Full wwPDB X-ray Structure Validation Report (i)

Aug 16, 2023 – 09:00 PM EDT

PDB ID	:	2BCC
Title	:	STIGMATELLIN-BOUND CYTOCHROME BC1 COMPLEX FROM CHICKEN
Authors	:	Zhang, Z.; Huang, L.; Shulmeister, V.M.; Chi, Y.I.; Kim, K.K.; Hung, L.W.; Crofts, A.R.; Berry, E.A.; Kim, S.H.
Deposited on	:	1998-09-18
Resolution	:	3.50 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

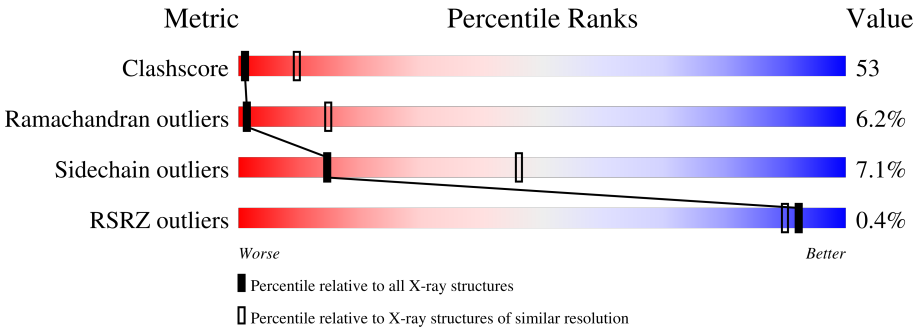
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

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 3.50 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)
RSRZ outliers	127900	1559 (3.60-3.40)

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 <=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	446	39% 53% 7%
2	B	422	35% 51% 10%
3	C	380	30% 57% 11%
4	D	241	42% 54%
5	E	196	2% 34% 56% 9%
6	F	109	50% 33% 8% 8%

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Mol	Chain	Length	Quality of chain
7	G	81	31% 54% 9%
8	H	78	46% 38% 15%
9	I	33	61% 39%
10	J	62	2% 42% 45% 5% 5%

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
12	U10	C	383	-	-	-	X
13	PEE	C	384	X	-	-	-
13	PEE	E	198	X	-	-	-

2 Entry composition (i)

There are 16 unique types of molecules in this entry. The entry contains 15754 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 UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	442	Total	C	N	O	S	0	0	0
			3423	2147	601	657	18			

- Molecule 2 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	406	Total	C	N	O	S	0	0	0
			2994	1878	518	591	7			

- Molecule 3 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	379	Total	C	N	O	S	0	0	0
			3002	2013	473	504	12			

- Molecule 4 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	241	Total	C	N	O	S	0	0	0
			1899	1214	326	345	14			

- Molecule 5 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	196	Total	C	N	O	S	0	0	0
			1512	953	266	285	8			

- Molecule 6 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	100	Total	C	N	O	S	0	0	0
			875	557	153	162	3			

- Molecule 7 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
7	G	78	Total	C	N	O	S	0	0	0
			626	411	114	100	1			

- Molecule 8 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	66	Total	C	N	O	S	0	0	0
			490	301	88	96	5			

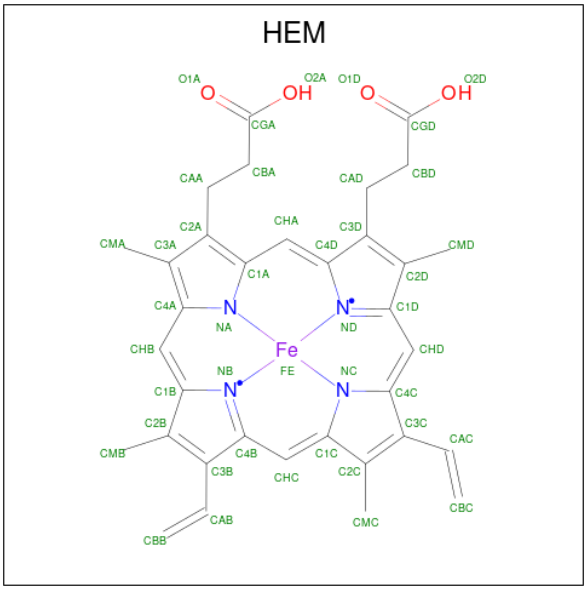
- Molecule 9 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
9	I	33	Total	C	N	O	0	0	0
			159	92	33	34			

- Molecule 10 is a protein called UBIQUINOL CYTOCHROME C OXIDOREDUCTASE.

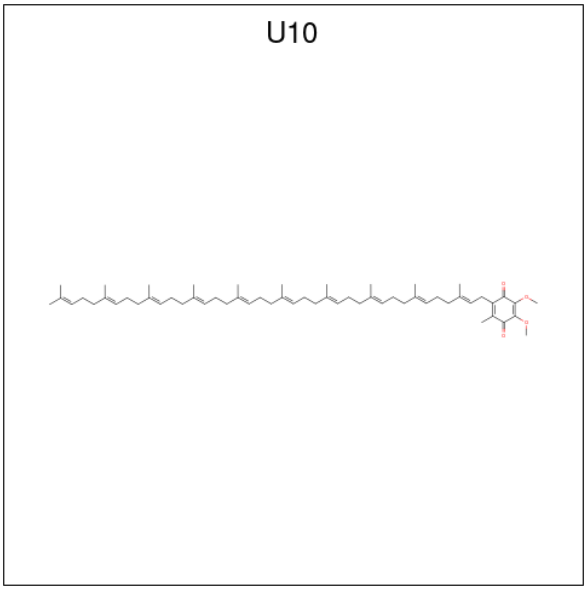
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
10	J	59	Total	C	N	O	0	0	0
			459	299	78	82			

- Molecule 11 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



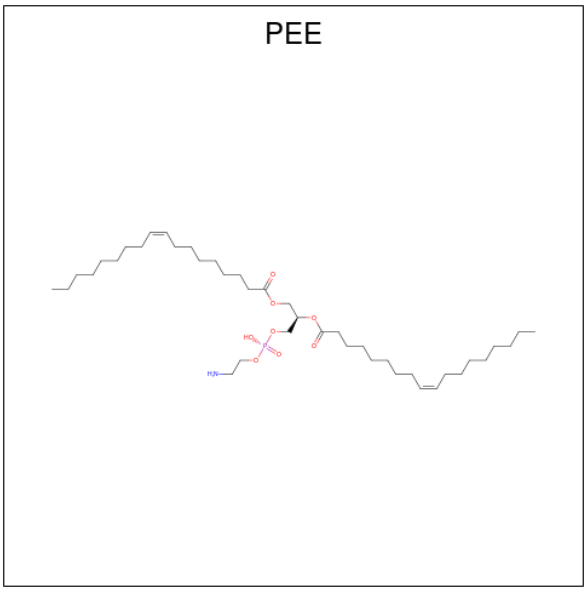
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
11	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
11	D	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 12 is UBIQUINONE-10 (three-letter code: U10) (formula: $C_{59}H_{90}O_4$).



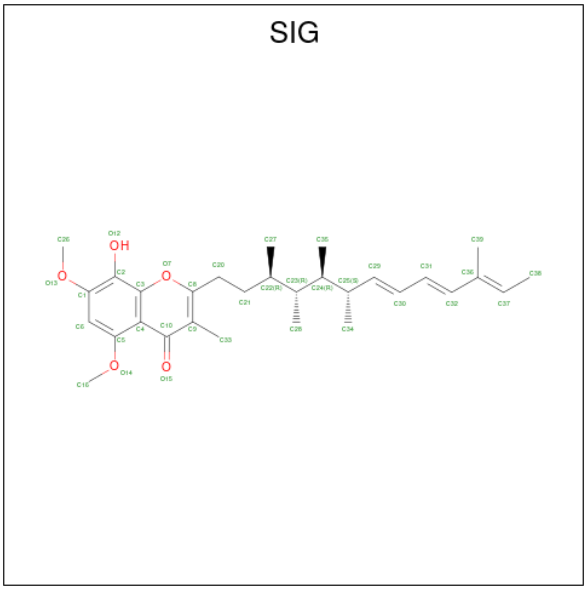
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
12	C	1	Total	C	O	0	0
			29	25	4		

- Molecule 13 is 1,2-dioleoyl-sn-glycero-3-phosphoethanolamine (three-letter code: PEE) (formula: $C_{41}H_{78}NO_8P$).



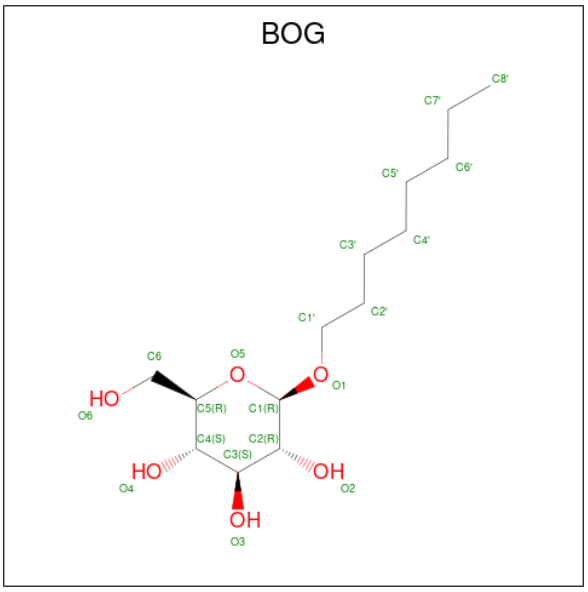
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	C	1	Total	C	N	O	P	0	0
			49	39	1	8	1		
13	E	1	Total	C	N	O	P	0	0
			49	39	1	8	1		

- Molecule 14 is STIGMATELLIN (three-letter code: SIG) (formula: $C_{30}H_{42}O_5$).



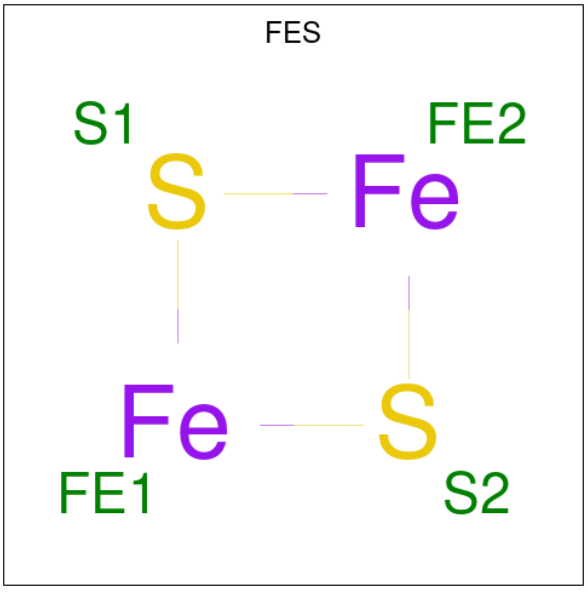
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
14	C	1	Total	C	O	0	0
			35	30	5		

- Molecule 15 is octyl beta-D-glucopyranoside (three-letter code: BOG) (formula: $C_{14}H_{28}O_6$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	D	1	Total C O 20 14 6	0	0

- Molecule 16 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



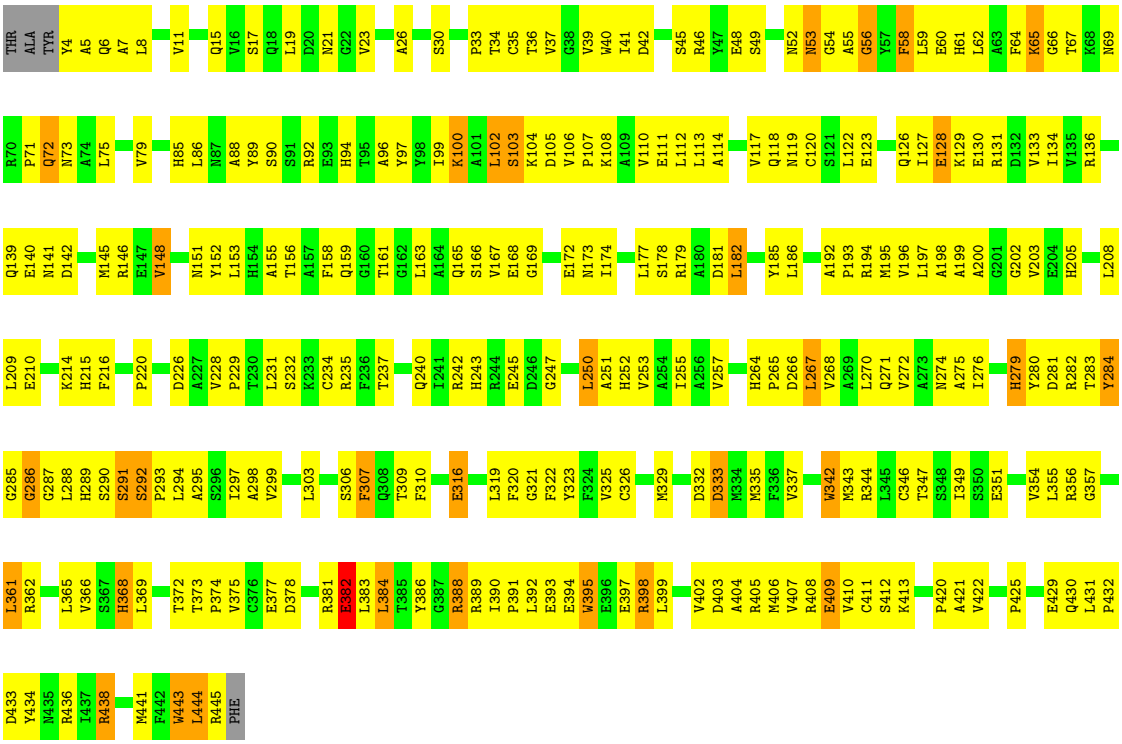
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	E	1	Total Fe S 4 2 2	0	0

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 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.

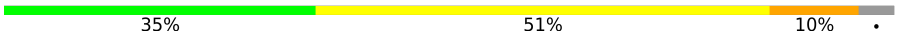
• Molecule 1: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

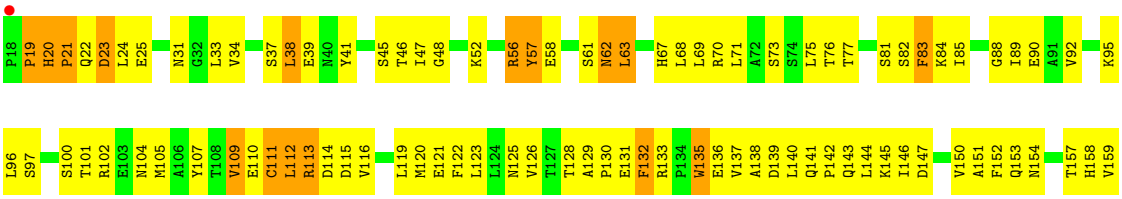
Chain A:

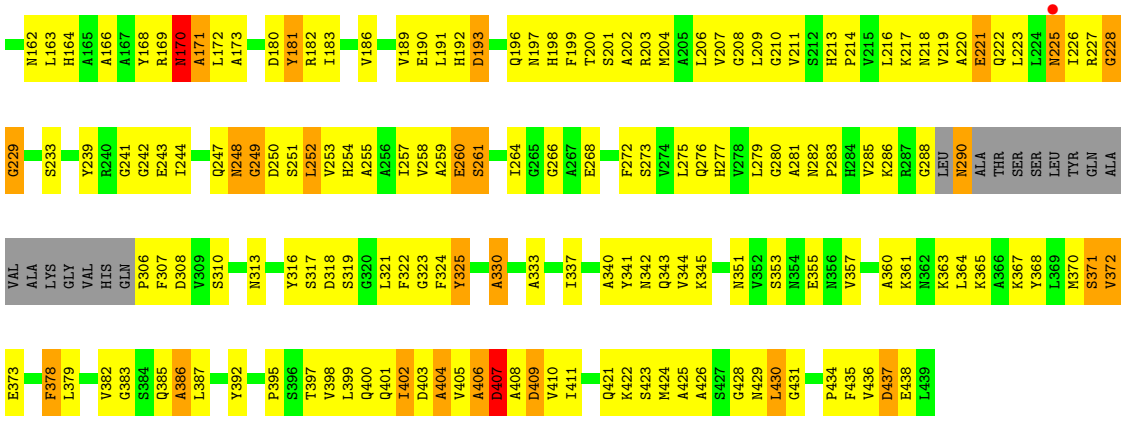


• Molecule 2: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain B:

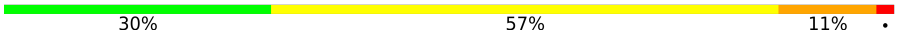


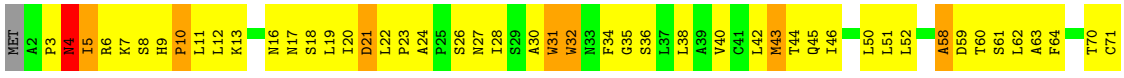


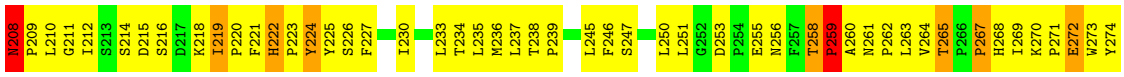


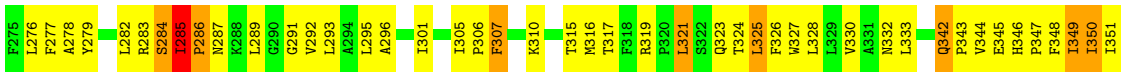
• Molecule 3: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

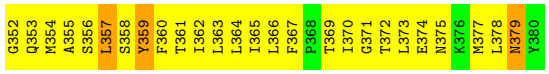
Chain C:





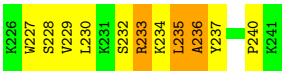






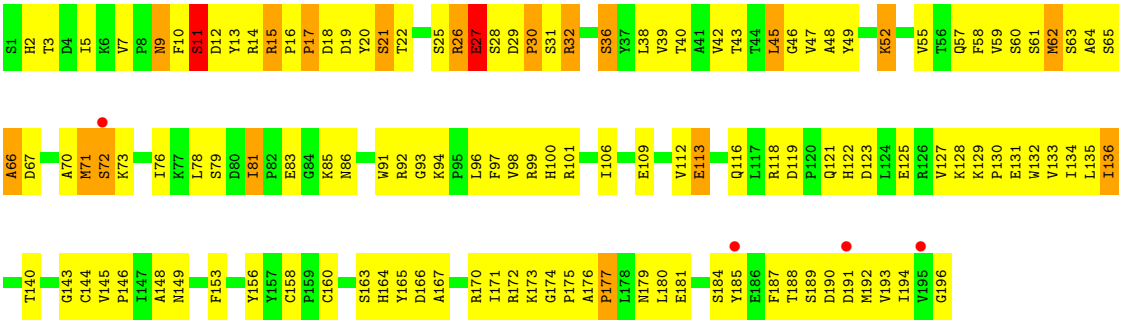
• Molecule 4: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain D:



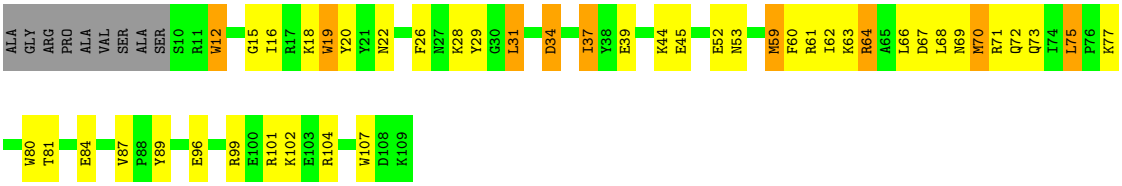
• Molecule 5: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain E:



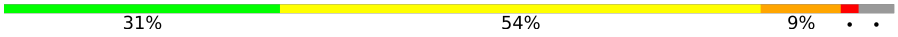
• Molecule 6: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

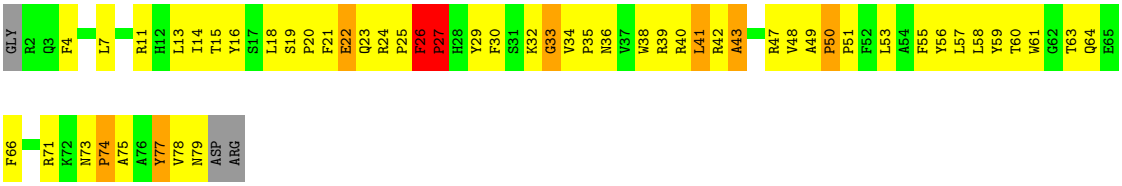
Chain F:



• Molecule 7: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain G:



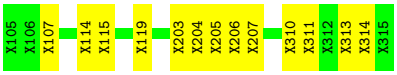


• Molecule 8: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

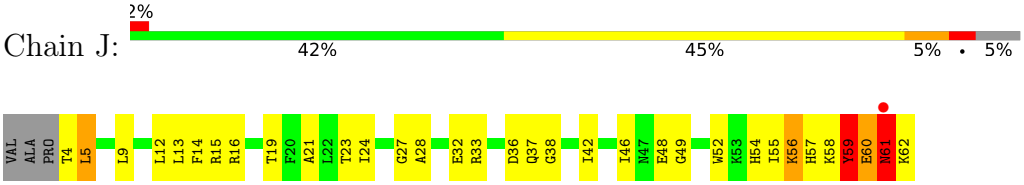
Chain H:

• Molecule 9: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE

Chain I:



• Molecule 10: UBIQUINOL CYTOCHROME C OXIDOREDUCTASE



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	173.46Å 182.45Å 241.33Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	12.00 – 3.50 87.05 – 3.02	Depositor EDS
% Data completeness (in resolution range)	85.6 (12.00-3.50) 62.8 (87.05-3.02)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	0.13	Depositor
$< I/\sigma(I) >$ [1]	1.61 (at 3.01Å)	Xtriage
Refinement program	CNS 0.1	Depositor
R, R_{free}	0.284 , 0.317 0.277 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	54.7	Xtriage
Anisotropy	0.276	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 21.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.29$, $< L^2 > = 0.12$	Xtriage
Estimated twinning fraction	0.229 for k,h,-l	Xtriage
F_o,F_c correlation	0.82	EDS
Total number of atoms	15754	wwPDB-VP
Average B, all atoms (Å^2)	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.65% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: BOG, PEE, HEM, SIG, FES, U10

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	0.45	0/3495	0.78	1/4742 (0.0%)
2	B	0.43	0/3046	0.73	0/4132
3	C	0.52	0/3104	0.85	5/4252 (0.1%)
4	D	0.50	0/1960	0.81	1/2665 (0.0%)
5	E	0.46	0/1548	0.78	1/2095 (0.0%)
6	F	0.49	0/896	0.76	0/1206
7	G	0.53	0/648	1.17	3/882 (0.3%)
8	H	0.44	0/495	0.69	0/669
10	J	0.52	0/470	0.80	1/635 (0.2%)
All	All	0.48	0/15662	0.81	12/21278 (0.1%)

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
3	C	0	1
10	J	0	1
All	All	0	2

There are no bond length outliers.

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	26	PHE	C-N-CD	-18.95	78.91	120.60
7	G	26	PHE	C-N-CA	13.72	179.63	122.00
7	G	27	PRO	CA-N-CD	-7.67	100.76	111.50
10	J	61	ASN	N-CA-C	6.56	128.72	111.00
3	C	267	PRO	N-CA-C	-6.18	96.03	112.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	235	LEU	CA-CB-CG	5.65	128.29	115.30
3	C	265	THR	N-CA-C	-5.50	96.16	111.00
3	C	104	TYR	CA-CB-CG	-5.33	103.28	113.40
3	C	35	GLY	N-CA-C	-5.32	99.79	113.10
5	E	143	GLY	N-CA-C	5.32	126.39	113.10
3	C	285	ILE	N-CA-C	-5.21	96.94	111.00
1	A	329	MET	N-CA-C	5.13	124.86	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	C	76	TYR	Sidechain
10	J	59	TYR	Sidechain

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	3423	0	3286	359	0
2	B	2994	0	2906	345	0
3	C	3002	0	3036	423	0
4	D	1899	0	1822	216	0
5	E	1512	0	1483	177	0
6	F	875	0	839	70	0
7	G	626	0	591	83	0
8	H	490	0	445	57	0
9	I	159	0	46	20	0
10	J	459	0	424	53	0
11	C	86	0	60	19	0
11	D	43	0	30	2	0
12	C	29	0	33	9	0
13	C	49	0	70	7	0
13	E	49	0	70	4	0
14	C	35	0	42	12	0
15	D	20	0	28	1	0
16	E	4	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	15754	0	15211	1654	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 53.

All (1654) 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)
3:C:166:TRP:HB2	3:C:175:THR:HB	1.22	1.17
1:A:36:THR:HG22	1:A:100:LYS:HB3	1.22	1.17
2:B:280:GLY:H	2:B:283:PRO:HD2	1.06	1.16
2:B:168:TYR:HB2	2:B:173:ALA:HB2	1.36	1.05
7:G:60:THR:HG22	7:G:64:GLN:HE21	1.19	1.01
3:C:52:LEU:HD13	3:C:80:ILE:HG22	1.43	0.99
2:B:337:ILE:HD11	2:B:434:PRO:HD2	1.41	0.99
3:C:342:GLN:HE21	3:C:343:PRO:HD2	1.27	0.98
10:J:57:HIS:HB2	10:J:61:ASN:C	1.84	0.98
1:A:349:ILE:HG22	1:A:408:ARG:HG3	1.45	0.97
3:C:138:GLN:NE2	3:C:261:ASN:H	1.62	0.97
4:D:158:ILE:HG22	4:D:160:MET:H	1.30	0.96
5:E:16:PRO:HG2	5:E:32:ARG:HH12	1.30	0.96
3:C:166:TRP:HB2	3:C:175:THR:CB	1.95	0.95
3:C:138:GLN:HE21	3:C:260:ALA:HA	1.32	0.95
3:C:207:ASN:O	3:C:208:ASN:HB3	1.66	0.93
3:C:327:TRP:HA	3:C:330:VAL:HG12	1.48	0.93
2:B:209:LEU:HG	2:B:379:LEU:HD23	1.51	0.93
3:C:138:GLN:HE22	3:C:261:ASN:H	1.03	0.93
7:G:26:PHE:H	7:G:26:PHE:HD1	1.17	0.92
5:E:13:TYR:O	5:E:14:ARG:HD3	1.69	0.92
2:B:258:VAL:HG11	2:B:321:LEU:HB3	1.49	0.92
1:A:297:ILE:HG21	1:A:337:VAL:HG11	1.52	0.91
3:C:107:SER:HB3	11:C:382:HEM:HBD1	1.52	0.91
5:E:101:ARG:HH22	5:E:127:VAL:HG21	1.36	0.91
1:A:245:GLU:HG3	7:G:11:ARG:HG2	1.50	0.91
3:C:202:HIS:CE1	12:C:383:U10:O2	2.24	0.91
3:C:166:TRP:CB	3:C:175:THR:HB	2.02	0.91
3:C:238:THR:OG1	4:D:212:MET:HG3	1.70	0.90
2:B:280:GLY:N	2:B:283:PRO:HD2	1.85	0.90
4:D:130:LEU:HD11	4:D:158:ILE:HD11	1.52	0.90
2:B:69:LEU:HD12	2:B:105:MET:HE1	1.54	0.90
3:C:120:LEU:HB3	11:C:382:HEM:HBB2	1.51	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:172:ASP:H	3:C:175:THR:HG23	1.37	0.90
2:B:76:THR:HG22	2:B:82:SER:H	1.37	0.90
5:E:16:PRO:HG2	5:E:32:ARG:NH1	1.87	0.90
1:A:391:PRO:HG2	1:A:394:GLU:HB2	1.53	0.89
5:E:72:SER:O	5:E:196:GLY:HA3	1.69	0.89
1:A:152:TYR:OH	5:E:5:ILE:HD12	1.73	0.88
1:A:250:LEU:HD21	1:A:325:VAL:HG13	1.54	0.88
3:C:261:ASN:HD21	3:C:264:VAL:HG23	1.35	0.88
4:D:224:ARG:HH22	7:G:27:PRO:HG3	1.34	0.88
5:E:9:ASN:ND2	5:E:11:SER:HB3	1.89	0.88
1:A:166:SER:OG	5:E:3:THR:HG23	1.73	0.87
4:D:75:ASN:HB2	4:D:77:ASP:H	1.39	0.87
4:D:83:ARG:NH1	4:D:86:LYS:HG3	1.89	0.86
1:A:333:ASP:O	1:A:337:VAL:HG23	1.73	0.86
2:B:25:GLU:HB2	2:B:213:HIS:ND1	1.90	0.86
4:D:165:TYR:O	4:D:168:VAL:HG23	1.76	0.85
2:B:122:PHE:O	2:B:126:VAL:HG23	1.77	0.85
3:C:283:ARG:O	3:C:283:ARG:HG3	1.77	0.85
3:C:342:GLN:NE2	3:C:343:PRO:HD2	1.90	0.85
4:D:132:THR:HA	4:D:179:MET:CE	2.07	0.84
2:B:92:VAL:HG11	2:B:115:ASP:HB3	1.57	0.84
2:B:399:LEU:HA	2:B:402:ILE:HG22	1.59	0.84
1:A:281:ASP:HB3	1:A:284:TYR:HE1	1.41	0.84
2:B:280:GLY:H	2:B:283:PRO:CD	1.87	0.83
3:C:272:GLU:N	3:C:272:GLU:OE1	2.10	0.83
5:E:122:HIS:O	5:E:125:GLU:HG2	1.76	0.83
10:J:56:LYS:O	10:J:60:GLU:HB2	1.78	0.83
3:C:142:TRP:CE3	3:C:265:THR:HG22	2.13	0.83
4:D:54:VAL:HG21	4:D:192:TRP:CZ3	2.14	0.83
2:B:154:ASN:O	2:B:157:THR:HG22	1.79	0.82
2:B:258:VAL:HG13	2:B:322:PHE:H	1.44	0.82
5:E:47:VAL:HG21	13:E:198:PEE:H24	1.60	0.82
10:J:57:HIS:O	10:J:61:ASN:N	2.13	0.82
3:C:31:TRP:CZ3	13:C:384:PEE:H17	2.15	0.82
1:A:250:LEU:C	1:A:250:LEU:HD22	1.98	0.82
3:C:27:ASN:HB2	6:F:69:ASN:HD22	1.44	0.82
3:C:245:LEU:O	4:D:201:ARG:HD3	1.79	0.82
8:H:47:ARG:HD3	8:H:48:SER:H	1.41	0.82
3:C:317:THR:HG23	13:C:384:PEE:O2P	1.80	0.81
3:C:316:MET:SD	3:C:319:ARG:HG3	2.19	0.81
4:D:158:ILE:HG22	4:D:159:GLY:N	1.94	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:GLN:OE1	2:B:146:ILE:HD11	1.80	0.81
5:E:62:MET:HG3	5:E:63:SER:H	1.46	0.81
5:E:189:SER:OG	5:E:192:MET:HB2	1.81	0.80
1:A:33:PRO:HG2	1:A:34:THR:H	1.46	0.80
2:B:62:ASN:HD22	2:B:63:LEU:N	1.79	0.80
3:C:295:LEU:HD21	14:C:385:SIG:H273	1.63	0.80
4:D:95:TYR:CD2	4:D:101:ALA:HA	2.17	0.80
1:A:56:GLY:HA2	1:A:185:TYR:CE2	2.17	0.80
3:C:120:LEU:CB	11:C:382:HEM:HBB2	2.11	0.79
3:C:342:GLN:HE21	3:C:342:GLN:HA	1.46	0.79
5:E:9:ASN:HD21	5:E:11:SER:HB3	1.46	0.79
1:A:90:SER:O	1:A:167:VAL:HG11	1.83	0.79
1:A:382:GLU:HG2	1:A:389:ARG:HA	1.62	0.79
1:A:281:ASP:HB3	1:A:284:TYR:CE1	2.18	0.79
1:A:49:SER:H	1:A:52:ASN:HB3	1.47	0.79
2:B:248:ASN:HD22	2:B:249:GLY:N	1.81	0.79
3:C:325:LEU:CD2	3:C:362:ILE:HG23	2.11	0.79
2:B:357:VAL:HG12	2:B:361:LYS:HD2	1.65	0.78
3:C:325:LEU:HD13	3:C:367:PHE:CD1	2.18	0.78
4:D:75:ASN:N	4:D:75:ASN:HD22	1.82	0.78
1:A:444:LEU:HD12	1:A:444:LEU:H	1.48	0.78
3:C:172:ASP:H	3:C:175:THR:CG2	1.95	0.78
1:A:361:LEU:HD13	1:A:399:LEU:HD22	1.66	0.78
1:A:65:LYS:NZ	9:I:311:UNK:HA	1.99	0.77
6:F:60:PHE:HD1	7:G:13:LEU:HD22	1.48	0.77
1:A:240:GLN:HB3	1:A:422:VAL:HG12	1.67	0.77
2:B:168:TYR:CB	2:B:173:ALA:HB2	2.14	0.77
4:D:132:THR:HA	4:D:179:MET:HE1	1.65	0.77
3:C:319:ARG:NH2	3:C:371:GLY:HA2	2.00	0.77
3:C:327:TRP:HA	3:C:330:VAL:CG1	2.14	0.77
1:A:142:ASP:OD1	5:E:2:HIS:HB3	1.85	0.76
4:D:57:THR:HB	4:D:60:GLU:HB2	1.66	0.76
1:A:37:VAL:HG12	1:A:199:ALA:HB1	1.67	0.76
5:E:29:ASP:C	5:E:31:SER:H	1.88	0.76
2:B:62:ASN:HD22	2:B:62:ASN:C	1.89	0.76
3:C:138:GLN:NE2	3:C:261:ASN:N	2.33	0.76
4:D:55:CYS:HG	4:D:56:TYR:HD1	1.33	0.76
1:A:42:ASP:HB2	1:A:384:LEU:HD21	1.66	0.76
2:B:24:LEU:H	2:B:24:LEU:HD23	1.50	0.76
4:D:30:PHE:CE2	4:D:64:LEU:HD21	2.20	0.76
4:D:164:ILE:HD11	4:D:182:VAL:HG22	1.66	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:68:LEU:HD21	6:F:75:LEU:HD13	1.68	0.76
2:B:146:ILE:HG13	2:B:147:ASP:N	2.01	0.75
3:C:212:ILE:HD12	6:F:62:ILE:HG23	1.67	0.75
2:B:258:VAL:HG12	2:B:259:ALA:N	2.01	0.75
1:A:237:THR:HG23	7:G:22:GLU:HG2	1.69	0.75
2:B:159:VAL:HG21	2:B:254:HIS:HB3	1.66	0.75
4:D:224:ARG:NH2	7:G:27:PRO:HG3	2.00	0.75
1:A:85:HIS:HA	9:I:314:UNK:HG1	1.67	0.75
2:B:260:GLU:O	2:B:261:SER:HB3	1.86	0.75
4:D:165:TYR:CE1	4:D:168:VAL:HG22	2.22	0.75
2:B:258:VAL:HG13	2:B:322:PHE:N	2.01	0.75
4:D:164:ILE:HD11	4:D:182:VAL:HG13	1.68	0.75
1:A:240:GLN:CB	1:A:422:VAL:HG12	2.17	0.74
2:B:341:TYR:OH	2:B:422:LYS:HE3	1.87	0.74
2:B:257:ILE:O	2:B:323:GLY:HA3	1.87	0.74
3:C:350:ILE:HD13	3:C:350:ILE:N	2.02	0.74
1:A:106:VAL:HG21	1:A:203:VAL:HG13	1.69	0.74
1:A:288:LEU:HD13	2:B:83:PHE:HA	1.70	0.74
3:C:73:ASN:O	5:E:66:ALA:HB3	1.88	0.74
7:G:29:TYR:O	7:G:30:PHE:HB2	1.88	0.74
1:A:67:THR:HB	1:A:119:ASN:O	1.86	0.74
2:B:181:TYR:CE1	2:B:182:ARG:HG3	2.23	0.73
3:C:131:GLY:HA2	3:C:134:LEU:HD13	1.69	0.73
4:D:225:HIS:HA	7:G:25:PRO:HB3	1.69	0.73
3:C:206:SER:OG	12:C:383:U10:H3M1	1.87	0.73
5:E:10:PHE:O	5:E:11:SER:O	2.05	0.73
1:A:250:LEU:HD21	1:A:325:VAL:CG1	2.18	0.73
2:B:109:VAL:HG22	2:B:119:LEU:HD11	1.68	0.73
3:C:31:TRP:O	3:C:101:ARG:HG3	1.87	0.73
3:C:172:ASP:O	3:C:175:THR:HG23	1.89	0.73
1:A:349:ILE:CG2	1:A:408:ARG:HG3	2.19	0.73
1:A:145:MET:HB2	1:A:252:HIS:NE2	2.03	0.73
2:B:264:ILE:HG12	2:B:316:TYR:O	1.89	0.73
2:B:337:ILE:HD11	2:B:434:PRO:CD	2.19	0.73
1:A:240:GLN:NE2	1:A:242:ARG:HE	1.87	0.72
3:C:90:PHE:HE1	3:C:236:MET:HB3	1.54	0.72
7:G:29:TYR:HD1	7:G:30:PHE:CD1	2.07	0.72
1:A:252:HIS:HB3	1:A:323:TYR:HE1	1.55	0.72
2:B:243:GLU:OE2	2:B:436:VAL:HG22	1.89	0.72
3:C:350:ILE:HD13	3:C:350:ILE:H	1.53	0.72
5:E:45:LEU:HD11	10:J:28:ALA:HA	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:88:ALA:HB1	1:A:96:ALA:O	1.89	0.72
4:D:21:LEU:HD13	4:D:26:ILE:HD11	1.72	0.72
3:C:104:TYR:CZ	3:C:316:MET:HB2	2.24	0.72
3:C:145:THR:O	3:C:149:ASN:HB2	1.90	0.72
2:B:89:ILE:HD13	2:B:96:LEU:HB2	1.72	0.72
3:C:138:GLN:NE2	3:C:260:ALA:HA	2.05	0.72
3:C:316:MET:HE3	3:C:319:ARG:HE	1.55	0.72
3:C:7:LYS:O	3:C:13:LYS:HD2	1.90	0.71
3:C:120:LEU:CG	11:C:382:HEM:HBB2	2.20	0.71
5:E:99:ARG:HB3	5:E:133:VAL:CG1	2.19	0.71
10:J:57:HIS:HA	10:J:60:GLU:C	2.09	0.71
1:A:35:CYS:HA	1:A:372:THR:HG21	1.72	0.71
1:A:250:LEU:HD13	1:A:250:LEU:N	2.05	0.71
3:C:142:TRP:CD2	3:C:265:THR:HG22	2.26	0.71
5:E:16:PRO:CG	5:E:32:ARG:HH12	2.02	0.71
7:G:78:VAL:C	7:G:79:ASN:HD22	1.93	0.71
1:A:62:LEU:HD11	1:A:127:ILE:HG12	1.72	0.71
2:B:273:SER:O	2:B:276:GLN:HB3	1.90	0.71
1:A:178:SER:HB2	1:A:181:ASP:OD1	1.91	0.71
1:A:291:SER:HB2	1:A:356:ARG:NH2	2.05	0.71
2:B:46:THR:HG22	2:B:110:GLU:HB2	1.72	0.71
2:B:250:ASP:O	2:B:252:LEU:HD23	1.89	0.71
1:A:39:VAL:HG11	1:A:117:VAL:HG11	1.73	0.71
3:C:226:SER:O	3:C:230:ILE:HG13	1.90	0.71
1:A:39:VAL:HG11	1:A:117:VAL:CG1	2.21	0.71
5:E:71:MET:O	5:E:73:LYS:N	2.23	0.71
1:A:349:ILE:HG22	1:A:408:ARG:CG	2.21	0.70
1:A:286:GLY:C	1:A:288:LEU:H	1.93	0.70
2:B:169:ARG:O	2:B:170:ASN:HB3	1.90	0.70
2:B:109:VAL:HG13	2:B:119:LEU:HD21	1.72	0.70
3:C:378:LEU:O	3:C:379:ASN:HB2	1.91	0.70
4:D:32:VAL:HG11	4:D:186:VAL:HG22	1.73	0.70
3:C:354:MET:HA	3:C:354:MET:CE	2.22	0.70
6:F:31:LEU:HD23	6:F:31:LEU:H	1.57	0.70
3:C:127:THR:HG22	3:C:186:LEU:HB3	1.72	0.70
3:C:327:TRP:CE3	3:C:330:VAL:HG11	2.26	0.70
1:A:102:LEU:C	1:A:104:LYS:H	1.94	0.70
3:C:101:ARG:HD2	3:C:101:ARG:C	2.12	0.70
3:C:12:LEU:O	3:C:12:LEU:HD23	1.91	0.70
1:A:45:SER:HA	1:A:48:GLU:HG3	1.72	0.69
1:A:276:ILE:CD1	1:A:349:ILE:HD11	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:261:ASN:HD21	3:C:264:VAL:CG2	2.02	0.69
5:E:140:THR:OG1	5:E:177:PRO:HD2	1.90	0.69
1:A:37:VAL:HG12	1:A:199:ALA:CB	2.22	0.69
5:E:62:MET:HG3	5:E:63:SER:N	2.06	0.69
2:B:286:LYS:CB	2:B:343:GLN:HG3	2.23	0.69
3:C:319:ARG:CZ	3:C:374:GLU:HB2	2.22	0.69
3:C:70:THR:HA	3:C:74:VAL:HG23	1.74	0.69
1:A:37:VAL:HG23	1:A:113:LEU:HD11	1.75	0.69
1:A:145:MET:HB3	1:A:252:HIS:CD2	2.27	0.69
3:C:325:LEU:HD11	3:C:366:LEU:HB3	1.74	0.69
2:B:144:LEU:HB2	2:B:183:ILE:HD12	1.75	0.69
3:C:13:LYS:O	3:C:17:ASN:HB2	1.93	0.69
3:C:120:LEU:HG	11:C:382:HEM:HBB2	1.75	0.68
8:H:17:LEU:HD11	8:H:21:ARG:NE	2.07	0.68
3:C:27:ASN:HB2	6:F:69:ASN:ND2	2.07	0.68
4:D:43:MET:HE2	4:D:46:VAL:HG21	1.73	0.68
8:H:17:LEU:HD11	8:H:21:ARG:HE	1.57	0.68
1:A:102:LEU:HD12	1:A:102:LEU:H	1.58	0.68
4:D:28:ARG:HD2	4:D:171:PHE:CE2	2.28	0.68
1:A:102:LEU:HD12	1:A:102:LEU:N	2.08	0.68
10:J:54:HIS:O	10:J:57:HIS:CD2	2.47	0.68
1:A:4:TYR:O	1:A:7:ALA:N	2.26	0.68
1:A:388:ARG:HD3	1:A:388:ARG:H	1.58	0.68
3:C:377:MET:HE1	6:F:20:TYR:HB2	1.75	0.68
5:E:29:ASP:O	5:E:32:ARG:N	2.26	0.68
1:A:65:LYS:HZ2	9:I:311:UNK:HA	1.59	0.68
2:B:81:SER:O	2:B:85:ILE:HG22	1.94	0.68
3:C:27:ASN:ND2	3:C:208:ASN:OD1	2.23	0.68
4:D:102:ARG:NH1	4:D:109:LEU:HB2	2.08	0.68
1:A:153:LEU:HD23	1:A:153:LEU:C	2.13	0.68
3:C:104:TYR:CE2	3:C:316:MET:HB2	2.29	0.68
3:C:120:LEU:HB3	11:C:382:HEM:CBB	2.22	0.68
8:H:73:LEU:O	8:H:73:LEU:HD23	1.94	0.68
2:B:162:ASN:HB3	2:B:244:ILE:HD11	1.75	0.67
5:E:52:LYS:C	5:E:52:LYS:HD3	2.14	0.67
2:B:19:PRO:C	2:B:21:PRO:HD3	2.14	0.67
3:C:142:TRP:CZ3	3:C:265:THR:HG22	2.29	0.67
1:A:19:LEU:C	1:A:21:ASN:H	1.97	0.67
1:A:156:THR:HA	5:E:7:VAL:HG21	1.75	0.67
4:D:83:ARG:HH12	4:D:86:LYS:HG3	1.59	0.67
3:C:348:PHE:O	3:C:350:ILE:N	2.28	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:16:ILE:O	6:F:19:TRP:HB3	1.94	0.67
1:A:36:THR:HG22	1:A:100:LYS:CB	2.14	0.67
1:A:321:GLY:HA2	1:A:342:TRP:CZ2	2.29	0.67
1:A:382:GLU:HG2	1:A:389:ARG:HD2	1.75	0.67
1:A:354:VAL:HG11	1:A:404:ALA:HA	1.76	0.67
3:C:90:PHE:CE1	3:C:236:MET:HB3	2.30	0.67
5:E:160:CYS:HB2	16:E:197:FES:S2	2.35	0.67
1:A:438:ARG:O	1:A:438:ARG:HD3	1.96	0.66
2:B:168:TYR:CE2	2:B:172:LEU:HD23	2.30	0.66
6:F:59:MET:HA	6:F:59:MET:CE	2.25	0.66
8:H:35:GLU:O	8:H:39:LEU:HD13	1.95	0.66
2:B:56:ARG:HH11	2:B:56:ARG:HG3	1.59	0.66
3:C:245:LEU:O	4:D:201:ARG:CD	2.44	0.66
3:C:350:ILE:H	3:C:350:ILE:CD1	2.08	0.66
2:B:56:ARG:NH2	2:B:318:ASP:OD2	2.29	0.66
2:B:370:MET:O	2:B:373:GLU:HG3	1.96	0.66
4:D:132:THR:HA	4:D:179:MET:HE2	1.78	0.66
5:E:99:ARG:HB3	5:E:133:VAL:HG12	1.78	0.66
5:E:43:THR:O	5:E:47:VAL:HG23	1.94	0.66
8:H:69:VAL:O	8:H:73:LEU:HB2	1.95	0.66
2:B:96:LEU:HD23	2:B:97:SER:N	2.10	0.66
3:C:123:THR:O	3:C:127:THR:HG23	1.96	0.66
3:C:131:GLY:CA	3:C:134:LEU:HD13	2.25	0.66
1:A:243:HIS:O	1:A:425:PRO:HA	1.96	0.66
1:A:433:ASP:OD1	1:A:436:ARG:HG2	1.96	0.66
3:C:133:VAL:CG1	3:C:144:ALA:HB2	2.24	0.66
12:C:383:U10:C8	12:C:383:U10:H1M1	2.26	0.66
2:B:207:VAL:HG21	2:B:383:GLY:HA2	1.77	0.66
3:C:146:VAL:HG23	3:C:147:ILE:N	2.10	0.66
5:E:93:GLY:O	5:E:94:LYS:HE3	1.96	0.66
10:J:13:LEU:HD12	10:J:13:LEU:N	2.11	0.66
3:C:222:HIS:HB3	3:C:223:PRO:HD2	1.78	0.65
4:D:180:SER:HB3	8:H:15:ASP:OD1	1.96	0.65
1:A:291:SER:O	1:A:292:SER:C	2.34	0.65
1:A:297:ILE:CG2	1:A:337:VAL:HG11	2.25	0.65
4:D:75:ASN:ND2	4:D:79:GLU:O	2.27	0.65
10:J:59:TYR:O	10:J:60:GLU:HG3	1.96	0.65
1:A:94:HIS:NE2	1:A:381:ARG:HG2	2.11	0.65
2:B:56:ARG:HG3	2:B:56:ARG:NH1	2.09	0.65
2:B:181:TYR:CZ	2:B:182:ARG:HG3	2.31	0.65
1:A:252:HIS:HD1	1:A:325:VAL:HG22	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:379:LEU:HD13	2:B:379:LEU:O	1.96	0.65
3:C:131:GLY:O	3:C:134:LEU:HB2	1.96	0.65
4:D:153:PHE:CG	4:D:158:ILE:HG12	2.31	0.65
10:J:55:ILE:O	10:J:57:HIS:N	2.29	0.65
2:B:61:SER:O	2:B:62:ASN:ND2	2.29	0.65
3:C:9:HIS:HB3	3:C:12:LEU:HB3	1.77	0.65
1:A:106:VAL:O	1:A:110:VAL:HG23	1.97	0.65
3:C:43:MET:CE	3:C:43:MET:HA	2.27	0.65
3:C:282:LEU:HD13	3:C:282:LEU:O	1.95	0.65
5:E:16:PRO:O	5:E:18:ASP:N	2.25	0.65
5:E:26:ARG:O	5:E:27:GLU:HG3	1.96	0.65
1:A:159:GLN:HE21	5:E:7:VAL:HG11	1.62	0.65
2:B:137:VAL:HG23	2:B:138:ALA:N	2.11	0.65
3:C:43:MET:HA	3:C:43:MET:HE2	1.78	0.65
2:B:272:PHE:O	2:B:276:GLN:N	2.29	0.65
3:C:377:MET:CE	6:F:20:TYR:HB2	2.26	0.65
12:C:383:U10:H1M1	12:C:383:U10:H8	1.78	0.65
1:A:403:ASP:OD2	1:A:405:ARG:HB3	1.97	0.65
2:B:63:LEU:HB2	2:B:182:ARG:HD3	1.79	0.65
2:B:101:THR:HG22	2:B:102:ARG:N	2.12	0.65
4:D:186:VAL:O	4:D:189:PHE:HB3	1.96	0.65
10:J:42:ILE:O	10:J:46:ILE:HG13	1.97	0.65
1:A:103:SER:C	1:A:105:ASP:H	1.97	0.65
4:D:43:MET:CE	4:D:46:VAL:HG21	2.26	0.65
5:E:36:SER:HG	7:G:21:PHE:HE1	1.43	0.65
2:B:385:GLN:O	2:B:387:LEU:N	2.30	0.64
3:C:233:LEU:CD1	3:C:237:LEU:HD22	2.27	0.64
2:B:62:ASN:C	2:B:62:ASN:ND2	2.48	0.64
3:C:235:LEU:O	3:C:239:PRO:HD3	1.98	0.64
1:A:100:LYS:HE3	2:B:370:MET:CE	2.27	0.64
1:A:293:PRO:O	1:A:297:ILE:N	2.26	0.64
3:C:301:ILE:HD11	3:C:364:LEU:HD11	1.79	0.64
1:A:161:THR:HG21	1:A:235:ARG:H	1.61	0.64
2:B:128:THR:C	2:B:130:PRO:HD3	2.17	0.64
3:C:349:ILE:HG22	3:C:350:ILE:HD13	1.79	0.64
4:D:44:ASP:O	4:D:90:TYR:HD2	1.80	0.64
1:A:291:SER:O	1:A:293:PRO:N	2.31	0.64
4:D:75:ASN:N	4:D:75:ASN:ND2	2.42	0.64
4:D:182:VAL:O	4:D:186:VAL:HG23	1.96	0.64
1:A:389:ARG:HD2	1:A:390:ILE:H	1.63	0.64
2:B:76:THR:CG2	2:B:82:SER:H	2.11	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:36:SER:O	3:C:40:VAL:HG23	1.97	0.64
3:C:347:PRO:HG3	7:G:66:PHE:CD1	2.32	0.64
2:B:33:LEU:HD21	2:B:223:LEU:HD23	1.80	0.64
3:C:130:VAL:HG12	3:C:183:HIS:HB2	1.79	0.64
3:C:138:GLN:HG2	3:C:258:THR:HG22	1.79	0.64
6:F:12:TRP:HA	6:F:12:TRP:CE3	2.32	0.64
1:A:15:GLN:HB3	1:A:205:HIS:ND1	2.13	0.64
1:A:86:LEU:HD13	1:A:99:ILE:CG1	2.27	0.64
2:B:166:ALA:HB1	2:B:242:GLY:C	2.18	0.64
3:C:20:ILE:O	3:C:21:ASP:HB2	1.97	0.64
3:C:261:ASN:ND2	3:C:264:VAL:HG23	2.11	0.64
4:D:75:ASN:ND2	4:D:75:ASN:H	1.96	0.64
4:D:102:ARG:HH11	4:D:109:LEU:HB2	1.62	0.64
4:D:178:THR:O	4:D:182:VAL:HG12	1.98	0.64
2:B:206:LEU:HG	2:B:216:LEU:HD11	1.80	0.64
2:B:258:VAL:HG12	2:B:259:ALA:H	1.63	0.64
3:C:222:HIS:O	3:C:223:PRO:C	2.34	0.64
5:E:29:ASP:O	5:E:31:SER:N	2.30	0.64
2:B:361:LYS:O	2:B:365:LYS:HG3	1.98	0.64
3:C:282:LEU:HD23	3:C:295:LEU:HB2	1.80	0.64
5:E:16:PRO:HD3	7:G:22:GLU:O	1.98	0.64
4:D:218:LEU:O	4:D:222:MET:HG3	1.98	0.63
1:A:146:ARG:HH21	9:I:206:UNK:CB	2.12	0.63
3:C:148:THR:HG21	3:C:166:TRP:CE3	2.33	0.63
5:E:113:GLU:OE2	5:E:116:GLN:HG3	1.98	0.63
1:A:321:GLY:HA2	1:A:342:TRP:HZ2	1.62	0.63
3:C:238:THR:OG1	4:D:212:MET:CG	2.44	0.63
3:C:316:MET:HE3	3:C:319:ARG:NE	2.12	0.63
4:D:165:TYR:CD1	4:D:168:VAL:HG22	2.33	0.63
1:A:382:GLU:OE2	1:A:390:ILE:HB	1.98	0.63
1:A:436:ARG:HD3	3:C:223:PRO:HD3	1.80	0.63
2:B:395:PRO:HA	2:B:398:VAL:CG1	2.28	0.63
1:A:61:HIS:HD2	1:A:134:ILE:HG12	1.63	0.63
1:A:102:LEU:O	1:A:104:LYS:N	2.31	0.63
3:C:113:THR:HG21	3:C:201:LEU:HA	1.81	0.63
4:D:54:VAL:HG11	4:D:192:TRP:CH2	2.33	0.63
5:E:5:ILE:HD13	7:G:14:ILE:CD1	2.29	0.63
7:G:60:THR:HG22	7:G:64:GLN:NE2	2.03	0.63
1:A:395:TRP:HA	1:A:395:TRP:CE3	2.34	0.63
5:E:119:ASP:HB3	5:E:179:ASN:ND2	2.13	0.63
1:A:235:ARG:HD3	5:E:21:SER:H	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:GLU:HG2	1:A:247:GLY:H	1.64	0.63
2:B:258:VAL:CG1	2:B:322:PHE:H	2.10	0.63
5:E:101:ARG:NH2	5:E:127:VAL:HG21	2.13	0.63
4:D:218:LEU:HD11	5:E:42:VAL:HG12	1.80	0.62
3:C:253:ASP:OD1	3:C:255:GLU:N	2.31	0.62
5:E:91:TRP:CE3	5:E:96:LEU:HD22	2.34	0.62
10:J:59:TYR:CD1	10:J:59:TYR:N	2.67	0.62
4:D:237:TYR:HB2	6:F:60:PHE:CD1	2.35	0.62
5:E:5:ILE:HD13	7:G:14:ILE:HD13	1.82	0.62
5:E:62:MET:O	5:E:64:ALA:O	2.17	0.62
1:A:444:LEU:O	1:A:445:ARG:O	2.17	0.62
3:C:16:ASN:OD1	3:C:16:ASN:O	2.16	0.62
1:A:15:GLN:HB3	1:A:205:HIS:CE1	2.35	0.62
2:B:248:ASN:HD21	2:B:428:GLY:HA2	1.64	0.62
3:C:27:ASN:HD22	6:F:69:ASN:ND2	1.97	0.62
3:C:325:LEU:HD13	3:C:367:PHE:HD1	1.65	0.62
4:D:95:TYR:HE2	4:D:104:ALA:HB3	1.63	0.62
7:G:71:ARG:NE	8:H:56:GLU:OE2	2.32	0.62
2:B:258:VAL:HG11	2:B:321:LEU:CB	2.28	0.62
3:C:52:LEU:HD13	3:C:80:ILE:CG2	2.25	0.62
1:A:295:ALA:O	1:A:298:ALA:HB3	2.00	0.62
3:C:325:LEU:HD22	3:C:362:ILE:HG23	1.81	0.62
7:G:29:TYR:HA	7:G:33:GLY:HA3	1.80	0.62
10:J:57:HIS:HB2	10:J:61:ASN:O	1.99	0.62
1:A:15:GLN:O	1:A:26:ALA:HA	2.01	0.61
1:A:86:LEU:HD13	1:A:99:ILE:HG13	1.82	0.61
1:A:151:ASN:ND2	5:E:2:HIS:NE2	2.48	0.61
1:A:399:LEU:C	1:A:399:LEU:HD12	2.19	0.61
8:H:66:ASP:HA	8:H:69:VAL:CG2	2.30	0.61
4:D:158:ILE:CG2	4:D:159:GLY:N	2.63	0.61
10:J:58:LYS:HB2	10:J:59:TYR:CE1	2.35	0.61
1:A:85:HIS:O	1:A:99:ILE:HA	2.00	0.61
1:A:297:ILE:HG22	1:A:303:LEU:HD11	1.82	0.61
6:F:60:PHE:CD1	7:G:13:LEU:HD22	2.33	0.61
1:A:267:LEU:O	1:A:271:GLN:HB2	2.01	0.61
4:D:144:ARG:HG3	4:D:147:LEU:HD23	1.83	0.61
1:A:307:PHE:CD1	1:A:307:PHE:C	2.73	0.61
2:B:38:LEU:HD23	2:B:378:PHE:HZ	1.64	0.61
2:B:19:PRO:C	2:B:21:PRO:CD	2.69	0.61
2:B:276:GLN:OE1	2:B:313:ASN:HB3	2.00	0.61
3:C:71:CYS:SG	3:C:81:ARG:HD3	2.40	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:362:ILE:HA	3:C:366:LEU:HD23	1.82	0.61
1:A:106:VAL:N	1:A:107:PRO:HD2	2.16	0.61
4:D:5:LEU:HB2	8:H:59:PHE:CD1	2.36	0.61
10:J:57:HIS:HB2	10:J:61:ASN:CA	2.30	0.61
6:F:12:TRP:HA	6:F:12:TRP:HE3	1.65	0.61
7:G:57:LEU:HD22	7:G:57:LEU:H	1.65	0.61
7:G:77:TYR:CE1	8:H:52:GLU:HB2	2.35	0.61
1:A:264:HIS:HD2	1:A:266:ASP:HB2	1.65	0.60
3:C:201:LEU:O	3:C:204:SER:O	2.19	0.60
8:H:47:ARG:HD3	8:H:48:SER:N	2.15	0.60
1:A:235:ARG:HB2	5:E:21:SER:HA	1.84	0.60
3:C:344:VAL:HG23	3:C:344:VAL:O	2.00	0.60
4:D:21:LEU:HD13	4:D:26:ILE:CD1	2.30	0.60
4:D:130:LEU:HD11	4:D:158:ILE:CD1	2.29	0.60
1:A:255:ILE:HA	1:A:421:ALA:O	2.02	0.60
2:B:162:ASN:HB3	2:B:244:ILE:CD1	2.31	0.60
3:C:301:ILE:CD1	3:C:364:LEU:HD11	2.31	0.60
3:C:319:ARG:HH22	3:C:371:GLY:HA2	1.64	0.60
10:J:13:LEU:HA	10:J:19:THR:CG2	2.31	0.60
1:A:436:ARG:HD3	3:C:223:PRO:CD	2.31	0.60
2:B:100:SER:OG	2:B:105:MET:HG2	2.01	0.60
2:B:399:LEU:CA	2:B:402:ILE:HG22	2.32	0.60
3:C:222:HIS:HB3	3:C:223:PRO:CD	2.31	0.60
4:D:117:VAL:HG12	4:D:191:ARG:NH2	2.16	0.60
6:F:61:ARG:HH21	6:F:89:TYR:HE2	1.47	0.60
2:B:426:ALA:HB1	2:B:430:LEU:HD21	1.83	0.60
3:C:319:ARG:NH1	3:C:374:GLU:HB2	2.16	0.60
5:E:148:ALA:O	5:E:149:ASN:HB2	2.02	0.60
5:E:163:SER:OG	5:E:175:PRO:HD2	2.00	0.60
6:F:61:ARG:NH2	6:F:89:TYR:CE2	2.69	0.60
3:C:3:PRO:HG2	3:C:4:ASN:H	1.67	0.60
8:H:73:LEU:HD23	8:H:73:LEU:C	2.22	0.60
3:C:147:ILE:O	3:C:150:LEU:HB3	2.01	0.60
3:C:307:PHE:N	3:C:307:PHE:CD1	2.69	0.60
1:A:40:TRP:CH2	1:A:377:GLU:HA	2.35	0.60
2:B:132:PHE:CE2	2:B:191:LEU:HB3	2.37	0.60
2:B:137:VAL:CG2	2:B:138:ALA:N	2.65	0.60
2:B:170:ASN:C	2:B:170:ASN:ND2	2.55	0.60
4:D:78:GLY:O	4:D:79:GLU:HG3	2.02	0.60
1:A:64:PHE:CE1	1:A:86:LEU:HG	2.37	0.59
2:B:128:THR:HG21	2:B:223:LEU:HD12	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:342:GLN:NE2	3:C:342:GLN:HA	2.16	0.59
5:E:106:ILE:HG12	5:E:130:PRO:O	2.02	0.59
1:A:40:TRP:HZ3	1:A:89:TYR:HH	1.50	0.59
1:A:145:MET:CB	1:A:252:HIS:CD2	2.84	0.59
1:A:286:GLY:C	1:A:288:LEU:N	2.56	0.59
2:B:101:THR:HB	2:B:104:ASN:OD1	2.02	0.59
2:B:109:VAL:HG13	2:B:119:LEU:CD2	2.31	0.59
5:E:184:SER:O	5:E:196:GLY:N	2.29	0.59
1:A:46:ARG:HD2	1:A:163:LEU:HD21	1.83	0.59
2:B:58:GLU:HB3	2:B:62:ASN:HD21	1.67	0.59
2:B:95:LYS:HB2	2:B:110:GLU:HG2	1.84	0.59
2:B:150:VAL:O	2:B:153:GLN:HG3	2.02	0.59
2:B:368:TYR:O	2:B:372:VAL:HG23	2.00	0.59
4:D:32:VAL:O	4:D:36:VAL:HG13	2.02	0.59
2:B:241:GLY:HA3	2:B:421:GLN:HE21	1.67	0.59
3:C:107:SER:CB	11:C:382:HEM:HBD1	2.31	0.59
7:G:50:PRO:HG2	7:G:51:PRO:HD2	1.82	0.59
3:C:230:ILE:HG21	13:E:198:PEE:H26	1.84	0.59
4:D:30:PHE:HE2	4:D:64:LEU:HD21	1.65	0.59
3:C:149:ASN:O	3:C:152:SER:HB3	2.03	0.59
3:C:289:LEU:HG	3:C:293:LEU:CD2	2.33	0.59
5:E:81:ILE:HD13	5:E:98:VAL:HG12	1.84	0.59
1:A:378:ASP:O	1:A:382:GLU:HB2	2.02	0.59
3:C:289:LEU:HG	3:C:293:LEU:HD23	1.83	0.59
4:D:158:ILE:HG22	4:D:159:GLY:H	1.67	0.59
4:D:164:ILE:HD11	4:D:182:VAL:CG2	2.32	0.59
4:D:211:MET:HG3	15:D:242:BOG:H5'1	1.85	0.59
4:D:149:PHE:CE1	4:D:156:GLN:HB3	2.38	0.59
1:A:123:GLU:OE1	1:A:123:GLU:HA	2.03	0.59
1:A:288:LEU:HD13	2:B:83:PHE:CA	2.32	0.59
1:A:443:TRP:C	1:A:445:ARG:H	2.06	0.59
2:B:166:ALA:HB1	2:B:242:GLY:HA3	1.85	0.59
2:B:255:ALA:O	2:B:325:TYR:HA	2.02	0.59
3:C:238:THR:CG2	4:D:212:MET:HG3	2.32	0.59
5:E:9:ASN:ND2	5:E:11:SER:H	2.01	0.59
5:E:45:LEU:O	5:E:48:ALA:HB3	2.03	0.59
1:A:85:HIS:CA	9:I:314:UNK:HG1	2.33	0.58
2:B:217:LYS:C	2:B:219:VAL:H	2.07	0.58
3:C:27:ASN:HD22	6:F:69:ASN:HD22	1.50	0.58
3:C:92:PHE:HA	3:C:95:ILE:HG22	1.84	0.58
2:B:109:VAL:CG2	2:B:119:LEU:HD11	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:271:PRO:HB3	14:C:385:SIG:C2	2.33	0.58
3:C:321:LEU:HD12	3:C:374:GLU:HG2	1.85	0.58
4:D:95:TYR:CE2	4:D:101:ALA:HA	2.38	0.58
4:D:134:TYR:O	4:D:135:CYS:HB3	2.03	0.58
4:D:230:LEU:HB3	6:F:70:MET:CE	2.34	0.58
5:E:11:SER:OG	5:E:12:ASP:N	2.36	0.58
2:B:101:THR:HG22	2:B:102:ARG:H	1.68	0.58
3:C:283:ARG:O	3:C:284:SER:HB3	2.03	0.58
4:D:224:ARG:NH1	7:G:25:PRO:O	2.36	0.58
6:F:61:ARG:HG3	6:F:61:ARG:HH11	1.68	0.58
1:A:290:SER:O	1:A:291:SER:C	2.42	0.58
1:A:146:ARG:NH2	9:I:206:UNK:CB	2.67	0.58
1:A:291:SER:HB2	1:A:356:ARG:HH22	1.68	0.58
2:B:113:ARG:HG3	2:B:114:ASP:N	2.19	0.58
2:B:248:ASN:HD22	2:B:248:ASN:C	2.04	0.58
1:A:153:LEU:CD2	1:A:319:LEU:HD13	2.33	0.58
1:A:242:ARG:O	7:G:14:ILE:HA	2.03	0.58
1:A:391:PRO:CG	1:A:394:GLU:HB2	2.29	0.58
2:B:397:THR:HA	2:B:400:GLN:HB3	1.86	0.58
3:C:6:ARG:HA	3:C:12:LEU:HD22	1.85	0.58
3:C:78:TRP:CG	4:D:197:GLU:HG2	2.37	0.58
1:A:272:VAL:O	1:A:275:ALA:HB3	2.03	0.58
1:A:351:GLU:O	1:A:354:VAL:HG22	2.03	0.58
1:A:85:HIS:CB	9:I:314:UNK:HG1	2.33	0.58
1:A:250:LEU:N	1:A:250:LEU:CD1	2.66	0.58
2:B:357:VAL:HG12	2:B:361:LYS:CD	2.33	0.58
4:D:181:GLN:HG2	8:H:77:LEU:HD22	1.84	0.58
6:F:18:LYS:O	6:F:22:ASN:ND2	2.37	0.58
3:C:61:SER:C	3:C:62:LEU:HD22	2.23	0.58
3:C:332:ASN:HD21	3:C:359:TYR:CA	2.16	0.58
3:C:18:SER:C	3:C:19:LEU:HD12	2.24	0.57
1:A:60:GLU:OE2	1:A:89:TYR:HA	2.03	0.57
2:B:193:ASP:O	2:B:197:ASN:ND2	2.37	0.57
2:B:280:GLY:C	2:B:282:ASN:N	2.56	0.57
3:C:104:TYR:O	3:C:105:TYR:CD2	2.57	0.57
4:D:233:ARG:O	6:F:71:ARG:NH2	2.37	0.57
2:B:228:GLY:O	2:B:229:GLY:C	2.42	0.57
2:B:243:GLU:CD	2:B:436:VAL:HG22	2.24	0.57
2:B:285:VAL:HG12	2:B:285:VAL:O	2.03	0.57
3:C:3:PRO:O	3:C:5:ILE:HG13	2.04	0.57
3:C:307:PHE:N	3:C:307:PHE:HD1	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:346:HIS:N	3:C:347:PRO:HD2	2.19	0.57
2:B:400:GLN:O	2:B:404:ALA:HB2	2.05	0.57
3:C:92:PHE:CZ	3:C:124:LEU:HD13	2.39	0.57
3:C:323:GLN:HE21	7:G:47:ARG:HD3	1.69	0.57
1:A:45:SER:HA	1:A:48:GLU:CG	2.35	0.57
1:A:75:LEU:O	1:A:79:VAL:HG23	2.05	0.57
1:A:351:GLU:OE1	1:A:351:GLU:HA	2.04	0.57
2:B:402:ILE:HD13	2:B:402:ILE:O	2.04	0.57
3:C:370:ILE:O	3:C:374:GLU:HG3	2.04	0.57
5:E:85:LYS:HG2	5:E:86:ASN:N	2.19	0.57
6:F:101:ARG:HA	6:F:104:ARG:HE	1.69	0.57
3:C:373:LEU:HD23	3:C:373:LEU:C	2.24	0.57
1:A:250:LEU:C	1:A:250:LEU:CD2	2.71	0.57
2:B:199:PHE:HA	2:B:204:MET:HE2	1.87	0.57
3:C:325:LEU:HD21	3:C:362:ILE:HG23	1.87	0.57
4:D:218:LEU:HD22	5:E:39:VAL:HG13	1.86	0.57
4:D:233:ARG:HB3	6:F:71:ARG:HH21	1.70	0.57
10:J:21:ALA:O	10:J:24:ILE:N	2.37	0.57
3:C:206:SER:OG	12:C:383:U10:C3M	2.53	0.57
2:B:258:VAL:CG1	2:B:259:ALA:N	2.68	0.57
4:D:28:ARG:HD2	4:D:171:PHE:CD2	2.40	0.57
4:D:212:MET:O	4:D:216:VAL:HG22	2.04	0.57
5:E:9:ASN:HD21	5:E:11:SER:CB	2.18	0.57
5:E:109:GLU:CG	5:E:167:ALA:HB3	2.35	0.57
1:A:250:LEU:HD13	1:A:250:LEU:H	1.67	0.57
1:A:395:TRP:HA	1:A:395:TRP:HE3	1.68	0.57
2:B:75:LEU:HD22	2:B:136:GLU:HB3	1.86	0.57
6:F:31:LEU:HD23	6:F:31:LEU:N	2.18	0.57
1:A:159:GLN:NE2	5:E:7:VAL:HG11	2.19	0.56
3:C:28:ILE:HG23	3:C:32:TRP:HB2	1.87	0.56
10:J:13:LEU:N	10:J:13:LEU:CD1	2.68	0.56
1:A:152:TYR:CZ	5:E:5:ILE:HD12	2.38	0.56
1:A:343:MET:O	1:A:347:THR:HG22	2.05	0.56
2:B:213:HIS:N	2:B:214:PRO:HD2	2.20	0.56
5:E:45:LEU:CD1	10:J:28:ALA:HA	2.34	0.56
1:A:59:LEU:HD11	1:A:186:LEU:HD11	1.87	0.56
1:A:196:VAL:HG11	1:A:383:LEU:HD12	1.86	0.56
1:A:250:LEU:CD2	1:A:325:VAL:HG13	2.31	0.56
1:A:270:LEU:HG	1:A:320:PHE:CE2	2.40	0.56
2:B:76:THR:HG22	2:B:82:SER:N	2.13	0.56
2:B:202:ALA:HB3	2:B:229:GLY:HA2	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:TYR:CD1	2:B:260:GLU:HB2	2.40	0.56
2:B:405:VAL:HG12	2:B:406:ALA:N	2.19	0.56
3:C:101:ARG:C	3:C:101:ARG:CD	2.74	0.56
3:C:182:LEU:HD22	14:C:385:SIG:H381	1.87	0.56
3:C:219:ILE:HG21	4:D:230:LEU:HD11	1.87	0.56
3:C:342:GLN:HB3	3:C:348:PHE:CE2	2.41	0.56
3:C:358:SER:O	3:C:362:ILE:HG13	2.05	0.56
3:C:366:LEU:HD22	3:C:366:LEU:H	1.70	0.56
5:E:153:PHE:HD2	5:E:172:ARG:NH1	2.04	0.56
1:A:250:LEU:HB2	1:A:326:CYS:O	2.06	0.56
3:C:22:LEU:HD21	12:C:383:U10:H3M2	1.86	0.56
3:C:105:TYR:CD1	3:C:209:PRO:HA	2.40	0.56
4:D:79:GLU:O	4:D:80:MET:C	2.44	0.56
4:D:178:THR:OG1	4:D:181:GLN:HB2	2.05	0.56
3:C:223:PRO:O	3:C:227:PHE:HD2	1.87	0.56
5:E:26:ARG:O	5:E:28:SER:N	2.31	0.56
5:E:32:ARG:HD3	5:E:32:ARG:C	2.26	0.56
9:I:310:UNK:O	9:I:311:UNK:C	2.53	0.56
1:A:23:VAL:HG23	1:A:192:ALA:CB	2.36	0.56
2:B:96:LEU:HD23	2:B:96:LEU:C	2.25	0.56
2:B:111:CYS:O	2:B:112:LEU:HB3	2.06	0.56
2:B:143:GLN:OE1	2:B:146:ILE:CD1	2.53	0.56
2:B:169:ARG:O	2:B:170:ASN:CB	2.53	0.56
4:D:43:MET:HE2	4:D:46:VAL:CG2	2.35	0.56
5:E:94:LYS:HE2	5:E:94:LYS:HA	1.87	0.56
1:A:293:PRO:O	1:A:294:LEU:C	2.44	0.56
3:C:319:ARG:NH2	3:C:374:GLU:OE2	2.38	0.56
4:D:153:PHE:CD2	4:D:158:ILE:HG12	2.41	0.56
1:A:159:GLN:OE1	5:E:15:ARG:NH2	2.35	0.56
2:B:132:PHE:CD2	2:B:191:LEU:HB3	2.41	0.56
3:C:133:VAL:HG11	3:C:144:ALA:HB2	1.87	0.56
3:C:293:LEU:O	3:C:296:ALA:HB3	2.06	0.56
4:D:97:ASN:OD1	4:D:99:GLU:HG2	2.06	0.56
4:D:215:LEU:O	4:D:219:VAL:HG22	2.05	0.56
5:E:85:LYS:HG2	5:E:86:ASN:H	1.71	0.56
10:J:57:HIS:CE1	10:J:62:LYS:C	2.79	0.56
1:A:103:SER:C	1:A:105:ASP:N	2.59	0.56
1:A:145:MET:HB3	1:A:252:HIS:HD2	1.71	0.56
3:C:219:ILE:HD13	4:D:230:LEU:HD11	1.88	0.56
6:F:28:LYS:O	6:F:75:LEU:HB2	2.06	0.56
1:A:108:LYS:HE3	1:A:108:LYS:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:ARG:O	2:B:116:VAL:HG23	2.06	0.56
2:B:168:TYR:HB2	2:B:173:ALA:CB	2.25	0.56
2:B:272:PHE:HA	2:B:275:LEU:HB3	1.87	0.56
2:B:397:THR:O	2:B:401:GLN:HG2	2.05	0.56
1:A:346:CYS:HB3	1:A:411:CYS:CB	2.36	0.55
2:B:150:VAL:HG23	2:B:151:ALA:N	2.21	0.55
3:C:104:TYR:CZ	3:C:316:MET:CB	2.88	0.55
3:C:261:ASN:ND2	3:C:264:VAL:CG2	2.67	0.55
4:D:55:CYS:SG	4:D:56:TYR:HD1	2.29	0.55
5:E:171:ILE:HD12	5:E:172:ARG:H	1.71	0.55
10:J:13:LEU:HA	10:J:19:THR:HG21	1.87	0.55
10:J:55:ILE:C	10:J:57:HIS:H	2.09	0.55
1:A:100:LYS:HE3	2:B:370:MET:HE2	1.88	0.55
1:A:145:MET:HA	1:A:148:VAL:CG1	2.35	0.55
2:B:409:ASP:O	2:B:411:ILE:N	2.40	0.55
3:C:4:ASN:O	3:C:5:ILE:HB	2.05	0.55
3:C:233:LEU:O	3:C:237:LEU:HB2	2.05	0.55
3:C:278:ALA:HB1	3:C:295:LEU:HD11	1.86	0.55
4:D:192:TRP:CD1	4:D:193:ALA:N	2.75	0.55
1:A:391:PRO:O	1:A:394:GLU:N	2.38	0.55
2:B:130:PRO:HB3	2:B:132:PHE:CE1	2.42	0.55
3:C:273:TRP:HA	3:C:276:LEU:CD1	2.37	0.55
5:E:65:SER:C	5:E:67:ASP:H	2.10	0.55
9:I:313:UNK:CB	9:I:314:UNK:CD	2.84	0.55
2:B:399:LEU:HA	2:B:402:ILE:CG2	2.32	0.55
3:C:283:ARG:O	3:C:283:ARG:CG	2.51	0.55
6:F:12:TRP:HB3	6:F:15:GLY:H	1.71	0.55
8:H:17:LEU:HD13	8:H:73:LEU:HD11	1.88	0.55
3:C:75:GLN:O	3:C:76:TYR:HB2	2.07	0.55
3:C:345:GLU:HB3	3:C:347:PRO:HD2	1.86	0.55
4:D:218:LEU:CD1	5:E:42:VAL:HG12	2.37	0.55
3:C:173:ASN:N	3:C:174:PRO:HD2	2.22	0.55
4:D:75:ASN:H	4:D:79:GLU:H	1.53	0.55
7:G:42:ARG:O	7:G:43:ALA:HB2	2.07	0.55
8:H:72:LYS:HA	8:H:75:ASN:ND2	2.22	0.55
2:B:395:PRO:HA	2:B:398:VAL:HG12	1.87	0.55
3:C:92:PHE:O	3:C:95:ILE:HG22	2.06	0.55
4:D:164:ILE:HD11	4:D:182:VAL:CG1	2.34	0.55
1:A:266:ASP:O	1:A:268:VAL:N	2.40	0.55
3:C:323:GLN:NE2	7:G:47:ARG:HD3	2.22	0.55
4:D:230:LEU:HB3	6:F:70:MET:HE1	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:14:PHE:N	10:J:14:PHE:CD1	2.71	0.55
8:H:57:GLU:CD	8:H:57:GLU:H	2.11	0.55
1:A:172:GLU:HA	1:A:172:GLU:OE1	2.07	0.55
1:A:250:LEU:HD22	1:A:251:ALA:N	2.21	0.55
1:A:297:ILE:HG21	1:A:337:VAL:CG1	2.32	0.55
4:D:164:ILE:CD1	4:D:182:VAL:HG13	2.37	0.55
1:A:158:PHE:CE2	1:A:319:LEU:HD21	2.42	0.54
1:A:365:LEU:HD21	1:A:395:TRP:CD1	2.42	0.54
3:C:295:LEU:CD2	14:C:385:SIG:H273	2.35	0.54
1:A:344:ARG:HA	1:A:347:THR:HG22	1.89	0.54
2:B:24:LEU:H	2:B:24:LEU:CD2	2.19	0.54
2:B:25:GLU:CB	2:B:213:HIS:ND1	2.67	0.54
2:B:402:ILE:HD13	2:B:402:ILE:C	2.27	0.54
3:C:42:LEU:HD22	3:C:190:ILE:HG22	1.88	0.54
3:C:130:VAL:HA	3:C:133:VAL:HG23	1.90	0.54
3:C:230:ILE:CG2	13:E:198:PEE:H26	2.37	0.54
2:B:129:ALA:N	2:B:130:PRO:HD3	2.23	0.54
2:B:260:GLU:O	2:B:261:SER:CB	2.56	0.54
2:B:370:MET:O	2:B:372:VAL:N	2.38	0.54
3:C:127:THR:CG2	3:C:186:LEU:HB3	2.37	0.54
3:C:359:TYR:HD2	3:C:360:PHE:CD1	2.25	0.54
4:D:144:ARG:CZ	4:D:147:LEU:HD21	2.37	0.54
4:D:218:LEU:HD11	5:E:42:VAL:CG1	2.37	0.54
2:B:68:LEU:HD23	2:B:186:VAL:HG11	1.89	0.54
5:E:26:ARG:C	5:E:28:SER:H	2.10	0.54
8:H:73:LEU:CD2	8:H:77:LEU:HD11	2.38	0.54
1:A:373:THR:HB	1:A:374:PRO:CD	2.38	0.54
3:C:130:VAL:HG12	3:C:131:GLY:N	2.23	0.54
1:A:42:ASP:HB3	1:A:194:ARG:HB3	1.89	0.54
3:C:166:TRP:CA	3:C:175:THR:HB	2.37	0.54
4:D:29:GLY:HA3	4:D:189:PHE:HB2	1.90	0.54
4:D:129:SER:HB3	4:D:152:TYR:CE2	2.42	0.54
5:E:32:ARG:HG3	5:E:32:ARG:HH11	1.72	0.54
5:E:96:LEU:HD12	5:E:135:LEU:O	2.08	0.54
8:H:16:PRO:O	8:H:20:VAL:HG23	2.08	0.54
10:J:57:HIS:CA	10:J:60:GLU:C	2.74	0.54
2:B:281:ALA:O	2:B:285:VAL:HB	2.07	0.54
3:C:270:LYS:O	3:C:270:LYS:HG3	2.06	0.54
1:A:445:ARG:NH1	10:J:16:ARG:HG2	2.23	0.54
2:B:52:LYS:HB2	2:B:203:ARG:HB2	1.90	0.54
5:E:190:ASP:OD1	5:E:190:ASP:N	2.40	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:31:ASN:HB3	2:B:201:SER:HB2	1.89	0.54
2:B:170:ASN:C	2:B:170:ASN:HD22	2.11	0.54
2:B:207:VAL:HG11	2:B:382:VAL:HG23	1.89	0.54
3:C:369:THR:C	3:C:371:GLY:N	2.60	0.54
1:A:41:ILE:HG23	1:A:195:MET:HG2	1.90	0.53
1:A:49:SER:HB2	1:A:52:ASN:HB3	1.89	0.53
2:B:20:HIS:N	2:B:21:PRO:CD	2.71	0.53
1:A:61:HIS:CD2	1:A:134:ILE:HG12	2.42	0.53
2:B:171:ALA:O	2:B:172:LEU:HB3	2.09	0.53
3:C:332:ASN:HD21	3:C:359:TYR:HA	1.72	0.53
5:E:29:ASP:C	5:E:31:SER:N	2.60	0.53
10:J:55:ILE:C	10:J:57:HIS:N	2.62	0.53
1:A:65:LYS:HD2	1:A:65:LYS:N	2.23	0.53
3:C:332:ASN:ND2	3:C:359:TYR:HA	2.23	0.53
7:G:25:PRO:O	7:G:26:PHE:C	2.47	0.53
7:G:53:LEU:O	7:G:56:TYR:HB3	2.08	0.53
1:A:294:LEU:O	1:A:298:ALA:N	2.38	0.53
2:B:24:LEU:HD23	2:B:24:LEU:N	2.22	0.53
6:F:52:GLU:OE2	7:G:11:ARG:NH1	2.41	0.53
7:G:77:TYR:CZ	8:H:52:GLU:HB2	2.44	0.53
10:J:12:LEU:O	10:J:19:THR:HG21	2.09	0.53
4:D:223:LYS:HD2	4:D:227:TRP:CD1	2.42	0.53
1:A:102:LEU:C	1:A:104:LYS:N	2.62	0.53
4:D:47:ALA:HB1	4:D:89:ASP:O	2.08	0.53
5:E:20:TYR:O	5:E:21:SER:O	2.27	0.53
1:A:134:ILE:CG2	1:A:174:ILE:HD13	2.39	0.53
1:A:290:SER:N	2:B:90:GLU:OE1	2.40	0.53
2:B:198:HIS:HD2	2:B:203:ARG:HH22	1.57	0.53
3:C:113:THR:HG22	3:C:201:LEU:N	2.24	0.53
3:C:142:TRP:HA	3:C:145:THR:OG1	2.08	0.53
5:E:52:LYS:HD3	5:E:52:LYS:O	2.08	0.53
1:A:19:LEU:C	1:A:21:ASN:N	2.61	0.53
1:A:410:VAL:O	1:A:413:LYS:HB3	2.09	0.53
2:B:166:ALA:HB1	2:B:242:GLY:CA	2.38	0.53
2:B:333:ALA:O	2:B:337:ILE:HG12	2.09	0.53
3:C:81:ARG:NH1	11:C:381:HEM:O2D	2.42	0.53
4:D:27:ARG:NH2	10:J:59:TYR:CE2	2.77	0.53
8:H:40:CYS:O	8:H:44:VAL:HG23	2.09	0.53
1:A:145:MET:CB	1:A:252:HIS:NE2	2.72	0.53
1:A:264:HIS:CD2	1:A:266:ASP:HB2	2.44	0.53
1:A:391:PRO:HG2	1:A:394:GLU:CB	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:372:VAL:HG12	2:B:372:VAL:O	2.09	0.53
3:C:146:VAL:HG23	3:C:147:ILE:H	1.72	0.53
4:D:27:ARG:NH2	10:J:59:TYR:HE2	2.07	0.53
1:A:362:ARG:HG3	1:A:399:LEU:HD11	1.91	0.53
2:B:202:ALA:CB	2:B:229:GLY:HA2	2.39	0.53
3:C:283:ARG:O	3:C:284:SER:CB	2.57	0.53
1:A:444:LEU:H	1:A:444:LEU:CD1	2.21	0.52
2:B:141:GLN:N	2:B:142:PRO:HD2	2.25	0.52
2:B:242:GLY:O	2:B:423:SER:HA	2.08	0.52
3:C:3:PRO:HG2	3:C:4:ASN:N	2.24	0.52
4:D:224:ARG:HH11	4:D:224:ARG:HB3	1.74	0.52
7:G:26:PHE:HD1	7:G:26:PHE:N	1.96	0.52
1:A:104:LYS:O	1:A:104:LYS:HG2	2.10	0.52
1:A:120:CYS:O	1:A:122:LEU:HG	2.09	0.52
1:A:159:GLN:OE1	1:A:237:THR:HG21	2.09	0.52
1:A:252:HIS:ND1	1:A:325:VAL:HG22	2.25	0.52
1:A:287:GLY:HA2	1:A:299:VAL:HG11	1.92	0.52
2:B:361:LYS:NZ	2:B:403:ASP:O	2.42	0.52
4:D:180:SER:HB2	8:H:17:LEU:HB2	1.91	0.52
5:E:21:SER:O	5:E:22:THR:HB	2.09	0.52
2:B:21:PRO:O	2:B:21:PRO:HG2	2.09	0.52
2:B:24:LEU:HG	2:B:24:LEU:O	2.09	0.52
3:C:105:TYR:HA	3:C:315:THR:HA	1.91	0.52
3:C:155:PRO:O	3:C:156:TYR:HB2	2.10	0.52
3:C:271:PRO:HB3	14:C:385:SIG:C3	2.39	0.52
3:C:325:LEU:HD12	3:C:370:ILE:HG13	1.90	0.52
5:E:144:CYS:HB2	5:E:158:CYS:SG	2.49	0.52
7:G:32:LYS:C	7:G:35:PRO:HD2	2.29	0.52
1:A:4:TYR:CG	2:B:113:ARG:HB3	2.44	0.52
1:A:36:THR:CG2	1:A:100:LYS:HB3	2.16	0.52
3:C:277:PHE:CG	3:C:278:ALA:N	2.76	0.52
5:E:28:SER:O	5:E:31:SER:HB3	2.08	0.52
10:J:57:HIS:CE1	10:J:58:LYS:HG3	2.45	0.52
1:A:294:LEU:HD23	1:A:307:PHE:CE1	2.45	0.52
2:B:219:VAL:C	2:B:221:GLU:H	2.13	0.52
3:C:43:MET:O	3:C:44:THR:C	2.48	0.52
3:C:101:ARG:HE	3:C:102:GLY:CA	2.22	0.52
3:C:105:TYR:CE1	3:C:209:PRO:HA	2.44	0.52
10:J:57:HIS:C	10:J:60:GLU:H	2.13	0.52
2:B:250:ASP:C	2:B:252:LEU:H	2.13	0.52
2:B:330:ALA:O	2:B:333:ALA:HB2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:107:SER:HB3	11:C:382:HEM:CBD	2.32	0.52
3:C:351:ILE:HG23	7:G:58:LEU:HD21	1.90	0.52
1:A:173:ASN:O	1:A:177:LEU:HG	2.09	0.52
2:B:57:TYR:N	2:B:57:TYR:CD1	2.78	0.52
2:B:111:CYS:SG	2:B:116:VAL:HA	2.50	0.52
2:B:406:ALA:O	2:B:408:ALA:N	2.43	0.52
3:C:28:ILE:HB	3:C:225:TYR:OH	2.10	0.52
3:C:31:TRP:CZ3	13:C:384:PEE:C13	2.89	0.52
3:C:136:TRP:CD1	3:C:176:LEU:HD13	2.44	0.52
4:D:29:GLY:HA2	4:D:32:VAL:HG12	1.92	0.52
5:E:123:ASP:O	5:E:127:VAL:HG22	2.09	0.52
2:B:258:VAL:CG1	2:B:259:ALA:H	2.22	0.52
2:B:385:GLN:CD	2:B:392:TYR:HA	2.29	0.52
2:B:405:VAL:CG1	2:B:409:ASP:OD1	2.57	0.52
3:C:169:PHE:O	3:C:170:SER:HB3	2.09	0.52
4:D:94:PRO:HB2	4:D:95:TYR:CD1	2.44	0.52
1:A:45:SER:HA	1:A:48:GLU:CD	2.29	0.52
1:A:146:ARG:NH2	9:I:206:UNK:HA	2.24	0.52
1:A:250:LEU:CD2	1:A:325:VAL:CG1	2.87	0.52
2:B:92:VAL:CG1	2:B:115:ASP:HB3	2.35	0.52
2:B:137:VAL:C	2:B:139:ASP:N	2.63	0.52
2:B:227:ARG:O	2:B:229:GLY:N	2.43	0.52
2:B:395:PRO:HA	2:B:398:VAL:HG11	1.92	0.52
3:C:222:HIS:CB	3:C:223:PRO:CD	2.86	0.52
6:F:26:PHE:O	6:F:31:LEU:HD23	2.10	0.52
1:A:72:GLN:O	1:A:73:ASN:C	2.47	0.52
2:B:146:ILE:HG13	2:B:147:ASP:H	1.72	0.52
2:B:290:ASN:CB	2:B:306:PRO:HD2	2.39	0.52
3:C:222:HIS:CG	3:C:223:PRO:N	2.77	0.52
3:C:342:GLN:HB3	3:C:348:PHE:CD2	2.44	0.52
4:D:217:PRO:HG2	4:D:218:LEU:H	1.75	0.52
7:G:56:TYR:O	7:G:59:TYR:HB3	2.10	0.52
7:G:73:ASN:O	7:G:75:ALA:N	2.43	0.52
2:B:248:ASN:C	2:B:248:ASN:ND2	2.63	0.51
4:D:95:TYR:CE2	4:D:104:ALA:HB3	2.44	0.51
4:D:139:THR:HG23	8:H:41:ASP:OD1	2.10	0.51
5:E:136:ILE:HG22	5:E:136:ILE:O	2.10	0.51
1:A:146:ARG:HG2	1:A:146:ARG:HH11	1.75	0.51
1:A:257:VAL:HG22	1:A:320:PHE:O	2.11	0.51
1:A:276:ILE:HD11	1:A:349:ILE:HD11	1.90	0.51
1:A:409:GLU:HA	1:A:409:GLU:OE1	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:310:SER:O	2:B:324:PHE:HB2	2.10	0.51
9:I:203:UNK:O	9:I:204:UNK:C	2.58	0.51
2:B:385:GLN:NE2	2:B:392:TYR:HA	2.25	0.51
3:C:95:ILE:HG23	3:C:96:PHE:N	2.25	0.51
4:D:117:VAL:CG1	4:D:191:ARG:HH21	2.22	0.51
5:E:171:ILE:HD12	5:E:172:ARG:N	2.25	0.51
8:H:50:THR:HG22	8:H:52:GLU:H	1.75	0.51
10:J:57:HIS:C	10:J:59:TYR:H	2.13	0.51
2:B:89:ILE:HD11	2:B:96:LEU:HD12	1.91	0.51
3:C:282:LEU:HD13	3:C:282:LEU:C	2.29	0.51
3:C:372:THR:HA	3:C:375:ASN:HD22	1.74	0.51
5:E:60:SER:C	5:E:62:MET:H	2.14	0.51
8:H:42:GLU:O	8:H:46:SER:HB3	2.11	0.51
1:A:136:ARG:O	1:A:139:GLN:N	2.43	0.51
3:C:95:ILE:HD13	3:C:121:LEU:CD1	2.40	0.51
3:C:131:GLY:N	3:C:134:LEU:HD13	2.26	0.51
4:D:57:THR:HB	4:D:60:GLU:CB	2.40	0.51
4:D:178:THR:HG21	8:H:16:PRO:HD2	1.93	0.51
5:E:21:SER:OG	5:E:22:THR:N	2.42	0.51
6:F:84:GLU:H	6:F:84:GLU:CD	2.14	0.51
1:A:127:ILE:O	1:A:129:LYS:N	2.44	0.51
1:A:389:ARG:HD2	1:A:390:ILE:N	2.25	0.51
2:B:61:SER:C	2:B:63:LEU:H	2.13	0.51
2:B:147:ASP:O	2:B:150:VAL:HG22	2.09	0.51
3:C:261:ASN:ND2	3:C:264:VAL:HB	2.25	0.51
3:C:327:TRP:HE3	3:C:330:VAL:HG11	1.75	0.51
5:E:62:MET:CG	5:E:63:SER:H	2.22	0.51
1:A:106:VAL:HB	1:A:107:PRO:CD	2.41	0.51
3:C:261:ASN:HD22	3:C:264:VAL:HB	1.74	0.51
4:D:32:VAL:CG1	4:D:186:VAL:HG22	2.40	0.51
6:F:59:MET:HA	6:F:59:MET:HE3	1.92	0.51
1:A:153:LEU:HD22	1:A:319:LEU:HD13	1.92	0.51
2:B:198:HIS:HD2	2:B:203:ARG:NH2	2.08	0.51
2:B:365:LYS:HE2	2:B:403:ASP:OD1	2.11	0.51
3:C:276:LEU:O	3:C:279:TYR:HB3	2.10	0.51
5:E:10:PHE:CD2	7:G:18:LEU:HD21	2.45	0.51
3:C:166:TRP:CD1	3:C:166:TRP:C	2.84	0.51
5:E:32:ARG:HD3	5:E:32:ARG:O	2.11	0.51
7:G:57:LEU:HD22	7:G:57:LEU:N	2.24	0.51
1:A:266:ASP:C	1:A:268:VAL:N	2.63	0.51
1:A:7:ALA:O	1:A:11:VAL:HG23	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:CYS:HB3	1:A:122:LEU:CD2	2.42	0.50
1:A:354:VAL:HG23	1:A:355:LEU:N	2.26	0.50
1:A:434:TYR:O	1:A:438:ARG:HB2	2.11	0.50
1:A:438:ARG:HD3	1:A:438:ARG:C	2.32	0.50
2:B:217:LYS:O	2:B:219:VAL:N	2.44	0.50
14:C:385:SIG:H201	14:C:385:SIG:H353	1.93	0.50
4:D:116:ILE:HG23	4:D:117:VAL:N	2.26	0.50
5:E:129:LYS:HB2	5:E:187:PHE:CZ	2.47	0.50
1:A:346:CYS:HB3	1:A:411:CYS:HB2	1.92	0.50
1:A:365:LEU:HD21	1:A:395:TRP:CB	2.41	0.50
3:C:22:LEU:HD12	3:C:23:PRO:CD	2.42	0.50
3:C:362:ILE:N	3:C:366:LEU:HD23	2.26	0.50
4:D:46:VAL:HG12	4:D:47:ALA:N	2.25	0.50
8:H:17:LEU:HD21	8:H:21:ARG:CZ	2.41	0.50
8:H:17:LEU:O	8:H:21:ARG:HG3	2.11	0.50
1:A:26:ALA:O	1:A:198:ALA:HA	2.10	0.50
4:D:213:GLY:O	4:D:217:PRO:HG3	2.10	0.50
1:A:36:THR:HG21	1:A:373:THR:OG1	2.12	0.50
1:A:228:VAL:O	1:A:228:VAL:HG13	2.10	0.50
3:C:32:TRP:HZ2	3:C:207:ASN:HB3	1.76	0.50
4:D:26:ILE:HD13	4:D:192:TRP:HB3	1.93	0.50
4:D:215:LEU:HD11	5:E:47:VAL:CG2	2.42	0.50
5:E:57:GLN:C	5:E:59:VAL:H	2.14	0.50
5:E:128:LYS:HB2	5:E:187:PHE:HE2	1.75	0.50
5:E:171:ILE:HG22	5:E:179:ASN:OD1	2.12	0.50
1:A:33:PRO:O	1:A:103:SER:OG	2.28	0.50
1:A:114:ALA:HA	1:A:216:PHE:CE1	2.47	0.50
3:C:219:ILE:HB	3:C:224:TYR:CD2	2.46	0.50
4:D:147:LEU:C	4:D:148:TYR:CD1	2.85	0.50
5:E:122:HIS:H	5:E:125:GLU:CD	2.15	0.50
10:J:57:HIS:HA	10:J:60:GLU:CA	2.41	0.50
2:B:63:LEU:HB2	2:B:182:ARG:CD	2.42	0.50
2:B:82:SER:O	2:B:85:ILE:CG2	2.60	0.50
2:B:105:MET:HE2	2:B:107:TYR:HE1	1.76	0.50
3:C:187:PRO:HG2	11:C:381:HEM:HMC3	1.94	0.50
4:D:117:VAL:CG1	4:D:191:ARG:NH2	2.75	0.50
5:E:62:MET:O	5:E:63:SER:C	2.49	0.50
5:E:112:VAL:HG21	5:E:170:ARG:NH2	2.26	0.50
1:A:4:TYR:HB2	2:B:113:ARG:CB	2.42	0.50
3:C:167:GLY:HA2	3:C:174:PRO:HB2	1.94	0.50
3:C:269:ILE:HG22	14:C:385:SIG:H263	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:148:ALA:HA	5:E:156:TYR:CD1	2.47	0.50
1:A:366:VAL:C	1:A:368:HIS:H	2.14	0.50
3:C:347:PRO:HG3	7:G:66:PHE:HD1	1.76	0.50
4:D:195:GLU:HG3	4:D:195:GLU:O	2.11	0.50
1:A:4:TYR:C	1:A:6:GLN:N	2.61	0.50
1:A:85:HIS:HA	9:I:314:UNK:CG	2.37	0.50
2:B:171:ALA:O	2:B:172:LEU:CB	2.60	0.50
2:B:406:ALA:O	2:B:407:ASP:C	2.50	0.50
3:C:133:VAL:HG13	3:C:144:ALA:HB2	1.92	0.50
3:C:167:GLY:H	3:C:175:THR:CB	2.24	0.50
3:C:234:THR:HG22	13:E:198:PEE:H31	1.94	0.50
4:D:41:HIS:HB3	4:D:113:LEU:HD13	1.93	0.50
4:D:54:VAL:HG13	4:D:55:CYS:N	2.27	0.50
5:E:106:ILE:HD11	5:E:131:GLU:HA	1.93	0.50
1:A:134:ILE:HG21	1:A:174:ILE:HD13	1.94	0.49
2:B:209:LEU:O	2:B:211:VAL:HG13	2.12	0.49
4:D:117:VAL:HG23	4:D:190:LEU:HB3	1.93	0.49
4:D:134:TYR:CG	4:D:162:PRO:HG3	2.46	0.49
4:D:216:VAL:N	4:D:217:PRO:HD2	2.27	0.49
10:J:4:THR:O	10:J:5:LEU:C	2.49	0.49
1:A:46:ARG:NH2	1:A:232:SER:O	2.43	0.49
1:A:100:LYS:HG3	2:B:370:MET:HE1	1.94	0.49
2:B:31:ASN:HB3	2:B:201:SER:CB	2.41	0.49
5:E:14:ARG:O	7:G:24:ARG:HG2	2.12	0.49
3:C:166:TRP:O	3:C:167:GLY:C	2.51	0.49
7:G:78:VAL:C	7:G:79:ASN:ND2	2.62	0.49
1:A:92:ARG:NH1	1:A:165:GLN:O	2.45	0.49
1:A:245:GLU:CG	7:G:11:ARG:HG2	2.35	0.49
2:B:133:ARG:HD3	2:B:135:TRP:CH2	2.48	0.49
2:B:316:TYR:HB2	2:B:319:SER:O	2.13	0.49
3:C:45:GLN:CB	11:C:381:HEM:HAB	2.43	0.49
3:C:131:GLY:H	3:C:134:LEU:HD13	1.78	0.49
8:H:15:ASP:O	8:H:17:LEU:N	2.45	0.49
1:A:92:ARG:HH12	1:A:166:SER:HA	1.77	0.49
1:A:365:LEU:HD13	1:A:392:LEU:HD22	1.93	0.49
1:A:443:TRP:C	1:A:445:ARG:N	2.64	0.49
2:B:24:LEU:HD21	2:B:392:TYR:CD2	2.47	0.49
2:B:150:VAL:CG2	2:B:151:ALA:N	2.75	0.49
3:C:101:ARG:NH1	11:C:382:HEM:O2A	2.32	0.49
4:D:237:TYR:HB2	6:F:60:PHE:CG	2.47	0.49
5:E:65:SER:O	5:E:67:ASP:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:97:PHE:O	5:E:134:ILE:HG23	2.13	0.49
1:A:86:LEU:HB2	1:A:99:ILE:HG12	1.94	0.49
1:A:298:ALA:HA	1:A:303:LEU:HD12	1.95	0.49
3:C:31:TRP:CE3	13:C:384:PEE:H13	2.47	0.49
3:C:101:ARG:HE	3:C:102:GLY:N	2.09	0.49
3:C:362:ILE:CA	3:C:366:LEU:HD23	2.42	0.49
5:E:25:SER:O	5:E:28:SER:HB3	2.13	0.49
8:H:17:LEU:HD13	8:H:73:LEU:CD1	2.43	0.49
1:A:34:THR:HA	1:A:102:LEU:HA	1.94	0.49
3:C:327:TRP:CA	3:C:330:VAL:HG12	2.32	0.49
7:G:36:ASN:O	7:G:40:ARG:HG3	2.13	0.49
2:B:146:ILE:O	2:B:147:ASP:C	2.50	0.49
2:B:318:ASP:O	2:B:319:SER:HB2	2.12	0.49
3:C:70:THR:HA	3:C:74:VAL:CG2	2.41	0.49
4:D:10:TYR:N	4:D:10:TYR:CD1	2.81	0.49
4:D:94:PRO:HB2	4:D:95:TYR:CE1	2.48	0.49
4:D:222:MET:HE1	5:E:40:THR:HG23	1.94	0.49
1:A:436:ARG:HH22	3:C:20:ILE:HG22	1.77	0.49
2:B:67:HIS:O	2:B:70:ARG:HB3	2.12	0.49
2:B:140:LEU:C	2:B:142:PRO:HD2	2.32	0.49
2:B:152:PHE:HA	2:B:157:THR:HG21	1.94	0.49
3:C:220:PRO:HG2	3:C:223:PRO:HG2	1.95	0.49
3:C:344:VAL:HB	3:C:349:ILE:HD11	1.95	0.49
6:F:61:ARG:HG3	6:F:61:ARG:NH1	2.28	0.49
7:G:25:PRO:HG2	7:G:26:PHE:HD1	1.77	0.49
7:G:36:ASN:OD1	7:G:39:ARG:NH1	2.46	0.49
1:A:443:TRP:O	1:A:445:ARG:N	2.36	0.49
2:B:385:GLN:C	2:B:387:LEU:H	2.16	0.49
2:B:429:ASN:O	2:B:431:GLY:N	2.46	0.49
4:D:97:ASN:HB2	4:D:98:PRO:HD2	1.95	0.49
4:D:235:LEU:CD1	6:F:64:ARG:HA	2.43	0.49
7:G:34:VAL:N	7:G:35:PRO:CD	2.76	0.49
1:A:403:ASP:OD1	1:A:406:MET:HB2	2.13	0.48
2:B:385:GLN:C	2:B:387:LEU:N	2.66	0.48
3:C:60:THR:HG23	3:C:136:TRP:CZ3	2.48	0.48
3:C:81:ARG:HG3	3:C:81:ARG:HH11	1.77	0.48
3:C:163:GLU:HB3	3:C:169:PHE:CD1	2.48	0.48
3:C:207:ASN:C	3:C:207:ASN:HD22	2.15	0.48
3:C:215:ASP:HB3	7:G:7:LEU:HB3	1.93	0.48
3:C:285:ILE:HG23	3:C:291:GLY:HA2	1.95	0.48
4:D:215:LEU:HD11	5:E:47:VAL:HG23	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:49:ALA:O	7:G:50:PRO:C	2.51	0.48
1:A:152:TYR:HA	1:A:155:ALA:HB3	1.94	0.48
2:B:120:MET:O	2:B:121:GLU:C	2.51	0.48
3:C:133:VAL:O	3:C:136:TRP:HD1	1.96	0.48
3:C:138:GLN:NE2	3:C:138:GLN:HA	2.28	0.48
4:D:14:HIS:CG	4:D:21:LEU:HD23	2.48	0.48
1:A:45:SER:HB3	1:A:167:VAL:HA	1.96	0.48
1:A:88:ALA:HB2	1:A:97:TYR:HA	1.95	0.48
1:A:369:LEU:HD22	1:A:375:VAL:HA	1.95	0.48
1:A:374:PRO:O	1:A:377:GLU:HB3	2.13	0.48
1:A:397:GLU:O	1:A:398:ARG:C	2.51	0.48
5:E:9:ASN:CG	5:E:11:SER:HB3	2.32	0.48
2:B:399:LEU:O	2:B:402:ILE:HG22	2.14	0.48
2:B:429:ASN:C	2:B:431:GLY:H	2.17	0.48
3:C:42:LEU:CD2	3:C:190:ILE:HG22	2.43	0.48
3:C:127:THR:HG22	3:C:186:LEU:CB	2.41	0.48
3:C:238:THR:CB	4:D:212:MET:HG3	2.43	0.48
3:C:305:ILE:HB	3:C:306:PRO:HD3	1.94	0.48
5:E:14:ARG:O	5:E:15:ARG:C	2.52	0.48
1:A:85:HIS:CG	9:I:314:UNK:HG1	2.49	0.48
2:B:84:LYS:O	2:B:88:GLY:N	2.44	0.48
3:C:167:GLY:CA	3:C:174:PRO:HB2	2.44	0.48
3:C:196:ILE:O	3:C:199:THR:HB	2.14	0.48
4:D:44:ASP:O	4:D:90:TYR:CD2	2.63	0.48
4:D:181:GLN:HE21	4:D:181:GLN:C	2.16	0.48
5:E:76:ILE:HB	5:E:193:VAL:HG13	1.94	0.48
1:A:240:GLN:HB2	1:A:422:VAL:HG12	1.93	0.48
3:C:157:ILE:O	3:C:161:LEU:HB2	2.12	0.48
3:C:207:ASN:C	3:C:207:ASN:ND2	2.65	0.48
3:C:361:THR:HA	3:C:365:ILE:HG22	1.95	0.48
5:E:65:SER:C	5:E:67:ASP:N	2.67	0.48
1:A:58:PHE:HD1	1:A:58:PHE:O	1.97	0.48
3:C:139:MET:HB2	3:C:256:ASN:OD1	2.14	0.48
3:C:283:ARG:NH2	3:C:342:GLN:O	2.46	0.48
5:E:156:TYR:HB2	5:E:165:TYR:HB2	1.96	0.48
6:F:101:ARG:CB	6:F:104:ARG:HH21	2.27	0.48
1:A:30:SER:O	1:A:202:GLY:HA2	2.13	0.48
1:A:444:LEU:O	1:A:445:ARG:C	2.52	0.48
2:B:47:ILE:HD11	2:B:116:VAL:CG1	2.44	0.48
2:B:113:ARG:HG3	2:B:114:ASP:H	1.77	0.48
2:B:131:GLU:O	2:B:132:PHE:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:214:LEU:O	4:D:217:PRO:HG2	2.14	0.48
5:E:83:GLU:HG3	5:E:100:HIS:NE2	2.29	0.48
10:J:61:ASN:O	10:J:62:LYS:CB	2.62	0.48
1:A:46:ARG:HG2	1:A:231:LEU:HD13	1.94	0.48
3:C:19:LEU:HD12	3:C:19:LEU:N	2.28	0.48
4:D:98:PRO:HG2	4:D:99:GLU:OE2	2.13	0.48
5:E:55:VAL:O	5:E:59:VAL:HG23	2.13	0.48
2:B:143:GLN:CD	2:B:146:ILE:HD11	2.33	0.48
2:B:275:LEU:O	2:B:279:LEU:HB2	2.13	0.48
3:C:219:ILE:HD13	4:D:230:LEU:CD1	2.43	0.48
3:C:285:ILE:N	3:C:286:PRO:HD3	2.29	0.48
4:D:165:TYR:H	4:D:168:VAL:CG2	2.26	0.48
4:D:232:SER:HB2	7:G:23:GLN:OE1	2.14	0.48
5:E:136:ILE:HB	5:E:181:GLU:HB3	1.94	0.48
1:A:166:SER:HG	5:E:3:THR:HG23	1.73	0.47
2:B:353:SER:C	2:B:355:GLU:H	2.17	0.47
2:B:395:PRO:C	2:B:398:VAL:HG12	2.35	0.47
3:C:182:LEU:CD2	14:C:385:SIG:H381	2.44	0.47
3:C:342:GLN:HE21	3:C:342:GLN:CA	2.11	0.47
4:D:51:LEU:O	4:D:54:VAL:HG12	2.14	0.47
5:E:119:ASP:HB3	5:E:179:ASN:CG	2.35	0.47
2:B:111:CYS:SG	2:B:119:LEU:HD23	2.54	0.47
2:B:406:ALA:C	2:B:408:ALA:N	2.66	0.47
5:E:15:ARG:NH1	5:E:19:ASP:HB3	2.29	0.47
5:E:62:MET:CG	5:E:63:SER:N	2.77	0.47
8:H:68:CYS:O	8:H:69:VAL:C	2.53	0.47
8:H:73:LEU:HD21	8:H:77:LEU:HD11	1.96	0.47
1:A:287:GLY:CA	1:A:299:VAL:HG11	2.44	0.47
2:B:89:ILE:CD1	2:B:96:LEU:HD12	2.44	0.47
4:D:158:ILE:HG22	4:D:160:MET:N	2.14	0.47
4:D:235:LEU:O	4:D:236:ALA:HB2	2.15	0.47
5:E:52:LYS:C	5:E:52:LYS:CD	2.82	0.47
5:E:171:ILE:HG12	5:E:176:ALA:HB3	1.96	0.47
2:B:144:LEU:CB	2:B:183:ILE:HD12	2.43	0.47
2:B:170:ASN:HD22	2:B:170:ASN:N	2.12	0.47
2:B:250:ASP:O	2:B:251:SER:HB3	2.15	0.47
4:D:147:LEU:HD22	4:D:147:LEU:N	2.29	0.47
7:G:63:THR:O	7:G:64:GLN:C	2.52	0.47
8:H:50:THR:HG22	8:H:52:GLU:N	2.29	0.47
1:A:382:GLU:O	1:A:386:TYR:N	2.43	0.47
2:B:288:GLY:O	2:B:290:ASN:CB	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:148:THR:HB	3:C:166:TRP:CZ3	2.49	0.47
3:C:167:GLY:H	3:C:175:THR:CA	2.27	0.47
7:G:25:PRO:HG2	7:G:26:PHE:CD1	2.49	0.47
1:A:145:MET:HA	1:A:148:VAL:HG13	1.96	0.47
1:A:152:TYR:O	1:A:155:ALA:HB3	2.13	0.47
1:A:253:VAL:HG11	1:A:335:MET:CE	2.45	0.47
3:C:32:TRP:CZ3	3:C:209:PRO:HD3	2.49	0.47
3:C:198:LEU:HD21	11:C:382:HEM:CMA	2.44	0.47
3:C:262:PRO:C	3:C:263:LEU:HD12	2.35	0.47
6:F:67:ASP:OD1	6:F:71:ARG:CZ	2.62	0.47
1:A:306:SER:HB2	9:I:206:UNK:CB	2.45	0.47
1:A:344:ARG:CA	1:A:347:THR:HG22	2.45	0.47
2:B:96:LEU:C	2:B:96:LEU:CD2	2.83	0.47
2:B:192:HIS:O	2:B:196:GLN:HG3	2.14	0.47
2:B:209:LEU:O	2:B:211:VAL:N	2.48	0.47
2:B:225:ASN:O	2:B:226:ILE:HG13	2.14	0.47
2:B:250:ASP:O	2:B:252:LEU:CD2	2.59	0.47
2:B:353:SER:C	2:B:355:GLU:N	2.68	0.47
3:C:92:PHE:CZ	3:C:124:LEU:CD1	2.97	0.47
3:C:162:VAL:O	3:C:164:TRP:N	2.42	0.47
3:C:356:SER:O	3:C:357:LEU:HB2	2.14	0.47
5:E:153:PHE:CD2	5:E:172:ARG:HG3	2.49	0.47
7:G:60:THR:O	7:G:61:TRP:C	2.52	0.47
10:J:57:HIS:CB	10:J:61:ASN:C	2.72	0.47
1:A:265:PRO:O	1:A:268:VAL:HG23	2.14	0.47
2:B:209:LEU:O	2:B:211:VAL:HG22	2.15	0.47
3:C:78:TRP:CD2	3:C:79:LEU:N	2.83	0.47
4:D:160:MET:HB2	11:D:243:HEM:C1D	2.50	0.47
5:E:164:HIS:CD2	5:E:173:LYS:HD3	2.50	0.47
7:G:29:TYR:O	7:G:30:PHE:CB	2.59	0.47
2:B:112:LEU:O	2:B:113:ARG:C	2.54	0.47
13:C:384:PEE:H12	6:F:69:ASN:OD1	2.15	0.47
4:D:14:HIS:HB3	4:D:21:LEU:HA	1.96	0.47
5:E:42:VAL:O	5:E:45:LEU:HB3	2.15	0.47
1:A:431:LEU:HD23	1:A:432:PRO:N	2.30	0.47
1:A:436:ARG:HH11	3:C:223:PRO:HD2	1.80	0.47
2:B:277:HIS:CE1	2:B:364:LEU:CD2	2.97	0.47
3:C:27:ASN:CB	6:F:69:ASN:HD22	2.20	0.47
3:C:295:LEU:HD11	14:C:385:SIG:H273	1.97	0.47
4:D:75:ASN:ND2	4:D:79:GLU:H	2.13	0.47
1:A:117:VAL:HG23	1:A:118:GLN:HG3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:ARG:HD3	5:E:21:SER:N	2.28	0.46
4:D:192:TRP:CD1	4:D:192:TRP:C	2.86	0.46
7:G:71:ARG:NH2	8:H:60:ASP:OD2	2.49	0.46
1:A:100:LYS:HZ2	1:A:100:LYS:HB2	1.80	0.46
1:A:420:PRO:HD3	1:A:441:MET:HG3	1.96	0.46
2:B:24:LEU:HD11	2:B:392:TYR:CG	2.49	0.46
2:B:199:PHE:C	2:B:204:MET:HE3	2.35	0.46
3:C:40:VAL:HG11	3:C:233:LEU:HD21	1.96	0.46
3:C:327:TRP:CE2	7:G:48:VAL:HG22	2.51	0.46
3:C:353:GLN:HA	3:C:356:SER:HB3	1.97	0.46
5:E:18:ASP:HB3	5:E:28:SER:OG	2.15	0.46
5:E:78:LEU:HB3	5:E:132:TRP:CZ2	2.50	0.46
2:B:82:SER:O	2:B:85:ILE:HG22	2.15	0.46
2:B:166:ALA:O	2:B:242:GLY:HA3	2.15	0.46
2:B:264:ILE:C	2:B:266:GLY:H	2.18	0.46
3:C:354:MET:HA	3:C:354:MET:HE3	1.94	0.46
4:D:138:PRO:HD3	8:H:58:LEU:CD2	2.46	0.46
10:J:32:GLU:O	10:J:33:ARG:C	2.53	0.46
1:A:250:LEU:CD2	1:A:251:ALA:N	2.77	0.46
2:B:307:PHE:CG	2:B:308:ASP:N	2.80	0.46
2:B:307:PHE:CD2	2:B:308:ASP:N	2.83	0.46
3:C:167:GLY:N	3:C:175:THR:HG22	2.31	0.46
4:D:165:TYR:CZ	4:D:168:VAL:HG22	2.50	0.46
5:E:57:GLN:O	5:E:59:VAL:N	2.47	0.46
7:G:78:VAL:HG12	7:G:78:VAL:O	2.15	0.46
10:J:49:GLY:N	10:J:54:HIS:ND1	2.61	0.46
2:B:248:ASN:HD21	2:B:428:GLY:CA	2.26	0.46
2:B:275:LEU:O	2:B:275:LEU:HD12	2.15	0.46
3:C:211:GLY:CA	3:C:315:THR:HG23	2.46	0.46
10:J:52:TRP:O	10:J:56:LYS:N	2.45	0.46
1:A:64:PHE:O	1:A:75:LEU:HD23	2.15	0.46
1:A:161:THR:HG21	1:A:235:ARG:N	2.29	0.46
3:C:30:ALA:C	3:C:32:TRP:H	2.19	0.46
3:C:95:ILE:CG2	3:C:96:PHE:N	2.78	0.46
3:C:103:LEU:C	3:C:103:LEU:HD13	2.35	0.46
3:C:168:GLY:O	3:C:169:PHE:HD1	1.98	0.46
3:C:369:THR:O	3:C:370:ILE:C	2.54	0.46
5:E:188:THR:CG2	5:E:194:ILE:HD12	2.45	0.46
1:A:436:ARG:HD3	3:C:223:PRO:HG3	1.98	0.46
3:C:102:GLY:HA2	3:C:107:SER:HB2	1.97	0.46
3:C:113:THR:O	3:C:197:HIS:CE1	2.69	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:26:PHE:N	7:G:26:PHE:CD1	2.68	0.46
1:A:39:VAL:HG22	1:A:41:ILE:HD13	1.98	0.46
1:A:120:CYS:HB3	1:A:122:LEU:HD21	1.97	0.46
2:B:170:ASN:O	2:B:171:ALA:O	2.33	0.46
3:C:147:ILE:O	3:C:150:LEU:CB	2.63	0.46
3:C:210:LEU:HB3	3:C:212:ILE:HG12	1.97	0.46
4:D:160:MET:HB2	11:D:243:HEM:C2D	2.51	0.46
5:E:32:ARG:HH22	7:G:25:PRO:HD2	1.81	0.46
5:E:36:SER:OG	7:G:21:PHE:HE1	1.99	0.46
1:A:106:VAL:HG13	1:A:208:LEU:HD13	1.98	0.46
1:A:399:LEU:HA	1:A:402:VAL:HG23	1.97	0.46
2:B:92:VAL:HG12	2:B:92:VAL:O	2.14	0.46
2:B:342:ASN:O	2:B:345:LYS:HB3	2.16	0.46
3:C:207:ASN:HB3	11:C:382:HEM:O1D	2.16	0.46
3:C:234:THR:HB	4:D:216:VAL:HG12	1.97	0.46
4:D:233:ARG:HB3	6:F:71:ARG:NH2	2.30	0.46
10:J:13:LEU:HG	10:J:23:THR:HG21	1.98	0.46
1:A:197:LEU:HD23	1:A:216:PHE:HE2	1.80	0.46
2:B:47:ILE:HG22	2:B:48:GLY:N	2.31	0.46
4:D:113:LEU:N	4:D:113:LEU:HD12	2.30	0.46
5:E:25:SER:O	5:E:26:ARG:O	2.34	0.46
5:E:38:LEU:O	5:E:42:VAL:HG23	2.16	0.46
2:B:38:LEU:O	2:B:38:LEU:HG	2.15	0.45
2:B:162:ASN:O	2:B:163:LEU:C	2.54	0.45
2:B:436:VAL:C	2:B:438:GLU:H	2.19	0.45
3:C:46:ILE:O	3:C:50:LEU:HB2	2.16	0.45
3:C:146:VAL:CG2	3:C:147:ILE:N	2.78	0.45
3:C:212:ILE:CD1	6:F:62:ILE:HG23	2.43	0.45
3:C:287:ASN:OD1	3:C:289:LEU:N	2.49	0.45
4:D:234:LYS:HE2	5:E:10:PHE:CE1	2.50	0.45
6:F:89:TYR:CD1	6:F:89:TYR:C	2.90	0.45
2:B:405:VAL:CG1	2:B:406:ALA:N	2.79	0.45
2:B:424:MET:HG2	2:B:425:ALA:N	2.31	0.45
4:D:149:PHE:CE2	4:D:151:PRO:HD3	2.51	0.45
5:E:45:LEU:HD21	10:J:28:ALA:N	2.30	0.45
6:F:29:TYR:HB2	6:F:31:LEU:HD21	1.98	0.45
6:F:70:MET:SD	6:F:70:MET:C	2.95	0.45
1:A:129:LYS:O	1:A:133:VAL:HG23	2.15	0.45
1:A:430:GLN:O	1:A:430:GLN:HG2	2.16	0.45
2:B:71:LEU:HD12	2:B:144:LEU:HD23	1.98	0.45
3:C:154:ILE:O	3:C:158:GLY:HA3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:324:THR:O	3:C:325:LEU:C	2.55	0.45
4:D:43:MET:HE1	4:D:189:PHE:CZ	2.52	0.45
5:E:78:LEU:HD22	5:E:132:TRP:CE2	2.52	0.45
5:E:118:ARG:NH1	5:E:174:GLY:O	2.38	0.45
1:A:4:TYR:HB2	2:B:113:ARG:HB3	1.97	0.45
1:A:266:ASP:C	1:A:268:VAL:H	2.18	0.45
1:A:332:ASP:O	1:A:333:ASP:C	2.53	0.45
1:A:394:GLU:O	1:A:395:TRP:C	2.54	0.45
2:B:152:PHE:HA	2:B:157:THR:CG2	2.47	0.45
2:B:372:VAL:O	2:B:378:PHE:HB2	2.16	0.45
3:C:72:ARG:NE	4:D:115:TYR:OH	2.50	0.45
3:C:130:VAL:CG1	3:C:183:HIS:HB2	2.47	0.45
3:C:285:ILE:HG13	3:C:285:ILE:O	2.17	0.45
3:C:369:THR:O	3:C:371:GLY:N	2.49	0.45
4:D:12:TRP:CZ2	4:D:124:GLU:HB2	2.51	0.45
4:D:213:GLY:O	4:D:217:PRO:CD	2.64	0.45
4:D:235:LEU:HD12	6:F:64:ARG:HA	1.98	0.45
5:E:29:ASP:N	5:E:30:PRO:HD2	2.31	0.45
5:E:76:ILE:O	5:E:193:VAL:HG12	2.17	0.45
5:E:128:LYS:HB2	5:E:187:PHE:CE2	2.52	0.45
1:A:33:PRO:CG	1:A:34:THR:H	2.20	0.45
1:A:349:ILE:HD12	1:A:407:VAL:HG11	1.99	0.45
2:B:277:HIS:HB2	2:B:360:ALA:HB1	1.99	0.45
2:B:437:ASP:OD1	2:B:438:GLU:HG3	2.16	0.45
3:C:277:PHE:CD2	3:C:278:ALA:N	2.85	0.45
3:C:350:ILE:HA	3:C:353:GLN:HE21	1.81	0.45
4:D:33:TYR:CD1	4:D:37:CYS:HB2	2.51	0.45
4:D:113:LEU:N	4:D:113:LEU:CD1	2.80	0.45
6:F:29:TYR:HB2	6:F:31:LEU:CD2	2.46	0.45
7:G:71:ARG:CZ	8:H:56:GLU:OE2	2.65	0.45
1:A:105:ASP:O	1:A:106:VAL:C	2.55	0.45
1:A:436:ARG:HD3	3:C:223:PRO:CG	2.47	0.45
2:B:135:TRP:CD1	2:B:135:TRP:N	2.84	0.45
3:C:12:LEU:HD23	3:C:12:LEU:C	2.37	0.45
3:C:101:ARG:HE	3:C:102:GLY:HA2	1.81	0.45
3:C:354:MET:O	3:C:357:LEU:HB3	2.16	0.45
4:D:232:SER:O	4:D:233:ARG:O	2.34	0.45
6:F:96:GLU:OE1	6:F:96:GLU:HA	2.16	0.45
1:A:210:GLU:O	1:A:214:LYS:HB2	2.17	0.45
1:A:346:CYS:HB2	1:A:412:SER:HB3	1.99	0.45
3:C:166:TRP:O	3:C:167:GLY:O	2.34	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:15:ASP:C	8:H:17:LEU:N	2.68	0.45
2:B:56:ARG:NH1	2:B:172:LEU:HD13	2.32	0.45
2:B:137:VAL:CG2	2:B:138:ALA:H	2.30	0.45
2:B:181:TYR:CE1	2:B:182:ARG:CG	2.99	0.45
1:A:292:SER:O	1:A:295:ALA:HB3	2.17	0.45
4:D:34:LYS:O	4:D:34:LYS:HG2	2.15	0.45
4:D:57:THR:HG22	4:D:58:GLU:N	2.32	0.45
4:D:195:GLU:HG3	4:D:198:HIS:HB2	1.98	0.45
5:E:134:ILE:HD12	5:E:185:TYR:CD1	2.52	0.45
1:A:127:ILE:HG22	1:A:128:GLU:N	2.32	0.45
1:A:444:LEU:C	1:A:445:ARG:O	2.53	0.45
2:B:24:LEU:HD11	2:B:392:TYR:CD2	2.51	0.45
2:B:200:THR:HG22	2:B:226:ILE:HG21	1.99	0.45
2:B:225:ASN:O	2:B:226:ILE:CG1	2.65	0.45
3:C:82:ASN:N	3:C:82:ASN:HD22	2.15	0.45
3:C:101:ARG:HD2	3:C:101:ARG:O	2.16	0.45
3:C:323:GLN:O	3:C:326:PHE:HB3	2.17	0.45
4:D:37:CYS:O	4:D:39:SER:N	2.50	0.45
4:D:124:GLU:O	4:D:125:ASP:C	2.55	0.45
5:E:16:PRO:CD	7:G:22:GLU:O	2.65	0.45
6:F:71:ARG:O	6:F:72:GLN:HB2	2.17	0.45
1:A:178:SER:O	1:A:182:LEU:HD23	2.17	0.44
2:B:38:LEU:C	2:B:38:LEU:HD12	2.37	0.44
4:D:72:ASP:O	4:D:73:GLY:O	2.34	0.44
4:D:168:VAL:HG12	4:D:168:VAL:O	2.17	0.44
6:F:12:TRP:CE3	6:F:12:TRP:CA	3.00	0.44
1:A:23:VAL:HG23	1:A:192:ALA:HB1	1.99	0.44
1:A:381:ARG:O	1:A:382:GLU:C	2.56	0.44
2:B:217:LYS:C	2:B:219:VAL:N	2.70	0.44
3:C:238:THR:N	3:C:239:PRO:CD	2.80	0.44
3:C:349:ILE:CG2	3:C:350:ILE:HD13	2.44	0.44
3:C:359:TYR:HD2	3:C:360:PHE:CE1	2.34	0.44
4:D:102:ARG:NH1	4:D:109:LEU:CB	2.77	0.44
5:E:15:ARG:HA	5:E:16:PRO:HD3	1.79	0.44
6:F:102:LYS:HB3	6:F:102:LYS:HE2	1.72	0.44
10:J:57:HIS:CE1	10:J:62:LYS:OXT	2.70	0.44
1:A:65:LYS:HZ1	9:I:311:UNK:HA	1.77	0.44
1:A:100:LYS:HG3	2:B:370:MET:CE	2.48	0.44
1:A:382:GLU:CG	1:A:389:ARG:HA	2.39	0.44
2:B:225:ASN:C	2:B:226:ILE:HG13	2.38	0.44
3:C:295:LEU:CG	14:C:385:SIG:H273	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:C:383:U10:H8	12:C:383:U10:C1M	2.47	0.44
4:D:33:TYR:HA	4:D:37:CYS:SG	2.58	0.44
1:A:178:SER:O	1:A:179:ARG:C	2.55	0.44
3:C:95:ILE:HD13	3:C:121:LEU:HD12	2.00	0.44
3:C:282:LEU:C	3:C:282:LEU:CD1	2.86	0.44
3:C:349:ILE:HG22	3:C:350:ILE:N	2.32	0.44
5:E:121:GLN:HA	5:E:125:GLU:OE2	2.17	0.44
10:J:48:GLU:HA	10:J:54:HIS:CE1	2.53	0.44
1:A:294:LEU:O	1:A:298:ALA:HB2	2.18	0.44
2:B:157:THR:HG23	2:B:158:HIS:N	2.32	0.44
2:B:241:GLY:HA3	2:B:421:GLN:NE2	2.32	0.44
3:C:109:LEU:C	3:C:111:LYS:H	2.21	0.44
3:C:139:MET:HE2	3:C:255:GLU:HB3	2.00	0.44
3:C:154:ILE:HG22	3:C:157:ILE:HG22	2.00	0.44
3:C:247:SER:O	3:C:250:LEU:HB2	2.17	0.44
3:C:267:PRO:O	3:C:268:HIS:HB2	2.17	0.44
7:G:73:ASN:O	7:G:74:PRO:C	2.56	0.44
10:J:13:LEU:HA	10:J:19:THR:HG22	1.98	0.44
1:A:140:GLU:O	1:A:142:ASP:N	2.51	0.44
1:A:290:SER:HB3	2:B:90:GLU:OE1	2.18	0.44
4:D:37:CYS:C	4:D:39:SER:H	2.21	0.44
5:E:109:GLU:HG3	5:E:167:ALA:HB3	1.99	0.44
5:E:165:TYR:CE2	5:E:180:LEU:HG	2.53	0.44
7:G:57:LEU:H	7:G:57:LEU:CD2	2.31	0.44
1:A:111:GLU:HB2	1:A:215:HIS:CD2	2.52	0.44
1:A:153:LEU:HD21	1:A:319:LEU:HD13	1.98	0.44
2:B:102:ARG:NE	2:B:164:HIS:CD2	2.86	0.44
2:B:112:LEU:HD23	2:B:112:LEU:N	2.33	0.44
3:C:22:LEU:HD12	3:C:23:PRO:HD2	1.99	0.44
3:C:30:ALA:O	3:C:32:TRP:N	2.51	0.44
4:D:95:TYR:CG	4:D:101:ALA:HB2	2.52	0.44
6:F:59:MET:HA	6:F:59:MET:HE2	1.97	0.44
6:F:71:ARG:O	6:F:72:GLN:CB	2.65	0.44
8:H:72:LYS:HA	8:H:75:ASN:HD21	1.81	0.44
10:J:38:GLY:O	10:J:42:ILE:HG13	2.18	0.44
10:J:52:TRP:O	10:J:56:LYS:HB2	2.18	0.44
2:B:199:PHE:CA	2:B:204:MET:HE2	2.46	0.44
2:B:213:HIS:HD2	2:B:213:HIS:O	2.01	0.44
2:B:258:VAL:CG1	2:B:322:PHE:N	2.75	0.44
3:C:100:GLY:O	3:C:101:ARG:C	2.56	0.44
3:C:132:TYR:HA	11:C:381:HEM:HAA2	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:271:PRO:HG2	3:C:276:LEU:HD23	2.00	0.44
2:B:111:CYS:C	2:B:112:LEU:HD23	2.37	0.44
2:B:253:VAL:HG12	2:B:254:HIS:N	2.33	0.44
3:C:87:GLY:O	3:C:88:ALA:C	2.56	0.44
3:C:133:VAL:HG13	3:C:140:SER:O	2.18	0.44
3:C:148:THR:HG22	3:C:162:VAL:HG13	2.00	0.44
4:D:221:TYR:CD2	5:E:39:VAL:HG21	2.52	0.44
7:G:24:ARG:HA	7:G:25:PRO:HD2	1.57	0.44
8:H:50:THR:CG2	8:H:52:GLU:H	2.31	0.44
2:B:120:MET:HE2	2:B:219:VAL:HG11	2.00	0.43
2:B:207:VAL:HG12	2:B:208:GLY:N	2.33	0.43
3:C:45:GLN:HB3	11:C:381:HEM:HAB	2.00	0.43
3:C:130:VAL:HA	3:C:133:VAL:CG2	2.47	0.43
3:C:142:TRP:CE2	3:C:265:THR:HG22	2.52	0.43
3:C:342:GLN:HE21	3:C:343:PRO:CD	2.13	0.43
4:D:29:GLY:O	4:D:32:VAL:HG12	2.18	0.43
4:D:148:TYR:CD1	4:D:148:TYR:N	2.86	0.43
5:E:188:THR:HG21	5:E:194:ILE:HD12	2.00	0.43
1:A:158:PHE:CZ	1:A:319:LEU:HD21	2.53	0.43
1:A:252:HIS:HB3	1:A:323:TYR:CE1	2.44	0.43
2:B:89:ILE:CD1	2:B:96:LEU:HB2	2.45	0.43
2:B:219:VAL:C	2:B:221:GLU:N	2.71	0.43
2:B:280:GLY:O	2:B:281:ALA:C	2.56	0.43
2:B:325:TYR:OH	9:I:119:UNK:HA	2.18	0.43
3:C:38:LEU:HD21	3:C:95:ILE:N	2.34	0.43
3:C:361:THR:C	3:C:363:LEU:N	2.71	0.43
4:D:129:SER:HB3	4:D:152:TYR:CD2	2.52	0.43
8:H:17:LEU:HD21	8:H:21:ARG:NH2	2.33	0.43
8:H:47:ARG:HD2	8:H:49:GLN:H	1.83	0.43
1:A:228:VAL:HA	1:A:229:PRO:HD2	1.82	0.43
3:C:214:SER:HA	6:F:66:LEU:HD11	2.01	0.43
3:C:354:MET:HA	3:C:354:MET:HE2	1.96	0.43
4:D:197:GLU:O	4:D:199:ASP:N	2.51	0.43
5:E:76:ILE:HD13	5:E:98:VAL:HG21	2.00	0.43
6:F:73:GLN:OE1	7:G:36:ASN:ND2	2.51	0.43
1:A:4:TYR:O	1:A:5:ALA:C	2.56	0.43
1:A:17:SER:OG	1:A:209:LEU:CD2	2.67	0.43
1:A:45:SER:CA	1:A:48:GLU:HG3	2.46	0.43
2:B:279:LEU:HD11	2:B:344:VAL:HG13	2.00	0.43
2:B:436:VAL:C	2:B:438:GLU:N	2.72	0.43
3:C:132:TYR:O	3:C:135:PRO:HD2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:328:LEU:HD12	3:C:328:LEU:HA	1.83	0.43
4:D:28:ARG:CD	4:D:171:PHE:CD2	3.01	0.43
10:J:57:HIS:C	10:J:59:TYR:N	2.72	0.43
1:A:126:GLN:O	1:A:130:GLU:HG2	2.19	0.43
1:A:131:ARG:HG3	1:A:131:ARG:HH11	1.83	0.43
1:A:281:ASP:O	1:A:284:TYR:CD1	2.71	0.43
12:C:383:U10:H161	12:C:383:U10:H121	1.89	0.43
5:E:148:ALA:HB2	5:E:156:TYR:HE1	1.82	0.43
10:J:13:LEU:CD1	10:J:13:LEU:H	2.31	0.43
1:A:53:ASN:HD22	1:A:54:GLY:N	2.15	0.43
1:A:156:THR:CA	5:E:7:VAL:HG21	2.47	0.43
1:A:365:LEU:HD21	1:A:395:TRP:CG	2.53	0.43
1:A:438:ARG:C	1:A:438:ARG:CD	2.87	0.43
2:B:111:CYS:SG	2:B:119:LEU:CD2	3.07	0.43
3:C:235:LEU:C	3:C:237:LEU:H	2.22	0.43
5:E:171:ILE:HD11	5:E:173:LYS:O	2.18	0.43
1:A:35:CYS:HB2	1:A:200:ALA:O	2.17	0.43
1:A:294:LEU:HG	1:A:307:PHE:CE2	2.54	0.43
2:B:22:GLN:O	2:B:23:ASP:C	2.57	0.43
6:F:73:GLN:HA	7:G:39:ARG:HH12	1.83	0.43
2:B:111:CYS:C	2:B:112:LEU:CD2	2.87	0.43
3:C:134:LEU:HD21	3:C:180:PHE:HD1	1.83	0.43
3:C:261:ASN:ND2	3:C:264:VAL:CB	2.82	0.43
5:E:145:VAL:HA	5:E:146:PRO:HD3	1.89	0.43
1:A:310:PHE:CE1	1:A:322:PHE:N	2.87	0.43
1:A:344:ARG:HG3	1:A:344:ARG:HH11	1.83	0.43
2:B:45:SER:OG	2:B:116:VAL:HG21	2.18	0.43
2:B:130:PRO:CB	2:B:132:PHE:CE1	3.02	0.43
2:B:137:VAL:C	2:B:139:ASP:H	2.22	0.43
2:B:170:ASN:O	2:B:173:ALA:HB3	2.19	0.43
2:B:253:VAL:CG1	2:B:254:HIS:N	2.81	0.43
2:B:371:SER:O	2:B:372:VAL:HG23	2.19	0.43
3:C:295:LEU:O	3:C:296:ALA:C	2.56	0.43
4:D:138:PRO:HD3	8:H:58:LEU:HD22	2.01	0.43
5:E:83:GLU:HG3	5:E:100:HIS:CE1	2.53	0.43
2:B:82:SER:C	2:B:85:ILE:HG22	2.39	0.43
2:B:259:ALA:O	2:B:260:GLU:C	2.58	0.43
3:C:5:ILE:HA	3:C:8:SER:OG	2.19	0.43
3:C:9:HIS:HA	3:C:10:PRO:HD2	1.83	0.43
3:C:58:ALA:O	3:C:59:ASP:HB2	2.19	0.43
3:C:108:TYR:HB2	3:C:306:PRO:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:171:VAL:HA	3:C:175:THR:HG21	2.01	0.43
3:C:210:LEU:HD23	3:C:210:LEU:HA	1.76	0.43
4:D:235:LEU:HD22	6:F:63:LYS:HE2	2.00	0.43
5:E:26:ARG:O	5:E:27:GLU:CG	2.67	0.43
7:G:71:ARG:NH2	8:H:56:GLU:OE2	2.52	0.43
8:H:35:GLU:O	8:H:39:LEU:CD1	2.67	0.43
10:J:36:ASP:O	10:J:37:GLN:C	2.56	0.43
1:A:19:LEU:HB2	1:A:21:ASN:HB3	2.00	0.42
1:A:163:LEU:HD23	1:A:163:LEU:HA	1.81	0.42
3:C:250:LEU:HB3	3:C:251:LEU:HD12	2.01	0.42
1:A:108:LYS:O	1:A:112:LEU:HG	2.19	0.42
2:B:189:VAL:O	2:B:191:LEU:N	2.52	0.42
3:C:88:ALA:O	3:C:91:PHE:HB3	2.19	0.42
3:C:366:LEU:HD22	3:C:366:LEU:N	2.33	0.42
4:D:47:ALA:HB2	4:D:90:TYR:HA	2.02	0.42
4:D:105:ASN:O	4:D:107:GLY:N	2.52	0.42
4:D:153:PHE:HB2	4:D:158:ILE:HD11	2.01	0.42
5:E:153:PHE:CD2	5:E:172:ARG:NH1	2.87	0.42
7:G:71:ARG:HH21	8:H:56:GLU:CG	2.32	0.42
1:A:120:CYS:CB	1:A:122:LEU:HD21	2.50	0.42
2:B:71:LEU:C	2:B:73:SER:H	2.22	0.42
2:B:170:ASN:O	2:B:171:ALA:C	2.57	0.42
3:C:24:ALA:O	3:C:218:LYS:HA	2.20	0.42
3:C:43:MET:CE	3:C:43:MET:CA	2.96	0.42
3:C:129:PHE:CE1	3:C:147:ILE:HD12	2.54	0.42
5:E:91:TRP:O	5:E:94:LYS:O	2.37	0.42
7:G:40:ARG:O	7:G:41:LEU:C	2.56	0.42
1:A:274:ASN:O	1:A:309:THR:HG21	2.20	0.42
2:B:22:GLN:O	2:B:23:ASP:O	2.37	0.42
2:B:120:MET:O	2:B:123:LEU:N	2.52	0.42
2:B:258:VAL:HA	2:B:322:PHE:O	2.20	0.42
3:C:158:GLY:O	3:C:160:THR:N	2.52	0.42
4:D:217:PRO:O	4:D:220:TYR:HB3	2.19	0.42
5:E:166:ASP:OD2	5:E:170:ARG:HB2	2.18	0.42
6:F:45:GLU:OE1	6:F:45:GLU:HA	2.19	0.42
8:H:66:ASP:HA	8:H:69:VAL:HG23	2.00	0.42
10:J:46:ILE:O	10:J:46:ILE:HG22	2.20	0.42
1:A:5:ALA:O	1:A:8:LEU:HB2	2.20	0.42
2:B:105:MET:CE	2:B:107:TYR:HE1	2.32	0.42
2:B:226:ILE:HG22	2:B:227:ARG:N	2.34	0.42
2:B:277:HIS:HD2	2:B:363:LYS:CB	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:20:ILE:O	3:C:21:ASP:CB	2.63	0.42
3:C:101:ARG:NE	3:C:102:GLY:N	2.67	0.42
3:C:349:ILE:HG22	3:C:353:GLN:NE2	2.35	0.42
4:D:158:ILE:CG2	4:D:159:GLY:H	2.27	0.42
6:F:31:LEU:N	6:F:31:LEU:CD2	2.81	0.42
6:F:39:GLU:O	6:F:44:LYS:HE3	2.19	0.42
8:H:57:GLU:OE1	8:H:57:GLU:N	2.43	0.42
1:A:283:THR:HG21	9:I:114:UNK:CB	2.48	0.42
2:B:39:GLU:HG3	2:B:41:TYR:CD1	2.54	0.42
2:B:340:ALA:O	2:B:344:VAL:HG23	2.19	0.42
3:C:148:THR:C	3:C:150:LEU:N	2.72	0.42
3:C:158:GLY:C	3:C:160:THR:N	2.71	0.42
3:C:163:GLU:OE1	3:C:169:PHE:CE1	2.73	0.42
1:A:39:VAL:HG22	1:A:41:ILE:CD1	2.49	0.42
1:A:40:TRP:CZ3	1:A:377:GLU:CD	2.93	0.42
1:A:280:TYR:CG	1:A:281:ASP:N	2.88	0.42
1:A:429:GLU:OE1	7:G:7:LEU:HD23	2.20	0.42
3:C:27:ASN:HA	6:F:70:MET:HB2	2.01	0.42
3:C:129:PHE:CD1	3:C:147:ILE:HD12	2.54	0.42
4:D:16:GLY:HA2	4:D:17:PRO:HD2	1.83	0.42
4:D:197:GLU:O	4:D:198:HIS:C	2.58	0.42
4:D:218:LEU:CD2	5:E:39:VAL:HG13	2.48	0.42
4:D:228:SER:O	4:D:229:VAL:C	2.58	0.42
5:E:14:ARG:O	5:E:15:ARG:O	2.37	0.42
5:E:148:ALA:HB2	5:E:156:TYR:CE1	2.55	0.42
10:J:9:LEU:O	10:J:13:LEU:HB2	2.19	0.42
1:A:268:VAL:O	1:A:272:VAL:HG23	2.20	0.42
2:B:69:LEU:CD1	2:B:105:MET:HE1	2.38	0.42
2:B:371:SER:O	2:B:372:VAL:CG2	2.67	0.42
2:B:397:THR:HA	2:B:400:GLN:CB	2.49	0.42
2:B:435:PHE:HD1	2:B:438:GLU:OE2	2.03	0.42
3:C:111:LYS:HE3	3:C:307:PHE:CE1	2.55	0.42
3:C:111:LYS:HE3	3:C:307:PHE:HE1	1.85	0.42
3:C:187:PRO:HG2	11:C:381:HEM:CMC	2.50	0.42
3:C:233:LEU:C	3:C:233:LEU:HD13	2.40	0.42
4:D:98:PRO:HG2	4:D:99:GLU:H	1.85	0.42
4:D:134:TYR:CD1	4:D:162:PRO:HG3	2.55	0.42
5:E:113:GLU:CD	5:E:116:GLN:HG3	2.40	0.42
7:G:57:LEU:O	7:G:58:LEU:C	2.58	0.42
9:I:205:UNK:O	9:I:207:UNK:N	2.53	0.42
10:J:57:HIS:CB	10:J:61:ASN:O	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:64:PHE:C	1:A:66:GLY:H	2.23	0.42
1:A:240:GLN:HB2	1:A:422:VAL:CG1	2.50	0.42
1:A:240:GLN:OE1	1:A:434:TYR:HB2	2.20	0.42
1:A:362:ARG:CG	1:A:399:LEU:HD11	2.49	0.42
1:A:436:ARG:HD2	1:A:436:ARG:HA	1.84	0.42
3:C:106:GLY:HA2	3:C:108:TYR:CE2	2.55	0.42
4:D:234:LYS:O	7:G:15:THR:HA	2.19	0.42
6:F:96:GLU:OE1	6:F:99:ARG:NE	2.53	0.42
1:A:46:ARG:NH1	1:A:316:GLU:OE2	2.43	0.42
1:A:59:LEU:CD1	1:A:186:LEU:HD11	2.49	0.42
1:A:391:PRO:C	1:A:393:GLU:N	2.72	0.42
2:B:371:SER:C	2:B:372:VAL:HG23	2.40	0.42
2:B:395:PRO:CA	2:B:398:VAL:HG12	2.48	0.42
3:C:346:HIS:O	3:C:347:PRO:C	2.58	0.42
4:D:43:MET:HE3	4:D:46:VAL:HG21	2.02	0.42
4:D:68:VAL:HG21	4:D:92:PRO:HG2	2.02	0.42
4:D:95:TYR:HA	4:D:96:PRO:HD3	1.73	0.42
5:E:16:PRO:HA	5:E:17:PRO:HD2	1.90	0.42
5:E:134:ILE:HD12	5:E:185:TYR:CG	2.55	0.42
7:G:49:ALA:N	7:G:50:PRO:HD2	2.35	0.42
1:A:163:LEU:HG	1:A:234:CYS:SG	2.60	0.41
2:B:268:GLU:O	2:B:268:GLU:HG2	2.19	0.41
3:C:27:ASN:CA	6:F:70:MET:HB2	2.50	0.41
3:C:364:LEU:N	3:C:364:LEU:HD12	2.35	0.41
5:E:171:ILE:N	5:E:179:ASN:OD1	2.46	0.41
7:G:38:TRP:C	7:G:40:ARG:N	2.73	0.41
9:I:107:UNK:HA	9:I:115:UNK:O	2.20	0.41
1:A:64:PHE:O	1:A:66:GLY:N	2.52	0.41
1:A:279:HIS:HA	1:A:307:PHE:CE1	2.55	0.41
2:B:146:ILE:CG1	2:B:147:ASP:N	2.79	0.41
2:B:180:ASP:O	2:B:182:ARG:N	2.54	0.41
3:C:156:TYR:C	3:C:158:GLY:H	2.23	0.41
3:C:282:LEU:HD22	3:C:291:GLY:O	2.19	0.41
4:D:29:GLY:O	4:D:30:PHE:C	2.58	0.41
4:D:43:MET:HE2	4:D:46:VAL:CB	2.50	0.41
4:D:54:VAL:HG21	4:D:192:TRP:CE3	2.55	0.41
2:B:111:CYS:SG	2:B:112:LEU:N	2.92	0.41
2:B:144:LEU:O	2:B:145:LYS:C	2.59	0.41
2:B:264:ILE:HD11	2:B:317:SER:HA	2.01	0.41
3:C:95:ILE:HD13	3:C:121:LEU:HD13	2.01	0.41
3:C:125:MET:HB3	14:C:385:SIG:H281	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:131:GLY:O	3:C:134:LEU:N	2.46	0.41
3:C:162:VAL:O	3:C:165:ALA:N	2.53	0.41
3:C:167:GLY:HA3	3:C:174:PRO:CG	2.50	0.41
3:C:167:GLY:HA3	3:C:175:THR:HG22	2.01	0.41
4:D:175:THR:HA	4:D:176:PRO:HD3	1.82	0.41
5:E:13:TYR:C	5:E:14:ARG:HD3	2.38	0.41
5:E:171:ILE:O	5:E:171:ILE:HG23	2.18	0.41
5:E:175:PRO:O	5:E:176:ALA:C	2.58	0.41
8:H:44:VAL:C	8:H:46:SER:H	2.23	0.41
8:H:72:LYS:O	8:H:75:ASN:ND2	2.54	0.41
1:A:169:GLY:O	5:E:3:THR:HG21	2.20	0.41
1:A:408:ARG:O	1:A:409:GLU:C	2.58	0.41
2:B:33:LEU:HD23	2:B:220:ALA:HB1	2.02	0.41
2:B:221:GLU:HG3	2:B:222:GLN:N	2.36	0.41
2:B:353:SER:OG	2:B:355:GLU:HB3	2.20	0.41
3:C:51:LEU:HD12	3:C:51:LEU:HA	1.74	0.41
3:C:103:LEU:HD12	3:C:326:PHE:CE1	2.56	0.41
3:C:104:TYR:O	3:C:105:TYR:CG	2.73	0.41
3:C:106:GLY:C	3:C:108:TYR:N	2.73	0.41
3:C:224:TYR:HB3	4:D:227:TRP:CZ2	2.54	0.41
3:C:278:ALA:HB1	3:C:295:LEU:CD1	2.49	0.41
3:C:355:ALA:O	3:C:357:LEU:N	2.53	0.41
8:H:47:ARG:CD	8:H:48:SER:N	2.82	0.41
13:C:384:PEE:O5	7:G:48:VAL:HG21	2.19	0.41
4:D:150:ASN:O	4:D:156:GLN:HA	2.21	0.41
4:D:151:PRO:HB2	8:H:59:PHE:HE1	1.84	0.41
5:E:78:LEU:HD13	5:E:132:TRP:NE1	2.34	0.41
6:F:64:ARG:HH11	6:F:64:ARG:HB3	1.85	0.41
8:H:15:ASP:C	8:H:17:LEU:H	2.23	0.41
10:J:54:HIS:O	10:J:57:HIS:NE2	2.53	0.41
1:A:46:ARG:CD	1:A:231:LEU:HD13	2.50	0.41
1:A:65:LYS:N	1:A:65:LYS:CD	2.83	0.41
1:A:264:HIS:HA	1:A:265:PRO:HD3	1.66	0.41
2:B:62:ASN:O	2:B:63:LEU:C	2.58	0.41
2:B:150:VAL:HA	2:B:153:GLN:HG3	2.01	0.41
2:B:277:HIS:CE1	2:B:364:LEU:HD21	2.56	0.41
2:B:436:VAL:HG23	2:B:437:ASP:N	2.36	0.41
3:C:377:MET:HE2	6:F:20:TYR:HB2	2.02	0.41
4:D:230:LEU:HB3	6:F:70:MET:HE3	2.01	0.41
5:E:129:LYS:HA	5:E:130:PRO:HD3	1.87	0.41
10:J:23:THR:O	10:J:27:GLY:N	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:382:GLU:HG2	1:A:390:ILE:H	1.85	0.41
2:B:111:CYS:O	2:B:112:LEU:CB	2.68	0.41
2:B:248:ASN:ND2	2:B:249:GLY:N	2.61	0.41
2:B:330:ALA:O	2:B:333:ALA:CB	2.68	0.41
3:C:64:PHE:CE2	3:C:259:PRO:HG3	2.56	0.41
3:C:113:THR:CG2	3:C:201:LEU:HA	2.48	0.41
3:C:246:PHE:O	4:D:201:ARG:NH1	2.54	0.41
3:C:373:LEU:C	3:C:373:LEU:CD2	2.89	0.41
4:D:227:TRP:O	4:D:228:SER:C	2.58	0.41
5:E:25:SER:C	5:E:26:ARG:O	2.56	0.41
6:F:34:ASP:O	6:F:37:ILE:HG13	2.21	0.41
1:A:39:VAL:HG13	1:A:39:VAL:O	2.20	0.41
2:B:280:GLY:C	2:B:282:ASN:H	2.24	0.41
3:C:31:TRP:HZ3	13:C:384:PEE:H22	1.86	0.41
3:C:220:PRO:O	3:C:221:PHE:C	2.58	0.41
4:D:83:ARG:HB2	4:D:84:PRO:HD2	2.03	0.41
4:D:113:LEU:HA	4:D:116:ILE:HB	2.02	0.41
8:H:73:LEU:C	8:H:73:LEU:CD2	2.88	0.41
1:A:23:VAL:N	1:A:192:ALA:HB1	2.34	0.41
1:A:153:LEU:C	1:A:153:LEU:CD2	2.86	0.41
1:A:158:PHE:O	1:A:159:GLN:C	2.59	0.41
2:B:101:THR:CG2	2:B:102:ARG:N	2.81	0.41
2:B:198:HIS:CD2	2:B:203:ARG:NH2	2.88	0.41
2:B:277:HIS:CD2	2:B:363:LYS:HB2	2.56	0.41
2:B:409:ASP:OD1	2:B:409:ASP:N	2.54	0.41
2:B:436:VAL:O	2:B:438:GLU:N	2.54	0.41
3:C:26:SER:HA	3:C:219:ILE:HD11	2.02	0.41
3:C:34:PHE:CZ	3:C:97:LEU:HD13	2.56	0.41
3:C:167:GLY:HA3	3:C:174:PRO:HG2	2.02	0.41
3:C:319:ARG:HH22	3:C:371:GLY:CA	2.30	0.41
14:C:385:SIG:H23	14:C:385:SIG:H343	1.79	0.41
4:D:225:HIS:CE1	7:G:20:PRO:HB2	2.55	0.41
5:E:32:ARG:NH2	7:G:25:PRO:HD2	2.36	0.41
6:F:34:ASP:OD1	6:F:34:ASP:N	2.54	0.41
6:F:77:LYS:HA	6:F:80:TRP:CE2	2.56	0.41
1:A:64:PHE:CZ	1:A:86:LEU:HG	2.56	0.41
1:A:253:VAL:O	1:A:323:TYR:HA	2.21	0.41
1:A:366:VAL:C	1:A:368:HIS:N	2.74	0.41
2:B:200:THR:HG22	2:B:226:ILE:CG2	2.51	0.41
3:C:27:ASN:ND2	6:F:69:ASN:HD22	2.18	0.41
4:D:21:LEU:CD1	4:D:192:TRP:HB2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:86:LYS:N	4:D:89:ASP:OD1	2.49	0.41
5:E:46:GLY:O	5:E:49:TYR:HB3	2.21	0.41
5:E:91:TRP:CE2	5:E:92:ARG:HG3	2.56	0.41
5:E:163:SER:HA	5:E:174:GLY:HA3	2.03	0.41
7:G:55:PHE:O	7:G:56:TYR:C	2.60	0.41
1:A:56:GLY:CA	1:A:185:TYR:CE2	2.97	0.40
1:A:388:ARG:HD3	1:A:388:ARG:N	2.31	0.40
2:B:280:GLY:O	2:B:282:ASN:N	2.54	0.40
2:B:405:VAL:HG11	2:B:409:ASP:CG	2.41	0.40
3:C:9:HIS:O	3:C:11:LEU:N	2.54	0.40
3:C:50:LEU:HD12	11:C:381:HEM:HBC1	2.02	0.40
3:C:346:HIS:ND1	3:C:346:HIS:C	2.74	0.40
4:D:81:PHE:CD1	4:D:81:PHE:C	2.94	0.40
4:D:116:ILE:HG21	4:D:190:LEU:HD13	2.01	0.40
8:H:47:ARG:CD	8:H:48:SER:H	2.22	0.40
1:A:65:LYS:NZ	9:I:311:UNK:CA	2.77	0.40
1:A:192:ALA:N	1:A:193:PRO:HD2	2.35	0.40
1:A:245:GLU:C	1:A:247:GLY:H	2.24	0.40
1:A:365:LEU:HD21	1:A:395:TRP:HB3	2.03	0.40
2:B:34:VAL:HG11	2:B:386:ALA:O	2.21	0.40
2:B:77:THR:CB	2:B:125:ASN:HB3	2.51	0.40
3:C:13:LYS:HE2	3:C:17:ASN:ND2	2.36	0.40
3:C:172:ASP:N	3:C:175:THR:HG23	2.19	0.40
3:C:202:HIS:HE1	12:C:383:U10:H1M3	1.86	0.40
3:C:211:GLY:HA3	3:C:315:THR:HG23	2.03	0.40
3:C:285:ILE:CG2	3:C:291:GLY:HA2	2.51	0.40
3:C:295:LEU:HD12	3:C:295:LEU:HA	1.82	0.40
4:D:207:LYS:O	4:D:211:MET:HG2	2.21	0.40
5:E:15:ARG:HH11	5:E:19:ASP:HB3	1.86	0.40
5:E:81:ILE:HD13	5:E:98:VAL:CG1	2.51	0.40
8:H:15:ASP:HA	8:H:16:PRO:HD2	1.97	0.40
1:A:253:VAL:HG11	1:A:335:MET:HE2	2.02	0.40
1:A:356:ARG:O	1:A:357:GLY:C	2.59	0.40
1:A:405:ARG:HG2	1:A:405:ARG:HH11	1.85	0.40
2:B:19:PRO:O	2:B:21:PRO:HD3	2.21	0.40
2:B:37:SER:O	2:B:38:LEU:CB	2.69	0.40
2:B:47:ILE:HD11	2:B:116:VAL:HG12	2.03	0.40
2:B:206:LEU:O	2:B:216:LEU:HD21	2.21	0.40
2:B:268:GLU:HG2	2:B:272:PHE:HE1	1.86	0.40
3:C:38:LEU:HD23	3:C:38:LEU:HA	1.89	0.40
3:C:292:VAL:O	3:C:295:LEU:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:327:TRP:HB2	7:G:51:PRO:HG3	2.03	0.40
3:C:361:THR:O	3:C:362:ILE:C	2.57	0.40
6:F:87:VAL:HG23	6:F:87:VAL:O	2.21	0.40
8:H:66:ASP:HA	8:H:69:VAL:HB	2.04	0.40
1:A:40:TRP:CE3	1:A:96:ALA:HB2	2.57	0.40
1:A:110:VAL:HA	1:A:113:LEU:HD12	2.03	0.40
1:A:346:CYS:HB3	1:A:411:CYS:HB3	2.03	0.40
3:C:59:ASP:O	3:C:60:THR:C	2.60	0.40
3:C:114:TRP:HE3	11:C:382:HEM:HMD1	1.87	0.40
3:C:163:GLU:HB3	3:C:169:PHE:CE1	2.57	0.40
4:D:147:LEU:N	4:D:147:LEU:CD2	2.84	0.40
4:D:232:SER:HB3	7:G:23:GLN:HE22	1.85	0.40
7:G:18:LEU:O	7:G:19:SER:C	2.59	0.40
7:G:79:ASN:ND2	7:G:79:ASN:N	2.69	0.40
1:A:40:TRP:N	1:A:40:TRP:CD1	2.89	0.40
2:B:367:LYS:O	2:B:371:SER:HB2	2.21	0.40
3:C:91:PHE:CE1	3:C:124:LEU:HG	2.56	0.40
3:C:222:HIS:O	3:C:224:TYR:N	2.55	0.40
3:C:310:LYS:HB3	3:C:372:THR:HG23	2.04	0.40
4:D:78:GLY:O	4:D:79:GLU:CG	2.68	0.40
4:D:195:GLU:OE2	4:D:201:ARG:NH2	2.55	0.40
8:H:69:VAL:CG1	8:H:73:LEU:HD12	2.51	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	440/446 (99%)	337 (77%)	85 (19%)	18 (4%)	3 23
2	B	404/422 (96%)	295 (73%)	78 (19%)	31 (8%)	1 10
3	C	377/380 (99%)	278 (74%)	68 (18%)	31 (8%)	1 9

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
4	D	239/241 (99%)	194 (81%)	34 (14%)	11 (5%)	2 21
5	E	194/196 (99%)	151 (78%)	28 (14%)	15 (8%)	1 10
6	F	98/109 (90%)	84 (86%)	12 (12%)	2 (2%)	7 39
7	G	76/81 (94%)	52 (68%)	18 (24%)	6 (8%)	1 10
8	H	64/78 (82%)	56 (88%)	7 (11%)	1 (2%)	9 43
10	J	57/62 (92%)	32 (56%)	20 (35%)	5 (9%)	1 8
All	All	1949/2015 (97%)	1479 (76%)	350 (18%)	120 (6%)	1 15

All (120) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	282	ARG
1	A	284	TYR
2	B	19	PRO
2	B	20	HIS
2	B	23	ASP
2	B	38	LEU
2	B	113	ARG
2	B	132	PHE
2	B	170	ASN
2	B	171	ALA
2	B	228	GLY
2	B	233	SER
2	B	290	ASN
2	B	410	VAL
3	C	5	ILE
3	C	111	LYS
3	C	167	GLY
3	C	208	ASN
3	C	222	HIS
3	C	284	SER
3	C	349	ILE
3	C	357	LEU
4	D	73	GLY
4	D	75	ASN
4	D	198	HIS
4	D	233	ARG
5	E	11	SER
5	E	21	SER
5	E	58	PHE

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Mol	Chain	Res	Type
5	E	72	SER
7	G	27	PRO
7	G	43	ALA
10	J	5	LEU
10	J	56	LYS
10	J	61	ASN
1	A	65	LYS
1	A	128	GLU
1	A	289	HIS
1	A	291	SER
2	B	210	GLY
2	B	218	ASN
2	B	229	GLY
2	B	261	SER
2	B	372	VAL
2	B	386	ALA
2	B	430	LEU
3	C	58	ALA
3	C	164	TRP
3	C	170	SER
4	D	38	SER
4	D	78	GLY
4	D	106	ASN
4	D	236	ALA
5	E	15	ARG
5	E	17	PRO
5	E	26	ARG
5	E	66	ALA
7	G	33	GLY
1	A	55	ALA
1	A	56	GLY
1	A	72	GLN
1	A	103	SER
1	A	141	ASN
1	A	267	LEU
1	A	285	GLY
2	B	63	LEU
2	B	111	CYS
2	B	181	TYR
2	B	190	GLU
2	B	330	ALA
2	B	371	SER

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Mol	Chain	Res	Type
2	B	407	ASP
3	C	31	TRP
3	C	105	TYR
3	C	207	ASN
3	C	286	PRO
5	E	30	PRO
6	F	53	ASN
10	J	60	GLU
1	A	71	PRO
1	A	292	SER
2	B	83	PHE
2	B	260	GLU
2	B	406	ALA
3	C	4	ASN
3	C	63	ALA
3	C	156	TYR
3	C	159	HIS
3	C	224	TYR
3	C	379	ASN
4	D	240	PRO
5	E	27	GLU
5	E	61	SER
1	A	286	GLY
1	A	382	GLU
1	A	398	ARG
2	B	404	ALA
3	C	10	PRO
3	C	202	HIS
3	C	321	LEU
3	C	359	TYR
5	E	62	MET
5	E	70	ALA
7	G	74	PRO
8	H	65	ARG
10	J	15	ARG
3	C	274	TYR
4	D	176	PRO
5	E	71	MET
5	E	177	PRO
6	F	19	TRP
2	B	249	GLY
3	C	158	GLY

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Mol	Chain	Res	Type
3	C	205	GLY
3	C	352	GLY
7	G	26	PHE
3	C	157	ILE
3	C	259	PRO
4	D	133	GLY
7	G	50	PRO

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	359/376 (96%)	333 (93%)	26 (7%)	14	45
2	B	307/336 (91%)	286 (93%)	21 (7%)	16	48
3	C	326/329 (99%)	298 (91%)	28 (9%)	10	38
4	D	201/207 (97%)	193 (96%)	8 (4%)	31	64
5	E	165/169 (98%)	153 (93%)	12 (7%)	14	45
6	F	90/98 (92%)	80 (89%)	10 (11%)	6	28
7	G	60/72 (83%)	53 (88%)	7 (12%)	5	26
8	H	51/74 (69%)	51 (100%)	0	100	100
10	J	41/52 (79%)	40 (98%)	1 (2%)	49	76
All	All	1600/1713 (93%)	1487 (93%)	113 (7%)	14	46

All (113) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	53	ASN
1	A	58	PHE
1	A	69	ASN
1	A	100	LYS
1	A	102	LEU
1	A	148	VAL
1	A	168	GLU

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Mol	Chain	Res	Type
1	A	182	LEU
1	A	220	PRO
1	A	226	ASP
1	A	250	LEU
1	A	279	HIS
1	A	307	PHE
1	A	316	GLU
1	A	333	ASP
1	A	342	TRP
1	A	361	LEU
1	A	368	HIS
1	A	382	GLU
1	A	384	LEU
1	A	388	ARG
1	A	395	TRP
1	A	409	GLU
1	A	438	ARG
1	A	443	TRP
1	A	444	LEU
2	B	21	PRO
2	B	56	ARG
2	B	57	TYR
2	B	62	ASN
2	B	109	VAL
2	B	112	LEU
2	B	135	TRP
2	B	170	ASN
2	B	193	ASP
2	B	221	GLU
2	B	225	ASN
2	B	247	GLN
2	B	248	ASN
2	B	252	LEU
2	B	325	TYR
2	B	351	ASN
2	B	378	PHE
2	B	402	ILE
2	B	407	ASP
2	B	409	ASP
2	B	437	ASP
3	C	4	ASN
3	C	21	ASP

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Mol	Chain	Res	Type
3	C	32	TRP
3	C	43	MET
3	C	104	TYR
3	C	129	PHE
3	C	133	VAL
3	C	136	TRP
3	C	145	THR
3	C	149	ASN
3	C	152	SER
3	C	164	TRP
3	C	166	TRP
3	C	175	THR
3	C	184	PHE
3	C	207	ASN
3	C	208	ASN
3	C	216	SER
3	C	219	ILE
3	C	258	THR
3	C	259	PRO
3	C	272	GLU
3	C	285	ILE
3	C	307	PHE
3	C	325	LEU
3	C	333	LEU
3	C	342	GLN
3	C	350	ILE
4	D	75	ASN
4	D	82	MET
4	D	136	GLU
4	D	163	PRO
4	D	181	GLN
4	D	192	TRP
4	D	209	LEU
4	D	224	ARG
5	E	9	ASN
5	E	11	SER
5	E	27	GLU
5	E	32	ARG
5	E	36	SER
5	E	45	LEU
5	E	52	LYS
5	E	79	SER

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Mol	Chain	Res	Type
5	E	81	ILE
5	E	113	GLU
5	E	136	ILE
5	E	191	ASP
6	F	12	TRP
6	F	31	LEU
6	F	34	ASP
6	F	37	ILE
6	F	59	MET
6	F	64	ARG
6	F	70	MET
6	F	75	LEU
6	F	81	THR
6	F	107	TRP
7	G	4	PHE
7	G	16	TYR
7	G	22	GLU
7	G	26	PHE
7	G	27	PRO
7	G	41	LEU
7	G	77	TYR
10	J	59	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (47) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	GLN
1	A	53	ASN
1	A	69	ASN
1	A	85	HIS
1	A	118	GLN
1	A	141	ASN
1	A	151	ASN
1	A	165	GLN
1	A	274	ASN
1	A	301	ASN
1	A	339	GLN
2	B	22	GLN
2	B	62	ASN
2	B	225	ASN
2	B	248	ASN
2	B	277	HIS

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Mol	Chain	Res	Type
2	B	342	ASN
2	B	343	GLN
2	B	351	ASN
2	B	356	ASN
2	B	421	GLN
2	B	429	ASN
3	C	4	ASN
3	C	16	ASN
3	C	17	ASN
3	C	82	ASN
3	C	86	ASN
3	C	138	GLN
3	C	207	ASN
3	C	261	ASN
3	C	323	GLN
3	C	332	ASN
3	C	342	GLN
3	C	353	GLN
4	D	35	GLN
4	D	75	ASN
4	D	105	ASN
4	D	156	GLN
4	D	225	HIS
5	E	9	ASN
5	E	57	GLN
5	E	86	ASN
6	F	69	ASN
7	G	64	GLN
7	G	79	ASN
8	H	75	ASN
10	J	57	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

9 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	$\#\|Z\| > 2$
15	BOG	D	242	-	20,20,20	1.16	2 (10%)	25,25,25	0.84	1 (4%)
13	PEE	C	384	-	48,48,50	2.63	11 (22%)	51,53,55	4.28	17 (33%)
11	HEM	C	382	3	41,50,50	1.73	9 (21%)	45,82,82	2.61	19 (42%)
12	U10	C	383	-	29,29,63	3.10	5 (17%)	35,38,79	1.99	8 (22%)
11	HEM	C	381	3	41,50,50	1.52	6 (14%)	45,82,82	2.50	20 (44%)
16	FES	E	197	5	0,4,4	-	-	-		
14	SIG	C	385	-	32,36,36	3.35	11 (34%)	40,50,50	2.36	12 (30%)
11	HEM	D	243	4	41,50,50	1.59	6 (14%)	45,82,82	2.59	14 (31%)
13	PEE	E	198	-	48,48,50	2.53	9 (18%)	51,53,55	4.32	18 (35%)

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
15	BOG	D	242	-	-	5/11/31/31	0/1/1/1
13	PEE	C	384	-	1/1/4/8	23/52/52/54	-
11	HEM	C	382	3	-	9/12/54/54	-
12	U10	C	383	-	-	7/23/47/87	0/1/1/1
11	HEM	C	381	3	-	6/12/54/54	-
16	FES	E	197	5	-	-	0/1/1/1
14	SIG	C	385	-	-	15/29/30/30	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
11	HEM	D	243	4	-	8/12/54/54	-
13	PEE	E	198	-	1/1/4/8	29/52/52/54	-

All (59) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	C	385	SIG	C24-C23	-14.79	1.47	1.56
12	C	383	U10	C13-C14	12.23	1.62	1.33
13	E	198	PEE	O5-C30	11.72	1.57	1.22
13	C	384	PEE	O5-C30	11.24	1.55	1.22
12	C	383	U10	C6-C1	7.27	1.48	1.35
13	C	384	PEE	O2-C10	6.34	1.52	1.34
12	C	383	U10	C7-C6	5.43	1.60	1.51
13	C	384	PEE	C18-C19	5.26	1.62	1.31
13	C	384	PEE	C39-C38	4.96	1.60	1.31
13	E	198	PEE	O2-C10	4.96	1.48	1.34
14	C	385	SIG	C37-C36	4.95	1.37	1.33
13	E	198	PEE	C39-C38	4.83	1.59	1.31
11	C	382	HEM	C3C-C2C	-4.75	1.33	1.40
13	E	198	PEE	C18-C19	4.74	1.59	1.31
14	C	385	SIG	O7-C8	4.57	1.41	1.35
11	C	381	HEM	C3C-CAC	-4.39	1.38	1.47
11	D	243	HEM	CBB-CAB	4.29	1.51	1.30
11	C	382	HEM	C3C-CAC	-4.19	1.39	1.47
13	C	384	PEE	C11-C10	4.19	1.63	1.50
14	C	385	SIG	O7-C3	3.89	1.42	1.36
13	E	198	PEE	C11-C10	3.69	1.61	1.50
14	C	385	SIG	O13-C1	3.68	1.43	1.37
14	C	385	SIG	O14-C5	3.61	1.43	1.36
12	C	383	U10	C3-C2	-3.58	1.38	1.48
11	C	381	HEM	CAB-C3B	-3.56	1.37	1.47
11	C	382	HEM	CAB-C3B	-3.53	1.37	1.47
11	D	243	HEM	CBC-CAC	3.31	1.51	1.29
13	C	384	PEE	C31-C30	-3.27	1.41	1.50
14	C	385	SIG	C21-C22	3.13	1.62	1.54
14	C	385	SIG	C6-C1	3.12	1.44	1.38
11	D	243	HEM	C3C-C2C	-3.12	1.36	1.40
13	E	198	PEE	C31-C30	-3.11	1.41	1.50
11	C	382	HEM	CAA-C2A	3.08	1.56	1.52
13	E	198	PEE	C21-C22	-3.05	1.34	1.51
11	D	243	HEM	C3C-CAC	3.03	1.54	1.47
13	E	198	PEE	C42-C41	-2.97	1.34	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	C	384	PEE	C42-C41	-2.95	1.35	1.51
13	C	384	PEE	C21-C22	-2.89	1.35	1.51
14	C	385	SIG	C31-C30	2.88	1.52	1.44
11	D	243	HEM	C1B-NB	-2.81	1.35	1.40
11	C	381	HEM	CAA-C2A	-2.71	1.48	1.52
11	C	382	HEM	C3B-C4B	2.56	1.50	1.44
15	D	242	BOG	C4-C5	2.53	1.58	1.53
14	C	385	SIG	C9-C8	2.50	1.42	1.39
13	C	384	PEE	P-O3P	2.47	1.69	1.59
15	D	242	BOG	O5-C1	2.46	1.48	1.41
12	C	383	U10	C8-C9	2.39	1.38	1.33
11	C	382	HEM	C1B-NB	-2.38	1.36	1.40
13	C	384	PEE	C1-C2	2.37	1.58	1.50
11	C	381	HEM	C1A-CHA	-2.34	1.34	1.41
11	C	381	HEM	CHD-C1D	-2.29	1.34	1.41
11	C	382	HEM	C2C-C1C	2.25	1.47	1.42
11	D	243	HEM	CAA-C2A	-2.24	1.48	1.52
11	C	382	HEM	C1A-CHA	-2.17	1.35	1.41
13	E	198	PEE	O2-C2	-2.13	1.41	1.46
11	C	382	HEM	C1D-C2D	2.13	1.48	1.44
13	C	384	PEE	O2-C2	-2.11	1.41	1.46
14	C	385	SIG	C6-C5	2.10	1.44	1.37
11	C	381	HEM	CHC-C4B	-2.07	1.35	1.41

All (109) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	C	384	PEE	O4-C10-C11	-18.62	51.07	123.73
13	E	198	PEE	O4-C10-C11	-18.59	51.22	123.73
13	E	198	PEE	O3-C30-C31	12.63	151.56	111.91
13	C	384	PEE	O3-C30-C31	12.57	151.35	111.91
13	C	384	PEE	O3-C30-O5	-11.28	95.11	123.59
13	E	198	PEE	O3-C30-O5	-11.28	95.11	123.59
11	D	243	HEM	C4A-C3A-C2A	-8.74	100.92	107.00
13	E	198	PEE	O2-C2-C3	8.03	137.47	108.40
14	C	385	SIG	C20-C8-C9	7.86	131.53	120.39
13	C	384	PEE	O2-C2-C3	7.68	136.21	108.40
11	C	382	HEM	CBA-CAA-C2A	7.50	125.43	112.62
13	E	198	PEE	O2-C10-C11	7.12	126.85	111.50
13	C	384	PEE	O2-C10-C11	7.00	126.60	111.50
13	E	198	PEE	C12-C11-C10	-6.62	89.54	113.62
11	D	243	HEM	CBA-CAA-C2A	6.42	123.57	112.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	C	385	SIG	C21-C20-C8	6.22	126.95	113.59
13	E	198	PEE	O2-C10-O4	-6.09	108.98	123.70
13	C	384	PEE	O2-C10-O4	-6.08	109.01	123.70
13	C	384	PEE	C12-C11-C10	-6.03	91.70	113.62
11	C	381	HEM	CMB-C2B-C1B	5.69	133.71	125.04
11	C	381	HEM	CAD-C3D-C4D	5.61	134.46	124.66
11	D	243	HEM	CMD-C2D-C1D	5.29	133.10	125.04
11	C	381	HEM	CBA-CAA-C2A	-5.21	103.73	112.62
11	C	382	HEM	C2B-C1B-NB	5.14	115.92	109.84
12	C	383	U10	C12-C13-C14	-5.03	115.54	127.66
11	D	243	HEM	CAD-C3D-C4D	4.85	133.14	124.66
11	C	381	HEM	CAD-C3D-C2D	-4.84	118.87	127.88
11	C	381	HEM	CMD-C2D-C1D	4.81	132.37	125.04
13	C	384	PEE	O3-C3-C2	4.66	121.99	108.43
14	C	385	SIG	C39-C36-C32	-4.65	110.75	118.08
13	E	198	PEE	O3-C3-C2	4.51	121.55	108.43
11	C	382	HEM	CHB-C1B-NB	-4.48	118.85	124.38
12	C	383	U10	C1-C6-C5	-4.17	115.66	119.58
11	D	243	HEM	CBB-CAB-C3B	-4.08	107.30	127.62
11	C	382	HEM	C3B-C2B-C1B	-4.07	103.47	106.49
11	D	243	HEM	CAD-C3D-C2D	-4.01	120.40	127.88
11	C	382	HEM	CHC-C4B-NB	-4.00	120.08	124.43
12	C	383	U10	C15-C14-C16	3.99	121.98	115.27
11	C	382	HEM	CMB-C2B-C1B	3.91	131.00	125.04
11	C	381	HEM	CBD-CAD-C3D	3.90	123.47	112.63
11	C	382	HEM	C4D-ND-C1D	-3.88	101.07	105.07
13	C	384	PEE	C42-C41-C40	3.86	130.59	113.79
13	E	198	PEE	C22-C21-C20	3.81	130.37	113.79
14	C	385	SIG	O7-C3-C2	3.77	120.86	116.12
13	E	198	PEE	C42-C41-C40	3.74	130.08	113.79
12	C	383	U10	O2-C2-C3	-3.71	113.06	120.93
12	C	383	U10	C15-C14-C13	-3.70	114.19	123.68
11	C	382	HEM	C3D-C4D-ND	3.66	114.24	110.17
12	C	383	U10	C10-C9-C8	-3.60	114.45	123.68
14	C	385	SIG	C35-C24-C23	3.45	114.25	111.23
11	C	382	HEM	CMD-C2D-C1D	3.38	130.18	125.04
13	C	384	PEE	C22-C21-C20	3.36	128.44	113.79
11	D	243	HEM	C4C-CHD-C1D	3.32	126.94	122.56
11	C	381	HEM	C1B-NB-C4B	-3.24	101.72	105.07
14	C	385	SIG	C33-C9-C10	-3.21	114.65	120.40
13	C	384	PEE	C12-C13-C14	-3.18	98.28	114.42
14	C	385	SIG	C33-C9-C8	3.14	126.79	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	382	HEM	CHD-C1D-ND	-3.14	121.03	124.43
11	C	381	HEM	C2C-C3C-C4C	-3.10	104.74	106.90
11	C	382	HEM	C1B-NB-C4B	-3.05	101.92	105.07
13	E	198	PEE	C34-C33-C32	-3.03	99.04	114.42
13	E	198	PEE	C33-C32-C31	2.99	123.95	113.19
15	D	242	BOG	C1'-O1-C1	2.97	118.77	113.84
13	C	384	PEE	C33-C32-C31	2.96	123.82	113.19
11	C	381	HEM	C4B-CHC-C1C	2.93	126.42	122.56
11	D	243	HEM	CMB-C2B-C1B	2.90	129.45	125.04
11	C	381	HEM	C4D-ND-C1D	-2.89	102.08	105.07
11	C	382	HEM	CAD-C3D-C4D	2.88	129.69	124.66
11	C	381	HEM	C4A-C3A-C2A	-2.82	105.03	107.00
11	C	381	HEM	CMB-C2B-C3B	-2.80	121.43	128.30
11	C	381	HEM	CHC-C4B-NB	-2.80	121.39	124.43
11	D	243	HEM	C2B-C1B-NB	2.79	113.15	109.84
13	C	384	PEE	C34-C33-C32	-2.76	100.39	114.42
13	E	198	PEE	C12-C13-C14	-2.73	100.58	114.42
12	C	383	U10	C10-C9-C11	2.72	119.85	115.27
11	C	382	HEM	C4C-CHD-C1D	2.69	126.10	122.56
11	D	243	HEM	C4B-CHC-C1C	2.68	126.09	122.56
11	C	381	HEM	CMC-C2C-C3C	2.67	129.67	124.68
13	E	198	PEE	O5-C30-C31	-2.67	113.32	123.73
14	C	385	SIG	C20-C21-C22	2.66	118.31	114.72
11	C	382	HEM	CAB-C3B-C2B	-2.66	119.84	128.60
11	D	243	HEM	CHD-C1D-ND	-2.65	121.55	124.43
13	C	384	PEE	O5-C30-C31	-2.65	113.41	123.73
11	C	382	HEM	CHC-C4B-C3B	2.61	128.56	124.57
11	C	382	HEM	C4B-CHC-C1C	2.57	125.95	122.56
11	C	382	HEM	C2C-C3C-C4C	-2.52	105.14	106.90
14	C	385	SIG	C5-C4-C3	2.48	120.36	115.15
13	E	198	PEE	C3-C2-C1	-2.45	106.00	111.79
11	C	381	HEM	C2B-C1B-NB	2.44	112.73	109.84
14	C	385	SIG	C5-C4-C10	-2.41	121.37	124.96
13	C	384	PEE	O2-C2-C1	2.41	117.11	108.40
11	D	243	HEM	CHC-C4B-NB	-2.40	121.83	124.43
13	E	198	PEE	C36-C35-C34	-2.39	102.32	114.42
11	D	243	HEM	CHA-C4D-ND	-2.31	121.52	124.38
14	C	385	SIG	O7-C8-C20	-2.28	109.21	111.91
12	C	383	U10	C11-C9-C8	2.26	125.69	121.12
14	C	385	SIG	C6-C1-C2	-2.26	118.38	120.60
11	C	382	HEM	CBD-CAD-C3D	2.26	118.90	112.63
13	C	384	PEE	C14-C15-C16	-2.25	102.99	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	E	198	PEE	O2-C2-C1	2.24	116.52	108.40
11	C	381	HEM	C3B-C2B-C1B	-2.22	104.84	106.49
11	C	381	HEM	C3D-C4D-ND	2.19	112.61	110.17
13	C	384	PEE	C3-C2-C1	-2.19	106.61	111.79
11	C	381	HEM	C2D-C1D-ND	2.17	112.48	109.88
11	C	381	HEM	CAB-C3B-C2B	-2.14	121.55	128.60
11	C	381	HEM	CHB-C1B-NB	-2.07	121.82	124.38
11	C	382	HEM	CMA-C3A-C4A	-2.05	125.32	128.46
13	E	198	PEE	C14-C15-C16	-2.03	104.13	114.42
11	D	243	HEM	CMD-C2D-C3D	-2.00	120.68	126.12

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	C	384	PEE	C2
13	E	198	PEE	C2

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
11	C	381	HEM	C2B-C3B-CAB-CBB
11	C	381	HEM	C4B-C3B-CAB-CBB
11	C	382	HEM	C1A-C2A-CAA-CBA
11	C	382	HEM	C3A-C2A-CAA-CBA
11	D	243	HEM	C1A-C2A-CAA-CBA
11	D	243	HEM	C3A-C2A-CAA-CBA
12	C	383	U10	C1-C6-C7-C8
12	C	383	U10	C5-C6-C7-C8
12	C	383	U10	C12-C11-C9-C10
12	C	383	U10	C14-C16-C17-C18
13	C	384	PEE	O4-C10-O2-C2
13	E	198	PEE	O4-C10-O2-C2
13	E	198	PEE	O5-C30-O3-C3
13	E	198	PEE	C31-C30-O3-C3
13	E	198	PEE	C37-C38-C39-C40
14	C	385	SIG	C21-C20-C8-C9
14	C	385	SIG	C8-C20-C21-C22
14	C	385	SIG	C21-C22-C23-C24
14	C	385	SIG	C21-C22-C23-C28
14	C	385	SIG	C27-C22-C23-C24
14	C	385	SIG	C27-C22-C23-C28
14	C	385	SIG	C22-C23-C24-C35

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Mol	Chain	Res	Type	Atoms
14	C	385	SIG	C28-C23-C24-C25
14	C	385	SIG	C28-C23-C24-C35
14	C	385	SIG	C31-C32-C36-C37
14	C	385	SIG	C31-C32-C36-C39
13	C	384	PEE	O5-C30-O3-C3
12	C	383	U10	C12-C11-C9-C8
13	C	384	PEE	C22-C23-C24-C25
13	E	198	PEE	C22-C23-C24-C25
13	C	384	PEE	C17-C18-C19-C20
13	C	384	PEE	C37-C38-C39-C40
13	C	384	PEE	C31-C30-O3-C3
13	E	198	PEE	C30-C31-C32-C33
15	D	242	BOG	O5-C1-O1-C1'
13	E	198	PEE	C12-C13-C14-C15
13	C	384	PEE	C3-C2-O2-C10
13	C	384	PEE	C13-C14-C15-C16
15	D	242	BOG	C2-C1-O1-C1'
13	C	384	PEE	C20-C21-C22-C23
13	E	198	PEE	C35-C36-C37-C38
13	E	198	PEE	C14-C15-C16-C17
15	D	242	BOG	C2'-C3'-C4'-C5'
13	E	198	PEE	C33-C34-C35-C36
13	E	198	PEE	C31-C32-C33-C34
13	E	198	PEE	C17-C18-C19-C20
13	E	198	PEE	C21-C22-C23-C24
15	D	242	BOG	C3'-C4'-C5'-C6'
13	E	198	PEE	C19-C20-C21-C22
13	E	198	PEE	C39-C40-C41-C42
13	E	198	PEE	C11-C12-C13-C14
13	C	384	PEE	C12-C13-C14-C15
13	E	198	PEE	C1-C2-C3-O3
13	C	384	PEE	C40-C41-C42-C43
11	C	382	HEM	C3D-CAD-CBD-CGD
13	E	198	PEE	C41-C42-C43-C44
13	E	198	PEE	O3P-C1-C2-O2
13	C	384	PEE	C39-C40-C41-C42
13	C	384	PEE	C41-C42-C43-C44
13	C	384	PEE	C23-C24-C25-C26
13	E	198	PEE	C42-C43-C44-C45
14	C	385	SIG	C20-C21-C22-C27
11	D	243	HEM	C2B-C3B-CAB-CBB
13	C	384	PEE	O3P-C1-C2-O2

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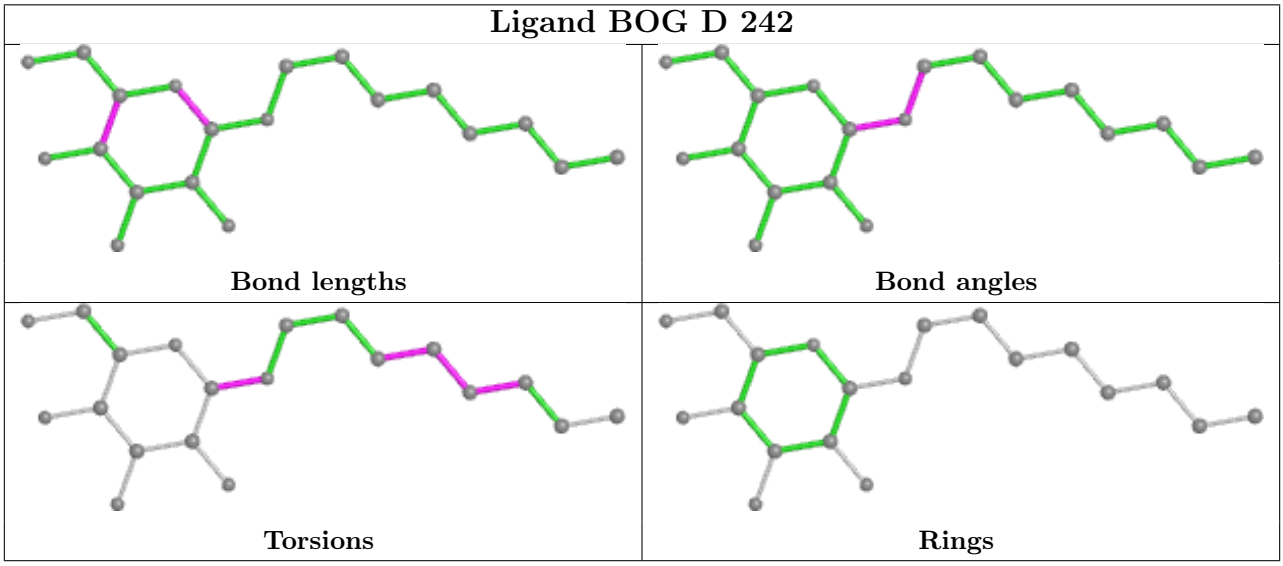
Mol	Chain	Res	Type	Atoms
13	C	384	PEE	C4-O4P-P-O3P
13	E	198	PEE	C4-O4P-P-O3P
14	C	385	SIG	C22-C23-C24-C25
13	C	384	PEE	O2-C2-C3-O3
13	C	384	PEE	C14-C15-C16-C17
13	E	198	PEE	C36-C37-C38-C39
14	C	385	SIG	C29-C30-C31-C32
13	C	384	PEE	C16-C17-C18-C19
13	E	198	PEE	C20-C21-C22-C23
11	C	382	HEM	C2A-CAA-CBA-CGA
11	C	381	HEM	CAA-CBA-CGA-O2A
13	E	198	PEE	C13-C14-C15-C16
14	C	385	SIG	C20-C21-C22-C23
11	C	382	HEM	C4D-C3D-CAD-CBD
13	E	198	PEE	C38-C39-C40-C41
11	C	381	HEM	CAA-CBA-CGA-O1A
11	C	381	HEM	CAD-CBD-CGD-O2D
11	C	381	HEM	CAD-CBD-CGD-O1D
11	D	243	HEM	CAD-CBD-CGD-O2D
11	D	243	HEM	CAD-CBD-CGD-O1D
11	D	243	HEM	C4B-C3B-CAB-CBB
13	C	384	PEE	C36-C37-C38-C39
15	D	242	BOG	C4'-C5'-C6'-C7'
11	C	382	HEM	CAA-CBA-CGA-O2A
11	D	243	HEM	CAA-CBA-CGA-O2A
12	C	383	U10	C16-C17-C18-C19
11	C	382	HEM	CAD-CBD-CGD-O2D
13	C	384	PEE	C4-O4P-P-O1P
13	E	198	PEE	O4P-C4-C5-N
11	C	382	HEM	CAA-CBA-CGA-O1A
11	C	382	HEM	CAD-CBD-CGD-O1D
12	C	383	U10	C5-C4-O4-C4M
11	D	243	HEM	CAA-CBA-CGA-O1A
13	C	384	PEE	C5-C4-O4P-P
13	E	198	PEE	C3-C2-O2-C10
13	E	198	PEE	O3-C30-C31-C32
13	E	198	PEE	O5-C30-C31-C32
13	C	384	PEE	O4-C10-C11-C12

There are no ring outliers.

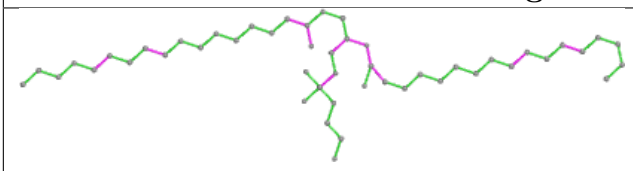
9 monomers are involved in 55 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	D	242	BOG	1	0
13	C	384	PEE	7	0
11	C	382	HEM	12	0
12	C	383	U10	9	0
11	C	381	HEM	7	0
16	E	197	FES	1	0
14	C	385	SIG	12	0
11	D	243	HEM	2	0
13	E	198	PEE	4	0

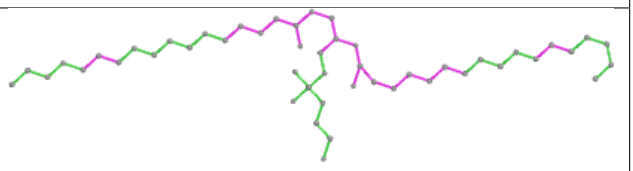
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.



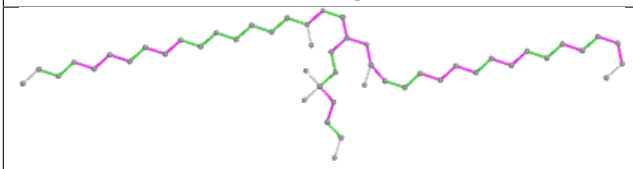
Ligand PEE C 384



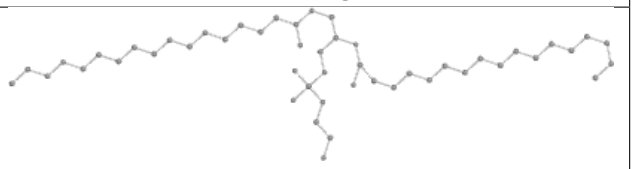
Bond lengths



Bond angles

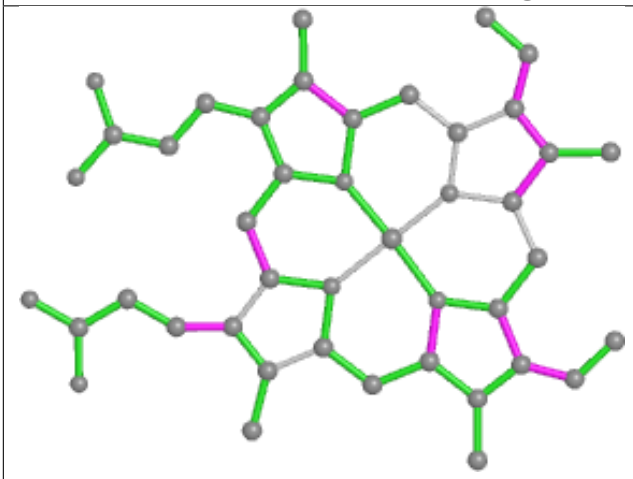


Torsions

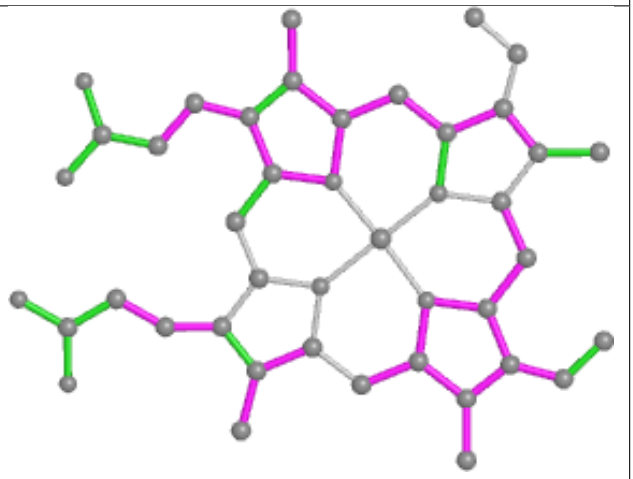


Rings

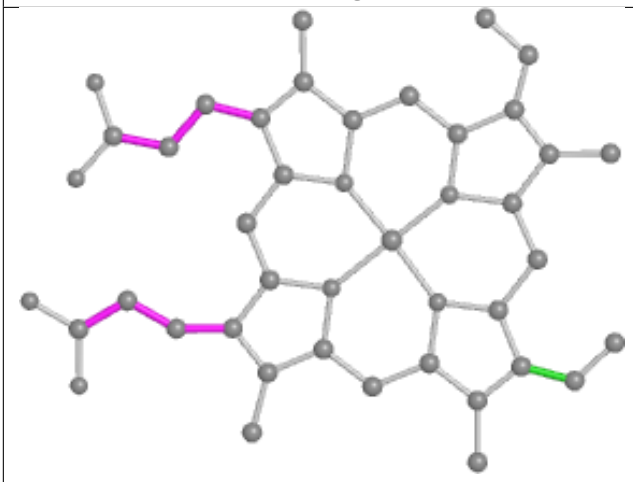
Ligand HEM C 382



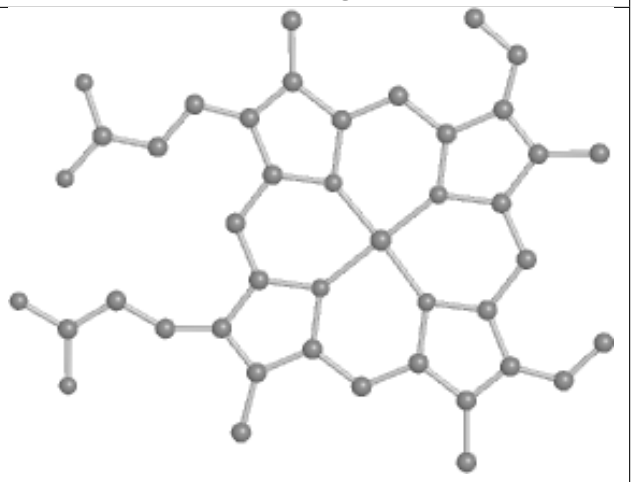
Bond lengths



Bond angles

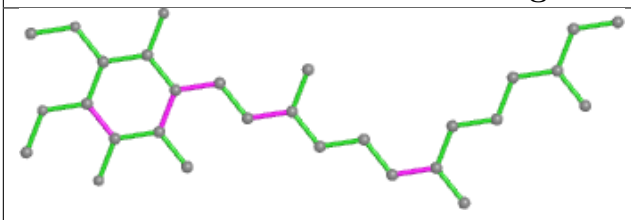


Torsions

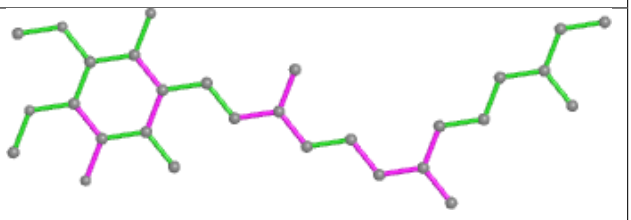


Rings

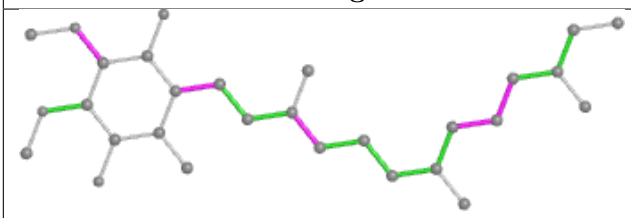
Ligand U10 C 383



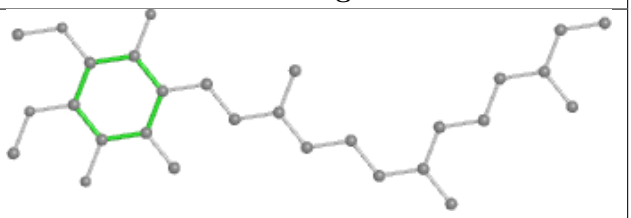
Bond lengths



Bond angles

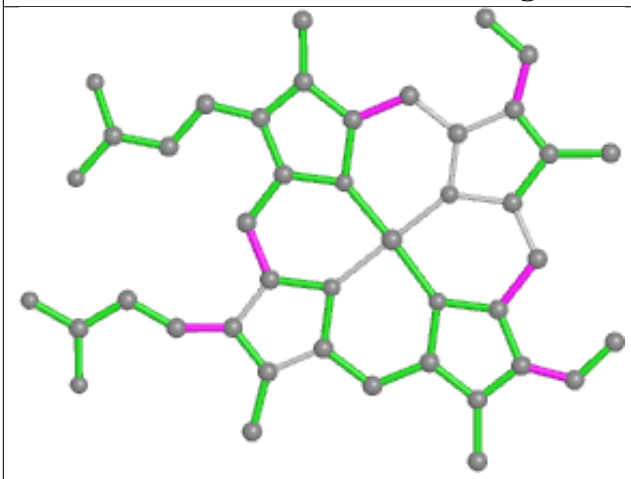


Torsions

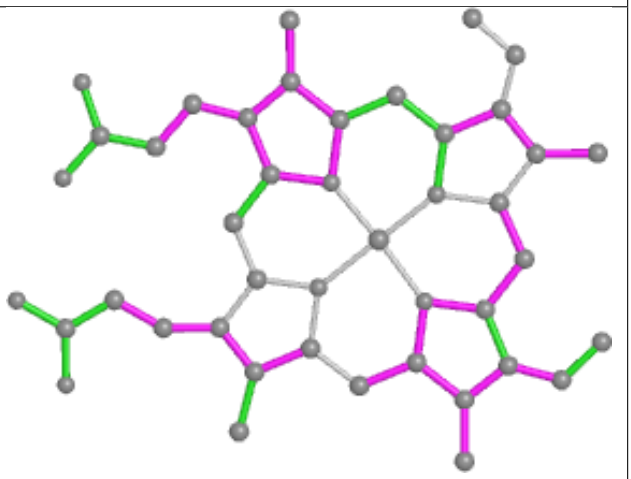


Rings

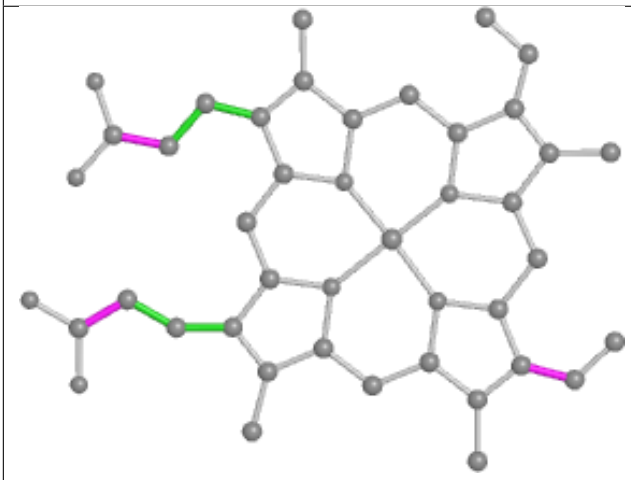
Ligand HEM C 381



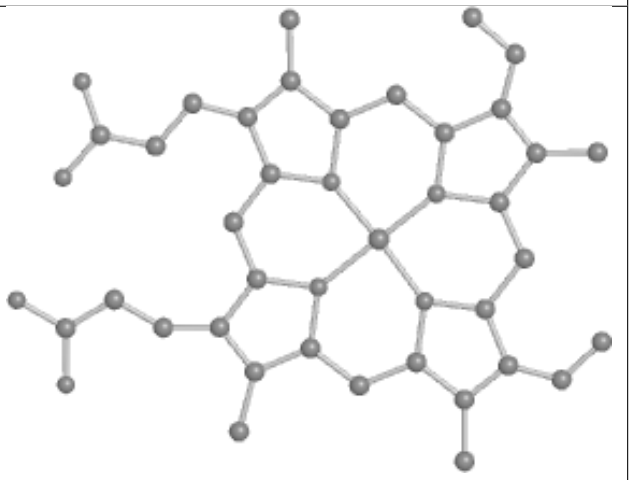
Bond lengths



Bond angles

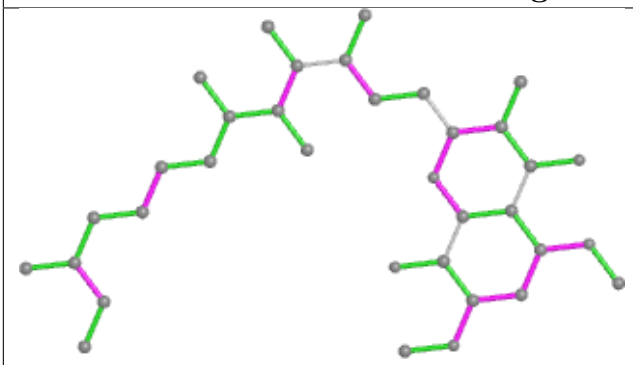


Torsions

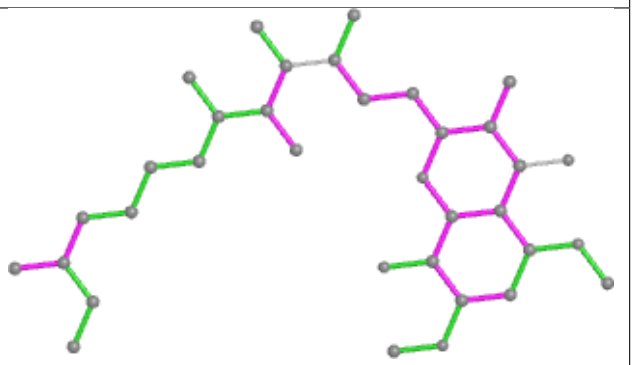


Rings

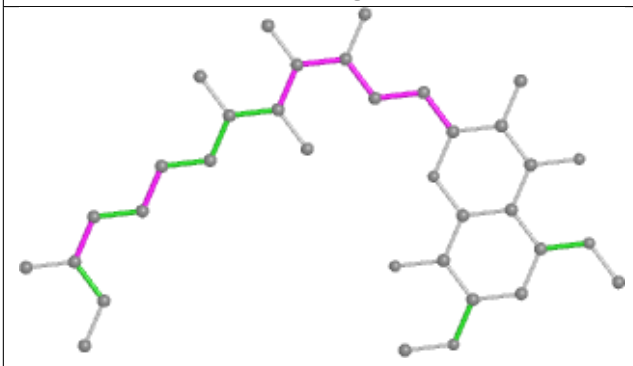
Ligand SIG C 385



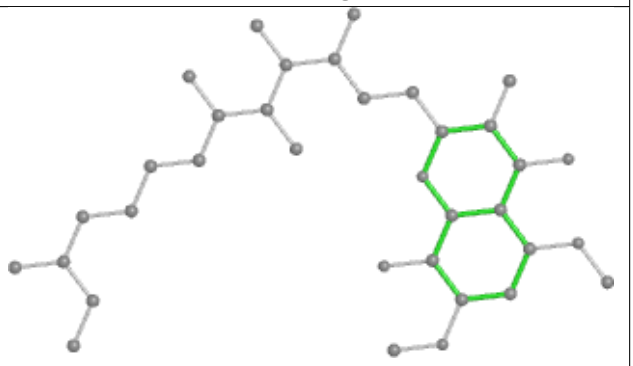
Bond lengths



Bond angles

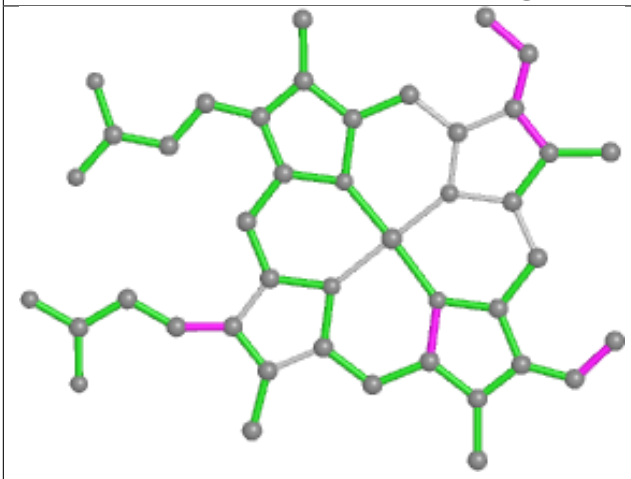


Torsions

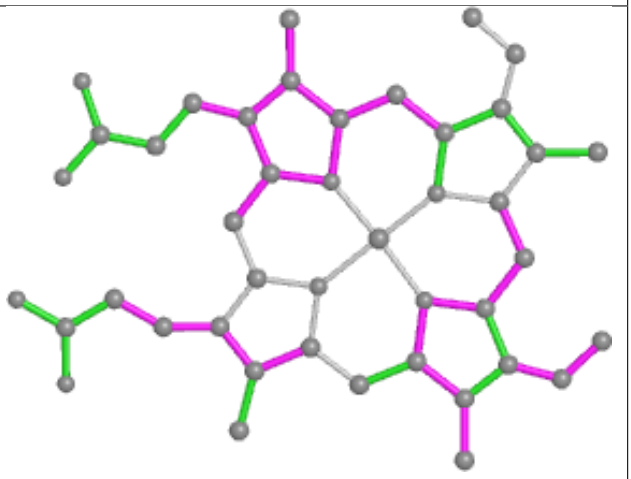


Rings

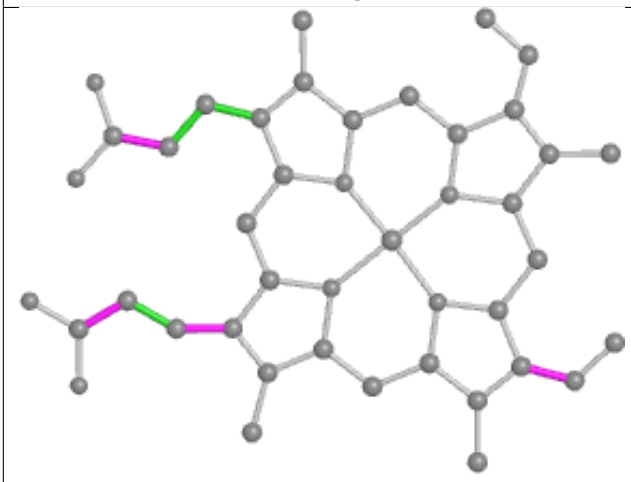
Ligand HEM D 243



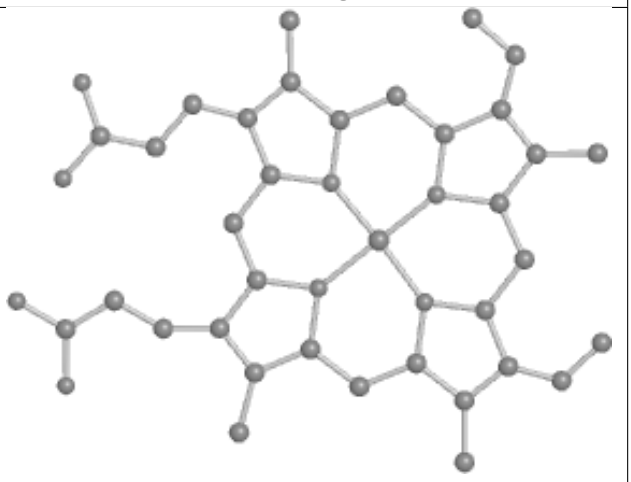
Bond lengths



Bond angles

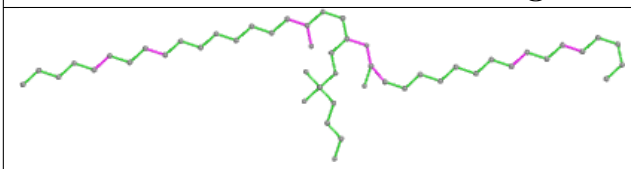


Torsions

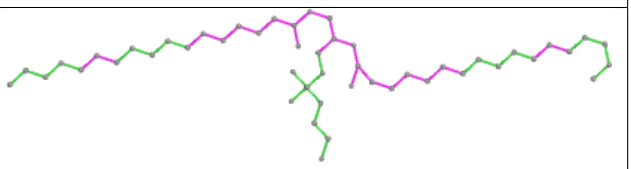


Rings

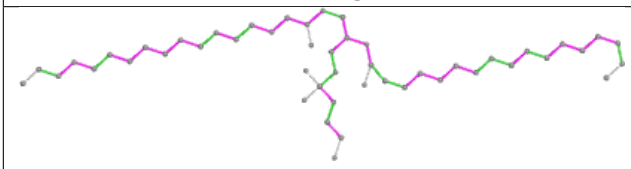
Ligand PEE E 198



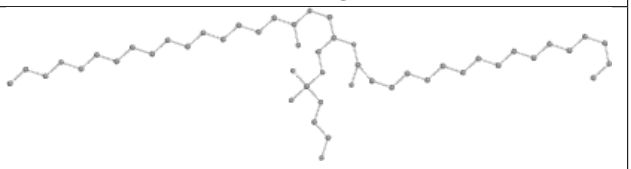
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

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
9	I	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	I	210:UNK	C	309:UNK	N	33.76
1	I	121:UNK	C	202:UNK	N	29.13

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	442/446 (99%)	-0.60	0 100 100	12, 58, 89, 100	0
2	B	406/422 (96%)	-0.53	2 (0%) 91 88	36, 71, 100, 100	0
3	C	379/380 (99%)	-0.74	0 100 100	4, 32, 71, 91	0
4	D	241/241 (100%)	-0.66	0 100 100	10, 41, 77, 100	0
5	E	196/196 (100%)	-0.25	4 (2%) 65 60	17, 76, 100, 100	0
6	F	100/109 (91%)	-0.68	0 100 100	18, 42, 74, 99	0
7	G	78/81 (96%)	-0.62	0 100 100	26, 54, 89, 100	0
8	H	66/78 (84%)	-0.62	0 100 100	27, 67, 86, 88	0
9	I	0/33	-	-	-	-
10	J	59/62 (95%)	-0.69	1 (1%) 70 64	37, 53, 86, 100	0
All	All	1967/2048 (96%)	-0.59	7 (0%) 92 90	4, 55, 98, 100	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	18	PRO	4.1
5	E	185	TYR	3.7
10	J	61	ASN	3.2
2	B	225	ASN	2.6
5	E	191	ASP	2.3
5	E	72	SER	2.2
5	E	195	VAL	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

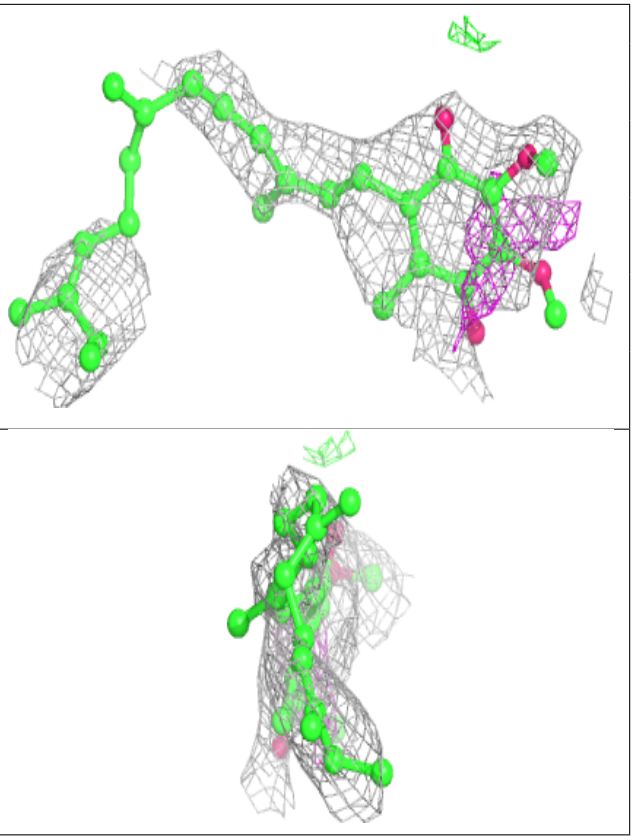
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

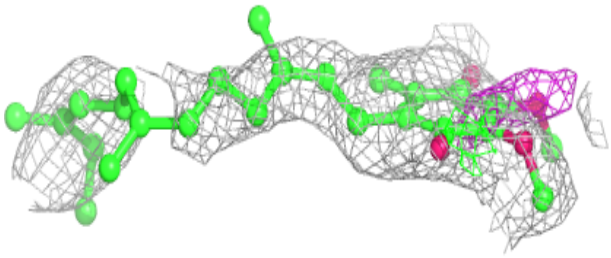
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
12	U10	C	383	29/63	0.72	0.48	72,88,100,100	0
13	PEE	E	198	49/51	0.81	0.36	43,80,98,100	0
13	PEE	C	384	49/51	0.88	0.42	42,58,76,87	0
15	BOG	D	242	20/20	0.88	0.23	35,68,81,81	0
14	SIG	C	385	35/35	0.95	0.20	2,17,26,29	0
11	HEM	D	243	43/43	0.97	0.16	10,21,32,35	0
11	HEM	C	381	43/43	0.97	0.20	6,24,32,43	0
11	HEM	C	382	43/43	0.97	0.20	8,20,32,41	0
16	FES	E	197	4/4	0.98	0.11	59,60,64,65	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 U10 C 383:

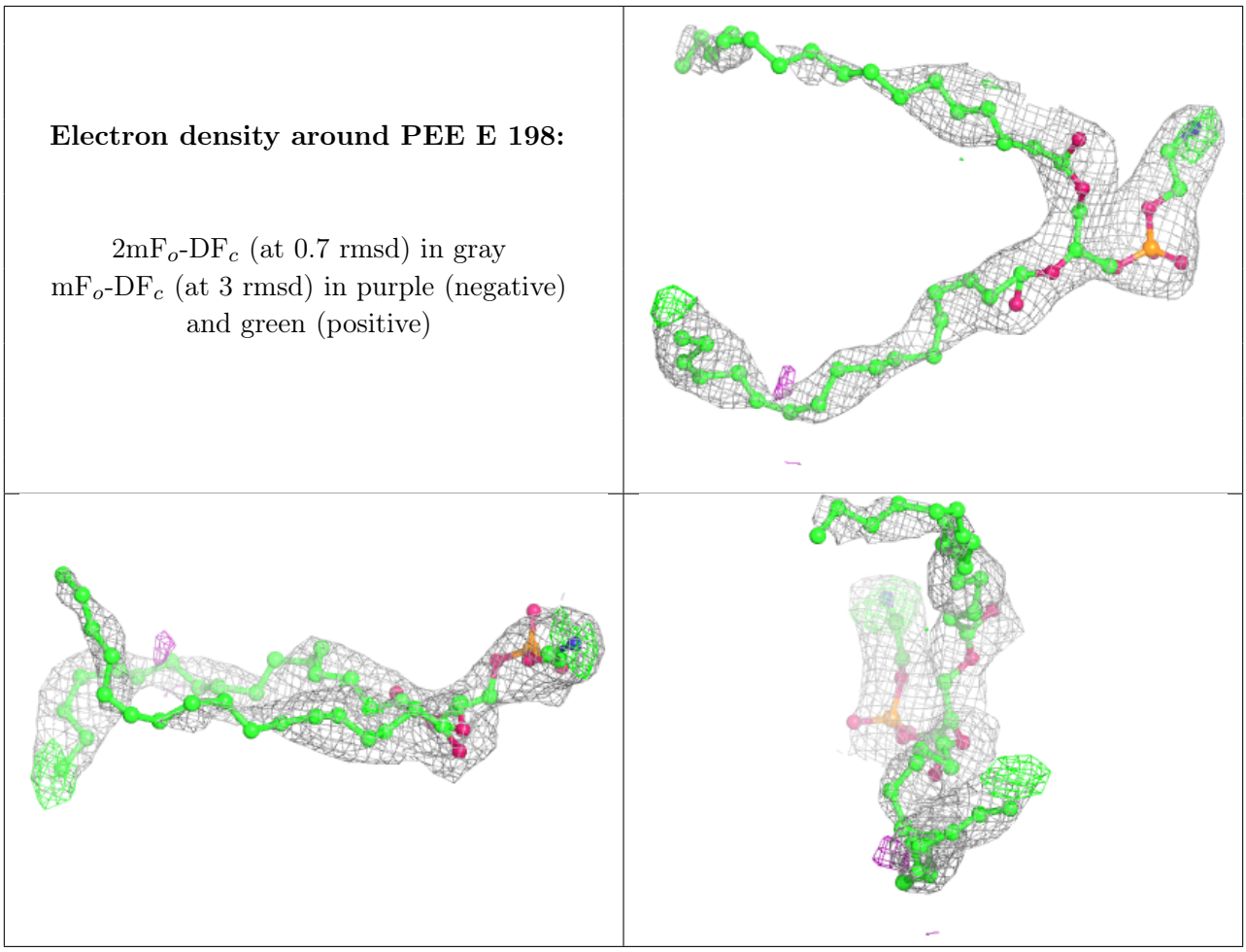
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





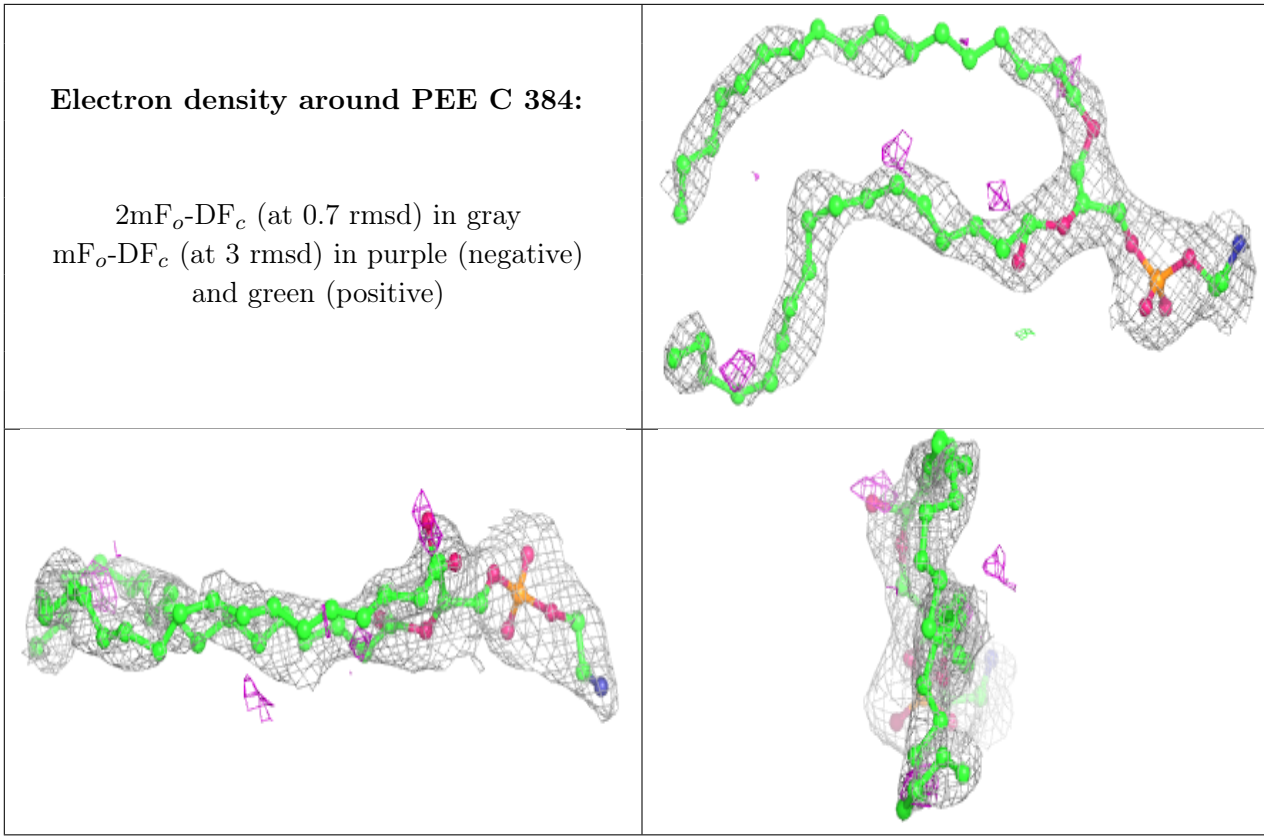
Electron density around PEE E 198:

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



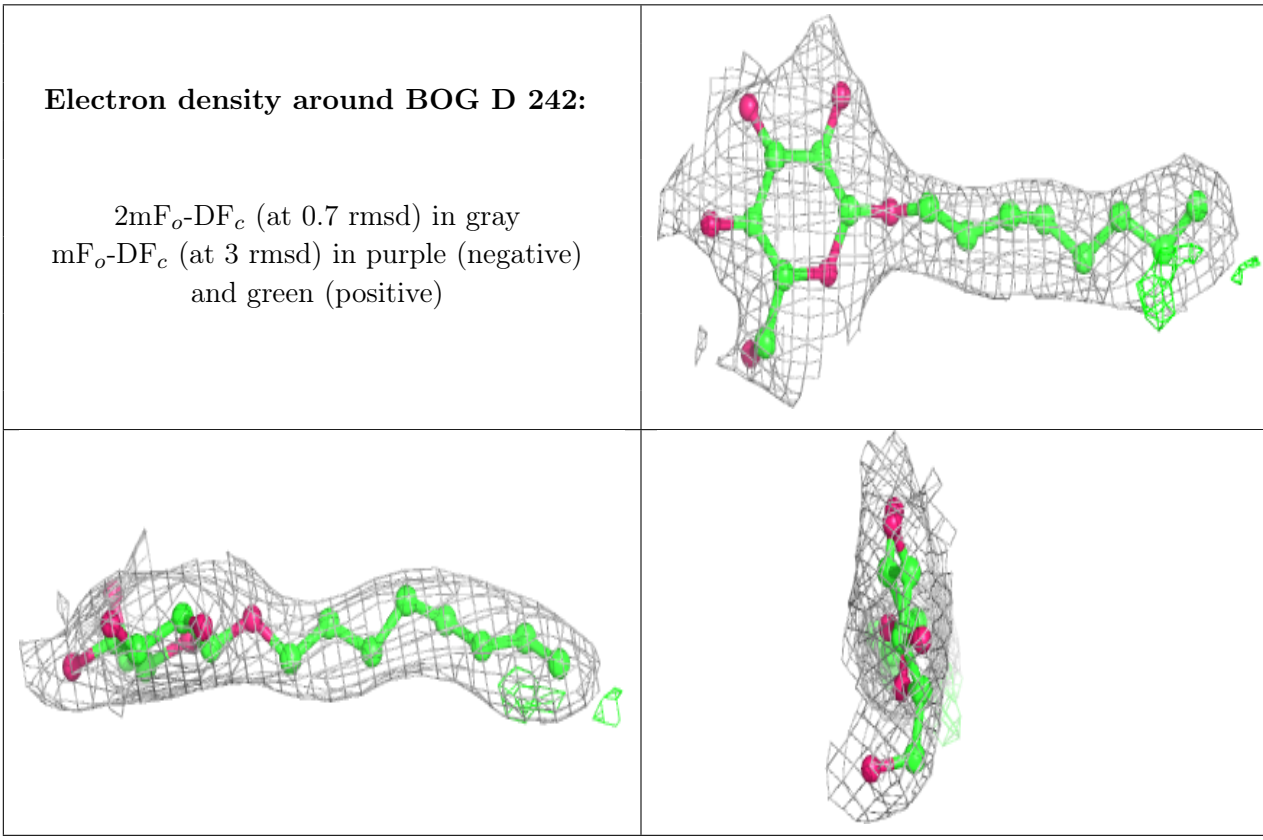
Electron density around PEE C 384:

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



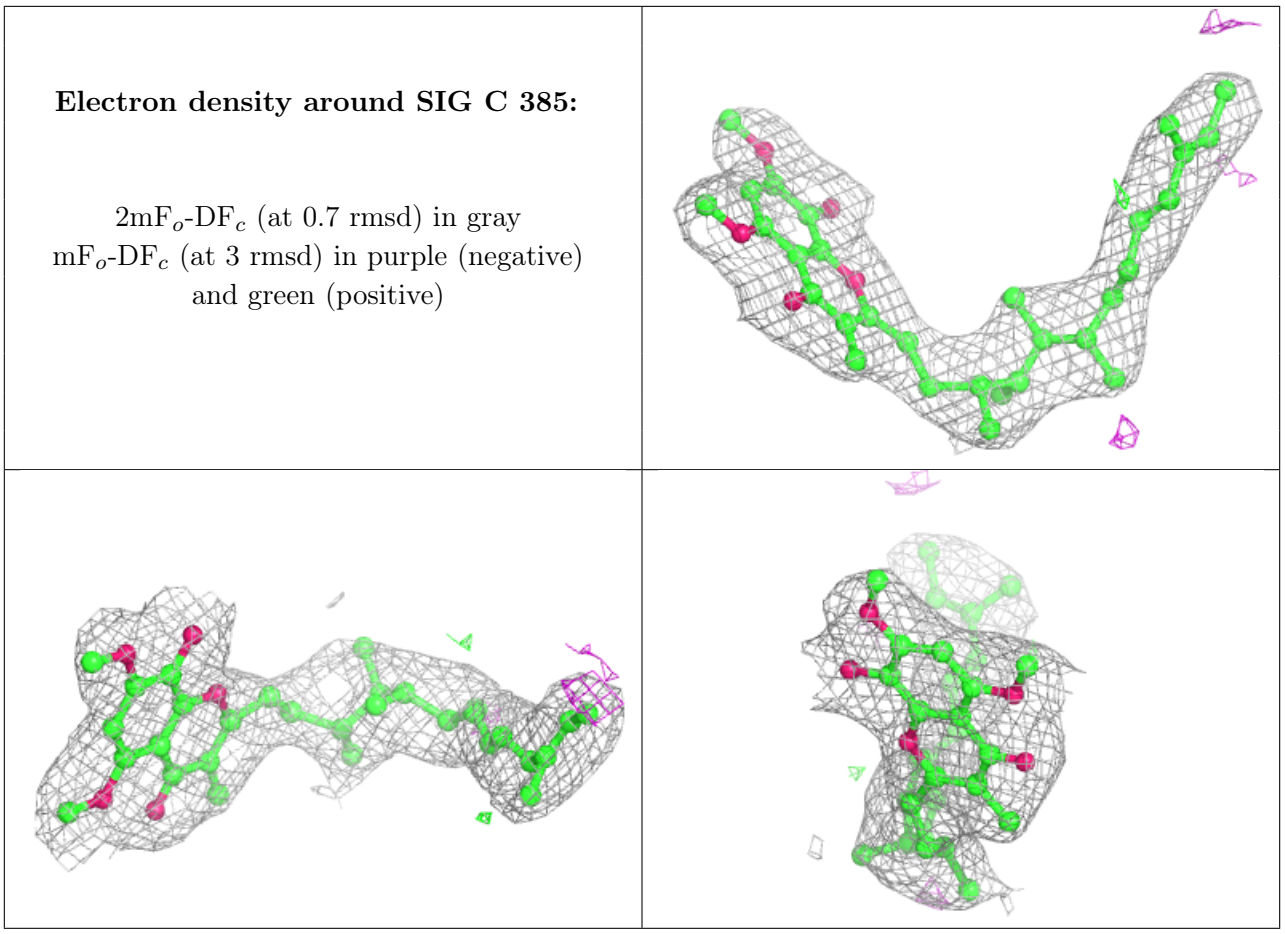
Electron density around BOG D 242:

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



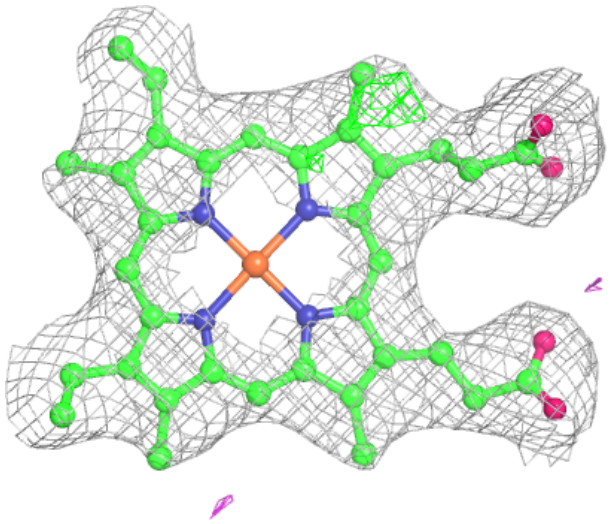
Electron density around SIG C 385:

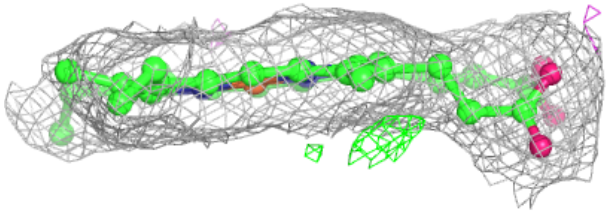
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

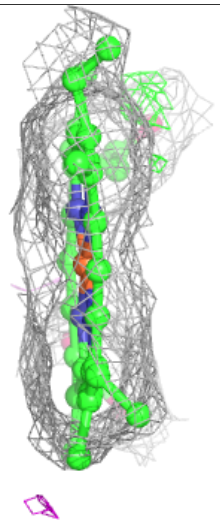


Electron density around HEM D 243:

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

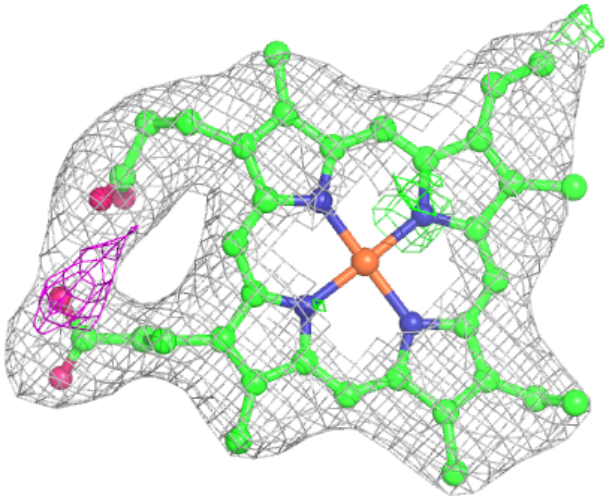


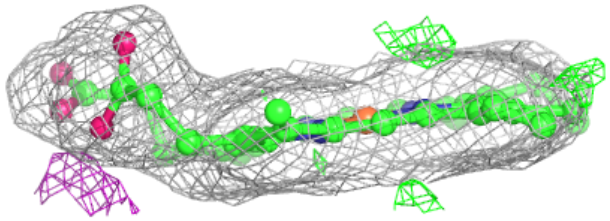


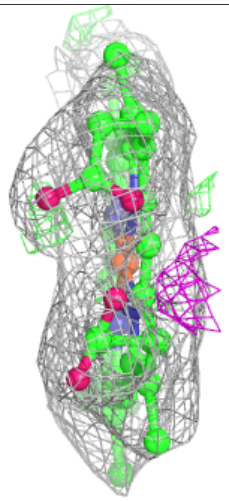


Electron density around HEM C 381:

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

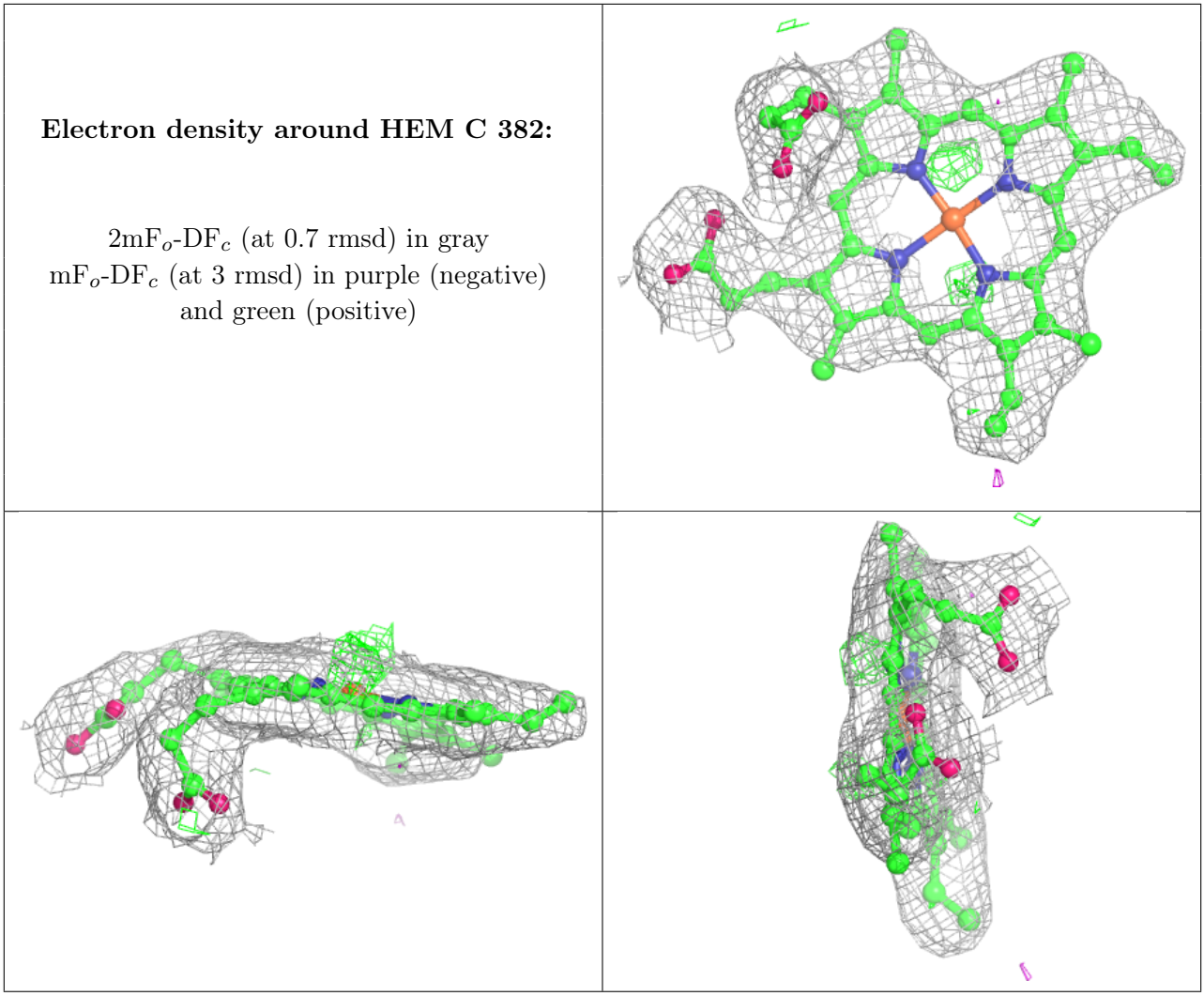






Electron density around HEM C 382:

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



6.5 Other polymers

There are no such residues in this entry.