



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 12, 2016 – 08:03 PM EDT

PDB ID : 5HPW
Title : Mode of binding of antithyroid drug, propylthiouracil to lactoperoxidase: Binding studies and structure determination
Authors : Singh, R.P.; Singh, A.; Sharma, P.; Kaur, P.; Sharma, S.; Singh, T.P.
Deposited on : 2016-01-21
Resolution : 2.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20027107
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20027107

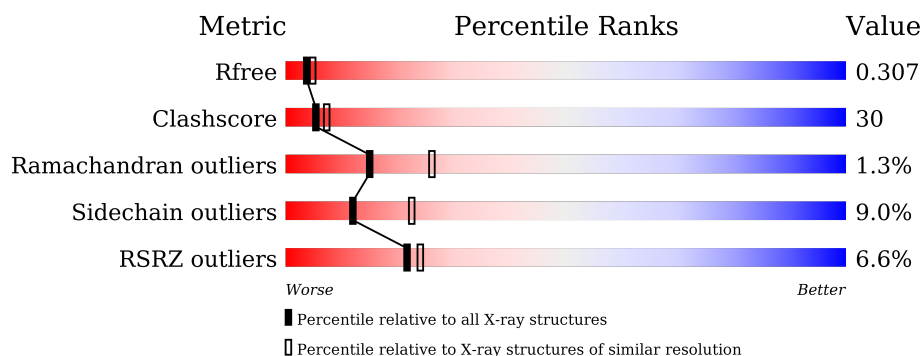
1 Overall quality at a glance

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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	595	<div> <div>5%</div> <div> <div></div> <div>50%</div> <div>45%</div> <div>• •</div> </div> </div>
1	B	595	<div> <div>6%</div> <div> <div></div> <div>55%</div> <div>42%</div> <div>•</div> </div> </div>
1	C	595	<div> <div>9%</div> <div> <div></div> <div>51%</div> <div>44%</div> <div>•</div> </div> </div>
1	D	595	<div> <div>7%</div> <div> <div></div> <div>47%</div> <div>48%</div> <div>5% •</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	601	-	-	-	X
4	NO3	A	606	-	-	-	X
4	NO3	A	608	-	-	-	X
4	NO3	B	607	-	-	-	X
4	NO3	C	606	-	-	-	X
4	NO3	C	608	-	-	X	X
4	NO3	D	606	-	-	X	-
4	NO3	D	607	-	-	X	-
4	NO3	D	608	-	-	X	X
5	3CJ	A	609	-	-	X	-
5	3CJ	B	609	-	-	X	-
5	3CJ	C	609	-	-	X	X
5	3CJ	D	609	-	-	X	X

2 Entry composition [i](#)

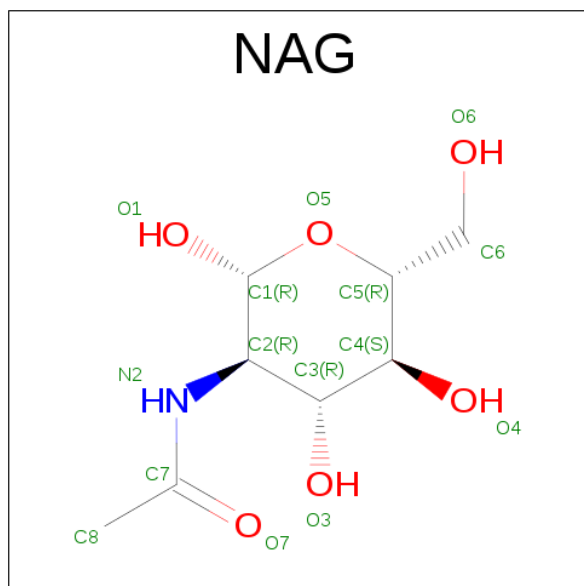
There are 7 unique types of molecules in this entry. The entry contains 20141 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



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

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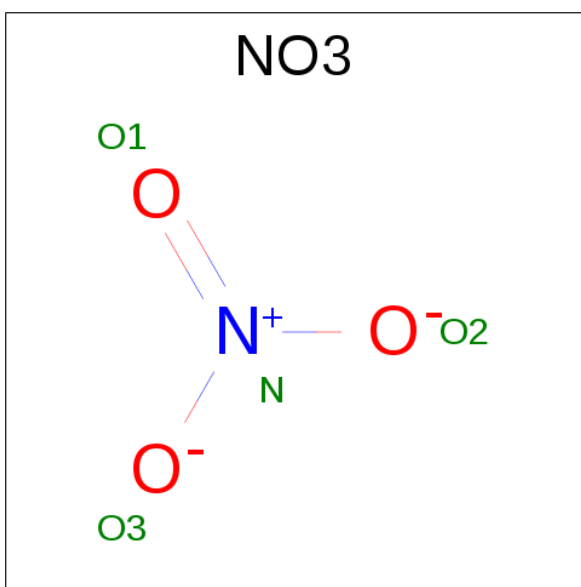
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
	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

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

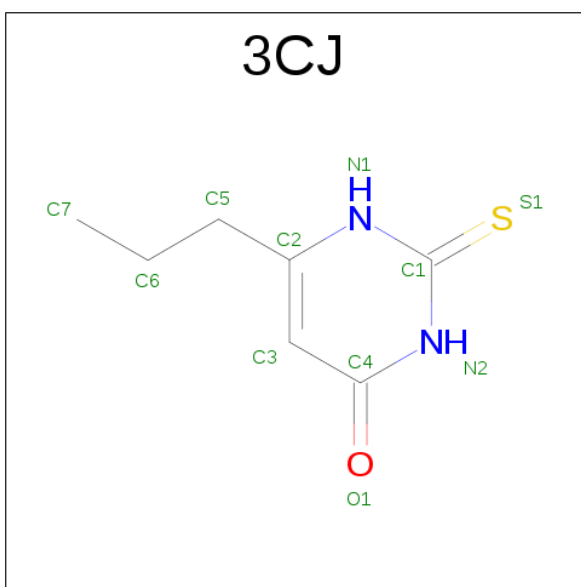
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Ca	0	0
			1	1		
3	A	1	Total	Ca	0	0
			1	1		
3	D	1	Total	Ca	0	0
			1	1		
3	C	1	Total	Ca	0	0
			1	1		

- Molecule 4 is NITRATE ION (three-letter code: NO3) (formula: NO₃).



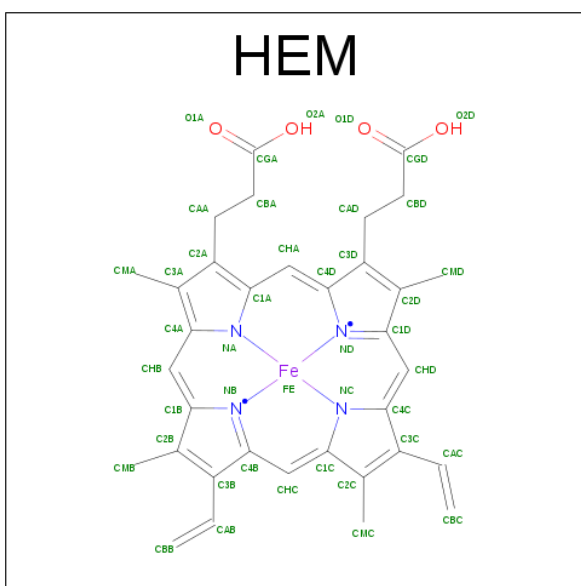
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	N	O	0	0
			4	1	3		
4	A	1	Total	N	O	0	0
			4	1	3		
4	A	1	Total	N	O	0	0
			4	1	3		
4	B	1	Total	N	O	0	0
			4	1	3		
4	B	1	Total	N	O	0	0
			4	1	3		
4	B	1	Total	N	O	0	0
			4	1	3		
4	C	1	Total	N	O	0	0
			4	1	3		
4	C	1	Total	N	O	0	0
			4	1	3		
4	C	1	Total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

- Molecule 5 is 6-propyl-2-thioxo-2,3-dihydropyrimidin-4(1H)-one (three-letter code: 3CJ) (formula: C₇H₁₀N₂OS).



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

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

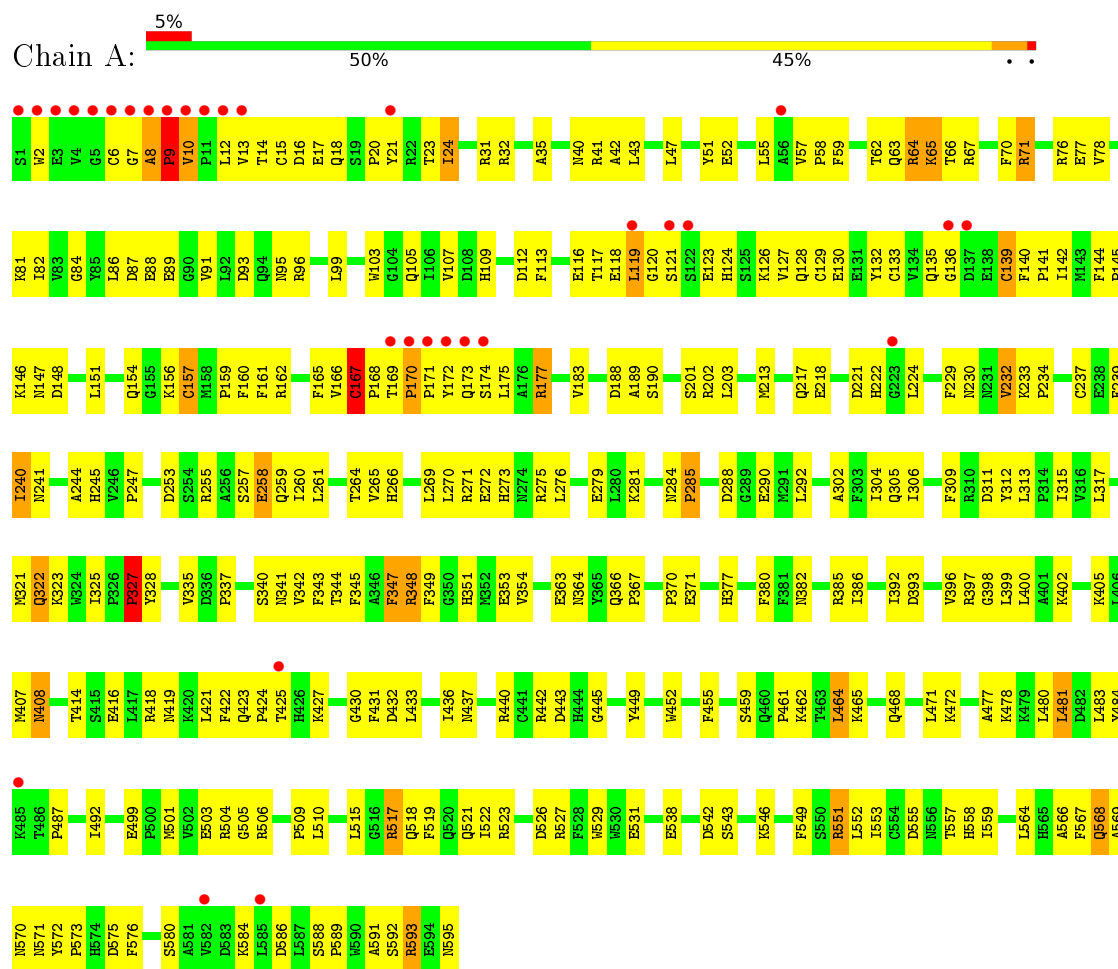
- Molecule 7 is water.

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

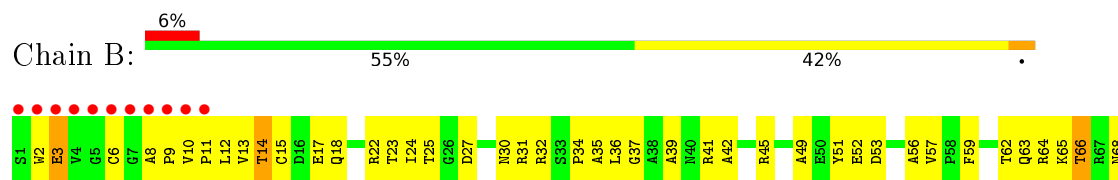
3 Residue-property plots

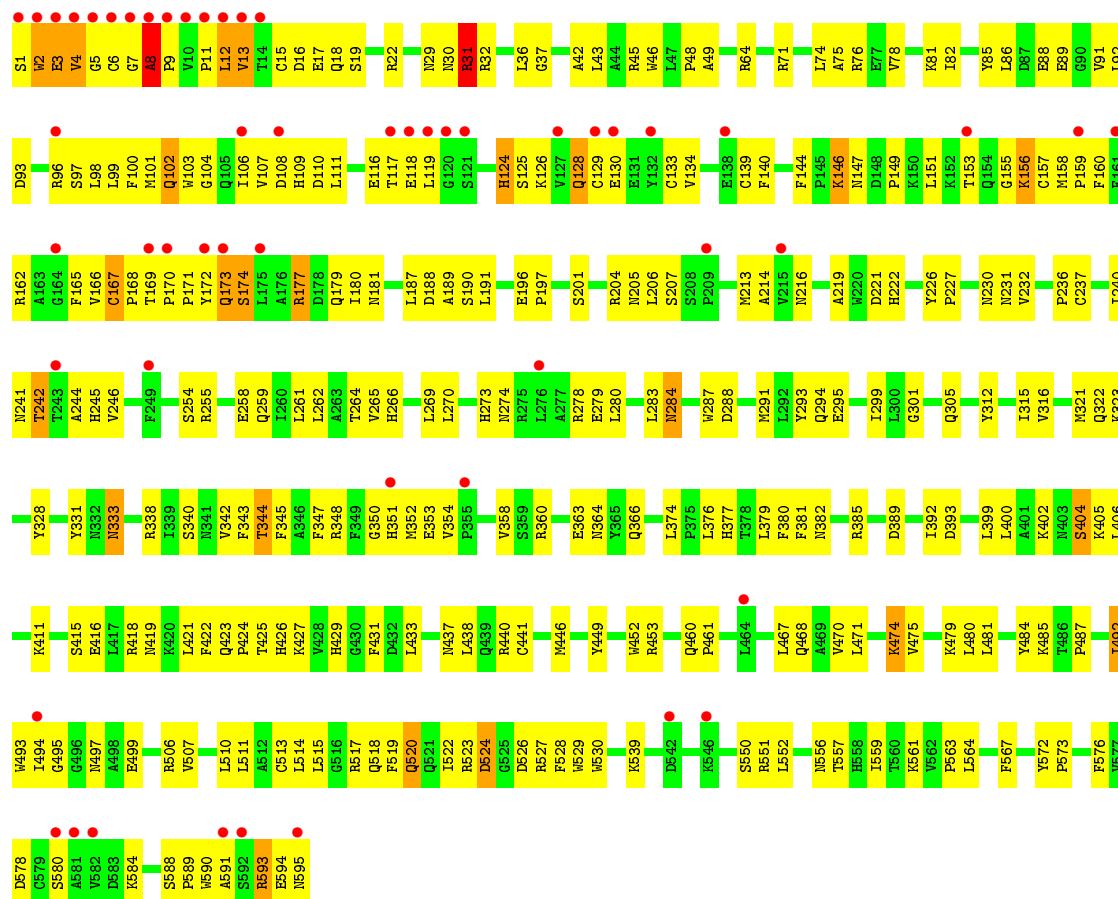
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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

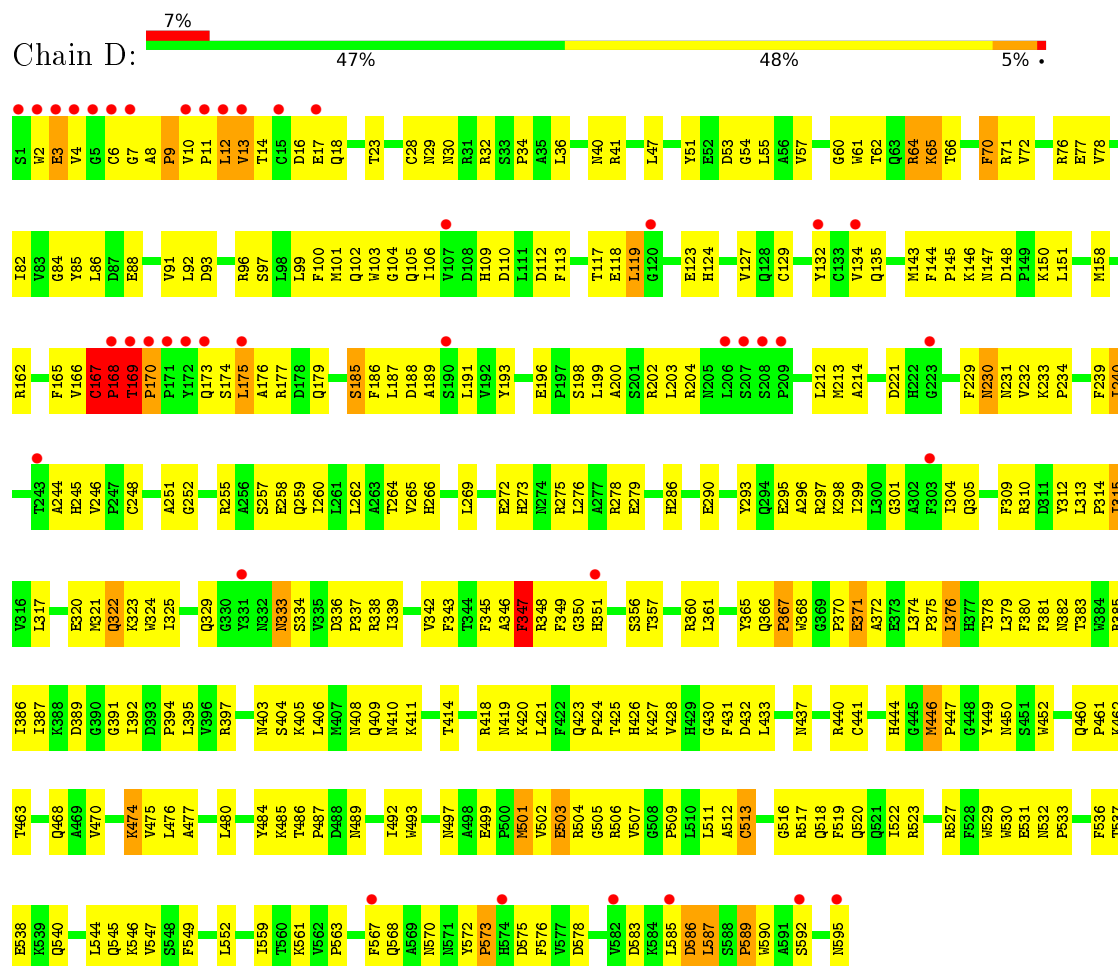


• Molecule 1: Lactoperoxidase





● Molecule 1: Lactoperoxidase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	80.22Å 82.59Å 95.08Å 80.91° 73.71° 89.96°	Depositor
Resolution (Å)	42.50 – 2.50 42.46 – 2.50	Depositor EDS
% Data completeness (in resolution range)	91.7 (42.50-2.50) 87.5 (42.46-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.19 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.260 , 0.311 0.254 , 0.307	Depositor DCC
R_{free} test set	3668 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	41.2	Xtriage
Anisotropy	0.744	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 49.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Outliers	0 of 73032 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.53	2/4882 (0.0%)	0.75	2/6632 (0.0%)
1	B	0.47	0/4882	0.76	0/6632
1	C	0.54	3/4882 (0.1%)	0.76	1/6632 (0.0%)
1	D	0.51	1/4882 (0.0%)	0.79	3/6632 (0.0%)
All	All	0.51	6/19528 (0.0%)	0.76	6/26528 (0.0%)

All (6) bond length outliers are listed below:

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

All (6) bond angle outliers are listed below:

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

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4753	0	4646	298	0
1	B	4753	0	4646	227	0
1	C	4753	0	4649	313	0
1	D	4753	0	4647	290	0
2	A	56	0	51	1	0
2	B	42	0	38	2	0
2	C	56	0	51	1	0
2	D	56	0	51	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	12	0	0	1	0
4	B	12	0	0	1	0
4	C	12	0	0	4	0
4	D	12	0	0	8	0
5	A	11	0	10	11	0
5	B	11	0	10	12	0
5	C	11	0	10	9	0
5	D	11	0	10	11	0
6	A	43	0	30	12	0
6	B	43	0	30	14	0
6	C	43	0	30	17	0
6	D	43	0	30	15	0
7	A	161	0	0	15	0
7	B	155	0	0	10	0
7	C	170	0	0	20	0
7	D	165	0	0	11	0
All	All	20141	0	18939	1151	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 30.

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:GLU:OE2	6:D:610:HEM:CMB	1.65	1.42
1:A:167:CYS:HB2	1:A:168:PRO:CD	1.55	1.32
1:D:258:GLU:OE2	6:D:610:HEM:HMB1	1.18	1.30
1:B:10:VAL:HG11	1:B:41:ARG:NH1	1.48	1.28
1:C:96:ARG:HD2	1:C:100:PHE:CD2	1.73	1.21
1:C:167:CYS:HB3	1:C:168:PRO:CD	1.68	1.17
1:C:96:ARG:HD2	1:C:100:PHE:CE2	1.79	1.16
1:A:62:THR:HG21	1:A:65:LYS:HB2	1.15	1.15
5:D:609:3CJ:H5	6:D:610:HEM:HAA1	1.25	1.13
1:C:96:ARG:NH1	1:C:100:PHE:HE2	1.45	1.12
1:D:169:THR:HB	1:D:170:PRO:HD3	1.32	1.10
1:A:62:THR:HG21	1:A:65:LYS:CB	1.83	1.08
1:C:167:CYS:HB3	1:C:168:PRO:HD2	1.29	1.08
1:B:167:CYS:HB3	1:B:168:PRO:HD2	1.11	1.07
1:A:167:CYS:HB2	1:A:168:PRO:HD3	1.24	1.07
2:B:602:NAG:O4	2:B:603: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	7:C:733:HOH:O	1.59	1.00
1:D:169:THR:CB	1:D:170:PRO:HD3	1.88	0.99
1:A:402:LYS:HD2	4:A:607:NO3:O3	1.61	0.98
1:B:42:ALA:HB2	1:B:166:VAL:HG11	1.46	0.98
1:A:167:CYS:CB	1:A:168:PRO:CD	2.38	0.98
1:A:169:THR:N	1:A:170:PRO:HD2	1.75	0.98
1:A:557:THR:OG1	1:A:559:ILE:HG12	1.65	0.97
1:C:167:CYS:CB	1:C:168:PRO:HD2	1.92	0.97
5:C:609:3CJ:H2	6:C:610:HEM:O1D	1.64	0.96
1:C:96:ARG:NH1	1:C:506:ARG:HG3	1.80	0.95
1:C:593:ARG:NH1	1:C:593:ARG:HB3	1.81	0.95
1:D:13:VAL:HG12	1:D:14:THR:H	1.29	0.95
1:B:10:VAL:HG11	1:B:41:ARG:HH12	1.12	0.93
1:B:10:VAL:CG1	1:B:41:ARG:HH12	1.81	0.93
1:A:62:THR:CG2	1:A:65:LYS:HB2	1.98	0.91
1:C:167:CYS:CB	1:C:168:PRO:CD	2.47	0.91
1:C:102:GLN:OE1	1:C:259:GLN:NE2	2.03	0.90
1:B:537:THR:OG1	1:B:540:GLN:HG3	1.71	0.90
1:D:258:GLU:OE2	6:D:610:HEM:HMB2	1.69	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:ALA:HB1	7:A:762:HOH:O	1.71	0.89
1:B:551:ARG:HD3	1:B:584:LYS:HA	1.53	0.89
1:C:96:ARG:CD	1:C:100:PHE:CE2	2.55	0.89
1:A:117:THR:HG22	1:A:162:ARG:O	1.72	0.89
1:C:312:TYR:O	1:C:315:ILE:HG12	1.73	0.89
1:A:129:CYS:O	1:A:133:CYS:HA	1.73	0.88
1:B:10:VAL:HG11	1:B:41:ARG:CZ	2.03	0.87
1:C:481:LEU:HD21	1:C:487:PRO:HG3	1.55	0.87
1:B:13:VAL:O	1:B:13:VAL:HG12	1.75	0.87
1:A:377:HIS:HB3	1:A:416:GLU:OE1	1.74	0.87
1:C:96:ARG:HH11	1:C:506:ARG:HG3	1.40	0.87
1:A:167:CYS:HB2	1:A:168:PRO:HD2	1.52	0.87
1:B:167:CYS:CB	1:B:168:PRO:CD	2.51	0.86
1:C:593:ARG:HB3	1:C:593:ARG:HH11	1.38	0.86
1:B:537:THR:HG23	1:B:540:GLN:OE1	1.75	0.86
1:D:403:ASN:HB2	4:D:607:NO3:O1	1.76	0.85
1:A:42:ALA:HB2	1:A:166:VAL:HG11	1.58	0.85
1:B:2:TRP:HH2	1:C:86:LEU:HD13	1.41	0.84
1:D:348:ARG:HH11	1:D:437:ASN:ND2	1.75	0.84
1:C:37:GLY:H	1:C:338:ARG:HG2	1.41	0.84
1:C:418:ARG:HG2	1:C:418:ARG:HH11	1.41	0.84
1:D:185:SER:HB3	1:D:339:ILE:HG12	1.58	0.84
1:D:530:TRP:CZ2	4:D:608:NO3:O2	2.30	0.84
1:C:421:LEU:HG	7:C:733:HOH:O	1.76	0.84
1:C:230:ASN:HD21	1:C:232:VAL:HG22	1.42	0.83
1:D:258:GLU:OE2	6:D:610:HEM:C2B	2.32	0.83
1:C:11:PRO:O	1:C:12:LEU:HB3	1.78	0.82
1:A:169:THR:N	1:A:170:PRO:CD	2.40	0.82
1:C:146:LYS:HG3	1:C:147:ASN:OD1	1.79	0.81
1:A:119:LEU:HD12	1:A:120:GLY:H	1.45	0.81
1:D:572:TYR:CE1	1:D:573:PRO:HB3	2.15	0.81
1:B:551:ARG:NH1	1:B:582:VAL:O	2.14	0.81
1:D:92:LEU:HD13	4:D:607:NO3:O1	1.80	0.81
1:D:310:ARG:O	1:D:314:PRO:HG2	1.81	0.81
1:B:276:LEU:O	1:B:280:LEU:HG	1.81	0.80
1:C:513:CYS:O	1:C:517:ARG:HG3	1.82	0.80
2:B:602:NAG:C4	2:B:603:NAG:HN2	1.95	0.79
1:B:332:ASN:OD1	1:B:334:SER:HB2	1.81	0.79
5:D:609:3CJ:C6	6:D:610: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	7:D:804:HOH:O	1.83	0.78
1:C:12:LEU:HG	1:C:13:VAL:H	1.48	0.77
1:A:322:GLN:H	1:A:322:GLN:HE21	1.30	0.77
1:C:468:GLN:HG2	1:C:474:LYS:HA	1.66	0.77
1:B:123:GLU:HB2	1:B:126:LYS:HG3	1.64	0.77
1:B:117:THR:OG1	1:B:119:LEU:HD23	1.83	0.77
5:C:609:3CJ:C6	6:C:610:HEM:HAA1	2.14	0.77
1:A:169:THR:H	1:A:170:PRO:CD	1.95	0.77
1:A:551:ARG:NH1	1:A:584:LYS:HG2	2.00	0.77
1:A:351:HIS:CE1	1:A:433:LEU:HD21	2.21	0.76
1:C:12:LEU:HG	1:C:13:VAL:N	1.99	0.76
1:D:295:GLU:O	1:D:299:ILE:HG13	1.86	0.76
1:C:125:SER:HA	1:C:128:GLN:HB3	1.67	0.76
1:C:96:ARG:NH1	1:C:506:ARG:CG	2.49	0.76
1:D:265:VAL:O	1:D:269:LEU:HG	1.86	0.75
1:B:551:ARG:HD2	1:B:583:ASP:O	1.85	0.75
1:C:146:LYS:HE3	1:C:147:ASN:HD21	1.52	0.75
1:C:348:ARG:HH11	1:C:437:ASN:ND2	1.84	0.75
1:C:452:TRP:HH2	4:C:608:NO3:O3	1.69	0.75
1:C:167:CYS:HB3	1:C:168:PRO:HD3	1.68	0.75
1:B:301:GLY:O	1:B:305:GLN:HG3	1.86	0.75
2:A:604:NAG:H62	2:A:604:NAG:O3	1.87	0.74
1:C:76:ARG:HH22	1:C:419:ASN:HD21	1.35	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
5:C:609:3CJ:H5	6:C:610:HEM:HAA1	1.70	0.74
1:C:159:PRO:HD2	1:C:431:PHE:HE1	1.50	0.73
1:C:348:ARG:HB2	1:C:493:TRP:CD1	2.23	0.73
1:C:96:ARG:HH21	1:C:406:LEU:HD12	1.51	0.73
1:D:113:PHE:CE1	5:D:609:3CJ:H6	2.23	0.73
1:C:519:PHE:HA	1:C:522:ILE:HG13	1.69	0.73
1:C:146:LYS:CE	1:C:147:ASN:HD21	2.02	0.73
1:C:348:ARG:HB2	1:C:493:TRP:NE1	2.02	0.73
1:A:260:ILE:HG23	1:A:261:LEU:HD23	1.70	0.73
1:A:588:SER:HB2	1:A:589:PRO:HD3	1.71	0.73
1:B:118:GLU:HG3	1:B:119:LEU:H	1.52	0.73
1:A:327:PRO:HA	7:A:719:HOH:O	1.89	0.73
1:C:170:PRO:HA	7:C:822:HOH:O	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:409:GLN:NE2	1:B:473:ASN:HD22	1.87	0.72
1:D:375:PRO:HG2	1:D:378:THR:HG23	1.70	0.72
1:A:421:LEU:HB3	1:A:431:PHE:HB2	1.72	0.72
6:B:608:HEM:HBB2	6:B:608:HEM:HMB1	1.72	0.72
1:C:552:LEU:HD12	1:C:556:ASN:ND2	2.05	0.72
1:C:348:ARG:CB	1:C:493:TRP:HE1	2.02	0.72
1:A:239:PHE:HZ	1:A:427:LYS:HB3	1.55	0.72
1:C:530:TRP:NE1	4:C:606:NO3:O2	2.22	0.72
1:B:2:TRP:CZ2	1:C:86:LEU:HD22	2.25	0.71
5:A:609:3CJ:H7	6:A:610:HEM:HBD2	1.73	0.71
1:C:528:PHE:HB3	7:C:840:HOH:O	1.89	0.71
1:C:452:TRP:CH2	4:C:608:NO3:O3	2.44	0.71
1:A:119:LEU:CD1	1:A:120:GLY:N	2.53	0.71
1:B:300:LEU:O	1:B:304:ILE:HD13	1.91	0.71
1:C:427:LYS:N	1:C:427:LYS:HD2	2.05	0.70
1:D:345:PHE:CD2	1:D:446:MET:SD	2.84	0.70
1:A:105:GLN:HG3	5:A:609:3CJ:S1	2.32	0.70
5:A:609:3CJ:H3	6:A:610:HEM:O1D	1.91	0.70
1:C:342:VAL:HB	1:C:452:TRP:CZ2	2.27	0.70
1:D:106:ILE:HG23	1:D:191:LEU:HD11	1.73	0.70
1:D:322:GLN:CD	1:D:322:GLN:H	1.91	0.70
1:B:213:MET:HG2	1:B:273:HIS:CD2	2.26	0.70
1:A:103:TRP:O	1:A:107:VAL:HG23	1.91	0.70
1:B:377:HIS:HA	1:B:380:PHE:CE2	2.26	0.70
1:A:230:ASN:HD21	1:A:232:VAL:HG22	1.55	0.70
1:A:340:SER:OG	1:A:343:PHE:HB2	1.92	0.70
1:B:139:CYS:SG	1:B:141:PRO:HD3	2.32	0.70
1:C:484:TYR:O	1:C:485:LYS:HB2	1.90	0.70
1:C:519:PHE:HA	1:C:522:ILE:CG1	2.21	0.70
1:A:148:ASP:O	1:A:151:LEU:HB2	1.91	0.70
1:A:119:LEU:HD12	1:A:120:GLY:N	2.06	0.70
1:B:39:ALA:HB1	1:B:182:ALA:O	1.92	0.70
1:B:257:SER:HB2	7:B:729:HOH:O	1.91	0.69
1:B:272:GLU:O	1:B:276:LEU:HG	1.93	0.69
1:C:188:ASP:OD1	1:C:190:SER:HB3	1.92	0.69
1:A:99:LEU:HD23	1:A:566:ALA:HB1	1.74	0.69
1:B:421:LEU:HD12	1:B:422:PHE:H	1.57	0.69
1:B:42:ALA:HB2	1:B:166:VAL:CG1	2.21	0.69
1:D:530:TRP:HZ2	4:D:608: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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	7:B:784:HOH:O	1.92	0.68
1:C:423:GLN:HB3	1:C:426:HIS:CD2	2.28	0.68
1:B:261:LEU:HD13	1:B:399:LEU:HD21	1.73	0.68
1:A:119:LEU:CD1	1:A:120:GLY:H	2.06	0.68
1:D:3:GLU:HG2	1:D:4:VAL:H	1.59	0.68
1:A:421:LEU:HB3	1:A:431:PHE:CB	2.24	0.68
1:D:196:GLU:HB3	7: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:30:ASN:O	1:D:34:PRO:HA	1.94	0.68
1:A:367:PRO:HB2	1:D:64:ARG:NH2	2.09	0.68
1:D:7:GLY:C	1:D:9:PRO:HD3	2.14	0.68
1:A:88:GLU:O	1:A:91:VAL:HG22	1.93	0.67
6:B:608:HEM:O1D	5:B:609:3CJ:H3	1.95	0.67
1:C:96:ARG:CZ	1:C:506:ARG:HD2	2.24	0.67
1:C:146:LYS:HE3	1:C:147:ASN:ND2	2.09	0.67
1:A:113:PHE:CE1	5:A:609:3CJ:H5	2.30	0.67
1:A:66:THR:HB	1:A:70:PHE:C	2.13	0.67
6:B:608:HEM:HHA	5:B:609:3CJ:H7	1.77	0.67
1:C:76:ARG:HH22	1:C:419:ASN:ND2	1.92	0.67
1:D:530:TRP:NE1	4:D:608:NO3:O2	2.26	0.67
1:A:464:LEU:HD12	1:A:464:LEU:O	1.94	0.67
1:A:322:GLN:H	1:A:322:GLN:NE2	1.92	0.67
1:C:418:ARG:NH1	1:C:418:ARG:HG2	2.02	0.67
1:D:350:GLY:HA3	6:D:610: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:280:LEU:O	1:B:284:ASN:N	2.28	0.66
1:B:113:PHE:CE1	5:B:609:3CJ:H5	2.30	0.66
1:C:146:LYS:NZ	1:C:147:ASN:HD21	1.93	0.66
1:C:76:ARG:NH1	1:C:418:ARG:HH12	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:370:PRO:HG2	1:D:371:GLU:OE1	1.95	0.66
1:A:2:TRP:HD1	1:A:175:LEU:HD23	1.60	0.66
1:C:345:PHE:O	1:C:493:TRP:HD1	1.79	0.66
1:A:188:ASP:OD1	1:A:190:SER:HB3	1.95	0.66
1:D:570:ASN:HB3	1:D:575:ASP:CB	2.26	0.66
1:C:287:TRP:HA	7:C:749:HOH:O	1.95	0.66
1:D:166:VAL:O	1:D:167:CYS:HB2	1.95	0.66
1:A:17:GLU:OE2	1:A:31:ARG:HG2	1.95	0.66
1:C:204:ARG:CZ	1:C:206:LEU:HD21	2.25	0.66
1:D:10:VAL:HG12	1:D:11:PRO:HD2	1.77	0.66
1:D:530:TRP:CE2	4:D:608:NO3:O2	2.47	0.66
1:B:51:TYR:HB3	1:B:57:VAL:O	1.96	0.65
1:D:11:PRO:O	1:D:13:VAL:HG23	1.96	0.65
1:C:348:ARG:HB2	1:C:493:TRP:HE1	1.58	0.65
1:D:123:GLU:HG3	7:D:804:HOH:O	1.95	0.65
1:A:167:CYS:HB3	1:A:168:PRO:HD3	1.77	0.65
1:A:253:ASP:OD2	1:A:255:ARG:HB2	1.96	0.65
1:A:165:PHE:CD2	1:A:177:ARG:HD2	2.32	0.65
1:A:322:GLN:N	1:A:322:GLN:HE21	1.94	0.65
1:C:37:GLY:N	1:C:338:ARG:HG2	2.11	0.65
1:C:98:LEU:HA	1:C:404:SER:OG	1.97	0.65
1:A:370:PRO:O	1:D:71:ARG:NH2	2.29	0.65
1:A:99:LEU:HG	1:A:567:PHE:HE1	1.61	0.65
1:B:407:MET:SD	1:B:408:ASN:N	2.69	0.65
1:C:201:SER:HA	7:C:816:HOH:O	1.95	0.65
1:C:109:HIS:HA	1:C:255:ARG:NH2	2.11	0.65
1:A:551:ARG:NH1	1:A:584:LYS:CG	2.60	0.65
1:B:94:GLN:O	1:B:569:ALA:HB3	1.96	0.65
1:A:71:ARG:CZ	1:A:71:ARG:HB3	2.24	0.65
1:D:463:THR:HB	7:D:714:HOH:O	1.94	0.65
1:D:105:GLN:NE2	5:D:609:3CJ:S1	2.60	0.65
1:A:95:ASN:O	1:A:96:ARG:HD3	1.97	0.65
1:B:145:PRO:O	1:B:148:ASP:HB2	1.97	0.65
1:B:10:VAL:HG21	1:B:41:ARG:HH12	1.62	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	7:C:720:HOH:O	1.98	0.64
1:D:408:ASN:O	1:D:411:LYS:N	2.28	0.64
1:A:123:GLU:HB2	1:A:126:LYS:HG3	1.78	0.64
1:A:348:ARG:HG2	6:A:610:HEM:C2D	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:ILE:HD12	1:A:160:PHE:HB2	1.77	0.64
1:A:546:LYS:HZ1	1:A:586:ASP:H	1.46	0.64
1:C:351:HIS:CE1	1:C:433:LEU:HD21	2.32	0.64
1:A:62:THR:CG2	1:A:65:LYS:H	2.10	0.64
1:C:393:ASP:OD1	1:C:557:THR:HB	1.96	0.64
1:D:112:ASP:OD1	6:D:610:HEM:O2D	2.16	0.64
1:B:265:VAL:O	1:B:269:LEU:HG	1.98	0.63
1:C:264:THR:HG23	1:C:392:ILE:HG23	1.81	0.63
1:D:368:TRP:O	1:D:372:ALA:HB2	1.98	0.63
1:D:424:PRO:O	1:D:425:THR:HB	1.96	0.63
1:B:145:PRO:HD2	1:B:148:ASP:OD2	1.96	0.63
1:A:8:ALA:HA	7:A:813:HOH:O	1.97	0.63
1:B:230:ASN:OD1	1:B:232:VAL:HG22	1.98	0.63
1:D:8:ALA:N	1:D:9:PRO:HD3	2.13	0.63
1:B:532:ASN:O	1:B:535:VAL:HG23	1.98	0.63
6:B:608:HEM:CHA	5:B:609:3CJ:H7	2.29	0.63
1:A:123:GLU:CB	1:A:126:LYS:HG3	2.29	0.63
1:B:167:CYS:SG	1:B:168:PRO:CD	2.87	0.63
1:A:121:SER:O	1:A:123:GLU:N	2.30	0.63
1:C:110:ASP:OD1	1:C:187:LEU:HA	1.99	0.63
1:D:167:CYS:HB3	1:D:168:PRO:CD	2.28	0.63
1:C:146:LYS:HE3	1:C:147:ASN:OD1	1.98	0.62
1:B:18:GLN:HG3	7: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	7:D:812:HOH:O	2.00	0.62
1:D:446:MET:HE3	4:D:606:NO3:O1	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:PHE:CZ	1:A:427:LYS:HB3	2.35	0.61
6:B:608:HEM:C1A	5:B:609:3CJ:N1	2.68	0.61
1:D:342:VAL:HB	1:D:446:MET:HE1	1.82	0.61
1:D:503:GLU:O	1:D:504:ARG:HB2	2.00	0.61
1:A:172:TYR:HE2	1:A:175:LEU:HB2	1.65	0.61
1:B:52:GLU:HG3	1:B:59:PHE:HA	1.81	0.61
1:C:425:THR:O	1:C:425:THR:HG22	2.01	0.61
1:D:309:PHE:HA	1:D:313:LEU:HD12	1.82	0.61
1:A: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	6:D:610:HEM:NC	2.69	0.61
1:A:174:SER:O	1:A:175:LEU:HG	2.01	0.61
1:D:240:ILE:HD13	1:D:382:ASN:HA	1.82	0.61
1:B:35:ALA:HB1	1:B:41:ARG:NE	2.16	0.61
1:D:101:MET:SD	1:D:101:MET:C	2.79	0.61
1:D:186:PHE:O	1:D:188:ASP:N	2.33	0.61
1:D:301:GLY:O	1:D:305:GLN:HG3	2.01	0.61
1:D:9:PRO:HG2	1:D:41:ARG:HH22	1.66	0.61
1:A:105:GLN:HB2	6:A:610:HEM:C2C	2.36	0.61
1:A:62:THR:HG21	1:A:65:LYS:H	1.66	0.61
1:D:325:ILE:O	1:D:325:ILE:HG22	2.01	0.61
1:D:113:PHE:HE1	5:D:609:3CJ:H6	1.66	0.61
1:A:165:PHE:CZ	1:A:169:THR:O	2.53	0.60
1:A:272:GLU:O	1:A:276:LEU:HG	2.01	0.60
1:C:168:PRO:HG3	1:C:172:TYR:HD2	1.67	0.60
1:C:539:LYS:HE2	1:C:589:PRO:HG3	1.81	0.60
1:C:151:LEU:HD11	1:C:156:LYS:HD2	1.82	0.60
1:C:169:THR:N	1:C:170:PRO:CD	2.64	0.60
1:D:144:PHE:CE1	1:D:158:MET:HG3	2.37	0.60
1:A:62:THR:HG21	1:A:65:LYS:N	2.16	0.60
1:B:110:ASP:OD2	1:B:189:ALA:HA	2.02	0.60
1:B:13:VAL:CG1	1:B:13:VAL:O	2.49	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
5:C:609:3CJ:H4	6:C:610:HEM:HAA1	1.82	0.60
1:D:586:ASP:O	1:D:589:PRO:HD2	2.02	0.60
5:D:609:3CJ:H2	6:D:610:HEM:O1D	2.02	0.60
1:A:81:LYS:HB2	1:A:483:LEU:HD11	1.84	0.60
1:D:7:GLY:HA2	1:D:166:VAL:HB	1.84	0.60
1:D:8:ALA:N	1:D:9:PRO:CD	2.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:325:ILE:O	1:A:325:ILE:HG22	2.02	0.60
1:D:492:ILE:HG23	1:D:493:TRP:N	2.17	0.60
1:B:258:GLU:O	1:B:380:PHE:HA	2.01	0.59
1:C:191:LEU:HD23	1:C:191:LEU:H	1.67	0.59
1:D:348:ARG:NH1	1:D:437:ASN:ND2	2.47	0.59
1:A:396:VAL:HA	1:A:399:LEU:HD12	1.84	0.59
1:A:342:VAL:HG11	1:A:452:TRP:CH2	2.37	0.59
1:C:12:LEU:O	1:C:13:VAL:HB	2.01	0.59
1:C:165:PHE:CG	1:C:177:ARG:HD2	2.37	0.59
6:D:610:HEM:HMC1	6:D:610:HEM:HBC2	1.84	0.59
1:B:409:GLN:HE22	1:B:473:ASN:HB2	1.66	0.59
1:C:169:THR:N	1:C:170:PRO:HD3	2.18	0.59
1:A:165:PHE:CG	1:A:177:ARG:HD2	2.37	0.59
1:A:392:ILE:O	1:A:396:VAL:HG23	2.01	0.59
1:C:165:PHE:CZ	1:C:169:THR:O	2.56	0.59
1:D:425:THR:O	1:D:425:THR:HG22	2.02	0.59
1:A:229:PHE:CD1	1:A:247:PRO:HG2	2.38	0.59
1:D:168:PRO:HB2	1:D:170:PRO:HD2	1.84	0.59
1:A:156:LYS:HG3	7:A:742:HOH:O	2.02	0.59
1:C:522:ILE:O	1:C:526:ASP:HB2	2.03	0.59
6:A:610:HEM:HMC2	6:A:610:HEM:HBC2	1.85	0.59
1:A:99:LEU:HG	1:A:567:PHE:CE1	2.38	0.59
1:C:557:THR:OG1	1:C:559:ILE:HG12	2.02	0.59
1:D:419:ASN:O	1:D:430:GLY:HA2	2.03	0.58
1:A:8:ALA:N	1:A:9:PRO:CD	2.66	0.58
1:D:106:ILE:HG23	1:D:191:LEU:CD1	2.33	0.58
1:D:96:ARG:HG3	1:D:506:ARG:HE	1.68	0.58
1:A:9:PRO:HB2	1:A:41:ARG:NH2	2.18	0.58
1:C:99:LEU:HA	1:C:399:LEU:HD22	1.85	0.58
1:D:117:THR:HG22	1:D:162:ARG:O	2.04	0.58
1:D:9:PRO:HG2	1:D:41:ARG:NH2	2.19	0.58
1:A:146:LYS:O	1:A:147:ASN:HB2	2.04	0.58
1:A:348:ARG:HG2	6:A:610:HEM:C3D	2.39	0.58
1:D:486:THR:HG23	1:D:489:ASN:H	1.69	0.58
1:D:501:MET:HA	1:D:507:VAL:O	2.03	0.58
1:A:504:ARG:HD3	7:A:831:HOH:O	2.02	0.58
1:A:66:THR:HB	1:A:70:PHE:O	2.03	0.58
1:D:199:LEU:HD12	1:D:199:LEU:O	2.04	0.58
1:B:348:ARG:HH11	1:B:437:ASN:ND2	2.02	0.58
1:B:62:THR:HB	1:B:65:LYS:HB2	1.84	0.58
1:C:124:HIS:HE1	1:C:128:GLN:HB2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:301:GLY:O	1:C:305:GLN:HG3	2.03	0.58
1:A:9:PRO:HB2	1:A:41:ARG:CZ	2.34	0.58
1:B:148:ASP:HB3	1:B:151:LEU:HD22	1.85	0.58
1:B:418:ARG:HG2	1:B:432:ASP:OD2	2.03	0.57
1:D:10:VAL:HG12	1:D:11:PRO:N	2.19	0.57
1:A:222:HIS:HB3	7:A:840:HOH:O	2.04	0.57
1:A:421:LEU:HG	1:A:422:PHE:N	2.18	0.57
1:D:10:VAL:CG1	1:D:11:PRO:CD	2.82	0.57
1:D:342:VAL:HB	1:D:446:MET:CE	2.33	0.57
1:C:196:GLU:HB3	7:C:707:HOH:O	2.03	0.57
1:C:2:TRP:N	1:C:2:TRP:CE3	2.73	0.57
1:D:361:LEU:HD13	1:D:365:TYR:O	2.05	0.57
1:A:233:LYS:NZ	1:B:322:GLN:HB2	2.20	0.57
1:C:197:PRO:HD2	7:C:707:HOH:O	2.03	0.57
1:D:234:PRO:HB2	7:D:821:HOH:O	2.04	0.57
1:B:66:THR:HB	1:B:70:PHE:O	2.05	0.57
1:C:258:GLU:O	1:C:380:PHE:HA	2.04	0.57
1:C:440:ARG:NH2	6:C:610:HEM:O1A	2.38	0.57
1:D:421:LEU:HD22	1:D:433:LEU:HB2	1.86	0.57
1:D:231:ASN:O	1:D:233:LYS:HE2	2.04	0.57
1:B:168:PRO:CG	1:B:172:TYR:HB3	2.35	0.57
1:B:392:ILE:O	1:B:396:VAL:HG23	2.05	0.57
1:B:425:THR:O	1:B:425:THR:HG22	2.05	0.57
1:C:167:CYS:HB2	1:C:168:PRO:HD2	1.85	0.57
1:C:299:ILE:HD11	1:C:590:TRP:NE1	2.20	0.57
1:A:71:ARG:HB3	1:A:71:ARG:NH1	2.20	0.57
1:D:119:LEU:HD22	1:D:169:THR:HG21	1.86	0.57
1:B:406:LEU:HG	1:B:407:MET:N	2.19	0.56
1:A:117:THR:O	1:A:161:PHE:HB3	2.05	0.56
5:A:609:3CJ:C5	6:A:610:HEM:HBD2	2.35	0.56
1:C:475:VAL:HG12	1:C:479:LYS:HE2	1.88	0.56
1:D:572:TYR:CD1	1:D:573:PRO:HB3	2.38	0.56
1:C:168:PRO:HB2	1:C:170:PRO:HD2	1.87	0.56
1:B:10:VAL:CG2	1:B:41:ARG:HH12	2.16	0.56
1:C:81:LYS:HB3	7:C:821:HOH:O	2.03	0.56
1:D:492:ILE:HG23	1:D:493:TRP:H	1.68	0.56
1:C:173:GLN:O	1:C:174:SER:HB2	2.04	0.56
1:D:109:HIS:HA	1:D:255:ARG:NH2	2.20	0.56
1:A:275:ARG:HD2	1:A:555:ASP:HB3	1.88	0.56
1:A:281:LYS:HD2	1:A:285:PRO:HA	1.87	0.56
1:A:62:THR:CG2	1:A:65:LYS:N	2.69	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ALA:HB2	1:A:304:ILE:HD12	1.87	0.56
1:C:204:ARG:CZ	1:C:206:LEU:CD2	2.84	0.56
1:C:517:ARG:HB3	1:C:517:ARG:HH21	1.70	0.56
1:A:144:PHE:CE2	1:A:157:CYS:N	2.74	0.56
1:A:465:LYS:HA	1:A:468:GLN:HE21	1.71	0.56
1:A:367:PRO:HB2	1:D:64:ARG:CZ	2.35	0.56
1:C:133:CYS:HB2	7:C:748:HOH:O	2.06	0.56
1:B:193:TYR:CE2	1:B:297:ARG:HG3	2.41	0.55
1:C:1:SER:C	1:C:2:TRP:CE3	2.80	0.55
1:D:96:ARG:HD2	1:D:100:PHE:CD2	2.40	0.55
1:D:29:ASN:HD21	1:D:527:ARG:H	1.53	0.55
1:A:393:ASP:OD2	1:A:558:HIS:HB2	2.06	0.55
1:A:169:THR:OG1	1:A:170:PRO:HD3	2.07	0.55
1:A:213:MET:CB	1:A:270:LEU:HD11	2.36	0.55
1:B:167:CYS:SG	1:B:168:PRO:HD2	2.46	0.55
1:B:193:TYR:CD2	1:B:297:ARG:HG3	2.41	0.55
1:D:529:TRP:CD1	1:D:531:GLU:HB2	2.40	0.55
1:A:109:HIS:NE2	5:A:609:3CJ:C1	2.70	0.55
1:A:13:VAL:HG12	1:A:14:THR:N	2.22	0.55
1:A:20:PRO:O	1:A:21:TYR:CD1	2.60	0.55
1:D:113:PHE:CD1	5:D:609:3CJ:H6	2.41	0.55
1:D:199:LEU:O	1:D:203:LEU:HG	2.06	0.55
1:D:146:LYS:O	1:D:147:ASN:HB2	2.06	0.55
1:B:113:PHE:HE1	5:B:609:3CJ:H5	1.71	0.55
1:C:125:SER:CA	1:C:128:GLN:HB3	2.36	0.55
1:A:87:ASP:OD1	1:A:89:GLU:HB2	2.07	0.55
1:B:118:GLU:HG3	7:B:716:HOH:O	2.07	0.55
1:C:134:VAL:HA	7:C:716:HOH:O	2.07	0.55
5:D:609:3CJ:H7	6:D:610:HEM:HBD2	1.89	0.55
1:A:43:LEU:HD13	1:A:341:ASN:HA	1.88	0.55
1:A:499:GLU:OE1	1:A:509:PRO:HG2	2.07	0.55
1:B:123:GLU:CB	1:B:126:LYS:HG3	2.34	0.55
1:C:381:PHE:CZ	1:C:424:PRO:HG3	2.43	0.54
6:C:610:HEM:HMB1	6:C:610:HEM:HBB2	1.88	0.54
1:D:167:CYS:CB	1:D:168:PRO:HD2	2.37	0.54
1:B:377:HIS:ND1	1:B:416:GLU:OE1	2.40	0.54
1:C:97:SER:O	1:C:98:LEU:C	2.46	0.54
1:D:333:ASN:HD22	1:D:333:ASN:N	2.03	0.54
1:A:367:PRO:HB2	1:D:64:ARG:HH21	1.70	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:GLU:O	1:D:276:LEU:HG	2.07	0.54
1:B:409:GLN:HE21	1:B:473:ASN:HD22	1.55	0.54
1:C:342:VAL:HG21	1:C:452:TRP:CE2	2.42	0.54
1:C:96:ARG:CZ	1:C:506:ARG:CD	2.85	0.54
1:D: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:A:203:LEU:HD13	1:A:213:MET:HE1	1.89	0.54
1:B:593:ARG:HG3	1:B:595:ASN:H	1.72	0.54
1:B:341:ASN:HB3	1:B:446:MET:HE1	1.89	0.54
6:B:608:HEM:HMC2	6:B:608:HEM:HBC2	1.89	0.54
1:C:7:GLY:O	1:C:8:ALA:HB3	2.07	0.54
1:A:62:THR:O	1:A:63:GLN:HB3	2.07	0.54
1:C:280:LEU:O	1:C:284:ASN:ND2	2.41	0.54
1:D:96:ARG:NH2	1:D:315:ILE:HB	2.23	0.54
1:C:1:SER:C	1:C:2:TRP:HE3	2.10	0.54
1:D:9:PRO:CG	1:D:41:ARG:NH2	2.71	0.54
1:A:408:ASN:C	1:A:408:ASN:OD1	2.46	0.53
1:C:259:GLN:OE1	1:C:261:LEU:HB2	2.08	0.53
1:C:213:MET:HG2	1:C:273:HIS:NE2	2.24	0.53
1:D:193:TYR:OH	1:D:297:ARG:HA	2.07	0.53
1:D:96:ARG:CZ	1:D:315:ILE:HB	2.38	0.53
1:C:82:ILE:HD12	1:C:480:LEU:HD23	1.91	0.53
1:D:103:TRP:O	1:D:106:ILE:N	2.36	0.53
1:D:9:PRO:HG3	1:D:41:ARG:CZ	2.39	0.53
1:B:117:THR:HG22	1:B:161:PHE:HB3	1.89	0.53
1:A:367:PRO:HB2	1:D:64:ARG:NE	2.24	0.53
1:B:30:ASN:O	1:B:34:PRO:HA	2.07	0.53
1:C:551:ARG:O	1:C:552:LEU:C	2.45	0.53
1:D:446:MET:CE	4:D:606:NO3:O1	2.56	0.53
1:D:589:PRO:HB2	1:D:590:TRP:CE3	2.43	0.53
1:D:214:ALA:HA	2:D:602:NAG:O7	2.08	0.53
1:A:15:CYS:HB3	7:A:747:HOH:O	2.09	0.53
1:A:99:LEU:CD2	1:A:566:ALA:HB1	2.39	0.53
1:A:62:THR:HG21	1:A:65:LYS:CA	2.37	0.53
1:B:117:THR:CG2	1:B:161:PHE:HB3	2.39	0.53
6:B:608:HEM:CHA	5:B:609:3CJ:N1	2.71	0.53
1:C:452:TRP:CD1	1:C:492:ILE:HG12	2.43	0.53
1:D:563:PRO:HD3	1:D:576:PHE:CE2	2.44	0.53
1:A:142:ILE:CD1	1:A:160:PHE:HB2	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:GLN:HG3	1:B:134:VAL:HG21	1.91	0.53
1:B:165:PHE:CZ	1:B:169:THR:O	2.62	0.53
1:B:522:ILE:HG13	1:B:523:ARG:N	2.22	0.53
1:C:205:ASN:HB2	1:C:214:ALA:HA	1.90	0.53
1:A:16:ASP:O	1:A:18:GLN:N	2.37	0.53
1:A:233:LYS:HZ2	1:B:322:GLN:HB2	1.73	0.53
1:C:237:CYS:HA	1:C:381:PHE:O	2.09	0.53
1:C:385:ARG:NH1	1:C:389:ASP:OD2	2.42	0.53
1:D:376:LEU:HD21	1:D:380:PHE:HE1	1.74	0.53
1:C:523:ARG:HG3	1:C:529:TRP:CE2	2.43	0.52
1:D:119:LEU:CD2	1:D:169:THR:HG21	2.39	0.52
1:C:11:PRO:O	1:C:12:LEU:CB	2.51	0.52
1:C:204:ARG:HB2	1:C:206:LEU:HG	1.91	0.52
1:D:6:CYS:O	1:D:167:CYS:SG	2.67	0.52
1:A:241:ASN:ND2	1:A:244:ALA:HB2	2.24	0.52
1:B:167:CYS:SG	1:B:168:PRO:HD3	2.49	0.52
1:C:144:PHE:HE1	1:C:158:MET:HG3	1.74	0.52
1:C:437:ASN:O	1:C:440:ARG:N	2.40	0.52
1:B:2:TRP:CH2	1:C:86:LEU:HD13	2.31	0.52
1:C:97:SER:O	1:C:99:LEU:N	2.42	0.52
1:A:13:VAL:HG12	1:A:14:THR:H	1.74	0.52
1:A:492:ILE:HD11	1:A:510:LEU:HD21	1.90	0.52
1:B:93:ASP:OD2	1:B:406:LEU:HD12	2.09	0.52
1:C:125:SER:O	1:C:128:GLN:HB3	2.08	0.52
1:D:397:ARG:HG3	1:D:559:ILE:HD12	1.91	0.52
1:D:424:PRO:O	1:D:425:THR:CB	2.58	0.52
1:D:513:CYS:O	1:D:517:ARG:HG2	2.09	0.52
1:C:96:ARG:CZ	1:C:100:PHE:CE2	2.92	0.52
1:C:400:LEU:HD13	1:C:563:PRO:HD2	1.91	0.52
1:D:348:ARG:HH22	1:D:440:ARG:HG2	1.73	0.52
1:A:168:PRO:HB2	1:A:170:PRO:O	2.10	0.52
1:C:117:THR:HG22	1:C:162:ARG:O	2.09	0.52
1:C:29:ASN:HD21	1:C:527:ARG:H	1.57	0.52
1:C:552:LEU:HD12	1:C:556:ASN:HD22	1.74	0.52
1:A:52:GLU:OE2	1:A:62:THR:HG22	2.09	0.52
1:B:352:MET:O	1:B:405:LYS:HD3	2.10	0.52
1:C:64:ARG:HA	1:C:71:ARG:NH2	2.25	0.52
1:A:128:GLN:HA	1:A:132:TYR:HD1	1.75	0.52
1:C:221:ASP:HB2	1:C:226:TYR:CZ	2.44	0.52
1:D:143:MET:HG2	7:D:725:HOH:O	2.09	0.52
1:B:418:ARG:HH11	1:B:418:ARG:HG2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:244:ALA:O	1:D:245:HIS:HB2	2.10	0.52
1:A:113:PHE:HE1	5:A:609:3CJ:H5	1.75	0.52
1:B:42:ALA:CB	1:B:166:VAL:HG11	2.30	0.52
1:B:551:ARG:CD	1:B:583:ASP:O	2.57	0.52
6:B:608:HEM:HAA1	5:B:609:3CJ:H4	1.92	0.52
1:C:29:ASN:HD21	1:C:527:ARG:N	2.08	0.52
1:D:16:ASP:O	1:D:17:GLU:HB3	2.10	0.52
1:C:288:ASP:OD1	1:C:291:MET:HB3	2.10	0.51
1:D:102:GLN:OE1	1:D:259:GLN:NE2	2.35	0.51
1:A:258:GLU:O	1:A:380:PHE:HA	2.09	0.51
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.46	0.51
1:B:10:VAL:CB	1:B:41:ARG:HH12	2.23	0.51
1:B:169:THR:N	1:B:170:PRO:HD2	2.26	0.51
1:D:257:SER:O	1:D:381:PHE:HA	2.11	0.51
1:A:340:SER:HG	1:A:343:PHE:HB2	1.75	0.51
1:A:551:ARG:HD2	1:A:584:LYS:HA	1.91	0.51
1:B:397:ARG:NH2	1:B:559:ILE:HD13	2.25	0.51
1:C:561:LYS:HD3	1:C:576:PHE:HB3	1.92	0.51
1:D:379:LEU:HA	1:D:382:ASN:HB2	1.91	0.51
1:A:8:ALA:N	1:A:9:PRO:HD2	2.26	0.51
1:C:146:LYS:HE3	1:C:147:ASN:CG	2.30	0.51
1:C:287:TRP:CZ3	1:C:295:GLU:HG3	2.45	0.51
1:C:75:ALA:HB1	1:C:438:LEU:HB2	1.92	0.51
1:B:25:THR:O	1:B:184:THR:HG22	2.10	0.51
1:B:37:GLY:H	1:B:338:ARG:HG2	1.76	0.51
1:C:348:ARG:CB	1:C:493:TRP:NE1	2.68	0.51
1:A:593:ARG:HD2	1:A:595:ASN:H	1.75	0.51
1:A:7:GLY:O	1:A:8:ALA:HB3	2.10	0.51
1:B:180:ILE:HG22	1:B:181:ASN:N	2.25	0.51
1:C:76:ARG:NH1	1:C:418:ARG:NH1	2.59	0.51
1:A:315:ILE:O	1:A:505:GLY:HA2	2.11	0.51
1:C:441:CYS:O	1:C:446:MET:HB2	2.10	0.51
1:D:349:PHE:CD1	1:D:349:PHE:C	2.84	0.51
1:D:499:GLU:OE1	1:D:509:PRO:HG2	2.11	0.51
1:C:116:GLU:O	1:C:117:THR:HB	2.10	0.51
1:D:349:PHE:CD1	1:D:350:GLY:N	2.78	0.51
1:B:447:PRO:HG2	1:B:452:TRP:NE1	2.25	0.51
1:B:503:GLU:O	1:B:504:ARG:HB2	2.10	0.51
1:B:530:TRP:CG	1:B:531:GLU:N	2.79	0.51
1:B:556:ASN:O	1:B:557:THR:HG23	2.10	0.51
1:B:56:ALA:O	1:B:162:ARG:NH1	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:321:MET:C	1:B:323:LYS:H	2.13	0.50
1:D:169:THR:HB	1:D:170:PRO:CD	2.22	0.50
1:D:474:LYS:HB3	1:D:474:LYS:NZ	2.26	0.50
1:A:245:HIS:CG	1:A:245:HIS:O	2.65	0.50
1:A:63:GLN:O	1:A:63:GLN:HG3	2.11	0.50
1:B:409:GLN:NE2	1:B:473:ASN:ND2	2.59	0.50
1:B:78:VAL:HA	1:B:483:LEU:HD13	1.93	0.50
1:C:358:VAL:HB	1:C:379:LEU:CD1	2.41	0.50
1:C:415:SER:HB2	7:C:800:HOH:O	2.11	0.50
1:D:167:CYS:HB2	1:D:168:PRO:HD2	1.91	0.50
1:A:312:TYR:O	1:A:315:ILE:HG12	2.12	0.50
1:D:221:ASP:OD1	1:D:221:ASP:C	2.50	0.50
1:D:312:TYR:N	1:D:567:PHE:HE2	2.09	0.50
1:C:125:SER:HA	1:C:128:GLN:CB	2.40	0.50
1:D:255:ARG:HH11	5:D:609:3CJ:H7	1.77	0.50
1:B:166:VAL:HG22	1:B:178:ASP:O	2.11	0.50
1:C:124:HIS:HD1	1:C:125:SER:N	2.09	0.50
1:C:259:GLN:HG3	1:C:262:LEU:HB3	1.94	0.50
1:D:204:ARG:HH22	1:D:290:GLU:HA	1.77	0.50
1:D:376:LEU:O	1:D:379:LEU:N	2.39	0.50
1:D:298:LYS:HG2	1:D:536:PHE:CZ	2.47	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	7: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	4:B:605:NO3:O1	2.12	0.49
1:C:227:PRO:HG3	1:C:270:LEU:HD22	1.93	0.49
1:C:481:LEU:O	1:C:485:LYS:N	2.36	0.49
5:C:609:3CJ:S1	6:C:610:HEM:ND	2.85	0.49
1:C:98:LEU:CD1	1:C:101:MET:HE2	2.42	0.49
1:D:84:GLY:HA2	7:D:775:HOH:O	2.11	0.49
1:A:139:CYS:SG	1:A:141:PRO:HD3	2.52	0.49
1:B:205:ASN:OD1	1:B:207:SER:OG	2.30	0.49
1:B:274:ASN:O	1:B:278:ARG:HG3	2.12	0.49
1:C:527:ARG:HH11	1:C:527:ARG:HG2	1.77	0.49
1:A:442:ARG:O	1:A:445:GLY:N	2.45	0.49
1:A:313:LEU:HD11	1:A:519:PHE:CD2	2.48	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:LEU:O	1:C:78:VAL:CG1	2.60	0.49
1:D:346:ALA:C	1:D:348:ARG:H	2.16	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:D:502:VAL:O	1:D:503:GLU:C	2.50	0.49
1:A:347:PHE:CE1	6:A:610:HEM:HBC1	2.48	0.49
1:D:450:ASN:HD21	1:D:487:PRO:HB2	1.78	0.49
1:D:343:PHE:CD1	1:D:518:GLN:HG2	2.47	0.49
1:A:168:PRO:HB3	1:A:170:PRO:HG2	1.95	0.49
1:A:284:ASN:HD21	1:A:591:ALA:HA	1.77	0.49
1:C:363:GLU:CD	1:C:363:GLU:H	2.15	0.49
1:D:246:VAL:HG11	1:D:387:ILE:HD12	1.95	0.49
1:D:317:LEU:HD12	1:D:321:MET:HA	1.95	0.49
1:D:62:THR:HB	1:D:65:LYS:HB2	1.95	0.49
1:A:551:ARG:CZ	1:A:584:LYS:HG2	2.41	0.49
1:C:1:SER:H2	1:C:2:TRP:HZ3	1.49	0.49
1:D:314:PRO:HD3	1:D:321:MET:HE1	1.94	0.49
1:D:110:ASP:OD2	1:D:189:ALA:N	2.45	0.49
1:A:42:ALA:HB2	1:A:166:VAL:CG1	2.37	0.48
1:A:347:PHE:O	1:A:347:PHE:HD1	1.95	0.48
1:A:62:THR:O	1:A:63:GLN:CB	2.61	0.48
1:B:554:CYS:SG	1:B:562:VAL:HG21	2.52	0.48
1:C:30:ASN:HD21	1:C:333:ASN:HB2	1.78	0.48
1:A:144:PHE:HD2	1:A:156:LYS:C	2.17	0.48
1:A: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:312:TYR:CE2	1:B:316:VAL:HG21	2.48	0.48
1:B:113:PHE:CD1	5:B:609:3CJ:H5	2.48	0.48
1:C:125:SER:O	1:C:126:LYS:C	2.51	0.48
1:C:151:LEU:HA	1:C:155:GLY:O	2.13	0.48
1:C:43:LEU:HD12	1:C:179:GLN:HB2	1.95	0.48
1:C:347:PHE:HB3	6:C:610:HEM:HMD3	1.95	0.48
1:D:119:LEU:CD2	1:D:169:THR:CG2	2.91	0.48
1:A:464:LEU:O	1:A:468:GLN:HG3	2.12	0.48
1:A:51:TYR:HB3	1:A:57:VAL:O	2.13	0.48
1:B:10:VAL:HG11	1:B:41:ARG:NH2	2.28	0.48
1:B:8:ALA:HB1	1:B:9:PRO:HD2	1.96	0.48
1:C:180:ILE:HG22	1:C:181:ASN:N	2.29	0.48
1:C:22:ARG:CZ	1:C:528:PHE:HB2	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:593:ARG:HB3	1:C:593:ARG:CZ	2.43	0.48
1:D:144:PHE:HE1	1:D:158:MET:HG3	1.75	0.48
1:D:380:PHE:HE2	1:D:420:LYS:O	1.96	0.48
1:A:244:ALA:O	1:A:245:HIS:HB3	2.14	0.48
1:A:275:ARG:CD	1:A:555:ASP:HB3	2.43	0.48
1:C:377:HIS:ND1	1:C:416:GLU:OE1	2.43	0.48
1:A:58:PRO:HG3	1:A:162:ARG:CZ	2.43	0.48
1:B:213:MET:HB3	1:B:270:LEU:HD11	1.94	0.48
1:B:140:PHE:CE2	1:B:439:GLN:HG3	2.48	0.48
1:C:102:GLN:HB2	1:C:399:LEU:HD21	1.96	0.48
1:D:150:LYS:HE2	1:D:419:ASN:HD22	1.78	0.48
1:A:317:LEU:HD12	1:A:321:MET:SD	2.53	0.48
1:A:481:LEU:HA	1:A:484:TYR:O	2.14	0.48
6:A:610:HEM:CMC	6:A:610:HEM:HBC2	2.43	0.48
1:B:137:ASP:CG	1:B:138:GLU:H	2.17	0.48
1:D:187:LEU:HD21	1:D:304:ILE:HG22	1.95	0.48
1:A:91:VAL:HA	7:A:777:HOH:O	2.12	0.48
5:C:609:3CJ:S1	6:C:610:HEM:C1D	3.07	0.48
1:D:193:TYR:CZ	1:D:297:ARG:HA	2.49	0.48
1:D:93:ASP:OD2	1:D:96:ARG:HG3	2.13	0.48
1:A:146:LYS:HB3	7:A:823:HOH:O	2.12	0.48
1:C:17:GLU:HB3	1:C:18:GLN:OE1	2.14	0.48
1:C:204:ARG:NE	1:C:206:LEU:HD21	2.29	0.48
1:D:275:ARG:O	1:D:279:GLU:HG2	2.14	0.48
1:D:408:ASN:HB3	1:D:411:LYS:HB2	1.95	0.48
1:A:165:PHE:CZ	1:A:169:THR:C	2.87	0.47
1:B:113:PHE:HB2	1:B:255:ARG:NH2	2.29	0.47
1:B:91:VAL:CG1	1:B:411:LYS:HD3	2.44	0.47
1:B:418:ARG:O	1:B:432:ASP:CB	2.62	0.47
1:D:357:THR:HB	1:D:374:LEU:O	2.14	0.47
1:A:109:HIS:NE2	5:A:609:3CJ: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: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:367:PRO:CB	1:D:64:ARG:NE	2.77	0.47
1:A:84:GLY:CA	1:A:418:ARG:NE	2.78	0.47
1:A:67:ARG:N	1:A:70:PHE:O	2.45	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:571:ASN:O	1:A:575:ASP:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:52:GLU:HG3	1:A:59:PHE:CD1	2.49	0.47
1:D:259:GLN:O	1:D:262:LEU:HB3	2.14	0.47
1:D:370:PRO:HG2	1:D:371:GLU:H	1.79	0.47
1:B:168:PRO:HG2	1:B:172:TYR:HB3	1.97	0.47
1:B:96:ARG:NH2	1:B:315:ILE:O	2.46	0.47
1:C:169:THR:HG22	7:C:736:HOH:O	2.13	0.47
1:C:322:GLN:HG3	7:C:810:HOH:O	2.13	0.47
1:C:22:ARG:NH1	1:C:528:PHE:HB2	2.29	0.47
1:D:264:THR:HG23	1:D:392:ILE:HG23	1.96	0.47
1:A:351:HIS:NE2	1:A:433:LEU:HD21	2.30	0.47
1:B:12:LEU:HD12	1:B:12:LEU:HA	1.79	0.47
1:C:230:ASN:ND2	1:C:232:VAL:HG22	2.22	0.47
1:C:423:GLN:CB	1:C:426:HIS:CD2	2.97	0.47
1:A:414:THR:HG22	7:A:721:HOH:O	2.15	0.47
1:A:76:ARG:HH22	1:A:419:ASN:ND2	2.13	0.47
1:B:30:ASN:ND2	1:B:36:LEU:HD12	2.29	0.47
1:B:544:LEU:O	1:B:547:VAL:HG22	2.14	0.47
1:C:221:ASP:O	1:C:222:HIS:C	2.53	0.47
1:C:511:LEU:O	1:C:515:LEU:HG	2.14	0.47
1:D:468:GLN:HG2	1:D:474:LYS:HA	1.96	0.47
1:A:224:LEU:HB2	1:A:271:ARG:NH2	2.30	0.47
1:A:363:GLU:HG2	7:A:816:HOH:O	2.15	0.47
1:B:466:GLY:HA3	7:B:749:HOH:O	2.14	0.47
1:C:96:ARG:CD	1:C:100:PHE:CD2	2.68	0.47
1:A:302:ALA:O	1:A:306:ILE:HG13	2.14	0.47
1:B:433:LEU:HD12	1:B:433:LEU:O	2.15	0.47
1:C:453:ARG:HD2	1:C:510:LEU:HD13	1.96	0.47
1:D:530:TRP:CE2	1:D:531:GLU:HG3	2.49	0.47
1:B:138:GLU:O	1:B:162:ARG:HG3	2.14	0.47
1:B:361:LEU:HB3	1:B:365:TYR:HA	1.96	0.47
1:B:376:LEU:HA	1:B:379:LEU:HD12	1.97	0.47
1:C:146:LYS:NZ	1:C:147:ASN:ND2	2.60	0.47
1:A: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
5:A:609:3CJ:H7	6:A:610:HEM:CBD	2.41	0.46
1:B:273:HIS:CD2	1:B:274:ASN:OD1	2.61	0.46
1:A:233:LYS:HA	1:A:234:PRO:C	2.34	0.46
1:A:265:VAL:O	1:A:269:LEU:HG	2.15	0.46
1:A:400:LEU:HD21	1:A:553:ILE:CD1	2.46	0.46
1:A:436:ILE:O	1:A:440:ARG:HB2	2.15	0.46
1:B:335:VAL:HG12	1:B:336:ASP:N	2.30	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:346:ALA:C	1:D:348:ARG:N	2.68	0.46
5:D:609:3CJ:C1	6:D:610:HEM:NA	2.78	0.46
1:B:185:SER:HB3	1:B:339:ILE:HG12	1.97	0.46
1:B:363:GLU:N	1:B:363:GLU:CD	2.67	0.46
6:B:608:HEM:HBB2	6:B:608:HEM:CMB	2.44	0.46
1:B:66:THR:HB	1:B:70:PHE:C	2.36	0.46
1:C:144:PHE:CE1	1:C:158:MET:HG3	2.50	0.46
1:C:30:ASN:ND2	1:C:333:ASN:HB2	2.30	0.46
1:C:572:TYR:HA	1:C:573:PRO:HA	1.62	0.46
1:D:113:PHE:CD1	1:D:255:ARG:HD3	2.50	0.46
1:D:313:LEU:HB2	1:D:314:PRO:HD3	1.97	0.46
1:A:113:PHE:CD1	5:A:609:3CJ:H5	2.50	0.46
1:A:62:THR:HG21	1:A:65:LYS:CG	2.43	0.46
1:B:303:PHE:HD2	1:B:304:ILE:HD12	1.80	0.46
1:B:557:THR:OG1	1:B:559:ILE:HG12	2.15	0.46
1:B:347:PHE:CE1	6:B:608:HEM:HBC1	2.51	0.46
1:C:236:PRO:CB	1:C:424:PRO:HB3	2.45	0.46
1:D:255:ARG:HD2	5:D:609:3CJ:C2	2.45	0.46
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.14	0.46
1:A:71:ARG:CB	1:A:71:ARG:NH1	2.79	0.46
1:C:171:PRO:HD3	7:C:822:HOH:O	2.15	0.46
1:D:99:LEU:HD21	1:D:549:PHE:CD2	2.50	0.46
1:D:54:GLY:HA2	7:D:853:HOH:O	2.15	0.46
1:A:112:ASP:HA	1:A:183:VAL:CG2	2.46	0.46
1:A:522:ILE:O	1:A:526:ASP:HB2	2.16	0.46
1:D:213:MET:HG2	1:D:273:HIS:NE2	2.31	0.46
1:A:113:PHE:HB2	1:A:255:ARG:CZ	2.46	0.46
1:A:9:PRO:O	1:A:10:VAL:C	2.52	0.46
1:D:148:ASP:O	1:D:151:LEU:CB	2.64	0.46
1:D:313:LEU:O	1:D:314:PRO:C	2.54	0.46
1:C:129:CYS:O	1:C:133:CYS:HA	2.15	0.46
1:C:213:MET:HG2	1:C:273:HIS:CD2	2.51	0.46
1:C:344:THR:HB	6:C:610:HEM:O2D	2.15	0.46
1:D:336:ASP:OD2	1:D:338:ARG:NH2	2.48	0.46
1:A:166:VAL:C	1:A:167:CYS:SG	2.94	0.46
1:A:213:MET:HB2	1:A:270:LEU:HD11	1.98	0.46
1:B:17:GLU:OE2	1:B:31:ARG:HG2	2.15	0.46
1:B:421:LEU:HD22	1:B:433:LEU:HB2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:93:ASP:CG	1:B:96:ARG:HB2	2.36	0.46
1:C:294:GLN:OE1	1:C:294:GLN:HA	2.15	0.46
1:C:108:ASP:HB2	1:C:347:PHE:CE2	2.50	0.46
1:D:351:HIS:HD2	6:D:610:HEM:C1C	2.34	0.46
1:D:570:ASN:HB3	1:D:575:ASP:HB3	1.98	0.46
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.51	0.46
1:C:423:GLN:HG3	1:C:431:PHE:CD2	2.51	0.46
1:C:449:TYR:OH	1:C:470:VAL:HG11	2.16	0.46
5:C:609:3CJ:H5	6:C:610:HEM:CAA	2.42	0.46
1:D:418:ARG:HG2	1:D:432:ASP:OD2	2.15	0.46
1:D:545:GLN:OE1	1:D:545:GLN:HA	2.16	0.46
1:A:260:ILE:HG23	1:A:261:LEU:N	2.31	0.45
1:B:324:TRP:CZ2	1:B:513:CYS:HB2	2.51	0.45
1:B:433:LEU:HA	1:B:436:ILE:HD12	1.97	0.45
2:C:603:NAG:H82	7:C:807:HOH:O	2.16	0.45
1:D:561:LYS:HE3	1:D:578:ASP:HA	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
1:A:419:ASN:O	1:A:430:GLY:HA2	2.17	0.45
1:A:47:LEU:HD21	1:A:455:PHE:HD2	1.81	0.45
1:A:82:ILE:HD13	1:A:480:LEU:HD23	1.98	0.45
1:A:86:LEU:HD23	1:D:55:LEU:HD23	1.98	0.45
1:B:257:SER:O	1:B:381:PHE:HA	2.16	0.45
1:B:418:ARG:NH1	1:B:418:ARG:HG2	2.31	0.45
1:C:244:ALA:HB1	1:C:246:VAL:HG23	1.97	0.45
1:C:31:ARG:H	1:C:31:ARG:HG2	1.59	0.45
1:C:350:GLY:HA3	6:C:610:HEM:CBC	2.47	0.45
1:D:239:PHE:CZ	1:D:427:LYS:CG	2.99	0.45
1:B:360:ARG:O	1:B:368:TRP:HB3	2.17	0.45
1:D:519:PHE:HA	1:D:522:ILE:HG12	1.97	0.45
1:A:418:ARG:HG2	1:A:418:ARG:HH11	1.81	0.45
1:C:100:PHE:HA	1:C:567:PHE:CD1	2.52	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: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:D:474:LYS:O	1:D:477:ALA:HB3	2.16	0.45
1:D:97:SER:O	1:D:100:PHE:HB3	2.15	0.45
1:A:353:GLU:HA	1:A:405:LYS:O	2.17	0.45
1:A:95:ASN:HA	1:A:569:ALA:HB3	1.97	0.45
1:B:348:ARG:NH1	1:B:437:ASN:ND2	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:GLY:O	1:B:455:PHE:C	2.55	0.45
1:B:528:PHE:HZ	7:B:748:HOH:O	1.99	0.45
1:C:344:THR:O	6:C:610:HEM:HAD2	2.16	0.45
1:D:246:VAL:CG1	1:D:387:ILE:HD12	2.46	0.45
1:D:484:TYR:O	1:D:485:LYS:HB2	2.17	0.45
1:D:561:LYS:CE	1:D:578:ASP:HA	2.47	0.45
1:A:392:ILE:HG22	1:A:396:VAL:CG2	2.47	0.45
1:B:35:ALA:HB1	1:B:41:ARG:HE	1.80	0.45
1:B:551:ARG:HD3	1:B:584:LYS:CA	2.37	0.45
1:C:130:GLU:HB2	1:C:159:PRO:HB3	1.99	0.45
1:C:552:LEU:O	1:C:556:ASN:ND2	2.46	0.45
1:D:590:TRP:HE3	1:D:590:TRP:H	1.65	0.45
1:A:135:GLN:HB3	1:A:135:GLN:HE21	1.49	0.45
1:A:173:GLN:O	1:A:174:SER:HB3	2.17	0.45
1:A:418:ARG:HG2	1:A:418:ARG:NH1	2.32	0.45
1:A:442:ARG:O	1:A:443:ASP:C	2.53	0.45
1:B:180:ILE:CG2	1:B:181:ASN:N	2.79	0.45
1:B:221:ASP:HB2	1:B:226:TYR:CZ	2.52	0.45
7:A:772:HOH:O	1:D:173:GLN:HB2	2.17	0.45
1:D:229:PHE:CZ	1:D:387:ILE:HD13	2.52	0.45
1:D:345:PHE:CE1	1:D:441:CYS:HA	2.52	0.45
1:D:546:LYS:NZ	1:D:546:LYS:HB2	2.31	0.45
1:A:59:PHE:CG	1:A:67:ARG:HD2	2.52	0.45
1:A:82:ILE:HD13	1:A:480:LEU:CD2	2.46	0.45
1:B:117:THR:HG21	1:B:138:GLU:OE1	2.17	0.45
1:C:527:ARG:NH1	1:C:527:ARG:HG2	2.31	0.45
1:D:12:LEU:C	1:D:13:VAL:HG23	2.37	0.45
1:D:144:PHE:HB2	1:D:151:LEU:HD13	1.98	0.45
1:D:175:LEU:HD23	1:D:176:ALA:H	1.82	0.45
1:A:400:LEU:HD21	1:A:553:ILE:HD13	1.99	0.45
1:C:168:PRO:HG3	1:C:172:TYR:CD2	2.49	0.45
1:C:29:ASN:ND2	1:C:527:ARG:H	2.14	0.45
1:D:10:VAL:HG13	1:D:11:PRO:HD2	1.98	0.45
1:A:449:TYR:HB3	1:A:487:PRO:O	2.18	0.44
1:B:563:PRO:HD3	1:B:576:PHE:CE2	2.51	0.44
1:C:551:ARG:HD3	1:C:584:LYS:HA	1.99	0.44
1:D:9:PRO:HG3	1:D:41:ARG:NH1	2.32	0.44
1:A:165:PHE:CE2	1:A:170:PRO:O	2.70	0.44
1:A:424:PRO:O	1:A:425:THR:HB	2.17	0.44
1:A:553:ILE:O	1:A:557:THR:HG23	2.17	0.44
1:B:188:ASP:N	1:B:188:ASP:OD1	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:ILE:HG13	1:B:382:ASN:O	2.17	0.44
1:C:517:ARG:CB	1:C:517:ARG:HH21	2.30	0.44
1:D:315:ILE:HD11	1:D:567:PHE:CD2	2.52	0.44
1:A:213:MET:HB3	1:A:270:LEU:HD11	1.98	0.44
1:B:393:ASP:OD1	1:B:557:THR:HB	2.18	0.44
1:B:76:ARG:NH2	7:B:702:HOH:O	2.50	0.44
1:C:124:HIS:O	1:C:125:SER:C	2.54	0.44
1:C:188:ASP:OD1	1:C:190:SER:CB	2.64	0.44
1:D:260:ILE:HD13	1:D:395:LEU:HD21	2.00	0.44
1:D:9:PRO:HG2	1:D:10:VAL:H	1.81	0.44
1:B:408:ASN:HB3	1:B:411:LYS:O	2.17	0.44
1:B:91:VAL:HG11	1:B:411:LYS:HD3	1.99	0.44
1:B:588:SER:HB2	1:B:589:PRO:HD3	2.00	0.44
1:C:188:ASP:CG	1:C:190:SER:HB3	2.37	0.44
1:C:2:TRP:CD2	1:C:2:TRP:N	2.84	0.44
1:C:468:GLN:CG	1:C:474:LYS:HA	2.40	0.44
1:C:29:ASN:O	1:C:527:ARG:HD3	2.18	0.44
1:C:88:GLU:O	1:C:91:VAL:HG22	2.17	0.44
1:A:123:GLU:HB3	1:A:126:LYS:HG3	1.99	0.44
1:A:145:PRO:O	1:A:148:ASP:HB2	2.17	0.44
1:A:313:LEU:HD11	1:A:519:PHE:CD1	2.53	0.44
1:A:559:ILE:HD13	1:A:559:ILE:N	2.33	0.44
1:C:421:LEU:HD22	1:C:433:LEU:HB2	1.98	0.44
1:A:328:TYR:CD2	1:A:531:GLU:HB3	2.52	0.44
1:A:462:LYS:HA	1:A:462:LYS:HE2	1.98	0.44
1:C:168:PRO:HD2	1:C:172:TYR:HE2	1.83	0.44
1:C:242:THR:O	1:C:245:HIS:CE1	2.71	0.44
1:C:279:GLU:O	1:C:283:LEU:HG	2.17	0.44
1:D:196:GLU:HG3	7:D:785:HOH:O	2.18	0.44
1:A:144:PHE:CD2	1:A:156:LYS:C	2.91	0.44
1:C:124:HIS:C	1:C:124:HIS:ND1	2.70	0.44
1:C:265:VAL:O	1:C:269:LEU:HG	2.18	0.44
1:C:402:LYS:HD3	4:C:607:NO3:O1	2.17	0.44
1:D:549:PHE:O	1:D:552:LEU:HB3	2.17	0.44
1:D:88:GLU:O	1:D:91:VAL:HG22	2.17	0.44
1:A:117:THR:O	1:A:117:THR:HG23	2.16	0.44
1:A:172:TYR:CE2	1:A:175:LEU:HB2	2.48	0.44
1:A:568:GLN:HG2	1:A:568:GLN:O	2.17	0.44
1:B:421:LEU:HD12	1:B:422:PHE:N	2.30	0.44
1:C:231:ASN:HB2	7:C:775:HOH:O	2.17	0.44
1:D:187:LEU:HD23	1:D:305:GLN:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:260:ILE:HG13	1:D:386:ILE:HD11	1.99	0.44
1:D:76:ARG:NH1	1:D:432:ASP:OD2	2.51	0.44
1:D:60:GLY:CA	1:D:72:VAL:HG21	2.48	0.44
1:A:203:LEU:HD22	7:A:775:HOH:O	2.17	0.44
1:A:363:GLU:CG	7:A:816:HOH:O	2.65	0.44
5:C:609:3CJ:C3	6:C:610:HEM:C2A	3.01	0.44
1:B:10:VAL:HG21	1:B:41:ARG:NH1	2.32	0.43
1:C:299:ILE:HD11	1:C:590:TRP:CD1	2.52	0.43
1:B:109:HIS:NE2	5:B:609:3CJ:S1	2.91	0.43
1:C:45:ARG:CZ	1:C:49:ALA:HB2	2.48	0.43
1:D:85:TYR:CE2	1:D:91:VAL:HG11	2.53	0.43
1:A:113:PHE:HB2	1:A:255:ARG:NH2	2.33	0.43
1:A:305:GLN:NE2	1:A:529:TRP:CE3	2.86	0.43
1:B:221:ASP:O	1:B:224:LEU:HB2	2.17	0.43
1:B:94:GLN:O	1:B:569:ALA:CB	2.66	0.43
1:C:342:VAL:HG13	1:C:343:PHE:N	2.33	0.43
1:C:74:LEU:O	1:C:78:VAL:HG13	2.18	0.43
1:C:91:VAL:HG23	1:C:92:LEU:HD23	2.01	0.43
1:D:28:CYS:O	1:D:29:ASN:C	2.57	0.43
1:A:382:ASN:ND2	1:A:385:ARG:HG3	2.34	0.43
1:A:55:LEU:HD13	1:A:173:GLN:HA	2.00	0.43
6:A:610:HEM:HBB2	6:A:610:HEM:HMB2	2.00	0.43
1:C:385:ARG:HA	1:C:385:ARG:HD3	1.86	0.43
1:C:520:GLN:O	1:C:524:ASP:HB2	2.19	0.43
1:D:497:ASN:OD1	1:D:511:LEU:HD11	2.18	0.43
1:D:82:ILE:HD13	1:D:480:LEU:CD2	2.49	0.43
1:B:518:GLN:O	1:B:522:ILE:HG23	2.19	0.43
1:C:328:TYR:CZ	1:C:529:TRP:CD1	3.07	0.43
1:D:187:LEU:HG	1:D:187:LEU:O	2.17	0.43
1:D:441:CYS:SG	1:D:492:ILE:CG2	3.07	0.43
1:D:320:GLU:HG3	1:D:512:ALA:HB1	2.00	0.43
1:B:222:HIS:HA	7:B:794:HOH:O	2.19	0.43
1:B:447:PRO:HG2	1:B:452:TRP:CE2	2.54	0.43
1:B:68:ASN:ND2	1:B:489:ASN:OD1	2.44	0.43
1:C:366:GLN:HA	1:C:366:GLN:OE1	2.18	0.43
1:C:353:GLU:HA	1:C:405:LYS:O	2.18	0.43
1:C:528:PHE:O	1:C:529:TRP:C	2.57	0.43
1:D:204:ARG:HG2	1:D:293:TYR:CE1	2.53	0.43
1:D:312:TYR:O	1:D:315:ILE:HG12	2.17	0.43
1:A:398:GLY:O	1:A:402:LYS:HB2	2.19	0.43
1:D:408:ASN:O	1:D:410:ASN:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:585:LEU:O	1:D:587:LEU:N	2.52	0.43
1:A:255:ARG:HH11	5:A:609:3CJ:H6	1.83	0.43
1:A:279:GLU:HA	1:A:279:GLU:OE2	2.19	0.43
1:A:519:PHE:HA	1:A:522:ILE:HG12	2.00	0.43
1:B:172:TYR:OH	1:B:177:ARG:HA	2.17	0.43
1:C:441:CYS:HB3	7:C:713:HOH:O	2.18	0.43
1:C:81:LYS:HE2	7:C:821:HOH:O	2.19	0.43
1:A:343:PHE:CE1	1:A:515:LEU:HD23	2.53	0.43
1:C:37:GLY:H	1:C:338:ARG:CG	2.20	0.43
1:D:119:LEU:HB3	7:D:773:HOH:O	2.19	0.43
1:D:312:TYR:O	1:D:315:ILE:CG1	2.67	0.43
1:D:391:GLY:O	1:D:394:PRO:HD2	2.19	0.43
1:A:239:PHE:CZ	1:A:427:LYS:CB	3.02	0.43
1:A:519:PHE:O	1:A:522:ILE:HG12	2.18	0.43
1:B:565:HIS:HB2	1:B:568:GLN:HG2	2.00	0.43
1:C:3:GLU:O	1:C:5:GLY:N	2.52	0.43
1:D:167:CYS:HB3	1:D:168:PRO:HD2	2.00	0.43
1:D:18:GLN:NE2	1:D:18:GLN:HA	2.33	0.43
1:A:112:ASP:HA	1:A:183:VAL:HG22	2.01	0.42
1:A:93:ASP:CG	1:A:96:ARG:HB2	2.39	0.42
1:C:110:ASP:OD2	1:C:189:ALA:N	2.49	0.42
1:C:227:PRO:HG3	1:C:270:LEU:CD2	2.48	0.42
1:C:467:LEU:HA	1:C:467:LEU:HD12	1.89	0.42
1:A:258:GLU:OE1	1:A:259:GLN:CG	2.66	0.42
1:A:84:GLY:HA2	1:A:418:ARG:NE	2.34	0.42
1:C:109:HIS:HA	1:C:255:ARG:HH22	1.81	0.42
1:C:16:ASP:O	1:C:18:GLN:HG2	2.19	0.42
1:A:165:PHE:CE1	1:A:177:ARG:CZ	3.01	0.42
1:A:543:SER:OG	1:A:589:PRO:HG2	2.19	0.42
1:B:116:GLU:HB3	7:B:746:HOH:O	2.18	0.42
1:B:191:LEU:H	1:B:191:LEU:HD23	1.85	0.42
1:C:283:LEU:HD13	1:C:591:ALA:HB2	2.00	0.42
1:C:108:ASP:HB2	1:C:347:PHE:CD2	2.54	0.42
5:C:609:3CJ:C4	6:C:610:HEM:C3A	3.02	0.42
1:D:146:LYS:O	1:D:147:ASN:CB	2.65	0.42
1:D:148:ASP:O	1:D:151:LEU:HB2	2.19	0.42
1:B:232:VAL:O	1:B:232:VAL:HG23	2.20	0.42
1:B:260:ILE:CG2	1:B:261:LEU:N	2.83	0.42
1:D:12:LEU:O	1:D:13:VAL:HB	2.20	0.42
1:D:474:LYS:HZ1	1:D:474:LYS:HB3	1.84	0.42
1:B:335:VAL:CG1	1:B:336:ASP:N	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:PRO:CG	1:C:172:TYR:CD2	3.03	0.42
1:C:348:ARG:NH2	6:C:610:HEM:HAD1	2.34	0.42
1:D:99:LEU:O	1:D:100:PHE:C	2.57	0.42
1:D:53:ASP:CG	1:D:57:VAL:HG23	2.40	0.42
1:A:281:LYS:HD3	1:A:292:LEU:HD11	2.02	0.42
1:A:65:LYS:HE3	1:A:65:LYS:HB3	1.61	0.42
1:A:77:GLU:O	1:A:81:LYS:HG3	2.19	0.42
1:B:246:VAL:HA	1:B:247:PRO:HD3	1.80	0.42
1:B:64:ARG:NH2	7:B:704:HOH:O	2.53	0.42
1:C:321:MET:HB3	1:C:322:GLN:OE1	2.19	0.42
1:D:376:LEU:HD21	1:D:380:PHE:CE1	2.53	0.42
1:A:363:GLU:OE2	1:A:397:ARG:NH1	2.52	0.42
1:A:572:TYR:CG	1:A:573:PRO:HA	2.55	0.42
1:A:57:VAL:HA	1:A:58:PRO:HD3	1.92	0.42
1:B:248:CYS:HB3	1:B:257:SER:OG	2.19	0.42
1:B:293:TYR:OH	1:B:297:ARG:HD2	2.18	0.42
1:B:313:LEU:N	1:B:314:PRO:CD	2.83	0.42
1:C:322:GLN:CD	1:C:322:GLN:H	2.23	0.42
1:C:36:LEU:CD2	1:C:338:ARG:HD3	2.50	0.42
1:D:272:GLU:O	1:D:276:LEU:CG	2.68	0.42
1:D:348:ARG:HH11	1:D:437:ASN:HD21	1.60	0.42
1:D:460:GLN:HA	1:D:461:PRO:HD2	1.91	0.42
1:A:124:HIS:O	1:A:127:VAL:HB	2.20	0.42
1:B:233:LYS:HB3	1:B:234:PRO:HA	2.01	0.42
1:C:180:ILE:CG2	1:C:181:ASN:N	2.83	0.42
1:C:101:MET:SD	1:C:354:VAL:HG22	2.60	0.42
1:C:529:TRP:O	1:C:530:TRP:C	2.58	0.42
1:C:550:SER:OG	1:C:563:PRO:O	2.26	0.42
1:D:446:MET:HA	1:D:447:PRO:HD3	1.93	0.42
1:A:464:LEU:HD12	1:A:464:LEU:C	2.40	0.42
6:B:608:HEM:O1D	5:B:609:3CJ:H6	2.19	0.42
1:C:106:ILE:HG13	1:C:265:VAL:HG11	2.02	0.42
1:C:348:ARG:HB3	1:C:493:TRP:HE1	1.80	0.42
1:A:24:ILE:HD13	1:A:24:ILE:HA	1.93	0.42
1:B:14:THR:HG22	1:B:15:CYS:N	2.35	0.42
1:B:166:VAL:CG2	1:B:178:ASP:HB2	2.50	0.42
1:B:215:VAL:O	1:B:217:GLN:NE2	2.53	0.42
1:B:281:LYS:HD2	1:B:285:PRO:HA	2.01	0.42
1:A:217:GLN:HA	1:A:217:GLN:OE1	2.20	0.41
1:A:237:CYS:O	1:A:240:ILE:HG13	2.20	0.41
1:B:113:PHE:O	1:B:181:ASN:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:45:ARG:NH1	1:B:49:ALA:HA	2.35	0.41
1:C:240:ILE:O	1:C:241:ASN:HB2	2.20	0.41
1:C:348:ARG:NH1	1:C:437:ASN:HD22	2.18	0.41
1:A:345:PHE:CE1	1:A:440:ARG:HG3	2.54	0.41
1:A:354:VAL:HG21	6:A:610:HEM:CAB	2.50	0.41
1:C:1:SER:N	1:C:2:TRP:CE3	2.82	0.41
1:D:103:TRP:O	1:D:104:GLY:C	2.58	0.41
1:D:60:GLY:HA2	1:D:72:VAL:CG2	2.50	0.41
1:B:31:ARG:O	1:B:32:ARG:C	2.59	0.41
1:C:333:ASN:HD22	1:C:333:ASN:H	1.67	0.41
1:C:494:ILE:HG23	1:C:495:GLY:N	2.36	0.41
1:D:132:TYR:HB3	1:D:134:VAL:HG23	2.02	0.41
1:D:532:ASN:HA	1:D:533:PRO:HD3	1.89	0.41
1:A:146:LYS:HE3	1:A:147:ASN:OD1	2.20	0.41
1:A:321:MET:C	1:A:323:LYS:H	2.22	0.41
1:A:522:ILE:HG13	1:A:523:ARG:N	2.36	0.41
1:B:117:THR:HG23	1:B:161:PHE:HD2	1.85	0.41
1:B:203:LEU:HD11	1:B:251:ALA:O	2.20	0.41
1:B:23:THR:O	1:B:297:ARG:NH2	2.44	0.41
1:B:588:SER:N	1:B:589:PRO:CD	2.83	0.41
1:C:101:MET:HB3	1:C:101:MET:HE2	1.52	0.41
1:A:140:PHE:N	1:A:141:PRO:HD3	2.34	0.41
1:A:335:VAL:O	1:A:337:PRO:HD3	2.20	0.41
1:A:423:GLN:HA	1:A:424:PRO:HD3	1.92	0.41
1:B:481:LEU:HD21	1:B:487:PRO:HG3	2.01	0.41
1:C:146:LYS:CE	1:C:147:ASN:ND2	2.73	0.41
1:C:17:GLU:O	1:C:31:ARG:NH2	2.54	0.41
1:C:216:ASN:OD1	1:C:219:ALA:N	2.31	0.41
1:D:336:ASP:OD1	1:D:338:ARG:HB2	2.21	0.41
1:D:91:VAL:HG12	1:D:411:LYS:HD3	2.02	0.41
1:D:3:GLU:CG	1:D:4:VAL:H	2.31	0.41
1:A:471:LEU:O	1:A:472:LYS:HB2	2.21	0.41
1:B:362:ASP:O	1:B:397:ARG:NE	2.53	0.41
1:B:529:TRP:CD1	1:B:531:GLU:HB3	2.55	0.41
1:C:82:ILE:HD12	1:C:480:LEU:CD2	2.51	0.41
1:D:96:ARG:HD2	1:D:100:PHE:CG	2.55	0.41
1:D:251:ALA:O	1:D:252:GLY:C	2.58	0.41
1:D:347:PHE:HA	1:D:347:PHE:HD1	1.73	0.41
1:D:91:VAL:HB	1:D:405:LYS:HG3	2.02	0.41
1:D:47:LEU:HD12	1:D:452:TRP:CZ3	2.56	0.41
1:D:9:PRO:O	1:D:10:VAL:CG2	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:572:TYR:HD2	1:A:576:PHE:CG	2.37	0.41
1:B:537:THR:HG23	1:B:540:GLN:CD	2.39	0.41
1:B:69:GLY:HA2	1:C:374:LEU:HD22	2.02	0.41
1:D:213:MET:CG	1:D:273:HIS:CD2	3.04	0.41
1:D:351:HIS:CD2	6:D:610:HEM:C1C	3.09	0.41
1:D:589:PRO:HB2	1:D:590:TRP:CZ3	2.56	0.41
1:A:165:PHE:HE2	1:A:170:PRO:O	2.03	0.41
1:A:501:MET:SD	1:A:506:ARG:HA	2.61	0.41
1:B:127:VAL:O	1:B:131:GLU:HB3	2.20	0.41
1:B:213:MET:HG2	1:B:273:HIS:NE2	2.35	0.41
1:B:106:ILE:HD11	1:B:265:VAL:HB	2.03	0.41
1:B:493:TRP:O	1:B:497:ASN:ND2	2.53	0.41
1:C:100:PHE:HA	1:C:567:PHE:HD1	1.85	0.41
1:C:149:PRO:C	1:C:151:LEU:N	2.73	0.41
1:C:46:TRP:CE2	1:C:340:SER:HB3	2.56	0.41
1:C:3:GLU:C	1:C:5:GLY:H	2.24	0.41
1:C:421:LEU:HD12	1:C:422:PHE:H	1.85	0.41
1:C:481:LEU:CD2	1:C:487:PRO:HG3	2.39	0.41
1:D:179:GLN:HG2	1:D:444:HIS:CD2	2.56	0.41
1:A:35:ALA:HB1	1:A:41:ARG:CD	2.50	0.41
1:A:424:PRO:O	1:A:425:THR:CB	2.69	0.41
1:A:418:ARG:O	1:A:432:ASP:HA	2.21	0.41
1:A:477:ALA:O	1:A:478:LYS:C	2.59	0.41
1:B:347:PHE:HB3	6:B:608:HEM:CMD	2.51	0.41
1:B:399:LEU:HA	1:B:399:LEU:HD23	1.92	0.41
1:C:506:ARG:HA	1:C:506:ARG:HD3	1.89	0.41
1:C:588:SER:N	1:C:589:PRO:CD	2.84	0.41
1:D:272:GLU:OE2	1:D:276:LEU:HG	2.20	0.41
1:D:28:CYS:HA	1:D:34:PRO:CB	2.51	0.41
1:D:423:GLN:O	1:D:426:HIS:HB2	2.20	0.41
1:D:51:TYR:HB3	1:D:57:VAL:O	2.20	0.41
1:D:523:ARG:HG3	1:D:529:TRP:CE2	2.56	0.41
1:A:121:SER:C	1:A:123:GLU:N	2.75	0.41
1:A:288:ASP:OD2	1:A:290:GLU:HB3	2.20	0.41
1:A:407:MET:SD	1:A:408:ASN:N	2.94	0.41
6:B:608:HEM:CHA	5:B:609:3CJ:H9	2.34	0.41
1:C:1:SER:N	1:C:2:TRP:CZ3	2.68	0.41
1:C:419:ASN:HD22	1:C:419:ASN:HA	1.70	0.41
6:C:610:HEM:HBC2	6:C:610:HEM:HMC2	2.02	0.41
1:D:366:GLN:HB3	1:D:367:PRO:CD	2.51	0.41
1:B:362:ASP:OD1	1:B:366:GLN:HB2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:HIS:HD1	1:C:125:SER:CA	2.34	0.40
1:C:424:PRO:O	1:C:425:THR:CB	2.69	0.40
1:C:460:GLN:HA	1:C:461:PRO:HD2	1.90	0.40
1:C:85:TYR:CD2	1:C:411:LYS:HA	2.57	0.40
1:D:165:PHE:CD1	1:D:165:PHE:N	2.89	0.40
1:A:221:ASP:HB3	1:A:224:LEU:HB2	2.03	0.40
1:A:517:ARG:NH2	1:A:521:GLN:OE1	2.54	0.40
1:B:24:ILE:HD13	1:B:24:ILE:HA	1.93	0.40
1:B:332:ASN:OD1	1:B:334:SER:N	2.45	0.40
1:B:468:GLN:HG2	1:B:474:LYS:HA	2.03	0.40
1:C:103:TRP:O	1:C:104:GLY:C	2.58	0.40
1:C:274:ASN:O	1:C:278:ARG:HG3	2.21	0.40
1:C:363:GLU:CD	1:C:363:GLU:N	2.75	0.40
1:C:382:ASN:OD1	1:C:385:ARG:HB2	2.21	0.40
1:C:497:ASN:HA	1:C:511:LEU:HD11	2.03	0.40
1:D:70:PHE:CD1	1:D:70:PHE:N	2.89	0.40
1:A:309:PHE:CZ	1:A:522:ILE:HD11	2.55	0.40
1:A:549:PHE:O	1:A:552:LEU:HB3	2.21	0.40
1:B:308:THR:HA	1:B:312:TYR:HB3	2.03	0.40
6:B:608:HEM:HBA2	6:B:608:HEM:HHA	2.02	0.40
1:C:471:LEU:HD23	1:C:499:GLU:HA	2.02	0.40
1:D:61:TRP:CE2	1:D:135:GLN:NE2	2.89	0.40
1:D:324:TRP:O	1:D:520:GLN:HB2	2.21	0.40
1:D:537:THR:OG1	1:D:540:GLN:HG3	2.21	0.40
1:D:572:TYR:HA	1:D:573:PRO:HA	1.75	0.40
1:A:367:PRO:HB2	1:D:64:ARG:HE	1.86	0.40
1:A:233:LYS:NZ	1:B:322:GLN:HE21	2.19	0.40
1:A:260:ILE:CG2	1:A:261:LEU:N	2.84	0.40
1:A:588:SER:N	1:A:589:PRO:CD	2.84	0.40
1:B:45:ARG:NH2	1:B:177:ARG:O	2.53	0.40
1:C:93:ASP:HB2	1:C:406:LEU:HB2	2.03	0.40
1:C:514:LEU:O	1:C:515:LEU:C	2.60	0.40
1:D:78:VAL:O	1:D:82:ILE:HB	2.21	0.40
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.86	0.40
1:A:518:GLN:O	1:A:522:ILE:HG23	2.21	0.40
1:A:568:GLN:O	1:A:570:ASN:ND2	2.54	0.40
1:A:77:GLU:CG	1:A:81:LYS:HD2	2.51	0.40
1:B:213:MET:CB	1:B:270:LEU:HD11	2.52	0.40
1:B:320:GLU:O	1:B:323:LYS:HB3	2.21	0.40
1:B:418:ARG:O	1:B:432:ASP:HB2	2.21	0.40
1:C:124:HIS:O	1:C:126:LYS:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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%)	24	41
1	B	593/595 (100%)	524 (88%)	63 (11%)	6 (1%)	19	34
1	C	593/595 (100%)	523 (88%)	61 (10%)	9 (2%)	13	22
1	D	593/595 (100%)	515 (87%)	67 (11%)	11 (2%)	10	16
All	All	2372/2380 (100%)	2082 (88%)	259 (11%)	31 (1%)	15	26

All (31) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	8	ALA
1	A	167	CYS
1	B	167	CYS
1	C	8	ALA
1	C	12	LEU
1	C	167	CYS
1	C	174	SER
1	D	13	VAL
1	D	167	CYS
1	D	174	SER
1	D	3	GLU
1	A	327	PRO
1	B	27	ASP

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

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	517/517 (100%)	471 (91%)	46 (9%)	12	23
1	B	517/517 (100%)	472 (91%)	45 (9%)	13	24
1	C	517/517 (100%)	475 (92%)	42 (8%)	15	27
1	D	517/517 (100%)	463 (90%)	54 (10%)	9	16
All	All	2068/2068 (100%)	1881 (91%)	187 (9%)	12	22

All (187) 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

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Mol	Chain	Res	Type
1	A	23	THR
1	A	24	ILE
1	A	32	ARG
1	A	40	ASN
1	A	64	ARG
1	A	65	LYS
1	A	71	ARG
1	A	78	VAL
1	A	116	GLU
1	A	118	GLU
1	A	119	LEU
1	A	139	CYS
1	A	154	GLN
1	A	157	CYS
1	A	167	CYS
1	A	177	ARG
1	A	201	SER
1	A	202	ARG
1	A	218	GLU
1	A	232	VAL
1	A	240	ILE
1	A	257	SER
1	A	258	GLU
1	A	266	HIS
1	A	311	ASP
1	A	322	GLN
1	A	327	PRO
1	A	344	THR
1	A	347	PHE
1	A	348	ARG
1	A	364	ASN
1	A	366	GLN
1	A	408	ASN
1	A	464	LEU
1	A	481	LEU
1	A	517	ARG
1	A	538	GLU
1	A	542	ASP
1	A	551	ARG
1	A	564	LEU
1	A	568	GLN
1	A	580	SER

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Mol	Chain	Res	Type
1	A	593	ARG
1	B	3	GLU
1	B	6	CYS
1	B	22	ARG
1	B	53	ASP
1	B	63	GLN
1	B	66	THR
1	B	78	VAL
1	B	86	LEU
1	B	95	ASN
1	B	118	GLU
1	B	119	LEU
1	B	125	SER
1	B	128	GLN
1	B	151	LEU
1	B	156	LYS
1	B	167	CYS
1	B	175	LEU
1	B	196	GLU
1	B	198	SER
1	B	202	ARG
1	B	231	ASN
1	B	242	THR
1	B	266	HIS
1	B	321	MET
1	B	322	GLN
1	B	337	PRO
1	B	347	PHE
1	B	356	SER
1	B	359	SER
1	B	360	ARG
1	B	371	GLU
1	B	383	THR
1	B	423	GLN
1	B	439	GLN
1	B	472	LYS
1	B	481	LEU
1	B	486	THR
1	B	513	CYS
1	B	522	ILE
1	B	542	ASP
1	B	551	ARG

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Mol	Chain	Res	Type
1	B	573	PRO
1	B	574	HIS
1	B	592	SER
1	B	593	ARG
1	C	2	TRP
1	C	3	GLU
1	C	4	VAL
1	C	6	CYS
1	C	19	SER
1	C	31	ARG
1	C	32	ARG
1	C	89	GLU
1	C	102	GLN
1	C	118	GLU
1	C	119	LEU
1	C	124	HIS
1	C	139	CYS
1	C	146	LYS
1	C	153	THR
1	C	156	LYS
1	C	157	CYS
1	C	173	GLN
1	C	177	ARG
1	C	207	SER
1	C	242	THR
1	C	254	SER
1	C	266	HIS
1	C	284	ASN
1	C	293	TYR
1	C	323	LYS
1	C	333	ASN
1	C	344	THR
1	C	360	ARG
1	C	364	ASN
1	C	376	LEU
1	C	404	SER
1	C	429	HIS
1	C	474	LYS
1	C	520	GLN
1	C	524	ASP
1	C	564	LEU
1	C	578	ASP

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Mol	Chain	Res	Type
1	C	580	SER
1	C	593	ARG
1	C	594	GLU
1	C	595	ASN
1	D	12	LEU
1	D	23	THR
1	D	32	ARG
1	D	36	LEU
1	D	40	ASN
1	D	64	ARG
1	D	65	LYS
1	D	66	THR
1	D	70	PHE
1	D	86	LEU
1	D	118	GLU
1	D	119	LEU
1	D	124	HIS
1	D	127	VAL
1	D	129	CYS
1	D	168	PRO
1	D	169	THR
1	D	175	LEU
1	D	177	ARG
1	D	185	SER
1	D	198	SER
1	D	202	ARG
1	D	230	ASN
1	D	240	ILE
1	D	266	HIS
1	D	286	HIS
1	D	315	ILE
1	D	322	GLN
1	D	323	LYS
1	D	329	GLN
1	D	333	ASN
1	D	334	SER
1	D	337	PRO
1	D	347	PHE
1	D	356	SER
1	D	360	ARG
1	D	371	GLU
1	D	376	LEU

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

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

Mol	Chain	Res	Type
1	A	128	GLN
1	A	135	GLN
1	A	230	ASN
1	A	250	GLN
1	A	322	GLN
1	A	366	GLN
1	A	419	ASN
1	A	437	ASN
1	A	468	GLN
1	A	565	HIS
1	B	217	GLN
1	B	231	ASN
1	B	273	HIS
1	B	305	GLN
1	B	322	GLN
1	B	409	GLN
1	B	410	ASN
1	B	429	HIS
1	B	437	ASN
1	B	468	GLN
1	B	545	GLN
1	B	574	HIS

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

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

Of 39 ligands modelled in this entry, 4 are monoatomic - leaving 35 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
2	NAG	A	601	1	14,14,15	0.96	0	15,19,21	2.30	7 (46%)
2	NAG	A	602	1	14,14,15	0.28	0	15,19,21	0.53	0
2	NAG	A	603	1,2	14,14,15	1.28	2 (14%)	15,19,21	1.58	1 (6%)
2	NAG	A	604	2	14,14,15	0.88	1 (7%)	15,19,21	2.72	5 (33%)
4	NO3	A	606	-	1,3,3	1.96	0	0,3,3	0.00	-
4	NO3	A	607	-	1,3,3	6.17	1 (100%)	0,3,3	0.00	-
4	NO3	A	608	-	1,3,3	0.40	0	0,3,3	0.00	-
5	3CJ	A	609	6	8,11,11	1.94	2 (25%)	9,14,14	3.38	5 (55%)
6	HEM	A	610	1,5	24,50,50	1.43	4 (16%)	16,82,82	2.00	3 (18%)
2	NAG	B	601	1	14,14,15	1.14	1 (7%)	15,19,21	1.80	6 (40%)
2	NAG	B	602	1,2	14,14,15	1.41	2 (14%)	15,19,21	2.19	6 (40%)
2	NAG	B	603	2	14,14,15	0.97	0	15,19,21	2.08	5 (33%)
4	NO3	B	605	-	1,3,3	0.41	0	0,3,3	0.00	-
4	NO3	B	606	-	1,3,3	6.20	1 (100%)	0,3,3	0.00	-
4	NO3	B	607	-	1,3,3	0.60	0	0,3,3	0.00	-
6	HEM	B	608	1	24,50,50	1.33	3 (12%)	16,82,82	1.76	2 (12%)
5	3CJ	B	609	-	8,11,11	2.51	3 (37%)	9,14,14	4.26	5 (55%)
2	NAG	C	601	1	14,14,15	0.29	0	15,19,21	0.54	0
2	NAG	C	602	2	14,14,15	0.28	0	15,19,21	0.54	0
2	NAG	C	603	1,2	14,14,15	0.25	0	15,19,21	0.62	0
2	NAG	C	604	1	14,14,15	0.27	0	15,19,21	0.54	0
4	NO3	C	606	-	1,3,3	0.40	0	0,3,3	0.00	-
4	NO3	C	607	-	1,3,3	6.01	1 (100%)	0,3,3	0.00	-
4	NO3	C	608	-	1,3,3	0.36	0	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	3CJ	C	609	-	8,11,11	2.18	2 (25%)	9,14,14	3.40	5 (55%)
6	HEM	C	610	1	24,50,50	1.01	2 (8%)	16,82,82	2.00	8 (50%)
2	NAG	D	601	1	14,14,15	0.79	0	15,19,21	1.74	3 (20%)
2	NAG	D	602	1	14,14,15	0.28	0	15,19,21	0.54	0
2	NAG	D	603	1,2	14,14,15	0.81	0	15,19,21	1.37	2 (13%)
2	NAG	D	604	2	14,14,15	0.70	0	15,19,21	1.94	5 (33%)
4	NO3	D	606	-	1,3,3	0.40	0	0,3,3	0.00	-
4	NO3	D	607	-	1,3,3	6.19	1 (100%)	0,3,3	0.00	-
4	NO3	D	608	-	1,3,3	0.42	0	0,3,3	0.00	-
5	3CJ	D	609	-	8,11,11	2.93	4 (50%)	9,14,14	5.03	6 (66%)
6	HEM	D	610	1	24,50,50	1.49	4 (16%)	16,82,82	2.23	6 (37%)

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	A	601	1	-	0/6/23/26	0/1/1/1
2	NAG	A	602	1	-	0/6/23/26	0/1/1/1
2	NAG	A	603	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	604	2	-	0/6/23/26	0/1/1/1
4	NO3	A	606	-	-	0/0/0/0	0/0/0/0
4	NO3	A	607	-	-	0/0/0/0	0/0/0/0
4	NO3	A	608	-	-	0/0/0/0	0/0/0/0
5	3CJ	A	609	6	-	0/3/3/3	0/1/1/1
6	HEM	A	610	1,5	-	0/6/54/54	0/0/8/8
2	NAG	B	601	1	-	0/6/23/26	0/1/1/1
2	NAG	B	602	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	603	2	-	0/6/23/26	0/1/1/1
4	NO3	B	605	-	-	0/0/0/0	0/0/0/0
4	NO3	B	606	-	-	0/0/0/0	0/0/0/0
4	NO3	B	607	-	-	0/0/0/0	0/0/0/0
6	HEM	B	608	1	-	0/6/54/54	0/0/8/8
5	3CJ	B	609	-	-	0/3/3/3	0/1/1/1
2	NAG	C	601	1	-	0/6/23/26	0/1/1/1
2	NAG	C	602	2	-	0/6/23/26	0/1/1/1
2	NAG	C	603	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	604	1	-	0/6/23/26	0/1/1/1
4	NO3	C	606	-	-	0/0/0/0	0/0/0/0
4	NO3	C	607	-	-	0/0/0/0	0/0/0/0

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NO3	C	608	-	-	0/0/0/0	0/0/0/0
5	3CJ	C	609	-	-	0/3/3/3	0/1/1/1
6	HEM	C	610	1	-	0/6/54/54	0/0/8/8
2	NAG	D	601	1	-	0/6/23/26	0/1/1/1
2	NAG	D	602	1	-	0/6/23/26	0/1/1/1
2	NAG	D	603	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	604	2	-	0/6/23/26	0/1/1/1
4	NO3	D	606	-	-	0/0/0/0	0/0/0/0
4	NO3	D	607	-	-	0/0/0/0	0/0/0/0
4	NO3	D	608	-	-	0/0/0/0	0/0/0/0
5	3CJ	D	609	-	-	0/3/3/3	0/1/1/1
6	HEM	D	610	1	-	0/6/54/54	0/0/8/8

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	610	HEM	C4D-ND	-3.65	1.31	1.36
6	A	610	HEM	C1B-NB	-3.60	1.31	1.36
6	D	610	HEM	C1B-NB	-3.52	1.32	1.36
6	B	608	HEM	C1B-NB	-3.06	1.32	1.36
6	D	610	HEM	C3B-C2B	-2.95	1.36	1.40
6	B	608	HEM	C3B-C2B	-2.85	1.36	1.40
2	A	603	NAG	C2-N2	-2.68	1.41	1.46
2	A	603	NAG	O5-C1	-2.65	1.39	1.43
6	C	610	HEM	C1B-NB	-2.48	1.33	1.36
6	B	608	HEM	C4D-ND	-2.40	1.33	1.36
2	A	604	NAG	C2-N2	-2.39	1.42	1.46
6	D	610	HEM	C4C-NC	-2.38	1.33	1.36
6	A	610	HEM	C1A-CHA	-2.27	1.34	1.40
6	C	610	HEM	C4D-ND	-2.22	1.33	1.36
2	B	601	NAG	C4-C5	-2.21	1.48	1.53
6	D	610	HEM	CAA-C2A	-2.06	1.48	1.52
2	B	602	NAG	O5-C1	-2.03	1.40	1.43
6	A	610	HEM	C3B-C2B	-2.03	1.37	1.40
5	D	609	3CJ	C4-N2	2.06	1.36	1.33
5	A	609	3CJ	C1-S1	2.26	1.71	1.66
5	B	609	3CJ	C4-N2	2.68	1.37	1.33
5	C	609	3CJ	C1-S1	2.69	1.72	1.66
2	B	602	NAG	C1-C2	2.89	1.56	1.52
5	D	609	3CJ	C2-N1	3.51	1.40	1.34
5	B	609	3CJ	C1-S1	3.72	1.74	1.66
5	A	609	3CJ	O1-C4	4.48	1.35	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	D	609	3CJ	C1-S1	4.84	1.76	1.66
5	B	609	3CJ	O1-C4	4.98	1.37	1.24
5	D	609	3CJ	O1-C4	5.16	1.37	1.24
5	C	609	3CJ	O1-C4	5.18	1.37	1.24
4	C	607	NO3	O1-N	6.01	1.40	1.23
4	A	607	NO3	O1-N	6.17	1.40	1.23
4	D	607	NO3	O1-N	6.19	1.40	1.23
4	B	606	NO3	O1-N	6.20	1.40	1.23

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	610	HEM	CBD-CAD-C3D	-6.34	101.34	112.47
5	B	609	3CJ	C3-C2-N1	-5.95	116.28	122.90
6	D	610	HEM	CBD-CAD-C3D	-5.72	102.43	112.47
2	A	603	NAG	C2-N2-C7	-4.92	116.70	123.11
2	B	603	NAG	C4-C3-C2	-4.69	104.06	111.34
6	B	608	HEM	CBD-CAD-C3D	-4.58	104.44	112.47
5	A	609	3CJ	C3-C2-N1	-4.53	117.86	122.90
5	D	609	3CJ	C3-C2-N1	-4.46	117.94	122.90
5	C	609	3CJ	C3-C4-N2	-4.27	119.50	124.02
2	A	601	NAG	C4-C3-C2	-4.23	104.78	111.34
2	D	601	NAG	C2-N2-C7	-4.11	117.76	123.11
2	D	604	NAG	C3-C4-C5	-4.06	102.98	110.23
5	C	609	3CJ	C3-C2-N1	-3.98	118.47	122.90
2	D	603	NAG	C2-N2-C7	-3.87	118.07	123.11
2	A	601	NAG	C2-N2-C7	-3.79	118.18	123.11
6	C	610	HEM	CBD-CAD-C3D	-3.69	105.99	112.47
2	A	604	NAG	O4-C4-C3	-3.69	102.04	110.36
5	D	609	3CJ	C5-C2-C3	-3.50	115.99	121.22
2	B	602	NAG	O4-C4-C3	-3.25	103.02	110.36
2	B	601	NAG	C2-N2-C7	-3.20	118.94	123.11
5	D	609	3CJ	C3-C4-N2	-3.17	120.66	124.02
2	A	601	NAG	C3-C4-C5	-3.08	104.73	110.23
2	D	604	NAG	O5-C5-C4	-3.06	105.07	110.13
6	B	608	HEM	CAA-C2A-C3A	-2.92	120.66	129.00
6	D	610	HEM	CBA-CAA-C2A	-2.84	107.50	112.49
2	B	601	NAG	O6-C6-C5	-2.66	102.42	111.30
5	A	609	3CJ	C3-C4-N2	-2.63	121.23	124.02
2	A	604	NAG	O3-C3-C4	-2.58	104.53	110.36
2	A	604	NAG	C2-N2-C7	-2.58	119.75	123.11
2	B	601	NAG	O5-C5-C4	-2.57	105.88	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	602	NAG	C6-C5-C4	-2.55	106.58	112.99
5	B	609	3CJ	C3-C4-N2	-2.53	121.35	124.02
6	C	610	HEM	CAA-C2A-C3A	-2.43	122.07	129.00
2	D	603	NAG	C6-C5-C4	-2.39	106.99	112.99
2	B	602	NAG	O4-C4-C5	-2.33	103.09	109.23
2	B	601	NAG	O3-C3-C4	-2.30	105.17	110.36
2	D	601	NAG	O3-C3-C4	-2.24	105.32	110.36
6	A	610	HEM	C3C-CAC-CBC	-2.22	121.94	126.40
2	B	601	NAG	C6-C5-C4	-2.21	107.45	112.99
2	D	601	NAG	C8-C7-N2	-2.13	112.00	116.10
2	A	601	NAG	O4-C4-C3	-2.09	105.64	110.36
6	C	610	HEM	C3B-CAB-CBB	-2.09	122.20	126.40
2	D	604	NAG	C4-C3-C2	-2.08	108.11	111.34
6	D	610	HEM	C3B-CAB-CBB	-2.06	122.26	126.40
6	C	610	HEM	C3B-C4B-NB	-2.06	106.55	109.21
6	C	610	HEM	CAA-CBA-CGA	-2.05	108.79	112.78
6	D	610	HEM	C3C-CAC-CBC	-2.00	122.37	126.40
2	B	603	NAG	C2-N2-C7	2.15	125.91	123.11
6	C	610	HEM	CMC-C2C-C3C	2.26	129.50	125.09
6	D	610	HEM	CMB-C2B-C3B	2.29	129.56	125.09
2	A	601	NAG	O5-C5-C6	2.38	112.43	107.34
2	B	603	NAG	O5-C5-C4	2.42	114.15	110.13
2	D	604	NAG	C1-O5-C5	2.47	115.77	112.14
6	A	610	HEM	CMD-C2D-C3D	2.62	130.71	125.24
2	B	603	NAG	C1-O5-C5	2.82	116.29	112.14
2	B	601	NAG	C1-O5-C5	2.84	116.32	112.14
6	C	610	HEM	CAD-CBD-CGD	3.05	118.72	112.78
5	A	609	3CJ	C5-C2-C3	3.06	125.80	121.22
2	B	602	NAG	C3-C4-C5	3.08	115.72	110.23
2	D	604	NAG	O5-C5-C6	3.11	113.99	107.34
2	A	601	NAG	C1-O5-C5	3.23	116.89	112.14
2	A	601	NAG	O4-C4-C5	3.23	117.75	109.23
6	C	610	HEM	CMB-C2B-C3B	3.37	131.69	125.09
5	B	609	3CJ	C5-C2-N1	3.54	121.09	115.71
2	B	602	NAG	O5-C5-C6	3.55	114.93	107.34
2	A	604	NAG	C4-C3-C2	3.73	117.14	111.34
5	C	609	3CJ	C5-C2-N1	3.87	121.60	115.71
6	D	610	HEM	CMC-C2C-C3C	3.94	132.79	125.09
2	B	603	NAG	O3-C3-C2	3.98	117.90	109.37
2	B	602	NAG	O3-C3-C2	4.62	119.27	109.37
5	C	609	3CJ	C1-N1-C2	4.71	120.41	115.39
5	A	609	3CJ	C4-N2-C1	4.76	118.94	114.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	609	3CJ	C4-N2-C1	5.43	119.54	114.68
5	C	609	3CJ	C4-N2-C1	5.52	119.62	114.68
5	A	609	3CJ	C1-N1-C2	6.29	122.08	115.39
5	D	609	3CJ	C5-C2-N1	6.73	125.94	115.71
5	D	609	3CJ	C1-N1-C2	6.94	122.78	115.39
2	A	604	NAG	C1-O5-C5	7.93	123.80	112.14
5	B	609	3CJ	C1-N1-C2	8.72	124.67	115.39
5	D	609	3CJ	C4-N2-C1	9.42	123.11	114.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

21 monomers are involved in 94 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	604	NAG	1	0
4	A	607	NO3	1	0
5	A	609	3CJ	11	0
6	A	610	HEM	12	0
2	B	602	NAG	2	0
2	B	603	NAG	2	0
4	B	605	NO3	1	0
6	B	608	HEM	14	0
5	B	609	3CJ	12	0
2	C	603	NAG	1	0
4	C	606	NO3	1	0
4	C	607	NO3	1	0
4	C	608	NO3	2	0
5	C	609	3CJ	9	0
6	C	610	HEM	17	0
2	D	602	NAG	1	0
4	D	606	NO3	2	0
4	D	607	NO3	2	0
4	D	608	NO3	4	0
5	D	609	3CJ	11	0
6	D	610	HEM	15	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	595/595 (100%)	0.24	31 (5%) 31 35	16, 42, 78, 117	0
1	B	595/595 (100%)	0.26	34 (5%) 27 31	20, 43, 76, 100	0
1	C	595/595 (100%)	0.43	53 (8%) 12 13	20, 43, 83, 100	0
1	D	595/595 (100%)	0.34	40 (6%) 21 23	14, 41, 79, 100	0
All	All	2380/2380 (100%)	0.32	158 (6%) 22 24	14, 42, 79, 117	0

All (158) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4	VAL	19.3
1	C	6	CYS	13.6
1	D	2	TRP	12.4
1	A	171	PRO	11.2
1	D	7	GLY	11.2
1	D	13	VAL	10.2
1	B	121	SER	9.8
1	D	1	SER	9.7
1	B	1	SER	9.7
1	A	2	TRP	9.4
1	A	5	GLY	9.1
1	B	2	TRP	8.9
1	D	3	GLU	8.9
1	A	1	SER	8.9
1	C	5	GLY	8.5
1	A	4	VAL	8.4
1	B	6	CYS	8.4
1	C	4	VAL	7.7
1	C	9	PRO	7.7
1	A	172	TYR	7.1
1	B	4	VAL	6.8

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Mol	Chain	Res	Type	RSRZ
1	B	5	GLY	6.7
1	C	7	GLY	6.7
1	C	1	SER	6.4
1	B	122	SER	6.3
1	D	11	PRO	6.3
1	C	121	SER	6.2
1	C	8	ALA	6.2
1	C	2	TRP	5.9
1	C	129	CYS	5.9
1	A	170	PRO	5.8
1	A	119	LEU	5.7
1	C	3	GLU	5.6
1	D	170	PRO	5.3
1	A	3	GLU	5.3
1	A	12	LEU	5.2
1	C	96	ARG	5.1
1	D	592	SER	5.1
1	C	132	TYR	5.0
1	A	6	CYS	5.0
1	B	3	GLU	4.9
1	B	120	GLY	4.8
1	D	120	GLY	4.8
1	A	121	SER	4.8
1	A	585	LEU	4.7
1	B	582	VAL	4.7
1	C	172	TYR	4.7
1	B	170	PRO	4.6
1	D	12	LEU	4.6
1	C	13	VAL	4.6
1	C	119	LEU	4.5
1	A	13	VAL	4.5
1	D	5	GLY	4.5
1	D	595	ASN	4.4
1	A	173	GLN	4.3
1	D	172	TYR	4.2
1	C	591	ALA	4.2
1	D	207	SER	4.2
1	D	169	THR	4.2
1	B	189	ALA	4.2
1	B	595	ASN	4.2
1	B	11	PRO	4.0
1	B	171	PRO	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	8	ALA	3.9
1	D	10	VAL	3.8
1	A	169	THR	3.8
1	D	6	CYS	3.7
1	C	249	PHE	3.7
1	C	161	PHE	3.7
1	A	9	PRO	3.6
1	B	8	ALA	3.6
1	A	223	GLY	3.5
1	A	136	GLY	3.5
1	A	122	SER	3.5
1	C	11	PRO	3.5
1	C	153	THR	3.5
1	C	10	VAL	3.4
1	C	580	SER	3.4
1	B	581	ALA	3.4
1	C	595	ASN	3.4
1	B	173	GLN	3.4
1	A	7	GLY	3.3
1	C	117	THR	3.3
1	B	172	TYR	3.3
1	C	138	GLU	3.3
1	B	530	TRP	3.2
1	B	369	GLY	3.2
1	B	262	LEU	3.1
1	D	209	PRO	3.0
1	D	132	TYR	3.0
1	B	9	PRO	3.0
1	B	137	ASP	3.0
1	B	583	ASP	3.0
1	C	209	PRO	2.9
1	D	190	SER	2.9
1	B	425	THR	2.9
1	C	106	ILE	2.9
1	B	282	ARG	2.8
1	C	169	THR	2.8
1	C	127	VAL	2.8
1	A	582	VAL	2.7
1	B	7	GLY	2.7
1	D	173	GLN	2.7
1	C	215	VAL	2.7
1	B	545	GLN	2.7

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Mol	Chain	Res	Type	RSRZ
1	D	175	LEU	2.7
1	C	351	HIS	2.6
1	D	574	HIS	2.6
1	D	171	PRO	2.6
1	C	464	LEU	2.6
1	A	174	SER	2.6
1	D	351	HIS	2.6
1	A	56	ALA	2.5
1	C	120	GLY	2.5
1	C	173	GLN	2.5
1	D	243	THR	2.5
1	B	593	ARG	2.4
1	C	175	LEU	2.4
1	D	585	LEU	2.4
1	C	542	ASP	2.4
1	C	118	GLU	2.4
1	A	137	ASP	2.4
1	D	107	VAL	2.4
1	D	134	VAL	2.4
1	A	425	THR	2.3
1	C	243	THR	2.3
1	D	17	GLU	2.3
1	C	130	GLU	2.3
1	C	14	THR	2.3
1	A	11	PRO	2.3
1	B	586	ASP	2.3
1	C	12	LEU	2.3
1	A	10	VAL	2.2
1	D	567	PHE	2.2
1	C	170	PRO	2.2
1	B	588	SER	2.2
1	D	223	GLY	2.2
1	A	21	TYR	2.1
1	C	581	ALA	2.1
1	C	494	ILE	2.1
1	C	592	SER	2.1
1	D	208	SER	2.1
1	A	485	LYS	2.1
1	C	582	VAL	2.1
1	D	582	VAL	2.1
1	C	355	PRO	2.1
1	D	303	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	351	HIS	2.1
1	B	10	VAL	2.1
1	C	108	ASP	2.0
1	C	164	GLY	2.0
1	D	15	CYS	2.0
1	C	159	PRO	2.0
1	D	168	PRO	2.0
1	C	546	LYS	2.0
1	C	276	LEU	2.0
1	D	331	TYR	2.0
1	D	206	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	NO3	C	606	4/4	0.92	0.59	10.60	24,27,29,31	0
4	NO3	D	608	4/4	0.94	0.46	10.37	23,23,26,30	0
4	NO3	B	607	4/4	0.91	0.66	7.83	24,24,24,28	0
4	NO3	A	608	4/4	0.96	0.42	6.79	23,24,26,27	0
4	NO3	C	608	4/4	0.87	0.25	4.44	24,28,29,30	0
4	NO3	A	606	4/4	0.96	0.30	3.77	23,23,24,26	0
2	NAG	A	601	14/15	0.74	0.20	3.27	64,79,81,81	0
5	3CJ	D	609	11/11	0.83	0.41	3.15	39,48,58,58	0
5	3CJ	C	609	11/11	0.74	0.36	2.31	69,79,84,85	0
4	NO3	B	605	4/4	0.89	0.20	1.77	22,25,27,28	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
4	NO3	D	606	4/4	0.95	0.22	1.67	21,24,24,26	0
6	HEM	A	610	43/43	0.95	0.23	1.41	31,39,44,49	0
2	NAG	C	603	14/15	0.86	0.24	1.25	20,20,20,20	0
2	NAG	B	601	14/15	0.91	0.15	1.10	55,63,73,75	0
6	HEM	B	608	43/43	0.94	0.23	1.02	33,42,54,62	0
5	3CJ	B	609	11/11	0.84	0.24	1.01	48,52,58,61	0
3	CA	C	605	1/1	0.94	0.23	0.66	46,46,46,46	0
3	CA	A	605	1/1	0.91	0.18	0.53	43,43,43,43	0
2	NAG	C	604	14/15	0.89	0.20	0.48	48,55,60,61	0
3	CA	D	605	1/1	0.97	0.24	0.21	36,36,36,36	0
2	NAG	B	602	14/15	0.85	0.19	0.15	36,50,59,66	0
2	NAG	C	601	14/15	0.64	0.39	-0.11	78,86,89,90	0
6	HEM	C	610	43/43	0.94	0.19	-0.16	35,45,51,53	0
6	HEM	D	610	43/43	0.95	0.19	-0.17	19,25,39,45	0
2	NAG	A	602	14/15	0.94	0.12	-0.38	38,46,51,54	0
5	3CJ	A	609	11/11	0.92	0.19	-0.38	47,50,55,56	0
2	NAG	A	603	14/15	0.93	0.14	-0.55	33,41,52,54	0
3	CA	B	604	1/1	0.93	0.14	-0.71	44,44,44,44	0
2	NAG	D	601	14/15	0.84	0.20	-0.72	52,60,65,66	0
2	NAG	D	602	14/15	0.82	0.17	-0.82	46,54,59,60	0
2	NAG	D	603	14/15	0.94	0.11	-0.95	70,79,82,85	0
2	NAG	B	603	14/15	0.81	0.27	-	45,53,55,58	14
2	NAG	A	604	14/15	0.88	0.20	-	43,50,51,52	14
2	NAG	C	602	14/15	0.83	0.21	-	49,56,63,63	14
4	NO3	C	607	4/4	0.86	0.43	-	24,24,27,31	0
4	NO3	B	606	4/4	0.90	0.40	-	26,26,27,29	0
2	NAG	D	604	14/15	0.84	0.20	-	61,67,70,70	14
4	NO3	D	607	4/4	0.90	0.38	-	25,26,27,28	0
4	NO3	A	607	4/4	0.97	0.17	-	24,26,28,32	0

6.5 Other polymers ⓘ

There are no such residues in this entry.