



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 10:35 AM EDT

PDB ID : 2RFC / pdb_00002rfc
Title : Ligand bound (4-phenylimidazole) Crystal Structure of a Cytochrome P450 from the Thermoacidophilic Archaeon *Picrophilus Torridus*
Authors : Ho, W.W.; Li, H.; Poulos, T.L.; Nishida, C.R.; Ortiz de Montellano, P.R.
Deposited on : 2007-09-28
Resolution : 3.10 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

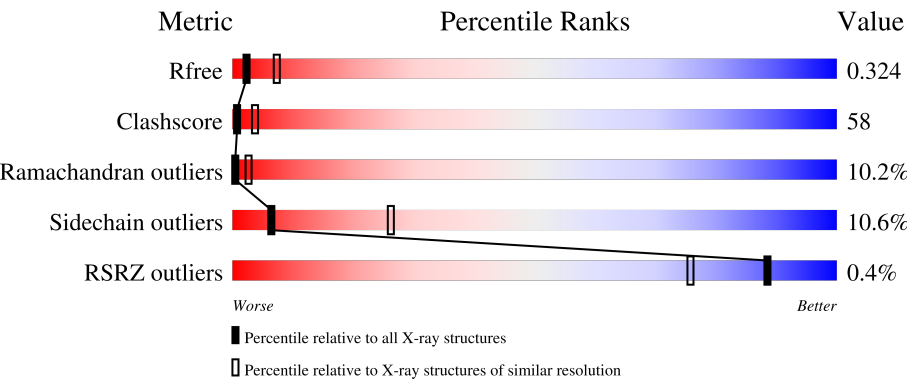
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

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 3.10 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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

Mol	Chain	Length	Quality of chain
1	A	343	% 25%58%15%..
1	B	343	24%56%17%..
1	C	343	22%57%18%..
1	D	343	22%55%20%..

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	PIM	A	411	-	X	-	-
3	PIM	B	411	-	X	-	-
3	PIM	C	411	-	X	-	-

2 Entry composition [i](#)

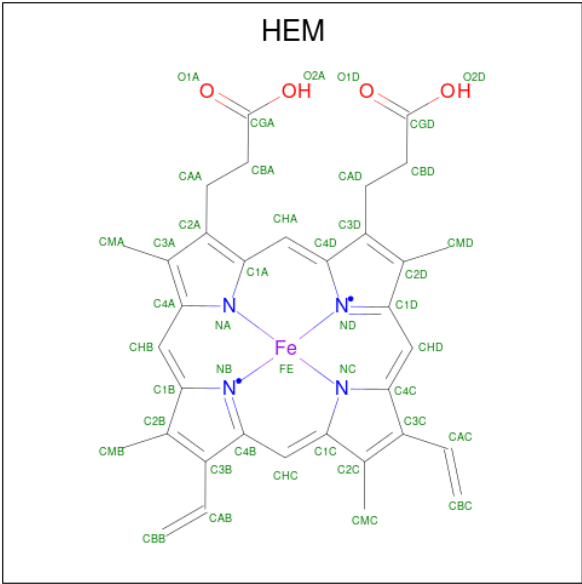
There are 4 unique types of molecules in this entry. The entry contains 11230 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cytochrome P450.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	338	Total	C	N	O	S	0	0	0
			2752	1763	467	511	11			
1	B	338	Total	C	N	O	S	0	0	0
			2752	1763	467	511	11			
1	C	338	Total	C	N	O	S	0	0	0
			2752	1763	467	511	11			
1	D	338	Total	C	N	O	S	0	0	0
			2739	1756	462	510	11			

- Molecule 2 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



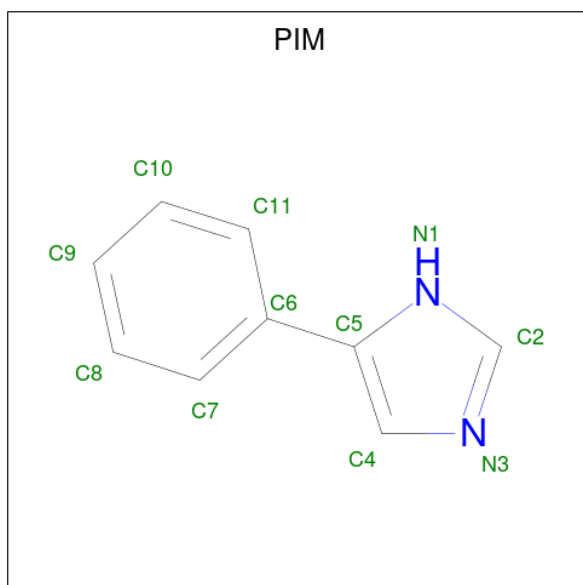
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		
2	B	1	Total	C	Fe	N O	0	0
			43	34	1	4 4		

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

- Molecule 3 is 4-PHENYL-1H-IMIDAZOLE (CCD ID: PIM) (formula: C₉H₈N₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	N	0	0
			11	9	2		
3	B	1	Total	C	N	0	0
			11	9	2		
3	C	1	Total	C	N	0	0
			11	9	2		
3	D	1	Total	C	N	0	0
			11	9	2		

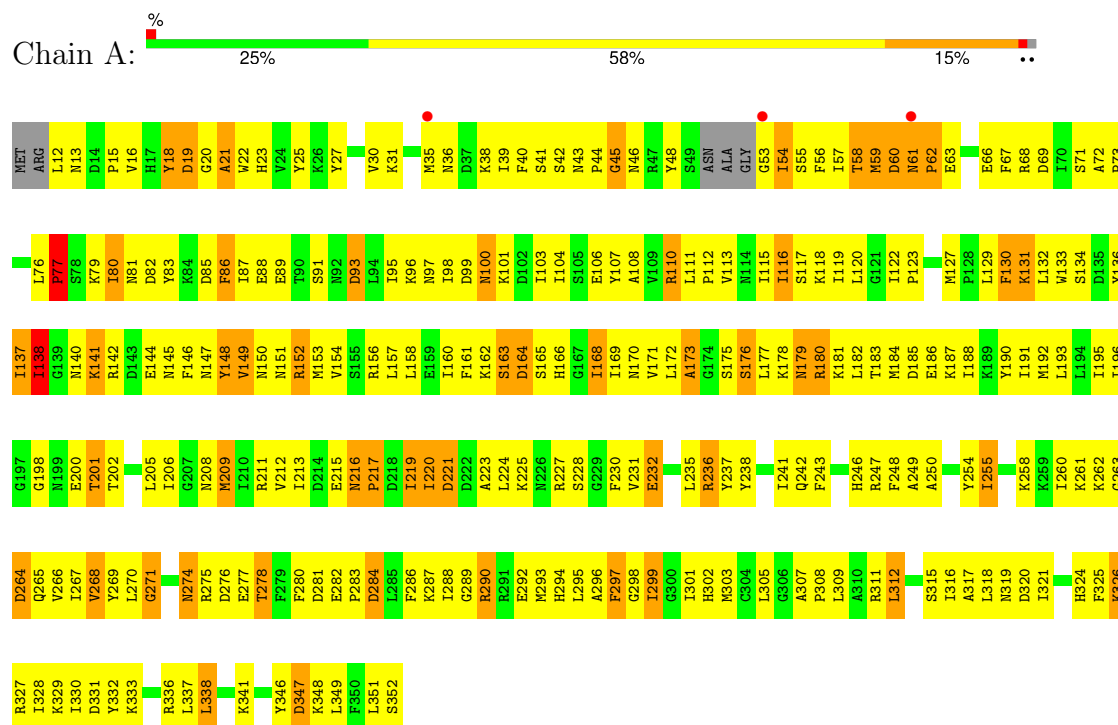
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	5	Total	O	0	0
			5	5		
4	B	5	Total	O	0	0
			5	5		
4	C	9	Total	O	0	0
			9	9		

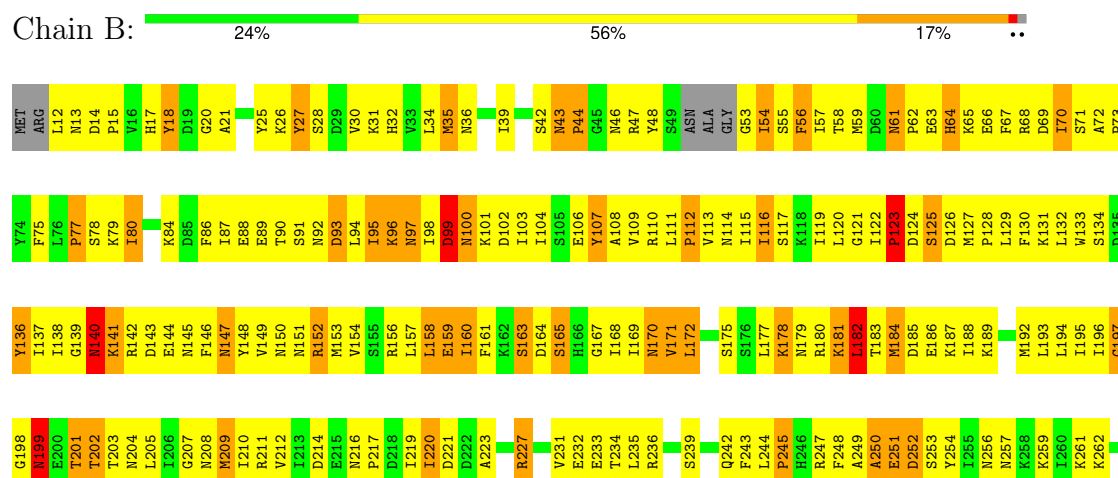
3 Residue-property plots

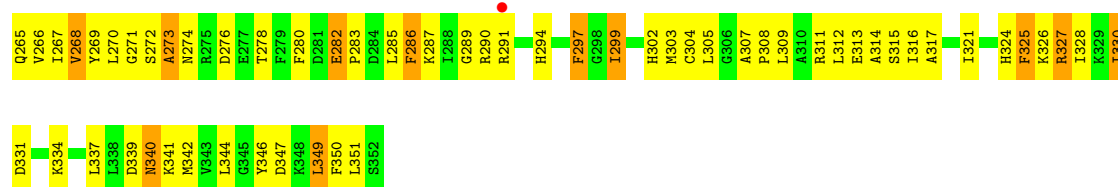
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: Cytochrome P450



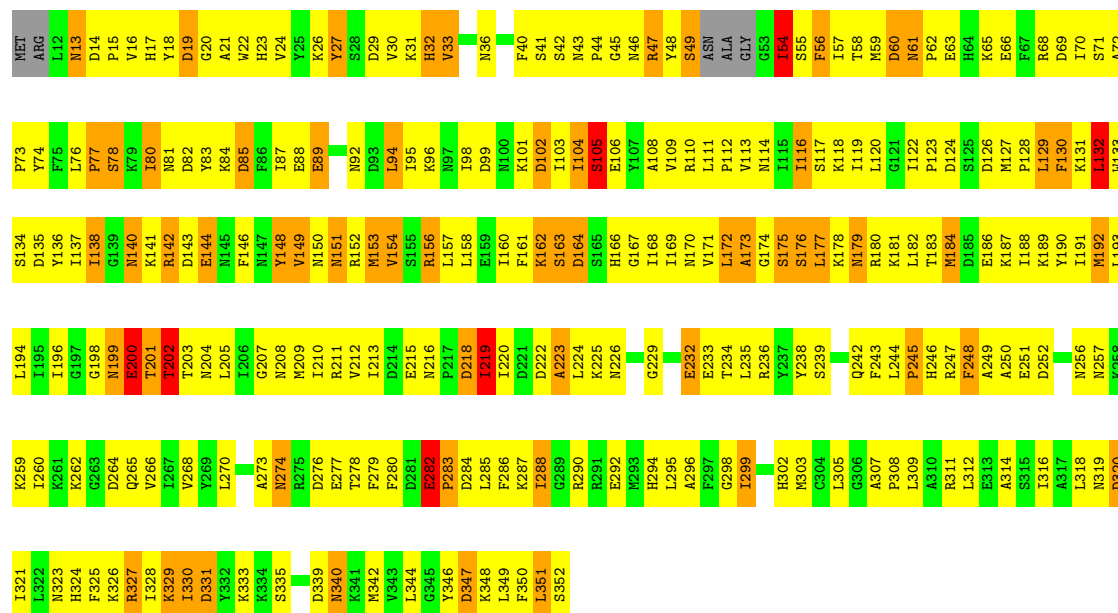
• Molecule 1: Cytochrome P450





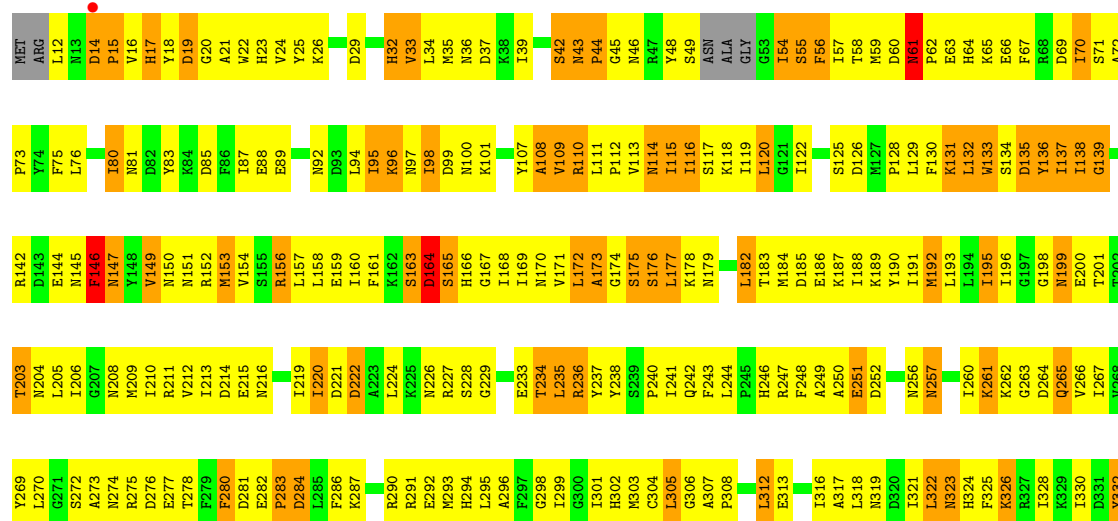
• Molecule 1: Cytochrome P450

Chain C: 22% 57% 18% ..



• Molecule 1: Cytochrome P450

Chain D: 22% 55% 20% ..



K333	K334	S335	R336	L337	L338	D339	M340	K341	M342	V343	L344	G345	Y346	D347	K348	L351	S352
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4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	48.52Å 141.01Å 101.03Å 90.00° 90.30° 90.00°	Depositor
Resolution (Å)	41.85 – 3.10 41.85 – 3.10	Depositor EDS
% Data completeness (in resolution range)	95.5 (41.85-3.10) 95.4 (41.85-3.10)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.82 (at 3.06Å)	Xtriage
Refinement program	CNS 1.2	Depositor
R, R_{free}	0.229 , 0.334 0.219 , 0.324	Depositor DCC
R_{free} test set	1141 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å ²)	49.3	Xtriage
Anisotropy	0.232	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 52.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.029 for h,-k,-l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	11230	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.88% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: PIM, HEM

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	0.57	0/2809	1.08	17/3785 (0.4%)
1	B	0.58	1/2809 (0.0%)	1.06	20/3785 (0.5%)
1	C	0.59	0/2809	1.11	21/3785 (0.6%)
1	D	0.57	0/2796	1.09	29/3770 (0.8%)
All	All	0.58	1/11223 (0.0%)	1.08	87/15125 (0.6%)

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	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	184	MET	SD-CE	6.33	1.95	1.79

All (87) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	166	HIS	N-CA-C	-10.35	99.74	114.12
1	C	199	ASN	N-CA-C	9.36	125.12	112.68
1	C	48	TYR	N-CA-C	-9.27	101.87	113.55
1	C	184	MET	N-CA-C	-8.57	101.93	111.28
1	C	149	VAL	N-CA-C	-8.41	101.03	110.62
1	A	216	ASN	CA-C-N	8.30	130.22	119.84
1	A	216	ASN	C-N-CA	8.30	130.22	119.84
1	C	130	PHE	N-CA-C	8.15	119.85	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	158	LEU	N-CA-C	-7.15	104.68	113.19
1	D	146	PHE	N-CA-C	-7.12	103.60	111.36
1	A	149	VAL	N-CA-C	-7.10	94.58	109.34
1	C	140	ASN	N-CA-C	-7.00	104.00	112.54
1	A	131	LYS	N-CA-C	-6.91	103.68	111.07
1	A	130	PHE	N-CA-C	6.79	119.26	111.11
1	C	170	ASN	N-CA-C	-6.76	104.84	113.23
1	C	43	ASN	N-CA-C	6.66	114.12	108.13
1	B	297	PHE	N-CA-C	-6.46	105.22	113.23
1	B	282	GLU	CA-C-N	6.46	126.39	119.28
1	B	282	GLU	C-N-CA	6.46	126.39	119.28
1	D	14	ASP	CA-C-N	6.41	127.85	119.84
1	D	14	ASP	C-N-CA	6.41	127.85	119.84
1	D	199	ASN	N-CA-C	6.37	118.24	108.12
1	B	186	GLU	N-CA-C	-6.33	104.43	111.71
1	D	110	ARG	N-CA-C	6.33	118.05	111.03
1	D	228	SER	N-CA-C	-6.27	104.44	111.28
1	A	58	THR	N-CA-C	-6.16	104.94	112.88
1	B	328	ILE	N-CA-C	6.14	116.95	107.99
1	C	172	LEU	N-CA-C	6.13	117.63	111.07
1	C	202	THR	N-CA-C	-6.06	104.75	111.36
1	A	144	GLU	N-CA-C	-6.05	104.60	112.23
1	D	42	SER	N-CA-C	-5.96	104.53	112.94
1	D	347	ASP	N-CA-C	-5.91	106.61	113.88
1	B	325	PHE	N-CA-C	5.87	118.18	108.49
1	A	219	ILE	N-CA-C	-5.87	106.01	113.22
1	A	60	ASP	N-CA-C	5.82	119.43	110.42
1	A	338	LEU	N-CA-C	-5.75	102.76	110.24
1	D	132	LEU	N-CA-C	-5.74	102.14	111.04
1	A	351	LEU	N-CA-C	5.67	118.73	110.17
1	A	347	ASP	N-CA-C	-5.67	103.88	112.04
1	D	120	LEU	N-CA-C	-5.66	104.73	111.69
1	D	56	PHE	N-CA-C	5.65	121.16	113.37
1	A	246	HIS	N-CA-C	5.64	118.45	108.24
1	D	305	LEU	N-CA-C	-5.64	105.66	112.54
1	C	347	ASP	N-CA-C	-5.62	104.42	112.13
1	B	103	ILE	N-CA-C	5.62	116.26	110.36
1	D	44	PRO	N-CA-C	-5.60	100.94	112.47
1	D	61	ASN	CA-C-N	5.59	124.78	118.97
1	D	61	ASN	C-N-CA	5.59	124.78	118.97
1	D	220	ILE	N-CA-C	5.58	120.95	109.34
1	D	291	ARG	N-CA-C	-5.54	106.68	113.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	184	MET	N-CA-C	-5.52	106.05	112.89
1	B	136	TYR	N-CA-C	-5.51	104.11	112.04
1	C	175	SER	N-CA-C	5.47	116.84	108.52
1	B	250	ALA	N-CA-C	-5.46	106.33	112.87
1	D	250	ALA	N-CA-C	-5.44	106.62	113.20
1	C	60	ASP	N-CA-C	5.43	116.89	109.18
1	C	56	PHE	N-CA-C	5.41	119.63	113.19
1	D	114	ASN	N-CA-C	-5.41	105.30	111.14
1	B	347	ASP	N-CA-C	-5.40	106.53	113.23
1	C	132	LEU	N-CA-C	-5.40	104.44	111.02
1	B	286	PHE	N-CA-C	-5.36	101.04	109.25
1	B	209	MET	N-CA-C	-5.36	105.35	111.14
1	D	131	LYS	N-CA-C	-5.30	105.92	112.38
1	B	14	ASP	CA-C-N	5.29	126.46	119.84
1	B	14	ASP	C-N-CA	5.29	126.46	119.84
1	D	303	MET	N-CA-C	-5.27	103.06	110.50
1	C	207	GLY	N-CA-C	-5.24	107.28	113.99
1	C	274	ASN	N-CA-C	-5.22	106.88	113.20
1	D	280	PHE	N-CA-C	5.21	116.91	108.41
1	C	27	TYR	N-CA-C	5.21	117.96	111.24
1	D	284	ASP	N-CA-C	5.21	118.94	112.59
1	B	79	LYS	N-CA-C	-5.20	106.13	113.20
1	A	297	PHE	N-CA-C	-5.18	106.80	113.02
1	A	255	ILE	N-CA-C	-5.17	98.58	109.34
1	D	304	CYS	CA-CB-SG	-5.16	102.53	114.40
1	A	106	GLU	N-CA-C	5.16	119.42	113.18
1	C	282	GLU	CA-C-N	5.14	126.27	119.84
1	C	282	GLU	C-N-CA	5.14	126.27	119.84
1	D	242	GLN	N-CA-C	5.12	116.95	111.36
1	D	176	SER	N-CA-C	5.12	115.81	108.74
1	D	322	LEU	N-CA-C	-5.12	107.20	113.50
1	B	167	GLY	N-CA-C	5.11	121.68	112.54
1	D	19	ASP	N-CA-C	-5.09	106.37	112.58
1	A	209	MET	N-CA-C	-5.09	105.43	111.69
1	B	86	PHE	N-CA-C	-5.08	105.74	111.28
1	B	171	VAL	N-CA-C	-5.06	105.91	110.82
1	C	200	GLU	N-CA-C	5.06	121.57	110.80

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2752	0	2756	294	0
1	B	2752	0	2756	332	0
1	C	2752	0	2756	342	0
1	D	2739	0	2730	337	0
2	A	43	0	30	6	0
2	B	43	0	30	6	0
2	C	43	0	30	10	0
2	D	43	0	30	11	0
3	A	11	0	8	1	0
3	B	11	0	8	0	0
3	C	11	0	8	0	0
3	D	11	0	8	1	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	9	0	0	0	0
All	All	11230	0	11150	1289	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 58.

All (1289) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:MET:HA	1:C:187:LYS:HE3	1.23	1.14
1:A:274:ASN:HD21	1:A:294:HIS:HB2	0.98	1.12
1:A:236:ARG:HA	1:A:274:ASN:ND2	1.71	1.06
1:B:183:THR:HG22	1:B:185:ASP:H	1.17	1.06
1:A:236:ARG:HA	1:A:274:ASN:HD22	1.11	1.05
1:C:126:ASP:HA	1:C:129:LEU:HD23	1.36	1.05
1:A:274:ASN:ND2	1:A:294:HIS:HB2	1.71	1.05
1:C:61:ASN:HB3	1:C:62:PRO:HD3	1.34	1.04

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:135:ASP:HA	1:D:138:ILE:HD12	1.39	1.04
1:C:177:LEU:HD12	1:C:178:LYS:H	1.17	1.02
1:C:176:SER:HB2	1:C:180:ARG:O	1.61	1.01
1:C:129:LEU:HD22	1:C:129:LEU:H	1.25	1.00
1:C:56:PHE:HA	1:C:59:MET:HG2	1.44	1.00
1:C:330:ILE:HG22	1:C:331:ASP:H	1.23	0.99
1:C:326:LYS:O	1:C:327:ARG:HG2	1.62	0.99
1:B:138:ILE:HD11	1:B:140:ASN:HB2	1.46	0.98
1:C:73:PRO:HG2	1:C:74:TYR:HD1	1.27	0.98
1:B:153:MET:HE2	1:B:157:LEU:HG	1.46	0.97
1:D:56:PHE:HA	1:D:59:MET:HG3	1.45	0.97
1:D:135:ASP:CG	1:D:136:TYR:H	1.66	0.96
1:A:299:ILE:HA	1:A:303:MET:HE3	1.44	0.96
1:A:166:HIS:HA	1:A:170:ASN:HD22	1.30	0.95
1:C:61:ASN:HB3	1:C:62:PRO:CD	1.96	0.94
1:A:183:THR:HB	1:A:186:GLU:HG3	1.49	0.93
1:D:208:ASN:HD22	1:D:238:TYR:HB3	1.32	0.93
1:B:259:LYS:HZ3	1:B:261:LYS:HE3	1.34	0.93
1:A:330:ILE:HD13	1:A:349:LEU:HD11	1.51	0.92
1:A:236:ARG:CA	1:A:274:ASN:HD22	1.82	0.92
1:D:70:ILE:HG12	1:D:177:LEU:HD21	1.52	0.92
1:C:130:PHE:HE2	1:C:153:MET:HE3	1.36	0.91
1:B:340:ASN:ND2	1:B:342:MET:H	1.68	0.91
1:B:53:GLY:HA3	1:B:58:THR:HG21	1.50	0.91
1:D:110:ARG:O	1:D:113:VAL:HG12	1.71	0.90
1:D:198:GLY:HA2	2:D:410:HEM:HMC2	1.52	0.89
1:B:116:ILE:O	1:B:120:LEU:HG	1.73	0.89
1:C:117:SER:HB2	1:C:127:MET:HE1	1.55	0.89
1:C:56:PHE:HA	1:C:59:MET:CG	2.02	0.88
1:B:138:ILE:HG13	1:B:139:GLY:N	1.89	0.87
1:A:87:ILE:HD12	1:A:312:LEU:HD13	1.57	0.86
1:B:251:GLU:HA	1:B:262:LYS:HB2	1.56	0.86
1:C:176:SER:HA	1:C:182:LEU:CD1	2.06	0.86
1:C:177:LEU:HD12	1:C:178:LYS:N	1.89	0.86
1:A:176:SER:HB2	1:A:181:LYS:HA	1.55	0.86
1:B:101:LYS:HB3	1:B:106:GLU:HG3	1.57	0.85
1:A:307:ALA:HB3	1:A:308:PRO:HD3	1.57	0.85
1:B:232:GLU:HA	1:B:235:LEU:HD12	1.58	0.85
1:C:73:PRO:HG2	1:C:74:TYR:CD1	2.12	0.84
1:C:116:ILE:HG21	1:C:199:ASN:HD21	1.42	0.84
1:D:183:THR:HB	1:D:186:GLU:HG3	1.58	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:PHE:H	1:B:56:PHE:HD2	1.23	0.84
1:C:126:ASP:CA	1:C:129:LEU:HD23	2.08	0.84
1:C:162:LYS:HA	1:C:162:LYS:NZ	1.92	0.84
1:B:133:TRP:O	1:B:137:ILE:HG12	1.78	0.84
1:B:138:ILE:HG13	1:B:139:GLY:H	1.42	0.84
1:D:54:ILE:O	1:D:193:LEU:HD13	1.77	0.82
1:D:157:LEU:HD23	1:D:188:ILE:HG23	1.61	0.82
1:A:183:THR:HB	1:A:186:GLU:CG	2.09	0.82
1:D:176:SER:C	1:D:177:LEU:HD22	2.04	0.82
1:A:27:TYR:CE2	1:A:31:LYS:HD2	2.15	0.81
1:A:274:ASN:HD21	1:A:294:HIS:CB	1.89	0.81
1:D:87:ILE:HG12	1:D:115:ILE:HD12	1.62	0.81
1:B:12:LEU:HD22	1:B:272:SER:OG	1.80	0.81
1:C:14:ASP:HB3	1:C:15:PRO:HD2	1.61	0.81
1:A:55:SER:HB3	1:A:193:LEU:HD22	1.61	0.81
1:A:166:HIS:HA	1:A:170:ASN:ND2	1.96	0.80
1:A:180:ARG:HD3	1:A:181:LYS:O	1.80	0.80
1:D:15:PRO:HA	1:D:23:HIS:O	1.79	0.80
1:D:287:LYS:HD3	1:D:290:ARG:NH2	1.96	0.80
1:C:85:ASP:O	1:C:89:GLU:HB2	1.81	0.80
1:C:136:TYR:HA	1:C:141:LYS:HB3	1.64	0.80
1:A:236:ARG:HH11	1:A:236:ARG:HB3	1.46	0.80
1:A:137:ILE:H	1:A:137:ILE:HD12	1.44	0.79
1:D:227:ARG:HG2	1:D:318:LEU:HD23	1.64	0.79
1:A:201:THR:HB	2:A:410:HEM:HAB	1.65	0.79
1:B:340:ASN:C	1:B:340:ASN:HD22	1.91	0.79
1:B:66:GLU:OE1	1:B:178:LYS:HB2	1.82	0.79
1:C:87:ILE:HG22	1:C:316:ILE:HG21	1.64	0.79
1:D:301:ILE:HG13	1:D:302:HIS:ND1	1.97	0.79
1:C:148:TYR:HD2	1:C:151:ASN:HB2	1.48	0.79
1:A:137:ILE:HG21	1:A:196:ILE:HD13	1.65	0.78
1:D:135:ASP:HA	1:D:138:ILE:CD1	2.13	0.78
1:A:176:SER:HB3	1:A:181:LYS:HD3	1.66	0.78
1:A:30:VAL:HG13	1:A:268:VAL:HG13	1.66	0.78
1:C:128:PRO:HA	1:C:131:LYS:HE2	1.63	0.78
1:D:137:ILE:HD12	1:D:196:ILE:HG12	1.64	0.78
1:D:136:TYR:CE1	1:D:149:VAL:HG21	2.20	0.77
1:A:66:GLU:OE1	1:A:178:LYS:HG3	1.85	0.77
1:C:351:LEU:H	1:C:351:LEU:HD12	1.48	0.77
1:D:164:ASP:O	1:D:165:SER:HB2	1.85	0.77
1:B:137:ILE:HG22	1:B:196:ILE:HG13	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:265:GLN:HE22	1:D:267:ILE:HG13	1.51	0.76
1:C:72:ALA:N	1:C:73:PRO:HD2	2.00	0.76
1:A:99:ASP:O	1:A:101:LYS:HG3	1.84	0.76
1:C:116:ILE:HG21	1:C:199:ASN:ND2	2.01	0.76
1:C:138:ILE:CD1	1:C:200:GLU:HB2	2.16	0.76
1:A:338:LEU:HD23	1:A:347:ASP:HB2	1.67	0.76
1:C:138:ILE:HD11	1:C:200:GLU:HB2	1.66	0.76
1:D:183:THR:HG22	1:D:185:ASP:H	1.50	0.76
1:C:276:ASP:OD1	1:C:278:THR:HB	1.86	0.75
1:A:150:ASN:O	1:A:154:VAL:HG23	1.87	0.75
1:C:226:ASN:ND2	1:C:229:GLY:H	1.84	0.75
1:A:176:SER:CB	1:A:181:LYS:HA	2.17	0.75
1:A:91:SER:O	1:A:95:ILE:HG22	1.87	0.75
1:A:120:LEU:O	1:A:169:ILE:HG13	1.87	0.75
1:B:55:SER:HB3	1:B:193:LEU:HD22	1.69	0.75
1:B:129:LEU:HD12	1:B:129:LEU:H	1.52	0.74
1:C:26:LYS:O	1:C:30:VAL:HG23	1.87	0.74
1:D:248:PHE:HA	1:D:264:ASP:O	1.87	0.74
1:A:220:ILE:HG22	1:A:221:ASP:N	2.02	0.74
1:C:328:ILE:H	1:C:328:ILE:HD12	1.52	0.74
1:D:227:ARG:NE	1:D:319:ASN:HD22	1.85	0.74
1:A:56:PHE:HA	1:A:59:MET:HB2	1.69	0.74
1:A:148:TYR:OH	1:C:303:MET:HE1	1.87	0.74
1:C:129:LEU:H	1:C:129:LEU:CD2	2.01	0.74
1:A:98:ILE:CD1	1:A:107:TYR:HB2	2.18	0.74
1:D:136:TYR:HE1	1:D:149:VAL:HG21	1.52	0.74
1:D:70:ILE:CG1	1:D:177:LEU:HD21	2.17	0.74
1:D:98:ILE:HD12	1:D:107:TYR:HB2	1.69	0.73
1:A:137:ILE:HD12	1:A:137:ILE:N	2.03	0.73
1:B:116:ILE:HA	1:B:119:ILE:HG22	1.69	0.73
1:C:111:LEU:HD23	1:C:111:LEU:C	2.13	0.73
1:C:330:ILE:HG22	1:C:331:ASP:N	2.00	0.73
1:B:157:LEU:C	1:B:159:GLU:H	1.97	0.73
1:D:75:PHE:HA	1:D:80:ILE:HD13	1.70	0.73
1:D:206:ILE:O	1:D:210:ILE:HG13	1.88	0.73
1:A:129:LEU:O	1:A:132:LEU:HB3	1.89	0.73
1:B:340:ASN:HD22	1:B:342:MET:H	1.35	0.73
1:C:153:MET:HE1	1:C:157:LEU:HD22	1.71	0.73
1:D:244:LEU:HD13	2:D:410:HEM:O1A	1.88	0.73
1:A:93:ASP:HA	1:A:96:LYS:HE3	1.71	0.72
1:C:116:ILE:HG13	1:C:198:GLY:HA3	1.68	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:MET:HB2	1:C:128:PRO:HD3	1.71	0.72
1:C:126:ASP:HA	1:C:129:LEU:CD2	2.19	0.72
1:D:108:ALA:O	1:D:112:PRO:HD2	1.90	0.72
1:A:18:TYR:C	1:A:18:TYR:HD1	1.96	0.72
1:C:183:THR:HB	1:C:186:GLU:HG3	1.72	0.72
1:D:135:ASP:CG	1:D:136:TYR:N	2.39	0.72
1:A:18:TYR:C	1:A:18:TYR:CD1	2.67	0.71
1:B:56:PHE:HD2	1:B:56:PHE:N	1.87	0.71
1:C:294:HIS:CE1	1:C:296:ALA:HB3	2.24	0.71
1:D:319:ASN:O	1:D:323:ASN:HB2	1.89	0.71
1:A:22:TRP:CZ3	1:A:258:LYS:HD2	2.26	0.71
1:C:176:SER:HB3	1:C:181:LYS:HD3	1.73	0.71
1:D:56:PHE:HA	1:D:59:MET:CG	2.20	0.71
1:B:87:ILE:HB	1:B:316:ILE:HD12	1.73	0.71
1:D:172:LEU:HD21	1:D:190:TYR:CD2	2.25	0.71
1:A:173:ALA:O	1:A:187:LYS:NZ	2.18	0.71
1:C:236:ARG:HG3	1:C:274:ASN:HB3	1.71	0.71
1:D:184:MET:O	1:D:188:ILE:HG12	1.90	0.71
1:D:211:ARG:O	1:D:215:GLU:HG3	1.91	0.71
1:D:226:ASN:ND2	1:D:229:GLY:H	1.88	0.71
1:A:280:PHE:O	1:A:283:PRO:HD3	1.91	0.71
1:C:184:MET:HA	1:C:187:LYS:CE	2.13	0.71
1:A:86:PHE:O	1:A:89:GLU:HB3	1.91	0.70
1:A:201:THR:HG21	1:A:241:ILE:HD11	1.74	0.70
1:A:309:LEU:HD23	2:A:410:HEM:HAC	1.72	0.70
1:B:161:PHE:CE2	1:B:169:ILE:HG23	2.26	0.70
1:D:22:TRP:O	1:D:267:ILE:N	2.24	0.70
1:D:198:GLY:HA2	2:D:410:HEM:CMC	2.19	0.70
1:A:137:ILE:H	1:A:137:ILE:CD1	2.04	0.70
1:A:188:ILE:O	1:A:192:MET:HG3	1.90	0.70
1:B:92:ASN:O	1:B:95:ILE:HG22	1.91	0.70
1:A:36:ASN:HB3	1:A:39:ILE:HD12	1.71	0.70
1:A:99:ASP:C	1:A:101:LYS:H	1.99	0.70
1:A:184:MET:O	1:A:188:ILE:HG12	1.92	0.70
1:C:103:ILE:HD11	1:C:351:LEU:HD11	1.73	0.70
1:C:319:ASN:ND2	1:C:323:ASN:HD21	1.89	0.70
1:D:80:ILE:HG23	1:D:312:LEU:HD12	1.74	0.70
1:D:265:GLN:HE22	1:D:267:ILE:CG1	2.04	0.70
1:A:18:TYR:O	1:A:20:GLY:N	2.24	0.70
1:A:138:ILE:HG12	1:A:200:GLU:HG3	1.72	0.70
1:C:109:VAL:O	1:C:113:VAL:HG12	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:132:LEU:O	1:D:135:ASP:OD1	2.10	0.70
1:D:183:THR:O	1:D:187:LYS:HG3	1.91	0.70
1:D:137:ILE:CD1	1:D:196:ILE:HG12	2.21	0.70
1:B:102:ASP:HB2	1:B:350:PHE:CZ	2.27	0.69
1:D:177:LEU:HD22	1:D:177:LEU:N	2.06	0.69
1:A:116:ILE:HG13	1:A:198:GLY:HA3	1.74	0.69
1:C:162:LYS:HA	1:C:162:LYS:HZ3	1.56	0.69
1:D:189:LYS:HA	1:D:192:MET:HG3	1.75	0.69
1:C:268:VAL:HG23	1:C:268:VAL:O	1.92	0.69
1:A:61:ASN:HB3	1:A:62:PRO:HD3	1.75	0.69
1:A:169:ILE:HG12	1:A:191:ILE:HD13	1.74	0.69
1:B:137:ILE:HG22	1:B:196:ILE:CG1	2.23	0.69
1:B:26:LYS:O	1:B:30:VAL:HG23	1.92	0.69
1:C:110:ARG:O	1:C:114:ASN:HB2	1.92	0.69
1:C:331:ASP:OD1	1:C:333:LYS:HB2	1.92	0.69
1:C:176:SER:HA	1:C:182:LEU:HD11	1.75	0.69
1:C:277:GLU:HA	1:C:283:PRO:HG3	1.74	0.69
1:D:130:PHE:CE2	1:D:153:MET:HE3	2.28	0.69
1:D:344:LEU:HD12	1:D:345:GLY:N	2.07	0.69
1:A:87:ILE:HG21	1:A:316:ILE:HD12	1.74	0.69
1:C:239:SER:O	1:C:242:GLN:NE2	2.26	0.69
1:A:93:ASP:OD2	1:A:93:ASP:N	2.26	0.68
1:C:282:GLU:OE1	1:C:285:LEU:HD11	1.93	0.68
1:A:118:LYS:HD3	1:A:118:LYS:C	2.18	0.68
1:B:57:ILE:HG23	1:B:58:THR:HG23	1.75	0.68
1:B:251:GLU:HA	1:B:262:LYS:CB	2.24	0.68
1:A:205:LEU:O	1:A:209:MET:HG3	1.93	0.68
1:B:36:ASN:HB3	1:B:39:ILE:HD12	1.76	0.68
1:C:110:ARG:HB3	1:C:110:ARG:NH1	2.08	0.68
1:D:201:THR:HG21	1:D:241:ILE:HD11	1.74	0.68
1:D:227:ARG:HD3	1:D:319:ASN:HB2	1.74	0.68
1:C:113:VAL:HG13	1:C:114:ASN:H	1.59	0.68
1:C:129:LEU:O	1:C:132:LEU:HB2	1.93	0.67
1:D:332:TYR:C	1:D:334:LYS:H	2.02	0.67
1:B:259:LYS:NZ	1:B:261:LYS:HE3	2.09	0.67
1:D:208:ASN:ND2	1:D:238:TYR:HB3	2.09	0.67
1:C:201:THR:HA	1:C:204:ASN:ND2	2.09	0.67
1:D:92:ASN:HA	1:D:95:ILE:HG22	1.77	0.67
1:B:98:ILE:HD13	1:B:106:GLU:HB2	1.76	0.67
1:C:176:SER:HA	1:C:182:LEU:HD12	1.77	0.67
1:A:208:ASN:O	1:A:212:VAL:HG23	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:ASN:HD22	1:D:44:PRO:CD	2.08	0.67
1:D:66:GLU:O	1:D:177:LEU:HG	1.95	0.67
1:A:137:ILE:HG21	1:A:196:ILE:CD1	2.24	0.66
1:A:299:ILE:CA	1:A:303:MET:HE3	2.21	0.66
1:B:112:PRO:HB2	1:B:199:ASN:HD22	1.58	0.66
1:D:129:LEU:O	1:D:132:LEU:HB3	1.95	0.66
1:D:221:ASP:HA	1:D:224:LEU:HD12	1.77	0.66
1:D:216:ASN:O	1:D:219:ILE:HG22	1.96	0.66
1:A:95:ILE:HG13	1:A:95:ILE:O	1.95	0.66
1:B:56:PHE:N	1:B:59:MET:HE3	2.11	0.66
1:C:134:SER:O	1:C:138:ILE:HB	1.95	0.66
1:C:202:THR:HA	2:C:410:HEM:CBB	2.26	0.66
1:B:75:PHE:HA	1:B:80:ILE:HD13	1.75	0.66
1:D:249:ALA:HB3	1:D:264:ASP:H	1.60	0.66
1:B:138:ILE:CG1	1:B:139:GLY:H	2.08	0.66
1:B:216:ASN:O	1:B:219:ILE:HG22	1.96	0.66
1:B:56:PHE:N	1:B:56:PHE:CD2	2.59	0.66
1:D:234:THR:O	1:D:237:TYR:N	2.29	0.66
1:A:156:ARG:O	1:A:160:ILE:HG12	1.96	0.66
1:D:17:HIS:ND1	1:D:18:TYR:N	2.42	0.66
1:A:30:VAL:HG13	1:A:268:VAL:CG1	2.26	0.65
1:B:12:LEU:HD13	1:B:25:TYR:O	1.96	0.65
1:D:98:ILE:CD1	1:D:107:TYR:HB2	2.25	0.65
1:C:71:SER:C	1:C:73:PRO:HD2	2.21	0.65
1:B:21:ALA:HB1	1:B:267:ILE:HD13	1.77	0.65
1:C:138:ILE:HG22	1:C:140:ASN:H	1.61	0.65
1:D:270:LEU:O	1:D:274:ASN:ND2	2.30	0.65
1:A:158:LEU:HD22	1:C:81:ASN:ND2	2.10	0.65
1:C:22:TRP:CD1	1:C:260:ILE:HG23	2.31	0.65
1:D:198:GLY:N	2:D:410:HEM:HAC	2.12	0.65
1:C:68:ARG:HE	1:C:305:LEU:HD13	1.62	0.65
1:C:251:GLU:HA	1:C:262:LYS:HB2	1.77	0.65
1:D:130:PHE:HE2	1:D:153:MET:HE3	1.61	0.65
1:B:144:GLU:HB3	1:D:35:MET:CE	2.27	0.65
1:B:156:ARG:O	1:B:160:ILE:HG13	1.95	0.65
1:C:326:LYS:O	1:C:327:ARG:CG	2.44	0.65
1:B:299:ILE:HA	1:B:303:MET:SD	2.36	0.65
1:A:276:ASP:OD1	1:A:278:THR:HG22	1.97	0.65
1:B:153:MET:HE3	1:B:156:ARG:HB3	1.78	0.65
1:A:302:HIS:HA	2:A:410:HEM:O2D	1.97	0.64
1:B:53:GLY:HA3	1:B:58:THR:CG2	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:ASP:HB3	1:C:259:LYS:NZ	2.11	0.64
1:B:95:ILE:O	1:B:98:ILE:HG22	1.97	0.64
1:D:134:SER:OG	1:D:135:ASP:N	2.22	0.64
1:C:157:LEU:O	1:C:161:PHE:HD1	1.81	0.64
1:D:138:ILE:HG22	1:D:138:ILE:O	1.97	0.64
1:A:42:SER:HA	1:A:247:ARG:CD	2.27	0.64
1:B:17:HIS:O	1:B:18:TYR:HB3	1.96	0.64
1:D:178:LYS:O	1:D:178:LYS:HG2	1.96	0.64
1:D:276:ASP:OD1	1:D:278:THR:HB	1.98	0.64
1:C:146:PHE:HA	1:C:149:VAL:HG23	1.78	0.64
1:A:89:GLU:O	1:A:93:ASP:OD2	2.15	0.64
1:C:329:LYS:HB2	1:C:329:LYS:NZ	2.12	0.64
1:A:38:LYS:H	1:A:38:LYS:HD2	1.62	0.64
1:B:138:ILE:CG1	1:B:139:GLY:N	2.60	0.64
1:C:329:LYS:HB2	1:C:329:LYS:HZ2	1.63	0.64
1:D:95:ILE:O	1:D:96:LYS:C	2.40	0.64
1:A:183:THR:HG22	1:A:186:GLU:H	1.63	0.64
1:B:183:THR:HG22	1:B:184:MET:N	2.13	0.64
1:D:43:ASN:HD22	1:D:44:PRO:HD2	1.62	0.64
1:D:73:PRO:O	1:D:76:LEU:HG	1.98	0.64
1:C:130:PHE:CE2	1:C:153:MET:HE3	2.26	0.63
1:A:98:ILE:HA	1:A:101:LYS:HD2	1.81	0.63
1:B:56:PHE:CE1	1:B:68:ARG:HA	2.32	0.63
1:B:299:ILE:HA	1:B:303:MET:CE	2.26	0.63
1:D:168:ILE:HA	1:D:171:VAL:CG2	2.29	0.63
1:A:67:PHE:CE2	1:A:182:LEU:HD11	2.33	0.63
1:C:116:ILE:CG2	1:C:199:ASN:HD21	2.10	0.63
1:C:192:MET:O	1:C:196:ILE:HD13	1.99	0.63
1:C:21:ALA:HB1	1:C:265:GLN:O	1.98	0.63
1:C:80:ILE:HD11	1:C:309:LEU:HD13	1.81	0.63
1:B:138:ILE:HG13	1:B:140:ASN:H	1.62	0.63
1:B:247:ARG:HB2	1:B:266:VAL:O	1.98	0.63
1:C:126:ASP:C	1:C:129:LEU:HD23	2.23	0.63
1:A:21:ALA:HB2	1:A:265:GLN:HB3	1.80	0.63
1:A:100:ASN:HD22	1:B:35:MET:HE2	1.64	0.63
1:B:61:ASN:O	1:B:62:PRO:C	2.40	0.63
1:D:22:TRP:NE1	1:D:260:ILE:HG23	2.13	0.63
1:D:157:LEU:CD2	1:D:188:ILE:HG23	2.27	0.63
1:C:24:VAL:HG11	1:C:29:ASP:O	1.99	0.62
1:C:123:PRO:HB2	1:C:126:ASP:OD2	1.99	0.62
1:D:332:TYR:C	1:D:334:LYS:N	2.55	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:332:TYR:HD1	1:D:332:TYR:H	1.46	0.62
1:B:55:SER:C	1:B:59:MET:HE3	2.24	0.62
1:C:162:LYS:HA	1:C:162:LYS:HZ2	1.64	0.62
2:C:410:HEM:HMC1	2:C:410:HEM:HBC2	1.82	0.62
1:D:168:ILE:HA	1:D:171:VAL:HG23	1.81	0.62
1:A:23:HIS:CE1	1:A:267:ILE:HD12	2.34	0.62
1:B:156:ARG:NH1	1:B:159:GLU:HG2	2.14	0.62
1:D:161:PHE:CE2	1:D:169:ILE:HG23	2.34	0.62
1:A:81:ASN:C	1:A:83:TYR:H	2.06	0.62
1:B:178:LYS:C	1:B:180:ARG:H	2.06	0.62
1:C:200:GLU:O	1:C:203:THR:N	2.33	0.62
1:D:111:LEU:O	1:D:115:ILE:HG12	1.99	0.62
1:D:244:LEU:HD13	2:D:410:HEM:CGA	2.30	0.62
1:A:328:ILE:HG22	1:A:328:ILE:O	2.00	0.61
1:A:68:ARG:O	1:A:72:ALA:HB2	1.99	0.61
1:C:66:GLU:OE1	1:C:177:LEU:HG	2.00	0.61
1:C:118:LYS:HD2	1:C:118:LYS:O	2.01	0.61
1:D:92:ASN:O	1:D:95:ILE:HG22	2.00	0.61
1:B:61:ASN:HA	1:B:64:HIS:HB3	1.81	0.61
1:D:156:ARG:HE	1:D:156:ARG:HA	1.66	0.61
1:B:236:ARG:NH2	1:B:283:PRO:O	2.33	0.61
1:C:156:ARG:O	1:C:160:ILE:HG12	2.00	0.61
1:B:178:LYS:O	1:B:180:ARG:N	2.26	0.61
1:B:244:LEU:HD13	2:B:410:HEM:HBA2	1.80	0.61
1:D:113:VAL:O	1:D:117:SER:CB	2.48	0.61
1:D:236:ARG:HB2	1:D:294:HIS:CB	2.31	0.61
1:B:92:ASN:HA	1:B:95:ILE:CG2	2.30	0.61
1:B:116:ILE:HG23	1:B:120:LEU:HD11	1.83	0.61
1:B:157:LEU:C	1:B:159:GLU:N	2.57	0.61
1:A:330:ILE:O	1:A:330:ILE:HG22	1.99	0.61
1:B:280:PHE:O	1:B:283:PRO:HD3	2.01	0.61
1:A:254:TYR:HA	1:A:258:LYS:O	2.01	0.61
1:C:163:SER:O	1:C:164:ASP:HB3	2.00	0.61
1:C:167:GLY:O	1:C:171:VAL:HG23	2.01	0.60
1:A:56:PHE:HE1	2:A:410:HEM:HBD2	1.65	0.60
1:A:62:PRO:HG2	1:A:63:GLU:H	1.66	0.60
1:A:138:ILE:HD12	1:A:138:ILE:H	1.65	0.60
1:B:69:ASP:O	1:B:71:SER:N	2.33	0.60
1:C:279:PHE:CE2	1:C:292:GLU:HB3	2.36	0.60
1:D:156:ARG:O	1:D:160:ILE:HG12	2.02	0.60
1:D:174:GLY:O	1:D:175:SER:HB3	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:MET:O	1:A:131:LYS:HG2	2.00	0.60
1:A:201:THR:HB	2:A:410:HEM:CAB	2.32	0.60
1:C:201:THR:C	2:C:410:HEM:HBB2	2.26	0.60
1:B:84:LYS:C	1:B:84:LYS:HD3	2.27	0.60
1:D:14:ASP:OD1	1:D:15:PRO:HD2	2.02	0.60
1:B:123:PRO:O	1:B:125:SER:N	2.29	0.60
1:C:68:ARG:NH2	1:C:305:LEU:HA	2.17	0.60
1:D:55:SER:C	1:D:59:MET:HE3	2.27	0.60
1:A:236:ARG:HH11	1:A:236:ARG:CB	2.12	0.60
1:C:41:SER:O	1:C:247:ARG:HD2	2.00	0.60
1:D:61:ASN:HB3	1:D:62:PRO:CD	2.31	0.60
1:B:130:PHE:CE1	1:B:195:ILE:HD11	2.37	0.59
1:B:144:GLU:O	1:D:35:MET:HE1	2.02	0.59
1:C:202:THR:HA	2:C:410:HEM:HBB1	1.84	0.59
1:C:226:ASN:HB3	1:C:288:ILE:HD13	1.83	0.59
1:D:172:LEU:HD21	1:D:190:TYR:CG	2.36	0.59
1:C:111:LEU:HB3	1:C:112:PRO:CD	2.32	0.59
1:B:72:ALA:N	1:B:73:PRO:HD2	2.17	0.59
1:B:92:ASN:C	1:B:95:ILE:HG22	2.28	0.59
1:C:135:ASP:OD2	1:C:141:LYS:HD3	2.01	0.59
1:C:136:TYR:CE2	1:C:143:ASP:HB2	2.36	0.59
1:D:135:ASP:O	1:D:137:ILE:N	2.36	0.59
1:C:252:ASP:HB3	1:C:259:LYS:CE	2.32	0.59
1:D:330:ILE:HG12	1:D:351:LEU:CD2	2.31	0.59
1:B:129:LEU:O	1:B:130:PHE:C	2.45	0.59
1:D:201:THR:HA	1:D:204:ASN:ND2	2.17	0.59
1:B:180:ARG:NH2	1:B:182:LEU:HA	2.17	0.59
1:C:135:ASP:OD2	1:C:141:LYS:HB2	2.03	0.59
1:C:148:TYR:HD2	1:C:151:ASN:CB	2.15	0.59
1:D:99:ASP:O	1:D:100:ASN:HB2	2.02	0.59
1:D:227:ARG:CD	1:D:319:ASN:HB2	2.31	0.59
1:A:205:LEU:HD22	1:A:235:LEU:HD21	1.85	0.59
1:B:153:MET:HG3	1:B:157:LEU:HD12	1.84	0.59
1:B:183:THR:O	1:B:187:LYS:HG3	2.01	0.59
1:D:12:LEU:HD13	1:D:25:TYR:O	2.02	0.59
1:D:136:TYR:C	1:D:138:ILE:N	2.57	0.59
1:D:172:LEU:HD11	1:D:190:TYR:CE2	2.37	0.59
1:A:116:ILE:HD12	1:A:120:LEU:HD11	1.83	0.59
1:B:72:ALA:HA	1:B:305:LEU:HD11	1.84	0.59
1:B:102:ASP:O	1:B:106:GLU:HG2	2.03	0.59
1:D:144:GLU:CD	1:D:144:GLU:H	2.10	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:184:MET:HE3	1:C:84:LYS:CE	2.33	0.59
1:A:249:ALA:O	1:A:263:GLY:N	2.36	0.58
1:B:133:TRP:C	1:B:137:ILE:HG12	2.28	0.58
1:A:22:TRP:CH2	1:A:258:LYS:HD2	2.38	0.58
1:B:227:ARG:O	1:B:231:VAL:HG23	2.04	0.58
1:D:43:ASN:HD22	1:D:44:PRO:N	2.01	0.58
1:B:30:VAL:HG21	1:B:273:ALA:HB2	1.86	0.58
1:B:156:ARG:HH11	1:B:159:GLU:HG2	1.68	0.58
1:B:340:ASN:ND2	1:B:340:ASN:C	2.61	0.58
1:C:256:ASN:O	1:C:257:ASN:HB2	2.03	0.58
1:A:88:GLU:HG3	1:A:316:ILE:HG23	1.86	0.58
1:B:66:GLU:OE1	1:B:178:LYS:CB	2.51	0.58
1:B:163:SER:OG	1:B:164:ASP:N	2.37	0.58
1:B:180:ARG:HG2	1:B:181:LYS:H	1.67	0.58
1:C:84:LYS:O	1:C:88:GLU:HG3	2.03	0.58
1:A:227:ARG:HD2	1:A:319:ASN:HD22	1.69	0.58
1:C:57:ILE:HG13	2:C:410:HEM:HBD1	1.85	0.58
1:C:270:LEU:HD22	1:C:295:LEU:O	2.03	0.58
1:A:18:TYR:C	1:A:20:GLY:H	2.12	0.58
1:A:247:ARG:HG2	1:A:247:ARG:HH11	1.69	0.58
1:C:116:ILE:CD1	1:C:120:LEU:HG	2.33	0.58
1:C:184:MET:O	1:C:187:LYS:HB2	2.04	0.58
1:C:204:ASN:C	1:C:208:ASN:HD22	2.12	0.58
1:C:325:PHE:HB2	1:C:328:ILE:HG13	1.84	0.58
1:C:347:ASP:OD2	1:C:348:LYS:HG2	2.03	0.58
1:B:84:LYS:HE2	1:B:88:GLU:OE2	2.03	0.58
1:B:119:ILE:C	1:B:120:LEU:HD23	2.29	0.58
1:D:332:TYR:N	1:D:332:TYR:CD1	2.72	0.58
1:D:340:ASN:OD1	1:D:342:MET:N	2.36	0.58
1:D:24:VAL:CG1	1:D:29:ASP:HB3	2.34	0.58
1:B:212:VAL:HG11	1:B:286:PHE:CE1	2.39	0.57
1:B:236:ARG:HG2	1:B:274:ASN:HB3	1.86	0.57
1:C:113:VAL:HG13	1:C:114:ASN:N	2.19	0.57
1:C:209:MET:HE1	1:C:314:ALA:O	2.04	0.57
1:B:208:ASN:O	1:B:212:VAL:HG23	2.04	0.57
1:C:259:LYS:O	1:C:259:LYS:HG3	2.04	0.57
1:D:132:LEU:C	1:D:134:SER:N	2.62	0.57
1:A:330:ILE:CD1	1:A:349:LEU:HD11	2.31	0.57
1:C:136:TYR:CE2	1:C:146:PHE:HB3	2.40	0.57
1:C:224:LEU:C	1:C:226:ASN:H	2.12	0.57
1:C:224:LEU:O	1:C:226:ASN:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:72:ALA:HA	1:D:305:LEU:HD11	1.86	0.57
1:B:324:HIS:ND1	1:B:324:HIS:O	2.37	0.57
1:C:247:ARG:HG2	1:C:247:ARG:HH11	1.68	0.57
1:D:280:PHE:O	1:D:283:PRO:HD3	2.04	0.57
1:A:111:LEU:HB3	1:A:112:PRO:CD	2.34	0.57
1:C:124:ASP:O	1:C:127:MET:HG2	2.03	0.57
1:A:227:ARG:CD	1:A:319:ASN:HD22	2.18	0.57
1:C:66:GLU:O	1:C:70:ILE:HG13	2.03	0.57
1:C:307:ALA:HB3	1:C:308:PRO:HD3	1.87	0.57
1:C:66:GLU:OE2	1:C:178:LYS:HD2	2.05	0.57
1:C:80:ILE:CG2	1:C:81:ASN:N	2.67	0.57
1:D:132:LEU:HG	1:D:149:VAL:HG11	1.87	0.57
1:D:234:THR:HA	1:D:286:PHE:HE1	1.69	0.57
1:C:153:MET:C	1:C:153:MET:HE2	2.29	0.57
1:B:127:MET:O	1:B:128:PRO:C	2.48	0.57
1:B:127:MET:HG3	1:B:131:LYS:HG3	1.86	0.57
1:A:55:SER:HB3	1:A:193:LEU:CD2	2.35	0.57
1:B:188:ILE:O	1:B:192:MET:HG3	2.04	0.57
1:B:265:GLN:HE21	1:B:267:ILE:HD11	1.69	0.57
1:D:183:THR:CB	1:D:186:GLU:HG3	2.34	0.57
1:A:216:ASN:O	1:A:219:ILE:HG22	2.05	0.56
1:A:79:LYS:O	1:A:82:ASP:HB2	2.04	0.56
1:D:294:HIS:CE1	1:D:296:ALA:HB3	2.40	0.56
1:A:21:ALA:CB	1:A:265:GLN:HB3	2.34	0.56
1:B:259:LYS:NZ	1:B:261:LYS:HG3	2.20	0.56
1:B:307:ALA:O	1:B:311:ARG:HG3	2.04	0.56
1:C:61:ASN:CB	1:C:62:PRO:CD	2.74	0.56
1:C:65:LYS:O	1:C:69:ASP:HB2	2.06	0.56
1:C:154:VAL:HG13	1:C:188:ILE:HG21	1.86	0.56
1:C:280:PHE:O	1:C:283:PRO:HD3	2.04	0.56
1:D:44:PRO:O	1:D:46:ASN:N	2.38	0.56
1:D:137:ILE:C	1:D:139:GLY:H	2.13	0.56
1:A:157:LEU:HD23	1:A:188:ILE:HG23	1.87	0.56
1:B:243:PHE:CD1	1:B:243:PHE:C	2.83	0.56
1:C:176:SER:O	1:C:177:LEU:HB2	2.05	0.56
1:C:236:ARG:CG	1:C:274:ASN:HB3	2.35	0.56
1:D:227:ARG:HG2	1:D:318:LEU:CD2	2.35	0.56
1:A:130:PHE:HD2	1:A:195:ILE:HD13	1.71	0.56
1:A:270:LEU:O	1:A:271:GLY:C	2.48	0.56
1:B:18:TYR:C	1:B:20:GLY:H	2.12	0.56
1:B:56:PHE:HE1	1:B:68:ARG:HA	1.70	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:PRO:HG2	1:C:246:HIS:H	1.71	0.56
1:A:20:GLY:O	1:A:21:ALA:HB2	2.05	0.56
1:A:99:ASP:O	1:A:101:LYS:N	2.38	0.56
1:B:154:VAL:O	1:B:158:LEU:HG	2.06	0.56
1:B:331:ASP:OD2	1:B:334:LYS:HE3	2.05	0.56
1:A:87:ILE:HG12	1:A:115:ILE:HD12	1.87	0.56
1:A:327:ARG:O	1:A:328:ILE:HG13	2.05	0.56
1:C:49:SER:C	1:C:246:HIS:HE2	2.13	0.56
1:D:95:ILE:O	1:D:96:LYS:O	2.24	0.56
1:D:125:SER:O	1:D:128:PRO:HD2	2.05	0.56
1:B:259:LYS:HZ1	1:B:261:LYS:HG3	1.71	0.56
1:D:17:HIS:HB2	1:D:22:TRP:CE3	2.41	0.56
1:D:57:ILE:CG2	1:D:193:LEU:HD11	2.35	0.56
1:A:12:LEU:HD13	1:A:25:TYR:O	2.06	0.56
1:C:141:LYS:O	1:C:142:ARG:HG3	2.06	0.56
1:C:245:PRO:HG2	1:C:246:HIS:ND1	2.21	0.56
1:D:247:ARG:HG2	1:D:247:ARG:HH11	1.71	0.56
1:D:302:HIS:HA	2:D:410:HEM:O2D	2.06	0.56
1:A:317:ALA:O	1:A:318:LEU:C	2.49	0.56
1:B:285:LEU:O	1:B:290:ARG:NH2	2.39	0.56
1:C:298:GLY:O	1:C:299:ILE:HB	2.06	0.56
1:D:113:VAL:O	1:D:117:SER:HB3	2.06	0.56
1:D:118:LYS:HD3	1:D:118:LYS:O	2.05	0.56
1:A:98:ILE:HD13	1:A:107:TYR:HB2	1.88	0.55
1:A:183:THR:O	1:A:187:LYS:HG3	2.06	0.55
1:A:215:GLU:C	1:A:217:PRO:HD3	2.32	0.55
1:B:65:LYS:O	1:B:69:ASP:CG	2.49	0.55
1:B:205:LEU:HA	1:B:208:ASN:HD22	1.70	0.55
1:A:110:ARG:O	1:A:113:VAL:HG12	2.06	0.55
1:C:250:ALA:O	1:C:262:LYS:HE3	2.06	0.55
1:D:37:ASP:OD2	1:D:61:ASN:ND2	2.39	0.55
1:A:40:PHE:CD2	1:A:266:VAL:HG21	2.42	0.55
1:A:164:ASP:OD1	1:A:165:SER:N	2.39	0.55
1:B:244:LEU:HD11	1:B:270:LEU:HD11	1.86	0.55
1:A:165:SER:OG	1:A:166:HIS:N	2.40	0.55
1:A:232:GLU:HA	1:A:232:GLU:OE1	2.06	0.55
1:B:126:ASP:C	1:B:128:PRO:HD2	2.32	0.55
1:B:139:GLY:O	1:B:142:ARG:NH2	2.40	0.55
1:B:144:GLU:HB3	1:D:35:MET:HE3	1.88	0.55
1:B:249:ALA:C	1:B:251:GLU:N	2.64	0.55
1:B:267:ILE:HD12	1:B:267:ILE:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:43:ASN:ND2	1:D:44:PRO:N	2.53	0.55
1:A:347:ASP:OD2	1:A:348:LYS:HG2	2.06	0.55
1:C:220:ILE:O	1:C:223:ALA:HB3	2.06	0.55
1:D:172:LEU:O	1:D:174:GLY:N	2.39	0.55
1:B:78:SER:C	1:B:80:ILE:H	2.14	0.55
1:B:96:LYS:O	1:B:99:ASP:OD1	2.23	0.55
1:B:143:ASP:OD2	1:B:145:ASN:OD1	2.25	0.55
1:C:133:TRP:HH2	1:C:192:MET:HB3	1.72	0.55
1:C:248:PHE:CD1	1:C:248:PHE:N	2.74	0.55
1:B:34:LEU:HD13	1:B:299:ILE:HG22	1.88	0.55
1:C:47:ARG:HG3	1:C:49:SER:OG	2.06	0.55
1:A:130:PHE:CD2	1:A:195:ILE:HD13	2.42	0.55
1:B:18:TYR:C	1:B:20:GLY:N	2.60	0.55
1:C:32:HIS:HD2	1:C:36:ASN:ND2	2.04	0.55
1:C:172:LEU:HD12	1:C:191:ILE:HD11	1.88	0.55
1:D:61:ASN:HB3	1:D:62:PRO:HD3	1.89	0.55
1:D:132:LEU:O	1:D:134:SER:N	2.39	0.55
1:A:99:ASP:C	1:A:101:LYS:N	2.62	0.54
1:B:42:SER:CB	1:B:302:HIS:NE2	2.69	0.54
1:B:111:LEU:O	1:B:115:ILE:HG12	2.06	0.54
1:C:183:THR:CB	1:C:186:GLU:HG3	2.36	0.54
1:B:66:GLU:OE2	1:B:178:LYS:HD2	2.08	0.54
1:B:119:ILE:HG23	1:B:120:LEU:HD23	1.89	0.54
1:B:130:PHE:O	1:B:131:LYS:C	2.50	0.54
1:A:54:ILE:O	1:A:57:ILE:HG22	2.08	0.54
1:C:62:PRO:HG2	1:C:63:GLU:H	1.72	0.54
1:C:153:MET:HE1	1:C:157:LEU:CD2	2.37	0.54
1:A:316:ILE:HG22	1:A:320:ASP:OD2	2.08	0.54
1:B:116:ILE:O	1:B:119:ILE:HG22	2.08	0.54
1:C:233:GLU:OE1	1:C:236:ARG:HD3	2.06	0.54
1:D:208:ASN:O	1:D:212:VAL:HG23	2.06	0.54
1:A:69:ASP:O	1:A:72:ALA:HB3	2.08	0.54
1:B:92:ASN:HA	1:B:95:ILE:HG22	1.89	0.54
1:B:245:PRO:HA	1:B:267:ILE:HG13	1.90	0.54
1:B:249:ALA:C	1:B:251:GLU:H	2.15	0.54
1:C:94:LEU:HD21	1:C:110:ARG:HB2	1.90	0.54
1:C:117:SER:CB	1:C:127:MET:HE1	2.34	0.54
1:A:200:GLU:O	1:A:202:THR:N	2.37	0.54
1:B:133:TRP:CZ2	1:B:192:MET:HE3	2.43	0.54
1:D:98:ILE:O	1:D:101:LYS:HB2	2.07	0.54
1:B:71:SER:O	1:B:72:ALA:C	2.50	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:233:GLU:OE1	1:B:287:LYS:O	2.26	0.54
1:C:56:PHE:HA	1:C:59:MET:HG3	1.86	0.54
1:A:98:ILE:HG23	1:A:98:ILE:O	2.08	0.54
1:A:312:LEU:HD22	1:A:316:ILE:HG13	1.90	0.54
1:B:134:SER:HA	1:B:137:ILE:CG1	2.38	0.54
1:C:205:LEU:O	1:C:208:ASN:HB2	2.08	0.54
1:C:339:ASP:O	1:C:340:ASN:C	2.50	0.54
1:C:232:GLU:HA	1:C:235:LEU:HD12	1.89	0.53
1:D:43:ASN:HB2	1:D:58:THR:O	2.08	0.53
1:D:312:LEU:O	1:D:316:ILE:HG13	2.07	0.53
1:B:36:ASN:CB	1:B:39:ILE:HD12	2.38	0.53
1:B:98:ILE:HD12	1:B:101:LYS:HB2	1.90	0.53
1:B:116:ILE:HD11	2:B:410:HEM:HBC1	1.90	0.53
1:B:127:MET:HG3	1:B:131:LYS:HD2	1.91	0.53
1:B:317:ALA:O	1:B:321:ILE:HG13	2.08	0.53
1:C:14:ASP:HB3	1:C:15:PRO:CD	2.33	0.53
1:C:134:SER:O	1:C:135:ASP:C	2.50	0.53
1:C:136:TYR:CE1	1:C:141:LYS:HE2	2.42	0.53
1:C:218:ASP:O	1:C:219:ILE:HB	2.08	0.53
1:D:115:ILE:O	1:D:119:ILE:HG13	2.08	0.53
1:B:42:SER:O	1:B:58:THR:HA	2.08	0.53
1:C:111:LEU:C	1:C:111:LEU:CD2	2.82	0.53
1:B:43:ASN:O	1:B:248:PHE:HD1	1.91	0.53
1:B:117:SER:HB3	1:B:130:PHE:CD2	2.43	0.53
1:C:335:SER:OG	1:C:349:LEU:HA	2.09	0.53
1:A:56:PHE:HE2	1:A:190:TYR:CZ	2.27	0.53
1:A:85:ASP:O	1:A:86:PHE:C	2.52	0.53
1:C:77:PRO:HA	1:C:80:ILE:HG22	1.89	0.53
1:C:176:SER:HB3	1:C:181:LYS:HA	1.90	0.53
1:D:73:PRO:HA	1:D:76:LEU:HG	1.89	0.53
1:D:120:LEU:O	1:D:169:ILE:HG13	2.07	0.53
1:D:129:LEU:HD11	1:D:152:ARG:HG3	1.90	0.53
1:D:208:ASN:HD21	1:D:344:LEU:HG	1.73	0.53
1:D:17:HIS:ND1	1:D:17:HIS:C	2.67	0.53
1:D:251:GLU:HA	1:D:262:LYS:HG3	1.91	0.53
1:A:216:ASN:N	1:A:217:PRO:HD3	2.24	0.53
1:B:100:ASN:N	1:B:100:ASN:HD22	2.06	0.53
1:B:330:ILE:HD13	1:B:349:LEU:HD21	1.91	0.53
1:C:99:ASP:OD2	1:C:324:HIS:NE2	2.41	0.53
1:D:184:MET:HA	1:D:187:LYS:HD2	1.89	0.53
1:A:161:PHE:CZ	1:A:191:ILE:HD12	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:206:ILE:HA	1:A:209:MET:HE2	1.89	0.53
1:A:261:LYS:HD2	1:A:264:ASP:OD1	2.09	0.53
1:B:158:LEU:HD22	1:B:184:MET:CG	2.39	0.53
1:B:219:ILE:O	1:B:220:ILE:C	2.51	0.53
1:C:182:LEU:HD12	1:C:182:LEU:H	1.74	0.53
1:D:59:MET:SD	1:D:63:GLU:HG2	2.49	0.53
1:B:307:ALA:HB3	1:B:308:PRO:HD3	1.89	0.53
1:D:157:LEU:HG	1:D:188:ILE:HD13	1.91	0.53
1:A:18:TYR:CE1	1:A:23:HIS:NE2	2.77	0.53
1:A:134:SER:O	1:A:138:ILE:HD12	2.08	0.53
1:B:70:ILE:O	1:B:70:ILE:HG22	2.07	0.53
1:B:134:SER:HA	1:B:137:ILE:HG12	1.91	0.53
1:B:136:TYR:O	1:B:137:ILE:C	2.52	0.52
1:B:156:ARG:CZ	1:D:226:ASN:CG	2.82	0.52
1:D:64:HIS:HE1	2:D:410:HEM:O2D	1.91	0.52
1:A:169:ILE:HG23	1:A:191:ILE:CD1	2.39	0.52
1:C:160:ILE:HG22	1:C:169:ILE:HG21	1.91	0.52
1:C:210:ILE:HD11	1:C:321:ILE:HD13	1.91	0.52
1:D:282:GLU:O	1:D:284:ASP:N	2.42	0.52
1:A:53:GLY:HA3	3:A:411:PIM:H10	1.91	0.52
1:A:276:ASP:OD1	1:A:278:THR:N	2.42	0.52
1:B:156:ARG:NH1	1:D:226:ASN:ND2	2.57	0.52
1:C:72:ALA:N	1:C:73:PRO:CD	2.71	0.52
1:D:177:LEU:N	1:D:177:LEU:CD2	2.72	0.52
1:B:107:TYR:CE2	1:B:111:LEU:HD22	2.45	0.52
1:B:248:PHE:CE2	1:B:265:GLN:HG3	2.44	0.52
1:D:42:SER:O	1:D:58:THR:HA	2.08	0.52
1:D:206:ILE:HA	1:D:209:MET:HE3	1.92	0.52
1:D:226:ASN:HD22	1:D:226:ASN:C	2.16	0.52
1:A:43:ASN:OD1	1:A:43:ASN:C	2.52	0.52
1:A:163:SER:OG	1:A:164:ASP:N	2.42	0.52
1:B:158:LEU:HD22	1:B:184:MET:HG3	1.91	0.52
1:A:116:ILE:HD12	1:A:120:LEU:CD1	2.40	0.52
1:B:161:PHE:HE2	1:B:169:ILE:HG23	1.71	0.52
1:B:184:MET:O	1:B:188:ILE:HG12	2.09	0.52
1:D:130:PHE:O	1:D:134:SER:N	2.42	0.52
1:C:178:LYS:O	1:C:179:ASN:C	2.53	0.52
1:C:268:VAL:O	1:C:268:VAL:CG2	2.58	0.52
1:B:34:LEU:CD1	1:B:299:ILE:HG22	2.40	0.52
1:B:153:MET:HE3	1:B:153:MET:HA	1.89	0.52
1:B:183:THR:HG22	1:B:185:ASP:N	2.03	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:276:ASP:OD1	1:B:278:THR:HB	2.10	0.52
1:C:68:ARG:NE	1:C:305:LEU:HD13	2.24	0.52
1:D:265:GLN:NE2	1:D:267:ILE:HG13	2.22	0.52
1:A:230:PHE:HD1	1:A:288:ILE:HD11	1.74	0.52
1:C:133:TRP:O	1:C:137:ILE:HG12	2.10	0.52
1:D:108:ALA:O	1:D:109:VAL:C	2.53	0.52
1:D:262:LYS:HG2	1:D:263:GLY:N	2.24	0.52
1:A:38:LYS:HD2	1:A:38:LYS:N	2.25	0.52
1:A:227:ARG:O	1:A:231:VAL:HG23	2.09	0.52
1:C:172:LEU:HD11	1:C:190:TYR:CD2	2.44	0.52
1:D:131:LYS:O	1:D:134:SER:OG	2.27	0.52
1:D:236:ARG:HB2	1:D:294:HIS:HB3	1.90	0.52
1:D:302:HIS:O	2:D:410:HEM:HAA2	2.10	0.52
1:A:227:ARG:HH11	1:A:227:ARG:HB3	1.75	0.51
1:D:256:ASN:O	1:D:257:ASN:C	2.53	0.51
1:A:280:PHE:HB3	1:A:290:ARG:NH1	2.25	0.51
1:D:201:THR:HA	1:D:204:ASN:HD22	1.74	0.51
1:B:129:LEU:O	1:B:133:TRP:N	2.41	0.51
1:D:306:GLY:C	1:D:308:PRO:HD2	2.35	0.51
1:A:108:ALA:O	1:A:112:PRO:HD2	2.11	0.51
1:A:118:LYS:HD3	1:A:118:LYS:O	2.11	0.51
1:B:12:LEU:HD12	1:B:26:LYS:HA	1.93	0.51
1:B:116:ILE:CA	1:B:119:ILE:HG22	2.39	0.51
1:B:183:THR:CG2	1:B:184:MET:N	2.72	0.51
1:C:146:PHE:HA	1:C:149:VAL:CG2	2.40	0.51
1:D:205:LEU:O	1:D:208:ASN:N	2.43	0.51
1:B:77:PRO:O	1:B:80:ILE:HG22	2.11	0.51
1:B:151:ASN:N	1:B:151:ASN:HD22	2.07	0.51
1:D:111:LEU:HB3	1:D:112:PRO:CD	2.40	0.51
1:D:135:ASP:O	1:D:138:ILE:HG13	2.10	0.51
1:B:325:PHE:O	1:B:326:LYS:C	2.54	0.51
1:B:250:ALA:O	1:B:251:GLU:HB3	2.11	0.51
1:C:60:ASP:O	1:C:61:ASN:C	2.53	0.51
1:D:92:ASN:HA	1:D:95:ILE:CG2	2.41	0.51
1:D:94:LEU:O	1:D:95:ILE:C	2.53	0.51
1:A:61:ASN:HB3	1:A:62:PRO:CD	2.39	0.51
1:C:133:TRP:CE2	1:C:137:ILE:HG13	2.46	0.51
1:D:57:ILE:HA	2:D:410:HEM:O1D	2.10	0.51
1:D:306:GLY:O	1:D:307:ALA:C	2.53	0.51
1:A:133:TRP:O	1:A:134:SER:C	2.54	0.51
1:B:87:ILE:CB	1:B:316:ILE:HD12	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:LEU:O	1:B:132:LEU:N	2.43	0.51
1:B:285:LEU:HD12	1:B:287:LYS:HE2	1.93	0.51
1:B:326:LYS:O	1:B:327:ARG:O	2.28	0.51
1:C:151:ASN:O	1:C:152:ARG:C	2.52	0.51
1:C:250:ALA:O	1:C:251:GLU:HB3	2.10	0.51
1:D:113:VAL:HG21	1:D:131:LYS:HG3	1.93	0.51
1:D:307:ALA:HB3	1:D:308:PRO:HD3	1.93	0.51
1:A:243:PHE:CB	1:A:269:TYR:HA	2.42	0.51
1:C:85:ASP:OD1	1:C:85:ASP:N	2.42	0.51
1:C:128:PRO:CA	1:C:131:LYS:HE2	2.37	0.51
1:D:146:PHE:O	1:D:149:VAL:HG23	2.11	0.51
1:A:319:ASN:O	1:A:320:ASP:C	2.55	0.50
1:B:214:ASP:HB2	1:B:330:ILE:HG13	1.93	0.50
1:B:244:LEU:CD1	2:B:410:HEM:HBA2	2.41	0.50
1:B:282:GLU:OE1	1:B:287:LYS:HE3	2.12	0.50
1:D:71:SER:C	1:D:73:PRO:HD2	2.36	0.50
1:B:21:ALA:HB1	1:B:267:ILE:CD1	2.41	0.50
1:B:121:GLY:O	1:B:122:ILE:C	2.52	0.50
1:B:133:TRP:CD2	1:B:153:MET:HG2	2.47	0.50
1:C:173:ALA:O	1:C:175:SER:N	2.43	0.50
1:D:135:ASP:O	1:D:138:ILE:N	2.34	0.50
1:B:259:LYS:HZ3	1:B:261:LYS:CE	2.13	0.50
1:C:168:ILE:HA	1:C:171:VAL:CG2	2.41	0.50
1:C:203:THR:O	1:C:204:ASN:C	2.53	0.50
1:C:247:ARG:HH11	1:C:247:ARG:CG	2.23	0.50
1:D:95:ILE:HG23	1:D:96:LYS:N	2.26	0.50
1:D:249:ALA:HB3	1:D:263:GLY:N	2.26	0.50
1:D:330:ILE:HG12	1:D:351:LEU:HD23	1.93	0.50
1:A:81:ASN:C	1:A:83:TYR:N	2.69	0.50
1:A:130:PHE:O	1:A:133:TRP:HB3	2.12	0.50
1:B:100:ASN:N	1:B:100:ASN:ND2	2.57	0.50
1:B:232:GLU:O	1:B:235:LEU:HB2	2.10	0.50
1:D:195:ILE:HG22	1:D:196:ILE:N	2.25	0.50
1:D:277:GLU:HG2	1:D:283:PRO:HG3	1.94	0.50
1:D:322:LEU:CD2	1:D:328:ILE:HD12	2.41	0.50
1:B:36:ASN:HB3	1:B:39:ILE:CD1	2.41	0.50
1:B:209:MET:HG2	1:B:234:THR:HG21	1.94	0.50
1:C:32:HIS:HD2	1:C:36:ASN:HD22	1.59	0.50
1:D:57:ILE:HG21	1:D:193:LEU:HD11	1.92	0.50
1:D:164:ASP:O	1:D:165:SER:CB	2.56	0.50
1:B:251:GLU:HA	1:B:262:LYS:HD3	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:188:ILE:C	1:C:190:TYR:N	2.69	0.50
1:C:244:LEU:HB2	1:C:268:VAL:HG22	1.94	0.50
1:A:62:PRO:HG2	1:A:63:GLU:N	2.27	0.50
1:C:213:ILE:HG21	1:C:328:ILE:HB	1.94	0.50
1:A:120:LEU:HD23	1:A:168:ILE:HB	1.93	0.50
1:B:340:ASN:HD22	1:B:341:LYS:N	2.08	0.50
1:D:322:LEU:HD23	1:D:328:ILE:CD1	2.42	0.50
1:A:42:SER:HA	1:A:247:ARG:HD3	1.92	0.50
1:A:263:GLY:O	1:A:264:ASP:C	2.54	0.50
1:B:177:LEU:O	1:B:178:LYS:HB3	2.12	0.50
1:C:134:SER:O	1:C:138:ILE:N	2.43	0.50
1:D:317:ALA:O	1:D:321:ILE:HG13	2.11	0.50
1:B:349:LEU:HD23	1:B:350:PHE:H	1.75	0.49
1:D:151:ASN:O	1:D:154:VAL:N	2.45	0.49
1:A:111:LEU:O	1:A:115:ILE:HG12	2.12	0.49
1:A:112:PRO:HB2	1:A:198:GLY:O	2.12	0.49
1:A:261:LYS:O	1:A:264:ASP:HB2	2.12	0.49
1:D:332:TYR:O	1:D:334:LYS:N	2.45	0.49
1:A:53:GLY:O	1:A:58:THR:HG23	2.13	0.49
1:B:299:ILE:HA	1:B:303:MET:HE1	1.92	0.49
1:B:302:HIS:O	1:B:303:MET:C	2.55	0.49
1:C:166:HIS:CG	1:C:166:HIS:O	2.64	0.49
1:A:274:ASN:ND2	1:A:294:HIS:CB	2.58	0.49
1:A:286:PHE:O	1:A:287:LYS:C	2.55	0.49
1:B:132:LEU:HD12	1:B:141:LYS:HE3	1.95	0.49
1:D:203:THR:HG22	1:D:204:ASN:N	2.27	0.49
1:A:281:ASP:O	1:A:282:GLU:C	2.55	0.49
1:C:72:ALA:O	1:C:73:PRO:C	2.54	0.49
1:C:163:SER:OG	1:C:164:ASP:N	2.42	0.49
1:C:330:ILE:CG2	1:C:331:ASP:H	2.01	0.49
1:D:133:TRP:HZ3	1:D:195:ILE:HG21	1.77	0.49
1:D:233:GLU:OE2	1:D:236:ARG:NH1	2.45	0.49
1:B:20:GLY:O	1:B:21:ALA:HB2	2.13	0.49
1:B:70:ILE:HG23	1:B:175:SER:HB2	1.94	0.49
1:B:129:LEU:H	1:B:129:LEU:CD1	2.23	0.49
1:C:41:SER:OG	1:C:60:ASP:OD2	2.30	0.49
1:C:76:LEU:O	1:C:77:PRO:C	2.55	0.49
1:C:110:ARG:HB3	1:C:110:ARG:HH11	1.75	0.49
1:A:325:PHE:O	1:A:326:LYS:C	2.56	0.49
1:A:337:LEU:O	1:A:338:LEU:C	2.54	0.49
1:C:218:ASP:OD2	1:C:218:ASP:N	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:224:LEU:C	1:C:226:ASN:N	2.66	0.49
1:D:136:TYR:C	1:D:138:ILE:H	2.21	0.49
1:D:198:GLY:H	2:D:410:HEM:HAC	1.75	0.49
1:D:325:PHE:CD1	1:D:351:LEU:HD12	2.46	0.49
1:A:176:SER:CB	1:A:182:LEU:H	2.26	0.49
1:A:312:LEU:HD22	1:A:316:ILE:CG1	2.42	0.49
1:B:43:ASN:C	1:B:248:PHE:CD1	2.91	0.49
1:B:90:THR:O	1:B:94:LEU:HD13	2.12	0.49
1:B:116:ILE:HD13	1:B:119:ILE:CG2	2.43	0.49
1:D:22:TRP:CD1	1:D:260:ILE:HG23	2.46	0.49
1:A:169:ILE:HA	1:A:191:ILE:HD11	1.95	0.49
1:A:176:SER:HA	1:A:182:LEU:HB2	1.95	0.49
1:A:236:ARG:CB	1:A:274:ASN:HD22	2.26	0.49
1:D:138:ILE:O	1:D:138:ILE:CG2	2.60	0.49
1:B:158:LEU:CD2	1:B:188:ILE:HD11	2.43	0.49
1:B:133:TRP:CE3	1:B:153:MET:HG2	2.48	0.48
1:B:178:LYS:O	1:B:178:LYS:HG2	2.13	0.48
1:C:27:TYR:HD1	1:C:273:ALA:O	1.96	0.48
1:C:148:TYR:HA	1:C:151:ASN:HB2	1.93	0.48
1:D:116:ILE:CG1	1:D:198:GLY:HA3	2.42	0.48
1:A:27:TYR:HE2	1:A:31:LYS:HD2	1.73	0.48
1:A:230:PHE:CD1	1:A:288:ILE:HD11	2.48	0.48
1:B:123:PRO:C	1:B:125:SER:N	2.72	0.48
1:D:69:ASP:O	1:D:71:SER:N	2.46	0.48
1:D:135:ASP:OD1	1:D:136:TYR:N	2.45	0.48
1:A:103:ILE:O	1:A:107:TYR:HB3	2.11	0.48
1:A:110:ARG:C	1:A:113:VAL:HG12	2.38	0.48
1:B:164:ASP:O	1:B:165:SER:HB3	2.13	0.48
1:C:157:LEU:HG	1:C:161:PHE:HE1	1.78	0.48
1:D:335:SER:O	1:D:336:ARG:HD3	2.13	0.48
1:A:111:LEU:HB3	1:A:112:PRO:HD3	1.95	0.48
1:A:172:LEU:O	1:A:173:ALA:O	2.30	0.48
1:C:163:SER:O	1:C:164:ASP:CB	2.61	0.48
1:C:176:SER:O	1:C:177:LEU:CB	2.60	0.48
1:C:274:ASN:OD1	1:C:294:HIS:HB2	2.14	0.48
1:D:132:LEU:C	1:D:134:SER:H	2.20	0.48
1:D:270:LEU:HD22	1:D:295:LEU:O	2.14	0.48
1:A:330:ILE:O	1:A:332:TYR:CD1	2.67	0.48
1:B:337:LEU:HD23	1:B:346:TYR:CD2	2.48	0.48
1:C:325:PHE:CB	1:C:328:ILE:HG13	2.44	0.48
1:D:208:ASN:HD22	1:D:238:TYR:CB	2.15	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:HIS:ND1	1:A:269:TYR:HE1	2.12	0.48
2:D:410:HEM:NB	3:D:411:PIM:H2	2.28	0.48
1:B:98:ILE:O	1:B:99:ASP:C	2.57	0.48
1:B:233:GLU:OE2	1:B:236:ARG:NH1	2.47	0.48
1:D:14:ASP:O	1:D:16:VAL:HG13	2.14	0.48
1:D:135:ASP:O	1:D:137:ILE:HG13	2.14	0.48
1:D:163:SER:C	1:D:164:ASP:CG	2.82	0.48
1:A:134:SER:O	1:A:137:ILE:N	2.47	0.48
1:B:44:PRO:HA	1:B:248:PHE:CD1	2.49	0.48
1:C:128:PRO:HA	1:C:131:LYS:CE	2.39	0.48
1:C:128:PRO:O	1:C:129:LEU:C	2.56	0.48
1:A:71:SER:C	1:A:73:PRO:HD2	2.39	0.48
1:A:287:LYS:HE2	1:A:290:ARG:HG2	1.96	0.48
1:B:87:ILE:CG2	1:B:316:ILE:HD12	2.43	0.48
1:B:282:GLU:HB3	1:B:285:LEU:HD12	1.96	0.48
1:C:57:ILE:HG13	2:C:410:HEM:CBD	2.44	0.48
1:C:252:ASP:HB3	1:C:259:LYS:HE2	1.94	0.48
1:C:307:ALA:HB1	1:C:311:ARG:NH1	2.28	0.48
1:C:18:TYR:CD1	1:C:19:ASP:CG	2.92	0.48
1:C:136:TYR:OH	1:C:143:ASP:HB2	2.14	0.48
1:C:335:SER:OG	1:C:350:PHE:N	2.42	0.48
1:D:151:ASN:O	1:D:152:ARG:C	2.57	0.48
1:A:200:GLU:C	1:A:202:THR:H	2.21	0.47
1:B:194:LEU:O	2:B:410:HEM:HBC2	2.13	0.47
1:C:103:ILE:HD11	1:C:351:LEU:HD21	1.96	0.47
1:C:18:TYR:HD1	1:C:19:ASP:CG	2.22	0.47
1:C:177:LEU:CD1	1:C:178:LYS:N	2.72	0.47
1:C:249:ALA:N	1:C:264:ASP:O	2.48	0.47
1:D:126:ASP:CG	1:D:156:ARG:HD3	2.40	0.47
1:A:56:PHE:CE2	1:A:190:TYR:CE1	3.01	0.47
1:A:147:ASN:OD1	1:A:148:TYR:CE1	2.67	0.47
1:B:30:VAL:HG22	1:B:268:VAL:HG22	1.97	0.47
1:B:56:PHE:HA	1:B:59:MET:HE3	1.96	0.47
1:B:104:ILE:HA	1:B:108:ALA:HB3	1.96	0.47
1:B:168:ILE:O	1:B:171:VAL:HB	2.14	0.47
1:B:272:SER:O	1:B:273:ALA:C	2.56	0.47
1:D:43:ASN:ND2	1:D:43:ASN:C	2.71	0.47
1:D:158:LEU:HD11	1:D:184:MET:CG	2.44	0.47
1:D:213:ILE:HG13	1:D:322:LEU:HD21	1.96	0.47
1:D:324:HIS:HD2	1:D:325:PHE:CE2	2.32	0.47
1:D:346:TYR:CD1	1:D:346:TYR:N	2.83	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:293:MET:CE	1:A:299:ILE:HD12	2.44	0.47
1:A:330:ILE:O	1:A:331:ASP:C	2.58	0.47
1:C:198:GLY:HA2	2:C:410:HEM:CMC	2.45	0.47
1:D:129:LEU:HD21	1:D:153:MET:HA	1.96	0.47
1:A:301:ILE:HG13	1:A:302:HIS:N	2.30	0.47
1:C:42:SER:O	1:C:58:THR:HA	2.15	0.47
1:C:226:ASN:HD21	1:C:229:GLY:H	1.60	0.47
1:D:66:GLU:OE1	1:D:178:LYS:HB3	2.13	0.47
1:D:115:ILE:HG21	1:D:313:GLU:OE2	2.14	0.47
1:D:192:MET:O	1:D:196:ILE:HG13	2.15	0.47
1:D:248:PHE:HE2	1:D:265:GLN:HG2	1.78	0.47
1:B:65:LYS:HG2	1:B:69:ASP:OD2	2.15	0.47
1:B:68:ARG:NH1	1:B:303:MET:O	2.32	0.47
1:B:287:LYS:HB2	1:B:290:ARG:HE	1.79	0.47
1:B:340:ASN:HD21	1:B:342:MET:CB	2.28	0.47
1:D:195:ILE:O	1:D:196:ILE:C	2.58	0.47
1:A:129:LEU:HD21	1:A:153:MET:HA	1.96	0.47
1:A:237:TYR:O	1:A:275:ARG:NH2	2.47	0.47
1:B:12:LEU:CD1	1:B:26:LYS:HA	2.44	0.47
1:B:140:ASN:HD22	1:B:140:ASN:HA	1.58	0.47
1:B:220:ILE:O	1:B:223:ALA:HB3	2.15	0.47
1:B:271:GLY:O	1:B:272:SER:C	2.58	0.47
1:C:250:ALA:C	1:C:262:LYS:HG3	2.40	0.47
1:D:32:HIS:O	1:D:33:VAL:C	2.58	0.47
1:D:157:LEU:HD23	1:D:188:ILE:HD12	1.97	0.47
1:D:204:ASN:O	1:D:208:ASN:OD1	2.32	0.47
1:D:281:ASP:OD1	1:D:282:GLU:HG2	2.14	0.47
1:D:348:LYS:HB2	1:D:348:LYS:NZ	2.29	0.47
1:B:99:ASP:O	1:B:100:ASN:HB2	2.15	0.47
1:B:127:MET:HG3	1:B:131:LYS:CG	2.44	0.47
1:B:291:ARG:O	1:B:291:ARG:HG3	2.14	0.47
1:C:68:ARG:HH21	1:C:305:LEU:HD12	1.79	0.47
1:C:80:ILE:HG22	1:C:81:ASN:N	2.30	0.47
1:C:98:ILE:O	1:C:98:ILE:HG13	2.14	0.47
1:D:147:ASN:O	1:D:150:ASN:HB3	2.14	0.47
1:D:170:ASN:O	1:D:171:VAL:C	2.57	0.47
1:A:162:LYS:O	1:A:163:SER:C	2.57	0.47
1:B:151:ASN:N	1:B:151:ASN:ND2	2.63	0.47
1:C:148:TYR:O	1:C:149:VAL:C	2.57	0.47
1:D:65:LYS:O	1:D:66:GLU:C	2.58	0.47
1:D:92:ASN:CA	1:D:95:ILE:HG22	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:LEU:HD13	1:D:191:ILE:HG23	1.97	0.47
1:B:132:LEU:O	1:B:133:TRP:C	2.57	0.47
1:A:236:ARG:NH2	1:A:283:PRO:O	2.48	0.46
1:A:289:GLY:O	1:A:290:ARG:C	2.58	0.46
1:B:272:SER:O	1:B:274:ASN:N	2.48	0.46
1:D:110:ARG:O	1:D:111:LEU:C	2.58	0.46
1:D:203:THR:O	1:D:204:ASN:C	2.56	0.46
1:D:211:ARG:O	1:D:214:ASP:HB3	2.15	0.46
1:D:12:LEU:HD11	1:D:272:SER:O	2.16	0.46
1:D:156:ARG:NH2	1:D:160:ILE:HD13	2.30	0.46
1:D:249:ALA:HB1	1:D:251:GLU:O	2.14	0.46
1:A:27:TYR:CE1	1:A:295:LEU:HG	2.51	0.46
1:C:138:ILE:HD13	1:C:200:GLU:HB2	1.96	0.46
1:B:93:ASP:O	1:B:94:LEU:C	2.59	0.46
1:C:102:ASP:O	1:C:106:GLU:HB2	2.15	0.46
1:C:131:LYS:O	1:C:132:LEU:C	2.57	0.46
1:C:198:GLY:HA2	2:C:410:HEM:HMC3	1.96	0.46
1:D:145:ASN:O	1:D:149:VAL:CG2	2.63	0.46
1:D:226:ASN:HD22	1:D:227:ARG:N	2.13	0.46
1:B:61:ASN:CA	1:B:64:HIS:HB3	2.43	0.46
1:B:94:LEU:CD2	1:B:110:ARG:HB2	2.46	0.46
1:B:203:THR:HG22	1:B:204:ASN:N	2.29	0.46
1:C:17:HIS:HE1	1:C:20:GLY:O	1.98	0.46
1:C:234:THR:HA	1:C:286:PHE:HE1	1.80	0.46
1:D:133:TRP:HZ3	1:D:195:ILE:CG2	2.28	0.46
1:D:269:TYR:CD1	1:D:269:TYR:N	2.84	0.46
1:A:79:LYS:HA	1:A:82:ASP:OD2	2.16	0.46
1:B:87:ILE:HD12	1:B:312:LEU:HD22	1.95	0.46
1:D:325:PHE:O	1:D:326:LYS:C	2.55	0.46
1:B:99:ASP:O	1:B:100:ASN:CB	2.63	0.46
1:C:73:PRO:HG2	1:C:74:TYR:H	1.81	0.46
1:C:116:ILE:CG2	1:C:117:SER:N	2.79	0.46
1:C:188:ILE:O	1:C:189:LYS:C	2.56	0.46
1:D:26:LYS:HG2	1:D:276:ASP:OD2	2.16	0.46
1:A:31:LYS:O	1:A:35:MET:HG2	2.15	0.46
1:A:202:THR:HA	2:A:410:HEM:HBB1	1.96	0.46
1:A:205:LEU:HD13	1:A:235:LEU:HD23	1.98	0.46
1:B:67:PHE:O	1:B:68:ARG:C	2.58	0.46
1:B:92:ASN:HA	1:B:95:ILE:HG21	1.96	0.46
1:B:96:LYS:O	1:B:98:ILE:N	2.48	0.46
1:B:164:ASP:HA	1:B:170:ASN:HD21	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:54:ILE:HB	1:C:55:SER:H	1.48	0.46
1:C:209:MET:CE	1:C:314:ALA:HB1	2.45	0.46
1:D:221:ASP:O	1:D:224:LEU:N	2.49	0.46
1:A:95:ILE:HG21	1:A:320:ASP:HB3	1.98	0.46
1:B:202:THR:HA	2:B:410:HEM:HBB1	1.97	0.46
1:C:302:HIS:ND1	2:C:410:HEM:O1D	2.47	0.46
1:D:18:TYR:CE1	1:D:23:HIS:CE1	3.04	0.46
1:D:81:ASN:C	1:D:83:TYR:H	2.23	0.46
1:C:77:PRO:O	1:C:78:SER:C	2.59	0.46
1:D:312:LEU:CD2	1:D:316:ILE:HD11	2.46	0.46
1:A:97:ASN:O	1:A:98:ILE:C	2.60	0.45
1:A:183:THR:HG22	1:A:185:ASP:N	2.32	0.45
1:A:312:LEU:HD22	1:A:316:ILE:HD11	1.98	0.45
1:C:32:HIS:O	1:C:33:VAL:C	2.58	0.45
1:C:61:ASN:CB	1:C:62:PRO:HD3	2.25	0.45
1:D:276:ASP:OD1	1:D:278:THR:CB	2.62	0.45
1:B:87:ILE:HD13	1:B:313:GLU:HG2	1.99	0.45
1:B:146:PHE:O	1:B:147:ASN:C	2.59	0.45
1:C:134:SER:C	1:C:138:ILE:HD12	2.41	0.45
1:C:211:ARG:O	1:C:212:VAL:C	2.59	0.45
1:C:294:HIS:HE1	1:C:296:ALA:HB3	1.78	0.45
1:B:69:ASP:C	1:B:71:SER:H	2.24	0.45
1:B:233:GLU:HG2	1:B:286:PHE:CD2	2.51	0.45
1:B:276:ASP:OD1	1:B:278:THR:N	2.48	0.45
1:C:66:GLU:HG2	1:C:177:LEU:CD2	2.46	0.45
1:C:247:ARG:CG	1:C:247:ARG:NH1	2.79	0.45
1:C:252:ASP:HB3	1:C:259:LYS:HZ1	1.81	0.45
1:C:330:ILE:HG23	1:C:349:LEU:HD12	1.97	0.45
1:D:195:ILE:O	1:D:199:ASN:ND2	2.50	0.45
1:D:214:ASP:OD2	1:D:330:ILE:HG13	2.16	0.45
1:D:252:ASP:OD2	1:D:262:LYS:N	2.49	0.45
1:D:322:LEU:HD23	1:D:328:ILE:HD12	1.97	0.45
1:A:164:ASP:CG	1:A:165:SER:H	2.25	0.45
1:B:43:ASN:C	1:B:248:PHE:HD1	2.23	0.45
1:B:113:VAL:C	1:B:115:ILE:H	2.24	0.45
1:B:149:VAL:O	1:B:150:ASN:C	2.59	0.45
1:C:153:MET:CE	1:C:157:LEU:HB2	2.47	0.45
1:D:113:VAL:O	1:D:117:SER:HB2	2.17	0.45
1:A:237:TYR:HE1	1:A:284:ASP:O	2.00	0.45
1:A:294:HIS:ND1	1:A:296:ALA:HB3	2.31	0.45
1:B:88:GLU:OE1	1:B:316:ILE:HG23	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:22:TRP:HB2	1:D:266:VAL:HA	1.99	0.45
1:D:330:ILE:HA	1:D:351:LEU:HA	1.98	0.45
1:B:189:LYS:HD3	1:B:189:LYS:HA	1.65	0.45
1:B:349:LEU:HD23	1:B:350:PHE:N	2.32	0.45
1:C:331:ASP:C	1:C:333:LYS:H	2.24	0.45
1:D:57:ILE:HG12	1:D:57:ILE:O	2.17	0.45
1:A:283:PRO:HG2	1:A:284:ASP:H	1.81	0.45
1:A:333:LYS:HA	1:B:257:ASN:OD1	2.17	0.45
1:A:337:LEU:HA	1:A:346:TYR:HA	1.99	0.45
1:B:136:TYR:OH	1:B:143:ASP:HB2	2.17	0.45
1:C:54:ILE:O	1:C:57:ILE:HG22	2.17	0.45
1:C:282:GLU:HB3	1:C:285:LEU:HD12	1.99	0.45
1:A:275:ARG:HG3	1:A:275:ARG:HH11	1.81	0.45
1:B:164:ASP:HA	1:B:170:ASN:OD1	2.17	0.45
1:A:242:GLN:O	1:A:243:PHE:HB3	2.17	0.45
1:B:67:PHE:O	1:B:70:ILE:N	2.49	0.45
1:B:92:ASN:CA	1:B:95:ILE:HG22	2.47	0.45
1:B:243:PHE:HB3	1:B:269:TYR:CD2	2.52	0.45
1:C:130:PHE:O	1:C:131:LYS:C	2.59	0.45
1:C:133:TRP:CZ3	1:C:196:ILE:HD11	2.51	0.45
1:C:340:ASN:ND2	1:C:342:MET:H	2.15	0.45
1:D:132:LEU:O	1:D:133:TRP:C	2.59	0.45
1:A:158:LEU:CD2	1:C:81:ASN:ND2	2.78	0.45
1:A:158:LEU:HD21	1:C:312:LEU:HD21	1.98	0.45
1:A:243:PHE:HB3	1:A:269:TYR:HA	1.99	0.45
1:A:299:ILE:O	1:A:299:ILE:HG23	2.17	0.45
1:B:120:LEU:HD23	1:B:120:LEU:N	2.33	0.45
1:B:132:LEU:CD1	1:B:141:LYS:NZ	2.80	0.45
1:B:282:GLU:HB3	1:B:285:LEU:CD1	2.47	0.45
1:C:13:ASN:OD1	1:C:14:ASP:N	2.50	0.45
1:D:75:PHE:HA	1:D:80:ILE:CD1	2.44	0.45
1:D:116:ILE:HG12	1:D:198:GLY:HA3	1.99	0.45
1:D:274:ASN:OD1	1:D:294:HIS:HB2	2.17	0.45
1:A:178:LYS:HE3	1:A:179:ASN:OD1	2.17	0.44
1:A:178:LYS:HB3	1:A:179:ASN:H	1.45	0.44
1:B:151:ASN:O	1:B:152:ARG:C	2.60	0.44
1:C:27:TYR:CE1	1:C:295:LEU:HD11	2.53	0.44
1:C:212:VAL:O	1:C:213:ILE:C	2.60	0.44
1:C:243:PHE:CD1	1:C:243:PHE:C	2.96	0.44
1:C:351:LEU:O	1:C:352:SER:HB2	2.16	0.44
1:D:243:PHE:CE2	1:D:342:MET:HA	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:GLY:O	1:A:299:ILE:HB	2.18	0.44
1:B:122:ILE:O	1:B:123:PRO:C	2.60	0.44
1:C:205:LEU:O	1:C:209:MET:N	2.50	0.44
1:D:60:ASP:O	1:D:62:PRO:HD2	2.16	0.44
1:D:185:ASP:OD1	1:D:189:LYS:CE	2.65	0.44
1:D:338:LEU:HD12	1:D:345:GLY:C	2.43	0.44
1:A:72:ALA:HA	1:A:305:LEU:HD11	2.00	0.44
1:A:236:ARG:O	1:A:274:ASN:HB3	2.16	0.44
1:A:237:TYR:CE2	1:A:238:TYR:CZ	3.06	0.44
1:B:61:ASN:N	1:B:64:HIS:HB3	2.32	0.44
1:C:260:ILE:HD13	1:C:260:ILE:N	2.32	0.44
1:D:32:HIS:ND1	1:D:36:ASN:ND2	2.66	0.44
1:D:48:TYR:O	1:D:49:SER:C	2.60	0.44
1:D:182:LEU:HG	1:D:186:GLU:OE1	2.17	0.44
1:A:292:GLU:OE1	1:A:292:GLU:HA	2.18	0.44
1:B:201:THR:HB	2:B:410:HEM:CAB	2.47	0.44
1:C:236:ARG:NH2	1:C:283:PRO:O	2.50	0.44
1:D:120:LEU:O	1:D:167:GLY:HA3	2.17	0.44
1:D:145:ASN:O	1:D:149:VAL:HG23	2.17	0.44
1:D:226:ASN:HD21	1:D:229:GLY:H	1.63	0.44
1:B:56:PHE:CA	1:B:59:MET:HE3	2.48	0.44
1:B:98:ILE:O	1:B:100:ASN:N	2.50	0.44
1:B:134:SER:CA	1:B:137:ILE:HG12	2.48	0.44
1:C:32:HIS:CD2	1:C:36:ASN:ND2	2.85	0.44
1:C:70:ILE:O	1:C:70:ILE:HG22	2.17	0.44
1:C:136:TYR:C	1:C:138:ILE:N	2.76	0.44
1:C:244:LEU:HB2	1:C:268:VAL:CG2	2.48	0.44
1:A:184:MET:HE3	1:C:84:LYS:HE2	1.99	0.44
1:B:90:THR:O	1:B:93:ASP:HB2	2.16	0.44
1:C:215:GLU:OE1	1:C:238:TYR:OH	2.28	0.44
1:A:76:LEU:O	1:A:77:PRO:C	2.61	0.44
1:A:227:ARG:NH1	1:A:315:SER:OG	2.47	0.44
1:B:119:ILE:HD13	1:B:309:LEU:HD22	1.99	0.44
1:B:148:TYR:CZ	1:D:293:MET:HG3	2.53	0.44
1:C:46:ASN:O	1:C:47:ARG:HB2	2.17	0.44
1:C:141:LYS:HG3	1:C:142:ARG:N	2.33	0.44
1:C:163:SER:HG	1:C:164:ASP:H	1.63	0.44
1:C:167:GLY:C	1:C:169:ILE:N	2.76	0.44
1:C:172:LEU:O	1:C:173:ALA:C	2.61	0.44
1:D:96:LYS:HB3	1:D:97:ASN:H	1.57	0.44
1:A:196:ILE:O	1:A:196:ILE:HG22	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:PHE:C	1:B:132:LEU:N	2.76	0.44
1:B:252:ASP:OD2	1:B:252:ASP:N	2.50	0.44
1:D:178:LYS:O	1:D:179:ASN:C	2.61	0.44
1:A:169:ILE:HG12	1:A:191:ILE:CD1	2.45	0.43
1:A:169:ILE:HG23	1:A:191:ILE:HD11	1.99	0.43
1:B:27:TYR:O	1:B:30:VAL:N	2.51	0.43
1:B:111:LEU:HB3	1:B:112:PRO:CD	2.48	0.43
1:B:140:ASN:O	1:B:141:LYS:C	2.60	0.43
1:C:30:VAL:HG13	1:C:268:VAL:HB	2.00	0.43
1:C:188:ILE:O	1:C:190:TYR:N	2.50	0.43
1:D:32:HIS:C	1:D:36:ASN:HD22	2.23	0.43
1:D:306:GLY:C	1:D:308:PRO:CD	2.91	0.43
1:A:134:SER:O	1:A:138:ILE:CD1	2.66	0.43
1:C:134:SER:O	1:C:138:ILE:CB	2.65	0.43
1:C:330:ILE:CG2	1:C:331:ASP:N	2.70	0.43
1:D:34:LEU:HD13	1:D:299:ILE:HG22	2.00	0.43
1:A:117:SER:HB3	1:A:122:ILE:O	2.18	0.43
1:A:250:ALA:C	1:A:262:LYS:HG3	2.43	0.43
1:B:172:LEU:O	1:B:187:LYS:NZ	2.51	0.43
1:D:72:ALA:N	1:D:73:PRO:HD2	2.34	0.43
1:D:273:ALA:C	1:D:275:ARG:H	2.27	0.43
1:A:41:SER:C	1:A:43:ASN:H	2.26	0.43
1:A:83:TYR:HE2	1:A:118:LYS:HD2	1.83	0.43
1:A:134:SER:C	1:A:138:ILE:HD11	2.44	0.43
1:A:158:LEU:HD22	1:C:81:ASN:HD21	1.81	0.43
1:B:131:LYS:O	1:B:134:SER:OG	2.36	0.43
1:C:15:PRO:HA	1:C:23:HIS:O	2.18	0.43
1:A:62:PRO:CG	1:A:63:GLU:H	2.32	0.43
1:A:236:ARG:CG	1:A:274:ASN:HD22	2.31	0.43
1:B:267:ILE:N	1:B:267:ILE:CD1	2.81	0.43
1:B:303:MET:O	1:B:304:CYS:C	2.61	0.43
1:C:135:ASP:CG	1:C:141:LYS:HB2	2.43	0.43
1:C:280:PHE:HB2	1:C:283:PRO:HB3	2.00	0.43
1:D:17:HIS:HB2	1:D:22:TRP:CZ3	2.53	0.43
1:D:156:ARG:HE	1:D:156:ARG:CA	2.27	0.43
1:D:282:GLU:N	1:D:283:PRO:CD	2.80	0.43
1:A:177:LEU:O	1:A:178:LYS:HB2	2.18	0.43
1:B:12:LEU:HD22	1:B:272:SER:HG	1.82	0.43
1:C:105:SER:HA	1:C:109:VAL:HB	2.00	0.43
1:C:320:ASP:HA	1:C:323:ASN:HD22	1.83	0.43
1:A:236:ARG:HH11	1:A:236:ARG:CG	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:260:ILE:N	1:A:260:ILE:HD13	2.33	0.43
1:B:207:GLY:O	1:B:210:ILE:HB	2.19	0.43
1:B:239:SER:O	1:B:242:GLN:NE2	2.48	0.43
1:B:297:PHE:HE2	1:B:311:ARG:CZ	2.32	0.43
1:D:60:ASP:O	1:D:62:PRO:CD	2.66	0.43
1:B:133:TRP:CE2	1:B:137:ILE:HD11	2.54	0.43
1:C:18:TYR:C	1:C:20:GLY:N	2.77	0.43
1:C:190:TYR:O	1:C:193:LEU:HB3	2.19	0.43
1:C:282:GLU:HB3	1:C:285:LEU:CD1	2.49	0.43
1:D:114:ASN:O	1:D:115:ILE:C	2.62	0.43
1:D:117:SER:OG	1:D:122:ILE:HB	2.18	0.43
1:D:226:ASN:ND2	1:D:226:ASN:C	2.77	0.43
1:A:31:LYS:HB2	1:A:295:LEU:HD11	1.99	0.43
1:A:88:GLU:HG3	1:A:316:ILE:CG2	2.48	0.43
1:A:289:GLY:O	1:A:290:ARG:O	2.37	0.43
1:B:53:GLY:O	1:B:54:ILE:HG23	2.19	0.43
1:D:56:PHE:HE2	1:D:190:TYR:CE1	2.36	0.43
1:D:158:LEU:HD11	1:D:184:MET:HG2	2.01	0.43
1:D:221:ASP:O	1:D:222:ASP:C	2.61	0.43
1:D:261:LYS:H	1:D:261:LYS:HG3	1.45	0.43
1:D:270:LEU:C	1:D:274:ASN:HD22	2.24	0.43
1:D:287:LYS:HB2	1:D:290:ARG:HE	1.84	0.43
1:D:344:LEU:HD12	1:D:344:LEU:C	2.44	0.43
1:A:18:TYR:HD1	1:A:18:TYR:O	2.02	0.43
1:B:67:PHE:C	1:B:69:ASP:N	2.75	0.43
1:B:71:SER:C	1:B:73:PRO:HD2	2.44	0.43
1:B:113:VAL:HG13	1:B:114:ASN:N	2.34	0.43
1:B:122:ILE:HG13	1:B:130:PHE:CD1	2.54	0.43
1:B:199:ASN:HD22	1:B:199:ASN:HA	1.60	0.43
1:C:98:ILE:O	1:C:101:LYS:HB2	2.19	0.43
1:C:191:ILE:O	1:C:192:MET:C	2.59	0.43
1:C:235:LEU:O	1:C:239:SER:HA	2.19	0.43
1:A:115:ILE:O	1:A:119:ILE:HG13	2.18	0.42
1:A:336:ARG:NH1	1:B:254:TYR:CE2	2.87	0.42
1:B:69:ASP:C	1:B:71:SER:N	2.77	0.42
1:C:56:PHE:CD1	1:C:56:PHE:C	2.96	0.42
1:C:210:ILE:O	1:C:213:ILE:HB	2.19	0.42
1:C:287:LYS:HD3	1:C:290:ARG:CZ	2.48	0.42
1:B:130:PHE:O	1:B:132:LEU:N	2.52	0.42
1:C:73:PRO:HG2	1:C:74:TYR:N	2.34	0.42
1:C:318:LEU:O	1:C:319:ASN:C	2.60	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:ASP:C	1:D:62:PRO:HD2	2.44	0.42
1:D:133:TRP:CZ3	1:D:195:ILE:HG21	2.54	0.42
1:A:297:PHE:CD2	1:A:311:ARG:NH2	2.87	0.42
1:B:99:ASP:OD1	1:B:99:ASP:N	2.50	0.42
1:C:88:GLU:O	1:C:92:ASN:HB2	2.19	0.42
1:C:156:ARG:HH21	1:C:160:ILE:HD13	1.84	0.42
1:D:153:MET:HE2	1:D:157:LEU:HD22	2.01	0.42
1:A:324:HIS:O	1:A:324:HIS:ND1	2.53	0.42
1:C:130:PHE:HE2	1:C:153:MET:CE	2.19	0.42
1:D:88:GLU:O	1:D:89:GLU:C	2.62	0.42
1:A:15:PRO:HA	1:A:23:HIS:O	2.19	0.42
1:A:56:PHE:HE2	1:A:190:TYR:CE1	2.37	0.42
1:A:176:SER:HB2	1:A:181:LYS:CA	2.37	0.42
1:B:78:SER:C	1:B:80:ILE:N	2.77	0.42
1:B:198:GLY:O	1:B:199:ASN:CB	2.67	0.42
1:B:54:ILE:O	1:B:55:SER:CB	2.67	0.42
1:B:227:ARG:NH1	1:B:315:SER:HB3	2.33	0.42
1:C:104:ILE:HA	1:C:108:ALA:HB3	2.02	0.42
1:C:104:ILE:HD11	1:C:346:TYR:HB2	2.02	0.42
1:C:174:GLY:O	1:C:175:SER:HB3	2.20	0.42
1:C:248:PHE:O	1:C:249:ALA:C	2.63	0.42
1:D:63:GLU:OE2	1:D:67:PHE:HE1	2.01	0.42
1:D:116:ILE:HG13	1:D:198:GLY:HA3	2.02	0.42
1:D:234:THR:O	1:D:235:LEU:C	2.62	0.42
1:A:227:ARG:HB3	1:A:227:ARG:NH1	2.35	0.42
1:B:112:PRO:O	1:B:115:ILE:N	2.51	0.42
1:B:129:LEU:HD12	1:B:129:LEU:N	2.26	0.42
1:B:172:LEU:HD23	1:B:172:LEU:HA	1.73	0.42
1:C:204:ASN:O	1:C:205:LEU:C	2.63	0.42
1:D:17:HIS:HA	1:D:21:ALA:O	2.19	0.42
1:D:151:ASN:C	1:D:153:MET:N	2.72	0.42
1:A:209:MET:O	1:A:213:ILE:HG12	2.20	0.42
1:B:28:SER:O	1:B:32:HIS:HB2	2.20	0.42
1:B:44:PRO:HA	1:B:248:PHE:CE1	2.55	0.42
1:B:196:ILE:O	1:B:197:GLY:C	2.61	0.42
1:B:311:ARG:O	1:B:314:ALA:HB3	2.20	0.42
1:C:80:ILE:HD12	1:C:80:ILE:HA	1.86	0.42
1:D:36:ASN:HB3	1:D:39:ILE:HD12	2.01	0.42
1:D:69:ASP:O	1:D:70:ILE:C	2.62	0.42
1:D:342:MET:O	1:D:342:MET:HG2	2.20	0.42
1:A:23:HIS:ND1	1:A:269:TYR:CE1	2.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LEU:O	1:A:173:ALA:C	2.63	0.42
1:B:178:LYS:C	1:B:180:ARG:N	2.72	0.42
1:B:182:LEU:HD13	1:B:187:LYS:CE	2.50	0.42
1:C:122:ILE:HD12	1:C:130:PHE:CE1	2.54	0.42
1:D:26:LYS:HB2	1:D:29:ASP:OD2	2.19	0.42
1:D:119:ILE:O	1:D:167:GLY:HA2	2.20	0.42
1:D:236:ARG:NH2	1:D:283:PRO:O	2.52	0.42
1:D:280:PHE:HD2	1:D:290:ARG:NH1	2.17	0.42
1:A:44:PRO:O	1:A:45:GLY:C	2.63	0.42
1:A:152:ARG:HD2	1:A:152:ARG:HA	1.88	0.42
1:B:31:LYS:HG3	1:B:299:ILE:HD13	2.02	0.42
1:B:236:ARG:HG3	1:B:294:HIS:HB3	2.02	0.42
1:C:83:TYR:CE1	1:C:119:ILE:HG12	2.55	0.42
1:C:243:PHE:CE2	1:C:342:MET:HA	2.55	0.42
1:D:211:ARG:NH2	1:D:238:TYR:OH	2.53	0.42
1:D:240:PRO:O	1:D:343:VAL:HA	2.20	0.42
1:D:248:PHE:CA	1:D:264:ASP:O	2.64	0.42
1:D:275:ARG:HG3	1:D:275:ARG:HH11	1.85	0.42
1:B:42:SER:HB2	1:B:302:HIS:NE2	2.35	0.41
1:C:65:LYS:O	1:C:69:ASP:CB	2.67	0.41
1:C:219:ILE:HD12	1:C:219:ILE:HA	1.73	0.41
1:C:238:TYR:HB3	1:C:344:LEU:HD23	2.01	0.41
1:D:296:ALA:C	1:D:298:GLY:H	2.28	0.41
1:A:87:ILE:CG2	1:A:316:ILE:HD12	2.46	0.41
1:A:153:MET:O	1:A:154:VAL:C	2.63	0.41
1:B:27:TYR:HA	1:B:273:ALA:HB1	2.02	0.41
1:C:55:SER:OG	1:C:56:PHE:N	2.52	0.41
1:C:200:GLU:O	1:C:202:THR:N	2.54	0.41
1:D:156:ARG:NH2	1:D:159:GLU:OE2	2.53	0.41
1:D:337:LEU:O	1:D:338:LEU:C	2.63	0.41
1:A:27:TYR:O	1:A:31:LYS:HB2	2.19	0.41
1:A:136:TYR:CE2	1:A:146:PHE:HB2	2.55	0.41
1:A:326:LYS:HD3	1:A:326:LYS:HA	1.87	0.41
1:B:138:ILE:CD1	1:B:140:ASN:HB2	2.32	0.41
1:C:77:PRO:O	1:C:80:ILE:HG22	2.20	0.41
1:D:126:ASP:OD1	1:D:156:ARG:HD3	2.18	0.41
1:A:18:TYR:CD1	1:A:19:ASP:HB2	2.55	0.41
1:A:120:LEU:CD2	1:A:168:ILE:HB	2.51	0.41
1:A:223:ALA:O	1:A:224:LEU:C	2.63	0.41
1:C:18:TYR:HD1	1:C:19:ASP:OD2	2.03	0.41
1:C:77:PRO:HD3	1:C:308:PRO:HG2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:ARG:NH1	1:A:227:ARG:CB	2.84	0.41
1:A:281:ASP:O	1:A:290:ARG:NH2	2.51	0.41
1:B:66:GLU:CD	1:B:178:LYS:HD2	2.46	0.41
1:C:27:TYR:CD1	1:C:273:ALA:O	2.73	0.41
1:C:40:PHE:CD2	1:C:266:VAL:HG21	2.55	0.41
1:C:245:PRO:HG2	1:C:246:HIS:N	2.34	0.41
1:D:92:ASN:C	1:D:94:LEU:N	2.78	0.41
1:D:174:GLY:O	1:D:175:SER:CB	2.66	0.41
1:D:227:ARG:CZ	1:D:319:ASN:HD22	2.31	0.41
1:D:277:GLU:H	1:D:277:GLU:HG3	1.72	0.41
1:A:236:ARG:HG3	1:A:274:ASN:ND2	2.35	0.41
1:A:336:ARG:NH1	1:B:254:TYR:CD2	2.89	0.41
1:B:243:PHE:HB2	1:B:268:VAL:O	2.21	0.41
1:C:183:THR:HB	1:C:186:GLU:H	1.84	0.41
1:C:259:LYS:O	1:C:259:LYS:CG	2.69	0.41
1:D:85:ASP:HA	1:D:88:GLU:OE1	2.21	0.41
1:A:117:SER:OG	1:A:127:MET:HG2	2.20	0.41
1:A:329:LYS:HD2	1:A:352:SER:OXT	2.20	0.41
1:B:172:LEU:HA	1:B:175:SER:OG	2.20	0.41
1:C:213:ILE:CG2	1:C:328:ILE:HB	2.51	0.41
1:C:347:ASP:O	1:C:348:LYS:HE3	2.20	0.41
1:D:12:LEU:CD1	1:D:25:TYR:O	2.68	0.41
1:D:205:LEU:O	1:D:206:ILE:C	2.63	0.41
1:D:233:GLU:HG3	1:D:286:PHE:CE1	2.55	0.41
1:A:23:HIS:CE1	1:A:267:ILE:CD1	3.02	0.41
1:A:133:TRP:CH2	1:A:196:ILE:HD11	2.56	0.41
1:A:178:LYS:CE	1:A:179:ASN:OD1	2.68	0.41
1:A:286:PHE:O	1:A:286:PHE:CD2	2.73	0.41
1:B:21:ALA:CB	1:B:267:ILE:HD13	2.48	0.41
1:C:44:PRO:HB3	1:C:248:PHE:CE2	2.56	0.41
1:C:92:ASN:HA	1:C:95:ILE:HG22	2.03	0.41
1:D:236:ARG:HD2	1:D:280:PHE:CE2	2.56	0.41
1:A:79:LYS:HA	1:A:79:LYS:HD3	1.83	0.41
1:A:80:ILE:CG2	1:A:81:ASN:N	2.82	0.41
1:A:98:ILE:HD11	1:A:107:TYR:HB2	1.98	0.41
1:A:140:ASN:O	1:A:141:LYS:HB2	2.21	0.41
1:A:162:LYS:O	1:A:163:SER:O	2.39	0.41
1:B:116:ILE:HG22	1:B:117:SER:N	2.34	0.41
1:B:153:MET:HG3	1:B:157:LEU:CD1	2.49	0.41
1:B:216:ASN:N	1:B:217:PRO:HD3	2.36	0.41
1:B:253:SER:C	1:B:254:TYR:CD1	2.99	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:349:LEU:CD2	1:B:350:PHE:N	2.84	0.41
1:C:120:LEU:HD21	1:C:194:LEU:HB3	2.03	0.41
1:C:136:TYR:CZ	1:C:143:ASP:HB2	2.55	0.41
1:C:202:THR:N	2:C:410:HEM:HBB2	2.35	0.41
1:C:212:VAL:O	1:C:216:ASN:N	2.50	0.41
1:C:226:ASN:C	1:C:226:ASN:HD22	2.28	0.41
1:D:116:ILE:CG2	1:D:117:SER:N	2.83	0.41
1:D:172:LEU:O	1:D:173:ALA:C	2.64	0.41
1:D:183:THR:HG22	1:D:184:MET:N	2.35	0.41
1:D:351:LEU:HB3	1:D:352:SER:H	1.66	0.41
1:B:34:LEU:O	1:B:36:ASN:N	2.54	0.41
1:B:127:MET:HG3	1:B:131:LYS:CD	2.51	0.41
1:B:142:ARG:H	1:B:142:ARG:HG2	1.72	0.41
1:C:143:ASP:O	1:C:144:GLU:C	2.64	0.41
1:C:223:ALA:O	1:C:224:LEU:C	2.63	0.41
1:D:131:LYS:C	1:D:134:SER:HB3	2.46	0.41
1:D:246:HIS:O	1:D:247:ARG:HD3	2.21	0.41
1:A:312:LEU:HD22	1:A:316:ILE:CD1	2.51	0.40
1:B:183:THR:CG2	1:B:184:MET:H	2.34	0.40
1:B:233:GLU:HG2	1:B:286:PHE:CE2	2.55	0.40
1:C:136:TYR:CD2	1:C:146:PHE:CB	3.04	0.40
1:C:136:TYR:HE2	1:C:143:ASP:HB2	1.83	0.40
1:D:17:HIS:HE1	1:D:20:GLY:HA2	1.85	0.40
1:A:140:ASN:OD1	1:A:338:LEU:HD13	2.21	0.40
1:A:183:THR:CB	1:A:186:GLU:HG3	2.33	0.40
1:C:148:TYR:C	1:C:150:ASN:N	2.75	0.40
1:D:336:ARG:HD3	1:D:336:ARG:HA	1.91	0.40
1:A:171:VAL:O	1:A:175:SER:OG	2.34	0.40
1:B:211:ARG:HB2	1:B:346:TYR:OH	2.22	0.40
1:B:299:ILE:HG13	1:B:303:MET:HE1	2.03	0.40
1:C:204:ASN:HB3	1:C:344:LEU:O	2.21	0.40
1:C:299:ILE:HA	1:C:303:MET:HG3	2.02	0.40
1:D:24:VAL:HG13	1:D:29:ASP:HB3	2.03	0.40
1:D:73:PRO:C	1:D:75:PHE:N	2.79	0.40
1:D:80:ILE:CG2	1:D:312:LEU:HD12	2.46	0.40
1:D:135:ASP:HA	1:D:138:ILE:CG1	2.52	0.40
1:D:144:GLU:HA	1:D:147:ASN:HB3	2.03	0.40
1:A:110:ARG:HA	1:A:113:VAL:CG1	2.52	0.40
1:A:211:ARG:O	1:A:212:VAL:C	2.63	0.40
1:A:221:ASP:O	1:A:225:LYS:HG3	2.21	0.40
1:A:247:ARG:HB2	1:A:266:VAL:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:329:LYS:HE2	1:A:352:SER:C	2.47	0.40
1:B:156:ARG:O	1:B:159:GLU:HB3	2.20	0.40
1:C:80:ILE:HG22	1:C:81:ASN:H	1.86	0.40
1:C:351:LEU:HD12	1:C:351:LEU:N	2.26	0.40
1:D:18:TYR:HD1	1:D:19:ASP:OD1	2.04	0.40
1:A:325:PHE:O	1:A:326:LYS:O	2.39	0.40
1:B:65:LYS:C	1:B:67:PHE:N	2.79	0.40
1:B:156:ARG:CZ	1:D:226:ASN:ND2	2.84	0.40
1:C:30:VAL:O	1:C:31:LYS:C	2.64	0.40
1:C:331:ASP:C	1:C:333:LYS:N	2.79	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	334/343 (97%)	242 (72%)	59 (18%)	33 (10%)	0	3
1	B	334/343 (97%)	216 (65%)	81 (24%)	37 (11%)	0	2
1	C	334/343 (97%)	230 (69%)	73 (22%)	31 (9%)	0	3
1	D	334/343 (97%)	229 (69%)	70 (21%)	35 (10%)	0	2
All	All	1336/1372 (97%)	917 (69%)	283 (21%)	136 (10%)	0	3

All (136) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	19	ASP
1	A	61	ASN
1	A	163	SER
1	A	164	ASP
1	A	173	ALA

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Mol	Chain	Res	Type
1	A	201	THR
1	A	220	ILE
1	B	35	MET
1	B	46	ASN
1	B	64	HIS
1	B	70	ILE
1	B	96	LYS
1	B	97	ASN
1	B	199	ASN
1	B	327	ARG
1	C	13	ASN
1	C	61	ASN
1	C	96	LYS
1	C	104	ILE
1	C	177	LEU
1	C	219	ILE
1	C	299	ILE
1	C	330	ILE
1	C	331	ASP
1	D	45	GLY
1	D	61	ASN
1	D	96	LYS
1	D	108	ALA
1	D	115	ILE
1	D	135	ASP
1	D	136	TYR
1	D	163	SER
1	D	173	ALA
1	D	175	SER
1	A	45	GLY
1	A	271	GLY
1	A	290	ARG
1	A	299	ILE
1	A	326	LYS
1	B	44	PRO
1	B	99	ASP
1	B	125	SER
1	B	141	LYS
1	B	165	SER
1	B	182	LEU
1	B	220	ILE
1	C	54	ILE

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Mol	Chain	Res	Type
1	C	78	SER
1	C	105	SER
1	C	144	GLU
1	C	164	ASP
1	C	176	SER
1	C	201	THR
1	C	225	LYS
1	C	327	ARG
1	C	340	ASN
1	D	15	PRO
1	D	70	ILE
1	D	109	VAL
1	D	138	ILE
1	D	142	ARG
1	D	165	SER
1	D	220	ILE
1	D	251	GLU
1	D	261	LYS
1	D	283	PRO
1	A	21	ALA
1	A	46	ASN
1	A	100	ASN
1	A	141	LYS
1	A	176	SER
1	A	217	PRO
1	A	221	ASP
1	A	264	ASP
1	A	321	ILE
1	B	27	TYR
1	B	80	ILE
1	B	89	GLU
1	B	107	TYR
1	B	124	ASP
1	B	140	ASN
1	B	179	ASN
1	B	273	ALA
1	C	19	ASP
1	C	32	HIS
1	C	45	GLY
1	C	47	ARG
1	C	179	ASN
1	C	245	PRO

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Mol	Chain	Res	Type
1	D	32	HIS
1	D	33	VAL
1	D	133	TRP
1	D	164	ASP
1	D	172	LEU
1	D	200	GLU
1	A	341	LYS
1	B	15	PRO
1	B	18	TYR
1	B	112	PRO
1	B	160	ILE
1	B	251	GLU
1	C	163	SER
1	C	223	ALA
1	D	95	ILE
1	D	234	THR
1	D	235	LEU
1	D	257	ASN
1	A	86	PHE
1	A	123	PRO
1	A	149	VAL
1	A	152	ARG
1	A	168	ILE
1	B	61	ASN
1	B	91	SER
1	B	93	ASP
1	B	123	PRO
1	B	178	LYS
1	B	289	GLY
1	B	299	ILE
1	C	142	ARG
1	C	173	ALA
1	C	283	PRO
1	D	326	LYS
1	D	333	LYS
1	D	338	LEU
1	A	284	ASP
1	D	139	GLY
1	A	77	PRO
1	A	138	ILE
1	C	33	VAL
1	A	104	ILE

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Mol	Chain	Res	Type
1	A	255	ILE
1	D	98	ILE
1	A	62	PRO
1	B	95	ILE
1	B	197	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	307/310 (99%)	279 (91%)	28 (9%)	9	32
1	B	307/310 (99%)	269 (88%)	38 (12%)	4	19
1	C	307/310 (99%)	271 (88%)	36 (12%)	5	22
1	D	304/310 (98%)	276 (91%)	28 (9%)	8	31
All	All	1225/1240 (99%)	1095 (89%)	130 (11%)	6	26

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	16	VAL
1	A	18	TYR
1	A	48	TYR
1	A	54	ILE
1	A	59	MET
1	A	60	ASP
1	A	77	PRO
1	A	80	ILE
1	A	93	ASP
1	A	110	ARG
1	A	116	ILE
1	A	137	ILE
1	A	138	ILE
1	A	142	ARG
1	A	145	ASN

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Mol	Chain	Res	Type
1	A	151	ASN
1	A	179	ASN
1	A	180	ARG
1	A	228	SER
1	A	232	GLU
1	A	236	ARG
1	A	248	PHE
1	A	268	VAL
1	A	274	ASN
1	A	277	GLU
1	A	278	THR
1	A	312	LEU
1	B	13	ASN
1	B	43	ASN
1	B	47	ARG
1	B	48	TYR
1	B	54	ILE
1	B	56	PHE
1	B	63	GLU
1	B	77	PRO
1	B	97	ASN
1	B	99	ASP
1	B	100	ASN
1	B	109	VAL
1	B	116	ILE
1	B	123	PRO
1	B	140	ASN
1	B	147	ASN
1	B	152	ARG
1	B	159	GLU
1	B	163	SER
1	B	170	ASN
1	B	172	LEU
1	B	181	LYS
1	B	182	LEU
1	B	199	ASN
1	B	201	THR
1	B	202	THR
1	B	221	ASP
1	B	227	ARG
1	B	245	PRO
1	B	252	ASP

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Mol	Chain	Res	Type
1	B	256	ASN
1	B	268	VAL
1	B	330	ILE
1	B	339	ASP
1	B	340	ASN
1	B	344	LEU
1	B	349	LEU
1	B	351	LEU
1	C	16	VAL
1	C	49	SER
1	C	54	ILE
1	C	77	PRO
1	C	80	ILE
1	C	82	ASP
1	C	85	ASP
1	C	89	GLU
1	C	94	LEU
1	C	102	ASP
1	C	105	SER
1	C	116	ILE
1	C	129	LEU
1	C	132	LEU
1	C	138	ILE
1	C	148	TYR
1	C	151	ASN
1	C	153	MET
1	C	154	VAL
1	C	156	ARG
1	C	158	LEU
1	C	162	LYS
1	C	192	MET
1	C	200	GLU
1	C	202	THR
1	C	218	ASP
1	C	219	ILE
1	C	222	ASP
1	C	232	GLU
1	C	248	PHE
1	C	282	GLU
1	C	284	ASP
1	C	288	ILE
1	C	320	ASP

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Mol	Chain	Res	Type
1	C	329	LYS
1	C	351	LEU
1	D	17	HIS
1	D	43	ASN
1	D	54	ILE
1	D	55	SER
1	D	80	ILE
1	D	116	ILE
1	D	137	ILE
1	D	146	PHE
1	D	147	ASN
1	D	149	VAL
1	D	153	MET
1	D	156	ARG
1	D	164	ASP
1	D	177	LEU
1	D	182	LEU
1	D	192	MET
1	D	195	ILE
1	D	203	THR
1	D	222	ASP
1	D	236	ARG
1	D	265	GLN
1	D	292	GLU
1	D	312	LEU
1	D	323	ASN
1	D	332	TYR
1	D	344	LEU
1	D	346	TYR
1	D	348	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (55) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	13	ASN
1	A	97	ASN
1	A	100	ASN
1	A	145	ASN
1	A	147	ASN
1	A	151	ASN
1	A	170	ASN
1	A	199	ASN

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Mol	Chain	Res	Type
1	A	226	ASN
1	A	246	HIS
1	A	256	ASN
1	A	274	ASN
1	A	319	ASN
1	B	64	HIS
1	B	100	ASN
1	B	140	ASN
1	B	145	ASN
1	B	151	ASN
1	B	199	ASN
1	B	208	ASN
1	B	242	GLN
1	B	265	GLN
1	B	340	ASN
1	C	32	HIS
1	C	36	ASN
1	C	43	ASN
1	C	46	ASN
1	C	114	ASN
1	C	140	ASN
1	C	179	ASN
1	C	199	ASN
1	C	204	ASN
1	C	208	ASN
1	C	226	ASN
1	C	302	HIS
1	C	319	ASN
1	C	323	ASN
1	C	340	ASN
1	D	36	ASN
1	D	43	ASN
1	D	61	ASN
1	D	97	ASN
1	D	100	ASN
1	D	147	ASN
1	D	150	ASN
1	D	166	HIS
1	D	199	ASN
1	D	204	ASN
1	D	208	ASN
1	D	226	ASN

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Mol	Chain	Res	Type
1	D	246	HIS
1	D	256	ASN
1	D	265	GLN
1	D	319	ASN
1	D	324	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

8 ligands 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	PIM	C	411	2	11,12,12	3.24	9 (81%)	14,15,15	2.02	5 (35%)
3	PIM	A	411	2	11,12,12	3.23	9 (81%)	14,15,15	1.93	4 (28%)
2	HEM	B	410	1,3	50,50,50	1.14	3 (6%)	67,82,82	1.42	8 (11%)
2	HEM	A	410	1,3	50,50,50	1.18	4 (8%)	67,82,82	1.46	12 (17%)
3	PIM	D	411	2	11,12,12	3.14	9 (81%)	14,15,15	1.82	4 (28%)
2	HEM	C	410	1,3	50,50,50	1.13	2 (4%)	67,82,82	1.18	6 (8%)
2	HEM	D	410	1,3	50,50,50	1.03	2 (4%)	67,82,82	1.30	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	PIM	B	411	2	11,12,12	3.76	9 (81%)	14,15,15	1.72	2 (14%)

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	PIM	C	411	2	-	0/4/4/4	0/2/2/2
3	PIM	A	411	2	-	4/4/4/4	0/2/2/2
2	HEM	B	410	1,3	-	5/14/54/54	-
2	HEM	A	410	1,3	-	6/14/54/54	-
3	PIM	D	411	2	-	0/4/4/4	0/2/2/2
2	HEM	C	410	1,3	-	7/14/54/54	-
2	HEM	D	410	1,3	-	6/14/54/54	-
3	PIM	B	411	2	-	4/4/4/4	0/2/2/2

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	411	PIM	C8-C7	5.63	1.48	1.38
3	B	411	PIM	C7-C6	5.61	1.47	1.39
3	A	411	PIM	C8-C7	5.04	1.47	1.38
3	D	411	PIM	C8-C7	4.75	1.47	1.38
3	C	411	PIM	C8-C7	4.63	1.46	1.38
3	B	411	PIM	C10-C11	4.54	1.46	1.38
3	C	411	PIM	C7-C6	4.51	1.46	1.39
3	D	411	PIM	C7-C6	4.40	1.46	1.39
3	A	411	PIM	C5-N1	-4.31	1.33	1.38
3	A	411	PIM	C7-C6	4.29	1.45	1.39
3	D	411	PIM	C10-C11	4.01	1.45	1.38
3	B	411	PIM	C10-C9	3.90	1.46	1.38
3	B	411	PIM	C2-N1	3.74	1.41	1.35
3	B	411	PIM	C6-C5	3.74	1.53	1.47
3	C	411	PIM	C10-C11	3.71	1.45	1.38
2	A	410	HEM	CAB-C3B	-3.69	1.37	1.47
3	D	411	PIM	C6-C5	3.69	1.53	1.47
3	A	411	PIM	C10-C11	3.69	1.45	1.38
2	C	410	HEM	CAC-C3C	-3.62	1.37	1.47
3	B	411	PIM	C5-N1	-3.62	1.34	1.38
3	C	411	PIM	C5-N1	-3.37	1.34	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	410	HEM	CAB-C3B	-3.31	1.38	1.47
3	C	411	PIM	C9-C8	3.23	1.45	1.38
3	C	411	PIM	C10-C9	3.21	1.45	1.38
2	B	410	HEM	FE-NC	3.19	2.05	1.95
2	A	410	HEM	CAC-C3C	-3.02	1.39	1.47
3	A	411	PIM	C4-N3	-3.01	1.32	1.37
2	D	410	HEM	CAB-C3B	-3.00	1.39	1.47
3	C	411	PIM	C4-N3	-2.99	1.32	1.37
3	C	411	PIM	C6-C5	2.98	1.52	1.47
3	D	411	PIM	C2-N1	2.94	1.39	1.35
3	D	411	PIM	C10-C9	2.91	1.44	1.38
3	B	411	PIM	C9-C8	2.82	1.44	1.38
3	A	411	PIM	C2-N1	2.80	1.39	1.35
3	A	411	PIM	C10-C9	2.77	1.44	1.38
3	D	411	PIM	C9-C8	2.69	1.44	1.38
2	B	410	HEM	CAC-C3C	-2.68	1.40	1.47
3	A	411	PIM	C9-C8	2.66	1.44	1.38
3	C	411	PIM	C2-N1	2.61	1.39	1.35
3	D	411	PIM	C4-N3	-2.57	1.33	1.37
3	A	411	PIM	C6-C5	2.57	1.51	1.47
3	B	411	PIM	C4-N3	-2.52	1.33	1.37
2	A	410	HEM	C3B-C2B	-2.37	1.32	1.37
2	A	410	HEM	CHC-C1C	2.29	1.42	1.38
3	D	411	PIM	C5-N1	-2.23	1.35	1.38
2	D	410	HEM	C4D-C3D	-2.05	1.41	1.45
2	B	410	HEM	CAB-C3B	-2.05	1.41	1.47

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	410	HEM	C3B-C4B-NB	3.96	112.31	109.47
2	D	410	HEM	C4C-C3C-C2C	-3.89	103.44	106.81
3	A	411	PIM	C2-N1-C5	-3.83	105.58	107.53
3	C	411	PIM	C2-N1-C5	-3.80	105.59	107.53
2	B	410	HEM	CMA-C3A-C4A	3.58	130.87	125.42
2	A	410	HEM	CAC-C3C-C4C	3.20	132.46	124.82
3	D	411	PIM	C2-N1-C5	-3.14	105.92	107.53
2	C	410	HEM	C3C-C2C-C1C	-3.12	104.09	107.05
2	B	410	HEM	CHD-C4C-NC	-3.09	121.08	124.45
2	D	410	HEM	C1D-C2D-C3D	-3.09	103.73	106.98
3	B	411	PIM	C6-C5-N1	3.08	127.30	123.72
3	B	411	PIM	C2-N1-C5	-2.93	106.03	107.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	410	HEM	C3B-C4B-NB	2.89	111.54	109.47
2	A	410	HEM	CBD-CAD-C3D	2.86	120.43	112.53
2	B	410	HEM	CBA-CAA-C2A	2.82	120.34	112.53
2	B	410	HEM	C4C-NC-C1C	-2.81	101.25	105.82
2	A	410	HEM	CMC-C2C-C1C	2.77	129.60	124.73
3	D	411	PIM	C6-C5-N1	2.65	126.80	123.72
2	A	410	HEM	CMC-C2C-C3C	-2.60	122.13	128.43
3	C	411	PIM	C9-C10-C11	-2.58	117.05	120.24
2	A	410	HEM	C2B-C1B-NB	2.57	112.80	109.84
2	C	410	HEM	CMD-C2D-C1D	2.56	129.04	125.03
3	A	411	PIM	C6-C5-N1	2.56	126.69	123.72
2	B	410	HEM	C2C-C1C-NC	2.51	114.28	109.64
2	B	410	HEM	CHC-C4B-C3B	-2.49	120.11	125.07
2	C	410	HEM	C1D-C2D-C3D	-2.46	104.40	106.98
2	A	410	HEM	CBA-CAA-C2A	2.45	119.30	112.53
2	D	410	HEM	CHD-C4C-C3C	-2.43	121.12	125.21
2	A	410	HEM	CAB-C3B-C2B	-2.41	120.58	128.43
2	A	410	HEM	CAC-C3C-C2C	-2.40	120.62	128.43
3	C	411	PIM	C6-C5-N1	2.35	126.44	123.72
2	C	410	HEM	CAD-C3D-C2D	-2.34	123.48	127.87
3	C	411	PIM	C4-C5-N1	2.33	108.74	104.68
2	D	410	HEM	C4D-C3D-C2D	2.31	110.26	106.89
3	A	411	PIM	C4-C5-N1	2.31	108.71	104.68
2	D	410	HEM	C2A-C1A-NA	2.31	112.71	110.15
2	A	410	HEM	CMB-C2B-C1B	2.29	128.61	125.03
2	D	410	HEM	CHD-C1D-C2D	-2.25	121.48	125.03
2	D	410	HEM	CBA-CAA-C2A	-2.21	106.41	112.53
2	A	410	HEM	CHA-C4D-C3D	-2.19	121.18	125.23
2	D	410	HEM	C4A-NA-C1A	-2.18	102.26	105.82
3	A	411	PIM	C9-C10-C11	-2.13	117.61	120.24
2	A	410	HEM	CAD-C3D-C4D	-2.12	121.00	124.70
2	A	410	HEM	C4A-NA-C1A	-2.11	102.38	105.82
2	C	410	HEM	C2C-C1C-NC	2.07	113.47	109.64
3	D	411	PIM	C9-C10-C11	-2.07	117.69	120.24
3	D	411	PIM	C4-C5-N1	2.06	108.28	104.68
2	B	410	HEM	CAC-C3C-C4C	2.06	129.73	124.82
3	C	411	PIM	C10-C9-C8	2.01	122.62	119.87

There are no chirality outliers.

All (32) torsion outliers are listed below:

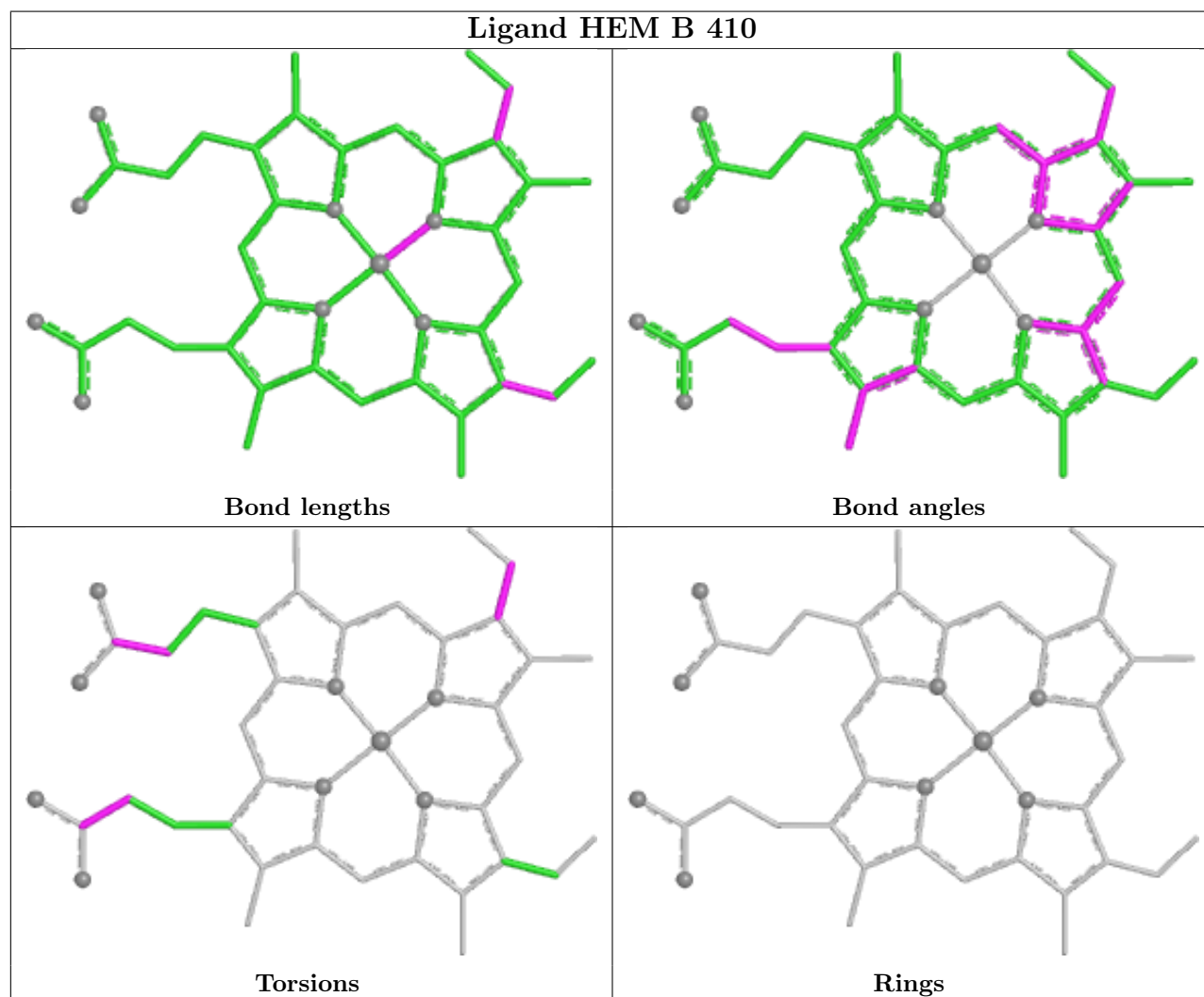
Mol	Chain	Res	Type	Atoms
2	B	410	HEM	C2C-C3C-CAC-CBC
2	C	410	HEM	C2B-C3B-CAB-CBB
2	C	410	HEM	C4B-C3B-CAB-CBB
2	D	410	HEM	C2C-C3C-CAC-CBC
2	D	410	HEM	C4C-C3C-CAC-CBC
3	A	411	PIM	N1-C5-C6-C7
3	A	411	PIM	N1-C5-C6-C11
3	A	411	PIM	C4-C5-C6-C7
3	A	411	PIM	C4-C5-C6-C11
3	B	411	PIM	N1-C5-C6-C7
3	B	411	PIM	N1-C5-C6-C11
3	B	411	PIM	C4-C5-C6-C7
3	B	411	PIM	C4-C5-C6-C11
2	A	410	HEM	C2B-C3B-CAB-CBB
2	A	410	HEM	C4B-C3B-CAB-CBB
2	B	410	HEM	C4C-C3C-CAC-CBC
2	C	410	HEM	C2D-C3D-CAD-CBD
2	D	410	HEM	CAD-CBD-CGD-O2D
2	B	410	HEM	CAA-CBA-CGA-O2A
2	C	410	HEM	CAD-CBD-CGD-O2D
2	D	410	HEM	CAD-CBD-CGD-O1D
2	A	410	HEM	CAD-CBD-CGD-O2D
2	B	410	HEM	CAA-CBA-CGA-O1A
2	C	410	HEM	CAA-CBA-CGA-O2A
2	D	410	HEM	CAA-CBA-CGA-O2A
2	D	410	HEM	CAA-CBA-CGA-O1A
2	C	410	HEM	CAA-CBA-CGA-O1A
2	C	410	HEM	CAD-CBD-CGD-O1D
2	A	410	HEM	CAA-CBA-CGA-O2A
2	A	410	HEM	CAD-CBD-CGD-O1D
2	A	410	HEM	CAA-CBA-CGA-O1A
2	B	410	HEM	CAD-CBD-CGD-O2D

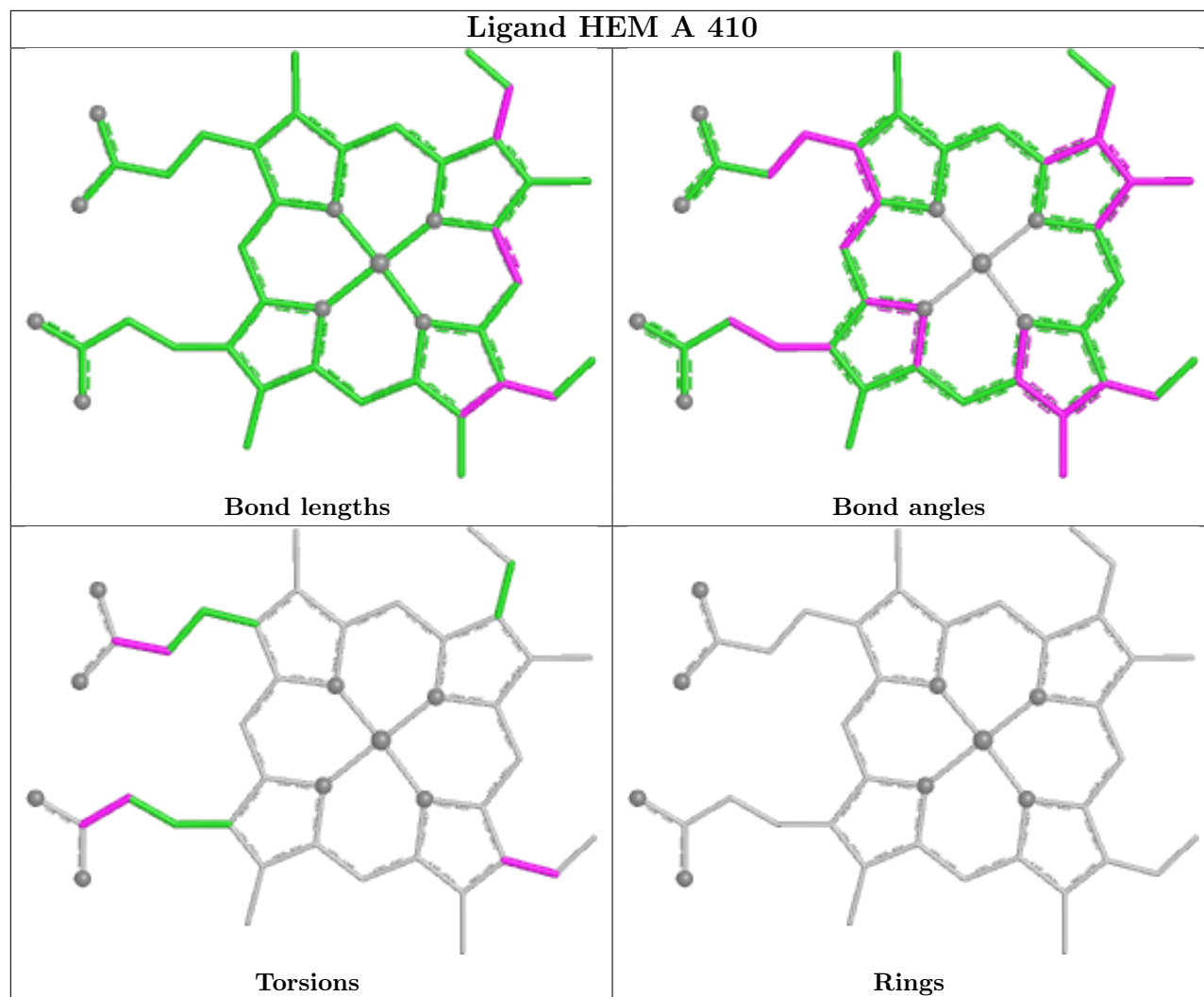
There are no ring outliers.

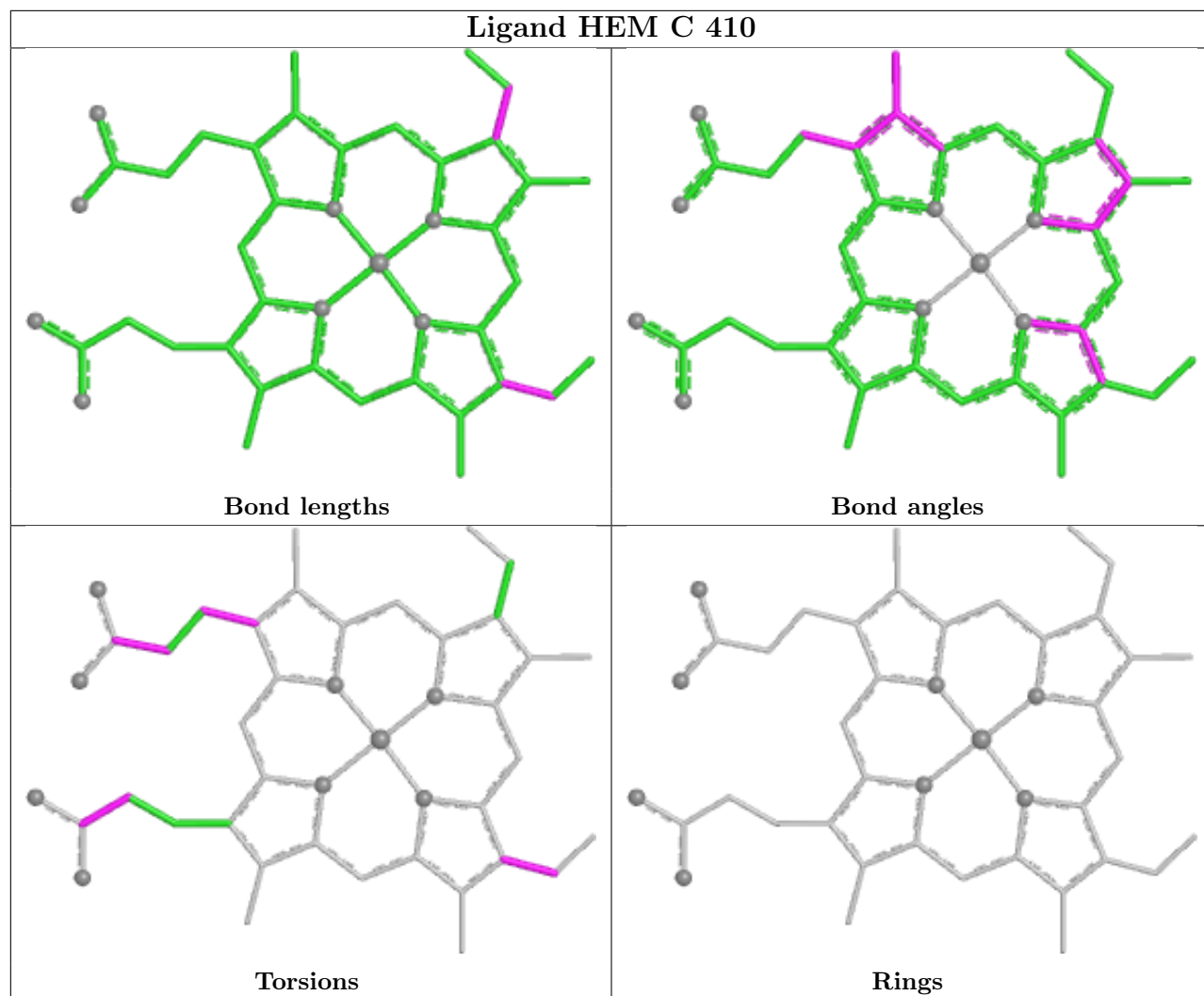
6 monomers are involved in 34 short contacts:

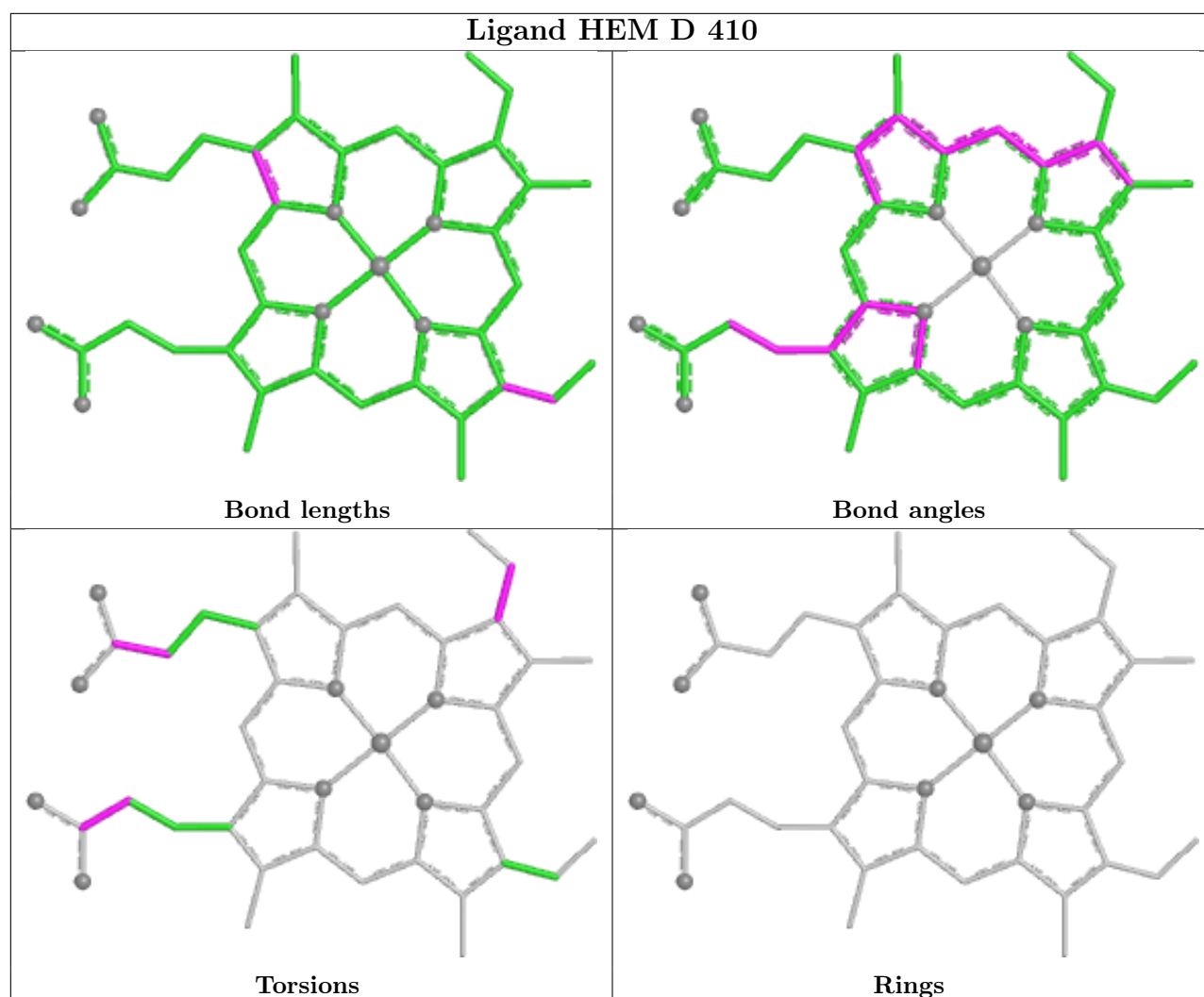
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	411	PIM	1	0
2	B	410	HEM	6	0
2	A	410	HEM	6	0
3	D	411	PIM	1	0
2	C	410	HEM	10	0
2	D	410	HEM	11	0

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









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	338/343 (98%)	-0.17	3 (0%) 81 63	16, 39, 65, 101	0
1	B	338/343 (98%)	-0.19	1 (0%) 90 80	14, 41, 61, 92	0
1	C	338/343 (98%)	-0.14	0 100 100	15, 41, 65, 89	0
1	D	338/343 (98%)	-0.11	1 (0%) 90 80	10, 41, 66, 103	0
All	All	1352/1372 (98%)	-0.15	5 (0%) 88 76	10, 40, 64, 103	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	53	GLY	3.7
1	D	14	ASP	3.1
1	A	35	MET	2.4
1	A	61	ASN	2.4
1	B	291	ARG	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

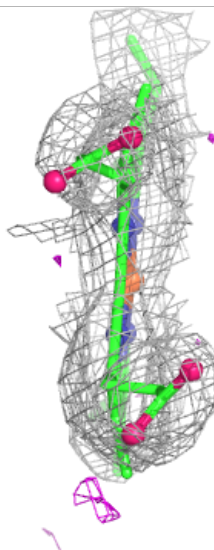
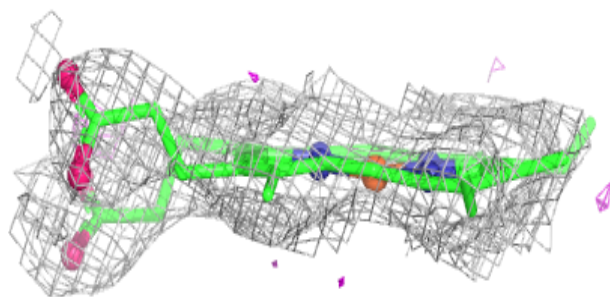
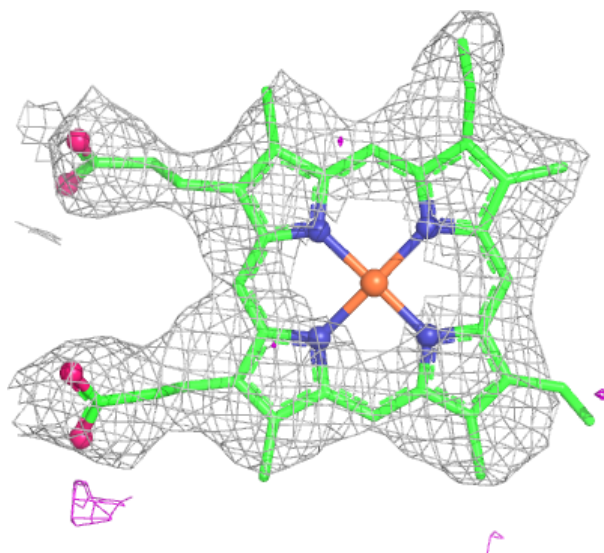
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	PIM	B	411	11/11	0.86	0.17	42,42,42,42	0
3	PIM	C	411	11/11	0.87	0.14	42,42,42,42	0
3	PIM	D	411	11/11	0.94	0.11	42,42,42,42	0
3	PIM	A	411	11/11	0.95	0.10	42,42,42,42	0
2	HEM	D	410	43/43	0.95	0.11	42,42,42,42	0
2	HEM	C	410	43/43	0.96	0.12	42,42,42,42	0
2	HEM	A	410	43/43	0.96	0.12	42,42,42,42	0
2	HEM	B	410	43/43	0.96	0.11	42,42,42,42	0

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

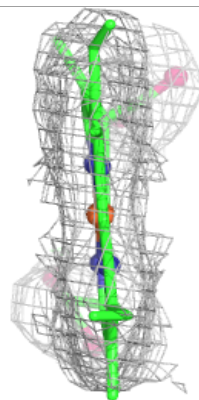
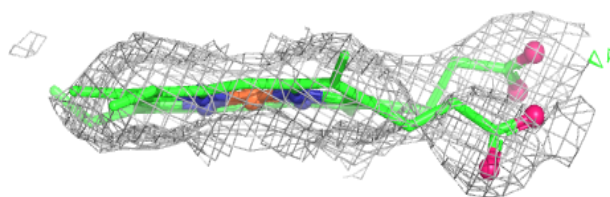
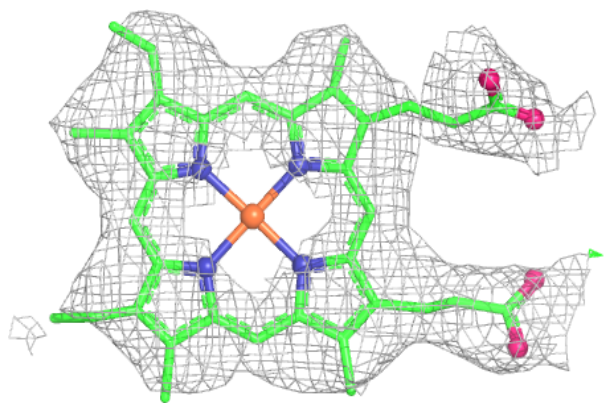
Electron density around HEM D 410:

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



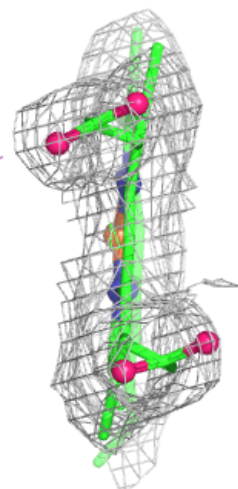
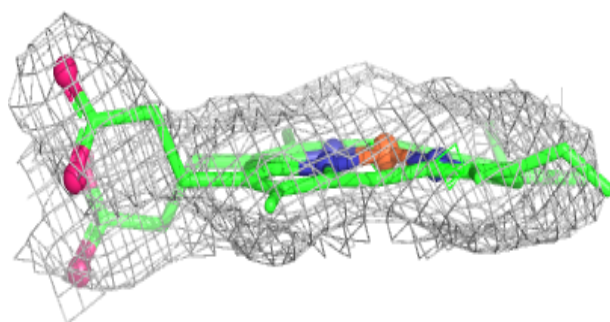
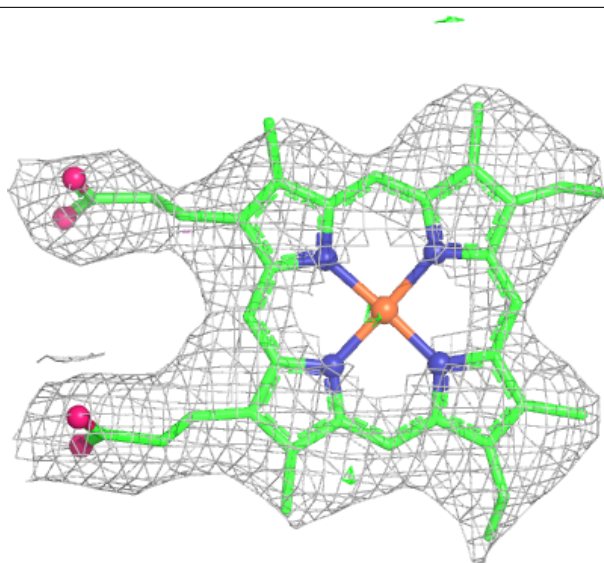
Electron density around HEM C 410:

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



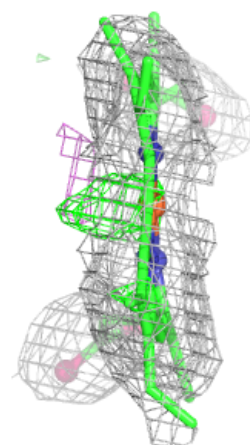
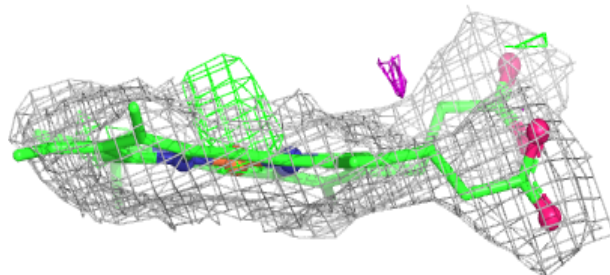
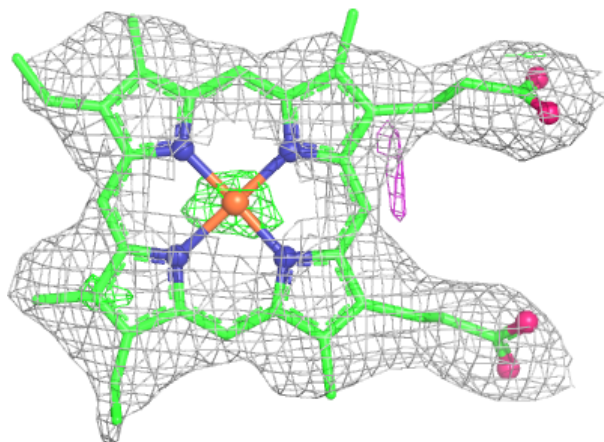
Electron density around HEM A 410:

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



Electron density around HEM B 410:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.