Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 11:52 PM BST

PDB ID	:	1MYP
Title	:	X-RAY CRYSTAL STRUCTURE OF CANINE MYELOPEROXIDASE AT 3 ANGSTROMS RESOLUTION
Authors	:	Fenna, R.E.; Zeng, J.
Deposited on	:	1992-04-15
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

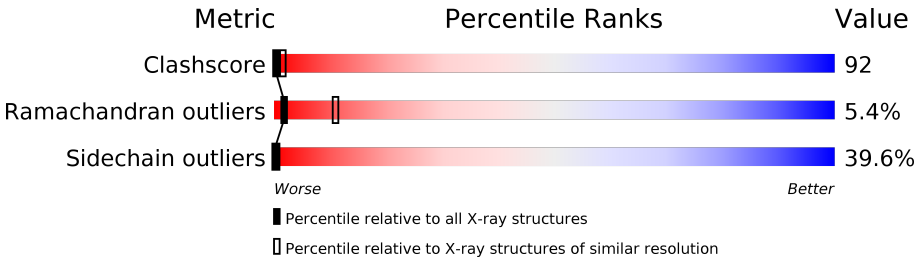
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	108	22% 32% 28% 14% .
1	B	108	19% 35% 27% 16% .
2	C	466	13% 40% 35% 12% .
2	D	466	16% 39% 33% 11% .
3	E	2	100%
3	F	2	100%
3	G	2	100%
3	H	2	50% 50%

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Mol	Chain	Length	Quality of chain
3	I	2	100%
3	J	2	100%

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	G	1	X	-	-	-
3	NAG	J	1	X	-	-	-
5	HEM	A	580	-	-	X	-
5	HEM	B	580	-	-	X	-

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 9134 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 MYELOPEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	104	Total	C	N	O	S	0	0	0
			830	525	147	153	5			
1	B	104	Total	C	N	O	S	0	0	0
			830	525	147	153	5			

- Molecule 2 is a protein called MYELOPEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	462	Total	C	N	O	S	0	0	0
			3609	2289	648	647	25			
2	D	462	Total	C	N	O	S	0	0	0
			3609	2289	648	647	25			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

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

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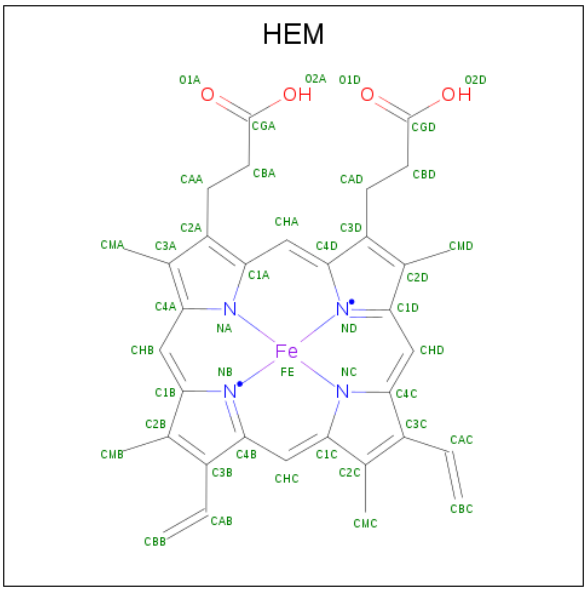
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
3	J	2	Total C N O 28 16 2 10	0	0	0

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

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

- Molecule 5 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

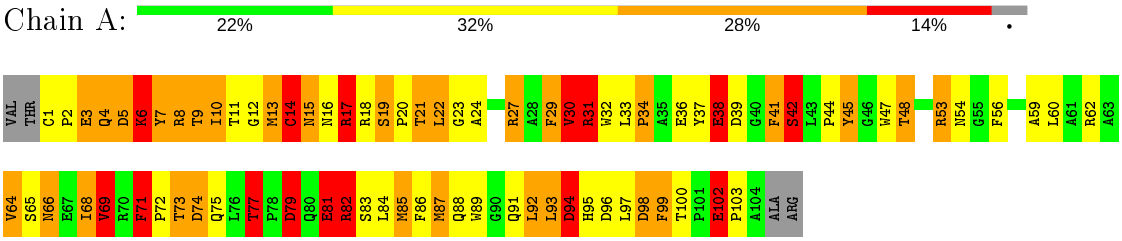
3 Residue-property plots (i)

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

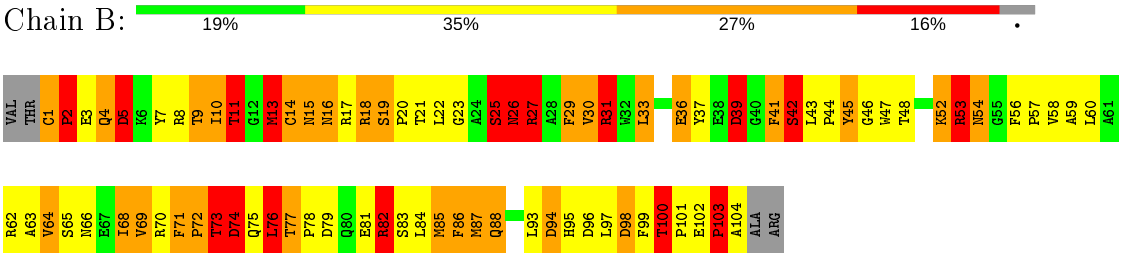
- Molecule 1: MYELOPEROXIDASE

Chain A:



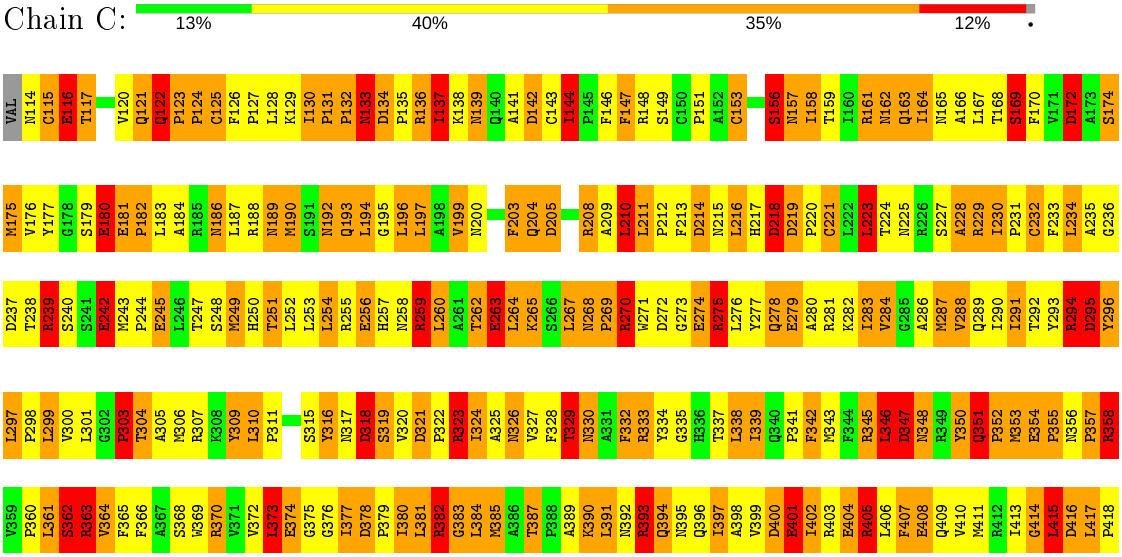
- Molecule 1: MYELOPEROXIDASE

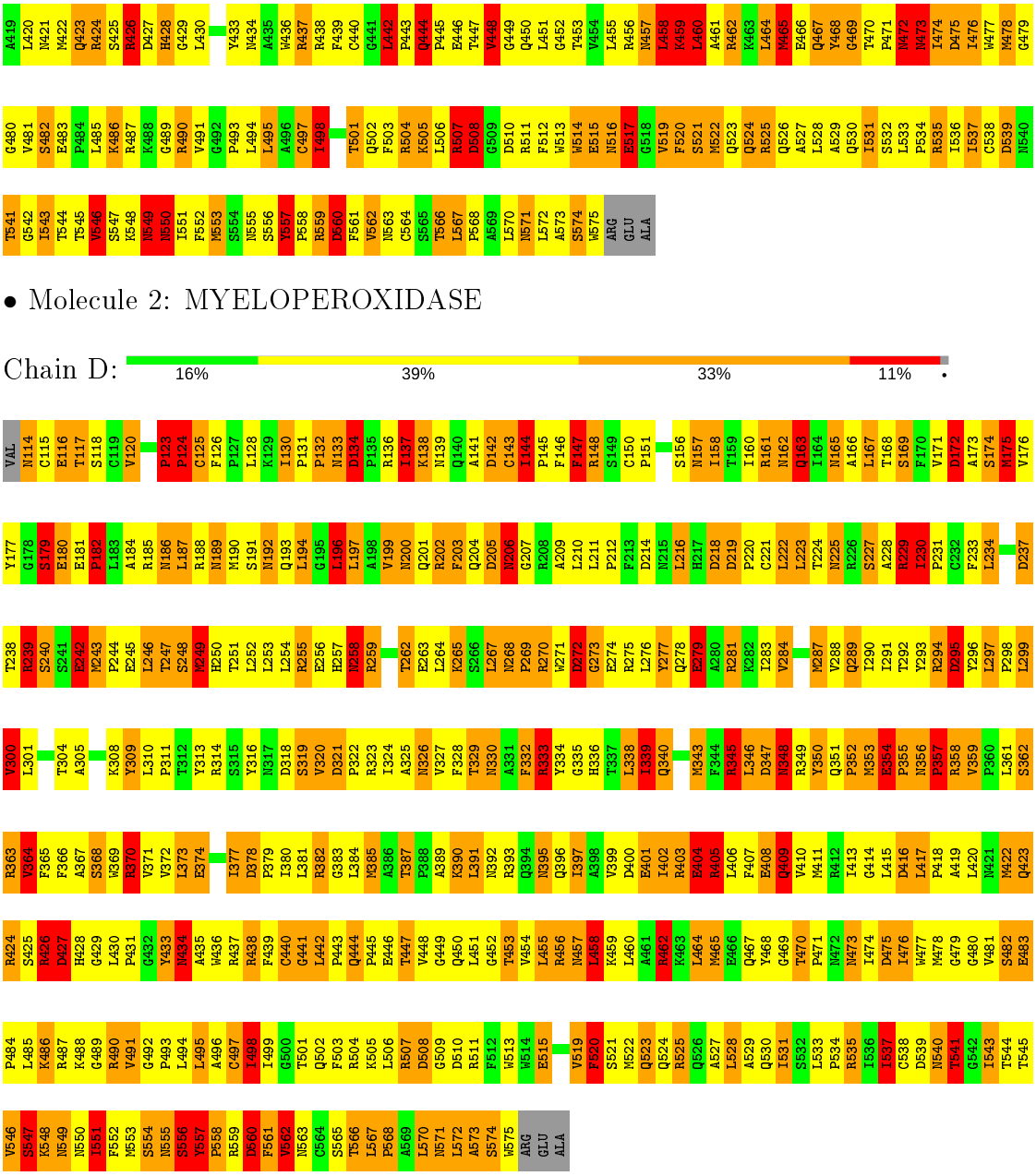
Chain B:



- Molecule 2: MYELOPEROXIDASE

Chain C:





• Molecule 2: MYELOPEROXIDASE

Chain D:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I:

• Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J:

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	133.00Å 133.00Å 203.60Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	(Not available) – 3.00	Depositor
% Data completeness (in resolution range)	(Not available) ((Not available)-3.00)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT	Depositor
R, R_{free}	0.257 , (Not available)	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	9134	wwPDB-VP
Average B, all atoms (Å^2)	15.0	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: HEM, CA, NAG

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	0.86	5/855 (0.6%)	1.98	27/1166 (2.3%)
1	B	1.30	12/854 (1.4%)	2.10	44/1163 (3.8%)
2	C	1.03	28/3695 (0.8%)	2.16	158/5030 (3.1%)
2	D	1.13	26/3695 (0.7%)	2.15	163/5030 (3.2%)
All	All	1.08	71/9099 (0.8%)	2.13	392/12389 (3.2%)

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	A	2	3
1	B	0	4
2	C	6	12
2	D	5	13
All	All	13	32

All (71) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	560	ASP	C-N	26.88	1.95	1.34
2	D	179	SER	C-N	20.67	1.81	1.34
2	D	557	TYR	C-N	20.42	1.73	1.34
2	D	560	ASP	C-N	19.45	1.78	1.34
2	D	203	PHE	C-N	17.63	1.74	1.34
2	C	516	ASN	C-N	16.76	1.72	1.34
2	D	556	SER	C-N	14.31	1.67	1.34
2	C	228	ALA	C-N	14.20	1.66	1.34
2	D	184	ALA	C-N	13.55	1.65	1.34
2	D	574	SER	C-N	-12.83	1.04	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	347	ASP	C-N	12.80	1.63	1.34
2	D	347	ASP	C-N	11.55	1.60	1.34
1	B	5	ASP	C-N	10.91	1.59	1.34
1	B	52	LYS	CB-CG	-10.39	1.24	1.52
1	B	26	ASN	C-N	10.18	1.57	1.34
1	B	54	ASN	C-N	9.73	1.50	1.33
1	B	52	LYS	C-N	9.57	1.56	1.34
2	D	354	GLU	C-N	8.99	1.51	1.34
1	A	66	ASN	C-N	8.93	1.54	1.34
1	B	14	CYS	CA-C	-8.57	1.30	1.52
2	D	529	ALA	C-N	8.12	1.52	1.34
1	B	101	PRO	C-N	8.08	1.52	1.34
2	C	204	GLN	C-N	7.94	1.52	1.34
2	C	487	ARG	CB-CG	-7.73	1.31	1.52
1	B	103	PRO	C-N	7.43	1.51	1.34
2	C	133	ASN	C-N	7.38	1.51	1.34
2	C	350	TYR	C-N	7.35	1.50	1.34
2	C	517	GLU	C-N	7.12	1.45	1.33
2	D	132	PRO	C-N	-7.07	1.17	1.34
2	D	199	VAL	C-N	-6.98	1.18	1.34
1	B	53	ARG	C-N	6.68	1.49	1.34
1	B	25	SER	C-N	6.53	1.49	1.34
2	C	256	GLU	CD-OE1	6.52	1.32	1.25
2	C	458	LEU	C-N	-6.52	1.19	1.34
2	D	275	ARG	C-N	-6.48	1.19	1.34
1	A	81	GLU	CD-OE2	6.42	1.32	1.25
2	D	263	GLU	CD-OE2	6.21	1.32	1.25
2	D	274	GLU	CD-OE1	6.17	1.32	1.25
2	C	180	GLU	CD-OE1	6.09	1.32	1.25
2	D	116	GLU	CD-OE1	6.04	1.32	1.25
2	C	279	GLU	CD-OE2	6.03	1.32	1.25
2	D	348	ASN	N-CA	-6.02	1.34	1.46
1	B	36	GLU	CD-OE2	6.01	1.32	1.25
2	C	274	GLU	CD-OE2	6.00	1.32	1.25
2	C	245	GLU	CD-OE1	5.93	1.32	1.25
2	C	242	GLU	CD-OE1	5.93	1.32	1.25
2	D	408	GLU	CD-OE1	5.91	1.32	1.25
2	C	116	GLU	CD-OE1	5.90	1.32	1.25
2	C	374	GLU	CD-OE1	5.87	1.32	1.25
2	D	348	ASN	C-N	5.85	1.47	1.34
1	B	81	GLU	CD-OE2	5.84	1.32	1.25
2	D	515	GLU	CD-OE1	5.79	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	263	GLU	CD-OE1	5.76	1.31	1.25
2	C	180	GLU	C-N	5.75	1.47	1.34
2	D	404	GLU	CD-OE1	5.72	1.31	1.25
2	C	404	GLU	CD-OE1	5.69	1.31	1.25
1	A	102	GLU	CD-OE2	5.67	1.31	1.25
2	D	279	GLU	CD-OE1	5.66	1.31	1.25
2	D	374	GLU	CD-OE1	5.66	1.31	1.25
2	C	132	PRO	C-N	5.54	1.46	1.34
2	D	245	GLU	CD-OE2	5.49	1.31	1.25
2	D	483	GLU	CD-OE2	5.43	1.31	1.25
2	C	401	GLU	CD-OE1	5.39	1.31	1.25
2	C	408	GLU	CD-OE1	5.38	1.31	1.25
2	C	362	SER	C-N	-5.36	1.21	1.34
1	A	38	GLU	CD-OE1	5.35	1.31	1.25
2	D	362	SER	C-N	5.30	1.46	1.34
2	C	522	MET	C-N	-5.30	1.21	1.34
2	C	483	GLU	CD-OE2	5.29	1.31	1.25
1	A	36	GLU	CD-OE2	5.29	1.31	1.25
2	C	515	GLU	CD-OE1	5.04	1.31	1.25

All (392) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	560	ASP	O-C-N	-21.52	88.26	122.70
2	C	560	ASP	O-C-N	-18.81	92.61	122.70
2	C	218	ASP	CB-CG-OD1	-18.33	101.80	118.30
2	D	202	ARG	O-C-N	-16.89	95.67	122.70
2	D	272	ASP	CB-CA-C	-16.82	76.77	110.40
2	C	560	ASP	CA-C-N	-15.42	83.28	117.20
2	D	405	ARG	NE-CZ-NH1	15.35	127.98	120.30
2	D	348	ASN	N-CA-CB	-15.08	83.46	110.60
1	B	5	ASP	O-C-N	-14.79	99.04	122.70
2	D	560	ASP	CA-C-N	-14.59	85.09	117.20
2	D	535	ARG	NE-CZ-NH2	-14.39	113.10	120.30
2	D	356	ASN	CB-CA-C	14.33	139.06	110.40
2	C	382	ARG	NE-CZ-NH2	-14.13	113.24	120.30
2	D	179	SER	C-N-CA	-13.59	87.73	121.70
2	D	348	ASN	CB-CA-C	-12.98	84.44	110.40
2	D	347	ASP	C-N-CA	-12.95	89.33	121.70
2	C	255	ARG	NE-CZ-NH1	12.90	126.75	120.30
2	C	382	ARG	NE-CZ-NH1	12.04	126.32	120.30
2	D	357	PRO	O-C-N	-11.91	103.65	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	172	ASP	CB-CG-OD2	-11.88	107.61	118.30
2	D	202	ARG	CA-C-N	11.86	143.28	117.20
2	C	517	GLU	O-C-N	-11.67	103.35	123.20
2	C	574	SER	O-C-N	-11.53	104.25	122.70
2	D	143	CYS	CB-CA-C	-11.30	87.80	110.40
2	D	557	TYR	CB-CG-CD2	-11.04	114.38	121.00
1	A	79	ASP	CB-CG-OD1	-11.02	108.38	118.30
2	D	192	ASN	CB-CA-C	-10.76	88.88	110.40
2	C	574	SER	C-N-CA	10.69	148.41	121.70
2	D	179	SER	N-CA-CB	10.68	126.52	110.50
2	D	229	ARG	CB-CA-C	-10.55	89.30	110.40
2	D	507	ARG	NE-CZ-NH1	10.37	125.49	120.30
1	B	14	CYS	N-CA-CB	-10.27	92.12	110.60
2	C	427	ASP	CB-CG-OD2	-10.17	109.15	118.30
2	C	507	ARG	NE-CZ-NH2	-10.13	115.23	120.30
2	C	516	ASN	C-N-CA	-10.06	96.54	121.70
2	C	295	ASP	CB-CG-OD1	-9.98	109.32	118.30
2	D	142	ASP	CB-CG-OD1	-9.96	109.33	118.30
2	D	270	ARG	NE-CZ-NH2	-9.94	115.33	120.30
2	D	141	ALA	CB-CA-C	9.91	124.97	110.10
1	A	8	ARG	NE-CZ-NH1	9.79	125.20	120.30
2	D	218	ASP	CB-CG-OD1	-9.75	109.53	118.30
1	B	18	ARG	NE-CZ-NH1	9.72	125.16	120.30
2	C	504	ARG	NE-CZ-NH1	9.71	125.15	120.30
2	C	354	GLU	N-CA-C	9.64	137.02	111.00
2	C	456	ARG	CG-CD-NE	-9.61	91.63	111.80
2	C	378	ASP	CB-CG-OD2	-9.59	109.67	118.30
1	B	54	ASN	O-C-N	-9.58	106.92	123.20
2	D	395	ASN	CB-CA-C	-9.44	91.53	110.40
2	C	218	ASP	CB-CG-OD2	9.44	126.79	118.30
2	D	440	CYS	N-CA-CB	9.37	127.47	110.60
2	D	199	VAL	O-C-N	-9.35	107.74	122.70
2	C	180	GLU	C-N-CA	-9.27	98.54	121.70
2	C	557	TYR	CB-CG-CD1	9.26	126.55	121.00
1	A	30	VAL	CA-CB-CG2	-9.19	97.11	110.90
2	C	557	TYR	CG-CD1-CE1	9.17	128.64	121.30
2	D	237	ASP	CB-CG-OD2	-9.17	110.05	118.30
2	C	355	PRO	N-CA-C	-9.16	88.28	112.10
1	B	52	LYS	C-N-CA	-9.08	99.00	121.70
2	C	550	ASN	N-CA-CB	9.03	126.85	110.60
1	B	8	ARG	CB-CA-C	-8.89	92.61	110.40
1	B	30	VAL	CB-CA-C	-8.89	94.52	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	132	PRO	C-N-CA	-8.85	99.57	121.70
2	D	275	ARG	NE-CZ-NH2	-8.85	115.87	120.30
2	D	508	ASP	CB-CG-OD1	8.84	126.26	118.30
2	D	172	ASP	CB-CG-OD1	8.84	126.25	118.30
2	C	507	ARG	NE-CZ-NH1	8.83	124.71	120.30
2	D	529	ALA	C-N-CA	-8.81	99.68	121.70
1	A	98	ASP	CB-CG-OD1	-8.75	110.42	118.30
2	C	475	ASP	CB-CG-OD2	8.73	126.16	118.30
2	C	393	ARG	NE-CZ-NH2	-8.71	115.95	120.30
2	C	574	SER	CA-C-N	8.70	136.35	117.20
2	C	136	ARG	NE-CZ-NH1	8.68	124.64	120.30
2	C	270	ARG	NE-CZ-NH2	-8.68	115.96	120.30
2	C	133	ASN	O-C-N	-8.66	108.85	122.70
2	D	538	CYS	CB-CA-C	-8.57	93.27	110.40
1	B	27	ARG	NE-CZ-NH2	-8.52	116.04	120.30
2	D	508	ASP	CB-CG-OD2	-8.49	110.66	118.30
2	C	504	ARG	NE-CZ-NH2	-8.47	116.06	120.30
2	D	557	TYR	CB-CA-C	-8.44	93.52	110.40
2	D	184	ALA	C-N-CA	-8.41	100.67	121.70
2	D	347	ASP	CB-CG-OD1	8.37	125.84	118.30
2	D	144	ILE	CB-CA-C	8.36	128.32	111.60
2	D	203	PHE	C-N-CA	-8.32	100.90	121.70
2	C	318	ASP	CB-CG-OD1	-8.31	110.82	118.30
1	B	14	CYS	CB-CA-C	8.31	127.03	110.40
2	C	487	ARG	CA-CB-CG	8.28	131.62	113.40
2	C	510	ASP	CB-CG-OD1	-8.21	110.91	118.30
2	D	556	SER	C-N-CA	-8.19	101.23	121.70
2	D	535	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	A	4	GLN	CB-CA-C	-8.17	94.06	110.40
2	D	348	ASN	O-C-N	-8.13	109.70	122.70
2	D	362	SER	C-N-CA	-8.12	101.40	121.70
2	C	346	LEU	C-N-CA	8.12	141.99	121.70
1	B	25	SER	CB-CA-C	-8.10	94.71	110.10
2	C	456	ARG	NE-CZ-NH2	8.07	124.34	120.30
2	D	281	ARG	NE-CZ-NH2	-8.00	116.30	120.30
2	C	291	ILE	CB-CA-C	-7.99	95.61	111.60
2	D	433	TYR	CB-CG-CD1	7.99	125.79	121.00
2	D	458	LEU	N-CA-CB	7.95	126.31	110.40
1	A	8	ARG	CB-CA-C	-7.95	94.50	110.40
2	C	156	SER	N-CA-CB	7.95	122.42	110.50
2	C	221	CYS	CB-CA-C	7.94	126.29	110.40
2	D	363	ARG	NE-CZ-NH2	7.90	124.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	94	ASP	CB-CG-OD1	7.88	125.39	118.30
1	B	42	SER	CB-CA-C	-7.86	95.18	110.10
1	A	7	TYR	CB-CG-CD1	-7.85	116.29	121.00
2	D	426	ARG	NE-CZ-NH1	7.82	124.21	120.30
2	C	295	ASP	CB-CG-OD2	7.81	125.33	118.30
2	C	382	ARG	N-CA-CB	-7.79	96.57	110.60
2	C	510	ASP	CB-CG-OD2	7.79	125.31	118.30
2	C	350	TYR	C-N-CA	-7.79	102.23	121.70
1	B	42	SER	N-CA-CB	-7.76	98.86	110.50
2	C	156	SER	CB-CA-C	7.70	124.72	110.10
2	C	520	PHE	N-CA-C	-7.68	90.27	111.00
2	D	229	ARG	NE-CZ-NH2	7.67	124.13	120.30
2	C	416	ASP	CB-CG-OD1	-7.63	111.43	118.30
2	C	227	SER	N-CA-CB	-7.63	99.05	110.50
2	D	137	ILE	CB-CA-C	7.63	126.85	111.60
2	D	456	ARG	NE-CZ-NH2	7.58	124.09	120.30
1	B	86	PHE	CB-CG-CD2	-7.57	115.50	120.80
2	C	253	LEU	CB-CA-C	7.55	124.54	110.20
2	D	462	ARG	CB-CA-C	7.54	125.48	110.40
2	D	561	PHE	CB-CA-C	-7.52	95.36	110.40
2	D	237	ASP	CB-CG-OD1	7.51	125.06	118.30
2	C	229	ARG	NE-CZ-NH2	7.50	124.05	120.30
2	C	309	TYR	CB-CG-CD1	-7.50	116.50	121.00
2	D	214	ASP	CB-CG-OD1	-7.48	111.57	118.30
2	C	237	ASP	CB-CG-OD2	-7.45	111.59	118.30
2	D	270	ARG	NE-CZ-NH1	7.45	124.02	120.30
1	B	70	ARG	NE-CZ-NH2	-7.40	116.60	120.30
2	C	318	ASP	CB-CG-OD2	7.39	124.95	118.30
2	C	442	LEU	CB-CA-C	7.39	124.23	110.20
2	C	358	ARG	NE-CZ-NH2	-7.34	116.63	120.30
2	C	309	TYR	CB-CG-CD2	7.33	125.40	121.00
2	D	205	ASP	CB-CG-OD2	7.32	124.89	118.30
2	C	508	ASP	CB-CG-OD2	-7.32	111.71	118.30
2	C	132	PRO	CA-C-N	-7.31	101.12	117.20
2	C	380	ILE	CB-CA-C	-7.30	97.00	111.60
2	C	350	TYR	CB-CG-CD2	-7.28	116.63	121.00
2	D	255	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	A	79	ASP	CB-CG-OD2	7.24	124.81	118.30
2	D	416	ASP	CB-CG-OD1	-7.23	111.79	118.30
1	A	99	PHE	CB-CG-CD1	-7.22	115.75	120.80
2	C	498	ILE	CB-CA-C	7.21	126.02	111.60
2	D	357	PRO	CA-C-N	7.16	132.94	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	426	ARG	NE-CZ-NH1	7.13	123.87	120.30
2	C	405	ARG	NE-CZ-NH1	7.13	123.86	120.30
1	B	53	ARG	NE-CZ-NH2	7.10	123.85	120.30
2	C	557	TYR	N-CA-CB	7.10	123.38	110.60
2	D	507	ARG	NE-CZ-NH2	-7.09	116.76	120.30
2	D	295	ASP	CB-CG-OD1	-7.05	111.96	118.30
2	D	539	ASP	CB-CG-OD1	-7.04	111.97	118.30
2	C	557	TYR	C-N-CD	-7.03	105.14	120.60
2	C	393	ARG	NE-CZ-NH1	7.02	123.81	120.30
2	C	383	GLY	N-CA-C	-7.00	95.61	113.10
2	C	147	PHE	CB-CA-C	-6.99	96.42	110.40
2	D	141	ALA	N-CA-CB	6.98	119.88	110.10
2	D	547	SER	N-CA-CB	-6.98	100.03	110.50
1	A	66	ASN	C-N-CA	-6.97	104.27	121.70
2	C	559	ARG	CB-CA-C	-6.96	96.48	110.40
2	D	539	ASP	CB-CG-OD2	6.96	124.56	118.30
2	C	363	ARG	NE-CZ-NH2	6.93	123.77	120.30
2	D	132	PRO	C-N-CA	-6.93	104.37	121.70
2	C	255	ARG	NE-CZ-NH2	-6.90	116.85	120.30
2	D	510	ASP	CB-CG-OD1	-6.84	112.15	118.30
2	C	444	GLN	C-N-CD	-6.83	105.59	120.60
2	D	196	LEU	N-CA-CB	-6.82	96.75	110.40
1	A	31	ARG	N-CA-CB	-6.81	98.35	110.60
2	D	475	ASP	CB-CG-OD1	-6.80	112.18	118.30
1	A	82	ARG	NE-CZ-NH1	6.77	123.68	120.30
2	C	323	ARG	NE-CZ-NH1	6.75	123.68	120.30
2	D	378	ASP	CB-CG-OD2	-6.75	112.23	118.30
2	C	517	GLU	C-N-CA	-6.75	108.13	122.30
2	C	132	PRO	O-C-N	6.73	133.47	122.70
1	B	82	ARG	NE-CZ-NH1	-6.73	116.94	120.30
2	C	438	ARG	NE-CZ-NH1	6.73	123.66	120.30
2	C	259	ARG	NE-CZ-NH1	6.71	123.66	120.30
2	D	168	THR	CB-CA-C	-6.71	93.47	111.60
2	C	189	ASN	CB-CA-C	6.70	123.81	110.40
2	D	273	GLY	O-C-N	-6.66	112.05	122.70
2	D	179	SER	O-C-N	6.65	133.34	122.70
2	D	350	TYR	CB-CG-CD2	-6.64	117.02	121.00
2	C	219	ASP	CB-CG-OD1	-6.61	112.35	118.30
1	B	100	THR	N-CA-CB	-6.57	97.81	110.30
2	D	142	ASP	CB-CG-OD2	6.56	124.20	118.30
2	C	466	GLU	CB-CA-C	-6.54	97.31	110.40
2	C	142	ASP	CB-CG-OD1	-6.53	112.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	199	VAL	N-CA-CB	-6.51	97.17	111.50
1	B	14	CYS	N-CA-C	6.50	128.55	111.00
2	D	321	ASP	CB-CG-OD1	-6.46	112.48	118.30
2	D	219	ASP	CB-CG-OD1	-6.46	112.49	118.30
2	D	370	ARG	NE-CZ-NH1	-6.44	117.08	120.30
1	A	77	THR	CA-CB-CG2	-6.43	103.39	112.40
2	D	265	LYS	N-CA-CB	6.41	122.14	110.60
2	D	350	TYR	CB-CG-CD1	6.41	124.85	121.00
1	B	39	ASP	CB-CG-OD2	-6.38	112.55	118.30
2	D	378	ASP	CB-CG-OD1	6.38	124.05	118.30
2	C	427	ASP	CB-CG-OD1	6.37	124.03	118.30
1	A	99	PHE	CB-CG-CD2	6.36	125.25	120.80
2	C	216	LEU	CB-CA-C	6.35	122.27	110.20
2	C	204	GLN	CA-C-N	-6.33	103.27	117.20
2	C	535	ARG	NE-CZ-NH2	-6.33	117.14	120.30
2	C	228	ALA	C-N-CA	-6.32	105.90	121.70
2	D	453	THR	CA-CB-CG2	-6.30	103.58	112.40
2	C	172	ASP	N-CA-C	-6.29	94.03	111.00
2	C	557	TYR	N-CA-C	6.28	127.96	111.00
2	C	428	HIS	CA-CB-CG	-6.24	102.99	113.60
2	D	227	SER	C-N-CA	6.24	137.31	121.70
1	B	30	VAL	N-CA-CB	-6.24	97.78	111.50
2	C	227	SER	CA-CB-OG	-6.24	94.36	111.20
2	D	347	ASP	CB-CG-OD2	-6.23	112.69	118.30
2	D	230	ILE	O-C-N	6.23	132.93	121.10
2	C	473	ASN	CB-CA-C	6.22	122.83	110.40
2	D	549	ASN	CB-CA-C	6.21	122.82	110.40
2	D	333	ARG	NE-CZ-NH1	6.21	123.40	120.30
2	D	201	GLN	CB-CA-C	6.21	122.81	110.40
2	D	374	GLU	CG-CD-OE1	-6.20	105.91	118.30
2	C	321	ASP	CB-CG-OD1	-6.19	112.73	118.30
2	C	303	PRO	N-CA-C	-6.17	96.07	112.10
2	C	121	GLN	C-N-CA	-6.16	106.30	121.70
2	D	433	TYR	CB-CG-CD2	-6.15	117.31	121.00
2	D	132	PRO	CA-C-N	-6.13	103.72	117.20
2	D	339	ILE	CB-CA-C	6.12	123.85	111.60
1	B	85	MET	CG-SD-CE	6.10	109.96	100.20
2	C	378	ASP	CB-CG-OD1	6.10	123.79	118.30
2	D	440	CYS	CA-CB-SG	6.09	124.96	114.00
2	C	125	CYS	CA-CB-SG	-6.09	103.04	114.00
2	C	465	MET	CA-CB-CG	-6.09	102.95	113.30
2	D	214	ASP	CB-CG-OD2	6.07	123.76	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	D	364	VAL	CB-CA-C	-6.05	99.91	111.40
2	D	407	PHE	CB-CA-C	-6.04	98.32	110.40
2	C	549	ASN	CB-CA-C	6.03	122.46	110.40
2	D	314	ARG	CB-CA-C	6.03	122.45	110.40
2	D	179	SER	CA-C-N	-6.01	103.98	117.20
2	D	258	ASN	N-CA-C	-6.01	94.78	111.00
2	D	405	ARG	NH1-CZ-NH2	-6.00	112.81	119.40
2	D	525	ARG	CB-CA-C	-6.00	98.41	110.40
2	C	239	ARG	NE-CZ-NH2	-5.99	117.30	120.30
2	C	566	THR	CA-CB-CG2	-5.99	104.02	112.40
2	D	148	ARG	NE-CZ-NH1	5.98	123.29	120.30
1	B	94	ASP	CB-CG-OD1	5.93	123.64	118.30
2	C	440	CYS	C-N-CA	-5.92	109.86	122.30
2	D	339	ILE	CG1-CB-CG2	-5.90	98.42	111.40
1	B	72	PRO	N-CA-CB	5.88	110.36	103.30
1	B	82	ARG	CD-NE-CZ	-5.87	115.38	123.60
2	D	239	ARG	NE-CZ-NH1	5.87	123.23	120.30
2	C	505	LYS	CB-CA-C	-5.87	98.67	110.40
2	C	414	GLY	O-C-N	-5.87	113.31	122.70
2	D	259	ARG	NE-CZ-NH1	5.86	123.23	120.30
2	D	203	PHE	CB-CG-CD1	-5.85	116.71	120.80
1	B	2	PRO	O-C-N	5.83	132.02	122.70
2	D	230	ILE	CA-C-N	-5.83	100.79	117.10
2	C	237	ASP	CB-CG-OD1	5.80	123.53	118.30
2	D	320	VAL	CB-CA-C	5.80	122.41	111.40
1	A	3	GLU	O-C-N	-5.77	113.47	122.70
2	C	144	ILE	N-CA-C	-5.76	95.45	111.00
2	C	204	GLN	O-C-N	-5.75	113.51	122.70
2	D	362	SER	CB-CA-C	-5.72	99.23	110.10
2	C	460	LEU	CB-CA-C	5.70	121.04	110.20
2	C	169	SER	N-CA-CB	-5.69	101.96	110.50
1	A	39	ASP	CB-CG-OD1	-5.69	113.18	118.30
2	C	459	LYS	O-C-N	-5.68	113.61	122.70
2	D	427	ASP	CB-CA-C	5.68	121.75	110.40
2	C	274	GLU	C-N-CA	-5.66	107.54	121.70
1	B	70	ARG	NE-CZ-NH1	5.66	123.13	120.30
2	C	364	VAL	CA-CB-CG1	-5.66	102.41	110.90
2	D	134	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	A	69	VAL	N-CA-CB	5.64	123.91	111.50
2	D	556	SER	CA-C-N	5.63	129.60	117.20
2	D	525	ARG	CD-NE-CZ	-5.62	115.72	123.60
2	D	374	GLU	C-N-CA	-5.62	110.50	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	270	ARG	NE-CZ-NH1	5.62	123.11	120.30
2	C	546	VAL	N-CA-CB	-5.61	99.15	111.50
2	C	137	ILE	CB-CA-C	5.61	122.82	111.60
2	D	537	ILE	N-CA-CB	5.61	123.70	110.80
1	A	64	VAL	CB-CA-C	5.61	122.05	111.40
2	C	393	ARG	CG-CD-NE	5.61	123.57	111.80
2	C	472	ASN	CB-CA-C	5.59	121.59	110.40
2	D	309	TYR	CB-CA-C	5.59	121.59	110.40
2	C	351	GLN	CB-CA-C	-5.59	99.22	110.40
2	D	199	VAL	CB-CA-C	-5.59	100.78	111.40
2	C	360	PRO	N-CA-CB	5.58	110.00	103.30
1	B	74	ASP	CB-CG-OD2	-5.58	113.28	118.30
2	C	357	PRO	N-CA-C	5.57	126.58	112.10
2	C	148	ARG	NE-CZ-NH2	5.57	123.08	120.30
2	D	358	ARG	N-CA-CB	-5.57	100.58	110.60
1	B	18	ARG	NE-CZ-NH2	-5.56	117.52	120.30
2	C	358	ARG	NE-CZ-NH1	5.54	123.07	120.30
2	D	249	MET	CA-CB-CG	-5.53	103.90	113.30
2	D	520	PHE	N-CA-CB	-5.53	100.66	110.60
2	D	345	ARG	CD-NE-CZ	-5.52	115.87	123.60
2	C	557	TYR	CD1-CE1-CZ	-5.51	114.84	119.80
2	C	210	LEU	CB-CA-C	5.51	120.67	110.20
2	D	242	GLU	CG-CD-OE1	5.50	129.31	118.30
2	D	295	ASP	CB-CG-OD2	5.50	123.25	118.30
2	D	475	ASP	CB-CG-OD2	5.50	123.25	118.30
2	C	172	ASP	CB-CG-OD1	5.49	123.24	118.30
1	B	98	ASP	CB-CG-OD1	-5.46	113.38	118.30
2	D	498	ILE	CB-CA-C	5.46	122.51	111.60
2	D	123	PRO	C-N-CD	-5.45	108.60	120.60
2	C	490	ARG	NE-CZ-NH1	-5.45	117.58	120.30
2	C	151	PRO	CA-N-CD	-5.44	103.88	111.50
2	C	400	ASP	CB-CG-OD2	-5.44	113.41	118.30
2	C	373	LEU	CB-CA-C	-5.43	99.89	110.20
2	D	458	LEU	CB-CG-CD1	5.43	120.23	111.00
2	D	562	VAL	CB-CA-C	-5.42	101.09	111.40
2	C	462	ARG	NE-CZ-NH2	-5.42	117.59	120.30
2	C	549	ASN	N-CA-CB	5.40	120.33	110.60
2	C	539	ASP	CB-CG-OD1	-5.40	113.44	118.30
2	C	458	LEU	C-N-CA	5.39	135.18	121.70
2	D	218	ASP	CB-CG-OD2	5.39	123.15	118.30
2	C	275	ARG	NE-CZ-NH1	5.37	122.98	120.30
2	D	188	ARG	N-CA-CB	-5.37	100.93	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	86	PHE	CB-CG-CD1	5.36	124.55	120.80
1	B	13	MET	N-CA-C	5.35	125.46	111.00
2	C	223	LEU	CB-CA-C	-5.35	100.03	110.20
2	D	566	THR	CA-CB-CG2	-5.34	104.92	112.40
2	D	202	ARG	C-N-CA	5.34	135.05	121.70
2	D	300	VAL	N-CA-C	-5.34	96.58	111.00
2	D	248	SER	CB-CA-C	5.32	120.21	110.10
1	B	27	ARG	NE-CZ-NH1	5.32	122.96	120.30
2	D	541	THR	N-CA-CB	5.31	120.40	110.30
1	B	54	ASN	C-N-CA	5.31	133.45	122.30
2	C	144	ILE	CB-CA-C	5.31	122.22	111.60
1	B	31	ARG	NE-CZ-NH1	5.30	122.95	120.30
2	C	329	THR	CA-CB-OG1	-5.30	97.87	109.00
1	B	76	LEU	CA-C-N	-5.30	105.54	117.20
2	D	573	ALA	N-CA-CB	5.30	117.52	110.10
2	D	548	LYS	N-CA-CB	5.29	120.13	110.60
2	C	294	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	C	232	CYS	CB-CA-C	5.26	120.91	110.40
1	B	98	ASP	CB-CG-OD2	5.25	123.03	118.30
2	C	387	THR	CA-CB-CG2	-5.25	105.05	112.40
2	D	147	PHE	O-C-N	-5.25	114.31	122.70
2	D	253	LEU	CB-CA-C	5.25	120.17	110.20
1	A	29	PHE	CB-CA-C	-5.24	99.91	110.40
2	D	205	ASP	N-CA-CB	5.24	120.02	110.60
2	D	161	ARG	NE-CZ-NH1	5.23	122.92	120.30
1	B	76	LEU	C-N-CA	-5.23	108.62	121.70
1	A	14	CYS	CB-CA-C	5.23	120.86	110.40
2	D	242	GLU	CG-CD-OE2	-5.23	107.85	118.30
2	C	214	ASP	CB-CG-OD2	5.22	123.00	118.30
2	D	294	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	D	362	SER	CA-C-N	-5.22	105.71	117.20
2	D	124	PRO	N-CA-CB	5.22	109.56	103.30
2	C	208	ARG	NE-CZ-NH2	-5.21	117.69	120.30
2	D	557	TYR	CA-C-N	-5.21	102.50	117.10
2	C	136	ARG	N-CA-CB	5.21	119.98	110.60
2	D	447	THR	N-CA-CB	-5.20	100.43	110.30
2	C	363	ARG	CA-C-N	-5.19	105.79	117.20
1	B	76	LEU	CB-CA-C	-5.18	100.35	110.20
2	D	163	GLN	CB-CA-C	5.18	120.76	110.40
2	D	462	ARG	CA-CB-CG	5.18	124.79	113.40
2	D	182	PRO	O-C-N	-5.18	114.42	122.70
2	C	355	PRO	C-N-CA	5.17	134.62	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	448	VAL	CA-CB-CG1	-5.16	103.15	110.90
2	C	205	ASP	CB-CG-OD1	5.16	122.94	118.30
2	C	507	ARG	N-CA-CB	-5.16	101.32	110.60
1	A	71	PHE	CB-CA-C	5.14	120.69	110.40
2	C	153	CYS	N-CA-CB	-5.14	101.34	110.60
2	C	468	TYR	N-CA-C	5.14	124.88	111.00
2	D	353	MET	CA-CB-CG	-5.14	104.56	113.30
2	C	458	LEU	O-C-N	-5.13	114.50	122.70
1	B	46	GLY	N-CA-C	-5.13	100.28	113.10
2	D	438	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	45	TYR	N-CA-CB	5.12	119.81	110.60
1	B	45	TYR	N-CA-C	-5.11	97.20	111.00
2	D	309	TYR	CA-CB-CG	-5.11	103.69	113.40
2	D	382	ARG	NE-CZ-NH1	-5.10	117.75	120.30
2	C	315	SER	CB-CA-C	-5.09	100.44	110.10
2	D	147	PHE	CB-CG-CD1	-5.08	117.24	120.80
2	C	409	GLN	CB-CA-C	5.08	120.56	110.40
2	D	551	ILE	CB-CA-C	-5.08	101.44	111.60
2	C	342	PHE	CB-CA-C	-5.07	100.26	110.40
1	B	1	CYS	CB-CA-C	-5.07	100.26	110.40
2	D	455	LEU	CB-CA-C	-5.07	100.57	110.20
2	C	296	TYR	CB-CG-CD2	5.07	124.04	121.00
2	C	190	MET	N-CA-CB	-5.06	101.49	110.60
2	C	391	LEU	CA-CB-CG	-5.06	103.67	115.30
1	B	39	ASP	CB-CA-C	-5.05	100.30	110.40
2	D	505	LYS	CB-CA-C	-5.05	100.30	110.40
2	D	240	SER	N-CA-CB	5.04	118.06	110.50
1	A	17	ARG	NE-CZ-NH1	5.03	122.82	120.30
2	C	508	ASP	CB-CG-OD1	5.03	122.83	118.30
1	A	98	ASP	CB-CG-OD2	5.03	122.83	118.30
2	D	199	VAL	CA-C-N	5.03	128.26	117.20
1	A	45	TYR	C-N-CA	-5.02	111.76	122.30
2	C	407	PHE	O-C-N	-5.02	114.67	122.70
1	A	6	LYS	CA-C-N	-5.02	106.16	117.20
2	D	289	GLN	CB-CA-C	-5.01	100.38	110.40
1	B	5	ASP	CB-CA-C	-5.00	100.39	110.40
1	B	11	THR	CA-CB-CG2	-5.00	105.39	112.40

All (13) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	A	14	CYS	CA

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Mol	Chain	Res	Type	Atom
1	A	69	VAL	CA
2	C	137	ILE	CA
2	C	156	SER	CA
2	C	460	LEU	CA
2	C	472	ASN	CA
2	C	473	ASN	CA
2	C	549	ASN	CA
2	D	123	PRO	CA
2	D	141	ALA	CA
2	D	356	ASN	CA
2	D	458	LEU	CA
2	D	549	ASN	CA

All (32) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	3	GLU	Mainchain
1	A	6	LYS	Mainchain
1	A	79	ASP	Sidechain
1	B	102	GLU	Mainchain
1	B	25	SER	Mainchain
1	B	5	ASP	Mainchain
1	B	54	ASN	Mainchain
2	C	122	GLN	Mainchain
2	C	133	ASN	Mainchain
2	C	180	GLU	Mainchain
2	C	182	PRO	Mainchain
2	C	203	PHE	Mainchain,Peptide
2	C	204	GLN	Mainchain
2	C	351	GLN	Mainchain
2	C	363	ARG	Mainchain
2	C	459	LYS	Mainchain
2	C	517	GLU	Mainchain
2	C	557	TYR	Peptide
2	D	114	ASN	Sidechain
2	D	182	PRO	Mainchain
2	D	185	ARG	Mainchain
2	D	230	ILE	Mainchain
2	D	348	ASN	Mainchain
2	D	355	PRO	Peptide
2	D	357	PRO	Mainchain
2	D	363	ARG	Sidechain,Mainchain

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Mol	Chain	Res	Type	Group
2	D	409	GLN	Mainchain
2	D	427	ASP	Sidechain
2	D	557	TYR	Sidechain
2	D	558	PRO	Peptide

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	830	0	785	198	0
1	B	830	0	784	186	0
2	C	3609	0	3529	859	0
2	D	3609	0	3529	605	0
3	E	28	0	25	2	0
3	F	28	0	25	1	0
3	G	28	0	25	5	0
3	H	28	0	25	1	0
3	I	28	0	25	6	0
3	J	28	0	25	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	43	0	30	35	0
5	B	43	0	30	32	0
All	All	9134	0	8837	1651	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 92.

All (1651) 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)
2:D:557:TYR:C	2:D:558:PRO:N	1.73	1.42
2:C:560:ASP:H	2:C:561:PHE:N	1.17	1.42
2:C:516:ASN:C	2:C:517:GLU:N	1.72	1.41
2:D:203:PHE:C	2:D:204:GLN:N	1.74	1.38
2:D:560:ASP:C	2:D:561:PHE:N	1.78	1.37

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:179:SER:C	2:D:180:GLU:N	1.81	1.31
1:B:4:GLN:NE2	1:B:17:ARG:HH22	1.26	1.29
1:B:3:GLU:O	1:B:4:GLN:HB2	1.21	1.26
5:A:580:HEM:HMC3	2:C:243:MET:SD	1.77	1.24
5:B:580:HEM:HBC1	2:D:365:PHE:CE1	1.74	1.21
2:C:560:ASP:N	2:C:561:PHE:N	1.89	1.20
2:C:560:ASP:C	2:C:561:PHE:N	1.95	1.19
1:B:3:GLU:O	1:B:4:GLN:CB	1.91	1.18
2:C:348:ASN:HA	2:C:382:ARG:HH22	1.00	1.17
1:B:94:ASP:OD2	5:B:580:HEM:HMA3	1.45	1.17
2:D:557:TYR:HB3	2:D:558:PRO:N	1.59	1.16
1:B:4:GLN:NE2	1:B:17:ARG:NH2	1.92	1.16
2:D:136:ARG:HG2	2:D:137:ILE:HG22	1.25	1.15
2:C:544:THR:HG23	2:C:545:THR:H	1.13	1.13
2:C:306:MET:HE3	2:C:310:LEU:HD23	1.19	1.12
2:C:230:ILE:HG21	2:C:372:VAL:HG21	1.32	1.11
1:A:31:ARG:HH11	2:C:162:ASN:ND2	1.50	1.10
1:A:22:LEU:HD11	2:C:323:ARG:HD2	1.29	1.08
2:C:467:GLN:HE21	2:C:467:GLN:HA	1.15	1.08
2:C:491:VAL:HG13	2:C:495:LEU:HB3	1.28	1.08
2:D:356:ASN:OD1	2:D:357:PRO:HD3	1.54	1.08
2:C:478:MET:HA	2:C:478:MET:HE3	1.29	1.07
5:B:580:HEM:HBC1	2:D:365:PHE:HE1	0.92	1.07
1:B:30:VAL:HG22	2:D:323:ARG:HG3	1.36	1.07
2:D:381:LEU:HA	2:D:384:LEU:HD12	1.35	1.07
2:C:541:THR:HB	2:C:543:ILE:HD13	1.37	1.06
2:C:122:GLN:HG3	2:C:123:PRO:HD2	1.27	1.06
2:D:192:ASN:HD22	2:D:194:LEU:HB2	1.13	1.06
2:C:446:GLU:H	2:C:450:GLN:NE2	1.55	1.05
2:C:229:ARG:O	2:C:229:ARG:HG3	1.31	1.05
2:C:447:THR:HB	2:C:450:GLN:HG3	1.05	1.04
3:J:1:NAG:H61	3:J:2:NAG:HN2	1.15	1.04
2:D:567:LEU:HD12	2:D:568:PRO:HD2	1.40	1.04
2:C:442:LEU:HB2	2:C:443:PRO:HD2	1.37	1.04
2:C:290:ILE:HG21	2:C:531:ILE:HD11	1.38	1.04
5:A:580:HEM:HBB2	5:A:580:HEM:HHC	1.40	1.03
1:A:66:ASN:HD22	2:C:403:ARG:NH1	1.54	1.03
1:A:30:VAL:HG21	2:C:323:ARG:HG3	1.41	1.02
2:C:348:ASN:HA	2:C:382:ARG:NH2	1.74	1.02
2:C:534:PRO:HG3	2:C:551:ILE:HD11	1.40	1.02
2:D:179:SER:C	2:D:180:GLU:CA	2.29	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:434:ASN:HD21	2:C:445:PRO:HD2	1.21	1.01
1:A:6:LYS:HG3	1:A:7:TYR:CE1	1.96	1.01
1:B:3:GLU:C	1:B:4:GLN:HB2	1.81	1.01
1:B:79:ASP:HB2	2:D:391:LEU:HB2	1.43	1.01
1:B:30:VAL:CG2	2:D:323:ARG:HG3	1.90	1.01
2:D:447:THR:HG22	2:D:449:GLY:H	1.25	1.00
2:C:136:ARG:HG3	2:C:137:ILE:HG22	1.42	1.00
1:B:30:VAL:HB	2:D:325:ALA:HA	1.43	1.00
2:D:540:ASN:N	2:D:540:ASN:HD22	1.55	1.00
2:C:415:LEU:HB3	2:C:420:LEU:HD11	1.43	1.00
1:A:99:PHE:HB3	2:C:167:LEU:HD13	1.44	1.00
1:A:77:THR:HG21	2:C:393:ARG:HD3	1.01	0.99
2:C:267:LEU:HD11	2:C:575:TRP:O	1.62	0.99
2:C:393:ARG:HG3	2:C:396:GLN:NE2	1.78	0.98
2:D:560:ASP:CA	2:D:561:PHE:N	2.26	0.98
1:A:77:THR:CG2	2:C:393:ARG:HD3	1.93	0.98
2:D:136:ARG:HE	2:D:404:GLU:HB3	1.27	0.98
1:A:30:VAL:CG2	2:C:323:ARG:HG3	1.93	0.98
2:D:465:MET:HE1	2:D:471:PRO:HD3	1.42	0.97
5:B:580:HEM:HBB2	5:B:580:HEM:HHC	1.43	0.97
1:A:66:ASN:ND2	2:C:403:ARG:HH12	1.61	0.97
5:A:580:HEM:HBC2	5:A:580:HEM:HMC2	1.46	0.97
1:B:4:GLN:HE21	1:B:17:ARG:HH22	0.98	0.96
2:C:447:THR:HG22	2:C:449:GLY:N	1.81	0.96
1:A:77:THR:HG21	2:C:393:ARG:CD	1.95	0.96
1:B:87:MET:SD	5:B:580:HEM:HBB1	2.05	0.96
2:D:130:ILE:HG21	2:D:137:ILE:HD11	1.43	0.96
2:C:390:LYS:HG3	2:C:391:LEU:N	1.80	0.95
2:C:447:THR:HG22	2:C:449:GLY:H	1.26	0.95
2:C:229:ARG:CG	2:C:229:ARG:O	2.11	0.94
2:C:544:THR:HG23	2:C:545:THR:HG22	1.47	0.94
1:B:4:GLN:HE22	1:B:17:ARG:NH2	1.65	0.94
2:C:491:VAL:CG1	2:C:495:LEU:HB3	1.96	0.94
2:D:555:ASN:N	2:D:560:ASP:OD1	1.99	0.94
2:D:557:TYR:CB	2:D:558:PRO:N	2.30	0.94
2:C:221:CYS:HB3	2:C:366:PHE:HB3	1.48	0.94
2:C:177:TYR:HE2	2:C:281:ARG:HA	1.31	0.94
2:D:216:LEU:H	2:D:216:LEU:HD22	1.33	0.94
2:C:348:ASN:CA	2:C:382:ARG:HH22	1.81	0.93
2:D:267:LEU:HD12	2:D:268:ASN:ND2	1.82	0.93
2:C:467:GLN:NE2	2:C:467:GLN:HA	1.77	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:348:ASN:N	2:D:348:ASN:OD1	1.94	0.93
5:B:580:HEM:HBC2	2:D:242:GLU:OE1	1.69	0.93
1:B:77:THR:HG21	2:D:393:ARG:HH11	1.31	0.92
2:C:541:THR:CB	2:C:543:ILE:HD13	2.00	0.92
2:C:240:SER:HB2	2:C:250:HIS:CD2	2.05	0.92
5:A:580:HEM:CAC	2:C:242:GLU:OE2	2.18	0.91
2:C:303:PRO:O	2:C:306:MET:HB3	1.70	0.91
2:C:516:ASN:C	2:C:517:GLU:CA	2.39	0.91
2:C:297:LEU:HA	2:C:300:VAL:CG1	2.00	0.91
2:D:197:LEU:H	2:D:258:ASN:HD21	1.12	0.91
1:B:100:THR:HG21	2:D:428:HIS:HE1	1.35	0.91
2:C:557:TYR:HB2	2:C:561:PHE:CE1	2.06	0.91
1:A:31:ARG:NH1	2:C:162:ASN:ND2	2.19	0.91
2:C:478:MET:HA	2:C:478:MET:CE	2.01	0.91
2:C:560:ASP:CA	2:C:561:PHE:N	2.34	0.91
2:D:556:SER:HB2	2:D:560:ASP:OD2	1.69	0.91
2:D:284:VAL:HA	2:D:287:MET:HG3	1.52	0.90
2:C:211:LEU:HD13	2:C:233:PHE:CD2	2.07	0.90
2:D:171:VAL:CG1	2:D:289:GLN:HG3	2.01	0.90
1:A:13:MET:O	1:A:14:CYS:HB3	1.70	0.90
2:D:385:MET:HE1	2:D:546:VAL:HA	1.54	0.90
1:A:62:ARG:NH2	2:C:136:ARG:HG2	1.87	0.89
2:C:139:ASN:HD22	2:C:141:ALA:H	1.20	0.89
2:C:477:TRP:O	2:C:481:VAL:HG22	1.73	0.89
2:D:320:VAL:HG13	2:D:509:GLY:HA2	1.52	0.89
2:D:267:LEU:HD12	2:D:268:ASN:HD21	1.32	0.89
2:C:181:GLU:N	2:C:182:PRO:CD	2.35	0.89
2:D:197:LEU:H	2:D:258:ASN:ND2	1.69	0.89
2:D:458:LEU:HD22	2:D:462:ARG:HH11	1.36	0.88
2:C:213:PHE:CE2	2:C:231:PRO:HD2	2.07	0.88
1:B:79:ASP:HB2	2:D:391:LEU:CB	2.03	0.88
2:D:179:SER:C	2:D:180:GLU:HA	1.94	0.87
2:C:350:TYR:HB2	2:C:557:TYR:CE2	2.08	0.87
5:B:580:HEM:CBC	2:D:365:PHE:HE1	1.83	0.87
2:D:192:ASN:ND2	2:D:194:LEU:HB2	1.89	0.87
2:D:292:THR:O	2:D:297:LEU:HD22	1.74	0.87
2:D:465:MET:CE	2:D:470:THR:HA	2.04	0.87
2:D:229:ARG:O	2:D:230:ILE:HD13	1.75	0.87
2:D:175:MET:HB2	2:D:250:HIS:HE1	1.37	0.87
2:D:353:MET:C	2:D:355:PRO:HD2	1.95	0.87
2:D:415:LEU:HD12	2:D:415:LEU:H	1.38	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:136:ARG:HH12	2:C:414:GLY:CA	1.86	0.87
2:C:186:ASN:C	2:C:187:LEU:HD12	1.95	0.87
2:C:342:PHE:CD1	2:C:358:ARG:HD3	2.09	0.87
2:D:557:TYR:O	2:D:558:PRO:C	2.12	0.86
1:A:27:ARG:NH2	1:B:41:PHE:HB3	1.90	0.86
5:A:580:HEM:CMC	2:C:243:MET:SD	2.63	0.86
2:C:348:ASN:HD22	2:C:348:ASN:H	1.24	0.86
3:I:1:NAG:H61	3:I:2:NAG:O5	1.76	0.85
2:C:541:THR:HB	2:C:543:ILE:CD1	2.06	0.85
2:D:290:ILE:HG21	2:D:531:ILE:HD11	1.59	0.84
1:B:103:PRO:O	1:B:104:ALA:O	1.94	0.84
2:C:415:LEU:H	2:C:415:LEU:HD22	1.41	0.84
2:C:122:GLN:CG	2:C:123:PRO:HD2	2.06	0.84
1:B:71:PHE:HZ	1:B:76:LEU:HD12	1.39	0.84
2:C:130:ILE:HG21	2:C:137:ILE:HD11	1.60	0.84
2:C:351:GLN:HB3	2:C:352:PRO:HD2	1.60	0.84
2:D:422:MET:O	2:D:425:SER:HB3	1.76	0.84
1:A:95:HIS:CE1	2:C:239:ARG:HE	1.96	0.84
1:B:99:PHE:HB3	2:D:167:LEU:HD13	1.57	0.84
2:C:556:SER:HB2	2:C:560:ASP:OD2	1.78	0.83
2:D:130:ILE:HD12	2:D:137:ILE:HG12	1.59	0.83
2:D:353:MET:O	2:D:355:PRO:HD2	1.77	0.83
2:D:383:GLY:O	2:D:387:THR:HG23	1.78	0.83
2:D:557:TYR:C	2:D:558:PRO:CA	2.45	0.83
1:B:3:GLU:C	1:B:4:GLN:N	2.32	0.83
2:C:348:ASN:ND2	2:C:348:ASN:H	1.75	0.83
1:A:31:ARG:NH2	2:C:428:HIS:O	2.09	0.83
2:D:372:VAL:HG12	2:D:373:LEU:HD13	1.60	0.83
2:D:130:ILE:HD12	2:D:137:ILE:CG1	2.08	0.83
2:C:321:ASP:OD1	2:C:323:ARG:HD3	1.79	0.83
1:B:85:MET:HG3	1:B:85:MET:O	1.76	0.82
2:D:313:TYR:CD1	2:D:507:ARG:HD3	2.14	0.82
1:A:22:LEU:CD1	2:C:323:ARG:HD2	2.08	0.82
2:C:407:PHE:CD2	2:C:415:LEU:HD23	2.13	0.82
2:C:491:VAL:HG13	2:C:495:LEU:CB	2.09	0.82
2:C:139:ASN:ND2	2:C:141:ALA:H	1.76	0.82
2:C:346:LEU:HA	2:C:353:MET:HB2	1.60	0.82
2:D:458:LEU:HD22	2:D:462:ARG:NH1	1.94	0.82
1:A:27:ARG:HH21	1:B:41:PHE:HB3	1.45	0.82
2:C:291:ILE:CG2	2:C:292:THR:N	2.42	0.82
1:A:30:VAL:HG23	2:C:324:ILE:O	1.80	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:251:THR:HG23	2:D:377:ILE:HD11	1.62	0.82
1:B:56:PHE:CD2	2:D:469:GLY:HA3	2.14	0.81
2:D:177:TYR:CD2	2:D:281:ARG:HG2	2.14	0.81
2:C:291:ILE:HG23	2:C:292:THR:N	1.92	0.81
2:C:196:LEU:CD1	2:C:258:ASN:HA	2.10	0.81
2:C:519:VAL:HG23	2:C:520:PHE:N	1.92	0.81
2:C:557:TYR:C	2:C:557:TYR:CD1	2.51	0.81
2:C:248:SER:O	2:C:377:ILE:HD11	1.79	0.81
2:C:474:ILE:HD11	2:C:478:MET:HB3	1.60	0.81
1:B:99:PHE:HB2	2:D:167:LEU:HD22	1.60	0.81
2:D:203:PHE:C	2:D:204:GLN:CA	2.48	0.81
2:C:365:PHE:HE2	2:C:406:LEU:HD12	1.45	0.81
2:C:544:THR:HG23	2:C:545:THR:N	1.96	0.81
1:A:84:LEU:HB3	2:C:384:LEU:CD2	2.10	0.81
2:C:541:THR:CB	2:C:543:ILE:CD1	2.58	0.81
2:D:528:LEU:O	2:D:531:ILE:HG23	1.80	0.81
1:A:77:THR:CG2	2:C:393:ARG:HH11	1.94	0.81
2:D:567:LEU:HD12	2:D:568:PRO:CD	2.11	0.81
2:D:559:ARG:CG	2:D:560:ASP:N	2.44	0.80
1:B:3:GLU:O	1:B:4:GLN:N	2.14	0.80
1:A:42:SER:HB2	2:C:161:ARG:HD2	1.64	0.80
2:D:175:MET:HB2	2:D:250:HIS:CE1	2.17	0.80
2:C:513:TRP:HE1	2:C:515:GLU:HB2	1.43	0.80
1:A:85:MET:HE1	2:C:533:LEU:HD21	1.64	0.80
2:C:177:TYR:CE2	2:C:281:ARG:HA	2.15	0.80
2:C:403:ARG:O	2:C:416:ASP:HA	1.81	0.80
2:C:346:LEU:HD12	2:C:353:MET:H	1.47	0.79
2:C:458:LEU:HD11	2:C:462:ARG:HE	1.44	0.79
1:A:99:PHE:HA	5:A:580:HEM:O2A	1.82	0.79
2:C:446:GLU:N	2:C:450:GLN:NE2	2.29	0.79
5:A:580:HEM:CMC	5:A:580:HEM:HBC2	2.10	0.79
1:A:30:VAL:HG21	2:C:323:ARG:CG	2.11	0.79
2:C:197:LEU:H	2:C:258:ASN:ND2	1.81	0.79
2:C:350:TYR:CD1	2:C:557:TYR:HE2	2.00	0.79
1:B:97:LEU:HB3	2:D:324:ILE:CD1	2.13	0.78
2:D:177:TYR:CE2	2:D:281:ARG:HG2	2.18	0.78
2:D:560:ASP:O	2:D:561:PHE:N	2.14	0.78
2:C:289:GLN:HE22	2:C:513:TRP:HA	1.46	0.78
1:B:66:ASN:HA	2:D:403:ARG:HH12	1.46	0.78
1:B:10:ILE:HG23	1:B:11:THR:HG22	1.65	0.78
2:C:244:PRO:HB2	2:C:343:MET:HE1	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:430:LEU:HD13	2:D:476:ILE:HD11	1.64	0.78
1:A:99:PHE:HB2	2:C:167:LEU:HD22	1.64	0.78
1:A:85:MET:CE	2:C:533:LEU:HD21	2.14	0.78
1:A:77:THR:O	2:C:391:LEU:HB3	1.83	0.78
2:C:522:MET:HA	2:C:525:ARG:HD3	1.65	0.78
2:D:130:ILE:HG21	2:D:137:ILE:CD1	2.12	0.78
2:C:519:VAL:CG2	2:C:520:PHE:N	2.47	0.77
2:C:195:GLY:O	2:C:196:LEU:HD13	1.85	0.77
2:D:187:LEU:HD12	2:D:234:LEU:HD21	1.65	0.77
2:C:330:ASN:O	2:C:333:ARG:HG2	1.84	0.77
2:C:467:GLN:CA	2:C:467:GLN:HE21	1.84	0.77
2:D:171:VAL:HG12	2:D:289:GLN:HG3	1.67	0.77
2:D:385:MET:CE	2:D:546:VAL:HA	2.15	0.77
1:B:16:ASN:ND2	1:B:19:SER:H	1.82	0.77
1:B:93:LEU:HD21	2:D:503:PHE:CZ	2.20	0.77
1:B:2:PRO:HB2	1:B:4:GLN:N	2.00	0.77
2:C:513:TRP:NE1	2:C:515:GLU:HB2	1.99	0.77
2:D:346:LEU:O	2:D:382:ARG:HD2	1.85	0.77
2:C:177:TYR:HE2	2:C:281:ARG:CA	1.97	0.77
2:C:365:PHE:CE2	2:C:406:LEU:HD12	2.19	0.77
2:C:417:LEU:HB3	2:C:418:PRO:HD3	1.67	0.77
2:D:320:VAL:HG13	2:D:509:GLY:CA	2.15	0.77
1:B:29:PHE:HE2	1:B:100:THR:HG23	1.50	0.77
1:B:3:GLU:O	1:B:4:GLN:CA	2.32	0.77
1:B:77:THR:HG21	2:D:393:ARG:NH1	1.99	0.77
2:C:136:ARG:NH1	2:C:414:GLY:O	2.18	0.77
2:D:557:TYR:HB3	2:D:558:PRO:CD	2.14	0.77
2:C:211:LEU:HD13	2:C:233:PHE:CG	2.20	0.76
2:C:330:ASN:HA	2:C:333:ARG:HD3	1.67	0.76
2:C:294:ARG:HG2	2:C:295:ASP:N	1.99	0.76
1:A:66:ASN:HA	2:C:403:ARG:HH12	1.48	0.76
2:C:176:VAL:HG23	2:C:177:TYR:CD1	2.21	0.76
2:C:347:ASP:N	2:C:353:MET:HG3	1.99	0.76
1:A:77:THR:HG21	2:C:393:ARG:HH11	1.47	0.76
2:D:320:VAL:CG1	2:D:509:GLY:HA2	2.14	0.76
2:D:223:LEU:HD13	2:D:223:LEU:N	1.99	0.76
5:A:580:HEM:C3A	2:C:333:ARG:HD2	2.21	0.76
1:B:94:ASP:CG	5:B:580:HEM:HMA3	2.06	0.76
2:D:247:THR:O	2:D:251:THR:HG22	1.86	0.76
3:G:2:NAG:O7	3:G:2:NAG:O3	2.01	0.76
2:D:381:LEU:HD12	2:D:384:LEU:CD1	2.15	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:102:GLU:HG2	2:C:147:PHE:HB2	1.68	0.76
5:A:580:HEM:HMD2	2:C:407:PHE:CZ	2.21	0.76
2:C:447:THR:HB	2:C:450:GLN:CG	2.01	0.75
2:C:434:ASN:HB2	2:C:472:ASN:HB3	1.68	0.75
2:D:229:ARG:C	2:D:230:ILE:HD13	2.06	0.75
2:D:445:PRO:O	2:D:471:PRO:HG2	1.87	0.75
2:D:118:SER:OG	2:D:120:VAL:HG12	1.87	0.75
3:J:1:NAG:O3	3:J:1:NAG:O7	2.04	0.75
2:C:289:GLN:O	2:C:292:THR:HG22	1.85	0.75
2:C:457:ASN:OD1	2:C:460:LEU:N	2.20	0.75
2:C:306:MET:HE3	2:C:310:LEU:CD2	2.08	0.75
2:D:123:PRO:O	2:D:125:CYS:N	2.20	0.75
2:D:528:LEU:O	2:D:531:ILE:HD13	1.87	0.75
2:C:175:MET:HB2	2:C:250:HIS:HE1	1.52	0.74
2:D:540:ASN:N	2:D:540:ASN:ND2	2.30	0.74
1:A:22:LEU:HD11	2:C:323:ARG:CD	2.13	0.74
1:B:87:MET:HG3	1:B:88:GLN:N	2.02	0.74
2:C:485:LEU:HD23	2:C:490:ARG:HD3	1.68	0.74
2:C:447:THR:CB	2:C:450:GLN:HG3	2.01	0.74
2:C:544:THR:CG2	2:C:545:THR:H	1.94	0.74
1:A:84:LEU:HD12	2:C:389:ALA:HA	1.67	0.74
1:A:66:ASN:ND2	2:C:403:ARG:HH22	1.85	0.74
1:A:95:HIS:CD2	2:C:239:ARG:HH21	2.06	0.74
2:C:256:GLU:HG3	2:C:260:LEU:HD22	1.68	0.74
2:C:338:LEU:O	2:C:390:LYS:HB3	1.87	0.74
2:C:399:VAL:CG2	2:C:400:ASP:N	2.51	0.74
2:C:196:LEU:HD12	2:C:258:ASN:HA	1.69	0.74
1:A:29:PHE:CE1	2:C:165:ASN:HB2	2.23	0.74
2:C:199:VAL:HG12	2:C:209:ALA:HB1	1.70	0.74
2:C:377:ILE:HD13	2:C:381:LEU:CD2	2.18	0.74
2:C:407:PHE:HD2	2:C:415:LEU:HD23	1.53	0.74
2:D:194:LEU:HB3	2:D:196:LEU:HD22	1.69	0.74
2:D:415:LEU:N	2:D:415:LEU:HD12	2.01	0.74
2:C:164:ILE:HD11	2:D:158:ILE:HD12	1.70	0.74
2:C:532:SER:C	2:C:534:PRO:HD2	2.08	0.73
2:D:332:PHE:CE1	2:D:334:TYR:HE1	2.06	0.73
2:D:224:THR:HG21	2:D:367:ALA:HB2	1.70	0.73
3:J:1:NAG:H61	3:J:2:NAG:N2	1.97	0.73
2:C:369:TRP:HB2	2:C:373:LEU:HD23	1.70	0.73
1:B:26:ASN:HD22	1:B:26:ASN:N	1.87	0.73
2:C:399:VAL:HG22	2:C:400:ASP:N	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:580:HEM:O1D	2:C:333:ARG:NH2	2.21	0.73
2:C:434:ASN:ND2	2:C:444:GLN:HB3	2.04	0.73
2:C:474:ILE:HD11	2:C:479:GLY:N	2.03	0.73
2:D:189:ASN:OD1	3:I:1:NAG:N2	2.22	0.73
2:D:278:GLN:O	2:D:281:ARG:HB2	1.89	0.73
1:B:64:VAL:HG21	2:D:422:MET:HE2	1.71	0.73
1:A:31:ARG:NH1	2:C:326:ASN:OD1	2.21	0.73
2:C:434:ASN:ND2	2:C:445:PRO:HD2	2.01	0.73
2:C:566:THR:O	2:C:567:LEU:HD13	1.88	0.73
2:D:221:CYS:HB3	2:D:366:PHE:O	1.88	0.73
2:D:171:VAL:HG11	2:D:289:GLN:HG3	1.69	0.73
1:B:94:ASP:OD2	5:B:580:HEM:CMA	2.31	0.73
2:C:136:ARG:CZ	2:C:414:GLY:O	2.35	0.73
2:D:540:ASN:H	2:D:540:ASN:HD22	1.33	0.73
1:B:66:ASN:HD22	2:D:403:ARG:NH1	1.87	0.73
2:C:164:ILE:HD11	2:D:158:ILE:CD1	2.18	0.73
2:C:252:LEU:HD11	2:C:537:ILE:HA	1.71	0.73
2:C:296:TYR:O	2:C:300:VAL:HG12	1.89	0.73
2:C:251:THR:HG23	2:C:377:ILE:HD11	1.71	0.73
2:C:497:CYS:O	2:C:501:THR:HG23	1.88	0.73
1:A:94:ASP:OD1	5:A:580:HEM:CMA	2.37	0.73
1:B:99:PHE:CB	2:D:167:LEU:HD13	2.19	0.73
2:C:264:LEU:CB	2:C:276:LEU:HD11	2.19	0.72
2:C:311:PRO:O	2:C:507:ARG:NH2	2.16	0.72
2:C:446:GLU:C	2:C:450:GLN:HE21	1.93	0.72
2:D:335:GLY:HA2	2:D:338:LEU:HD22	1.70	0.72
1:B:64:VAL:HG21	2:D:422:MET:CE	2.20	0.72
1:A:42:SER:HB2	2:C:161:ARG:CD	2.19	0.72
1:A:15:ASN:HD21	2:C:511:ARG:H	1.37	0.72
2:D:465:MET:HE3	2:D:470:THR:HA	1.69	0.72
5:A:580:HEM:HMD3	2:C:406:LEU:HD21	1.72	0.72
1:B:103:PRO:C	1:B:104:ALA:O	2.27	0.72
1:B:39:ASP:HB3	1:B:41:PHE:CD1	2.25	0.72
1:A:99:PHE:HB2	2:C:167:LEU:CD2	2.20	0.72
1:B:65:SER:HA	1:B:69:VAL:HG13	1.72	0.72
2:D:557:TYR:C	2:D:558:PRO:C	2.46	0.72
2:C:169:SER:HB3	2:C:324:ILE:HD12	1.72	0.72
2:C:345:ARG:NH2	2:C:374:GLU:OE1	2.23	0.71
2:D:287:MET:O	2:D:291:ILE:HG13	1.89	0.71
2:C:153:CYS:SG	2:C:156:SER:HB2	2.31	0.71
2:C:447:THR:CG2	2:C:449:GLY:H	2.02	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:29:PHE:CE2	1:B:100:THR:HG23	2.25	0.71
2:D:365:PHE:O	2:D:409:GLN:NE2	2.23	0.71
2:D:454:VAL:HG12	2:D:455:LEU:N	2.05	0.71
1:A:53:ARG:HD2	2:C:473:ASN:HB2	1.72	0.71
2:C:223:LEU:HD23	2:C:410:VAL:HG23	1.71	0.71
1:A:99:PHE:CB	2:C:167:LEU:HD13	2.19	0.71
1:A:9:THR:OG1	1:A:10:ILE:N	2.23	0.71
2:C:423:GLN:HE21	2:C:423:GLN:HA	1.54	0.71
2:C:572:LEU:O	2:C:575:TRP:HB2	1.91	0.71
2:C:337:THR:O	2:C:390:LYS:HE3	1.91	0.71
2:D:321:ASP:OD2	2:D:323:ARG:NH1	2.24	0.71
2:C:131:PRO:HB2	2:C:132:PRO:CD	2.20	0.71
2:D:385:MET:HE3	2:D:546:VAL:HG22	1.73	0.71
1:A:10:ILE:HG21	2:C:181:GLU:HG3	1.70	0.70
2:C:248:SER:O	2:C:251:THR:HG23	1.91	0.70
2:C:260:LEU:O	2:C:264:LEU:HD22	1.91	0.70
1:B:15:ASN:HD21	2:D:511:ARG:H	1.37	0.70
2:D:557:TYR:CA	2:D:558:PRO:N	2.53	0.70
2:D:572:LEU:HA	2:D:575:TRP:CE3	2.25	0.70
2:C:131:PRO:HD2	2:C:134:ASP:OD2	1.91	0.70
2:D:244:PRO:O	2:D:247:THR:HG22	1.91	0.70
1:B:16:ASN:C	1:B:16:ASN:HD22	1.94	0.70
2:C:380:ILE:O	2:C:384:LEU:HB2	1.91	0.70
2:C:415:LEU:HD13	2:C:415:LEU:N	2.06	0.70
2:D:416:ASP:HB3	2:D:419:ALA:HB3	1.74	0.70
1:A:97:LEU:HB3	2:C:324:ILE:HD11	1.73	0.70
2:C:350:TYR:CB	2:C:557:TYR:CE2	2.74	0.70
2:C:533:LEU:O	2:C:537:ILE:HG22	1.92	0.70
2:D:257:HIS:O	2:D:258:ASN:ND2	2.22	0.70
2:C:562:VAL:HG23	2:C:563:ASN:N	2.06	0.70
2:D:257:HIS:O	2:D:257:HIS:ND1	2.24	0.70
2:D:571:ASN:HD22	2:D:573:ALA:H	1.40	0.70
1:A:66:ASN:HA	2:C:403:ARG:NH1	2.07	0.70
1:B:77:THR:CG2	2:D:396:GLN:HE22	2.05	0.70
2:D:224:THR:HG23	2:D:409:GLN:OE1	1.91	0.70
1:A:29:PHE:CE2	1:A:100:THR:HG22	2.26	0.70
1:B:4:GLN:HA	1:B:4:GLN:HE21	1.57	0.70
2:C:282:LYS:HG2	2:C:520:PHE:CZ	2.27	0.70
1:B:26:ASN:HD22	1:B:26:ASN:H	1.37	0.69
1:B:45:TYR:CE2	1:B:53:ARG:HA	2.27	0.69
2:C:350:TYR:CG	2:C:557:TYR:CE2	2.80	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:428:HIS:O	2:D:430:LEU:N	2.25	0.69
2:C:128:LEU:N	2:C:128:LEU:HD12	2.07	0.69
2:C:337:THR:O	2:C:390:LYS:HG2	1.91	0.69
2:C:534:PRO:CG	2:C:551:ILE:HD11	2.21	0.69
1:B:79:ASP:OD2	2:D:490:ARG:NH1	2.25	0.69
5:A:580:HEM:HAA2	2:C:333:ARG:NH1	2.07	0.69
1:B:85:MET:CG	1:B:85:MET:O	2.40	0.69
2:C:130:ILE:HG21	2:C:137:ILE:CD1	2.22	0.69
2:D:130:ILE:HD11	2:D:139:ASN:O	1.92	0.69
2:C:442:LEU:HD22	2:C:442:LEU:H	1.55	0.69
2:C:126:PHE:O	2:C:146:PHE:HB3	1.92	0.69
2:C:181:GLU:N	2:C:182:PRO:HD2	2.04	0.69
2:C:223:LEU:CD2	2:C:410:VAL:HG23	2.23	0.69
2:D:535:ARG:HG3	2:D:535:ARG:O	1.93	0.69
1:B:13:MET:HG3	1:B:14:CYS:N	1.97	0.69
5:A:580:HEM:HMA1	2:C:329:THR:O	1.92	0.69
1:A:77:THR:HB	2:C:393:ARG:NH1	2.08	0.69
5:A:580:HEM:HAC	2:C:242:GLU:OE2	1.91	0.69
1:A:66:ASN:ND2	2:C:403:ARG:NH1	2.28	0.69
1:B:16:ASN:ND2	1:B:18:ARG:N	2.41	0.69
2:C:229:ARG:C	2:C:230:ILE:HD13	2.13	0.69
2:D:200:ASN:ND2	2:D:203:PHE:H	1.91	0.69
1:A:84:LEU:O	1:A:87:MET:N	2.26	0.69
2:C:342:PHE:CE1	2:C:358:ARG:HD3	2.28	0.69
2:C:549:ASN:ND2	2:C:550:ASN:H	1.90	0.69
2:D:237:ASP:OD2	2:D:239:ARG:HG2	1.92	0.69
1:A:66:ASN:HD22	2:C:403:ARG:HH12	0.78	0.69
2:D:428:HIS:O	2:D:430:LEU:HG	1.93	0.69
5:A:580:HEM:HBB2	5:A:580:HEM:CHC	2.17	0.69
1:A:29:PHE:CZ	1:A:100:THR:HG22	2.28	0.69
1:B:5:ASP:OD1	1:B:5:ASP:N	2.26	0.69
1:B:71:PHE:CZ	1:B:76:LEU:HD12	2.25	0.69
1:A:68:ILE:HD12	2:C:464:LEU:HD13	1.75	0.69
2:D:415:LEU:H	2:D:415:LEU:CD1	2.06	0.69
2:C:309:TYR:O	2:C:311:PRO:HD2	1.92	0.68
1:A:44:PRO:HB2	2:C:126:PHE:CZ	2.29	0.68
2:C:197:LEU:N	2:C:258:ASN:HD21	1.92	0.68
2:C:335:GLY:HA2	2:C:338:LEU:HD22	1.75	0.68
2:D:251:THR:O	2:D:255:ARG:HG3	1.91	0.68
1:A:99:PHE:CD1	2:C:239:ARG:NH1	2.62	0.68
2:C:200:ASN:HD21	2:C:213:PHE:HE1	1.40	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:370:ARG:HG3	2:C:374:GLU:OE1	1.93	0.68
2:C:197:LEU:N	2:C:258:ASN:ND2	2.41	0.68
2:C:434:ASN:HB2	2:C:472:ASN:CB	2.23	0.68
1:A:5:ASP:OD1	1:A:5:ASP:N	2.25	0.68
1:A:6:LYS:C	1:A:7:TYR:CD1	2.67	0.68
2:C:248:SER:OG	2:C:381:LEU:HD22	1.94	0.68
2:C:262:THR:O	2:C:265:LYS:HB3	1.93	0.68
1:B:66:ASN:HD22	2:D:403:ARG:HH12	1.40	0.67
2:C:350:TYR:CD2	2:C:557:TYR:HD2	2.13	0.67
2:C:136:ARG:NH2	2:C:414:GLY:O	2.27	0.67
1:A:94:ASP:OD1	5:A:580:HEM:HMA3	1.94	0.67
2:C:382:ARG:HA	2:C:385:MET:HE2	1.76	0.67
2:C:434:ASN:HD22	2:C:444:GLN:HB3	1.59	0.67
2:C:229:ARG:O	2:C:231:PRO:HD3	1.93	0.67
2:C:330:ASN:HD22	2:C:333:ARG:HD3	1.59	0.67
2:C:368:SER:O	2:C:372:VAL:HG23	1.94	0.67
5:B:580:HEM:CBC	2:D:242:GLU:OE1	2.42	0.67
2:D:251:THR:HG23	2:D:377:ILE:CD1	2.25	0.67
2:D:521:SER:O	2:D:525:ARG:HG2	1.94	0.67
2:C:228:ALA:HB2	3:G:1:NAG:H61	1.75	0.67
2:C:193:GLN:NE2	2:C:273:GLY:H	1.91	0.67
1:A:30:VAL:HG22	2:C:323:ARG:HG3	1.76	0.67
2:C:345:ARG:HA	2:C:379:PRO:O	1.94	0.67
2:C:164:ILE:CD1	2:D:158:ILE:HD12	2.25	0.67
1:A:77:THR:CB	2:C:393:ARG:HH11	2.07	0.67
2:D:362:SER:HA	2:D:365:PHE:CE2	2.29	0.67
1:B:94:ASP:OD1	5:B:580:HEM:HMA2	1.95	0.67
2:C:123:PRO:HB2	2:C:124:PRO:HD3	1.76	0.67
1:A:71:PHE:HD1	1:A:72:PRO:HD2	1.59	0.66
2:C:142:ASP:OD1	2:C:143:CYS:N	2.28	0.66
2:D:434:ASN:ND2	2:D:444:GLN:HB3	2.09	0.66
2:C:382:ARG:HA	2:C:385:MET:CE	2.25	0.66
2:C:304:THR:O	2:C:307:ARG:N	2.27	0.66
2:C:523:GLN:OE1	2:C:523:GLN:N	2.28	0.66
1:A:7:TYR:CD2	2:C:278:GLN:HB3	2.30	0.66
2:C:415:LEU:H	2:C:415:LEU:CD2	2.00	0.66
2:D:256:GLU:OE2	2:D:259:ARG:HD3	1.95	0.66
1:A:16:ASN:HD22	1:A:19:SER:H	1.41	0.66
2:C:297:LEU:HA	2:C:300:VAL:HG11	1.76	0.66
1:B:19:SER:HB3	1:B:22:LEU:HD13	1.77	0.66
2:C:114:ASN:OD1	2:C:115:CYS:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:282:LYS:HB3	2:C:520:PHE:HZ	1.60	0.66
1:B:44:PRO:HD3	2:D:148:ARG:NH2	2.11	0.66
2:D:197:LEU:N	2:D:258:ASN:HD21	1.89	0.66
2:D:347:ASP:O	2:D:382:ARG:HD3	1.96	0.66
1:A:84:LEU:O	1:A:86:PHE:N	2.29	0.66
1:B:3:GLU:N	1:B:4:GLN:N	2.42	0.66
2:C:370:ARG:NE	2:C:374:GLU:OE1	2.27	0.66
2:D:492:GLY:O	2:D:496:ALA:HB2	1.96	0.66
2:C:196:LEU:HD11	2:C:258:ASN:HA	1.77	0.66
2:C:325:ALA:H	2:C:502:GLN:HE22	1.42	0.65
2:C:442:LEU:HB2	2:C:443:PRO:CD	2.22	0.65
1:B:45:TYR:HE2	1:B:53:ARG:HA	1.59	0.65
2:C:393:ARG:CG	2:C:396:GLN:NE2	2.58	0.65
1:B:97:LEU:HB3	2:D:324:ILE:HD11	1.77	0.65
2:C:244:PRO:HB2	2:C:343:MET:CE	2.25	0.65
2:D:381:LEU:HD12	2:D:384:LEU:HD12	1.77	0.65
5:B:580:HEM:HMD3	2:D:406:LEU:HD21	1.77	0.65
1:A:97:LEU:HB3	2:C:324:ILE:CD1	2.27	0.65
2:D:523:GLN:H	2:D:523:GLN:HE21	1.44	0.65
2:D:523:GLN:N	2:D:523:GLN:HE21	1.94	0.65
1:B:94:ASP:OD1	5:B:580:HEM:CMA	2.45	0.65
2:C:350:TYR:CD1	2:C:557:TYR:CE2	2.84	0.65
2:C:378:ASP:HB2	2:C:379:PRO:HD3	1.79	0.65
2:C:350:TYR:CG	2:C:557:TYR:CD2	2.85	0.65
2:D:348:ASN:C	2:D:350:TYR:H	1.97	0.65
2:C:254:LEU:HG	2:C:254:LEU:O	1.88	0.65
2:C:434:ASN:HD21	2:C:445:PRO:CD	2.02	0.65
2:D:311:PRO:O	2:D:507:ARG:NH2	2.30	0.65
2:C:404:GLU:O	2:C:405:ARG:HD3	1.96	0.65
2:C:507:ARG:HD2	2:C:508:ASP:OD1	1.97	0.65
2:D:347:ASP:OD1	2:D:351:GLN:N	2.29	0.65
3:I:2:NAG:O7	3:I:2:NAG:O3	2.08	0.65
2:C:144:ILE:CD1	2:C:416:ASP:H	2.11	0.64
1:A:31:ARG:NH1	2:C:162:ASN:HD22	1.92	0.64
1:A:31:ARG:HH11	2:C:162:ASN:HD21	1.44	0.64
2:C:221:CYS:CB	2:C:366:PHE:HB3	2.25	0.64
1:A:71:PHE:CD2	2:C:396:GLN:HA	2.33	0.64
2:C:556:SER:O	2:C:561:PHE:CE1	2.50	0.64
2:D:405:ARG:HH11	2:D:405:ARG:CG	2.10	0.64
2:C:433:TYR:CD1	2:C:494:LEU:HD22	2.33	0.64
2:D:479:GLY:O	2:D:483:GLU:HG3	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:220:PRO:HA	2:D:223:LEU:HD22	1.79	0.64
1:A:66:ASN:ND2	2:C:403:ARG:NH2	2.46	0.64
2:C:478:MET:HE3	2:C:481:VAL:CG2	2.28	0.64
1:A:87:MET:SD	2:C:339:ILE:HG22	2.38	0.64
2:D:216:LEU:N	2:D:216:LEU:HD22	2.08	0.64
2:C:321:ASP:CG	2:C:323:ARG:HD3	2.18	0.64
1:B:4:GLN:HE21	1:B:17:ARG:NH2	1.73	0.64
1:A:10:ILE:HG21	2:C:181:GLU:CG	2.27	0.64
2:C:346:LEU:CA	2:C:353:MET:HB2	2.27	0.63
2:C:383:GLY:O	2:C:387:THR:HG22	1.98	0.63
5:B:580:HEM:HAC	2:D:406:LEU:HD11	1.79	0.63
2:D:546:VAL:HG13	2:D:547:SER:N	2.13	0.63
1:B:15:ASN:O	2:D:511:ARG:NE	2.26	0.63
2:C:177:TYR:OH	2:C:284:VAL:HG11	1.98	0.63
2:C:364:VAL:HG13	2:C:364:VAL:O	1.98	0.63
2:D:392:ASN:C	2:D:392:ASN:OD1	2.35	0.63
2:D:362:SER:O	2:D:409:GLN:HG2	1.99	0.63
1:B:16:ASN:HD21	1:B:19:SER:H	1.45	0.63
1:B:4:GLN:HA	1:B:4:GLN:NE2	2.12	0.63
1:B:88:GLN:OE1	1:B:88:GLN:HA	1.98	0.63
2:C:240:SER:HB2	2:C:250:HIS:HD2	1.62	0.63
2:C:382:ARG:HB2	2:C:385:MET:CE	2.28	0.63
2:D:453:THR:HG22	2:D:454:VAL:N	2.11	0.63
2:D:565:SER:C	2:D:567:LEU:H	1.99	0.63
2:C:139:ASN:HD22	2:C:139:ASN:C	2.02	0.63
2:C:144:ILE:HD12	2:C:416:ASP:H	1.62	0.63
2:C:220:PRO:HB3	2:C:410:VAL:HG21	1.79	0.63
2:C:527:ALA:O	2:C:530:GLN:HB2	1.98	0.63
2:D:165:ASN:HD22	2:D:166:ALA:N	1.96	0.63
2:C:249:MET:HE2	2:C:381:LEU:HD11	1.80	0.63
2:C:428:HIS:N	2:C:428:HIS:CD2	2.63	0.63
2:D:465:MET:CE	2:D:471:PRO:HD3	2.21	0.63
2:C:256:GLU:OE2	2:C:260:LEU:HD11	1.98	0.63
2:C:291:ILE:HD11	2:C:533:LEU:HB2	1.80	0.63
2:C:535:ARG:HD2	2:C:568:PRO:O	1.99	0.63
2:D:313:TYR:HD1	2:D:507:ARG:HD3	1.62	0.63
1:A:30:VAL:HG13	2:C:323:ARG:CZ	2.29	0.63
2:D:465:MET:HE1	2:D:471:PRO:CD	2.25	0.63
1:A:7:TYR:CE1	2:C:279:GLU:OE2	2.52	0.62
2:D:171:VAL:HG12	2:D:171:VAL:O	1.98	0.62
1:A:59:ALA:O	2:C:426:ARG:NH2	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:33:LEU:HD22	2:D:436:TRP:CZ3	2.35	0.62
2:C:251:THR:O	2:C:254:LEU:HB3	1.98	0.62
2:D:132:PRO:HD2	2:D:133:ASN:OD1	2.00	0.62
2:D:200:ASN:ND2	2:D:203:PHE:N	2.47	0.62
1:B:9:THR:HG21	1:B:13:MET:H	1.65	0.62
2:C:177:TYR:HH	2:C:284:VAL:HG11	1.64	0.62
5:B:580:HEM:C3C	2:D:242:GLU:OE2	2.52	0.62
2:D:364:VAL:O	2:D:364:VAL:HG23	1.95	0.62
5:B:580:HEM:HAC	2:D:406:LEU:CD1	2.29	0.62
2:D:434:ASN:HD21	2:D:445:PRO:HD2	1.64	0.62
2:C:264:LEU:HB3	2:C:276:LEU:HD11	1.79	0.62
2:C:458:LEU:CD1	2:C:462:ARG:HE	2.10	0.62
2:D:192:ASN:ND2	2:D:194:LEU:HD22	2.14	0.62
2:D:445:PRO:CG	2:D:451:LEU:HD13	2.29	0.62
1:B:29:PHE:HE2	1:B:100:THR:CG2	2.12	0.62
2:C:283:ILE:O	2:C:287:MET:HG2	2.00	0.62
2:D:355:PRO:O	2:D:356:ASN:HB2	1.98	0.62
2:D:390:LYS:HG3	2:D:390:LYS:O	1.97	0.62
2:D:385:MET:HE3	2:D:547:SER:H	1.65	0.62
2:D:570:LEU:HD23	2:D:571:ASN:H	1.64	0.62
1:A:99:PHE:CB	2:C:167:LEU:HD22	2.29	0.62
2:C:544:THR:CG2	2:C:545:THR:HG22	2.27	0.62
2:D:136:ARG:HE	2:D:404:GLU:CB	2.07	0.62
2:D:519:VAL:CG2	2:D:520:PHE:N	2.62	0.62
1:B:13:MET:O	1:B:20:PRO:O	2.17	0.62
2:C:557:TYR:HB2	2:C:561:PHE:CD1	2.34	0.62
2:C:303:PRO:HD2	2:C:304:THR:HG22	1.82	0.62
2:C:303:PRO:O	2:C:306:MET:CB	2.46	0.62
2:D:326:ASN:HD21	2:D:428:HIS:HB3	1.64	0.62
1:A:87:MET:HE1	1:A:88:GLN:HE22	1.65	0.61
1:B:71:PHE:CD2	2:D:396:GLN:HB3	2.35	0.61
2:C:131:PRO:HB2	2:C:132:PRO:HD2	1.82	0.61
2:C:264:LEU:HB2	2:C:276:LEU:HD11	1.80	0.61
2:D:219:ASP:HB3	2:D:222:LEU:HD23	1.80	0.61
2:C:123:PRO:O	2:C:124:PRO:C	2.35	0.61
1:B:99:PHE:HB2	2:D:167:LEU:CD2	2.30	0.61
1:B:53:ARG:N	1:B:56:PHE:O	2.33	0.61
1:A:98:ASP:C	2:C:167:LEU:HD22	2.21	0.61
2:C:260:LEU:HD21	2:C:287:MET:HE1	1.82	0.61
2:C:407:PHE:HD2	2:C:415:LEU:CD2	2.12	0.61
2:C:548:LYS:CG	2:C:560:ASP:O	2.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:79:ASP:OD2	1:B:82:ARG:HB2	2.01	0.61
2:C:290:ILE:HD12	2:C:514:TRP:CZ2	2.36	0.61
2:C:430:LEU:CD1	2:C:476:ILE:HD11	2.30	0.61
2:C:501:THR:O	2:C:505:LYS:HG3	2.00	0.61
2:D:544:THR:HG23	2:D:545:THR:HG23	1.81	0.61
2:C:269:PRO:O	2:C:271:TRP:N	2.34	0.61
2:C:393:ARG:HG3	2:C:396:GLN:HE21	1.62	0.61
2:C:468:TYR:O	2:C:470:THR:N	2.32	0.61
2:C:249:MET:HE2	2:C:381:LEU:CD1	2.30	0.61
1:B:98:ASP:OD1	5:B:580:HEM:HBA1	2.01	0.61
2:C:262:THR:HG22	2:C:263:GLU:N	2.16	0.61
2:C:361:LEU:HB2	2:C:401:GLU:HG2	1.82	0.60
2:D:533:LEU:O	2:D:537:ILE:HG23	2.00	0.60
2:D:524:GLN:HG2	2:D:575:TRP:CE2	2.36	0.60
2:C:251:THR:HG23	2:C:377:ILE:CD1	2.31	0.60
2:C:350:TYR:CB	2:C:557:TYR:CD2	2.84	0.60
2:C:490:ARG:O	2:C:491:VAL:HG23	2.02	0.60
2:D:187:LEU:CD1	2:D:234:LEU:HD21	2.31	0.60
1:B:30:VAL:HG12	1:B:31:ARG:N	2.14	0.60
2:C:121:GLN:HG3	2:C:127:PRO:HD2	1.84	0.60
2:C:350:TYR:CG	2:C:557:TYR:HE2	2.20	0.60
2:C:300:VAL:HG22	2:C:300:VAL:O	2.00	0.60
2:C:524:GLN:CA	2:C:524:GLN:HE21	2.13	0.60
2:C:306:MET:CE	2:C:310:LEU:HD23	2.13	0.60
2:D:128:LEU:CB	2:D:144:ILE:HG12	2.30	0.60
2:D:248:SER:HA	2:D:251:THR:HG22	1.82	0.60
2:D:405:ARG:HH11	2:D:405:ARG:HG3	1.67	0.60
2:C:181:GLU:N	2:C:182:PRO:HD3	2.14	0.60
2:D:179:SER:CA	2:D:180:GLU:N	2.63	0.60
2:D:244:PRO:HB2	2:D:343:MET:HE3	1.83	0.60
2:C:543:ILE:H	2:C:543:ILE:HD13	1.66	0.60
2:D:138:LYS:O	2:D:138:LYS:HG2	2.00	0.60
2:D:415:LEU:HD23	2:D:420:LEU:HD21	1.83	0.60
1:A:65:SER:O	2:C:403:ARG:NH1	2.35	0.60
2:C:186:ASN:O	2:C:187:LEU:HD12	2.01	0.60
2:C:365:PHE:HE2	2:C:406:LEU:CD1	2.13	0.60
2:C:183:LEU:CD1	2:C:187:LEU:HD11	2.32	0.59
2:C:256:GLU:HG2	2:C:287:MET:CE	2.32	0.59
2:C:418:PRO:HB3	2:C:477:TRP:CH2	2.37	0.59
1:B:100:THR:HG21	2:D:428:HIS:CE1	2.27	0.59
1:B:1:CYS:O	1:B:2:PRO:O	2.20	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:220:PRO:O	2:C:223:LEU:HB2	2.02	0.59
2:C:309:TYR:O	2:C:310:LEU:HD13	2.02	0.59
2:C:516:ASN:C	2:C:517:GLU:HA	2.22	0.59
2:C:136:ARG:HH12	2:C:414:GLY:N	2.00	0.59
2:D:256:GLU:OE2	2:D:259:ARG:NH1	2.33	0.59
2:D:267:LEU:O	2:D:269:PRO:HD3	2.02	0.59
2:D:332:PHE:HE1	2:D:334:TYR:HE1	1.50	0.59
1:A:53:ARG:HD2	2:C:473:ASN:CB	2.32	0.59
2:D:345:ARG:HH22	2:D:374:GLU:CD	2.06	0.59
2:D:478:MET:O	2:D:482:SER:HB3	2.02	0.59
1:B:16:ASN:HD21	1:B:18:ARG:N	1.99	0.59
2:C:193:GLN:HE22	2:C:273:GLY:H	1.48	0.59
1:B:62:ARG:NH2	2:D:134:ASP:OD2	2.33	0.59
2:C:533:LEU:N	2:C:534:PRO:CD	2.66	0.59
2:D:362:SER:HA	2:D:365:PHE:HE2	1.68	0.59
2:D:545:THR:HG22	2:D:563:ASN:HA	1.85	0.59
1:A:75:GLN:O	2:C:396:GLN:OE1	2.20	0.59
5:B:580:HEM:NB	2:D:336:HIS:NE2	2.51	0.59
2:C:229:ARG:O	2:C:230:ILE:HD13	2.02	0.59
2:C:375:GLY:O	2:C:379:PRO:HG2	2.03	0.59
2:C:458:LEU:HD11	2:C:462:ARG:NE	2.16	0.59
5:B:580:HEM:HMC3	2:D:243:MET:SD	2.43	0.59
2:C:327:VAL:HG23	2:C:476:ILE:CD1	2.32	0.59
2:C:486:LYS:HD3	2:C:493:PRO:HD3	1.82	0.59
2:C:399:VAL:CG2	2:C:400:ASP:H	2.14	0.58
2:C:516:ASN:CA	2:C:517:GLU:N	2.65	0.58
2:D:326:ASN:ND2	2:D:430:LEU:HD21	2.17	0.58
1:B:10:ILE:CG2	1:B:11:THR:HG22	2.34	0.58
2:C:243:MET:HB3	2:C:245:GLU:HG2	1.85	0.58
2:C:405:ARG:HG3	2:C:408:GLU:CD	2.23	0.58
2:C:560:ASP:O	2:C:561:PHE:N	2.36	0.58
2:D:128:LEU:HB2	2:D:144:ILE:HG12	1.85	0.58
2:D:157:ASN:HB3	2:D:158:ILE:HG23	1.85	0.58
2:D:381:LEU:HD23	2:D:541:THR:HG21	1.85	0.58
2:C:457:ASN:OD1	2:C:460:LEU:HD12	2.03	0.58
2:D:437:ARG:NH1	2:D:443:PRO:O	2.37	0.58
2:D:328:PHE:CZ	2:D:332:PHE:CD2	2.91	0.58
2:D:460:LEU:HG	2:D:464:LEU:HD22	1.86	0.58
1:B:97:LEU:HB3	2:D:324:ILE:HD13	1.83	0.58
2:C:244:PRO:HA	2:C:247:THR:HG22	1.85	0.58
2:C:175:MET:HB2	2:C:250:HIS:CE1	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:328:PHE:HB2	2:C:502:GLN:HE21	1.69	0.58
2:D:430:LEU:CD1	2:D:476:ILE:HD11	2.33	0.58
2:D:434:ASN:HA	2:D:437:ARG:HB2	1.84	0.58
2:C:187:LEU:HD12	2:C:187:LEU:N	2.15	0.58
2:C:280:ALA:O	2:C:284:VAL:HG12	2.04	0.58
2:D:502:GLN:O	2:D:502:GLN:HG3	2.03	0.58
1:B:83:SER:O	1:B:86:PHE:HB3	2.03	0.58
2:D:355:PRO:O	2:D:356:ASN:CB	2.52	0.58
2:D:395:ASN:CB	2:D:396:GLN:HG3	2.34	0.58
2:D:439:PHE:O	3:E:2:NAG:O3	2.21	0.58
2:D:258:ASN:O	2:D:262:THR:HB	2.03	0.57
2:D:174:SER:O	2:D:177:TYR:O	2.22	0.57
1:B:29:PHE:HB3	2:D:326:ASN:HB2	1.86	0.57
2:D:497:CYS:O	2:D:501:THR:OG1	2.16	0.57
1:B:16:ASN:C	1:B:16:ASN:ND2	2.57	0.57
2:C:128:LEU:CD1	2:C:146:PHE:HB2	2.35	0.57
2:C:345:ARG:O	2:C:346:LEU:HD13	2.04	0.57
2:C:436:TRP:HA	2:C:439:PHE:HB3	1.84	0.57
2:D:177:TYR:OH	2:D:257:HIS:CD2	2.58	0.57
1:A:74:ASP:OD1	1:A:74:ASP:N	2.28	0.57
1:B:66:ASN:HA	2:D:403:ARG:NH1	2.18	0.57
2:D:162:ASN:HD22	2:D:163:GLN:H	1.52	0.57
1:A:6:LYS:HE3	2:C:282:LYS:NZ	2.20	0.57
2:C:460:LEU:HD22	2:C:464:LEU:HD22	1.85	0.57
2:D:179:SER:O	2:D:180:GLU:HA	2.05	0.57
2:D:297:LEU:N	2:D:298:PRO:HD2	2.19	0.57
2:C:168:THR:HG23	2:C:179:SER:HB2	1.85	0.57
2:C:474:ILE:CD1	2:C:478:MET:HB3	2.33	0.57
2:D:572:LEU:HA	2:D:575:TRP:HE3	1.68	0.57
1:B:94:ASP:CG	5:B:580:HEM:CMA	2.73	0.57
2:C:130:ILE:HG23	2:C:142:ASP:O	2.05	0.57
2:C:418:PRO:HB3	2:C:477:TRP:CZ3	2.39	0.57
2:D:248:SER:HA	2:D:251:THR:CG2	2.35	0.57
3:I:1:NAG:H61	3:I:2:NAG:O6	2.05	0.57
2:C:131:PRO:CB	2:C:132:PRO:CD	2.83	0.57
2:C:205:ASP:HB2	2:C:210:LEU:HD13	1.85	0.57
2:C:244:PRO:CD	2:C:364:VAL:HG13	2.35	0.57
2:D:370:ARG:O	2:D:374:GLU:HB3	2.04	0.57
2:D:433:TYR:CE1	2:D:437:ARG:CG	2.88	0.57
1:A:77:THR:HB	2:C:393:ARG:HH11	1.68	0.56
1:A:93:LEU:HD23	2:C:296:TYR:HE2	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:321:ASP:OD2	2:C:323:ARG:NH1	2.33	0.56
2:D:177:TYR:OH	2:D:257:HIS:HD2	1.88	0.56
1:A:84:LEU:HB3	2:C:384:LEU:HD23	1.84	0.56
2:D:174:SER:O	2:D:176:VAL:N	2.37	0.56
2:D:291:ILE:HD13	2:D:533:LEU:HB2	1.87	0.56
1:B:4:GLN:HE22	1:B:17:ARG:CZ	2.18	0.56
2:C:162:ASN:ND2	2:C:163:GLN:H	2.04	0.56
2:C:351:GLN:HB3	2:C:352:PRO:CD	2.34	0.56
2:C:410:VAL:HG22	2:C:410:VAL:O	2.05	0.56
2:C:422:MET:CE	2:C:478:MET:HB2	2.36	0.56
2:D:209:ALA:O	2:D:255:ARG:NH2	2.39	0.56
2:D:251:THR:CG2	2:D:377:ILE:HD11	2.32	0.56
2:D:309:TYR:O	2:D:504:ARG:HD3	2.05	0.56
1:A:82:ARG:HB3	2:C:552:PHE:O	2.06	0.56
1:A:89:TRP:O	1:A:93:LEU:HB2	2.04	0.56
2:C:230:ILE:HG13	2:C:369:TRP:HA	1.87	0.56
2:D:350:TYR:HB2	2:D:557:TYR:CZ	2.41	0.56
2:C:244:PRO:CG	2:C:343:MET:HE3	2.34	0.56
2:C:556:SER:O	2:C:561:PHE:HE1	1.88	0.56
1:B:36:GLU:CD	2:D:431:PRO:HB3	2.25	0.56
1:B:47:TRP:HD1	1:B:48:THR:HG23	1.71	0.56
5:B:580:HEM:HHC	5:B:580:HEM:CBB	2.28	0.56
2:C:351:GLN:CB	2:C:352:PRO:CD	2.83	0.56
2:D:247:THR:HG21	2:D:371:VAL:HG21	1.88	0.56
2:C:362:SER:OG	2:C:363:ARG:NH1	2.38	0.56
2:D:566:THR:O	2:D:567:LEU:HD13	2.06	0.56
2:C:262:THR:O	2:C:265:LYS:N	2.39	0.56
2:D:399:VAL:HG22	2:D:401:GLU:H	1.70	0.56
2:D:465:MET:O	2:D:468:TYR:O	2.24	0.56
2:C:288:VAL:O	2:C:291:ILE:HG22	2.05	0.56
2:C:380:ILE:C	2:C:382:ARG:N	2.56	0.56
2:C:532:SER:CB	2:C:534:PRO:HD2	2.35	0.56
2:D:321:ASP:OD1	2:D:323:ARG:HG2	2.06	0.56
2:D:395:ASN:HB3	2:D:396:GLN:HG3	1.86	0.56
5:A:580:HEM:C4A	2:C:333:ARG:HB3	2.41	0.56
2:C:234:LEU:HG	2:C:235:ALA:N	2.20	0.56
2:C:326:ASN:O	2:C:329:THR:HB	2.06	0.56
2:C:248:SER:OG	2:C:377:ILE:HG12	2.06	0.55
2:C:400:ASP:O	2:C:402:ILE:N	2.39	0.55
2:C:433:TYR:HD1	2:C:494:LEU:HD22	1.70	0.55
1:B:103:PRO:HD2	2:D:148:ARG:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:434:ASN:ND2	2:D:444:GLN:CB	2.68	0.55
1:A:27:ARG:NH2	1:B:41:PHE:CB	2.68	0.55
5:A:580:HEM:CBB	5:A:580:HEM:HHC	2.22	0.55
2:C:177:TYR:CD2	2:C:281:ARG:HD2	2.41	0.55
2:C:177:TYR:CD2	2:C:281:ARG:HG3	2.41	0.55
2:C:345:ARG:C	2:C:346:LEU:HD13	2.26	0.55
2:C:348:ASN:CA	2:C:382:ARG:NH2	2.55	0.55
2:C:400:ASP:HA	2:C:403:ARG:HB3	1.87	0.55
2:C:468:TYR:CD1	2:C:474:ILE:HA	2.42	0.55
2:D:548:LYS:HB3	2:D:562:VAL:HG22	1.88	0.55
3:J:1:NAG:C7	3:J:1:NAG:HO3	2.14	0.55
1:A:88:GLN:OE1	1:A:91:GLN:NE2	2.40	0.55
2:C:123:PRO:O	2:C:125:CYS:N	2.39	0.55
2:C:256:GLU:HG2	2:C:287:MET:HE3	1.88	0.55
1:B:95:HIS:CE1	2:D:239:ARG:HG3	2.41	0.55
2:D:308:LYS:HD3	2:D:309:TYR:CZ	2.41	0.55
2:D:137:ILE:HD12	2:D:413:ILE:HD11	1.87	0.55
2:C:240:SER:CB	2:C:250:HIS:CD2	2.87	0.55
2:C:382:ARG:CA	2:C:385:MET:HE2	2.36	0.55
2:C:361:LEU:O	2:C:401:GLU:HG3	2.07	0.55
5:B:580:HEM:C4C	2:D:242:GLU:OE2	2.60	0.55
1:A:88:GLN:HG3	1:A:88:GLN:O	2.05	0.55
2:C:305:ALA:O	2:C:309:TYR:N	2.37	0.55
2:D:519:VAL:HG23	2:D:520:PHE:N	2.20	0.55
1:A:77:THR:CB	2:C:393:ARG:NH1	2.67	0.55
2:C:123:PRO:HB2	2:C:124:PRO:CD	2.36	0.55
2:C:244:PRO:HG2	2:C:343:MET:HE3	1.89	0.55
2:C:399:VAL:HG22	2:C:401:GLU:H	1.72	0.55
5:A:580:HEM:CMD	2:C:407:PHE:CZ	2.88	0.55
2:C:480:GLY:C	2:C:495:LEU:HD22	2.27	0.55
2:C:296:TYR:HB2	2:C:552:PHE:CE2	2.41	0.55
2:C:264:LEU:HD11	2:C:572:LEU:HB3	1.88	0.55
2:C:208:ARG:NH2	2:C:542:GLY:CA	2.70	0.55
2:C:522:MET:CB	2:C:523:GLN:OE1	2.55	0.55
2:C:299:LEU:HD21	2:C:550:ASN:ND2	2.22	0.55
2:D:199:VAL:HG13	2:D:209:ALA:HB1	1.87	0.55
2:D:355:PRO:O	2:D:356:ASN:ND2	2.40	0.55
2:D:433:TYR:CE1	2:D:494:LEU:HD22	2.42	0.55
1:A:81:GLU:C	1:A:82:ARG:HG2	2.26	0.55
1:B:83:SER:OG	2:D:551:ILE:O	2.17	0.55
2:C:256:GLU:HG3	2:C:260:LEU:CD2	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:7:TYR:OH	2:D:279:GLU:OE1	2.24	0.55
2:C:534:PRO:HG3	2:C:551:ILE:CD1	2.27	0.55
2:D:279:GLU:O	2:D:283:ILE:HD12	2.07	0.55
2:D:345:ARG:NH2	2:D:374:GLU:HG2	2.22	0.55
2:C:347:ASP:OD1	2:C:351:GLN:N	2.40	0.54
2:C:415:LEU:HD22	2:C:415:LEU:N	2.18	0.54
2:C:474:ILE:CD1	2:C:479:GLY:N	2.69	0.54
2:D:165:ASN:C	2:D:165:ASN:HD22	2.10	0.54
1:B:56:PHE:CG	2:D:469:GLY:HA3	2.41	0.54
2:C:363:ARG:N	2:C:363:ARG:CD	2.69	0.54
2:D:353:MET:HG2	2:D:355:PRO:HD3	1.89	0.54
2:C:181:GLU:H	2:C:182:PRO:HD3	1.72	0.54
2:C:345:ARG:HH22	2:C:374:GLU:CD	2.11	0.54
2:C:534:PRO:HA	2:C:537:ILE:HG23	1.88	0.54
2:D:447:THR:HG22	2:D:449:GLY:N	2.10	0.54
1:A:13:MET:O	1:A:20:PRO:O	2.26	0.54
2:C:183:LEU:HD12	2:C:187:LEU:HD11	1.88	0.54
2:C:495:LEU:HA	2:C:498:ILE:HG22	1.89	0.54
1:A:94:ASP:OD2	5:A:580:HEM:HMA3	2.07	0.54
1:B:41:PHE:CD1	1:B:41:PHE:N	2.76	0.54
2:D:480:GLY:O	2:D:495:LEU:HD22	2.08	0.54
2:C:114:ASN:OD1	2:C:116:GLU:N	2.41	0.54
2:C:244:PRO:HG2	2:C:364:VAL:HG22	1.89	0.54
2:D:203:PHE:C	2:D:204:GLN:HA	2.27	0.54
2:D:272:ASP:O	2:D:276:LEU:HB2	2.08	0.54
2:C:114:ASN:OD1	2:C:114:ASN:C	2.45	0.54
2:C:282:LYS:HB3	2:C:520:PHE:CZ	2.42	0.54
2:D:278:GLN:O	2:D:281:ARG:N	2.41	0.54
2:C:197:LEU:HD22	2:C:257:HIS:CG	2.43	0.54
2:C:249:MET:CE	2:C:381:LEU:HD11	2.37	0.54
2:C:519:VAL:CG2	2:C:520:PHE:H	2.19	0.54
2:D:326:ASN:ND2	2:D:326:ASN:O	2.26	0.54
2:D:523:GLN:H	2:D:523:GLN:NE2	2.04	0.54
2:D:567:LEU:O	2:D:568:PRO:O	2.26	0.54
3:J:1:NAG:O3	3:J:1:NAG:C7	2.54	0.54
1:B:93:LEU:HD21	2:D:503:PHE:HZ	1.71	0.54
2:D:181:GLU:HB2	2:D:182:PRO:HD3	1.89	0.54
2:D:557:TYR:C	2:D:559:ARG:N	2.61	0.54
1:A:22:LEU:HD12	1:A:23:GLY:N	2.23	0.54
1:A:72:PRO:O	1:A:74:ASP:N	2.41	0.54
1:A:94:ASP:CG	5:A:580:HEM:HMA3	2.29	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:157:ASN:OD1	2:C:158:ILE:HG23	2.08	0.54
2:C:304:THR:HG23	2:C:305:ALA:H	1.72	0.54
5:A:580:HEM:CMC	2:C:339:ILE:HD12	2.38	0.54
2:C:461:ALA:O	2:C:465:MET:HB2	2.08	0.54
2:C:534:PRO:O	2:C:537:ILE:HG23	2.08	0.54
5:A:580:HEM:CBC	5:A:580:HEM:HMC2	2.27	0.53
2:C:136:ARG:HH12	2:C:414:GLY:HA3	1.69	0.53
2:C:361:LEU:HB3	2:C:401:GLU:HG3	1.89	0.53
2:D:326:ASN:HD22	2:D:326:ASN:C	2.11	0.53
1:A:21:THR:O	1:A:24:ALA:HB3	2.09	0.53
5:B:580:HEM:HBB2	5:B:580:HEM:CHC	2.21	0.53
2:C:347:ASP:N	2:C:353:MET:CG	2.70	0.53
1:A:66:ASN:CA	2:C:403:ARG:HH12	2.19	0.53
2:D:200:ASN:ND2	2:D:202:ARG:H	2.06	0.53
2:D:267:LEU:CD1	2:D:268:ASN:HD21	2.14	0.53
2:D:486:LYS:HB2	2:D:491:VAL:O	2.08	0.53
2:C:286:ALA:O	2:C:290:ILE:HG22	2.08	0.53
2:C:146:PHE:CE2	2:C:424:ARG:NH1	2.76	0.53
2:D:439:PHE:CG	2:D:439:PHE:O	2.60	0.53
2:D:559:ARG:CG	2:D:560:ASP:HB3	2.38	0.53
2:C:213:PHE:CE2	2:C:231:PRO:CD	2.86	0.53
2:D:251:THR:HG21	2:D:377:ILE:HG13	1.89	0.53
2:D:416:ASP:O	2:D:419:ALA:HB3	2.09	0.53
1:A:84:LEU:C	1:A:86:PHE:N	2.60	0.53
2:C:377:ILE:HD13	2:C:381:LEU:HD22	1.91	0.53
2:C:422:MET:HE2	2:C:478:MET:HB2	1.91	0.53
2:C:423:GLN:HE21	2:C:423:GLN:CA	2.17	0.53
2:D:417:LEU:HB3	2:D:418:PRO:HD3	1.91	0.53
2:C:290:ILE:HD11	2:C:529:ALA:HA	1.91	0.53
2:C:428:HIS:N	2:C:428:HIS:HD2	2.04	0.53
2:C:470:THR:OG1	2:C:471:PRO:HD2	2.09	0.53
1:B:14:CYS:O	2:D:511:ARG:NH2	2.42	0.53
2:C:136:ARG:NH2	2:C:413:ILE:HG12	2.24	0.53
2:C:570:LEU:HD13	2:C:572:LEU:HD11	1.90	0.53
5:A:580:HEM:CAC	2:C:242:GLU:CD	2.77	0.53
2:C:193:GLN:HE22	2:C:272:ASP:HB2	1.72	0.53
2:C:391:LEU:HD12	2:C:392:ASN:N	2.24	0.53
2:C:446:GLU:CA	2:C:450:GLN:NE2	2.72	0.53
1:B:45:TYR:CE2	1:B:53:ARG:HG3	2.43	0.53
2:C:220:PRO:CB	2:C:410:VAL:HG21	2.38	0.53
2:C:293:TYR:CD2	2:C:513:TRP:HZ3	2.27	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:327:VAL:O	2:D:330:ASN:N	2.26	0.53
2:D:354:GLU:O	2:D:356:ASN:ND2	2.42	0.53
1:A:71:PHE:CZ	2:C:396:GLN:HG2	2.43	0.52
1:B:19:SER:CB	1:B:22:LEU:HD13	2.39	0.52
2:C:287:MET:O	2:C:290:ILE:HG22	2.09	0.52
2:C:350:TYR:CD2	2:C:557:TYR:CD2	2.96	0.52
2:C:571:ASN:C	2:C:573:ALA:N	2.60	0.52
2:D:223:LEU:HB2	2:D:410:VAL:HG22	1.91	0.52
2:D:533:LEU:N	2:D:534:PRO:HD2	2.23	0.52
2:C:330:ASN:HD22	2:C:333:ARG:CD	2.21	0.52
2:C:446:GLU:N	2:C:450:GLN:HE21	2.06	0.52
1:B:82:ARG:NH2	2:D:299:LEU:HD12	2.24	0.52
2:D:224:THR:CG2	2:D:369:TRP:HE1	2.22	0.52
1:A:11:THR:HG23	1:A:13:MET:H	1.74	0.52
1:A:71:PHE:HD1	1:A:72:PRO:CD	2.21	0.52
2:D:167:LEU:N	2:D:167:LEU:CD1	2.71	0.52
2:D:560:ASP:N	2:D:561:PHE:N	2.56	0.52
1:A:66:ASN:ND2	2:C:403:ARG:CZ	2.72	0.52
1:A:96:ASP:OD2	2:C:172:ASP:O	2.28	0.52
2:C:177:TYR:HD2	2:C:281:ARG:CD	2.22	0.52
2:C:300:VAL:HG23	2:C:334:TYR:OH	2.09	0.52
2:C:415:LEU:HB3	2:C:420:LEU:CD1	2.30	0.52
2:D:216:LEU:H	2:D:216:LEU:CD2	2.14	0.52
1:A:72:PRO:HG2	1:A:75:GLN:OE1	2.10	0.52
1:A:79:ASP:HB2	2:C:391:LEU:HB2	1.90	0.52
1:B:26:ASN:ND2	1:B:26:ASN:N	2.56	0.52
2:C:381:LEU:O	2:C:385:MET:HE2	2.10	0.52
2:C:416:ASP:OD1	2:C:418:PRO:HD2	2.10	0.52
1:A:27:ARG:NH2	1:B:41:PHE:CG	2.77	0.52
1:B:60:LEU:HB3	1:B:63:ALA:HB2	1.91	0.52
2:C:259:ARG:NH2	2:C:539:ASP:HB3	2.24	0.52
2:C:260:LEU:HD21	2:C:287:MET:CE	2.40	0.52
2:C:430:LEU:HD12	2:C:476:ILE:HD11	1.92	0.52
1:A:5:ASP:OD2	2:C:511:ARG:NH2	2.41	0.52
2:C:128:LEU:N	2:C:128:LEU:CD1	2.72	0.52
2:C:139:ASN:HD22	2:C:141:ALA:N	2.01	0.52
2:C:248:SER:HA	2:C:251:THR:CG2	2.40	0.52
2:C:342:PHE:CE1	2:C:358:ARG:CD	2.93	0.52
2:C:521:SER:OG	2:C:523:GLN:HB2	2.10	0.52
2:D:497:CYS:SG	2:D:498:ILE:N	2.82	0.52
2:C:165:ASN:ND2	2:C:166:ALA:N	2.58	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:369:TRP:HB2	2:C:373:LEU:CD2	2.39	0.52
2:D:378:ASP:O	2:D:379:PRO:C	2.47	0.52
1:A:41:PHE:H	1:A:41:PHE:HD1	1.58	0.52
2:C:301:LEU:HG	2:C:305:ALA:HB3	1.91	0.52
2:C:361:LEU:CB	2:C:401:GLU:HG2	2.40	0.52
2:C:524:GLN:HG3	2:C:575:TRP:CZ3	2.45	0.52
2:D:203:PHE:O	2:D:204:GLN:HA	2.09	0.52
2:D:416:ASP:O	2:D:420:LEU:HD12	2.10	0.52
2:C:139:ASN:HD21	2:C:141:ALA:HB3	1.75	0.52
2:C:348:ASN:HD22	2:C:348:ASN:N	2.01	0.52
2:D:157:ASN:C	2:D:158:ILE:CG2	2.79	0.52
2:D:143:CYS:O	2:D:413:ILE:HD13	2.10	0.52
1:A:38:GLU:OE2	1:A:48:THR:OG1	2.27	0.51
2:C:211:LEU:HB2	2:C:233:PHE:HB3	1.93	0.51
2:C:197:LEU:HD22	2:C:257:HIS:ND1	2.25	0.51
2:C:293:TYR:CD2	2:C:513:TRP:CZ3	2.98	0.51
2:C:399:VAL:HG23	2:C:400:ASP:H	1.75	0.51
2:D:222:LEU:C	2:D:223:LEU:HD13	2.30	0.51
1:B:87:MET:SD	2:D:339:ILE:HG22	2.49	0.51
2:D:423:GLN:HA	2:D:426:ARG:HD3	1.92	0.51
2:D:533:LEU:HB3	2:D:551:ILE:HD11	1.92	0.51
2:C:327:VAL:O	2:C:330:ASN:N	2.39	0.51
2:C:430:LEU:HD13	2:C:476:ILE:HD11	1.90	0.51
2:D:347:ASP:OD1	2:D:351:GLN:HB2	2.10	0.51
2:D:440:CYS:O	2:D:442:LEU:HD13	2.11	0.51
2:C:196:LEU:HD11	2:C:258:ASN:CA	2.41	0.51
2:C:290:ILE:HG23	2:C:291:ILE:N	2.25	0.51
2:D:240:SER:HA	2:D:246:LEU:HD13	1.91	0.51
1:B:71:PHE:CE2	2:D:396:GLN:HB3	2.46	0.51
2:D:433:TYR:CE1	2:D:437:ARG:HG2	2.46	0.51
2:D:446:GLU:H	2:D:450:GLN:NE2	2.08	0.51
1:B:68:ILE:CG2	2:D:460:LEU:HD11	2.39	0.51
1:A:95:HIS:HA	2:C:239:ARG:NH2	2.26	0.51
2:C:541:THR:OG1	2:C:543:ILE:CD1	2.59	0.51
1:B:62:ARG:NE	2:D:134:ASP:OD1	2.43	0.51
2:D:136:ARG:NE	2:D:404:GLU:HB3	2.10	0.51
2:D:417:LEU:O	2:D:420:LEU:N	2.44	0.51
2:C:209:ALA:O	2:C:210:LEU:HD12	2.11	0.51
2:C:244:PRO:CG	2:C:364:VAL:HG22	2.41	0.51
2:C:300:VAL:O	2:C:300:VAL:CG2	2.58	0.51
2:C:348:ASN:ND2	2:C:348:ASN:N	2.51	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:482:SER:O	2:C:482:SER:OG	2.26	0.51
2:D:408:GLU:C	2:D:410:VAL:N	2.64	0.51
1:A:91:GLN:O	1:A:95:HIS:HB2	2.11	0.51
1:B:87:MET:SD	5:B:580:HEM:CBB	2.91	0.51
2:C:197:LEU:H	2:C:258:ASN:HD22	1.55	0.51
2:C:391:LEU:HD12	2:C:392:ASN:H	1.74	0.51
2:C:208:ARG:NH2	2:C:542:GLY:HA3	2.26	0.51
2:C:571:ASN:HD22	2:C:573:ALA:CB	2.22	0.51
2:D:128:LEU:HD23	2:D:144:ILE:HD11	1.92	0.51
1:B:9:THR:OG1	1:B:10:ILE:N	2.41	0.51
2:C:165:ASN:ND2	2:C:165:ASN:C	2.63	0.51
2:C:165:ASN:HD22	2:C:166:ALA:N	2.07	0.51
2:C:196:LEU:HD12	2:C:258:ASN:HD22	1.75	0.51
2:C:268:ASN:HB2	2:C:271:TRP:CD2	2.45	0.51
2:D:128:LEU:HD22	2:D:144:ILE:CG1	2.40	0.51
2:D:200:ASN:HD22	2:D:203:PHE:H	1.56	0.51
2:D:300:VAL:CG1	2:D:334:TYR:OH	2.59	0.51
1:A:17:ARG:HH11	2:C:511:ARG:NH1	2.09	0.51
2:C:446:GLU:CA	2:C:450:GLN:HE21	2.23	0.51
2:C:556:SER:O	2:C:560:ASP:CB	2.59	0.51
2:D:436:TRP:CE3	2:D:436:TRP:HA	2.45	0.51
1:B:22:LEU:HD23	2:D:322:PRO:CD	2.41	0.51
2:C:397:ILE:HG22	2:C:398:ALA:N	2.26	0.51
2:C:537:ILE:O	2:C:543:ILE:HD11	2.11	0.51
5:B:580:HEM:O2D	2:D:424:ARG:NH1	2.45	0.51
2:D:181:GLU:CD	2:D:181:GLU:H	2.14	0.50
2:D:247:THR:HG22	2:D:248:SER:N	2.26	0.50
2:D:494:LEU:O	2:D:498:ILE:HB	2.11	0.50
1:A:99:PHE:HB2	2:C:239:ARG:HH12	1.74	0.50
1:A:79:ASP:CG	2:C:490:ARG:HH12	2.14	0.50
2:C:533:LEU:HD12	2:C:536:ILE:HB	1.92	0.50
2:C:549:ASN:ND2	2:C:550:ASN:N	2.58	0.50
1:A:32:TRP:CE2	2:C:325:ALA:HB2	2.47	0.50
2:C:442:LEU:N	2:C:442:LEU:HD22	2.21	0.50
1:A:15:ASN:ND2	2:C:511:ARG:H	2.07	0.50
2:D:205:ASP:OD1	2:D:205:ASP:O	2.30	0.50
2:D:257:HIS:NE2	2:D:277:TYR:CD1	2.80	0.50
2:D:345:ARG:HH22	2:D:374:GLU:CG	2.24	0.50
2:C:136:ARG:HH22	2:C:414:GLY:C	2.14	0.50
2:C:468:TYR:CE1	2:C:474:ILE:HA	2.46	0.50
2:C:534:PRO:HA	2:C:537:ILE:CG2	2.40	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:350:TYR:CE2	2:D:561:PHE:CZ	3.00	0.50
2:D:440:CYS:O	2:D:442:LEU:N	2.44	0.50
1:A:41:PHE:N	1:A:41:PHE:CD1	2.79	0.50
2:C:445:PRO:O	2:C:471:PRO:HG2	2.12	0.50
2:D:244:PRO:HB2	2:D:343:MET:CE	2.41	0.50
2:C:144:ILE:HD12	2:C:416:ASP:N	2.26	0.50
2:C:146:PHE:CZ	2:C:423:GLN:HG3	2.46	0.50
2:C:476:ILE:O	2:C:480:GLY:N	2.38	0.50
2:D:417:LEU:HB3	2:D:418:PRO:CD	2.41	0.50
1:B:85:MET:CE	2:D:249:MET:SD	3.00	0.50
2:C:175:MET:HG2	2:C:176:VAL:N	2.26	0.50
2:C:270:ARG:HH11	2:C:270:ARG:CG	2.25	0.50
2:C:343:MET:SD	2:C:364:VAL:HG21	2.52	0.50
2:D:114:ASN:HD22	2:D:117:THR:HB	1.76	0.50
5:B:580:HEM:CBC	2:D:242:GLU:CD	2.81	0.50
1:B:44:PRO:CB	2:D:126:PHE:CE2	2.94	0.50
2:C:177:TYR:HE2	2:C:281:ARG:CB	2.25	0.50
2:C:247:THR:O	2:C:251:THR:HG22	2.12	0.50
2:C:382:ARG:CA	2:C:385:MET:CE	2.88	0.50
2:D:297:LEU:O	2:D:298:PRO:C	2.49	0.50
5:A:580:HEM:HMC1	2:C:339:ILE:HD12	1.94	0.49
2:C:351:GLN:CB	2:C:352:PRO:HD2	2.27	0.49
2:C:380:ILE:C	2:C:382:ARG:H	2.15	0.49
2:D:165:ASN:ND2	2:D:167:LEU:H	2.08	0.49
2:D:200:ASN:ND2	2:D:202:ARG:N	2.59	0.49
2:D:491:VAL:HG22	2:D:495:LEU:HB3	1.93	0.49
1:B:10:ILE:HG23	1:B:11:THR:N	2.26	0.49
2:C:177:TYR:CE2	2:C:281:ARG:CB	2.95	0.49
2:C:334:TYR:CG	2:C:335:GLY:N	2.80	0.49
2:C:382:ARG:CB	2:C:385:MET:CE	2.91	0.49
2:C:385:MET:CE	2:C:537:ILE:HD11	2.41	0.49
1:A:81:GLU:O	2:C:553:MET:HG2	2.12	0.49
1:B:39:ASP:HB3	1:B:41:PHE:H	1.78	0.49
2:C:224:THR:HG21	2:C:369:TRP:HE1	1.77	0.49
2:D:293:TYR:HA	2:D:297:LEU:HD23	1.94	0.49
2:D:233:PHE:CE2	2:D:368:SER:HB3	2.48	0.49
2:D:136:ARG:HH21	2:D:404:GLU:HA	1.77	0.49
2:D:447:THR:HG22	2:D:448:VAL:N	2.27	0.49
5:A:580:HEM:HAC	2:C:406:LEU:HD11	1.93	0.49
1:B:47:TRP:CD1	1:B:48:THR:HG23	2.47	0.49
2:C:177:TYR:OH	2:C:257:HIS:CD2	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:414:GLY:O	2:C:415:LEU:C	2.48	0.49
2:D:361:LEU:O	2:D:365:PHE:CE2	2.66	0.49
2:D:524:GLN:O	2:D:527:ALA:HB3	2.13	0.49
2:D:350:TYR:CZ	2:D:561:PHE:CE2	3.00	0.49
1:A:87:MET:HE1	1:A:88:GLN:NE2	2.25	0.49
1:B:16:ASN:ND2	1:B:18:ARG:H	2.09	0.49
2:C:136:ARG:CG	2:C:137:ILE:HG22	2.28	0.49
2:C:187:LEU:CD1	2:C:187:LEU:N	2.76	0.49
2:D:130:ILE:HD12	2:D:137:ILE:CD1	2.42	0.49
2:D:455:LEU:O	2:D:456:ARG:HB2	2.13	0.49
1:A:9:THR:HG23	1:A:12:GLY:HA2	1.94	0.49
2:C:378:ASP:N	2:C:379:PRO:HD2	2.28	0.49
1:A:69:VAL:O	1:A:69:VAL:HG23	2.13	0.49
2:C:247:THR:HG23	2:C:248:SER:N	2.28	0.49
2:C:347:ASP:CA	2:C:353:MET:HG3	2.41	0.49
1:B:62:ARG:HE	2:D:134:ASP:CG	2.16	0.49
1:B:44:PRO:HD3	2:D:148:ARG:CZ	2.41	0.49
2:D:557:TYR:O	2:D:558:PRO:CA	2.59	0.49
2:C:229:ARG:C	2:C:231:PRO:HD3	2.32	0.49
2:C:297:LEU:HA	2:C:300:VAL:HG12	1.92	0.49
2:C:434:ASN:ND2	2:C:444:GLN:HA	2.28	0.49
2:D:385:MET:CE	2:D:546:VAL:HG22	2.41	0.49
2:D:560:ASP:HA	2:D:561:PHE:N	2.23	0.49
1:A:30:VAL:CG1	2:C:323:ARG:CZ	2.91	0.49
1:A:37:TYR:CE1	2:C:429:GLY:HA3	2.48	0.49
2:C:433:TYR:HD1	2:C:494:LEU:CD2	2.24	0.49
2:C:452:GLY:O	2:C:453:THR:C	2.51	0.49
2:D:565:SER:C	2:D:567:LEU:N	2.65	0.49
2:C:131:PRO:CB	2:C:132:PRO:HD3	2.43	0.49
2:C:220:PRO:HD2	2:C:232:CYS:SG	2.52	0.49
2:C:395:ASN:O	2:C:396:GLN:HG3	2.13	0.49
2:C:434:ASN:HD21	2:C:444:GLN:HA	1.78	0.49
2:D:378:ASP:O	2:D:380:ILE:N	2.46	0.49
2:C:284:VAL:O	2:C:287:MET:N	2.46	0.48
1:A:89:TRP:CZ2	2:C:291:ILE:HG21	2.48	0.48
2:C:556:SER:O	2:C:561:PHE:CD1	2.65	0.48
2:C:571:ASN:ND2	2:C:573:ALA:HB2	2.28	0.48
2:D:422:MET:HG2	2:D:475:ASP:OD2	2.12	0.48
2:D:521:SER:OG	2:D:524:GLN:NE2	2.46	0.48
2:D:554:SER:CA	2:D:560:ASP:OD1	2.61	0.48
1:A:98:ASP:OD1	5:A:580:HEM:HBA1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:130:ILE:CG2	2:C:137:ILE:HD11	2.37	0.48
2:C:216:LEU:HD11	2:C:219:ASP:HA	1.95	0.48
2:C:329:THR:O	2:C:333:ARG:HD3	2.12	0.48
2:C:136:ARG:HH22	2:C:414:GLY:N	2.12	0.48
2:C:546:VAL:O	2:C:561:PHE:HB3	2.12	0.48
2:D:297:LEU:O	2:D:301:LEU:HB2	2.13	0.48
1:B:87:MET:CE	2:D:339:ILE:HG22	2.43	0.48
2:C:230:ILE:CG2	2:C:372:VAL:HG21	2.22	0.48
2:C:382:ARG:HA	2:C:385:MET:HB2	1.94	0.48
1:A:84:LEU:C	1:A:86:PHE:H	2.16	0.48
2:C:220:PRO:HA	2:C:223:LEU:HD22	1.95	0.48
2:D:147:PHE:N	2:D:147:PHE:CD1	2.81	0.48
2:D:247:THR:CG2	2:D:248:SER:N	2.72	0.48
1:A:86:PHE:CD1	2:C:552:PHE:HB3	2.48	0.48
1:A:93:LEU:HD23	2:C:296:TYR:CE2	2.48	0.48
1:B:37:TYR:O	1:B:45:TYR:HE1	1.97	0.48
2:C:175:MET:O	2:C:236:GLY:HA3	2.14	0.48
2:C:297:LEU:N	2:C:298:PRO:CD	2.76	0.48
1:A:77:THR:HG22	2:C:396:GLN:OE1	2.13	0.48
2:D:116:GLU:HA	2:D:145:PRO:HB3	1.96	0.48
1:B:84:LEU:HD13	2:D:389:ALA:HA	1.95	0.48
2:C:127:PRO:C	2:C:128:LEU:HD12	2.34	0.48
2:C:571:ASN:HD22	2:C:573:ALA:HB2	1.77	0.48
2:D:131:PRO:C	2:D:133:ASN:H	2.17	0.48
2:D:197:LEU:O	2:D:199:VAL:HG23	2.14	0.48
2:D:330:ASN:HD21	2:D:477:TRP:HB2	1.78	0.48
2:C:221:CYS:SG	2:C:232:CYS:N	2.87	0.48
5:A:580:HEM:CAA	2:C:333:ARG:NH1	2.75	0.48
2:C:478:MET:HE3	2:C:481:VAL:HG21	1.95	0.48
2:C:533:LEU:O	2:C:536:ILE:N	2.47	0.48
2:D:157:ASN:C	2:D:158:ILE:HG23	2.34	0.48
2:D:300:VAL:HG11	2:D:334:TYR:OH	2.13	0.48
2:D:434:ASN:ND2	2:D:445:PRO:HD2	2.28	0.48
2:D:465:MET:HE3	2:D:470:THR:CA	2.41	0.48
2:D:482:SER:O	2:D:482:SER:OG	2.31	0.48
2:D:483:GLU:HB3	2:D:484:PRO:HD2	1.95	0.48
1:A:96:ASP:OD1	2:C:174:SER:OG	2.32	0.48
1:A:62:ARG:HH21	2:C:136:ARG:HG2	1.72	0.48
2:C:136:ARG:HH12	2:C:414:GLY:C	2.18	0.48
2:C:244:PRO:HG2	2:C:343:MET:CE	2.43	0.48
2:C:383:GLY:O	2:C:387:THR:CG2	2.60	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:490:ARG:HA	2:D:490:ARG:HD3	1.60	0.48
1:B:71:PHE:C	1:B:71:PHE:CD1	2.86	0.48
2:C:177:TYR:HH	2:C:257:HIS:HB2	1.79	0.48
1:A:7:TYR:CZ	2:C:279:GLU:OE2	2.67	0.48
2:C:338:LEU:HD12	2:C:338:LEU:HA	1.47	0.48
2:C:437:ARG:O	2:C:442:LEU:HD23	2.13	0.48
2:C:556:SER:HB2	2:C:560:ASP:CG	2.33	0.48
2:C:544:THR:O	2:C:564:CYS:SG	2.71	0.48
1:B:85:MET:HE1	2:D:249:MET:SD	2.54	0.48
1:B:60:LEU:HB3	1:B:63:ALA:CB	2.44	0.47
2:C:486:LYS:HD2	2:C:486:LYS:HA	1.51	0.47
2:C:521:SER:HG	2:C:524:GLN:H	1.61	0.47
1:A:82:ARG:HA	2:C:553:MET:HA	1.95	0.47
1:B:18:ARG:HH21	2:D:318:ASP:HB3	1.79	0.47
5:B:580:HEM:O1D	2:D:424:ARG:HG3	2.13	0.47
2:D:433:TYR:O	2:D:433:TYR:CG	2.67	0.47
2:D:457:ASN:HD22	2:D:457:ASN:HA	1.40	0.47
2:D:471:PRO:HA	2:D:474:ILE:HD12	1.96	0.47
1:A:22:LEU:HA	1:A:22:LEU:HD13	1.61	0.47
2:C:177:TYR:CD2	2:C:281:ARG:CG	2.97	0.47
2:C:244:PRO:HD3	2:C:364:VAL:HG13	1.95	0.47
2:C:533:LEU:N	2:C:534:PRO:HD2	2.29	0.47
2:C:417:LEU:HB3	2:C:418:PRO:CD	2.40	0.47
2:D:433:TYR:CD1	2:D:494:LEU:HD22	2.49	0.47
2:C:262:THR:CG2	2:C:263:GLU:N	2.76	0.47
2:C:424:ARG:HD3	2:C:424:ARG:HA	1.63	0.47
2:D:340:GLN:HB2	2:D:340:GLN:HE21	1.53	0.47
2:D:493:PRO:O	2:D:497:CYS:HB3	2.14	0.47
2:D:385:MET:CE	2:D:546:VAL:CG2	2.92	0.47
1:B:9:THR:HG21	1:B:13:MET:N	2.29	0.47
1:A:29:PHE:CZ	2:C:165:ASN:HB2	2.49	0.47
2:C:177:TYR:OH	2:C:284:VAL:CG1	2.62	0.47
2:C:338:LEU:HD13	2:C:338:LEU:N	2.29	0.47
2:C:562:VAL:HG23	2:C:566:THR:OG1	2.14	0.47
1:B:96:ASP:OD2	2:D:172:ASP:O	2.32	0.47
2:D:199:VAL:CG1	2:D:209:ALA:HB1	2.44	0.47
2:D:571:ASN:O	2:D:575:TRP:HZ3	1.98	0.47
1:A:99:PHE:CB	2:C:167:LEU:CD1	2.90	0.47
1:B:9:THR:CG2	1:B:13:MET:H	2.26	0.47
2:C:177:TYR:CE2	2:C:281:ARG:HG3	2.49	0.47
2:C:180:GLU:C	2:C:182:PRO:HD2	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:234:LEU:O	2:C:235:ALA:HB2	2.15	0.47
1:A:87:MET:HE1	2:C:243:MET:CE	2.44	0.47
2:C:433:TYR:O	2:C:437:ARG:HB2	2.15	0.47
2:C:437:ARG:HD3	2:C:443:PRO:O	2.15	0.47
2:C:513:TRP:CD1	2:C:515:GLU:HB2	2.49	0.47
2:C:350:TYR:CE2	2:C:561:PHE:CE2	3.03	0.47
2:D:435:ALA:O	2:D:438:ARG:HB3	2.15	0.47
1:A:29:PHE:HE2	1:A:100:THR:HG22	1.77	0.47
1:A:1:CYS:SG	1:A:20:PRO:HB3	2.55	0.47
1:A:41:PHE:HD2	1:B:27:ARG:HH22	1.61	0.47
2:C:211:LEU:HD12	2:C:211:LEU:H	1.79	0.47
2:C:177:TYR:OH	2:C:257:HIS:HB2	2.15	0.47
2:C:221:CYS:HB2	2:C:366:PHE:O	2.15	0.47
1:A:44:PRO:CB	2:C:126:PHE:CE2	2.97	0.47
2:C:139:ASN:ND2	2:C:141:ALA:N	2.55	0.47
2:C:199:VAL:CG1	2:C:209:ALA:HB1	2.43	0.47
1:A:32:TRP:CZ2	2:C:325:ALA:HB2	2.50	0.47
1:B:64:VAL:O	1:B:64:VAL:HG23	2.12	0.47
2:C:541:THR:HG1	2:C:543:ILE:HD11	1.79	0.47
2:C:541:THR:OG1	2:C:543:ILE:HD11	2.14	0.47
1:A:13:MET:O	1:A:13:MET:SD	2.73	0.47
2:C:214:ASP:OD1	2:C:215:ASN:N	2.43	0.47
2:C:267:LEU:HD12	2:C:268:ASN:ND2	2.30	0.47
2:C:269:PRO:C	2:C:271:TRP:H	2.18	0.47
2:C:282:LYS:CG	2:C:520:PHE:CZ	2.97	0.47
2:C:356:ASN:HA	2:C:356:ASN:HD22	1.36	0.47
2:D:225:ASN:OD1	2:D:369:TRP:CE2	2.68	0.47
2:C:267:LEU:HD12	2:C:267:LEU:O	2.14	0.47
2:C:249:MET:CE	2:C:381:LEU:CD1	2.93	0.47
2:C:387:THR:O	2:C:387:THR:HG23	2.15	0.47
2:C:556:SER:O	2:C:560:ASP:HB3	2.14	0.47
2:D:295:ASP:HB2	2:D:552:PHE:HE2	1.81	0.47
2:D:310:LEU:HD11	2:D:504:ARG:HA	1.97	0.47
1:A:56:PHE:CD1	2:C:469:GLY:HA3	2.49	0.46
2:C:559:ARG:CG	2:C:560:ASP:N	2.78	0.46
2:D:353:MET:HG2	2:D:355:PRO:CD	2.44	0.46
2:D:350:TYR:HB2	2:D:557:TYR:CE1	2.50	0.46
1:A:41:PHE:N	1:A:41:PHE:HD1	2.12	0.46
2:C:457:ASN:OD1	2:C:460:LEU:CA	2.62	0.46
2:C:531:ILE:HG23	2:C:531:ILE:H	1.29	0.46
2:D:177:TYR:CE1	2:D:197:LEU:HD21	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:465:MET:HE2	2:D:470:THR:HA	1.90	0.46
1:A:86:PHE:HD1	2:C:552:PHE:HB3	1.80	0.46
1:B:99:PHE:CD1	1:B:100:THR:N	2.83	0.46
2:C:177:TYR:CD1	2:C:177:TYR:N	2.82	0.46
2:C:321:ASP:OD2	2:C:323:ARG:HD3	2.15	0.46
2:C:439:PHE:HA	3:H:2:NAG:O7	2.16	0.46
2:C:447:THR:CG2	2:C:448:VAL:N	2.78	0.46
2:C:551:ILE:CD1	2:C:551:ILE:N	2.78	0.46
2:D:192:ASN:ND2	2:D:194:LEU:CD2	2.79	0.46
1:A:94:ASP:OD1	5:A:580:HEM:HHB	2.16	0.46
1:B:71:PHE:HZ	1:B:76:LEU:CD1	2.19	0.46
2:C:176:VAL:HG23	2:C:177:TYR:CE1	2.51	0.46
2:C:400:ASP:O	2:C:401:GLU:C	2.51	0.46
1:B:66:ASN:ND2	2:D:403:ARG:HH12	2.09	0.46
2:D:405:ARG:NH1	2:D:405:ARG:CG	2.73	0.46
2:D:489:GLY:O	2:D:490:ARG:NE	2.48	0.46
1:A:87:MET:HB3	2:C:338:LEU:HB3	1.96	0.46
1:A:87:MET:HE1	2:C:243:MET:HE2	1.98	0.46
2:D:327:VAL:CG1	2:D:328:PHE:N	2.79	0.46
1:B:68:ILE:HD12	2:D:464:LEU:HD13	1.98	0.46
2:D:422:MET:HE1	2:D:478:MET:SD	2.56	0.46
2:C:192:ASN:CG	2:C:194:LEU:HB2	2.36	0.46
2:D:216:LEU:N	2:D:216:LEU:CD2	2.76	0.46
5:B:580:HEM:NB	2:D:336:HIS:CD2	2.83	0.46
2:D:348:ASN:O	2:D:350:TYR:N	2.49	0.46
1:A:77:THR:HG21	2:C:393:ARG:NH1	2.23	0.46
1:A:8:ARG:HG2	2:C:512:PHE:CD2	2.51	0.46
2:D:194:LEU:CD1	2:D:194:LEU:N	2.77	0.46
2:D:212:PRO:O	2:D:233:PHE:HA	2.16	0.46
2:D:310:LEU:CD1	2:D:504:ARG:HA	2.46	0.46
2:D:380:ILE:HG22	2:D:381:LEU:N	2.31	0.46
2:D:392:ASN:OD1	2:D:393:ARG:N	2.48	0.46
2:D:492:GLY:O	2:D:496:ALA:CB	2.63	0.46
1:A:99:PHE:O	2:C:165:ASN:ND2	2.47	0.46
2:C:194:LEU:HD12	2:C:194:LEU:HA	1.47	0.46
2:C:306:MET:O	2:C:310:LEU:N	2.48	0.46
2:C:498:ILE:HD13	2:C:498:ILE:HG21	1.63	0.46
2:D:136:ARG:CZ	2:D:414:GLY:O	2.63	0.46
2:D:338:LEU:N	2:D:338:LEU:HD13	2.31	0.46
2:D:350:TYR:CG	2:D:557:TYR:CE1	3.04	0.46
2:D:433:TYR:CE1	2:D:437:ARG:HG3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:320:VAL:CG1	2:D:509:GLY:CA	2.87	0.46
2:C:158:ILE:HA	1:B:27:ARG:NH2	2.30	0.46
1:A:62:ARG:HH22	2:C:136:ARG:HG2	1.72	0.46
2:C:361:LEU:HB3	2:C:401:GLU:CG	2.46	0.46
2:C:571:ASN:ND2	2:C:573:ALA:CB	2.78	0.46
2:D:345:ARG:NH2	2:D:374:GLU:CG	2.79	0.46
2:D:385:MET:CE	2:D:546:VAL:CA	2.92	0.46
1:A:79:ASP:OD2	1:A:82:ARG:CG	2.63	0.45
1:B:77:THR:CG2	2:D:396:GLN:NE2	2.78	0.45
2:C:400:ASP:C	2:C:402:ILE:N	2.69	0.45
2:C:485:LEU:CD1	2:C:485:LEU:N	2.79	0.45
2:D:405:ARG:NH1	2:D:405:ARG:HG3	2.31	0.45
2:D:531:ILE:HG23	2:D:531:ILE:HD13	1.69	0.45
2:D:537:ILE:O	2:D:541:THR:HG23	2.16	0.45
1:B:44:PRO:HB2	2:D:126:PHE:CE2	2.51	0.45
2:D:336:HIS:ND1	2:D:417:LEU:HG	2.32	0.45
2:D:533:LEU:N	2:D:534:PRO:CD	2.79	0.45
2:C:434:ASN:ND2	2:C:444:GLN:CB	2.77	0.45
2:C:460:LEU:HD22	2:C:464:LEU:CD2	2.46	0.45
1:A:85:MET:CE	2:C:533:LEU:CD2	2.92	0.45
2:C:213:PHE:CD2	2:C:231:PRO:HD2	2.50	0.45
2:C:248:SER:C	2:C:377:ILE:HD11	2.36	0.45
2:C:420:LEU:O	2:C:424:ARG:N	2.48	0.45
2:C:422:MET:HG2	2:C:475:ASP:HB2	1.99	0.45
2:C:489:GLY:C	2:C:490:ARG:HG2	2.37	0.45
5:B:580:HEM:HHA	2:D:333:ARG:NH2	2.32	0.45
1:A:71:PHE:CD1	1:A:72:PRO:N	2.85	0.45
1:A:84:LEU:O	1:A:85:MET:C	2.55	0.45
2:C:316:TYR:CD2	2:C:511:ARG:HA	2.51	0.45
2:C:442:LEU:CB	2:C:443:PRO:HD2	2.22	0.45
2:C:557:TYR:CG	2:C:557:TYR:O	2.67	0.45
2:C:570:LEU:HD13	2:C:572:LEU:CD1	2.47	0.45
2:C:572:LEU:N	2:C:572:LEU:CD1	2.78	0.45
2:D:257:HIS:NE2	2:D:277:TYR:HD1	2.14	0.45
2:D:372:VAL:HG12	2:D:373:LEU:CD1	2.39	0.45
2:D:408:GLU:C	2:D:410:VAL:H	2.17	0.45
2:D:424:ARG:HH11	2:D:424:ARG:CG	2.28	0.45
2:C:262:THR:HG22	2:C:263:GLU:H	1.80	0.45
1:B:66:ASN:ND2	2:D:403:ARG:NH1	2.60	0.45
1:A:72:PRO:O	1:A:73:THR:C	2.54	0.45
2:C:165:ASN:HD21	2:C:167:LEU:H	1.65	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:291:ILE:HG23	2:C:292:THR:CA	2.47	0.45
2:C:339:ILE:HG21	2:C:339:ILE:HD12	1.74	0.45
2:C:365:PHE:CD1	2:C:365:PHE:N	2.84	0.45
2:C:170:PHE:HB2	2:C:172:ASP:OD2	2.16	0.45
2:C:248:SER:CB	2:C:377:ILE:HG12	2.47	0.45
5:A:580:HEM:CMA	2:C:333:ARG:HD2	2.47	0.45
2:C:339:ILE:HD11	2:C:402:ILE:HD12	1.99	0.45
2:C:297:LEU:HD21	2:C:503:PHE:CG	2.51	0.45
2:D:163:GLN:HG3	2:D:428:HIS:ND1	2.32	0.45
2:D:437:ARG:HH11	2:D:437:ARG:HD2	1.59	0.45
2:C:415:LEU:CD1	2:C:415:LEU:N	2.68	0.45
2:C:541:THR:CB	2:C:543:ILE:HD11	2.46	0.45
2:C:350:TYR:CG	2:C:557:TYR:HD2	2.30	0.45
2:D:223:LEU:HB2	2:D:410:VAL:CG2	2.46	0.45
2:D:477:TRP:O	2:D:481:VAL:HG22	2.17	0.45
2:D:543:ILE:HG23	2:D:543:ILE:HD13	1.61	0.45
2:D:556:SER:O	2:D:557:TYR:C	2.51	0.45
3:I:1:NAG:C6	3:I:2:NAG:O5	2.56	0.45
1:A:98:ASP:O	2:C:167:LEU:HD22	2.16	0.45
2:C:264:LEU:HA	2:C:264:LEU:HD12	1.50	0.45
2:D:400:ASP:O	2:D:402:ILE:N	2.50	0.45
1:A:87:MET:O	5:A:580:HEM:HBB1	2.17	0.44
2:C:167:LEU:N	2:C:167:LEU:CD1	2.79	0.44
2:C:213:PHE:HE2	2:C:231:PRO:CD	2.25	0.44
2:C:270:ARG:HG2	2:C:270:ARG:NH1	2.31	0.44
2:C:295:ASP:CB	2:C:550:ASN:ND2	2.80	0.44
2:C:378:ASP:O	2:C:382:ARG:HB3	2.17	0.44
2:D:174:SER:O	2:D:175:MET:C	2.54	0.44
2:D:223:LEU:HA	2:D:223:LEU:HD12	1.41	0.44
2:D:381:LEU:HA	2:D:384:LEU:CD1	2.24	0.44
1:B:36:GLU:OE2	2:D:431:PRO:HB3	2.17	0.44
2:D:546:VAL:O	2:D:561:PHE:HD2	1.99	0.44
5:B:580:HEM:CHD	2:D:242:GLU:OE2	2.65	0.44
1:A:41:PHE:O	2:C:161:ARG:HB2	2.18	0.44
2:C:165:ASN:ND2	2:C:167:LEU:H	2.15	0.44
2:C:421:ASN:HD22	2:C:421:ASN:HA	1.41	0.44
2:D:179:SER:N	2:D:180:GLU:N	2.65	0.44
2:D:211:LEU:HB2	2:D:233:PHE:CD1	2.52	0.44
2:D:493:PRO:HA	2:D:496:ALA:HB3	1.98	0.44
2:D:544:THR:HG23	2:D:545:THR:N	2.31	0.44
1:A:83:SER:O	1:A:86:PHE:HB3	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:370:ARG:HE	2:C:374:GLU:CD	2.19	0.44
2:C:382:ARG:HA	2:C:385:MET:HE3	1.98	0.44
2:C:399:VAL:O	2:C:403:ARG:HB2	2.17	0.44
2:C:415:LEU:H	2:C:415:LEU:CD1	2.30	0.44
1:A:44:PRO:HB2	2:C:126:PHE:CE2	2.52	0.44
2:C:244:PRO:HA	2:C:247:THR:CG2	2.47	0.44
5:A:580:HEM:CMD	2:C:406:LEU:HD21	2.43	0.44
5:B:580:HEM:C4B	2:D:336:HIS:CD2	3.05	0.44
1:A:99:PHE:HD2	2:C:166:ALA:HB3	1.82	0.44
1:B:56:PHE:HA	1:B:57:PRO:HD3	1.85	0.44
1:A:79:ASP:CG	2:C:490:ARG:NH1	2.71	0.44
2:C:480:GLY:C	2:C:495:LEU:CD2	2.86	0.44
2:D:142:ASP:OD1	2:D:143:CYS:N	2.46	0.44
2:D:294:ARG:HG2	2:D:295:ASP:OD1	2.18	0.44
2:D:332:PHE:CD1	2:D:334:TYR:HE1	2.34	0.44
2:D:356:ASN:CG	2:D:357:PRO:HD3	2.31	0.44
2:D:543:ILE:HG21	2:D:543:ILE:HD12	1.66	0.44
2:C:297:LEU:O	2:C:300:VAL:HG13	2.17	0.44
2:C:317:ASN:O	2:C:319:SER:N	2.51	0.44
2:C:326:ASN:HD21	2:C:428:HIS:HB3	1.83	0.44
2:C:521:SER:HG	2:C:523:GLN:HB2	1.82	0.44
2:C:537:ILE:CG1	2:C:537:ILE:O	2.65	0.44
2:C:208:ARG:HH22	2:C:542:GLY:HA3	1.83	0.44
2:D:301:LEU:HA	2:D:301:LEU:HD12	1.66	0.44
2:D:403:ARG:HG2	2:D:416:ASP:OD1	2.17	0.44
2:D:424:ARG:O	2:D:425:SER:C	2.54	0.44
1:B:41:PHE:N	1:B:41:PHE:HD1	2.16	0.44
2:C:130:ILE:HD13	2:C:137:ILE:O	2.18	0.44
2:C:216:LEU:HD12	2:C:218:ASP:H	1.82	0.44
2:C:267:LEU:CD2	2:C:572:LEU:O	2.66	0.44
2:C:278:GLN:HE21	2:C:278:GLN:HB2	1.30	0.44
2:C:310:LEU:HD11	2:C:504:ARG:HA	2.00	0.44
2:D:128:LEU:CD2	2:D:144:ILE:HD11	2.48	0.44
1:A:29:PHE:CE2	1:A:100:THR:CG2	2.99	0.44
2:C:230:ILE:HG21	2:C:372:VAL:CG2	2.23	0.44
2:C:270:ARG:HG2	2:C:270:ARG:HH11	1.82	0.44
2:C:346:LEU:HA	2:C:346:LEU:HD12	1.68	0.44
2:D:150:CYS:HA	2:D:151:PRO:HD3	1.77	0.44
2:D:182:PRO:O	2:D:186:ASN:HB2	2.17	0.44
2:D:347:ASP:HA	2:D:382:ARG:NH1	2.33	0.44
2:D:362:SER:OG	2:D:401:GLU:OE1	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:68:ILE:CG2	2:D:460:LEU:CD1	2.96	0.44
1:A:44:PRO:O	1:A:47:TRP:N	2.51	0.44
1:B:47:TRP:C	1:B:47:TRP:CD1	2.91	0.44
2:C:350:TYR:HB2	2:C:557:TYR:HE2	1.76	0.44
2:C:514:TRP:HA	2:C:519:VAL:HG21	2.00	0.44
2:C:519:VAL:HG22	2:C:520:PHE:H	1.81	0.44
2:D:264:LEU:HA	2:D:264:LEU:HD12	1.86	0.44
2:D:320:VAL:O	2:D:322:PRO:HD3	2.18	0.44
2:D:327:VAL:HG13	2:D:328:PHE:N	2.33	0.44
2:D:440:CYS:O	2:D:441:GLY:C	2.56	0.44
2:D:513:TRP:CD1	2:D:515:GLU:HB2	2.53	0.44
2:D:554:SER:C	2:D:560:ASP:OD1	2.56	0.44
2:D:225:ASN:OD1	3:J:1:NAG:N2	2.51	0.44
2:D:206:ASN:HA	2:D:206:ASN:HD22	1.39	0.43
2:D:297:LEU:O	2:D:301:LEU:N	2.51	0.43
2:D:377:ILE:HD12	2:D:377:ILE:HG21	1.38	0.43
2:D:422:MET:O	2:D:426:ARG:HD3	2.18	0.43
2:D:447:THR:CG2	2:D:448:VAL:N	2.81	0.43
2:D:498:ILE:HD13	2:D:498:ILE:HG21	1.71	0.43
1:A:94:ASP:HB3	1:A:95:HIS:HD2	1.83	0.43
2:C:363:ARG:N	2:C:363:ARG:HD3	2.32	0.43
2:C:378:ASP:CB	2:C:379:PRO:HD3	2.48	0.43
2:C:474:ILE:HD11	2:C:479:GLY:H	1.82	0.43
2:D:177:TYR:CE2	2:D:281:ARG:CG	2.96	0.43
2:D:385:MET:SD	2:D:537:ILE:HD11	2.58	0.43
2:D:447:THR:HB	2:D:450:GLN:HB2	1.98	0.43
1:B:79:ASP:CG	2:D:490:ARG:NH1	2.72	0.43
1:A:77:THR:O	2:C:391:LEU:N	2.52	0.43
1:B:72:PRO:HB2	1:B:75:GLN:HG3	1.99	0.43
2:C:162:ASN:ND2	2:C:163:GLN:N	2.67	0.43
2:C:260:LEU:HA	2:C:260:LEU:HD12	1.72	0.43
2:C:297:LEU:CA	2:C:300:VAL:CG1	2.86	0.43
2:C:264:LEU:CD1	2:C:572:LEU:HD23	2.48	0.43
3:G:2:NAG:O3	3:G:2:NAG:C7	2.65	0.43
2:C:199:VAL:CG1	2:C:209:ALA:CB	2.96	0.43
2:C:378:ASP:N	2:C:379:PRO:CD	2.81	0.43
2:C:223:LEU:HD22	2:C:410:VAL:HG23	1.99	0.43
1:B:11:THR:CG2	2:D:181:GLU:OE2	2.67	0.43
2:D:370:ARG:O	2:D:374:GLU:CB	2.67	0.43
1:B:68:ILE:H	1:B:68:ILE:HG12	1.54	0.43
2:C:480:GLY:CA	2:C:495:LEU:HD22	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:193:GLN:O	2:D:273:GLY:HA2	2.19	0.43
2:D:291:ILE:O	2:D:295:ASP:N	2.45	0.43
1:B:22:LEU:HD23	2:D:322:PRO:HD2	1.99	0.43
1:B:79:ASP:CB	2:D:391:LEU:HB2	2.31	0.43
2:D:436:TRP:CE3	2:D:498:ILE:HD11	2.54	0.43
3:E:1:NAG:O4	3:E:2:NAG:O7	2.36	0.43
1:A:10:ILE:HG21	2:C:181:GLU:CD	2.38	0.43
1:A:94:ASP:OD1	5:A:580:HEM:CHB	2.67	0.43
1:B:85:MET:HG3	2:D:552:PHE:CE1	2.53	0.43
1:A:47:TRP:CE3	2:C:121:GLN:OE1	2.72	0.43
2:C:287:MET:HA	2:C:531:ILE:HD11	2.01	0.43
2:D:264:LEU:HD12	2:D:267:LEU:HD11	2.00	0.43
2:D:400:ASP:C	2:D:402:ILE:H	2.22	0.43
2:D:491:VAL:HG11	2:D:496:ALA:HA	2.00	0.43
2:C:162:ASN:HD22	2:C:162:ASN:HA	1.24	0.43
2:C:284:VAL:C	2:C:286:ALA:N	2.71	0.43
2:C:551:ILE:HD12	2:C:551:ILE:N	2.33	0.43
2:D:377:ILE:HG23	2:D:377:ILE:HD13	1.43	0.43
2:D:486:LYS:HA	2:D:486:LYS:HD2	1.68	0.43
2:D:534:PRO:HB3	2:D:546:VAL:CG1	2.49	0.43
2:C:130:ILE:CG2	2:C:137:ILE:CD1	2.96	0.43
2:C:299:LEU:HD21	2:C:550:ASN:CG	2.39	0.43
1:A:84:LEU:CB	2:C:384:LEU:HD23	2.48	0.43
2:C:437:ARG:O	2:C:442:LEU:CD2	2.66	0.43
1:A:68:ILE:HD11	2:C:467:GLN:HG3	2.00	0.43
2:C:571:ASN:C	2:C:573:ALA:H	2.21	0.43
2:D:486:LYS:HG3	2:D:486:LYS:HZ3	1.14	0.43
2:D:550:ASN:O	2:D:553:MET:N	2.46	0.43
1:B:72:PRO:O	1:B:74:ASP:N	2.52	0.43
2:C:524:GLN:HG3	2:C:575:TRP:CH2	2.54	0.43
2:D:196:LEU:HD12	2:D:258:ASN:HA	2.00	0.43
2:D:467:GLN:HA	2:D:467:GLN:NE2	2.34	0.43
1:B:10:ILE:HG23	1:B:11:THR:CG2	2.44	0.43
1:B:13:MET:CG	1:B:14:CYS:N	2.73	0.43
2:C:528:LEU:HA	2:C:528:LEU:HD12	1.72	0.43
2:C:528:LEU:O	2:C:531:ILE:HG23	2.19	0.43
2:D:200:ASN:HD22	2:D:202:ARG:N	2.16	0.43
2:D:268:ASN:OD1	2:D:271:TRP:CZ3	2.72	0.43
1:B:22:LEU:HD23	2:D:322:PRO:HD3	2.00	0.43
2:D:350:TYR:CZ	2:D:561:PHE:HE2	2.37	0.43
1:A:6:LYS:HE3	2:C:282:LYS:HZ2	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:306:MET:CE	2:C:310:LEU:HB2	2.49	0.42
2:C:345:ARG:NH2	2:C:374:GLU:CD	2.72	0.42
2:C:417:LEU:O	2:C:420:LEU:N	2.46	0.42
2:D:251:THR:CG2	2:D:377:ILE:CD1	2.93	0.42
2:D:422:MET:O	2:D:426:ARG:CD	2.67	0.42
2:D:457:ASN:HB3	2:D:460:LEU:HB3	2.00	0.42
2:C:244:PRO:CB	2:C:343:MET:CE	2.95	0.42
2:C:361:LEU:CB	2:C:401:GLU:CG	2.96	0.42
2:C:458:LEU:C	2:C:458:LEU:HD12	2.40	0.42
2:C:516:ASN:HB3	2:C:519:VAL:CG1	2.49	0.42
2:D:224:THR:HG21	2:D:367:ALA:CB	2.46	0.42
2:D:257:HIS:CE1	2:D:277:TYR:HD1	2.37	0.42
2:C:183:LEU:HD11	2:C:187:LEU:HD11	2.00	0.42
2:C:264:LEU:HD13	2:C:572:LEU:HD23	2.01	0.42
1:A:84:LEU:CD1	2:C:389:ALA:HA	2.41	0.42
2:D:219:ASP:HB3	2:D:222:LEU:CD2	2.48	0.42
2:D:295:ASP:N	2:D:295:ASP:OD1	2.50	0.42
2:D:557:TYR:HB3	2:D:558:PRO:HD3	1.95	0.42
1:B:42:SER:OG	1:B:42:SER:O	2.28	0.42
2:C:183:LEU:HG	2:C:184:ALA:N	2.34	0.42
2:C:383:GLY:H	2:C:385:MET:H	1.68	0.42
2:C:474:ILE:CD1	2:C:479:GLY:H	2.32	0.42
2:C:567:LEU:HA	2:C:567:LEU:HD12	1.87	0.42
2:D:433:TYR:CD1	2:D:494:LEU:CD2	3.03	0.42
3:G:2:NAG:HO3	3:G:2:NAG:C7	2.23	0.42
2:C:158:ILE:HG21	2:C:158:ILE:HD12	1.71	0.42
2:C:361:LEU:HD13	2:C:365:PHE:CE1	2.54	0.42
2:C:434:ASN:ND2	2:C:444:GLN:CA	2.83	0.42
2:C:485:LEU:HG	2:C:490:ARG:HA	2.02	0.42
2:D:370:ARG:HA	2:D:374:GLU:HB2	2.02	0.42
2:C:350:TYR:HE1	2:C:545:THR:HG23	1.84	0.42
2:C:567:LEU:HA	2:C:568:PRO:HD2	1.94	0.42
2:D:297:LEU:O	2:D:299:LEU:N	2.52	0.42
2:D:339:ILE:HD13	2:D:339:ILE:HG23	1.68	0.42
2:D:487:ARG:O	2:D:488:LYS:HB3	2.19	0.42
2:D:507:ARG:HD2	2:D:508:ASP:OD1	2.18	0.42
1:A:18:ARG:HD3	2:C:318:ASP:OD2	2.20	0.42
2:C:117:THR:HG22	2:C:117:THR:H	1.35	0.42
2:C:146:PHE:HZ	2:C:424:ARG:HA	1.84	0.42
2:C:177:TYR:CD2	2:C:281:ARG:CD	2.99	0.42
2:C:274:GLU:OE1	2:C:278:GLN:NE2	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:321:ASP:HA	2:C:322:PRO:HD3	1.63	0.42
2:C:169:SER:CB	2:C:324:ILE:HD12	2.46	0.42
2:C:422:MET:O	2:C:426:ARG:HD3	2.20	0.42
2:C:544:THR:HG23	2:C:545:THR:CG2	2.35	0.42
2:D:144:ILE:HD12	2:D:144:ILE:HG21	1.58	0.42
5:B:580:HEM:CMC	2:D:243:MET:SD	3.07	0.42
1:B:71:PHE:CD2	2:D:396:GLN:HA	2.54	0.42
2:D:534:PRO:CB	2:D:546:VAL:HG11	2.50	0.42
1:B:10:ILE:CG2	1:B:11:THR:CG2	2.98	0.42
1:B:30:VAL:CG1	1:B:31:ARG:N	2.80	0.42
2:C:225:ASN:OD1	3:G:1:NAG:C5	2.68	0.42
2:D:197:LEU:HD12	2:D:197:LEU:HA	1.44	0.42
2:D:339:ILE:HD12	2:D:339:ILE:HG21	1.82	0.42
1:A:91:GLN:O	1:A:92:LEU:C	2.55	0.42
1:B:103:PRO:O	1:B:104:ALA:C	2.58	0.42
1:B:23:GLY:HA2	2:D:169:SER:OG	2.20	0.42
1:B:76:LEU:O	1:B:78:PRO:HD3	2.20	0.42
2:C:294:ARG:HE	2:C:295:ASP:CG	2.22	0.42
2:D:163:GLN:HG3	2:D:428:HIS:CG	2.55	0.42
2:D:403:ARG:HG3	2:D:418:PRO:HG2	2.00	0.42
2:D:458:LEU:O	2:D:462:ARG:HD2	2.20	0.42
1:B:16:ASN:ND2	1:B:19:SER:N	2.61	0.42
1:B:56:PHE:CD1	1:B:56:PHE:N	2.88	0.42
1:A:99:PHE:CB	2:C:239:ARG:HH12	2.33	0.42
2:C:287:MET:HA	2:C:531:ILE:CD1	2.50	0.42
2:D:144:ILE:HA	2:D:145:PRO:HD2	1.58	0.42
2:D:297:LEU:O	2:D:301:LEU:CB	2.68	0.42
2:D:395:ASN:C	2:D:396:GLN:HG3	2.39	0.42
1:B:53:ARG:CB	2:D:473:ASN:HD21	2.33	0.42
2:D:537:ILE:HD13	2:D:537:ILE:HG23	1.67	0.42
2:D:557:TYR:O	2:D:558:PRO:O	2.38	0.42
1:B:60:LEU:HD12	1:B:60:LEU:HA	1.61	0.41
1:B:72:PRO:C	1:B:74:ASP:H	2.23	0.41
2:C:300:VAL:H	2:C:300:VAL:HG12	1.53	0.41
2:C:444:GLN:HA	2:C:445:PRO:HD3	1.85	0.41
2:C:537:ILE:HG21	2:C:537:ILE:HD13	1.89	0.41
2:D:199:VAL:HG12	2:D:200:ASN:N	2.35	0.41
2:D:230:ILE:HA	2:D:231:PRO:HD2	1.83	0.41
2:D:177:TYR:CE1	2:D:257:HIS:CD2	3.07	0.41
2:D:406:LEU:HB3	2:D:415:LEU:HB2	2.02	0.41
2:D:494:LEU:HD12	2:D:494:LEU:HA	1.83	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:PHE:HZ	1:A:100:THR:HG22	1.80	0.41
1:A:44:PRO:O	1:A:47:TRP:HB3	2.20	0.41
1:A:85:MET:SD	2:C:551:ILE:HG21	2.59	0.41
1:A:89:TRP:HD1	2:C:296:TYR:CD2	2.37	0.41
2:C:197:LEU:HD23	2:C:257:HIS:HB3	2.02	0.41
2:C:316:TYR:HB3	2:C:516:ASN:OD1	2.20	0.41
2:C:244:PRO:HD2	2:C:364:VAL:CG1	2.50	0.41
2:C:407:PHE:HB2	2:C:415:LEU:CD2	2.50	0.41
1:B:31:ARG:HH11	2:D:162:ASN:ND2	2.18	0.41
2:D:171:VAL:HG11	2:D:289:GLN:HA	2.01	0.41
2:D:177:TYR:HE1	2:D:197:LEU:HD21	1.84	0.41
2:D:299:LEU:HD21	2:D:553:MET:CE	2.50	0.41
2:D:547:SER:HB3	2:D:551:ILE:HG23	2.02	0.41
1:A:10:ILE:HG23	1:A:11:THR:N	2.36	0.41
1:A:33:LEU:O	1:A:34:PRO:O	2.39	0.41
1:A:83:SER:O	1:A:86:PHE:CB	2.69	0.41
2:C:175:MET:C	2:C:236:GLY:HA3	2.41	0.41
2:C:244:PRO:HD2	2:C:364:VAL:HG13	2.01	0.41
2:C:267:LEU:CD1	2:C:268:ASN:HD21	2.33	0.41
2:C:309:TYR:C	2:C:311:PRO:HD2	2.41	0.41
2:C:369:TRP:O	2:C:373:LEU:HB2	2.20	0.41
2:C:447:THR:N	2:C:450:GLN:HE21	2.19	0.41
2:D:292:THR:HA	2:D:296:TYR:HB3	2.02	0.41
2:D:146:PHE:CZ	2:D:424:ARG:CZ	3.04	0.41
2:D:445:PRO:HA	2:D:450:GLN:HB3	2.02	0.41
2:D:451:LEU:HD12	2:D:451:LEU:HA	1.88	0.41
3:F:1:NAG:H61	3:F:2:NAG:O5	2.19	0.41
1:B:62:ARG:NH2	2:D:136:ARG:HB3	2.36	0.41
2:C:264:LEU:HD11	2:C:572:LEU:CG	2.51	0.41
2:C:470:THR:C	2:C:472:ASN:N	2.72	0.41
2:C:485:LEU:HD23	2:C:490:ARG:CD	2.45	0.41
2:C:520:PHE:HD1	2:C:520:PHE:HA	1.79	0.41
2:C:570:LEU:HA	2:C:570:LEU:HD23	1.77	0.41
2:D:126:PHE:CD1	2:D:126:PHE:C	2.91	0.41
2:D:346:LEU:HD12	2:D:352:PRO:HA	2.02	0.41
1:B:77:THR:HG23	2:D:396:GLN:NE2	2.36	0.41
2:D:471:PRO:C	2:D:473:ASN:N	2.74	0.41
1:B:31:ARG:NH1	2:D:162:ASN:ND2	2.69	0.41
2:C:136:ARG:NH2	2:C:414:GLY:C	2.73	0.41
2:C:213:PHE:HE2	2:C:231:PRO:N	2.18	0.41
2:C:332:PHE:HD1	2:C:332:PHE:HA	1.81	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:130:ILE:HD12	2:D:137:ILE:HD11	2.02	0.41
2:D:194:LEU:HD13	2:D:194:LEU:N	2.35	0.41
2:D:447:THR:H	2:D:450:GLN:HB2	1.85	0.41
2:D:458:LEU:CD2	2:D:462:ARG:NH1	2.75	0.41
1:A:17:ARG:NH1	2:C:511:ARG:NH1	2.67	0.41
1:A:88:GLN:HE22	2:C:243:MET:HE2	1.86	0.41
2:C:196:LEU:HA	2:C:196:LEU:HD12	1.74	0.41
2:C:244:PRO:CA	2:C:247:THR:HG22	2.51	0.41
1:B:95:HIS:O	2:D:167:LEU:HD23	2.21	0.41
2:D:177:TYR:HH	2:D:284:VAL:HG11	1.84	0.41
2:D:348:ASN:C	2:D:350:TYR:N	2.70	0.41
2:D:417:LEU:O	2:D:418:PRO:C	2.56	0.41
2:D:531:ILE:HG12	2:D:531:ILE:O	2.10	0.41
2:C:223:LEU:HD12	2:C:223:LEU:HA	1.78	0.41
2:C:287:MET:O	2:C:290:ILE:CG2	2.69	0.41
1:A:87:MET:CB	2:C:338:LEU:HB3	2.51	0.41
2:D:173:ALA:HB1	2:D:176:VAL:HG13	2.01	0.41
2:D:177:TYR:OH	2:D:284:VAL:HG11	2.20	0.41
2:D:248:SER:CA	2:D:251:THR:HG22	2.49	0.41
2:D:327:VAL:C	2:D:329:THR:N	2.72	0.41
2:D:491:VAL:HG21	2:D:499:ILE:HD12	2.02	0.41
1:A:94:ASP:OD1	5:A:580:HEM:HMA2	2.18	0.41
2:C:177:TYR:HD2	2:C:281:ARG:HG3	1.83	0.41
2:D:130:ILE:CD1	2:D:137:ILE:HG12	2.42	0.41
2:D:175:MET:N	2:D:175:MET:SD	2.94	0.41
2:D:433:TYR:CE1	2:D:483:GLU:OE2	2.74	0.41
2:D:528:LEU:HD12	2:D:528:LEU:HA	1.72	0.41
2:D:544:THR:CG2	2:D:545:THR:N	2.84	0.41
2:D:567:LEU:HA	2:D:567:LEU:HD12	1.47	0.41
1:A:41:PHE:CD1	1:A:42:SER:N	2.88	0.41
2:C:291:ILE:HG22	2:C:292:THR:N	2.30	0.41
2:C:322:PRO:HD2	2:C:323:ARG:H	1.85	0.41
2:D:189:ASN:OD1	3:I:1:NAG:C2	2.69	0.41
2:D:197:LEU:HB3	2:D:254:LEU:CD1	2.51	0.41
2:D:417:LEU:HD12	2:D:417:LEU:HA	1.81	0.41
2:D:571:ASN:C	2:D:571:ASN:HD22	2.24	0.41
1:B:52:LYS:O	1:B:53:ARG:O	2.38	0.41
2:C:282:LYS:HE2	2:C:520:PHE:CE1	2.56	0.41
2:C:321:ASP:OD1	2:C:322:PRO:CD	2.69	0.41
2:C:385:MET:HG2	2:C:547:SER:OG	2.21	0.41
2:D:244:PRO:HD2	2:D:364:VAL:HG21	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:VAL:HG22	2:D:323:ARG:CG	2.26	0.41
1:B:64:VAL:HG21	2:D:422:MET:HE1	2.00	0.41
1:B:73:THR:HG22	1:B:73:THR:H	1.63	0.41
2:C:196:LEU:HD12	2:C:258:ASN:ND2	2.36	0.41
2:C:197:LEU:HB3	2:C:254:LEU:HD12	2.03	0.41
2:C:269:PRO:C	2:C:271:TRP:N	2.74	0.41
1:A:7:TYR:OH	2:C:279:GLU:OE2	2.23	0.41
2:C:177:TYR:HD2	2:C:281:ARG:HD2	1.83	0.41
2:C:382:ARG:HB2	2:C:385:MET:HE1	1.99	0.41
2:C:448:VAL:H	2:C:448:VAL:HG12	1.57	0.41
2:C:293:TYR:CE2	2:C:513:TRP:HZ3	2.39	0.41
2:D:137:ILE:HD12	2:D:137:ILE:HG21	1.63	0.41
1:B:10:ILE:CG2	1:B:11:THR:N	2.84	0.40
2:C:256:GLU:HG2	2:C:287:MET:HE2	2.02	0.40
2:C:271:TRP:NE1	2:C:275:ARG:NH1	2.69	0.40
2:C:290:ILE:CG2	2:C:291:ILE:N	2.84	0.40
2:C:381:LEU:HD13	2:C:381:LEU:HA	1.66	0.40
2:C:537:ILE:O	2:C:541:THR:OG1	2.31	0.40
2:D:123:PRO:O	2:D:124:PRO:C	2.59	0.40
2:D:304:THR:HG23	2:D:305:ALA:N	2.36	0.40
1:B:18:ARG:NH2	2:D:319:SER:OG	2.51	0.40
2:D:345:ARG:HH11	2:D:345:ARG:HD3	1.48	0.40
2:D:224:THR:HG21	2:D:369:TRP:HE1	1.86	0.40
2:D:295:ASP:O	2:D:552:PHE:CD2	2.74	0.40
1:B:79:ASP:HB3	2:D:389:ALA:O	2.22	0.40
2:C:346:LEU:C	2:C:353:MET:HB2	2.42	0.40
2:C:224:THR:CG2	2:C:369:TRP:HE1	2.34	0.40
2:D:385:MET:HE3	2:D:547:SER:N	2.34	0.40
2:D:522:MET:HA	2:D:525:ARG:HG3	2.03	0.40
2:C:137:ILE:HG12	2:C:137:ILE:O	2.19	0.40
2:C:290:ILE:HD12	2:C:514:TRP:CH2	2.56	0.40
2:C:346:LEU:HD12	2:C:353:MET:N	2.24	0.40
2:C:248:SER:CA	2:C:377:ILE:HD11	2.52	0.40
1:A:82:ARG:HA	2:C:552:PHE:O	2.22	0.40
2:D:128:LEU:HB3	2:D:144:ILE:HG12	2.03	0.40
2:D:295:ASP:HB2	2:D:552:PHE:CE2	2.56	0.40
2:D:400:ASP:C	2:D:402:ILE:N	2.74	0.40
1:A:102:GLU:OE2	2:C:424:ARG:NH2	2.55	0.40
2:C:177:TYR:HD2	2:C:281:ARG:CG	2.34	0.40
2:C:281:ARG:HD3	2:C:281:ARG:HH11	1.60	0.40
2:C:393:ARG:CD	2:C:396:GLN:HE22	2.34	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:476:ILE:HD13	2:C:476:ILE:HG21	1.84	0.40
2:C:538:CYS:O	2:C:539:ASP:C	2.60	0.40
2:D:330:ASN:HA	2:D:333:ARG:HD2	2.02	0.40
2:D:343:MET:HB3	2:D:359:VAL:HG13	2.03	0.40
2:C:519:VAL:H	2:C:519:VAL:HG13	1.65	0.40
2:D:252:LEU:HD21	2:D:537:ILE:HG22	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	102/108 (94%)	75 (74%)	22 (22%)	5 (5%)	2 13
1	B	100/108 (93%)	80 (80%)	13 (13%)	7 (7%)	1 6
2	C	460/466 (99%)	349 (76%)	84 (18%)	27 (6%)	1 9
2	D	460/466 (99%)	356 (77%)	82 (18%)	22 (5%)	2 13
All	All	1122/1148 (98%)	860 (77%)	201 (18%)	61 (5%)	2 11

All (61) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	C	123	PRO
2	C	303	PRO
2	C	352	PRO
2	C	376	GLY
2	C	560	ASP
2	D	123	PRO
2	D	124	PRO
2	D	354	GLU
2	D	429	GLY

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Mol	Chain	Res	Type
2	D	555	ASN
2	D	568	PRO
1	A	73	THR
1	A	85	MET
2	C	135	PRO
2	C	218	ASP
2	C	270	ARG
2	C	354	GLU
2	C	362	SER
2	C	397	ILE
2	C	469	GLY
2	C	550	ASN
2	C	558	PRO
1	B	53	ARG
1	B	59	ALA
1	B	73	THR
2	D	175	MET
2	D	270	ARG
2	D	441	GLY
1	A	42	SER
2	C	269	PRO
2	C	394	GLN
2	C	415	LEU
2	C	457	ASN
1	B	26	ASN
1	B	42	SER
2	D	206	ASN
2	D	207	GLY
2	D	258	ASN
2	D	434	ASN
1	A	34	PRO
1	A	103	PRO
2	C	514	TRP
2	D	228	ALA
2	D	349	ARG
2	D	352	PRO
2	D	397	ILE
2	C	212	PRO
2	C	355	PRO
2	C	401	GLU
1	B	103	PRO
2	D	401	GLU

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Mol	Chain	Res	Type
2	D	549	ASN
2	C	417	LEU
1	B	2	PRO
2	C	341	PRO
2	C	131	PRO
2	C	124	PRO
2	C	357	PRO
2	D	417	LEU
2	D	269	PRO
2	D	452	GLY

5.3.2 Protein sidechains (i)

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	88/93 (95%)	52 (59%)	36 (41%)	0 0
1	B	88/93 (95%)	56 (64%)	32 (36%)	0 1
2	C	386/411 (94%)	228 (59%)	158 (41%)	0 0
2	D	386/411 (94%)	237 (61%)	149 (39%)	0 0
All	All	948/1008 (94%)	573 (60%)	375 (40%)	0 0

All (375) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	PRO
1	A	4	GLN
1	A	5	ASP
1	A	9	THR
1	A	10	ILE
1	A	13	MET
1	A	14	CYS
1	A	15	ASN
1	A	17	ARG
1	A	19	SER
1	A	21	THR

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Mol	Chain	Res	Type
1	A	22	LEU
1	A	27	ARG
1	A	30	VAL
1	A	31	ARG
1	A	38	GLU
1	A	41	PHE
1	A	42	SER
1	A	45	TYR
1	A	48	THR
1	A	53	ARG
1	A	54	ASN
1	A	60	LEU
1	A	64	VAL
1	A	68	ILE
1	A	69	VAL
1	A	71	PHE
1	A	74	ASP
1	A	77	THR
1	A	81	GLU
1	A	82	ARG
1	A	87	MET
1	A	92	LEU
1	A	93	LEU
1	A	94	ASP
1	A	102	GLU
2	C	115	CYS
2	C	116	GLU
2	C	117	THR
2	C	120	VAL
2	C	122	GLN
2	C	129	LYS
2	C	130	ILE
2	C	133	ASN
2	C	134	ASP
2	C	137	ILE
2	C	138	LYS
2	C	139	ASN
2	C	144	ILE
2	C	149	SER
2	C	156	SER
2	C	157	ASN
2	C	158	ILE

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Mol	Chain	Res	Type
2	C	159	THR
2	C	161	ARG
2	C	162	ASN
2	C	163	GLN
2	C	164	ILE
2	C	169	SER
2	C	172	ASP
2	C	174	SER
2	C	175	MET
2	C	181	GLU
2	C	186	ASN
2	C	188	ARG
2	C	189	ASN
2	C	190	MET
2	C	192	ASN
2	C	193	GLN
2	C	194	LEU
2	C	196	LEU
2	C	197	LEU
2	C	199	VAL
2	C	203	PHE
2	C	210	LEU
2	C	211	LEU
2	C	217	HIS
2	C	218	ASP
2	C	223	LEU
2	C	230	ILE
2	C	234	LEU
2	C	238	THR
2	C	239	ARG
2	C	242	GLU
2	C	249	MET
2	C	251	THR
2	C	254	LEU
2	C	259	ARG
2	C	260	LEU
2	C	262	THR
2	C	263	GLU
2	C	264	LEU
2	C	265	LYS
2	C	267	LEU
2	C	268	ASN

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Mol	Chain	Res	Type
2	C	270	ARG
2	C	275	ARG
2	C	277	TYR
2	C	278	GLN
2	C	283	ILE
2	C	284	VAL
2	C	287	MET
2	C	288	VAL
2	C	294	ARG
2	C	295	ASP
2	C	297	LEU
2	C	299	LEU
2	C	304	THR
2	C	310	LEU
2	C	316	TYR
2	C	318	ASP
2	C	319	SER
2	C	320	VAL
2	C	323	ARG
2	C	324	ILE
2	C	326	ASN
2	C	329	THR
2	C	330	ASN
2	C	332	PHE
2	C	333	ARG
2	C	338	LEU
2	C	339	ILE
2	C	345	ARG
2	C	346	LEU
2	C	347	ASP
2	C	348	ASN
2	C	351	GLN
2	C	353	MET
2	C	358	ARG
2	C	361	LEU
2	C	362	SER
2	C	363	ARG
2	C	370	ARG
2	C	373	LEU
2	C	377	ILE
2	C	381	LEU
2	C	382	ARG

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Mol	Chain	Res	Type
2	C	384	LEU
2	C	385	MET
2	C	390	LYS
2	C	393	ARG
2	C	394	GLN
2	C	402	ILE
2	C	405	ARG
2	C	411	MET
2	C	415	LEU
2	C	423	GLN
2	C	424	ARG
2	C	425	SER
2	C	426	ARG
2	C	437	ARG
2	C	442	LEU
2	C	444	GLN
2	C	448	VAL
2	C	451	LEU
2	C	455	LEU
2	C	458	LEU
2	C	459	LYS
2	C	460	LEU
2	C	464	LEU
2	C	465	MET
2	C	467	GLN
2	C	472	ASN
2	C	473	ASN
2	C	474	ILE
2	C	476	ILE
2	C	478	MET
2	C	482	SER
2	C	486	LYS
2	C	495	LEU
2	C	497	CYS
2	C	498	ILE
2	C	501	THR
2	C	506	LEU
2	C	507	ARG
2	C	508	ASP
2	C	519	VAL
2	C	521	SER
2	C	524	GLN

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Mol	Chain	Res	Type
2	C	525	ARG
2	C	526	GLN
2	C	531	ILE
2	C	537	ILE
2	C	541	THR
2	C	543	ILE
2	C	546	VAL
2	C	549	ASN
2	C	553	MET
2	C	555	ASN
2	C	560	ASP
2	C	562	VAL
2	C	567	LEU
2	C	571	ASN
2	C	574	SER
1	B	4	GLN
1	B	5	ASP
1	B	9	THR
1	B	10	ILE
1	B	11	THR
1	B	13	MET
1	B	15	ASN
1	B	16	ASN
1	B	19	SER
1	B	21	THR
1	B	25	SER
1	B	26	ASN
1	B	27	ARG
1	B	29	PHE
1	B	31	ARG
1	B	33	LEU
1	B	39	ASP
1	B	41	PHE
1	B	43	LEU
1	B	58	VAL
1	B	64	VAL
1	B	68	ILE
1	B	69	VAL
1	B	71	PHE
1	B	73	THR
1	B	74	ASP
1	B	76	LEU

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Mol	Chain	Res	Type
1	B	77	THR
1	B	82	ARG
1	B	87	MET
1	B	88	GLN
1	B	100	THR
2	D	115	CYS
2	D	117	THR
2	D	120	VAL
2	D	125	CYS
2	D	130	ILE
2	D	133	ASN
2	D	134	ASP
2	D	137	ILE
2	D	138	LYS
2	D	144	ILE
2	D	147	PHE
2	D	156	SER
2	D	157	ASN
2	D	158	ILE
2	D	160	ILE
2	D	161	ARG
2	D	162	ASN
2	D	163	GLN
2	D	165	ASN
2	D	167	LEU
2	D	169	SER
2	D	172	ASP
2	D	174	SER
2	D	175	MET
2	D	179	SER
2	D	180	GLU
2	D	186	ASN
2	D	187	LEU
2	D	189	ASN
2	D	190	MET
2	D	191	SER
2	D	194	LEU
2	D	196	LEU
2	D	197	LEU
2	D	200	ASN
2	D	206	ASN
2	D	210	LEU

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Mol	Chain	Res	Type
2	D	216	LEU
2	D	218	ASP
2	D	222	LEU
2	D	223	LEU
2	D	225	ASN
2	D	227	SER
2	D	229	ARG
2	D	230	ILE
2	D	234	LEU
2	D	238	THR
2	D	239	ARG
2	D	242	GLU
2	D	243	MET
2	D	246	LEU
2	D	247	THR
2	D	249	MET
2	D	258	ASN
2	D	262	THR
2	D	265	LYS
2	D	267	LEU
2	D	268	ASN
2	D	272	ASP
2	D	277	TYR
2	D	279	GLU
2	D	284	VAL
2	D	287	MET
2	D	288	VAL
2	D	295	ASP
2	D	297	LEU
2	D	299	LEU
2	D	300	VAL
2	D	316	TYR
2	D	319	SER
2	D	326	ASN
2	D	329	THR
2	D	330	ASN
2	D	332	PHE
2	D	333	ARG
2	D	338	LEU
2	D	339	ILE
2	D	340	GLN
2	D	343	MET

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Mol	Chain	Res	Type
2	D	345	ARG
2	D	346	LEU
2	D	348	ASN
2	D	357	PRO
2	D	358	ARG
2	D	359	VAL
2	D	364	VAL
2	D	368	SER
2	D	370	ARG
2	D	373	LEU
2	D	377	ILE
2	D	385	MET
2	D	387	THR
2	D	390	LYS
2	D	391	LEU
2	D	397	ILE
2	D	402	ILE
2	D	403	ARG
2	D	404	GLU
2	D	405	ARG
2	D	409	GLN
2	D	411	MET
2	D	422	MET
2	D	423	GLN
2	D	424	ARG
2	D	426	ARG
2	D	427	ASP
2	D	434	ASN
2	D	442	LEU
2	D	444	GLN
2	D	457	ASN
2	D	458	LEU
2	D	459	LYS
2	D	462	ARG
2	D	464	LEU
2	D	465	MET
2	D	470	THR
2	D	473	ASN
2	D	476	ILE
2	D	482	SER
2	D	485	LEU
2	D	486	LYS

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Mol	Chain	Res	Type
2	D	490	ARG
2	D	491	VAL
2	D	495	LEU
2	D	497	CYS
2	D	498	ILE
2	D	506	LEU
2	D	519	VAL
2	D	520	PHE
2	D	523	GLN
2	D	528	LEU
2	D	530	GLN
2	D	531	ILE
2	D	537	ILE
2	D	540	ASN
2	D	541	THR
2	D	543	ILE
2	D	546	VAL
2	D	547	SER
2	D	551	ILE
2	D	554	SER
2	D	556	SER
2	D	560	ASP
2	D	562	VAL
2	D	567	LEU
2	D	570	LEU
2	D	571	ASN
2	D	572	LEU
2	D	574	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (66) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	ASN
1	A	16	ASN
1	A	66	ASN
1	A	88	GLN
1	A	91	GLN
1	A	95	HIS
2	C	121	GLN
2	C	139	ASN
2	C	162	ASN
2	C	163	GLN

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Mol	Chain	Res	Type
2	C	165	ASN
2	C	192	ASN
2	C	193	GLN
2	C	250	HIS
2	C	257	HIS
2	C	258	ASN
2	C	278	GLN
2	C	289	GLN
2	C	330	ASN
2	C	348	ASN
2	C	356	ASN
2	C	392	ASN
2	C	394	GLN
2	C	421	ASN
2	C	423	GLN
2	C	434	ASN
2	C	444	GLN
2	C	450	GLN
2	C	467	GLN
2	C	472	ASN
2	C	502	GLN
2	C	524	GLN
2	C	549	ASN
2	C	571	ASN
1	B	4	GLN
1	B	15	ASN
1	B	16	ASN
1	B	26	ASN
1	B	66	ASN
1	B	95	HIS
2	D	114	ASN
2	D	121	GLN
2	D	139	ASN
2	D	162	ASN
2	D	163	GLN
2	D	165	ASN
2	D	192	ASN
2	D	200	ASN
2	D	206	ASN
2	D	250	HIS
2	D	258	ASN
2	D	268	ASN

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Mol	Chain	Res	Type
2	D	289	GLN
2	D	326	ASN
2	D	330	ASN
2	D	340	GLN
2	D	396	GLN
2	D	421	ASN
2	D	434	ASN
2	D	450	GLN
2	D	457	ASN
2	D	467	GLN
2	D	523	GLN
2	D	524	GLN
2	D	540	ASN
2	D	571	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

12 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	NAG	E	1	3,2	14,14,15	1.09	1 (7%)	17,19,21	1.84	4 (23%)
3	NAG	E	2	3	14,14,15	1.82	2 (14%)	17,19,21	1.02	1 (5%)
3	NAG	F	1	3,2	14,14,15	1.04	1 (7%)	17,19,21	1.57	3 (17%)
3	NAG	F	2	3	14,14,15	1.08	1 (7%)	17,19,21	1.05	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
3	NAG	G	1	3,2	14,14,15	1.00	1 (7%)	17,19,21	1.84	2 (11%)
3	NAG	G	2	3	14,14,15	1.10	1 (7%)	17,19,21	0.93	1 (5%)
3	NAG	H	1	3,2	14,14,15	1.16	1 (7%)	17,19,21	1.68	3 (17%)
3	NAG	H	2	3	14,14,15	1.09	1 (7%)	17,19,21	0.99	1 (5%)
3	NAG	I	1	3,2	14,14,15	0.98	1 (7%)	17,19,21	1.64	2 (11%)
3	NAG	I	2	3	14,14,15	0.93	1 (7%)	17,19,21	0.90	1 (5%)
3	NAG	J	1	3,2	14,14,15	1.07	1 (7%)	17,19,21	1.54	4 (23%)
3	NAG	J	2	3	14,14,15	0.97	1 (7%)	17,19,21	0.83	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	E	2	3	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	4/6/23/26	0/1/1/1
3	NAG	G	1	3,2	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	G	2	3	-	4/6/23/26	0/1/1/1
3	NAG	H	1	3,2	-	2/6/23/26	0/1/1/1
3	NAG	H	2	3	-	2/6/23/26	0/1/1/1
3	NAG	I	1	3,2	-	0/6/23/26	0/1/1/1
3	NAG	I	2	3	-	3/6/23/26	0/1/1/1
3	NAG	J	1	3,2	1/1/5/7	2/6/23/26	0/1/1/1
3	NAG	J	2	3	-	0/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	NAG	O4-C4	5.75	1.56	1.43
3	F	2	NAG	C8-C7	3.46	1.57	1.50
3	E	1	NAG	C8-C7	3.38	1.57	1.50
3	F	1	NAG	C8-C7	3.37	1.57	1.50
3	H	1	NAG	C8-C7	3.37	1.57	1.50
3	G	1	NAG	C8-C7	3.36	1.57	1.50
3	J	2	NAG	C8-C7	3.36	1.57	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2	NAG	C8-C7	3.35	1.57	1.50
3	I	2	NAG	C8-C7	3.34	1.57	1.50
3	I	1	NAG	C8-C7	3.33	1.57	1.50
3	G	2	NAG	C8-C7	3.32	1.57	1.50
3	H	2	NAG	C8-C7	3.24	1.57	1.50
3	J	1	NAG	C8-C7	3.23	1.57	1.50

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	G	1	NAG	O4-C4-C5	-5.85	94.78	109.30
3	I	1	NAG	O4-C4-C5	5.77	123.63	109.30
3	H	1	NAG	O5-C5-C6	-5.16	99.11	107.20
3	F	1	NAG	O4-C4-C5	4.87	121.39	109.30
3	E	1	NAG	O4-C4-C5	-4.74	97.53	109.30
3	E	1	NAG	O5-C5-C6	-4.38	100.34	107.20
3	J	1	NAG	O4-C4-C5	3.70	118.48	109.30
3	G	1	NAG	O5-C5-C6	3.42	112.56	107.20
3	J	1	NAG	O5-C5-C6	-2.98	102.53	107.20
3	H	2	NAG	C1-O5-C5	2.63	115.75	112.19
3	H	1	NAG	O5-C1-C2	-2.60	107.18	111.29
3	F	1	NAG	O5-C5-C6	-2.48	103.32	107.20
3	E	2	NAG	O5-C5-C6	2.44	111.02	107.20
3	H	1	NAG	C1-O5-C5	2.33	115.35	112.19
3	G	2	NAG	C1-O5-C5	2.32	115.34	112.19
3	J	1	NAG	C1-O5-C5	2.32	115.33	112.19
3	E	1	NAG	O5-C1-C2	-2.31	107.64	111.29
3	F	1	NAG	C1-O5-C5	2.25	115.23	112.19
3	F	2	NAG	C1-O5-C5	2.22	115.19	112.19
3	I	1	NAG	C1-O5-C5	2.17	115.14	112.19
3	E	1	NAG	C1-O5-C5	2.17	115.14	112.19
3	J	1	NAG	O5-C1-C2	-2.16	107.87	111.29
3	F	2	NAG	O3-C3-C4	-2.11	105.46	110.35
3	J	2	NAG	O4-C4-C5	-2.07	104.16	109.30
3	I	2	NAG	C1-O5-C5	2.02	114.93	112.19

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	G	1	NAG	C1
3	J	1	NAG	C1

All (25) torsion outliers are listed below:

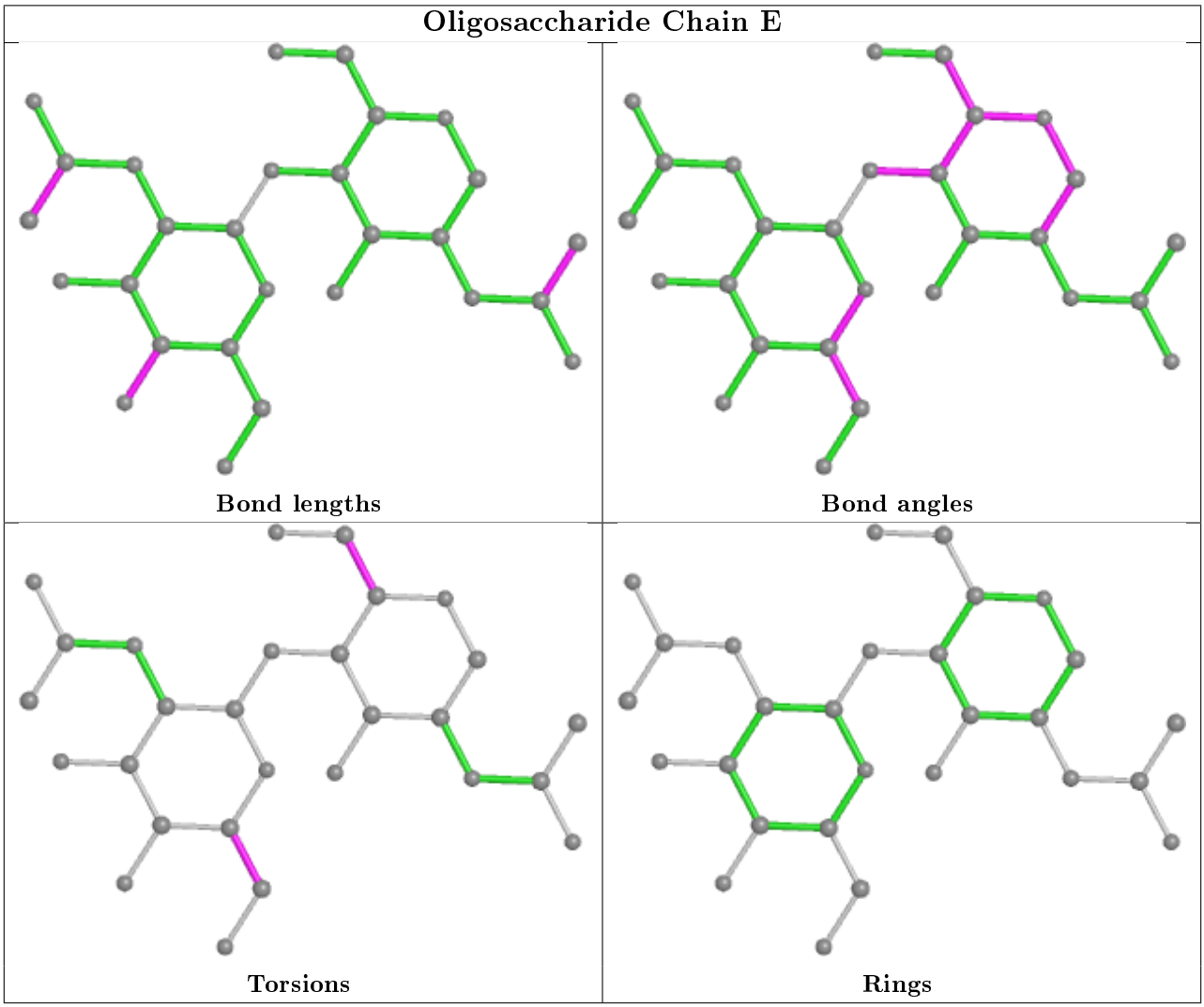
Mol	Chain	Res	Type	Atoms
3	I	2	NAG	C3-C2-N2-C7
3	J	1	NAG	C1-C2-N2-C7
3	G	2	NAG	C1-C2-N2-C7
3	H	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	I	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C4-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	I	2	NAG	C4-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6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

There are no ring outliers.

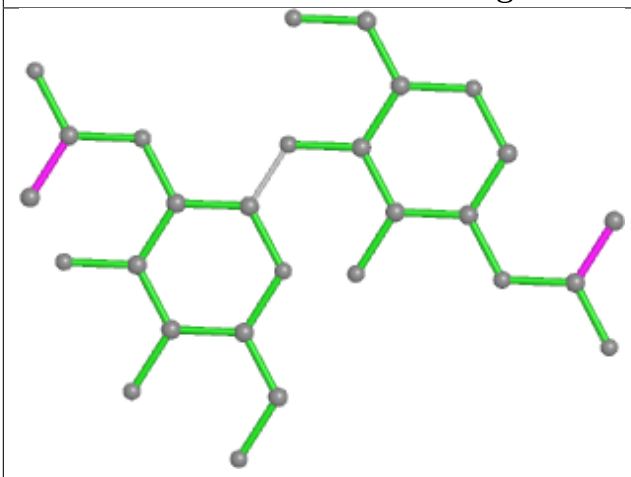
11 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	G	1	NAG	2	0
3	J	2	NAG	2	0
3	E	2	NAG	2	0
3	H	2	NAG	1	0
3	F	2	NAG	1	0
3	F	1	NAG	1	0
3	I	2	NAG	4	0
3	J	1	NAG	6	0
3	G	2	NAG	3	0
3	I	1	NAG	5	0
3	E	1	NAG	1	0

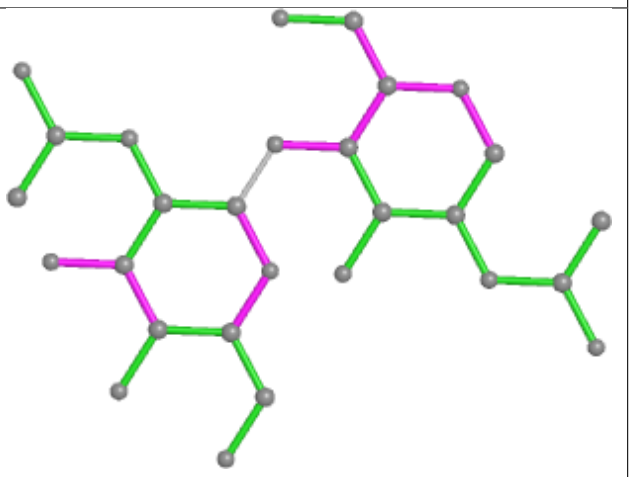
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



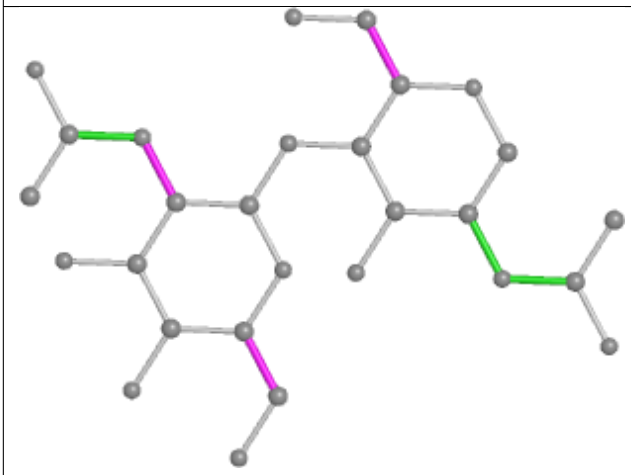
Oligosaccharide Chain F



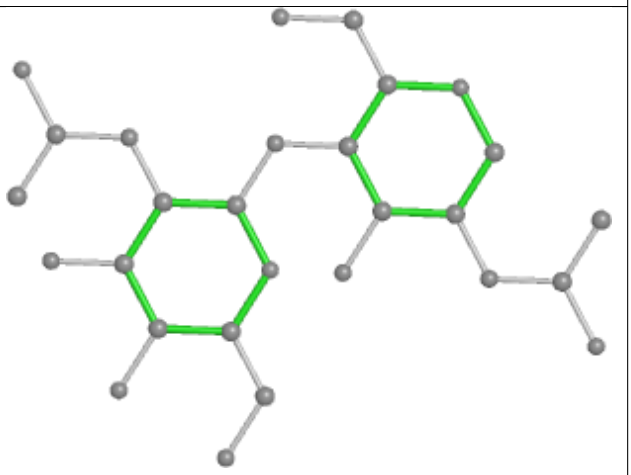
Bond lengths



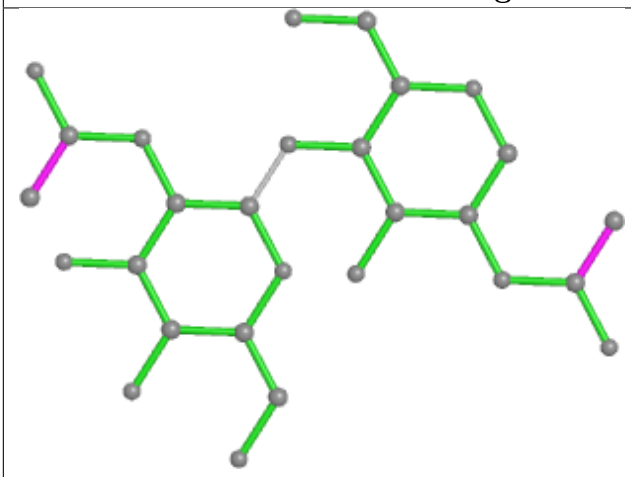
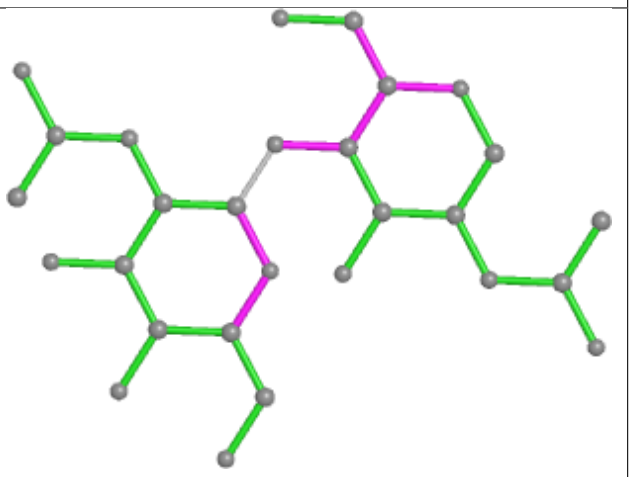
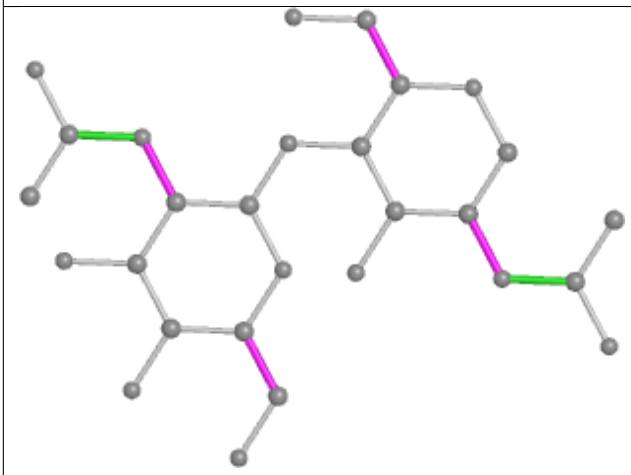
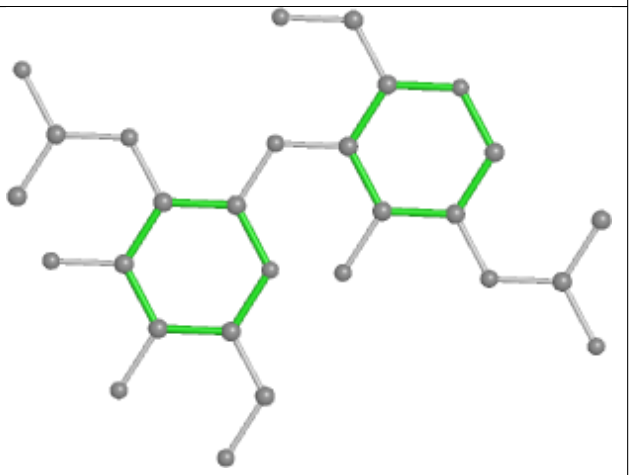
Bond angles



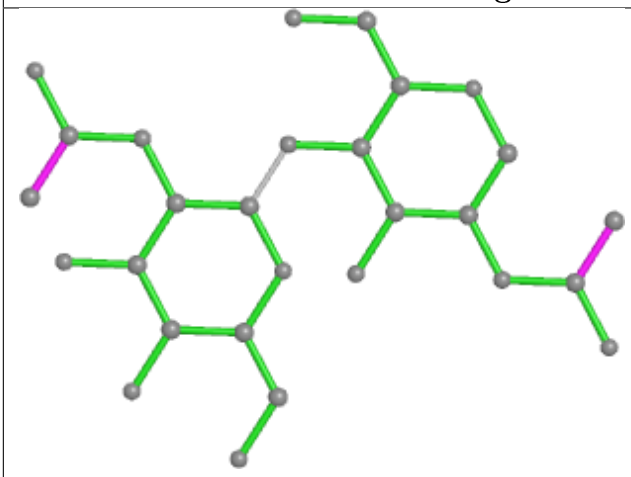
Torsions



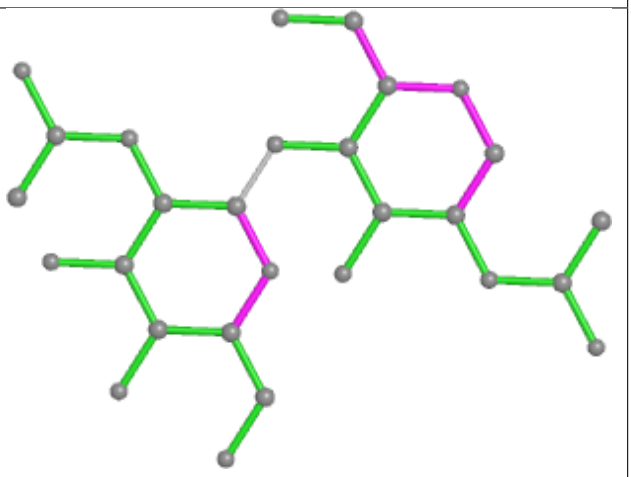
Rings

Oligosaccharide Chain G	
 Bond lengths	 Bond angles
 Torsions	 Rings

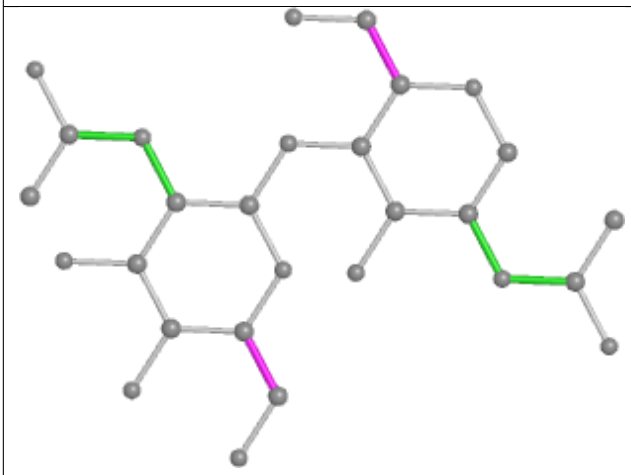
Oligosaccharide Chain H



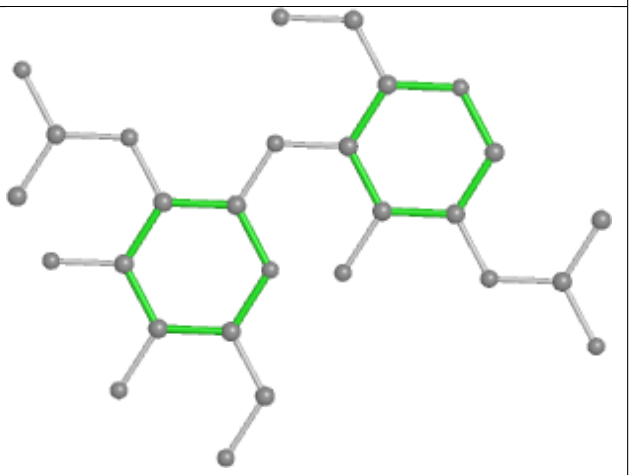
Bond lengths



Bond angles

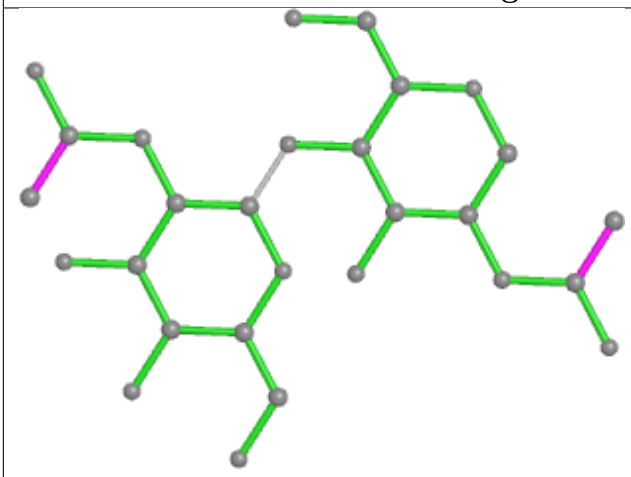


Torsions

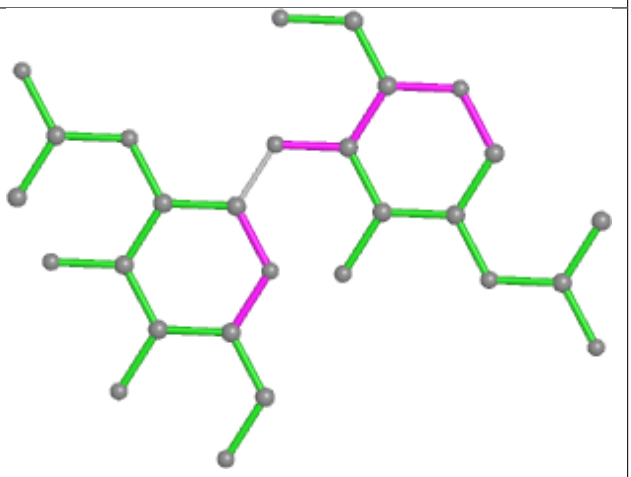


Rings

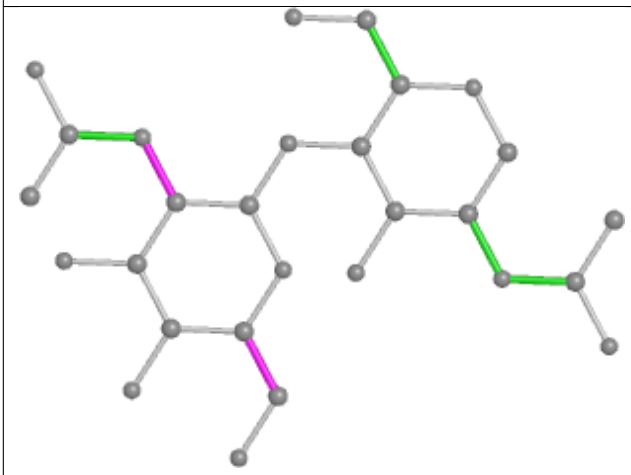
Oligosaccharide Chain I



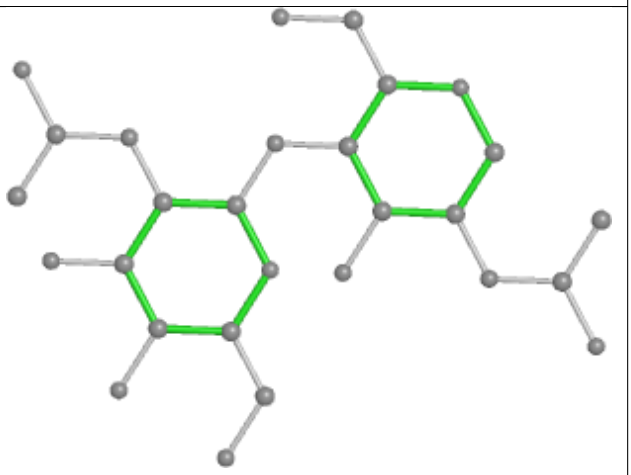
Bond lengths



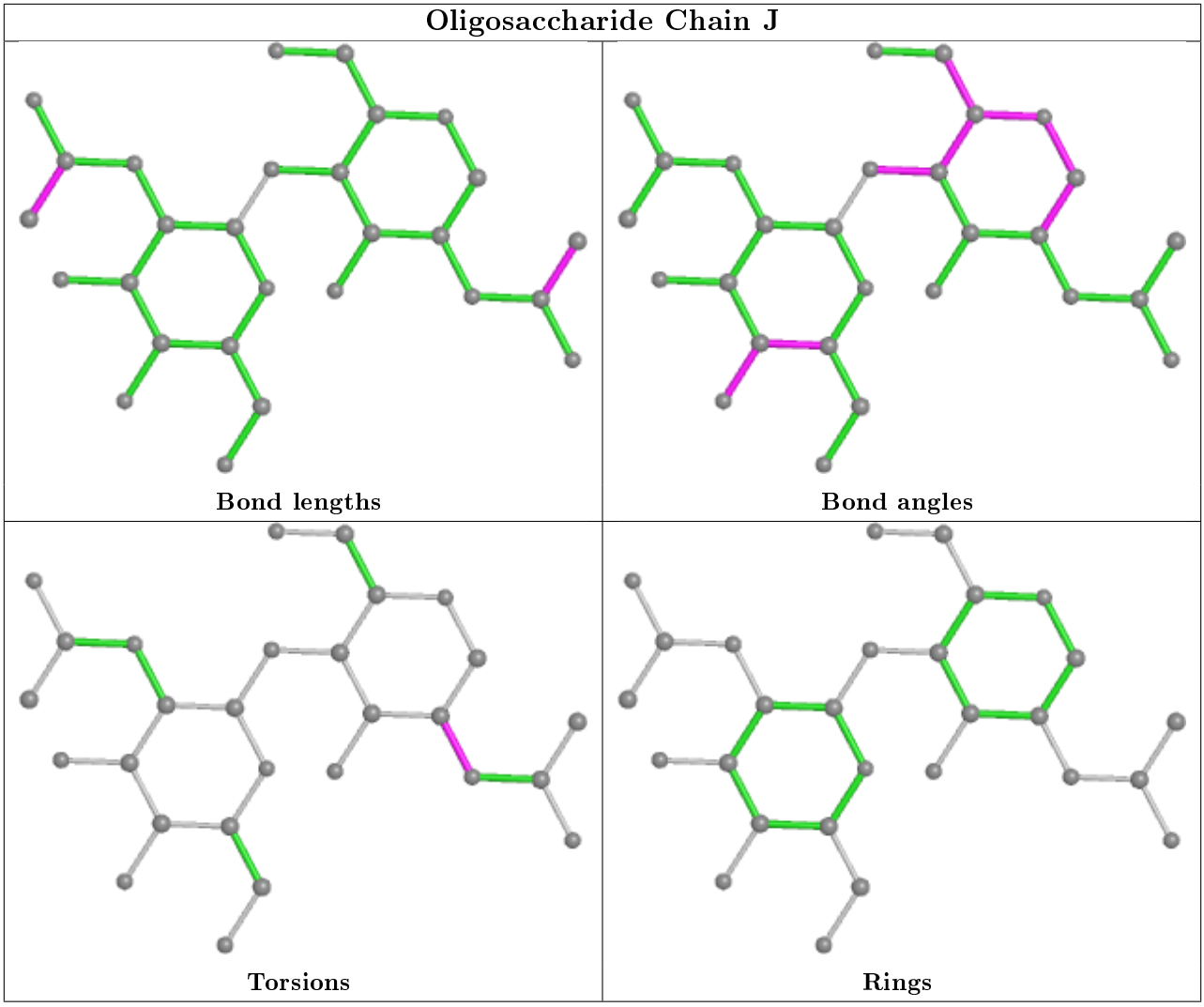
Bond angles



Torsions



Rings



5.6 Ligand geometry (i)

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	HEM	A	580	2	27,50,50	1.53	3 (11%)	17,82,82	1.45	4 (23%)
5	HEM	B	580	2	27,50,50	1.60	4 (14%)	17,82,82	1.41	4 (23%)

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	HEM	A	580	2	-	2/6/54/54	-
5	HEM	B	580	2	-	0/6/54/54	-

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	580	HEM	C3C-C2C	-3.95	1.34	1.40
5	B	580	HEM	C3C-C2C	-3.85	1.35	1.40
5	A	580	HEM	C3B-C2B	-3.75	1.35	1.40
5	B	580	HEM	C3B-C2B	-3.68	1.35	1.40
5	B	580	HEM	C1D-CHD	-3.66	1.30	1.41
5	A	580	HEM	C1A-NA	2.30	1.40	1.36
5	B	580	HEM	C1C-C2C	2.04	1.47	1.42

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	580	HEM	CAD-CBD-CGD	-2.81	107.96	112.67
5	A	580	HEM	CAD-CBD-CGD	-2.77	108.02	112.67
5	B	580	HEM	CAA-CBA-CGA	-2.72	108.10	112.67
5	A	580	HEM	CAA-CBA-CGA	-2.71	108.12	112.67
5	A	580	HEM	CBA-CAA-C2A	-2.56	107.77	112.49
5	B	580	HEM	CBD-CAD-C3D	-2.45	107.97	112.48
5	A	580	HEM	CBD-CAD-C3D	-2.39	108.07	112.48
5	B	580	HEM	CBA-CAA-C2A	-2.38	108.10	112.49

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	580	HEM	C3A-C2A-CAA-CBA
5	A	580	HEM	C3D-CAD-CBD-CGD

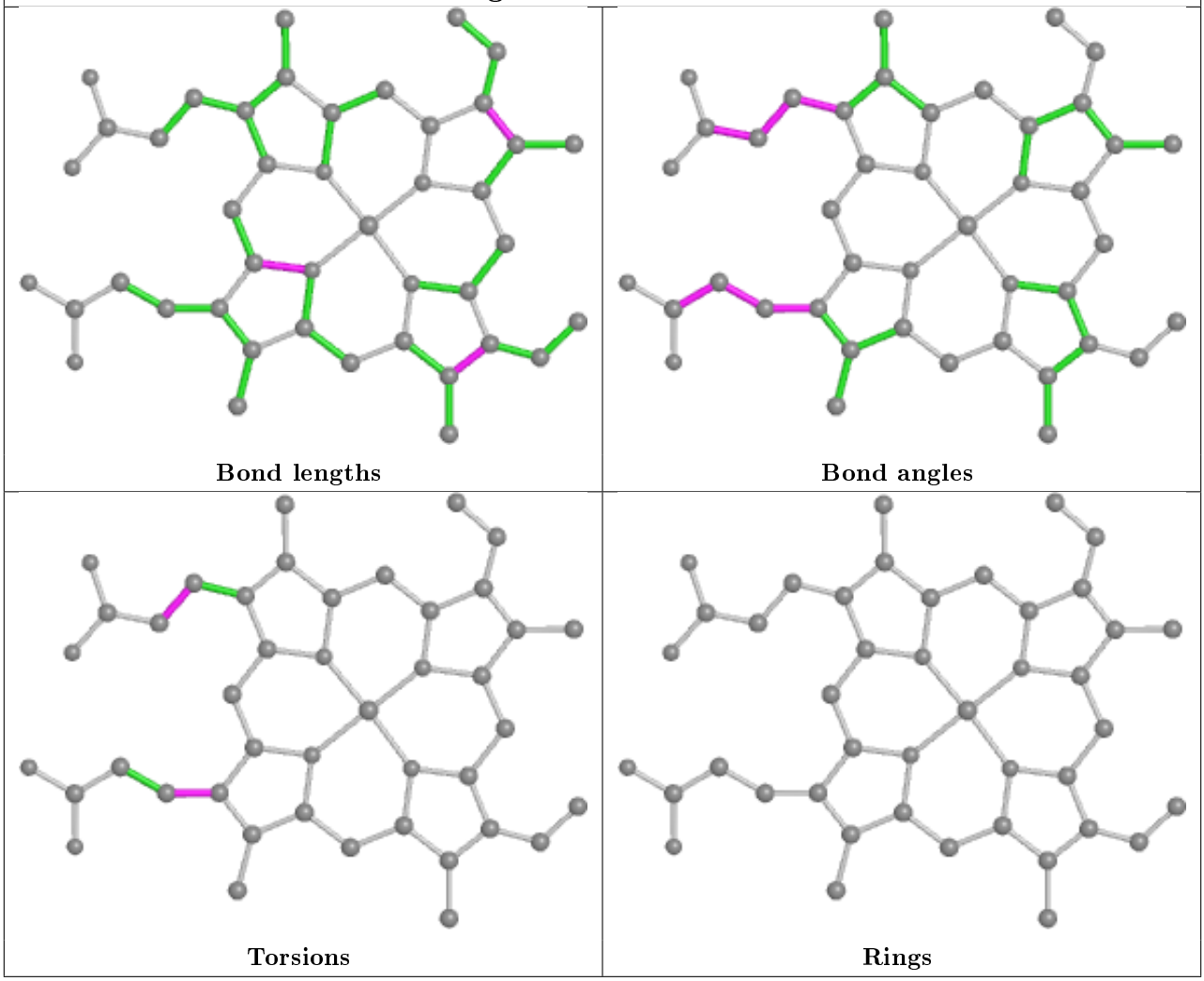
There are no ring outliers.

2 monomers are involved in 67 short contacts:

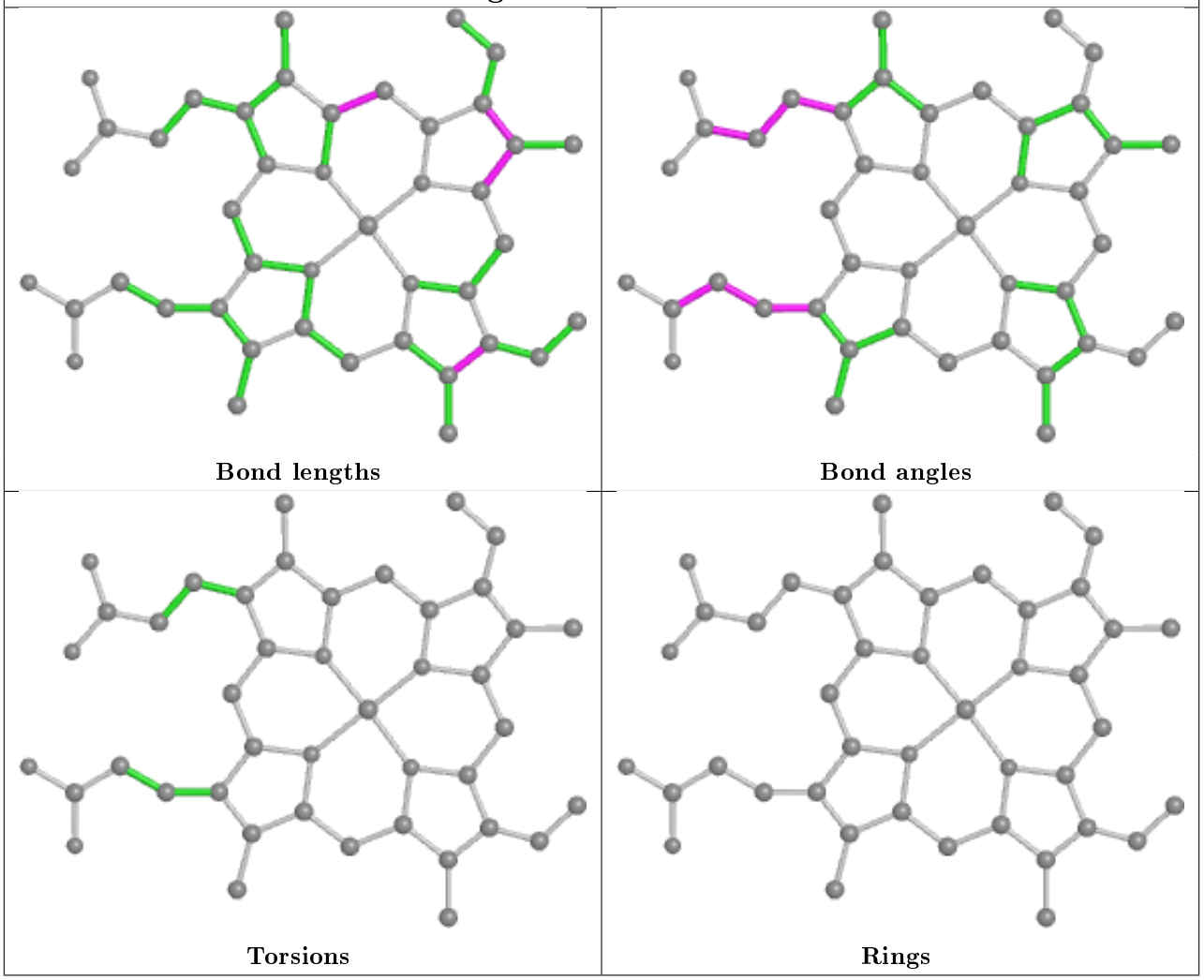
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	580	HEM	35	0
5	B	580	HEM	32	0

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

Ligand HEM A 580



Ligand HEM B 580



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	D	11
2	C	5
1	B	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	3:GLU	C	4:GLN	N	2.32
1	C	560:ASP	C	561:PHE	N	1.95
1	D	179:SER	C	180:GLU	N	1.81
1	D	560:ASP	C	561:PHE	N	1.78
1	D	203:PHE	C	204:GLN	N	1.74
1	D	557:TYR	C	558:PRO	N	1.73
1	C	516:ASN	C	517:GLU	N	1.72
1	D	556:SER	C	557:TYR	N	1.67
1	C	228:ALA	C	229:ARG	N	1.66
1	D	184:ALA	C	185:ARG	N	1.65
1	C	347:ASP	C	348:ASN	N	1.63
1	D	347:ASP	C	348:ASN	N	1.60
1	C	458:LEU	C	459:LYS	N	1.19
1	D	275:ARG	C	276:LEU	N	1.19
1	D	199:VAL	C	200:ASN	N	1.18
1	D	132:PRO	C	133:ASN	N	1.17
1	D	574:SER	C	575:TRP	N	1.04

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.