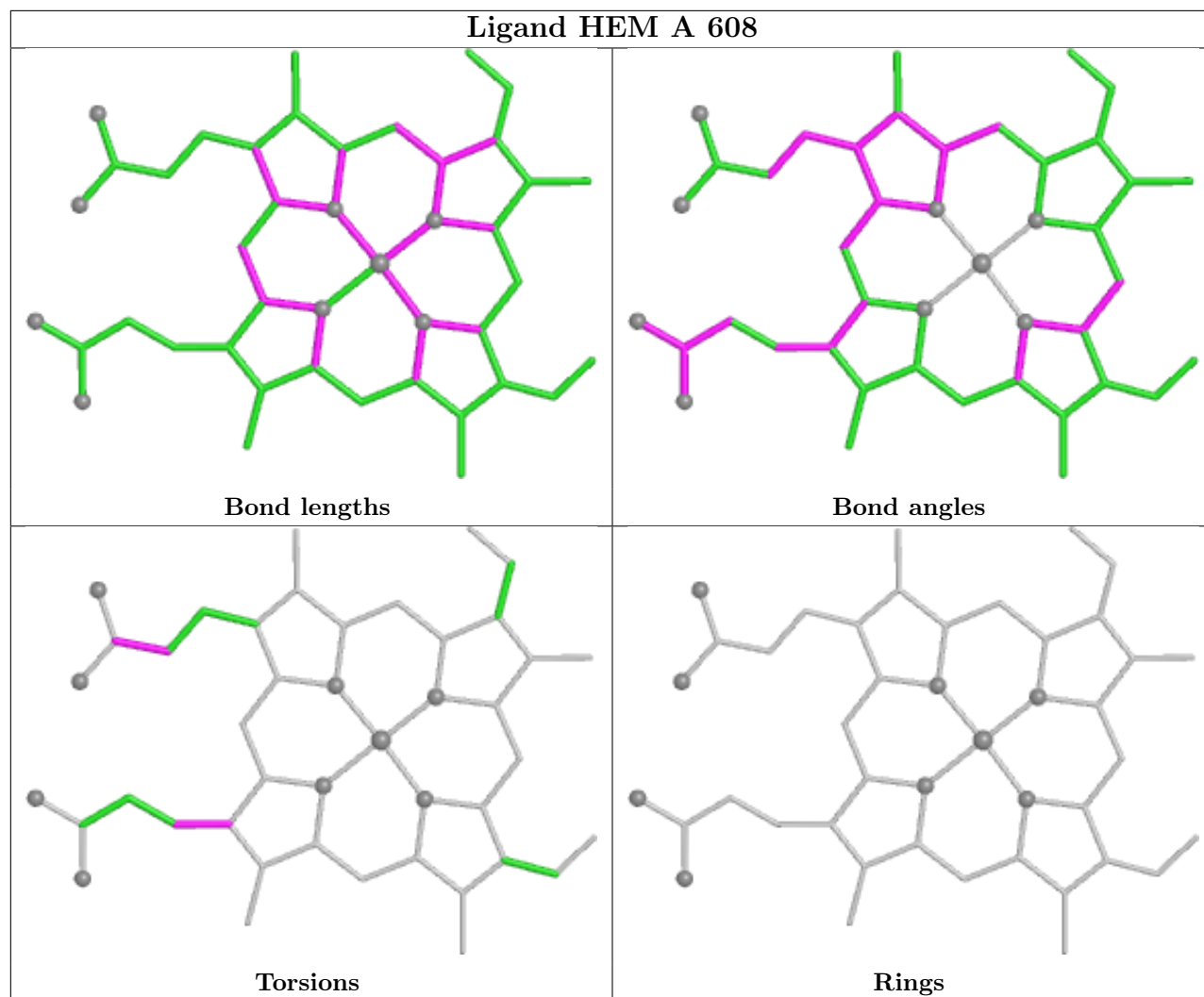
18 monomers are involved in 92 short contacts:

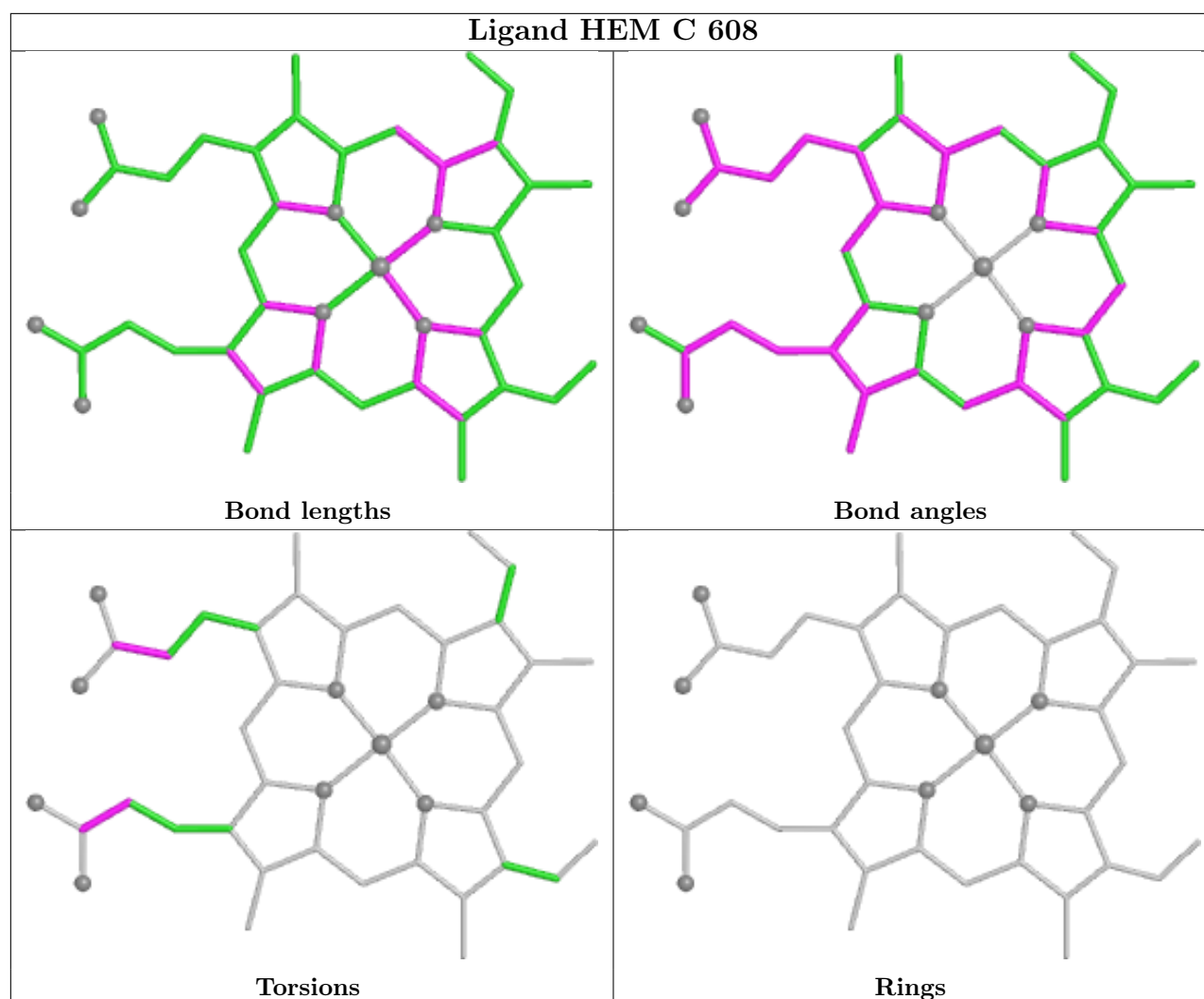
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	D	606	NO3	4	0
6	C	605	NO3	1	0
6	C	604	NO3	1	0
4	B	601	NAG	1	0
8	B	606	HEM	14	0
8	D	608	HEM	15	0
8	A	608	HEM	12	0
8	C	608	HEM	17	0
6	D	605	NO3	2	0
6	D	604	NO3	2	0
6	B	603	NO3	2	0
4	D	602	NAG	1	0
7	C	607	3CJ	9	0
7	B	607	3CJ	12	0
6	A	605	NO3	1	0
6	C	606	NO3	2	0
7	A	607	3CJ	11	0
7	D	607	3CJ	11	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%)	0.40	23 (3%) 43 38	16, 42, 78, 117	0
1	B	595/595 (100%)	0.39	18 (3%) 52 48	20, 43, 76, 100	0
1	C	595/595 (100%)	0.47	32 (5%) 31 27	20, 43, 83, 100	0
1	D	595/595 (100%)	0.45	31 (5%) 33 29	14, 41, 79, 100	0
All	All	2380/2380 (100%)	0.43	104 (4%) 39 34	14, 42, 79, 117	0

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4	VAL	7.4
1	D	2	TRP	6.1
1	A	171	PRO	6.0
1	B	189	ALA	5.2
1	C	96	ARG	5.1
1	C	4	VAL	4.7
1	B	4	VAL	4.7
1	D	13	VAL	4.5
1	D	207	SER	4.5
1	A	5	GLY	4.2
1	A	56	ALA	3.9
1	C	10	VAL	3.8
1	C	9	PRO	3.8
1	C	153	THR	3.7
1	B	2	TRP	3.6
1	D	169	THR	3.6
1	B	121	SER	3.6
1	C	95	ASN	3.6
1	B	171	PRO	3.4
1	B	122	SER	3.4
1	C	132	TYR	3.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	494	ILE	3.3
1	C	249	PHE	3.3
1	B	582	VAL	3.3
1	C	115	PRO	3.2
1	D	170	PRO	3.1
1	D	7	GLY	3.1
1	C	169	THR	3.1
1	A	223	GLY	3.1
1	D	11	PRO	3.0
1	D	168	PRO	3.0
1	A	170	PRO	3.0
1	A	21	TYR	3.0
1	A	172	TYR	3.0
1	C	6	CYS	3.0
1	C	592	SER	2.9
1	A	547	VAL	2.9
1	D	153	THR	2.9
1	C	1	SER	2.9
1	D	205	ASN	2.9
1	D	592	SER	2.9
1	A	2	TRP	2.9
1	D	3	GLU	2.9
1	C	121	SER	2.8
1	D	359	SER	2.8
1	C	5	GLY	2.7
1	C	567	PHE	2.7
1	B	425	THR	2.7
1	B	1	SER	2.7
1	B	170	PRO	2.6
1	B	137	ASP	2.6
1	D	5	GLY	2.6
1	D	1	SER	2.6
1	C	172	TYR	2.6
1	A	425	THR	2.5
1	B	5	GLY	2.5
1	C	236	PRO	2.5
1	A	174	SER	2.5
1	C	519	PHE	2.5
1	D	567	PHE	2.5
1	B	434	ALA	2.5
1	C	37	GLY	2.5
1	C	175	LEU	2.5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	168	PRO	2.4
1	B	6	CYS	2.4
1	A	10	VAL	2.4
1	A	464	LEU	2.4
1	D	392	ILE	2.4
1	D	17	GLU	2.4
1	A	135	GLN	2.4
1	C	215	VAL	2.4
1	B	530	TRP	2.4
1	C	534	GLY	2.3
1	A	13	VAL	2.3
1	C	2	TRP	2.3
1	D	121	SER	2.3
1	D	6	CYS	2.3
1	C	209	PRO	2.3
1	A	485	LYS	2.3
1	C	355	PRO	2.3
1	C	49	ALA	2.2
1	D	8	ALA	2.2
1	D	331	TYR	2.2
1	B	120	GLY	2.2
1	C	125	SER	2.2
1	A	431	PHE	2.2
1	C	8	ALA	2.2
1	D	39	ALA	2.2
1	A	169	THR	2.2
1	A	6	CYS	2.2
1	B	11	PRO	2.2
1	C	171	PRO	2.2
1	D	120	GLY	2.1
1	D	164	GLY	2.1
1	D	560	THR	2.1
1	A	133	CYS	2.1
1	C	211	GLY	2.1
1	D	533	PRO	2.1
1	A	4	VAL	2.1
1	A	582	VAL	2.1
1	D	332	ASN	2.1
1	B	9	PRO	2.1
1	D	522	ILE	2.1
1	D	446	MET	2.0

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

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

6.3 Carbohydrates ⓘ

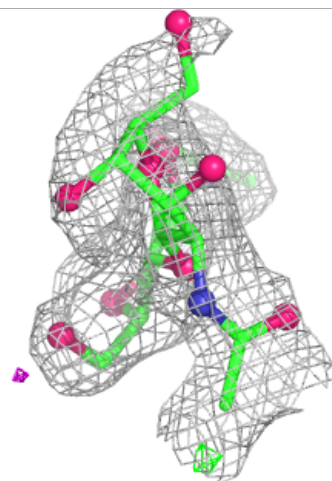
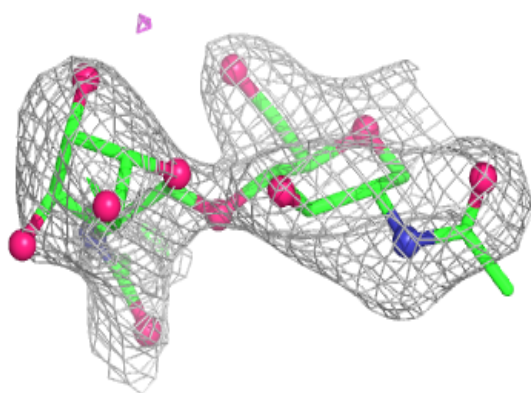
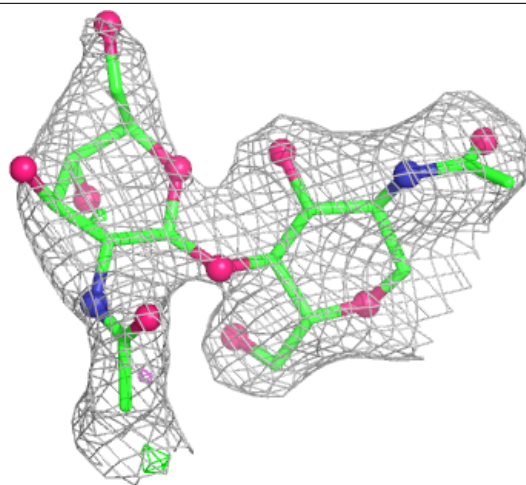
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	E	2	14/15	0.73	0.14	43,50,51,52	14
2	NAG	G	2	14/15	0.74	0.12	49,56,63,63	14
2	NAG	H	2	14/15	0.75	0.13	61,67,70,70	14
3	NAG	F	2	14/15	0.75	0.14	45,53,55,58	14
2	NAG	G	1	14/15	0.82	0.14	20,20,20,20	0
3	NAG	F	1	14/15	0.87	0.12	36,50,59,66	0
2	NAG	H	1	14/15	0.88	0.11	70,79,82,85	0
2	NAG	E	1	14/15	0.89	0.10	33,41,52,54	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.

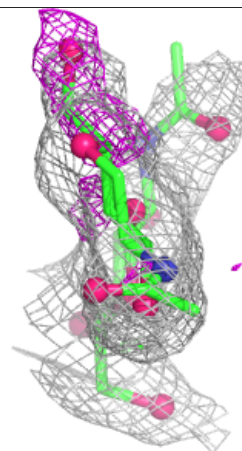
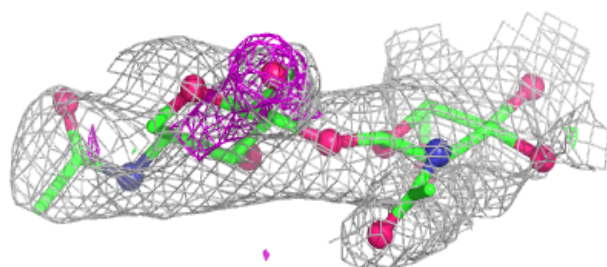
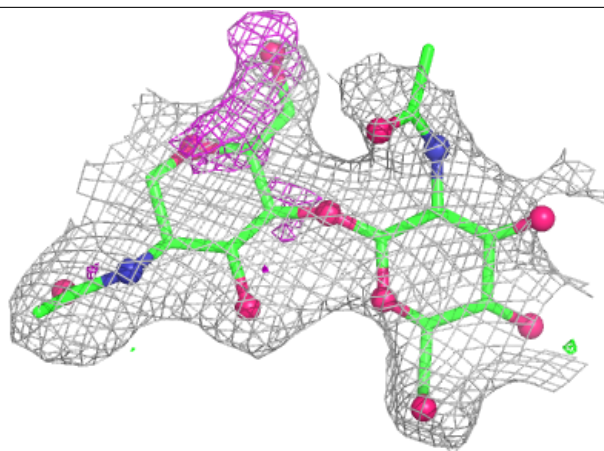
Electron density around Chain E:

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



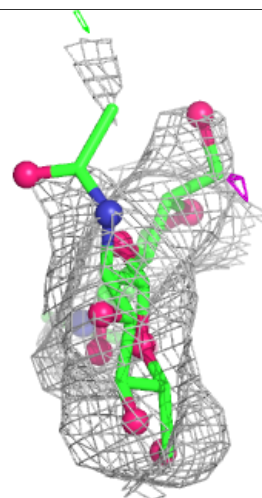
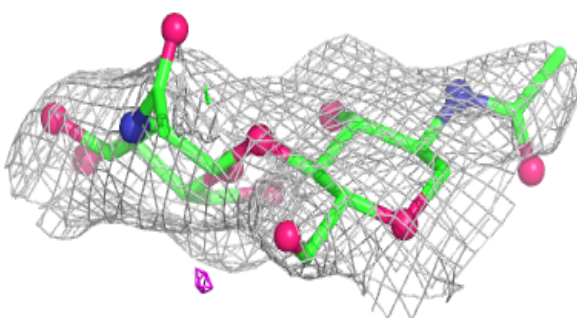
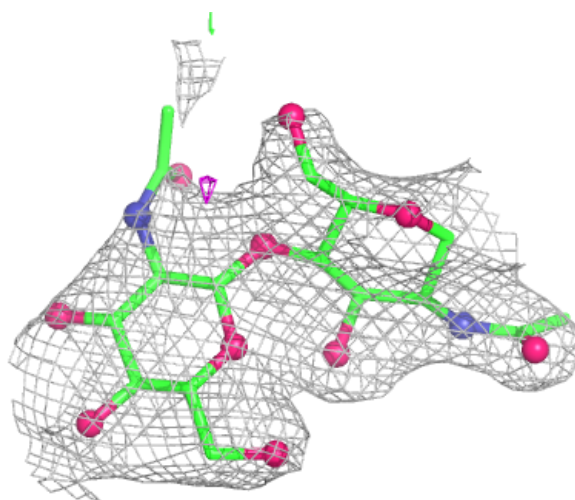
Electron density around Chain G:

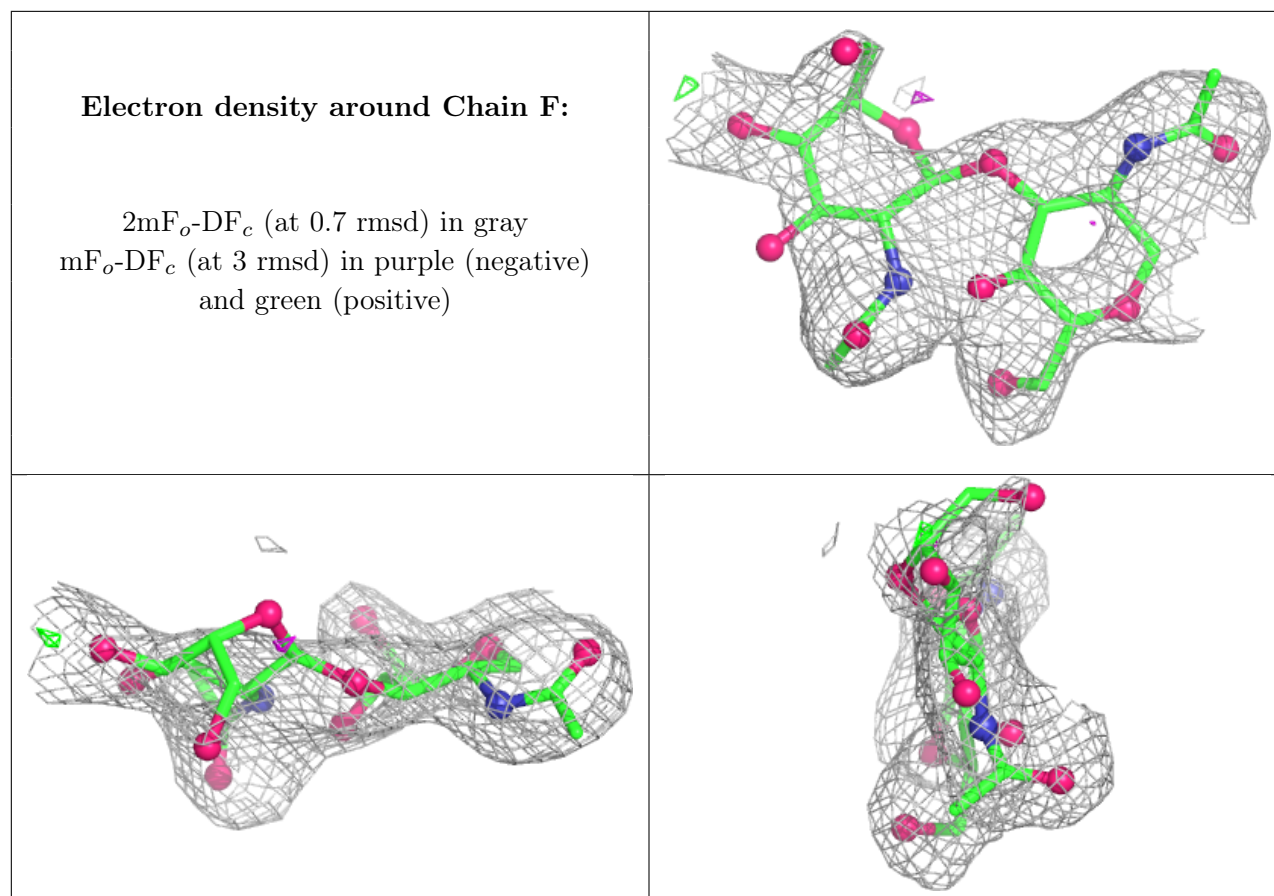
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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 ⓘ

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	A	601	14/15	0.55	0.14	64,79,81,81	0
4	NAG	C	601	14/15	0.63	0.17	78,86,89,90	0
6	NO3	C	605	4/4	0.67	0.31	24,24,27,31	0
4	NAG	D	602	14/15	0.75	0.13	46,54,59,60	0
7	3CJ	C	607	11/11	0.75	0.16	69,79,84,85	0
6	NO3	B	605	4/4	0.76	0.37	24,24,24,28	0
6	NO3	B	603	4/4	0.77	0.13	22,25,27,28	0
4	NAG	C	602	14/15	0.77	0.13	48,55,60,61	0
6	NO3	C	606	4/4	0.78	0.22	24,28,29,30	0
4	NAG	D	601	14/15	0.79	0.10	52,60,65,66	0
7	3CJ	B	607	11/11	0.79	0.12	48,52,58,61	0
6	NO3	B	604	4/4	0.79	0.25	26,26,27,29	0
7	3CJ	D	607	11/11	0.79	0.12	39,48,58,58	0

Continued on next page...

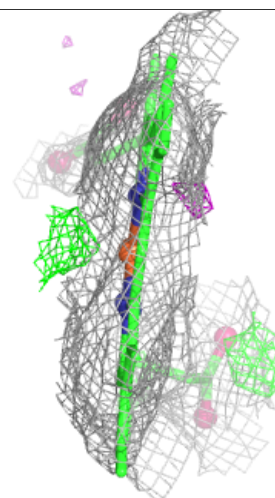
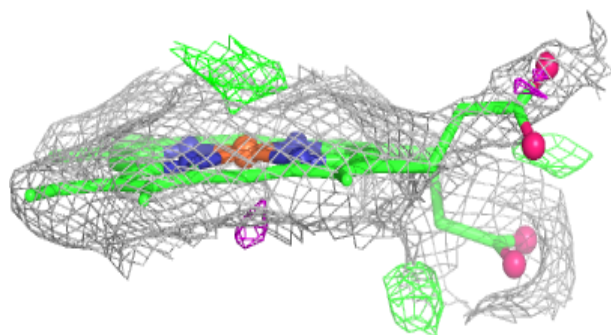
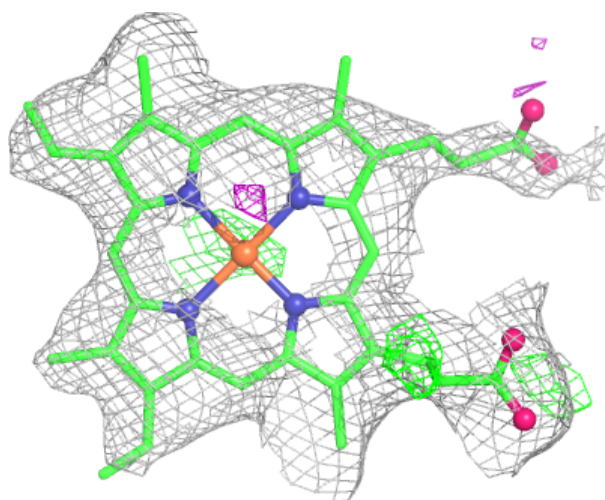
Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	NO3	D	605	4/4	0.82	0.27	25,26,27,28	0
6	NO3	C	604	4/4	0.82	0.35	24,27,29,31	0
6	NO3	D	606	4/4	0.85	0.24	23,23,26,30	0
6	NO3	A	604	4/4	0.86	0.21	23,23,24,26	0
4	NAG	B	601	14/15	0.87	0.13	55,63,73,75	0
7	3CJ	A	607	11/11	0.88	0.09	47,50,55,56	0
6	NO3	A	606	4/4	0.88	0.21	23,24,26,27	0
6	NO3	A	605	4/4	0.89	0.15	24,26,28,32	0
4	NAG	A	602	14/15	0.89	0.08	38,46,51,54	0
6	NO3	D	604	4/4	0.89	0.13	21,24,24,26	0
5	CA	C	603	1/1	0.91	0.07	46,46,46,46	0
8	HEM	B	606	43/43	0.93	0.11	33,42,54,62	0
5	CA	B	602	1/1	0.94	0.04	44,44,44,44	0
8	HEM	C	608	43/43	0.94	0.09	35,45,51,53	0
8	HEM	A	608	43/43	0.95	0.08	31,39,44,49	0
5	CA	A	603	1/1	0.95	0.05	43,43,43,43	0
5	CA	D	603	1/1	0.95	0.09	36,36,36,36	0
8	HEM	D	608	43/43	0.95	0.09	19,25,39,45	0

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

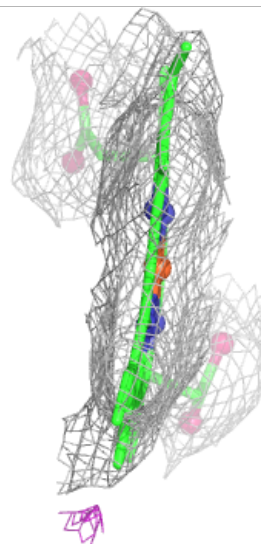
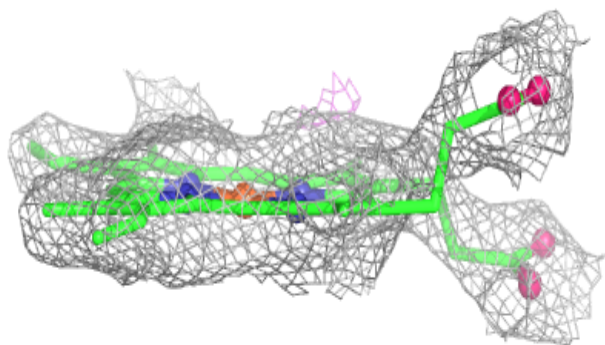
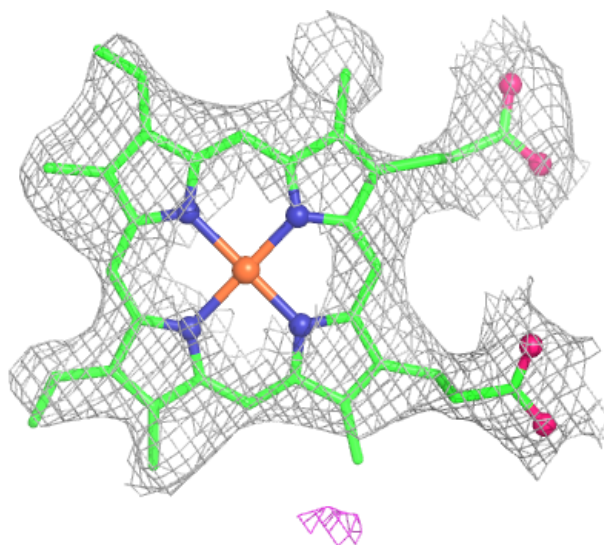
Electron density around HEM B 606:

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



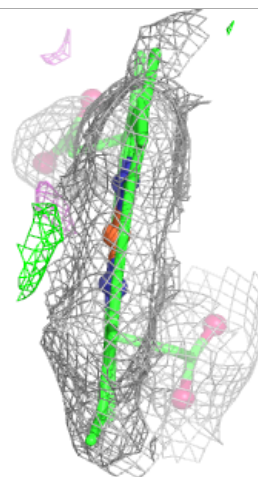
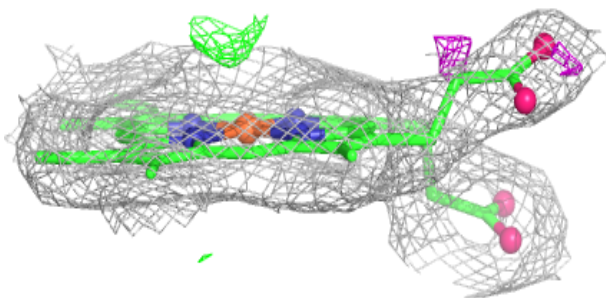
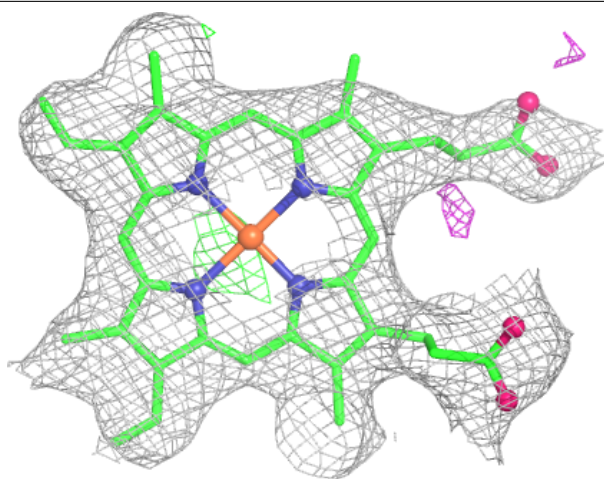
Electron density around HEM C 608:

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



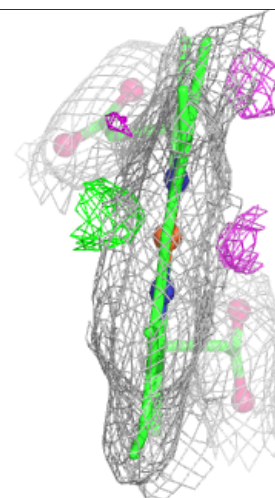
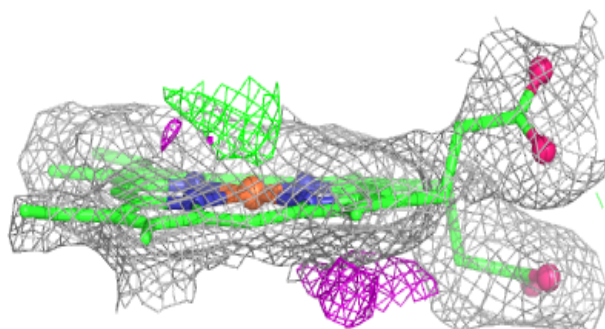
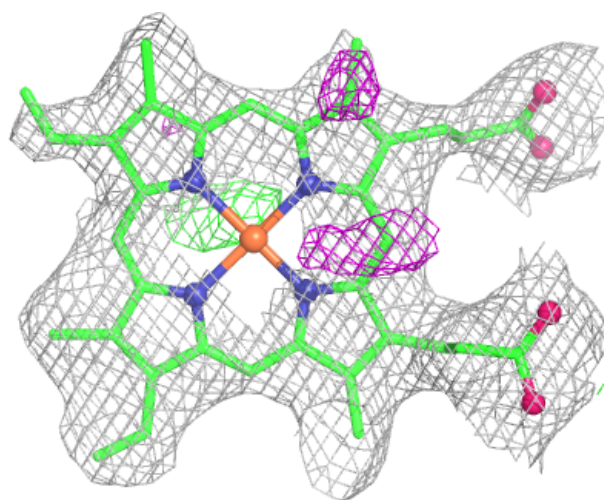
Electron density around HEM A 608:

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



Electron density around HEM D 608:

$2mF_o-DF_c$ (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.