



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 9, 2017 – 03:25 AM EDT

PDB ID : 2IKC
Title : Crystal structure of sheep lactoperoxidase at 3.25 Å resolution reveals the binding sites for formate
Authors : Sheikh, I.A.; Singh, N.; Singh, A.K.; Sharma, S.; Singh, T.P.
Deposited on : unknown
Resolution : 3.25 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030345

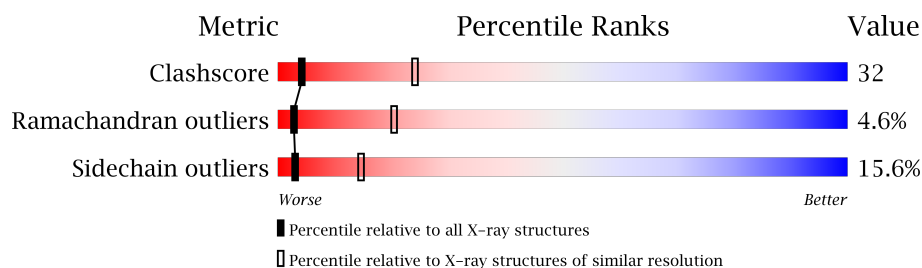
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.25 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	112137	2036 (3.32-3.20)
Ramachandran outliers	110173	2000 (3.32-3.20)
Sidechain outliers	110143	1998 (3.32-3.20)

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.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	595	
1	B	595	

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
7	FMT	A	3002	-	-	X	-

2 Entry composition [i](#)

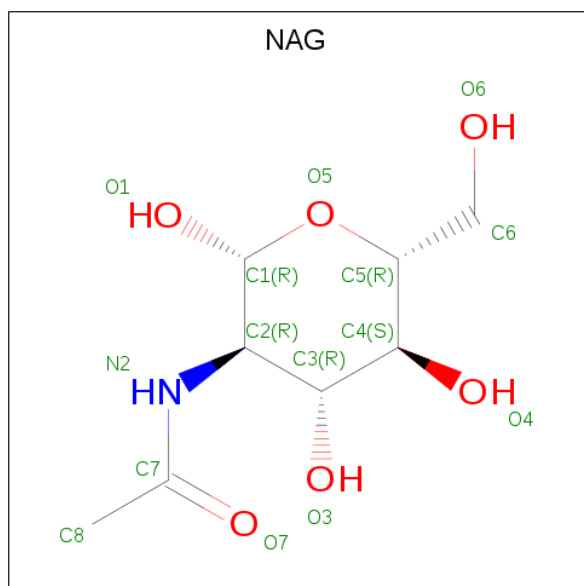
There are 8 unique types of molecules in this entry. The entry contains 10008 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 milk lactoperoxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	0	0
			4764	3024	853	861	26			
1	B	595	Total	C	N	O	S	0	0	0
			4764	3024	853	861	26			

- Molecule 2 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



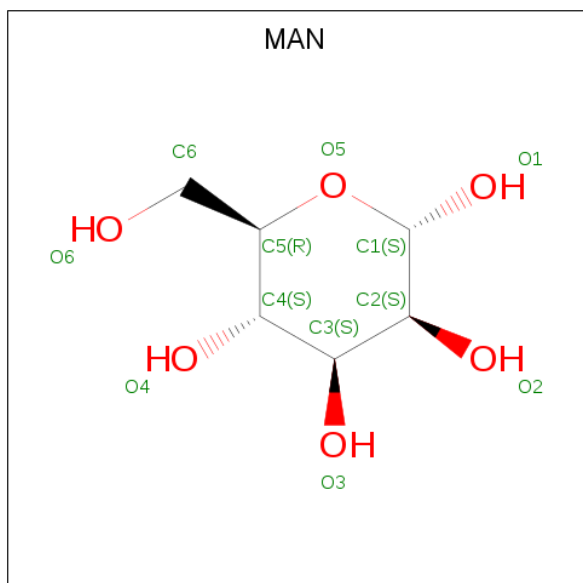
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	A	1	Total	C	N	O	0	0
			14	8	1	5		

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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	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	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		

- Molecule 3 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			11	6	5		

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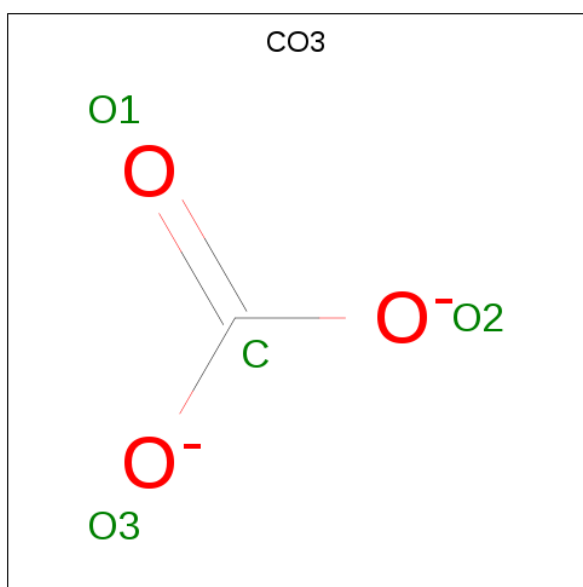
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			11	6	5		

- Molecule 4 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Ca	0	0
			1	1		
4	A	1	Total	Ca	0	0
			1	1		

- Molecule 5 is CARBONATE ION (three-letter code: CO3) (formula: CO₃).



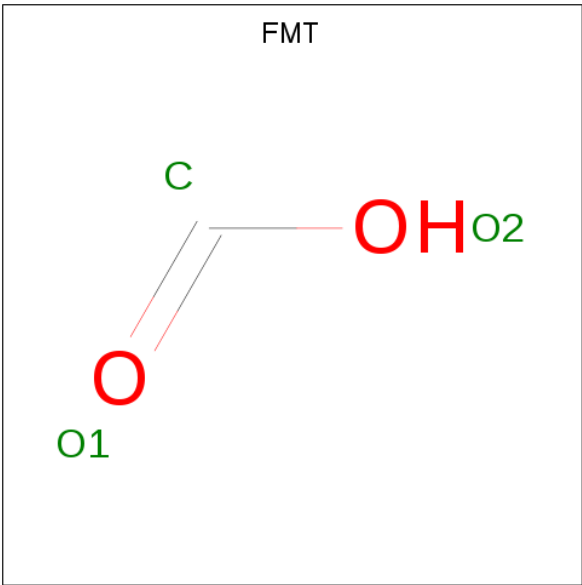
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			4	1	3		
5	B	1	Total	C	O	0	0
			4	1	3		

- Molecule 6 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

- Molecule 7 is FORMIC ACID (three-letter code: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			3	1	2		
7	A	1	Total	C	O	0	0
			3	1	2		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			3	1	2		
7	B	1	Total	C	O	0	0
			3	1	2		
7	B	1	Total	C	O	0	0
			3	1	2		
7	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 8 is water.

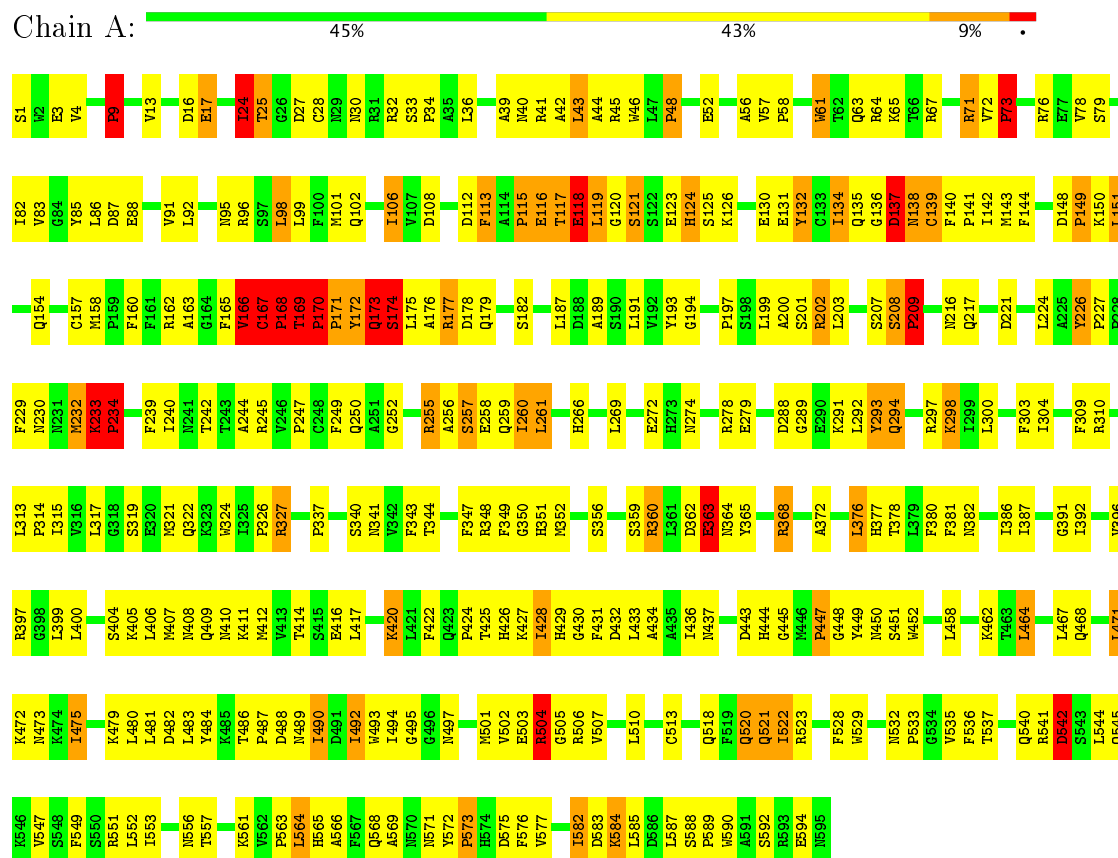
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	86	Total	O	0	0
			86	86		
8	B	62	Total	O	0	0
			62	62		

3 Residue-property plots

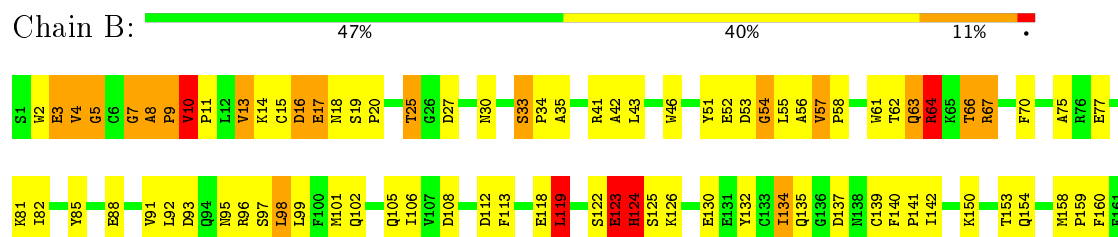
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are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

Note EDS was not executed.

- Molecule 1: milk lactoperoxidase



- Molecule 1: milk lactoperoxidase





4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	59.08 Å 72.59 Å 84.47 Å 85.20° 84.07° 75.41°	Depositor
Resolution (Å)	19.97 – 3.25	Depositor
% Data completeness (in resolution range)	96.4 (19.97-3.25)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.187 , 0.230	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10008	wwPDB-VP
Average B, all atoms (Å ²)	11.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CO3, NAG, FMT, HEM, CA, MAN

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	0.64	7/4889 (0.1%)	1.10	36/6629 (0.5%)
1	B	0.64	3/4889 (0.1%)	1.04	24/6629 (0.4%)
All	All	0.64	10/9778 (0.1%)	1.07	60/13258 (0.5%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	67	ARG	N-CA	18.38	1.83	1.46
1	A	24	ILE	N-CA	6.80	1.59	1.46
1	A	9	PRO	N-CA	6.63	1.58	1.47
1	A	172	TYR	N-CA	6.18	1.58	1.46
1	A	118	GLU	N-CA	-5.61	1.35	1.46
1	B	123	GLU	N-CA	5.52	1.57	1.46
1	A	173	GLN	N-CA	5.51	1.57	1.46
1	B	573	PRO	N-CA	5.28	1.56	1.47
1	A	171	PRO	CA-C	5.10	1.63	1.52
1	A	209	PRO	CA-C	-5.04	1.42	1.52

All (60) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	233	LYS	C-N-CD	-19.31	78.12	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	67	ARG	N-CA-CB	-17.09	79.85	110.60
1	A	233	LYS	C-N-CD	-14.78	88.09	120.60
1	A	172	TYR	CB-CG-CD2	-14.67	112.20	121.00
1	A	172	TYR	CB-CG-CD1	14.37	129.62	121.00
1	B	573	PRO	CA-N-CD	-13.86	92.10	111.50
1	B	571	ASN	CB-CA-C	11.30	133.01	110.40
1	A	171	PRO	CA-C-N	11.02	141.44	117.20
1	B	233	LYS	C-N-CA	10.40	165.67	122.00
1	A	172	TYR	CA-CB-CG	10.38	133.12	113.40
1	A	171	PRO	N-CA-C	9.80	137.59	112.10
1	B	66	THR	C-N-CA	-9.07	99.01	121.70
1	A	209	PRO	CA-N-CD	-8.41	99.73	111.50
1	A	172	TYR	CB-CA-C	-8.33	93.74	110.40
1	B	234	PRO	CA-N-CD	-8.21	100.00	111.50
1	A	171	PRO	O-C-N	-7.75	110.31	122.70
1	A	173	GLN	N-CA-C	7.68	131.75	111.00
1	B	122	SER	CB-CA-C	7.53	124.40	110.10
1	B	124	HIS	CA-CB-CG	7.45	126.27	113.60
1	A	166	VAL	N-CA-C	7.33	130.79	111.00
1	A	24	ILE	N-CA-C	7.24	130.54	111.00
1	B	7	GLY	N-CA-C	7.23	131.17	113.10
1	B	174	SER	N-CA-C	7.08	130.12	111.00
1	B	119	LEU	N-CA-C	-7.07	91.91	111.00
1	B	573	PRO	N-CA-C	7.04	130.41	112.10
1	A	149	PRO	CA-N-CD	-6.93	101.79	111.50
1	A	234	PRO	CA-N-CD	-6.85	101.92	111.50
1	B	171	PRO	C-N-CA	6.85	138.81	121.70
1	A	115	PRO	C-N-CA	-6.55	105.33	121.70
1	B	122	SER	N-CA-C	-6.54	93.36	111.00
1	A	167	CYS	C-N-CD	-6.48	106.35	120.60
1	B	375	PRO	CA-N-CD	-6.34	102.62	111.50
1	A	115	PRO	CA-N-CD	-6.28	102.71	111.50
1	A	86	LEU	CB-CA-C	-6.09	98.63	110.20
1	A	48	PRO	CA-N-CD	-6.04	103.05	111.50
1	B	122	SER	C-N-CA	5.98	136.65	121.70
1	A	166	VAL	CB-CA-C	-5.91	100.18	111.40
1	A	172	TYR	N-CA-C	5.90	126.94	111.00
1	B	464	LEU	CA-CB-CG	5.84	128.72	115.30
1	A	293	TYR	CA-CB-CG	5.80	124.42	113.40
1	A	168	PRO	C-N-CA	5.72	136.01	121.70
1	A	209	PRO	CA-C-N	-5.70	104.67	117.20
1	A	9	PRO	CA-N-CD	-5.69	103.53	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	41	ARG	C-N-CA	-5.65	107.58	121.70
1	B	571	ASN	CA-C-N	5.61	129.53	117.20
1	B	123	GLU	N-CA-C	5.59	126.08	111.00
1	A	169	THR	N-CA-C	-5.56	95.98	111.00
1	A	24	ILE	N-CA-CB	-5.43	98.31	110.80
1	B	119	LEU	C-N-CA	-5.41	110.94	122.30
1	A	73	PRO	CA-N-CD	-5.34	104.03	111.50
1	A	118	GLU	CA-C-N	-5.23	105.69	117.20
1	B	572	TYR	N-CA-CB	5.22	120.00	110.60
1	A	112	ASP	CA-CB-CG	5.20	124.84	113.40
1	A	584	LYS	N-CA-C	5.17	124.94	111.00
1	A	43	LEU	CB-CA-C	-5.16	100.40	110.20
1	A	208	SER	C-N-CD	-5.16	109.25	120.60
1	B	584	LYS	N-CA-C	5.12	124.83	111.00
1	A	170	PRO	C-N-CD	-5.04	109.51	120.60
1	A	166	VAL	CA-C-N	5.02	128.25	117.20
1	B	573	PRO	N-CD-CG	5.02	110.73	103.20

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	570	ASN	Mainchain

5.2 Too-close contacts [i](#)

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	4764	0	4684	315	0
1	B	4764	0	4683	304	0
2	A	98	0	87	13	0
2	B	98	0	87	0	0
3	A	11	0	10	1	0
3	B	11	0	10	1	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	4	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	B	4	0	0	0	0
6	A	43	0	30	8	0
6	B	43	0	30	16	0
7	A	9	0	4	2	0
7	B	9	0	3	1	0
8	A	86	0	0	10	0
8	B	62	0	0	4	0
All	All	10008	0	9628	631	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 (631) 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:B:67:ARG:CA	1:B:67:ARG:N	1.83	1.40
1:A:108:ASP:OD2	6:A:605:HEM:HMD1	1.25	1.33
1:A:233:LYS:HB3	1:A:234:PRO:HD2	1.31	1.11
1:A:167:CYS:HB2	1:A:168:PRO:HD2	1.13	1.10
1:A:209:PRO:O	1:A:289:GLY:HA2	1.50	1.08
1:B:67:ARG:N	1:B:67:ARG:CB	2.17	1.07
1:A:360:ARG:HH11	1:A:360:ARG:HB2	1.21	1.05
1:A:167:CYS:HB2	1:A:168:PRO:CD	1.85	1.04
1:A:294:GLN:HA	1:A:297:ARG:HB3	1.37	1.04
1:A:172:TYR:HB3	1:A:173:GLN:HG2	1.35	1.03
1:A:175:LEU:HD23	1:A:176:ALA:N	1.73	1.01
1:B:158:MET:HE2	1:B:431:PHE:HA	1.40	1.00
1:B:381:PHE:CZ	1:B:424:PRO:HG3	1.95	1.00
1:A:42:ALA:HB2	1:A:166:VAL:CG1	1.95	0.96
1:B:327:ARG:H	1:B:327:ARG:HD2	1.34	0.93
1:B:179:GLN:HG3	1:B:444:HIS:CE1	2.04	0.92
1:A:233:LYS:CB	1:A:234:PRO:HD2	1.97	0.91
1:B:551:ARG:HD3	1:B:583:ASP:O	1.71	0.90
1:A:24:ILE:HD13	1:A:200:ALA:HB1	1.53	0.90
1:B:179:GLN:HG3	1:B:444:HIS:ND1	1.87	0.89
1:A:169:THR:HB	1:A:170:PRO:CD	2.01	0.89
1:A:167:CYS:CB	1:A:168:PRO:HD2	1.98	0.88
1:A:108:ASP:OD2	6:A:605:HEM:HMD2	1.72	0.88
1:B:66:THR:C	1:B:67:ARG:CA	2.43	0.88
1:A:42:ALA:CB	1:A:166:VAL:HG11	2.04	0.87
1:A:123:GLU:HG3	1:A:125:SER:H	1.40	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:119:LEU:N	1:B:119:LEU:HD13	1.89	0.87
1:A:167:CYS:CB	1:A:168:PRO:CD	2.49	0.87
1:A:175:LEU:HD23	1:A:176:ALA:H	1.36	0.86
1:A:64:ARG:HA	1:A:71:ARG:NH2	1.90	0.86
1:A:42:ALA:CB	1:A:166:VAL:CG1	2.54	0.85
1:A:209:PRO:O	1:A:289:GLY:CA	2.24	0.84
1:A:344:THR:HB	6:A:605:HEM:O1D	1.76	0.84
1:A:119:LEU:CD2	1:A:120:GLY:H	1.90	0.84
1:A:260:ILE:HB	8:A:3060:HOH:O	1.78	0.83
1:A:119:LEU:HD23	1:A:120:GLY:H	1.42	0.82
1:B:42:ALA:HB2	1:B:166:VAL:CG1	2.10	0.82
1:B:362:ASP:HB3	1:B:368:ARG:HB3	1.61	0.82
1:B:588:SER:OG	1:B:589:PRO:HD3	1.78	0.82
1:A:42:ALA:HB3	1:A:166:VAL:HG11	1.58	0.82
1:A:432:ASP:O	1:A:436:ILE:HG12	1.79	0.82
1:B:130:GLU:HG3	1:B:159:PRO:HG3	1.62	0.82
1:B:505:GLY:O	1:B:506:ARG:HD3	1.81	0.81
1:B:595:ASN:HD22	1:B:595:ASN:N	1.78	0.81
1:A:24:ILE:HD11	1:A:293:TYR:OH	1.82	0.80
1:B:572:TYR:CD2	1:B:573:PRO:HD3	2.15	0.80
1:A:25:THR:HG22	1:A:27:ASP:H	1.46	0.79
1:B:67:ARG:N	1:B:67:ARG:HB2	1.96	0.79
1:B:123:GLU:OE2	1:B:125:SER:HB2	1.82	0.79
1:B:360:ARG:NH1	1:B:372:ALA:HA	1.98	0.78
1:A:341:ASN:HB3	7:A:3002:FMT:H	1.66	0.78
1:A:279:GLU:HG2	1:A:587:LEU:HD12	1.66	0.77
1:A:30:ASN:HB3	1:A:33:SER:O	1.85	0.77
1:B:295:GLU:O	1:B:299:ILE:HG12	1.83	0.77
1:A:272:GLU:HA	1:A:272:GLU:OE1	1.83	0.77
1:A:96:ARG:NH2	1:A:315:ILE:HB	2.00	0.76
1:B:377:HIS:HB3	1:B:416:GLU:OE2	1.85	0.76
1:A:368:ARG:HH11	1:A:368:ARG:HG3	1.49	0.76
1:A:260:ILE:HD11	1:A:386:ILE:HG13	1.68	0.76
1:A:52:GLU:HB3	1:A:57:VAL:HG23	1.67	0.76
1:B:327:ARG:N	1:B:327:ARG:HD2	2.02	0.75
1:A:230:ASN:ND2	1:A:232:MET:HB3	2.01	0.75
1:A:169:THR:HB	1:A:170:PRO:HD2	1.69	0.74
1:B:8:ALA:HB1	1:B:10:VAL:CG1	2.17	0.74
1:B:204:ARG:HB3	1:B:206:LEU:HG	1.70	0.74
1:B:300:LEU:O	1:B:303:PHE:HB3	1.88	0.73
1:A:170:PRO:HB3	1:A:171:PRO:HD2	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:THR:HB	1:A:426:HIS:CD2	2.24	0.73
1:B:173:GLN:HG3	1:B:174:SER:N	2.04	0.73
1:B:16:ASP:O	1:B:17:GLU:HB2	1.88	0.73
1:B:400:LEU:HD11	1:B:553:ILE:HD13	1.71	0.73
1:B:173:GLN:HG3	1:B:174:SER:H	1.54	0.73
1:A:230:ASN:HD21	1:A:232:MET:HB3	1.53	0.72
1:B:42:ALA:HB2	1:B:166:VAL:HG11	1.71	0.72
1:A:368:ARG:O	1:A:368:ARG:HG3	1.91	0.71
1:B:400:LEU:HD11	1:B:553:ILE:CD1	2.21	0.71
1:A:169:THR:HB	1:A:170:PRO:HD3	1.71	0.70
1:A:288:ASP:HB3	1:A:291:LYS:H	1.56	0.70
1:A:360:ARG:HB2	1:A:360:ARG:NH1	2.03	0.70
1:A:76:ARG:NH2	1:A:150:LYS:HG3	2.06	0.70
1:B:381:PHE:HZ	1:B:424:PRO:HG3	1.54	0.70
1:A:467:LEU:HG	1:A:471:LEU:HD22	1.73	0.70
1:A:464:LEU:O	1:A:468:GLN:HG3	1.92	0.69
1:A:260:ILE:CD1	1:A:386:ILE:HG13	2.22	0.69
1:B:544:LEU:O	1:B:547:VAL:HG22	1.93	0.69
1:B:172:TYR:N	1:B:172:TYR:CD1	2.60	0.69
1:A:56:ALA:O	1:A:58:PRO:HD3	1.93	0.68
1:A:362:ASP:HB2	1:A:368:ARG:CB	2.22	0.68
1:A:475:ILE:HD11	1:A:479:LYS:HE3	1.75	0.68
1:A:368:ARG:HG3	1:A:368:ARG:NH1	2.05	0.68
1:A:408:ASN:O	1:A:410:ASN:N	2.26	0.68
1:B:279:GLU:O	1:B:282:ARG:HG2	1.94	0.68
1:B:464:LEU:HD22	1:B:464:LEU:O	1.95	0.67
1:B:258:GLU:O	1:B:381:PHE:N	2.27	0.67
1:A:260:ILE:HD11	1:A:386:ILE:CG1	2.24	0.67
1:A:360:ARG:HH11	1:A:360:ARG:CB	2.05	0.67
1:A:298:LYS:HG2	1:A:536:PHE:CZ	2.30	0.67
1:A:137:ASP:OD1	1:A:138:ASN:N	2.28	0.67
1:A:327:ARG:HD2	1:A:327:ARG:H	1.60	0.67
1:B:8:ALA:HB1	1:B:10:VAL:HG13	1.76	0.67
1:A:139:CYS:SG	1:A:141:PRO:HD3	2.34	0.66
1:A:360:ARG:HH12	1:A:372:ALA:HA	1.60	0.66
1:B:218:GLU:HG3	8:B:3060:HOH:O	1.94	0.66
1:B:10:VAL:HG23	1:B:10:VAL:O	1.94	0.66
1:A:588:SER:N	1:A:589:PRO:HD2	2.10	0.66
1:A:191:LEU:H	1:A:191:LEU:HD23	1.61	0.66
1:B:64:ARG:HG2	1:B:64:ARG:O	1.96	0.66
1:A:24:ILE:HD13	1:A:200:ALA:CB	2.22	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:PRO:HG2	1:A:249:PHE:CG	2.31	0.66
1:B:123:GLU:HB3	1:B:126:LYS:HE3	1.77	0.66
1:A:549:PHE:CE1	1:A:552:LEU:HD23	2.30	0.65
1:B:370:PRO:HG3	3:B:602:MAN:H62	1.76	0.65
1:B:166:VAL:HG23	1:B:167:CYS:SG	2.37	0.65
1:A:445:GLY:O	1:A:447:PRO:HD3	1.95	0.65
1:A:123:GLU:HB3	1:A:126:LYS:NZ	2.12	0.65
1:A:391:GLY:HA3	8:A:3007:HOH:O	1.95	0.64
1:A:294:GLN:CA	1:A:297:ARG:HB3	2.21	0.64
1:A:377:HIS:CE1	1:A:378:THR:HG23	2.33	0.64
1:B:410:ASN:O	1:B:410:ASN:ND2	2.31	0.64
1:B:407:MET:HB3	1:B:501:MET:CE	2.27	0.64
1:B:258:GLU:O	1:B:380:PHE:HA	1.98	0.64
1:A:368:ARG:HH11	1:A:368:ARG:CG	2.10	0.64
1:B:432:ASP:O	1:B:436:ILE:HG13	1.97	0.64
1:A:362:ASP:HB2	1:A:368:ARG:HB3	1.81	0.63
1:B:579:CYS:O	1:B:582:ILE:HG23	1.98	0.63
1:B:7:GLY:O	1:B:8:ALA:HB2	1.98	0.63
1:B:2:TRP:HD1	1:B:4:VAL:CG1	2.12	0.63
1:A:259:GLN:OE1	1:A:261:LEU:HB2	1.98	0.63
1:A:73:PRO:HG3	1:A:483:LEU:O	1.99	0.63
1:B:113:PHE:HA	6:B:605:HEM:O2D	1.99	0.63
1:B:169:THR:N	1:B:170:PRO:CD	2.62	0.63
1:A:44:ALA:O	1:A:340:SER:HA	1.99	0.62
1:A:327:ARG:HD2	1:A:327:ARG:N	2.14	0.62
1:B:359:SER:HB3	1:B:373:GLU:HG2	1.81	0.62
1:A:324:TRP:O	1:A:326:PRO:HD3	1.99	0.62
1:B:158:MET:HE2	1:B:431:PHE:CA	2.26	0.62
1:A:504:ARG:NH2	2:A:597:NAG:H5	2.14	0.62
1:B:257:SER:O	1:B:258:GLU:C	2.35	0.62
1:B:91:VAL:HG22	1:B:91:VAL:O	2.00	0.62
1:A:382:ASN:HB3	8:A:3060:HOH:O	1.99	0.62
1:A:492:ILE:CG2	1:A:493:TRP:N	2.63	0.62
1:B:4:VAL:O	1:B:4:VAL:HG23	1.99	0.62
1:A:91:VAL:HG22	1:A:91:VAL:O	1.98	0.61
1:B:123:GLU:HG3	1:B:124:HIS:N	2.15	0.61
1:B:10:VAL:CG2	1:B:10:VAL:O	2.49	0.61
1:B:3:GLU:O	1:B:5:GLY:N	2.33	0.61
1:B:2:TRP:HD1	1:B:4:VAL:HG11	1.65	0.61
1:B:368:ARG:O	1:B:372:ALA:HB2	2.00	0.61
1:B:453:ARG:NH2	1:B:458:LEU:HB3	2.15	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:53:ASP:CG	1:B:57:VAL:HG13	2.21	0.61
1:A:179:GLN:NE2	1:A:444:HIS:HA	2.15	0.61
1:A:46:TRP:CE2	1:A:340:SER:HB3	2.36	0.61
1:B:173:GLN:CG	1:B:174:SER:N	2.62	0.61
1:A:42:ALA:HB1	1:A:179:GLN:O	2.00	0.61
1:A:229:PHE:CG	1:A:247:PRO:HG2	2.36	0.61
1:B:343:PHE:CD1	1:B:518:GLN:HG2	2.36	0.61
1:B:407:MET:HB3	1:B:501:MET:HE3	1.82	0.61
1:A:123:GLU:HB3	1:A:126:LYS:HZ2	1.66	0.61
1:A:169:THR:CB	1:A:170:PRO:HD2	2.30	0.61
1:B:169:THR:OG1	1:B:170:PRO:HD3	2.01	0.61
1:A:362:ASP:O	1:A:364:ASN:N	2.34	0.60
1:B:342:VAL:HB	1:B:446:MET:HE1	1.82	0.60
1:B:467:LEU:HD23	1:B:477:ALA:HA	1.82	0.60
1:A:119:LEU:CD2	1:A:120:GLY:N	2.64	0.60
1:A:377:HIS:HB3	1:A:416:GLU:OE2	2.01	0.60
1:A:98:LEU:O	1:A:98:LEU:HD22	2.02	0.60
1:A:274:ASN:HB3	1:A:278:ARG:NH2	2.16	0.60
1:B:170:PRO:HB3	1:B:171:PRO:HD2	1.83	0.60
1:B:420:LYS:HA	1:B:429:HIS:O	2.01	0.60
1:A:362:ASP:N	1:A:368:ARG:HB3	2.17	0.59
1:A:407:MET:SD	1:A:408:ASN:N	2.75	0.59
1:A:310:ARG:HG2	1:A:310:ARG:O	2.02	0.59
1:B:361:LEU:HB3	1:B:365:TYR:HA	1.84	0.59
1:B:408:ASN:HB3	1:B:411:LYS:HB2	1.85	0.59
1:A:449:TYR:HB2	1:A:490:ILE:HG22	1.85	0.59
1:A:313:LEU:N	1:A:314:PRO:CD	2.64	0.59
1:B:119:LEU:CD1	1:B:119:LEU:N	2.61	0.59
1:A:142:ILE:O	1:A:157:CYS:HB2	2.02	0.58
1:A:450:ASN:HD21	1:A:487:PRO:HB2	1.68	0.58
1:B:98:LEU:HD13	1:B:399:LEU:HD23	1.85	0.58
1:A:537:THR:OG1	1:A:540:GLN:HG3	2.03	0.58
1:A:58:PRO:HG3	1:A:443:ASP:HA	1.84	0.58
1:A:17:GLU:O	1:A:17:GLU:HG3	2.02	0.58
1:B:187:LEU:HB3	1:B:305:GLN:HG3	1.84	0.58
1:A:351:HIS:CE1	1:A:433:LEU:HD21	2.38	0.58
1:A:221:ASP:O	1:A:224:LEU:HB2	2.04	0.57
1:B:105:GLN:NE2	6:B:605:HEM:C4B	2.71	0.57
1:A:202:ARG:NH2	1:A:250:GLN:HE22	2.03	0.57
1:A:27:ASP:O	1:A:28:CYS:HB2	2.03	0.57
1:A:481:LEU:C	1:A:483:LEU:N	2.57	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:504:ARG:HH21	2:A:597:NAG:H5	1.69	0.57
1:A:150:LYS:HD3	1:A:154:GLN:OE1	2.04	0.57
2:A:601:NAG:H61	2:A:601:NAG:H2	1.85	0.57
2:A:601:NAG:H5	3:A:602:MAN:H2	1.85	0.57
1:A:501:MET:HE2	1:A:506:ARG:HA	1.86	0.57
1:B:287:TRP:CE2	1:B:291:LYS:HE3	2.39	0.57
1:B:417:LEU:HD11	6:B:605:HEM:HBB2	1.87	0.57
1:A:169:THR:CB	1:A:170:PRO:CD	2.74	0.56
1:B:323:LYS:HD3	1:B:324:TRP:NE1	2.20	0.56
1:B:9:PRO:CG	1:B:10:VAL:H	2.18	0.56
1:B:9:PRO:HG2	1:B:10:VAL:H	1.70	0.56
1:A:229:PHE:CD1	1:A:247:PRO:HG2	2.40	0.56
1:B:377:HIS:CD2	1:B:377:HIS:C	2.79	0.56
1:A:102:GLN:OE1	1:A:261:LEU:HB3	2.05	0.56
1:B:362:ASP:O	1:B:364:ASN:N	2.38	0.56
1:B:480:LEU:O	1:B:483:LEU:HB2	2.04	0.56
1:A:473:ASN:OD1	1:A:475:ILE:HG23	2.06	0.56
1:B:191:LEU:HD23	1:B:191:LEU:H	1.70	0.56
1:A:492:ILE:HG23	1:A:493:TRP:N	2.21	0.56
1:B:327:ARG:H	1:B:327:ARG:CD	2.14	0.56
1:B:299:ILE:HD11	1:B:590:TRP:NE1	2.20	0.56
1:B:53:ASP:C	1:B:55:LEU:H	2.09	0.56
1:A:356:SER:HA	1:A:414:THR:HG21	1.86	0.56
2:A:598:NAG:H61	8:A:3023:HOH:O	2.06	0.56
1:B:276:LEU:O	1:B:280:LEU:HG	2.06	0.55
1:A:587:LEU:C	1:A:589:PRO:HD2	2.26	0.55
1:B:362:ASP:O	1:B:362:ASP:OD2	2.24	0.55
1:B:494:ILE:CG2	1:B:495:GLY:N	2.69	0.55
1:A:551:ARG:CA	1:A:582:ILE:HD11	2.36	0.55
1:A:293:TYR:C	1:A:294:GLN:HG2	2.27	0.55
1:B:481:LEU:C	1:B:483:LEU:N	2.59	0.55
1:A:377:HIS:CE1	1:A:378:THR:CG2	2.89	0.55
1:A:158:MET:HB2	1:A:431:PHE:CE2	2.42	0.55
1:B:168:PRO:HB3	1:B:170:PRO:HD2	1.89	0.55
1:B:595:ASN:ND2	1:B:595:ASN:N	2.50	0.55
1:A:542:ASP:HA	1:A:545:GLN:NE2	2.21	0.54
1:A:584:LYS:O	1:A:585:LEU:HB3	2.07	0.54
1:A:494:ILE:HG23	1:A:495:GLY:H	1.73	0.54
1:B:66:THR:O	1:B:67:ARG:CA	2.55	0.54
1:A:501:MET:CE	1:A:506:ARG:HD2	2.37	0.54
1:A:119:LEU:N	1:A:119:LEU:HD13	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:108:ASP:CG	6:A:605:HEM:HMD1	2.18	0.54
1:B:216:ASN:ND2	8:B:3060:HOH:O	2.41	0.54
1:B:354:VAL:HG11	6:B:605:HEM:HBB1	1.88	0.54
1:A:564:LEU:HD22	8:A:3079:HOH:O	2.07	0.54
1:B:27:ASP:OD1	1:B:35:ALA:HA	2.08	0.54
1:A:61:TRP:C	1:A:61:TRP:CD1	2.81	0.54
1:A:217:GLN:NE2	2:A:598:NAG:H83	2.23	0.54
1:A:412:MET:HB2	8:A:3062:HOH:O	2.07	0.54
1:B:165:PHE:CG	1:B:177:ARG:HD2	2.43	0.54
1:B:106:ILE:HD11	1:B:265:VAL:HB	1.89	0.54
1:B:106:ILE:HG23	1:B:191:LEU:HD11	1.90	0.53
1:B:260:ILE:HG21	1:B:379:LEU:HD22	1.90	0.53
1:B:75:ALA:HB2	1:B:439:GLN:HG3	1.89	0.53
1:A:360:ARG:NH1	1:A:372:ALA:HA	2.23	0.53
1:A:588:SER:N	1:A:589:PRO:CD	2.70	0.53
1:A:162:ARG:HB3	1:A:443:ASP:OD1	2.08	0.53
1:A:85:TYR:CD2	1:A:411:LYS:HB3	2.43	0.53
1:B:142:ILE:HA	1:B:439:GLN:HE22	1.72	0.53
1:B:242:THR:O	1:B:245:ARG:HG3	2.09	0.53
1:B:360:ARG:HH11	1:B:372:ALA:HA	1.73	0.53
1:A:189:ALA:HB2	1:A:304:ILE:HG13	1.90	0.53
1:B:360:ARG:HB2	1:B:360:ARG:HH11	1.74	0.53
1:B:66:THR:HB	1:B:70:PHE:N	2.24	0.53
1:B:105:GLN:HB2	6:B:605:HEM:HMC3	1.91	0.53
1:A:201:SER:HA	8:A:3072:HOH:O	2.09	0.53
1:A:258:GLU:O	1:A:380:PHE:HA	2.08	0.53
1:A:501:MET:HE2	1:A:506:ARG:HD2	1.90	0.53
1:B:108:ASP:OD2	6:B:605:HEM:HHD	2.07	0.53
1:B:77:GLU:OE2	1:B:81:LYS:NZ	2.42	0.53
1:A:226:TYR:CE1	1:A:387:ILE:HG12	2.43	0.53
1:A:309:PHE:CD1	1:A:529:TRP:HH2	2.27	0.53
1:B:328:TYR:OH	1:B:532:ASN:HB2	2.09	0.53
1:B:2:TRP:C	1:B:4:VAL:H	2.11	0.53
6:B:605:HEM:HMC1	6:B:605:HEM:HBC2	1.91	0.53
1:A:131:GLU:HB2	1:A:132:TYR:CE1	2.44	0.53
1:A:322:GLN:HE21	1:A:327:ARG:HH21	1.57	0.53
1:A:25:THR:HG21	1:A:27:ASP:OD2	2.09	0.52
2:A:600:NAG:H62	2:A:601:NAG:N2	2.24	0.52
1:B:16:ASP:OD2	1:B:19:SER:HB2	2.10	0.52
1:B:267:THR:O	1:B:271:ARG:HG3	2.08	0.52
1:A:494:ILE:HG23	1:A:495:GLY:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:LEU:HD13	1:B:399:LEU:CD2	2.38	0.52
1:B:142:ILE:HA	1:B:439:GLN:NE2	2.24	0.52
1:B:481:LEU:C	1:B:483:LEU:H	2.10	0.52
1:A:113:PHE:HB3	1:A:182:SER:OG	2.10	0.52
1:B:360:ARG:HH12	1:B:372:ALA:HA	1.73	0.52
1:A:362:ASP:CA	1:A:368:ARG:HB3	2.39	0.52
1:B:9:PRO:O	1:B:10:VAL:HG22	2.10	0.52
1:A:52:GLU:OE1	1:A:65:LYS:HD2	2.10	0.52
1:B:165:PHE:CE2	1:B:172:TYR:HB3	2.44	0.52
1:B:213:MET:HG2	1:B:273:HIS:CD2	2.45	0.52
1:B:386:ILE:HG23	1:B:392:ILE:HG22	1.91	0.52
1:B:342:VAL:CB	1:B:446:MET:HE1	2.40	0.52
1:B:410:ASN:O	1:B:411:LYS:HG3	2.10	0.52
1:B:101:MET:HE2	6:B:605:HEM:HMC2	1.91	0.52
1:A:124:HIS:HB3	8:A:3080:HOH:O	2.09	0.52
1:A:242:THR:HB	1:A:245:ARG:NH2	2.25	0.52
1:B:173:GLN:HG3	1:B:174:SER:OG	2.10	0.52
1:B:52:GLU:HB3	1:B:57:VAL:HG22	1.90	0.52
1:A:132:TYR:N	1:A:132:TYR:CD1	2.78	0.51
1:A:193:TYR:OH	1:A:300:LEU:HD23	2.10	0.51
1:B:179:GLN:HG3	1:B:444:HIS:HD1	1.70	0.51
1:B:142:ILE:HG12	1:B:439:GLN:NE2	2.25	0.51
1:B:351:HIS:HD1	1:B:437:ASN:HD21	1.58	0.51
1:B:61:TRP:O	1:B:135:GLN:NE2	2.43	0.51
1:B:362:ASP:O	1:B:365:TYR:N	2.43	0.51
1:A:137:ASP:OD1	1:A:137:ASP:C	2.48	0.51
1:A:16:ASP:O	1:A:17:GLU:CB	2.59	0.51
1:B:186:PHE:O	1:B:188:ASP:N	2.42	0.51
1:B:283:LEU:C	1:B:285:PRO:HD3	2.31	0.51
1:A:381:PHE:CZ	1:A:424:PRO:HB3	2.46	0.51
1:B:253:ASP:OD2	1:B:255:ARG:HD3	2.11	0.51
1:B:393:ASP:N	1:B:394:PRO:HD2	2.25	0.51
1:B:95:ASN:O	1:B:96:ARG:HD3	2.09	0.51
1:A:175:LEU:CD2	1:A:176:ALA:N	2.62	0.51
1:B:13:VAL:HG21	1:B:25:THR:HG21	1.92	0.51
1:A:362:ASP:CB	1:A:368:ARG:HB3	2.40	0.51
1:A:396:VAL:CG1	1:A:553:ILE:HD12	2.40	0.51
1:B:208:SER:HB2	1:B:210:LEU:HD21	1.92	0.51
1:A:255:ARG:O	1:A:257:SER:N	2.43	0.50
1:A:571:ASN:N	1:A:575:ASP:OD2	2.41	0.50
1:B:475:ILE:HD11	1:B:479:LYS:NZ	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:LEU:HD12	1:B:499:GLU:HA	1.92	0.50
1:B:453:ARG:CZ	1:B:458:LEU:HB3	2.41	0.50
1:B:298:LYS:HG2	1:B:536:PHE:CZ	2.46	0.50
1:B:66:THR:HB	1:B:70:PHE:H	1.77	0.50
1:A:585:LEU:HG	1:A:585:LEU:O	2.11	0.50
1:B:112:ASP:HA	1:B:183:VAL:CG2	2.41	0.50
1:B:258:GLU:OE1	6:B:605:HEM:C2B	2.64	0.50
1:A:522:ILE:HD12	8:A:3064:HOH:O	2.12	0.50
1:B:30:ASN:HB3	1:B:33:SER:O	2.12	0.50
1:A:400:LEU:HD13	1:A:563:PRO:HD3	1.93	0.50
1:A:564:LEU:HB2	1:A:565:HIS:CD2	2.47	0.50
1:B:368:ARG:HG3	1:B:368:ARG:O	2.11	0.50
1:B:165:PHE:HA	1:B:179:GLN:HA	1.92	0.50
1:B:169:THR:H	1:B:170:PRO:CD	2.25	0.50
1:B:362:ASP:OD2	1:B:362:ASP:C	2.49	0.50
1:A:341:ASN:CB	7:A:3002:FMT:H	2.39	0.50
1:A:505:GLY:O	1:A:506:ARG:HD3	2.11	0.50
2:A:596:NAG:O3	2:A:596:NAG:C7	2.60	0.50
1:A:88:GLU:OE1	1:A:356:SER:HB3	2.12	0.50
1:B:208:SER:HB2	1:B:210:LEU:CD2	2.42	0.50
1:B:187:LEU:HD13	1:B:305:GLN:HA	1.93	0.50
1:A:42:ALA:HB2	1:A:166:VAL:HG12	1.90	0.49
1:B:245:ARG:HD2	8:B:3017:HOH:O	2.13	0.49
1:B:93:ASP:CA	1:B:406:LEU:HB2	2.43	0.49
1:B:82:ILE:HD13	1:B:480:LEU:HD13	1.94	0.49
1:A:556:ASN:C	1:A:557:THR:HG23	2.33	0.49
1:B:454:GLY:O	1:B:456:CYS:N	2.45	0.49
1:A:406:LEU:HD12	1:A:407:MET:H	1.76	0.49
1:A:230:ASN:HD21	1:A:232:MET:CB	2.22	0.49
1:A:351:HIS:CD2	1:A:433:LEU:HD21	2.48	0.49
1:A:408:ASN:C	1:A:410:ASN:H	2.15	0.49
1:A:148:ASP:O	1:A:151:LEU:HB2	2.13	0.49
1:A:365:TYR:CE1	1:A:397:ARG:HB3	2.48	0.49
1:A:420:LYS:HA	1:A:429:HIS:O	2.13	0.49
1:A:42:ALA:HB2	1:A:166:VAL:HG13	1.90	0.49
1:A:481:LEU:C	1:A:483:LEU:H	2.14	0.49
1:B:170:PRO:CB	1:B:171:PRO:HD2	2.42	0.49
1:B:546:LYS:HD3	1:B:583:ASP:OD2	2.13	0.49
1:A:116:GLU:HA	1:A:163:ALA:HA	1.94	0.49
1:B:365:TYR:CE2	1:B:397:ARG:HD3	2.48	0.49
1:B:579:CYS:O	1:B:582:ILE:CG2	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:TYR:HB2	1:A:134:ILE:HG13	1.95	0.48
1:A:119:LEU:HD22	1:A:119:LEU:H	1.78	0.48
1:A:170:PRO:CB	1:A:171:PRO:HD2	2.35	0.48
1:A:244:ALA:HB2	2:A:600:NAG:O6	2.12	0.48
1:A:362:ASP:HB2	1:A:368:ARG:HB2	1.95	0.48
1:A:148:ASP:C	1:A:148:ASP:OD1	2.52	0.48
1:A:556:ASN:O	1:A:557:THR:CG2	2.62	0.48
1:A:589:PRO:HG2	1:A:590:TRP:CE3	2.49	0.48
1:B:123:GLU:HG2	1:B:126:LYS:H	1.76	0.48
1:B:168:PRO:CB	1:B:170:PRO:HD2	2.42	0.48
1:B:282:ARG:HG3	1:B:283:LEU:N	2.29	0.48
1:A:432:ASP:C	1:A:432:ASP:OD1	2.51	0.48
1:B:221:ASP:O	1:B:224:LEU:HB2	2.12	0.48
1:B:280:LEU:CD2	1:B:587:LEU:HD13	2.44	0.48
1:A:137:ASP:OD1	1:A:138:ASN:HB2	2.14	0.48
1:A:422:PHE:HE1	1:A:427:LYS:O	1.95	0.48
1:B:180:ILE:CG2	1:B:181:ASN:N	2.76	0.48
1:B:343:PHE:CG	1:B:518:GLN:HG2	2.49	0.48
1:B:62:THR:HG22	1:B:62:THR:O	2.13	0.48
1:B:283:LEU:O	1:B:285:PRO:HD3	2.14	0.48
1:B:82:ILE:HD13	1:B:480:LEU:CD1	2.44	0.48
1:B:66:THR:HB	1:B:70:PHE:O	2.12	0.48
1:A:541:ARG:O	1:A:544:LEU:N	2.46	0.48
1:B:365:TYR:CZ	1:B:397:ARG:HD3	2.49	0.48
1:B:560:THR:HB	7:B:3004:FMT:O1	2.14	0.48
1:A:274:ASN:HB3	1:A:278:ARG:HH22	1.79	0.48
1:A:300:LEU:O	1:A:303:PHE:HB3	2.12	0.48
1:A:351:HIS:NE2	1:A:433:LEU:HD21	2.28	0.48
1:B:64:ARG:O	1:B:64:ARG:CG	2.60	0.48
1:B:97:SER:OG	1:B:99:LEU:HB3	2.14	0.48
1:B:302:ALA:O	1:B:306:ILE:HG13	2.14	0.47
1:B:150:LYS:HE3	1:B:430:GLY:O	2.14	0.47
1:A:520:GLN:HG2	1:A:521:GLN:N	2.29	0.47
1:A:116:GLU:H	1:A:116:GLU:HG3	1.58	0.47
1:A:119:LEU:O	1:A:126:LYS:HE3	2.15	0.47
1:A:396:VAL:HG11	1:A:553:ILE:HD12	1.96	0.47
1:B:99:LEU:HG	1:B:567:PHE:CE1	2.49	0.47
1:A:167:CYS:CB	1:A:168:PRO:HD3	2.40	0.47
1:B:139:CYS:SG	1:B:141:PRO:HD3	2.54	0.47
1:B:475:ILE:HG13	1:B:475:ILE:O	2.14	0.47
1:B:560:THR:HG23	1:B:578:ASP:OD1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:PHE:CZ	1:B:172:TYR:HB3	2.49	0.47
1:B:332:ASN:O	1:B:334:SER:N	2.47	0.47
1:B:98:LEU:HB3	1:B:399:LEU:HD23	1.95	0.47
1:B:484:TYR:O	1:B:485:LYS:HB2	2.14	0.47
1:B:43:LEU:HD23	1:B:181:ASN:HB2	1.95	0.47
1:A:96:ARG:NH2	1:A:315:ILE:O	2.48	0.47
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.49	0.47
1:B:560:THR:HG22	1:B:561:LYS:CD	2.45	0.47
1:A:362:ASP:OD1	1:A:363:GLU:N	2.48	0.47
1:B:159:PRO:HD2	8:B:3023:HOH:O	2.13	0.47
1:B:450:ASN:HD21	1:B:487:PRO:HB2	1.80	0.47
1:B:467:LEU:HG	1:B:471:LEU:HD22	1.97	0.47
1:B:91:VAL:HG13	1:B:92:LEU:HD12	1.94	0.47
1:B:35:ALA:HB1	1:B:41:ARG:CZ	2.45	0.47
6:B:605:HEM:HMB1	6:B:605:HEM:CBB	2.45	0.47
1:A:144:PHE:HE2	1:A:158:MET:HE3	1.79	0.47
1:A:165:PHE:N	1:A:165:PHE:CD1	2.83	0.47
1:B:123:GLU:HG2	1:B:126:LYS:HB2	1.96	0.47
1:B:471:LEU:HD12	1:B:471:LEU:HA	1.75	0.46
1:A:16:ASP:O	1:A:17:GLU:HB3	2.14	0.46
1:A:406:LEU:HD12	1:A:407:MET:N	2.29	0.46
1:A:368:ARG:O	1:A:368:ARG:CG	2.62	0.46
1:A:462:LYS:NZ	1:A:488:ASP:OD2	2.48	0.46
2:A:596:NAG:O3	2:A:596:NAG:O7	2.34	0.46
1:B:118:GLU:C	1:B:119:LEU:HD13	2.36	0.46
1:A:131:GLU:HB2	1:A:132:TYR:CD1	2.50	0.46
1:A:199:LEU:O	1:A:199:LEU:HD12	2.15	0.46
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.96	0.46
1:A:350:GLY:HA3	6:A:605:HEM:HBC2	1.97	0.46
1:B:132:TYR:HB3	1:B:134:ILE:CD1	2.45	0.46
1:A:85:TYR:HD1	1:A:87:ASP:O	1.98	0.46
1:B:258:GLU:OE2	6:B:605:HEM:HHB	2.14	0.46
1:B:376:LEU:HD13	1:B:380:PHE:CZ	2.49	0.46
1:A:130:GLU:O	1:A:130:GLU:HG2	2.16	0.46
1:A:475:ILE:O	1:A:475:ILE:HD12	2.16	0.46
1:A:510:LEU:O	1:A:513:CYS:HB3	2.15	0.46
1:B:272:GLU:OE2	1:B:276:LEU:HD13	2.15	0.46
1:B:342:VAL:HG13	1:B:343:PHE:N	2.31	0.46
1:B:53:ASP:O	1:B:55:LEU:N	2.48	0.46
1:A:272:GLU:OE1	1:A:272:GLU:CA	2.56	0.46
1:A:492:ILE:CG2	1:A:493:TRP:H	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:PHE:CD1	1:B:350:GLY:N	2.84	0.46
1:A:101:MET:SD	1:A:101:MET:C	2.94	0.46
1:A:203:LEU:HD21	1:A:252:GLY:HA2	1.97	0.46
1:B:170:PRO:O	1:B:172:TYR:N	2.41	0.46
1:B:212:LEU:HD22	1:B:274:ASN:OD1	2.16	0.46
1:B:130:GLU:OE1	1:B:426:HIS:ND1	2.49	0.46
1:A:91:VAL:HG22	1:A:405:LYS:HG2	1.97	0.46
1:B:187:LEU:HA	1:B:187:LEU:HD23	1.66	0.46
1:B:287:TRP:NE1	1:B:291:LYS:HE3	2.31	0.45
1:B:375:PRO:O	1:B:376:LEU:C	2.54	0.45
1:B:464:LEU:HD22	1:B:464:LEU:C	2.35	0.45
1:A:45:ARG:NE	1:A:178:ASP:OD1	2.39	0.45
1:B:253:ASP:OD1	1:B:255:ARG:NH1	2.48	0.45
1:B:358:VAL:HB	1:B:379:LEU:HD11	1.98	0.45
1:A:249:PHE:CZ	1:A:387:ILE:HD11	2.51	0.45
1:A:257:SER:O	1:A:381:PHE:HA	2.16	0.45
1:A:343:PHE:CG	1:A:518:GLN:HG2	2.51	0.45
1:B:93:ASP:HA	1:B:406:LEU:HB2	1.98	0.45
1:B:261:LEU:HA	1:B:261:LEU:HD12	1.83	0.45
1:B:288:ASP:O	1:B:291:LYS:HB3	2.17	0.45
1:B:480:LEU:HD12	1:B:480:LEU:HA	1.84	0.45
1:B:494:ILE:HG23	1:B:495:GLY:N	2.31	0.45
1:B:99:LEU:HD23	1:B:566:ALA:HB1	1.98	0.45
1:B:467:LEU:HD23	1:B:477:ALA:CA	2.46	0.45
1:A:350:GLY:HA3	6:A:605:HEM:CBC	2.47	0.45
1:B:503:GLU:HG2	1:B:504:ARG:HG3	1.98	0.45
1:A:226:TYR:N	8:A:3063:HOH:O	2.50	0.45
1:A:362:ASP:O	1:A:365:TYR:N	2.47	0.45
1:A:85:TYR:CD1	1:A:87:ASP:O	2.70	0.45
1:B:418:ARG:O	1:B:418:ARG:HG2	2.17	0.45
1:B:305:GLN:HG2	1:B:529:TRP:CZ3	2.51	0.45
1:A:106:ILE:HG23	1:A:191:LEU:HD11	1.99	0.45
1:B:377:HIS:CD2	1:B:378:THR:HG22	2.52	0.45
1:B:130:GLU:CD	1:B:426:HIS:HD1	2.20	0.45
1:B:57:VAL:HA	1:B:58:PRO:HD3	1.72	0.45
1:A:464:LEU:HD13	1:A:468:GLN:OE1	2.17	0.45
1:A:88:GLU:OE2	1:A:414:THR:HG23	2.17	0.45
1:B:180:ILE:HG22	1:B:181:ASN:N	2.32	0.45
1:B:58:PRO:HG3	1:B:162:ARG:NH2	2.32	0.44
1:A:39:ALA:O	1:A:40:ASN:HB2	2.18	0.44
1:A:492:ILE:HG22	1:A:493:TRP:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ASP:CG	1:B:17:GLU:N	2.69	0.44
1:A:233:LYS:HB3	1:A:234:PRO:CD	2.23	0.44
1:B:165:PHE:N	1:B:165:PHE:CD1	2.86	0.44
1:B:62:THR:O	1:B:63:GLN:C	2.55	0.44
1:B:358:VAL:HB	1:B:379:LEU:CD1	2.48	0.44
1:B:7:GLY:O	1:B:8:ALA:CB	2.62	0.44
1:B:102:GLN:OE1	1:B:259:GLN:NE2	2.47	0.44
1:B:306:ILE:O	1:B:310:ARG:HB3	2.17	0.44
1:B:52:GLU:C	1:B:54:GLY:H	2.21	0.44
1:A:173:GLN:HB2	1:A:174:SER:H	1.38	0.44
1:A:260:ILE:HG23	1:A:261:LEU:N	2.32	0.44
1:A:67:ARG:HD3	1:A:489:ASN:OD1	2.18	0.44
1:B:458:LEU:HD21	1:B:509:PRO:HB3	2.00	0.44
1:B:368:ARG:O	1:B:368:ARG:CG	2.66	0.44
1:B:101:MET:CE	6:B:605:HEM:HMC2	2.47	0.44
1:B:299:ILE:HD11	1:B:590:TRP:CE2	2.52	0.44
1:A:106:ILE:HG23	1:A:191:LEU:CD1	2.48	0.44
1:A:433:LEU:O	1:A:437:ASN:ND2	2.51	0.43
1:A:551:ARG:N	1:A:582:ILE:HD11	2.32	0.43
1:A:556:ASN:C	1:A:557:THR:CG2	2.87	0.43
1:B:541:ARG:O	1:B:544:LEU:N	2.51	0.43
1:B:62:THR:O	1:B:64:ARG:N	2.51	0.43
1:A:78:VAL:HG13	1:A:82:ILE:HD12	2.00	0.43
1:B:246:VAL:HG11	1:B:387:ILE:HG13	2.00	0.43
1:B:493:TRP:O	1:B:497:ASN:ND2	2.50	0.43
1:B:258:GLU:OE2	6:B:605:HEM:CHB	2.66	0.43
1:A:25:THR:HG22	1:A:27:ASP:N	2.25	0.43
1:B:251:ALA:O	1:B:253:ASP:N	2.52	0.43
1:B:584:LYS:O	1:B:585:LEU:HB3	2.18	0.43
1:B:588:SER:OG	1:B:589:PRO:CD	2.59	0.43
6:B:605:HEM:CMC	6:B:605:HEM:HBC2	2.48	0.43
1:A:194:GLY:HA2	1:A:252:GLY:O	2.18	0.43
1:B:14:LYS:O	1:B:15:CYS:HB2	2.18	0.43
1:B:91:VAL:HG13	1:B:91:VAL:O	2.17	0.43
1:A:249:PHE:CE1	1:A:387:ILE:HD11	2.54	0.43
1:A:428:ILE:HG12	1:A:430:GLY:H	1.83	0.43
1:A:436:ILE:HG12	1:A:436:ILE:H	1.71	0.43
1:A:319:SER:OG	1:A:503:GLU:HB3	2.18	0.43
1:B:335:VAL:O	1:B:337:PRO:HD3	2.18	0.43
1:B:101:MET:HE2	6:B:605:HEM:CMC	2.48	0.43
1:B:233:LYS:CB	1:B:234:PRO:HD2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:GLN:O	1:A:298:LYS:HB2	2.18	0.43
1:A:85:TYR:CG	1:A:411:LYS:HB3	2.53	0.43
1:A:136:GLY:O	1:A:138:ASN:N	2.41	0.43
1:A:556:ASN:O	1:A:557:THR:HG22	2.19	0.43
1:B:191:LEU:CD2	1:B:191:LEU:H	2.32	0.43
1:A:226:TYR:CE1	1:A:387:ILE:CG1	3.01	0.43
1:A:417:LEU:HD11	6:A:605:HEM:HBB2	2.01	0.43
1:A:64:ARG:HA	1:A:71:ARG:HH22	1.77	0.43
1:B:187:LEU:HD11	1:B:308:THR:HG21	2.00	0.43
1:A:175:LEU:O	1:A:176:ALA:C	2.57	0.42
1:A:24:ILE:CD1	1:A:200:ALA:HB1	2.35	0.42
1:A:227:PRO:HG2	1:A:249:PHE:CD2	2.53	0.42
1:A:408:ASN:C	1:A:410:ASN:N	2.73	0.42
1:A:448:GLY:O	1:A:452:TRP:CD1	2.73	0.42
1:B:569:ALA:O	1:B:570:ASN:ND2	2.52	0.42
1:B:16:ASP:O	1:B:17:GLU:CB	2.64	0.42
1:B:274:ASN:O	1:B:275:ARG:C	2.56	0.42
1:B:476:LEU:O	1:B:480:LEU:HB2	2.19	0.42
1:A:92:LEU:HD22	1:A:404:SER:O	2.19	0.42
1:B:584:LYS:O	1:B:584:LYS:HG3	2.19	0.42
1:A:475:ILE:HD11	1:A:479:LYS:CE	2.46	0.42
1:B:126:LYS:HE3	1:B:126:LYS:HB2	1.85	0.42
1:B:153:THR:HG22	1:B:154:GLN:HG3	2.02	0.42
1:B:88:GLU:O	1:B:91:VAL:HG12	2.20	0.42
1:A:170:PRO:CB	1:A:171:PRO:CD	2.96	0.42
1:A:407:MET:C	1:A:407:MET:SD	2.98	0.42
2:A:601:NAG:H61	2:A:601:NAG:C2	2.47	0.42
1:B:98:LEU:HB3	1:B:399:LEU:HA	2.02	0.42
1:B:85:TYR:CD2	1:B:411:LYS:HA	2.55	0.42
1:B:99:LEU:HD21	1:B:549:PHE:CD2	2.54	0.42
1:A:179:GLN:N	1:A:179:GLN:OE1	2.53	0.42
1:A:532:ASN:HA	1:A:533:PRO:HD3	1.92	0.42
1:B:160:PHE:CD1	1:B:160:PHE:C	2.93	0.42
1:B:346:ALA:HB1	1:B:511:LEU:HD12	2.01	0.42
1:B:130:GLU:CD	1:B:426:HIS:ND1	2.73	0.42
1:B:351:HIS:CE1	1:B:433:LEU:HD21	2.55	0.42
1:A:239:PHE:O	1:A:240:ILE:C	2.58	0.42
1:B:170:PRO:CB	1:B:171:PRO:CD	2.97	0.42
1:B:260:ILE:HG13	1:B:386:ILE:HD11	2.01	0.42
1:A:260:ILE:HD11	1:A:386:ILE:HG12	2.00	0.42
1:A:572:TYR:HA	1:A:573:PRO:HA	1.86	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:345:PHE:HZ	1:B:444:HIS:CD2	2.38	0.42
1:B:51:TYR:CD2	1:B:56:ALA:HA	2.54	0.42
1:A:501:MET:HE2	1:A:506:ARG:CA	2.50	0.41
1:B:299:ILE:CD1	1:B:590:TRP:CE2	3.03	0.41
1:A:433:LEU:HG	1:A:437:ASN:HD21	1.85	0.41
1:B:140:PHE:N	1:B:141:PRO:HD3	2.36	0.41
1:B:351:HIS:HD1	1:B:437:ASN:ND2	2.18	0.41
1:B:362:ASP:HB3	1:B:368:ARG:CB	2.40	0.41
1:A:36:LEU:HD12	1:A:36:LEU:HA	1.79	0.41
1:B:293:TYR:CD2	1:B:294:GLN:HG2	2.55	0.41
1:B:571:ASN:O	1:B:576:PHE:HE1	2.03	0.41
1:A:118:GLU:HG3	1:A:119:LEU:H	1.85	0.41
1:A:502:VAL:HG13	1:A:507:VAL:O	2.20	0.41
1:A:535:VAL:HG12	1:A:536:PHE:CD1	2.55	0.41
1:B:472:LYS:HE3	1:B:472:LYS:HB2	1.76	0.41
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.85	0.41
1:A:99:LEU:HA	1:A:399:LEU:HD22	2.02	0.41
1:A:426:HIS:CD2	1:A:426:HIS:N	2.88	0.41
1:B:233:LYS:HB3	1:B:234:PRO:CD	2.50	0.41
1:A:260:ILE:CD1	1:A:386:ILE:CG1	2.92	0.41
1:A:484:TYR:CD2	1:A:490:ILE:HG13	2.55	0.41
1:A:528:PHE:O	1:A:529:TRP:C	2.58	0.41
1:A:83:VAL:O	1:A:412:MET:HB2	2.20	0.41
1:B:108:ASP:OD2	6:B:605:HEM:CHD	2.69	0.41
1:B:475:ILE:HD11	1:B:479:LYS:HZ1	1.83	0.41
1:A:229:PHE:HE1	1:A:387:ILE:CD1	2.34	0.41
1:A:233:LYS:HD2	1:A:233:LYS:HA	1.84	0.41
1:A:551:ARG:HA	1:A:582:ILE:HD11	2.02	0.41
1:A:95:ASN:HA	1:A:569:ALA:HB2	2.03	0.41
1:B:264:THR:O	1:B:267:THR:HB	2.20	0.41
1:A:165:PHE:CG	1:A:177:ARG:HD2	2.55	0.41
1:A:561:LYS:HA	1:A:577:VAL:O	2.20	0.41
1:B:53:ASP:C	1:B:55:LEU:N	2.72	0.41
1:B:85:TYR:CG	1:B:411:LYS:HG2	2.55	0.41
1:A:120:GLY:O	1:A:121:SER:HB2	2.21	0.41
1:A:400:LEU:HD13	1:A:563:PRO:CD	2.50	0.41
1:A:352:MET:SD	1:A:412:MET:HG2	2.61	0.41
1:A:544:LEU:O	1:A:547:VAL:HG22	2.20	0.41
1:B:123:GLU:HG3	1:B:125:SER:H	1.85	0.41
1:B:19:SER:HA	1:B:20:PRO:HD3	1.76	0.41
1:A:140:PHE:O	1:A:160:PHE:HB3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ILE:HD12	1:A:386:ILE:HG13	2.02	0.41
2:A:601:NAG:C6	2:A:601:NAG:H2	2.50	0.41
1:B:511:LEU:HD13	1:B:511:LEU:HA	1.82	0.41
1:A:549:PHE:O	1:A:553:ILE:HG12	2.21	0.41
1:A:572:TYR:CE2	1:A:573:PRO:HB3	2.56	0.41
1:B:150:LYS:HG2	1:B:154:GLN:OE1	2.21	0.41
1:B:438:LEU:HA	1:B:438:LEU:HD23	1.77	0.41
1:A:258:GLU:HG2	1:A:258:GLU:O	2.21	0.40
1:A:414:THR:HG22	1:A:416:GLU:H	1.86	0.40
1:A:484:TYR:C	1:A:486:THR:H	2.23	0.40
1:A:568:GLN:H	1:A:568:GLN:HG2	1.69	0.40
1:A:348:ARG:NH1	6:A:605:HEM:O2A	2.48	0.40
1:A:88:GLU:CD	1:A:356:SER:HB3	2.42	0.40
1:B:172:TYR:H	1:B:172:TYR:HD1	1.66	0.40
1:B:312:TYR:CD2	1:B:312:TYR:C	2.94	0.40
1:B:542:ASP:O	1:B:545:GLN:HG3	2.20	0.40
1:A:260:ILE:CG2	1:A:261:LEU:N	2.84	0.40
1:A:376:LEU:C	1:A:376:LEU:CD2	2.89	0.40
1:A:434:ALA:HA	1:A:437:ASN:HD22	1.86	0.40
1:A:464:LEU:CD1	1:A:468:GLN:OE1	2.69	0.40
1:A:537:THR:O	1:A:541:ARG:HG3	2.21	0.40
1:A:576:PHE:N	1:A:576:PHE:CD1	2.89	0.40
2:A:601:NAG:C6	2:A:601:NAG:C2	2.99	0.40
1:B:134:ILE:O	1:B:134:ILE:HG22	2.22	0.40
1:B:160:PHE:HE2	1:B:436:ILE:HG23	1.86	0.40
1:A:545:GLN:HB2	1:A:545:GLN:HE21	1.67	0.40
1:A:85:TYR:CE2	1:A:411:LYS:HB3	2.56	0.40
1:B:46:TRP:NE1	1:B:340:SER:HB3	2.36	0.40
1:A:216:ASN:HB2	1:A:227:PRO:O	2.21	0.40
1:B:95:ASN:HA	1:B:569:ALA:CB	2.52	0.40
1:B:95:ASN:HA	1:B:569:ALA:HB2	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%)	494 (83%)	75 (13%)	24 (4%)	3	24
1	B	593/595 (100%)	492 (83%)	70 (12%)	31 (5%)	2	17
All	All	1186/1190 (100%)	986 (83%)	145 (12%)	55 (5%)	3	20

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	117	THR
1	A	137	ASP
1	A	169	THR
1	A	174	SER
1	A	234	PRO
1	A	256	ALA
1	A	409	GLN
1	A	594	GLU
1	B	4	VAL
1	B	9	PRO
1	B	17	GLU
1	B	63	GLN
1	B	123	GLU
1	B	167	CYS
1	B	168	PRO
1	B	169	THR
1	B	171	PRO
1	B	172	TYR
1	B	174	SER
1	B	234	PRO
1	B	363	GLU
1	A	170	PRO
1	A	232	MET
1	A	363	GLU
1	A	504	ARG
1	A	583	ASP
1	B	5	GLY
1	B	8	ALA
1	B	64	ARG
1	B	211	GLY
1	B	231	ASN
1	B	232	MET

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Mol	Chain	Res	Type
1	B	455	PHE
1	B	594	GLU
1	A	9	PRO
1	A	168	PRO
1	B	10	VAL
1	B	54	GLY
1	B	170	PRO
1	B	333	ASN
1	B	473	ASN
1	A	63	GLN
1	A	566	ALA
1	B	411	LYS
1	A	17	GLU
1	A	121	SER
1	A	167	CYS
1	A	542	ASP
1	B	34	PRO
1	B	173	GLN
1	B	252	GLY
1	A	166	VAL
1	A	34	PRO
1	B	260	ILE

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	518/518 (100%)	430 (83%)	88 (17%)	2	12
1	B	518/518 (100%)	444 (86%)	74 (14%)	4	18
All	All	1036/1036 (100%)	874 (84%)	162 (16%)	3	14

All (162) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER

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Mol	Chain	Res	Type
1	A	3	GLU
1	A	4	VAL
1	A	9	PRO
1	A	13	VAL
1	A	24	ILE
1	A	25	THR
1	A	32	ARG
1	A	48	PRO
1	A	61	TRP
1	A	71	ARG
1	A	72	VAL
1	A	73	PRO
1	A	79	SER
1	A	98	LEU
1	A	106	ILE
1	A	113	PHE
1	A	115	PRO
1	A	116	GLU
1	A	117	THR
1	A	118	GLU
1	A	119	LEU
1	A	124	HIS
1	A	132	TYR
1	A	134	ILE
1	A	135	GLN
1	A	137	ASP
1	A	138	ASN
1	A	139	CYS
1	A	143	MET
1	A	149	PRO
1	A	151	LEU
1	A	169	THR
1	A	173	GLN
1	A	174	SER
1	A	177	ARG
1	A	187	LEU
1	A	197	PRO
1	A	202	ARG
1	A	207	SER
1	A	208	SER
1	A	209	PRO
1	A	226	TYR

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Mol	Chain	Res	Type
1	A	233	LYS
1	A	234	PRO
1	A	255	ARG
1	A	257	SER
1	A	260	ILE
1	A	261	LEU
1	A	266	HIS
1	A	269	LEU
1	A	292	LEU
1	A	294	GLN
1	A	298	LYS
1	A	317	LEU
1	A	321	MET
1	A	327	ARG
1	A	337	PRO
1	A	347	PHE
1	A	359	SER
1	A	360	ARG
1	A	363	GLU
1	A	368	ARG
1	A	376	LEU
1	A	392	ILE
1	A	420	LYS
1	A	428	ILE
1	A	447	PRO
1	A	451	SER
1	A	458	LEU
1	A	464	LEU
1	A	471	LEU
1	A	472	LYS
1	A	475	ILE
1	A	480	LEU
1	A	482	ASP
1	A	490	ILE
1	A	492	ILE
1	A	504	ARG
1	A	520	GLN
1	A	521	GLN
1	A	522	ILE
1	A	523	ARG
1	A	542	ASP
1	A	564	LEU

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Mol	Chain	Res	Type
1	A	573	PRO
1	A	582	ILE
1	A	592	SER
1	B	3	GLU
1	B	10	VAL
1	B	11	PRO
1	B	13	VAL
1	B	16	ASP
1	B	18	ASN
1	B	25	THR
1	B	33	SER
1	B	57	VAL
1	B	64	ARG
1	B	98	LEU
1	B	119	LEU
1	B	124	HIS
1	B	134	ILE
1	B	137	ASP
1	B	165	PHE
1	B	169	THR
1	B	172	TYR
1	B	175	LEU
1	B	177	ARG
1	B	179	GLN
1	B	185	SER
1	B	187	LEU
1	B	191	LEU
1	B	198	SER
1	B	204	ARG
1	B	207	SER
1	B	210	LEU
1	B	215	VAL
1	B	216	ASN
1	B	232	MET
1	B	234	PRO
1	B	242	THR
1	B	246	VAL
1	B	255	ARG
1	B	261	LEU
1	B	265	VAL
1	B	275	ARG
1	B	288	ASP

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Mol	Chain	Res	Type
1	B	304	ILE
1	B	314	PRO
1	B	317	LEU
1	B	327	ARG
1	B	329	GLN
1	B	333	ASN
1	B	359	SER
1	B	360	ARG
1	B	373	GLU
1	B	375	PRO
1	B	376	LEU
1	B	377	HIS
1	B	389	ASP
1	B	392	ILE
1	B	404	SER
1	B	410	ASN
1	B	451	SER
1	B	462	LYS
1	B	464	LEU
1	B	471	LEU
1	B	474	LYS
1	B	475	ILE
1	B	481	LEU
1	B	494	ILE
1	B	511	LEU
1	B	520	GLN
1	B	523	ARG
1	B	537	THR
1	B	545	GLN
1	B	547	VAL
1	B	550	SER
1	B	561	LYS
1	B	573	PRO
1	B	582	ILE
1	B	595	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	94	GLN
1	A	128	GLN
1	A	147	ASN

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Mol	Chain	Res	Type
1	A	217	GLN
1	A	230	ASN
1	A	250	GLN
1	A	322	GLN
1	A	364	ASN
1	A	377	HIS
1	A	450	ASN
1	A	497	ASN
1	A	520	GLN
1	A	545	GLN
1	A	558	HIS
1	A	565	HIS
1	A	570	ASN
1	B	18	ASN
1	B	63	GLN
1	B	128	GLN
1	B	179	GLN
1	B	216	ASN
1	B	322	GLN
1	B	329	GLN
1	B	341	ASN
1	B	410	ASN
1	B	439	GLN
1	B	468	GLN
1	B	595	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 28 ligands modelled in this entry, 2 are monoatomic - leaving 26 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$
5	CO3	A	2001	-	0,3,3	0.00	-	0,3,3	0.00	-
7	FMT	A	3001	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	A	3002	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	A	3003	-	0,2,2	0.00	-	0,1,1	0.00	-
2	NAG	A	596	1,2	14,14,15	1.10	1 (7%)	15,19,21	2.70	5 (33%)
2	NAG	A	597	2	14,14,15	1.24	1 (7%)	15,19,21	2.13	3 (20%)
2	NAG	A	598	1,2	14,14,15	0.66	0	15,19,21	1.03	0
2	NAG	A	599	2	14,14,15	0.75	0	15,19,21	0.80	0
2	NAG	A	600	1,2	14,14,15	0.55	0	15,19,21	0.89	0
2	NAG	A	601	3,2	14,14,15	0.85	0	15,19,21	0.89	1 (6%)
3	MAN	A	602	2	11,11,12	0.64	0	13,15,17	0.34	0
2	NAG	A	603	1	14,14,15	0.80	0	15,19,21	1.59	2 (13%)
6	HEM	A	605	1	28,50,50	2.38	9 (32%)	17,82,82	2.50	7 (41%)
5	CO3	B	2002	-	0,3,3	0.00	-	0,3,3	0.00	-
7	FMT	B	3004	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	B	3005	-	0,2,2	0.00	-	0,1,1	0.00	-
7	FMT	B	3006	-	0,2,2	0.00	-	0,1,1	0.00	-
2	NAG	B	596	1,2	14,14,15	0.64	0	15,19,21	0.76	0
2	NAG	B	597	2	14,14,15	0.64	0	15,19,21	1.63	2 (13%)
2	NAG	B	598	1,2	14,14,15	0.66	0	15,19,21	0.91	0
2	NAG	B	599	2	14,14,15	0.84	1 (7%)	15,19,21	0.86	0
2	NAG	B	600	1,2	14,14,15	0.76	1 (7%)	15,19,21	1.47	2 (13%)
2	NAG	B	601	3,2	14,14,15	0.83	0	15,19,21	1.64	3 (20%)
3	MAN	B	602	2	11,11,12	0.81	0	13,15,17	1.74	2 (15%)
2	NAG	B	603	1	14,14,15	0.82	1 (7%)	15,19,21	1.48	2 (13%)
6	HEM	B	605	1	28,50,50	2.45	11 (39%)	17,82,82	2.21	7 (41%)

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
5	CO3	A	2001	-	-	0/0/0/0	0/0/0/0
7	FMT	A	3001	-	-	0/0/0/0	0/0/0/0
7	FMT	A	3002	-	-	0/0/0/0	0/0/0/0
7	FMT	A	3003	-	-	0/0/0/0	0/0/0/0
2	NAG	A	596	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	597	2	-	0/6/23/26	0/1/1/1
2	NAG	A	598	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	599	2	-	0/6/23/26	0/1/1/1
2	NAG	A	600	1,2	-	0/6/23/26	0/1/1/1
2	NAG	A	601	3,2	-	0/6/23/26	0/1/1/1
3	MAN	A	602	2	-	0/2/19/22	1/1/1/1
2	NAG	A	603	1	-	0/6/23/26	0/1/1/1
6	HEM	A	605	1	-	0/6/54/54	0/0/8/8
5	CO3	B	2002	-	-	0/0/0/0	0/0/0/0
7	FMT	B	3004	-	-	0/0/0/0	0/0/0/0
7	FMT	B	3005	-	-	0/0/0/0	0/0/0/0
7	FMT	B	3006	-	-	0/0/0/0	0/0/0/0
2	NAG	B	596	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	597	2	-	0/6/23/26	0/1/1/1
2	NAG	B	598	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	599	2	-	0/6/23/26	0/1/1/1
2	NAG	B	600	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	601	3,2	-	0/6/23/26	0/1/1/1
3	MAN	B	602	2	-	0/2/19/22	1/1/1/1
2	NAG	B	603	1	-	0/6/23/26	0/1/1/1
6	HEM	B	605	1	-	0/6/54/54	0/0/8/8

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	605	HEM	C3B-C2B	-3.98	1.35	1.40
6	B	605	HEM	C3B-C2B	-3.05	1.36	1.40
6	A	605	HEM	C1C-NC	2.08	1.39	1.36
2	B	603	NAG	C4-C3	2.09	1.57	1.52
6	B	605	HEM	C1D-ND	2.11	1.40	1.36
2	B	600	NAG	C4-C5	2.19	1.57	1.53
6	A	605	HEM	CAD-C3D	2.40	1.56	1.52
2	B	599	NAG	C1-C2	2.42	1.55	1.52
2	A	596	NAG	C1-C2	2.48	1.55	1.52
6	B	605	HEM	CMC-C2C	2.57	1.57	1.51
6	B	605	HEM	C4D-ND	2.58	1.39	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	605	HEM	CAA-C2A	2.65	1.56	1.52
2	A	597	NAG	C3-C2	2.72	1.58	1.52
6	A	605	HEM	CMC-C2C	2.95	1.57	1.51
6	B	605	HEM	CAD-C3D	3.15	1.58	1.52
6	B	605	HEM	C4C-NC	3.60	1.41	1.36
6	A	605	HEM	C3B-CAB	3.89	1.55	1.47
6	A	605	HEM	C1B-NB	4.04	1.41	1.36
6	A	605	HEM	C4C-NC	4.21	1.41	1.36
6	B	605	HEM	C1B-NB	4.26	1.41	1.36
6	B	605	HEM	C3B-CAB	4.45	1.56	1.47
6	A	605	HEM	C3C-CAC	4.59	1.56	1.47
6	B	605	HEM	C3C-CAC	5.18	1.58	1.47
6	B	605	HEM	C3D-C2D	5.37	1.53	1.37
6	A	605	HEM	C3D-C2D	5.44	1.53	1.37

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	596	NAG	C2-N2-C7	-5.29	115.23	122.94
2	A	596	NAG	C4-C3-C2	-5.27	103.30	111.02
6	A	605	HEM	CAD-CBD-CGD	-5.01	104.09	112.66
6	A	605	HEM	CBA-CAA-C2A	-4.39	104.10	112.48
6	B	605	HEM	CAD-CBD-CGD	-4.34	105.25	112.66
2	B	601	NAG	C2-N2-C7	-4.27	116.71	122.94
2	A	597	NAG	O5-C1-C2	-3.84	106.13	111.47
6	B	605	HEM	C3B-C4B-NB	-3.64	104.51	109.21
6	B	605	HEM	C4C-C3C-C2C	-3.62	104.37	106.90
6	A	605	HEM	CMD-C2D-C1D	-3.57	122.97	128.46
6	A	605	HEM	C3B-C4B-NB	-3.51	104.67	109.21
2	A	596	NAG	C3-C4-C5	-3.34	104.34	110.22
6	A	605	HEM	C4C-C3C-C2C	-3.31	104.59	106.90
6	B	605	HEM	CBA-CAA-C2A	-3.05	106.64	112.48
6	B	605	HEM	CMD-C2D-C1D	-2.99	123.86	128.46
2	B	600	NAG	O4-C4-C3	-2.55	104.80	110.36
2	B	600	NAG	C2-N2-C7	-2.54	119.24	122.94
6	B	605	HEM	C4A-C3A-C2A	-2.44	105.30	107.00
6	A	605	HEM	C4A-C3A-C2A	-2.42	105.31	107.00
2	A	596	NAG	C8-C7-N2	2.06	119.83	116.11
2	A	601	NAG	C1-O5-C5	2.09	115.05	112.17
2	A	597	NAG	C4-C3-C2	2.30	114.39	111.02
2	B	603	NAG	C3-C4-C5	2.31	114.30	110.22
6	B	605	HEM	CMD-C2D-C3D	2.49	129.64	124.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	601	NAG	C1-O5-C5	2.52	115.64	112.17
2	A	603	NAG	C3-C4-C5	2.92	115.36	110.22
2	B	601	NAG	C6-C5-C4	2.92	119.83	113.00
3	B	602	MAN	C1-C2-C3	3.12	113.61	109.65
6	A	605	HEM	CMD-C2D-C3D	3.23	131.04	124.94
2	B	597	NAG	C3-C4-C5	3.34	116.10	110.22
2	B	603	NAG	C4-C3-C2	4.24	117.23	111.02
2	B	597	NAG	C4-C3-C2	4.33	117.36	111.02
2	A	596	NAG	C1-C2-N2	4.79	118.67	110.49
2	A	603	NAG	C4-C3-C2	4.80	118.05	111.02
3	B	602	MAN	C1-O5-C5	5.07	119.15	112.17
2	A	597	NAG	C3-C4-C5	5.38	119.69	110.22

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	MAN	C1-C2-C3-C4-C5-O5
3	A	602	MAN	C1-C2-C3-C4-C5-O5

11 monomers are involved in 41 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	3002	FMT	2	0
2	A	596	NAG	2	0
2	A	597	NAG	2	0
2	A	598	NAG	2	0
2	A	600	NAG	2	0
2	A	601	NAG	6	0
3	A	602	MAN	1	0
6	A	605	HEM	8	0
7	B	3004	FMT	1	0
3	B	602	MAN	1	0
6	B	605	HEM	16	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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.