Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 09:40 am BST

PDB ID	:	2D2C
Title	:	Crystal Structure Of Cytochrome B6F Complex with DBMIB From M. Laminosus
Authors	:	Yan, J.; Kurisu, G.; Cramer, W.A.
Deposited on	:	2005-09-07
Resolution	:	3.80 Å(reported)

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

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

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

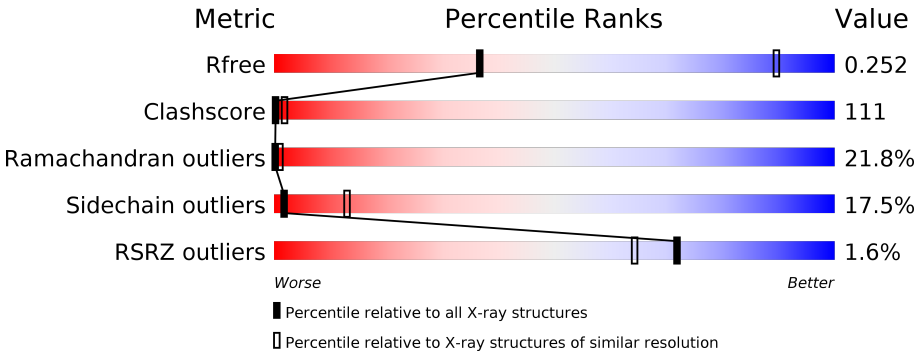
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 3.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1212 (4.00-3.60)
Clashscore	141614	1288 (4.00-3.60)
Ramachandran outliers	138981	1243 (4.00-3.60)
Sidechain outliers	138945	1237 (4.00-3.60)
RSRZ outliers	127900	1121 (4.00-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% 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	215	6% 58% 27% • 6%
1	N	215	9% 54% 26% 5% 6%
2	B	160	12% 44% 26% • 14%
2	O	160	% 5% 48% 25% 8% 14%
3	C	289	3% 17% 56% 24% • •
3	P	289	2% 14% 59% 22% • •

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Mol	Chain	Length	Quality of chain
4	D	179	4% 18% 51% 23% 6%
4	Q	179	% 15% 56% 22% 6%
5	E	32	6% 6% 59% 28% 6%
5	R	32	6% 59% 28% 6%
6	F	35	14% 57% 26%
6	S	35	20% 54% 23%
7	G	37	43% 24% 27%
7	T	37	3% 43% 30% 27%
8	H	29	24% 52% 17% 7%
8	U	29	24% 52% 17% 7%

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
11	OPC	B	305	-	-	X	-
12	BNT	B	309	-	-	X	-
12	BNT	O	1309	-	-	X	-
13	CLA	B	201	X	-	-	-
13	CLA	O	1201	X	-	-	-
14	FES	D	201	-	-	X	-
14	FES	Q	201	-	-	X	-
15	BCR	R	1101	-	-	-	X

2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 14984 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Cytochrome b6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	202	Total	C	N	O	S	0	0	0
			1593	1062	253	268	10			
1	N	202	Total	C	N	O	S	0	0	0
			1593	1062	253	268	10			

- Molecule 2 is a protein called Cytochrome b6-f complex subunit 4.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	137	Total	C	N	O	S	0	0	0
			1067	721	164	177	5			
2	O	137	Total	C	N	O	S	0	0	0
			1067	721	164	177	5			

- Molecule 3 is a protein called Apocytochrome f.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	286	Total	C	N	O	S	0	0	0
			2200	1406	366	421	7			
3	P	286	Total	C	N	O	S	0	0	0
			2200	1406	366	421	7			

- Molecule 4 is a protein called Cytochrome b6-f complex iron-sulfur subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	168	Total	C	N	O	S	0	0	0
			1280	815	223	235	7			
4	Q	168	Total	C	N	O	S	0	0	0
			1280	815	223	235	7			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	138	ARG	LYS	CONFLICT	UNP P83794
Q	138	ARG	LYS	CONFLICT	UNP P83794

- Molecule 5 is a protein called Cytochrome b6-f complex subunit VI.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	E	32	Total	C	N	O	S	0	0	0
			248	179	34	34	1			
5	R	32	Total	C	N	O	S	0	0	0
			248	179	34	34	1			

- Molecule 6 is a protein called Cytochrome b6-f complex subunit VII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	35	Total	C	N	O	S	0	0	0
			270	181	39	48	2			
6	S	35	Total	C	N	O	S	0	0	0
			270	181	39	48	2			

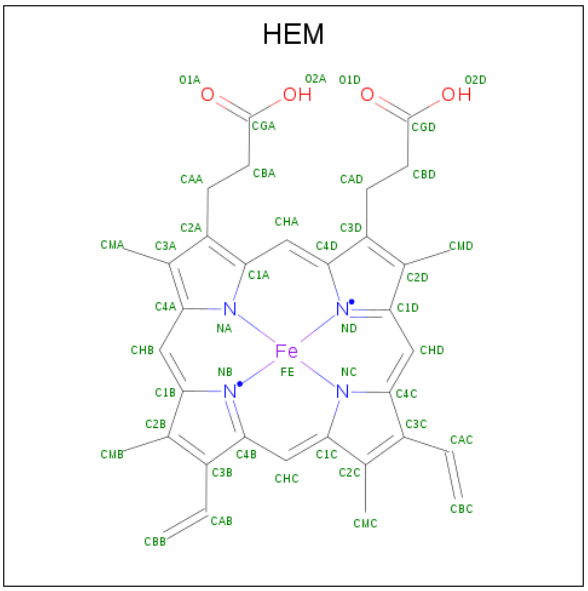
- Molecule 7 is a protein called Cytochrome b6-f complex subunit V.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	27	Total	C	N	O	0	0	0
			216	146	34	36			
7	T	27	Total	C	N	O	0	0	0
			216	146	34	36			

- Molecule 8 is a protein called Cytochrome b6-f complex subunit VIII.

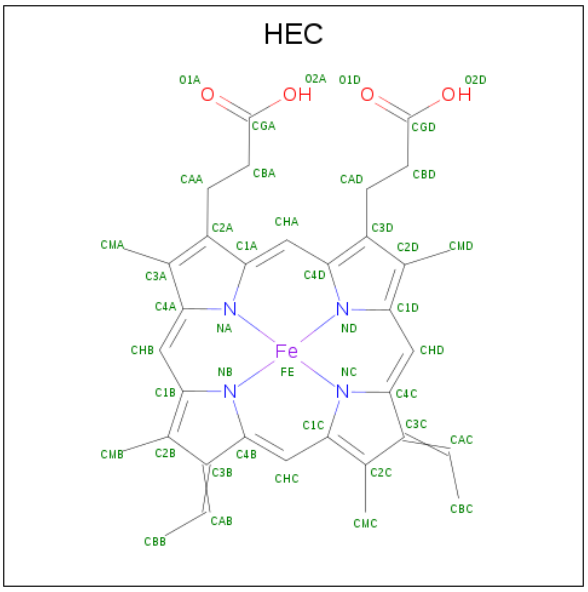
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	27	Total	C	N	O	S	0	0	0
			214	146	34	33	1			
8	U	27	Total	C	N	O	S	0	0	0
			214	146	34	33	1			

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



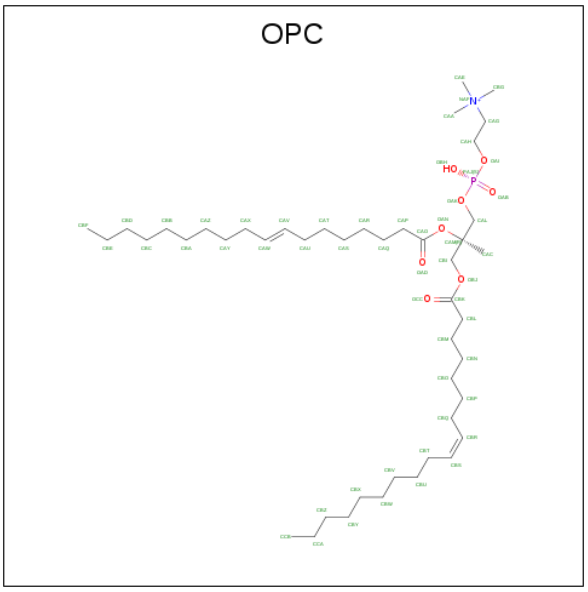
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	C	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	N	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		
9	P	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

- Molecule 10 is HEME C (three-letter code: HEC) (formula: $C_{34}H_{34}FeN_4O_4$).



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

- Molecule 11 is (7R,17E)-4-HYDROXY-N,N,N,7-TETRAMETHYL-7-[(8E)-OCTADEC-8-ENOYLOXY]-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOS-17-EN-1-AMINIUM 4-OXIDE (three-letter code: OPC) (formula: $C_{45}H_{87}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	B	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

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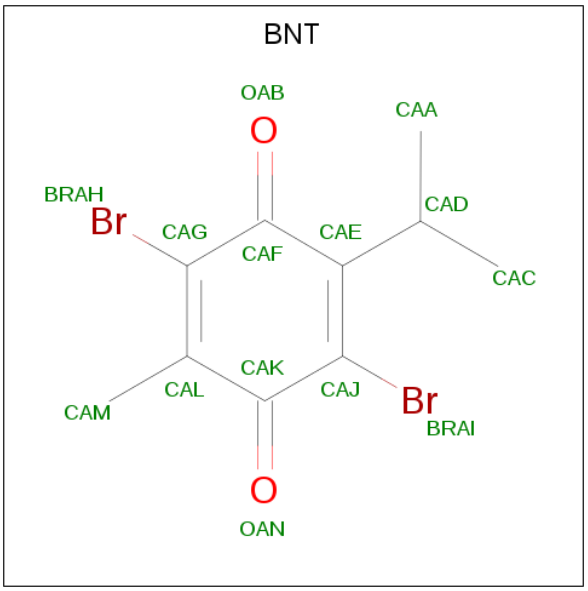
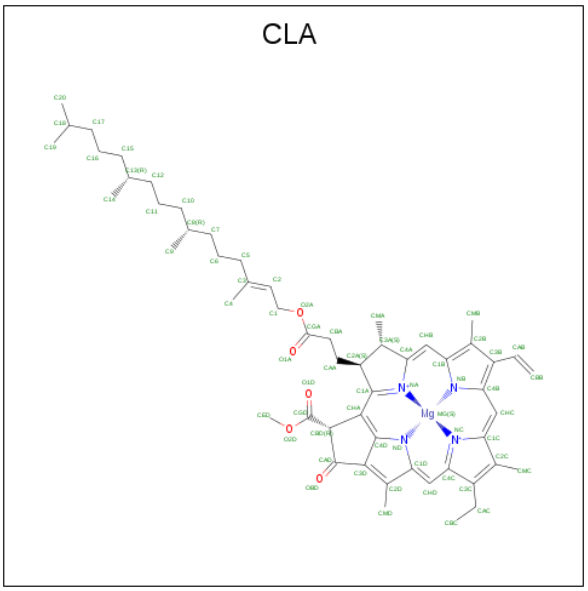
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
11	C	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
11	N	1	Total	C	N	O	P	0	0
			54	44	1	8	1		
11	O	1	Total	C	N	O	P	0	0
			54	44	1	8	1		

- Molecule 12 is 2,5-DIBROMO-3-ISOPROPYL-6-METHYLBENZO-1,4-QUINONE (three-letter code: BNT) (formula: $C_{10}H_{10}Br_2O_2$).



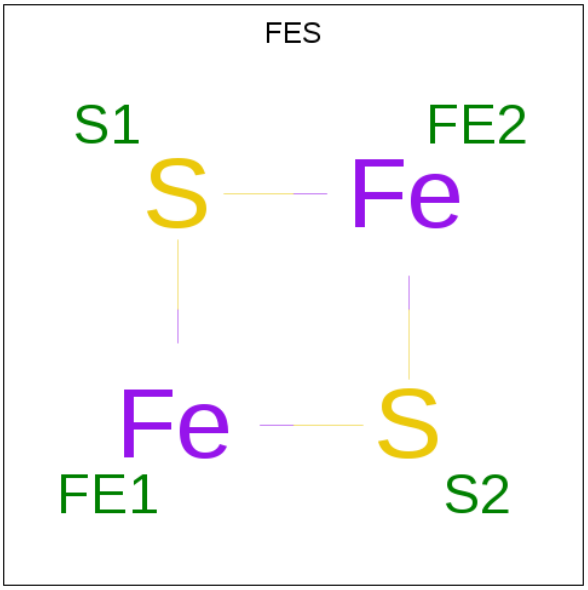
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
12	B	1	Total	Br	C	O	0	0
			14	2	10	2		
12	O	1	Total	Br	C	O	0	0
			14	2	10	2		

- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$).



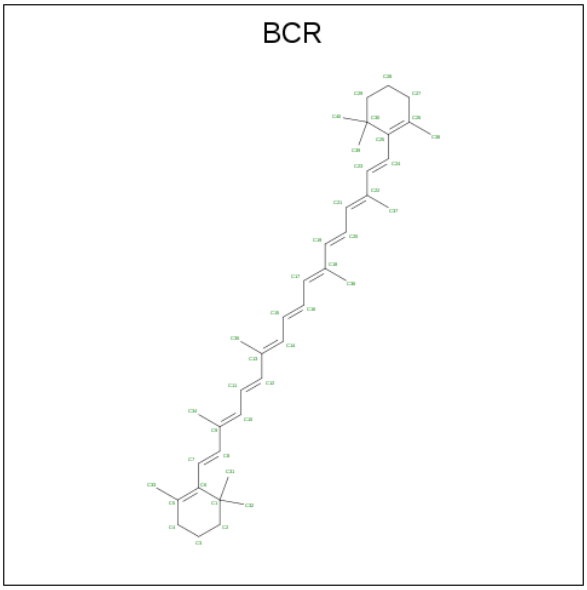
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	O	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe_2S_2).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
14	D	1	Total	Fe	S		0	0
			4	2	2			
14	Q	1	Total	Fe	S		0	0
			4	2	2			

- Molecule 15 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
15	E	1	Total C 40 40	0	0
15	R	1	Total C 40 40	0	0

- Molecule 16 is water.

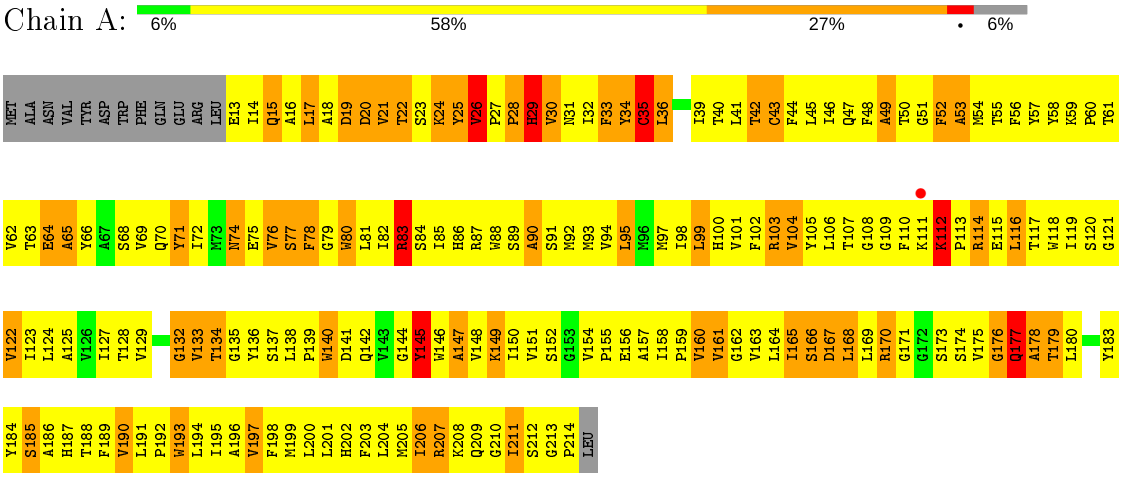
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
16	A	1	Total O 1 1	0	0
16	N	1	Total O 1 1	0	0

3 Residue-property plots (i)

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

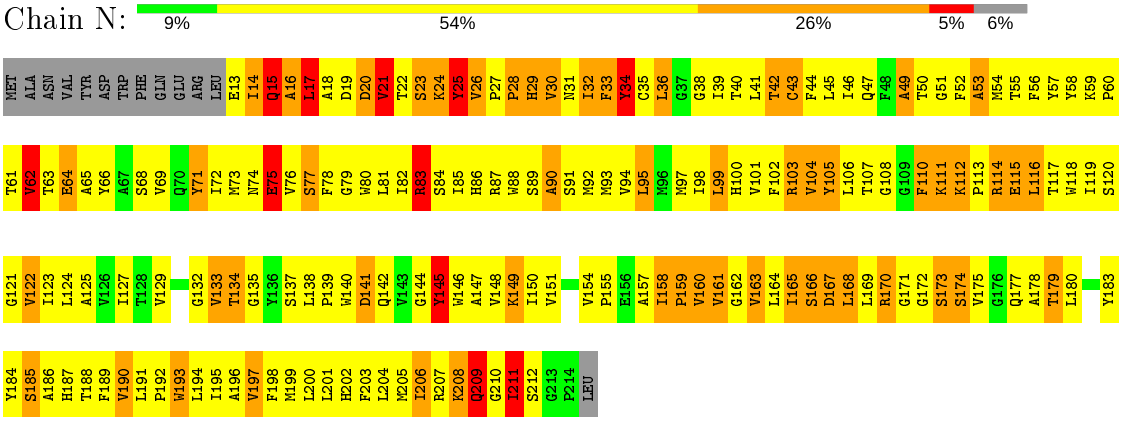
- Molecule 1: Cytochrome b6

Chain A:



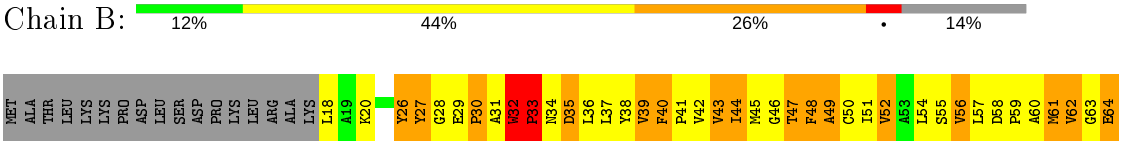
- Molecule 1: Cytochrome b6

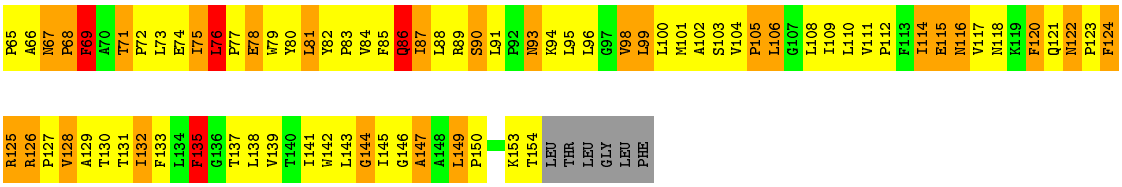
Chain N:

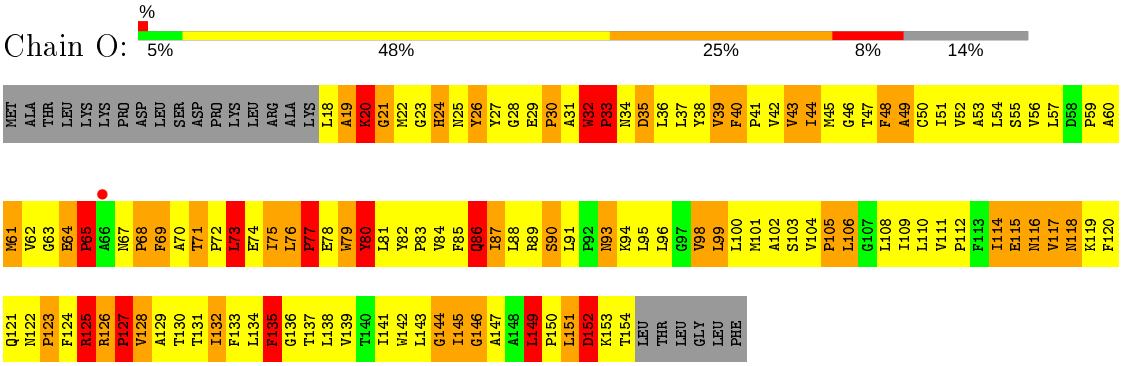


- Molecule 2: Cytochrome b6-f complex subunit 4

Chain B:

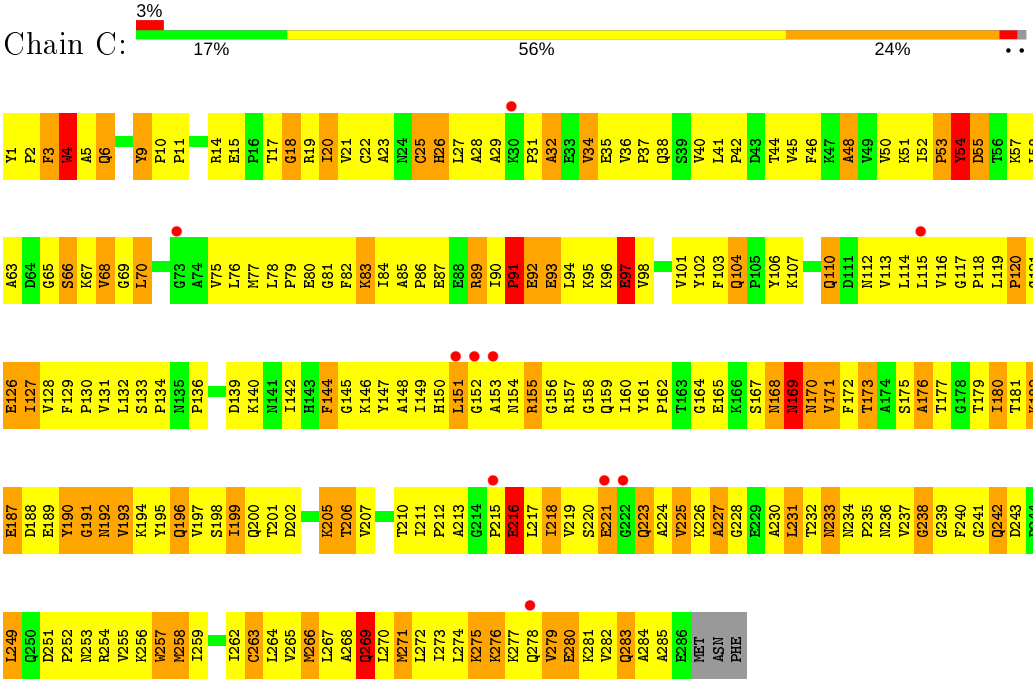




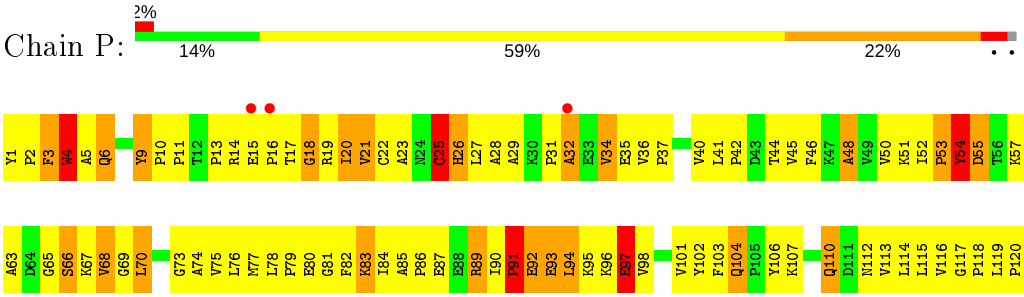


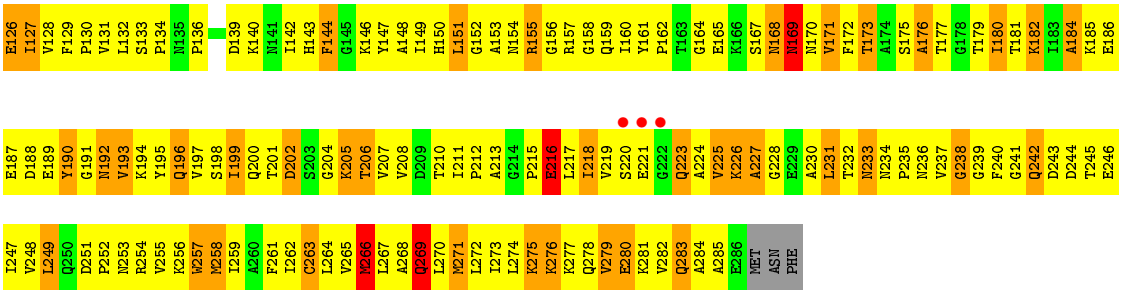
• Molecule 2: Cytochrome b6-f complex subunit 4

• Molecule 3: Apocytochrome f

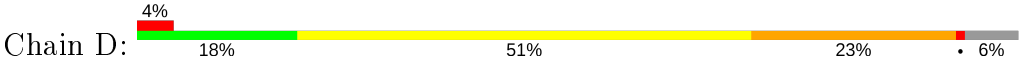


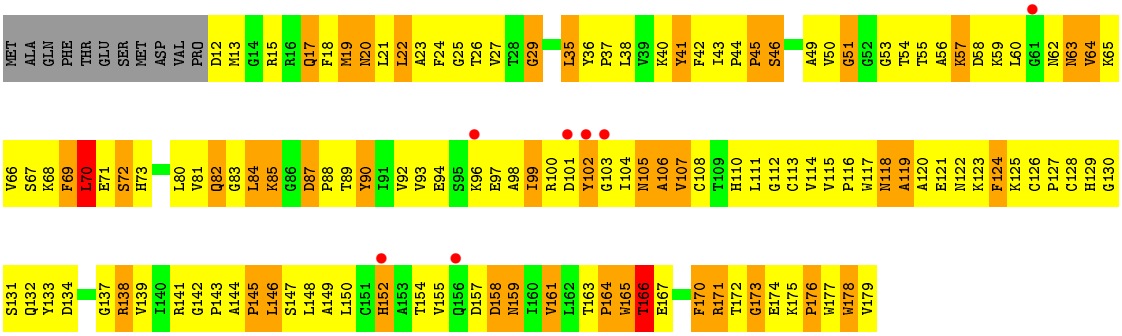
• Molecule 3: Apocytochrome f



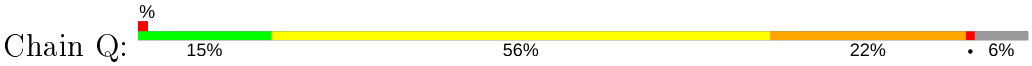


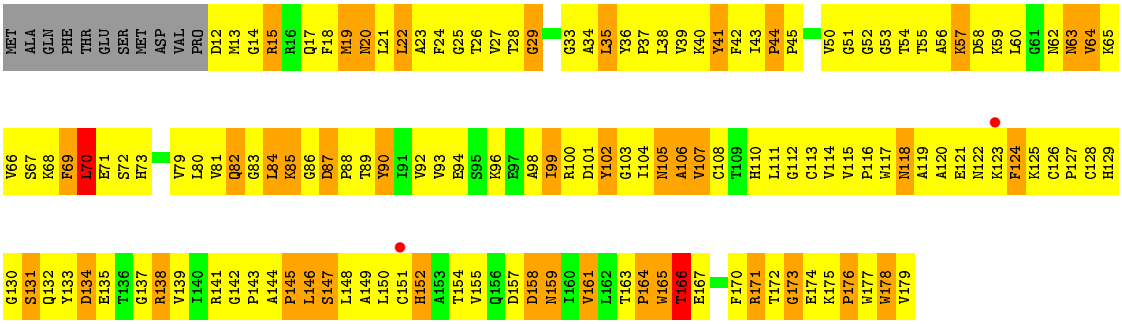
• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit





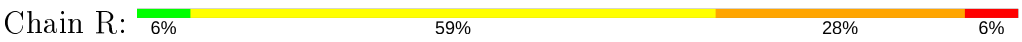
• Molecule 4: Cytochrome b6-f complex iron-sulfur subunit





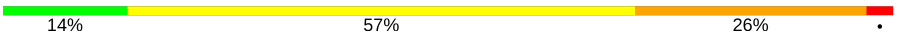
• Molecule 5: Cytochrome b6-f complex subunit VI

• Molecule 5: Cytochrome b6-f complex subunit VI



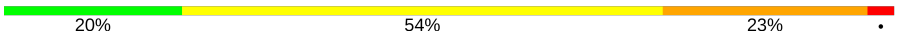
• Molecule 6: Cytochrome b6-f complex subunit VII

Chain F:



• Molecule 6: Cytochrome b6-f complex subunit VII

Chain S:

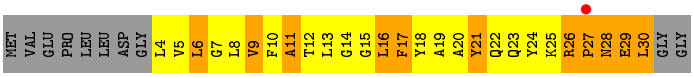


• Molecule 7: Cytochrome b6-f complex subunit V

Chain G:

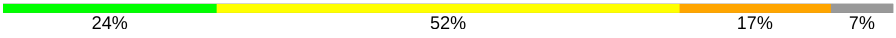
• Molecule 7: Cytochrome b6-f complex subunit V

Chain T:



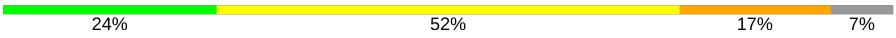
• Molecule 8: Cytochrome b6-f complex subunit VIII

Chain H:



• Molecule 8: Cytochrome b6-f complex subunit VIII

Chain U:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	156.59Å 156.59Å 361.79Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	24.76 – 3.80 49.31 – 3.79	Depositor EDS
% Data completeness (in resolution range)	(Not available) (24.76-3.80) 92.5 (49.31-3.79)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.04 (at 3.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.276 , 0.378 0.263 , 0.252	Depositor DCC
R_{free} test set	1490 reflections (3.15%)	wwPDB-VP
Wilson B-factor (Å^2)	103.0	Xtriage
Anisotropy	0.039	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.28 , 89.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	0.499 for h,-h-k,-l	Xtriage
F_o,F_c correlation	0.87	EDS
Total number of atoms	14984	wwPDB-VP
Average B, all atoms (Å^2)	80.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.22% 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: OPC, CLA, BNT, FES, HEC, HEM, BCR

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	0.58	0/1641	0.80	1/2239 (0.0%)
1	N	0.56	0/1641	0.80	1/2239 (0.0%)
2	B	0.61	0/1102	0.97	3/1515 (0.2%)
2	O	0.65	0/1102	1.04	5/1515 (0.3%)
3	C	0.54	0/2248	0.76	0/3061
3	P	0.57	0/2248	0.75	0/3061
4	D	0.63	0/1312	0.80	0/1786
4	Q	0.59	0/1312	0.81	0/1786
5	E	0.68	0/253	0.88	0/340
5	R	0.71	0/253	0.87	0/340
6	F	0.64	0/274	0.77	0/366
6	S	0.61	0/274	0.77	0/366
7	G	0.71	0/221	0.97	1/299 (0.3%)
7	T	0.73	0/221	0.87	0/299
8	H	0.62	0/220	0.83	0/301
8	U	0.61	0/220	0.83	0/301
All	All	0.60	0/14542	0.83	11/19814 (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
1	A	0	1
2	O	0	1
All	All	0	2

There are no bond length outliers.

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	144	GLY	N-CA-C	-7.42	94.56	113.10
2	O	144	GLY	N-CA-C	-6.42	97.05	113.10
2	O	149	LEU	CA-CB-CG	5.70	128.41	115.30
2	O	21	GLY	N-CA-C	5.70	127.35	113.10
2	B	69	PHE	N-CA-C	5.60	126.13	111.00
2	O	126	ARG	C-N-CA	-5.51	98.84	122.00
2	O	40	PHE	N-CA-C	-5.38	96.46	111.00
1	N	209	GLN	N-CA-C	5.25	125.18	111.00
2	B	40	PHE	N-CA-C	-5.20	96.96	111.00
7	G	27	PRO	N-CA-C	5.14	125.47	112.10
1	A	207	ARG	N-CA-C	-5.06	97.33	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	25	TYR	Sidechain
2	O	80	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	1593	0	1623	444	0
1	N	1593	0	1623	469	0
2	B	1067	0	1106	356	0
2	O	1067	0	1106	382	0
3	C	2200	0	2216	423	0
3	P	2200	0	2216	470	0
4	D	1280	0	1265	223	0
4	Q	1280	0	1265	218	0
5	E	248	0	284	135	0
5	R	248	0	284	120	0
6	F	270	0	282	93	0
6	S	270	0	282	75	0
7	G	216	0	220	89	0
7	T	216	0	220	99	0
8	H	214	0	224	37	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	U	214	0	224	35	0
9	A	86	0	60	12	0
9	C	43	0	30	4	0
9	N	86	0	60	11	0
9	P	43	0	30	5	0
10	A	43	0	31	4	0
10	N	43	0	31	10	0
11	B	54	0	83	34	0
11	C	54	0	83	20	0
11	N	54	0	83	14	0
11	O	54	0	83	17	0
12	B	14	0	10	9	0
12	O	14	0	10	7	0
13	B	65	0	70	6	0
13	O	65	0	70	8	0
14	D	4	0	0	3	0
14	Q	4	0	0	2	0
15	E	40	0	56	11	0
15	R	40	0	56	8	0
16	A	1	0	0	1	0
16	N	1	0	0	2	0
All	All	14984	0	15286	3367	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 111.

All (3367) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:34:TYR:HA	1:A:103:ARG:HH11	1.06	1.18
1:N:162:GLY:O	1:N:165:ILE:HG22	1.45	1.16
1:A:106:LEU:HG	5:E:18:ILE:HD12	1.22	1.16
3:C:171:VAL:HG13	3:C:234:ASN:HB2	1.22	1.14
3:P:271:MET:HB3	4:Q:23:ALA:HA	1.15	1.14
1:N:87:ARG:HD2	2:O:61:MET:HE1	1.29	1.14
5:E:18:ILE:HA	5:E:22:ILE:HG22	1.31	1.13
1:A:34:TYR:HA	1:A:103:ARG:NH1	1.62	1.12
1:A:124:LEU:HB3	9:A:302:HEM:HBB2	1.19	1.11
1:N:112:LYS:H	1:N:113:PRO:HD2	1.09	1.11
2:B:149:LEU:HD13	6:F:3:THR:HG23	1.22	1.11
3:C:173:THR:HG22	3:C:230:ALA:HA	1.34	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:89:ARG:HG3	2:O:90:SER:H	1.16	1.10
2:B:150:PRO:HB3	2:B:153:LYS:HB2	1.28	1.09
5:R:14:LEU:O	5:R:18:ILE:HG12	1.53	1.09
1:N:167:ASP:HA	1:N:170:ARG:HE	1.08	1.08
1:N:32:ILE:HG22	1:N:33:PHE:H	1.20	1.07
11:O:1306:OPC:HAL2	11:O:1306:OPC:HAP2	1.36	1.07
2:B:125:ARG:HA	2:B:125:ARG:HH11	1.15	1.06
2:B:149:LEU:HD21	6:F:2:MET:N	1.71	1.05
7:G:26:ARG:HD3	7:G:27:PRO:HD3	1.36	1.05
5:R:18:ILE:HA	5:R:22:ILE:HG22	1.35	1.05
3:P:171:VAL:HG13	3:P:234:ASN:HB2	1.31	1.04
4:Q:53:GLY:HA2	4:Q:57:LYS:HD3	1.35	1.04
1:A:148:VAL:HA	1:A:151:VAL:HG22	1.36	1.04
2:B:122:ASN:ND2	2:B:124:PHE:HB3	1.71	1.04
1:N:142:GLN:N	2:O:64:GLU:HG2	1.71	1.04
3:P:173:THR:HG22	3:P:230:ALA:HA	1.36	1.03
1:A:66:TYR:CE2	2:B:66:ALA:HA	1.93	1.03
1:A:161:VAL:HG12	1:A:164:LEU:HD12	1.39	1.03
5:E:14:LEU:O	5:E:18:ILE:HG12	1.59	1.02
1:A:62:VAL:HG13	1:A:177:GLN:HG2	1.36	1.02
2:B:89:ARG:HG3	2:B:90:SER:H	1.23	1.02
3:P:36:VAL:HG12	3:P:48:ALA:HA	1.39	1.02
1:N:142:GLN:H	2:O:64:GLU:HG2	1.18	1.02
1:N:148:VAL:HA	1:N:151:VAL:HG22	1.41	1.02
2:O:117:VAL:HG13	2:O:118:ASN:H	1.20	1.02
1:A:26:VAL:HB	2:B:29:GLU:HG3	1.38	1.02
2:B:79:TRP:CZ3	5:E:1:MET:HA	1.95	1.01
4:D:53:GLY:HA2	4:D:57:LYS:HD3	1.41	1.01
1:N:28:PRO:HG2	2:O:32:TRP:HB3	1.43	1.01
3:P:271:MET:CB	4:Q:23:ALA:HA	1.90	1.01
4:D:154:THR:HG22	4:D:155:VAL:H	1.24	1.00
1:N:74:ASN:O	1:N:75:GLU:HB2	1.58	1.00
4:D:124:PHE:HB2	4:D:133:TYR:HB2	1.42	0.99
4:Q:124:PHE:HB2	4:Q:133:TYR:HB2	1.41	0.99
4:D:51:GLY:N	4:D:84:LEU:HD21	1.78	0.99
1:A:28:PRO:HD2	2:B:33:PRO:HD3	1.43	0.99
2:B:42:VAL:HG22	3:C:272:LEU:HB3	1.46	0.98
1:N:209:GLN:HE22	2:O:28:GLY:N	1.60	0.98
2:O:125:ARG:HB3	2:O:125:ARG:NH1	1.79	0.98
1:N:105:TYR:OH	2:O:129:ALA:HB1	1.62	0.98
2:O:34:ASN:ND2	2:O:35:ASP:H	1.62	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:154:THR:HG22	4:Q:155:VAL:H	1.25	0.98
3:P:171:VAL:HG12	3:P:231:LEU:HD11	1.45	0.98
1:A:113:PRO:HA	1:N:16:ALA:HB2	1.45	0.97
3:C:36:VAL:HG12	3:C:48:ALA:HA	1.45	0.97
3:C:102:TYR:N	3:C:118:PRO:HG3	1.78	0.97
2:O:64:GLU:HG3	2:O:65:PRO:HD3	1.46	0.97
5:E:5:ALA:HB1	6:F:10:ALA:HB2	1.46	0.97
3:C:171:VAL:HG12	3:C:231:LEU:HD11	1.45	0.97
3:C:172:PHE:O	3:C:231:LEU:HB3	1.64	0.96
1:N:191:LEU:H	1:N:191:LEU:HD12	1.30	0.96
4:Q:60:LEU:HB2	4:Q:62:ASN:ND2	1.81	0.96
5:E:2:ILE:HA	6:F:6:MET:HB3	1.44	0.95
1:N:23:SER:HA	1:N:25:TYR:CZ	2.01	0.95
3:P:102:TYR:H	3:P:118:PRO:HG3	1.30	0.95
5:R:5:ALA:HB1	6:S:10:ALA:HB2	1.47	0.95
2:B:34:ASN:ND2	2:B:35:ASP:H	1.64	0.95
3:P:101:VAL:HB	3:P:118:PRO:CG	1.95	0.95
2:O:32:TRP:N	2:O:33:PRO:HD2	1.80	0.95
3:P:172:PHE:O	3:P:231:LEU:HB3	1.66	0.95
2:O:51:ILE:HD12	2:O:51:ILE:H	1.32	0.95
1:A:33:PHE:CE1	5:E:18:ILE:HD13	2.01	0.94
3:C:171:VAL:CG1	3:C:234:ASN:HB2	1.97	0.94
3:P:102:TYR:N	3:P:118:PRO:HG3	1.81	0.94
3:C:102:TYR:H	3:C:118:PRO:HG3	1.26	0.94
1:A:36:LEU:H	1:A:36:LEU:HD22	1.30	0.94
3:P:273:ILE:HG21	7:T:22:GLN:HB3	1.48	0.94
1:A:114:ARG:NH1	1:A:114:ARG:H	1.65	0.94
1:N:123:ILE:H	1:N:123:ILE:HD12	1.30	0.94
2:B:32:TRP:N	2:B:33:PRO:HD2	1.81	0.94
2:O:38:TYR:HB2	3:P:276:LYS:HD3	1.47	0.94
6:F:27:LEU:HD11	8:H:15:TRP:HE1	1.30	0.94
4:Q:67:SER:HA	4:Q:70:LEU:HD21	1.50	0.94
6:S:28:LEU:HA	6:S:31:GLN:HE21	1.32	0.94
6:S:8:TYR:O	6:S:12:LEU:HB2	1.67	0.94
3:C:101:VAL:HB	3:C:118:PRO:CG	1.97	0.93
1:A:114:ARG:HH11	1:A:114:ARG:N	1.66	0.93
5:R:2:ILE:HA	6:S:6:MET:HB3	1.51	0.93
7:T:21:TYR:HA	7:T:24:TYR:CD1	2.04	0.93
1:A:123:ILE:H	1:A:123:ILE:HD12	1.31	0.93
4:D:110:HIS:HB2	4:D:144:ALA:HA	1.49	0.93
2:O:125:ARG:HH11	2:O:126:ARG:H	1.02	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:146:LYS:HG2	3:C:248:VAL:HG22	1.51	0.92
12:O:1309:BNT:HAM2	3:P:148:ALA:N	1.83	0.92
1:N:211:ILE:HD13	1:N:212:SER:H	1.35	0.92
11:O:1306:OPC:HAL2	11:O:1306:OPC:HAT2	1.48	0.92
3:C:31:PRO:HB2	3:C:53:PRO:HG3	1.50	0.92
1:A:191:LEU:H	1:A:191:LEU:HD12	1.31	0.92
1:A:47:GLN:OE1	1:A:86:HIS:HA	1.69	0.92
1:A:142:GLN:HE21	2:B:68:PRO:HB2	1.34	0.92
2:B:150:PRO:CB	2:B:153:LYS:HB2	1.98	0.92
2:O:43:VAL:HG22	7:T:23:GLN:OE1	1.70	0.92
7:G:6:LEU:H	7:G:6:LEU:HD22	1.35	0.92
4:Q:110:HIS:HB2	4:Q:144:ALA:HA	1.51	0.92
11:N:1305:OPC:HAT1	11:N:1305:OPC:HAX1	1.51	0.92
1:A:39:ILE:HD12	2:B:47:THR:HG21	1.51	0.91
1:A:158:ILE:HG23	1:A:159:PRO:HD2	1.52	0.91
1:N:158:ILE:HG22	1:N:161:VAL:HG23	1.50	0.91
6:S:27:LEU:HD11	8:U:15:TRP:HE1	1.35	0.91
1:A:33:PHE:HE1	5:E:18:ILE:HD13	1.32	0.91
2:O:42:VAL:HG13	3:P:269:GLN:HB2	1.51	0.91
3:P:146:LYS:HG2	3:P:248:VAL:HG22	1.53	0.91
1:N:77:SER:OG	4:Q:41:TYR:HA	1.69	0.90
4:D:81:VAL:HG12	4:D:82:GLN:H	1.36	0.90
2:B:50:CYS:O	2:B:54:LEU:HG	1.71	0.90
6:F:8:TYR:O	6:F:12:LEU:HB2	1.70	0.90
1:N:47:GLN:OE1	1:N:86:HIS:HA	1.70	0.90
1:A:140:TRP:CZ3	2:B:67:ASN:HA	2.06	0.90
3:P:40:VAL:HG13	3:P:247:ILE:HD11	1.51	0.90
1:A:113:PRO:HA	1:N:16:ALA:CB	2.00	0.89
4:D:38:LEU:O	4:D:41:TYR:HB3	1.72	0.89
7:G:21:TYR:HA	7:G:24:TYR:CD1	2.07	0.89
1:N:140:TRP:HE1	1:N:180:LEU:HD13	1.37	0.89
1:A:14:ILE:HD12	1:A:15:GLN:N	1.88	0.89
1:A:214:PRO:HG3	5:E:29:ILE:HD13	1.53	0.89
7:T:21:TYR:HA	7:T:24:TYR:CE1	2.06	0.89
2:B:65:PRO:HB3	2:B:68:PRO:HB3	1.54	0.88
4:D:51:GLY:HA2	4:D:54:THR:HB	1.55	0.88
4:Q:81:VAL:HG12	4:Q:82:GLN:H	1.37	0.88
1:A:62:VAL:HG23	1:A:63:THR:H	1.37	0.88
3:C:188:ASP:H	3:C:193:VAL:HG22	1.36	0.88
1:N:119:ILE:HG23	2:O:109:ILE:HD11	1.55	0.88
11:O:1306:OPC:HAP2	11:O:1306:OPC:HAT2	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:7:PHE:HA	5:R:10:VAL:HG12	1.56	0.88
3:C:40:VAL:HG13	3:C:247:ILE:HD11	1.54	0.88
2:B:42:VAL:CG2	3:C:272:LEU:HB3	2.03	0.88
3:P:274:LEU:O	3:P:278:GLN:HB2	1.74	0.88
3:P:31:PRO:HB2	3:P:53:PRO:HG3	1.54	0.88
1:A:47:GLN:HE22	1:A:89:SER:HB3	1.38	0.88
2:O:89:ARG:HG3	2:O:90:SER:N	1.87	0.88
5:R:11:PHE:HA	5:R:14:LEU:HD23	1.56	0.88
3:P:101:VAL:HG23	3:P:103:PHE:CE2	2.08	0.88
8:H:4:LEU:C	8:H:6:TRP:H	1.78	0.87
3:C:149:ILE:HB	3:C:245:THR:HG23	1.57	0.87
1:N:167:ASP:HA	1:N:170:ARG:NE	1.88	0.87
3:P:233:ASN:HD22	3:P:234:ASN:H	1.23	0.87
3:P:199:ILE:HG22	3:P:200:GLN:H	1.38	0.87
4:Q:149:ALA:HB2	4:Q:178:TRP:CZ2	2.09	0.87
1:A:21:VAL:HG12	1:A:22:THR:H	1.40	0.87
2:O:75:ILE:HG22	2:O:76:LEU:H	1.39	0.87
2:B:32:TRP:O	2:B:32:TRP:HE3	1.56	0.87
7:G:21:TYR:HA	7:G:24:TYR:CE1	2.10	0.87
2:B:89:ARG:HG3	2:B:90:SER:N	1.90	0.87
2:O:124:PHE:HE1	5:R:26:ILE:HG21	1.37	0.87
1:N:32:ILE:HG22	1:N:33:PHE:N	1.90	0.87
11:N:1305:OPC:HAP1	11:N:1305:OPC:HBI1	1.54	0.86
1:N:32:ILE:CG2	1:N:33:PHE:H	1.88	0.86
2:O:32:TRP:HE3	2:O:32:TRP:O	1.56	0.86
7:T:20:ALA:HB1	7:T:24:TYR:OH	1.75	0.86
8:U:4:LEU:C	8:U:6:TRP:H	1.78	0.86
6:F:28:LEU:HA	6:F:31:GLN:HE21	1.38	0.86
1:N:31:ASN:HB3	1:N:34:TYR:HE2	1.38	0.86
5:E:7:PHE:HA	5:E:10:VAL:HG12	1.54	0.86
2:B:62:VAL:HG23	2:B:63:GLY:H	1.39	0.86
1:N:47:GLN:HE22	1:N:89:SER:HB3	1.39	0.86
4:Q:154:THR:HB	4:Q:161:VAL:CG2	2.06	0.86
3:P:101:VAL:HB	3:P:118:PRO:HG3	1.57	0.86
1:N:195:ILE:O	1:N:199:MET:HG3	1.76	0.86
4:D:67:SER:HA	4:D:70:LEU:HD21	1.55	0.85
6:F:27:LEU:CD1	8:H:15:TRP:HE1	1.88	0.85
3:P:171:VAL:CG1	3:P:234:ASN:HB2	2.06	0.85
3:P:272:LEU:HD21	4:Q:24:PHE:CE1	2.10	0.85
7:G:20:ALA:HB1	7:G:24:TYR:OH	1.75	0.85
5:R:2:ILE:HG23	5:R:3:LEU:H	1.42	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:176:ALA:HB3	3:C:199:ILE:HG21	1.57	0.85
3:P:271:MET:HB3	4:Q:23:ALA:CA	2.03	0.85
4:Q:93:VAL:HA	4:Q:99:ILE:HG22	1.56	0.85
2:O:38:TYR:HB2	3:P:276:LYS:CD	2.07	0.85
5:R:9:ILE:HG21	6:S:10:ALA:O	1.77	0.85
5:E:11:PHE:HA	5:E:14:LEU:HD23	1.59	0.84
1:N:69:VAL:HA	1:N:72:ILE:HD13	1.59	0.84
1:A:53:ALA:HA	4:D:42:PHE:HZ	1.42	0.84
5:E:2:ILE:HG23	5:E:3:LEU:H	1.41	0.84
1:N:14:ILE:HB	1:N:17:LEU:HD11	1.58	0.84
3:P:101:VAL:HG23	3:P:103:PHE:HE2	1.42	0.84
3:C:101:VAL:HG23	3:C:103:PHE:CE2	2.11	0.84
7:G:28:ASN:HD21	7:G:30:LEU:HD22	1.42	0.84
1:N:62:VAL:HG13	1:N:177:GLN:OE1	1.77	0.84
2:B:125:ARG:O	2:B:127:PRO:HD3	1.76	0.84
3:C:101:VAL:HG23	3:C:103:PHE:HE2	1.41	0.84
3:C:233:ASN:HD22	3:C:234:ASN:H	1.20	0.84
3:C:274:LEU:O	3:C:278:GLN:HB2	1.77	0.84
2:O:122:ASN:C	2:O:124:PHE:H	1.78	0.84
1:A:39:ILE:HG23	2:B:47:THR:HG21	1.60	0.84
2:O:31:ALA:HB1	7:T:30:LEU:HB2	1.59	0.84
2:O:81:LEU:HD23	2:O:84:VAL:HG23	1.60	0.84
4:Q:105:ASN:O	4:Q:148:LEU:HD22	1.77	0.84
4:D:125:LYS:HA	4:D:131:SER:O	1.77	0.84
1:A:195:ILE:O	1:A:199:MET:HG3	1.78	0.84
4:D:60:LEU:HB2	4:D:62:ASN:ND2	1.92	0.84
1:N:112:LYS:H	1:N:113:PRO:CD	1.90	0.84
3:P:188:ASP:H	3:P:193:VAL:HG22	1.43	0.84
3:P:176:ALA:HB3	3:P:199:ILE:HG21	1.56	0.83
1:N:101:VAL:HG11	13:O:1201:CLA:HMA2	1.60	0.83
2:B:125:ARG:NH1	2:B:125:ARG:HA	1.93	0.83
2:O:34:ASN:HD22	2:O:35:ASP:H	1.27	0.83
1:A:213:GLY:HA2	5:E:30:LYS:HZ1	1.43	0.83
2:O:124:PHE:O	2:O:125:ARG:HB2	1.77	0.83
1:A:114:ARG:O	1:A:116:LEU:N	2.11	0.83
1:A:202:HIS:O	1:A:206:ILE:HG13	1.77	0.83
3:P:55:ASP:OD1	3:P:57:LYS:HD2	1.79	0.83
1:A:140:TRP:O	2:B:68:PRO:HG3	1.79	0.83
4:D:118:ASN:OD1	4:D:121:GLU:HG2	1.77	0.83
4:D:35:LEU:H	4:D:37:PRO:HD2	1.43	0.83
1:N:83:ARG:NH1	2:O:60:ALA:HB1	1.94	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:27:LEU:CD1	8:U:15:TRP:HE1	1.92	0.83
2:B:75:ILE:O	2:B:77:PRO:HD3	1.78	0.83
3:C:199:ILE:HG22	3:C:200:GLN:H	1.44	0.83
4:D:73:HIS:CB	4:D:93:VAL:HG21	2.09	0.83
2:O:64:GLU:CG	2:O:65:PRO:HD3	2.09	0.83
1:A:52:PHE:O	1:A:55:THR:HG23	1.78	0.83
2:B:123:PRO:HB2	2:B:129:ALA:HB3	1.60	0.83
3:C:164:GLY:O	3:C:165:GLU:HG3	1.78	0.83
11:B:305:OPC:HBA1	11:C:306:OPC:HBX2	1.60	0.82
7:G:26:ARG:N	7:G:27:PRO:HD2	1.93	0.82
4:Q:35:LEU:H	4:Q:37:PRO:HD2	1.44	0.82
1:A:29:HIS:HB3	1:A:211:ILE:HD12	1.58	0.82
3:C:55:ASP:O	3:C:58:LEU:HD13	1.79	0.82
3:P:164:GLY:O	3:P:165:GLU:HG3	1.79	0.82
3:C:101:VAL:HB	3:C:118:PRO:HG3	1.61	0.82
7:G:5:VAL:HG13	7:G:8:LEU:HB3	1.60	0.82
4:Q:129:HIS:HB2	14:Q:201:FES:S1	2.19	0.82
1:N:112:LYS:N	1:N:113:PRO:HD2	1.94	0.82
1:N:52:PHE:O	1:N:55:THR:HG23	1.79	0.82
3:P:98:VAL:HB	3:P:128:VAL:HG21	1.60	0.82
2:O:79:TRP:HB2	2:O:80:TYR:CE2	2.15	0.81
2:O:124:PHE:CE1	5:R:26:ILE:HG21	2.15	0.81
2:O:125:ARG:NH1	2:O:126:ARG:H	1.77	0.81
2:O:129:ALA:O	2:O:132:ILE:HG13	1.80	0.81
2:O:53:ALA:O	2:O:57:LEU:HB2	1.80	0.81
11:O:1306:OPC:HAP2	11:O:1306:OPC:CAL	2.09	0.81
2:B:75:ILE:O	2:B:75:ILE:HG22	1.78	0.81
4:D:149:ALA:HB2	4:D:178:TRP:CZ2	2.14	0.81
1:N:28:PRO:HD2	2:O:33:PRO:HD3	1.62	0.81
7:T:9:VAL:HG23	7:T:10:PHE:H	1.43	0.81
1:A:53:ALA:HA	4:D:42:PHE:CZ	2.16	0.81
3:C:233:ASN:ND2	3:C:234:ASN:H	1.77	0.81
1:A:155:PRO:HG2	1:A:166:SER:HB3	1.61	0.81
4:D:36:TYR:N	4:D:37:PRO:HD2	1.94	0.81
2:O:91:LEU:CD2	2:O:96:LEU:HD12	2.11	0.81
4:Q:36:TYR:N	4:Q:37:PRO:HD2	1.94	0.81
4:Q:38:LEU:O	4:Q:41:TYR:HB3	1.81	0.81
7:G:9:VAL:HG23	7:G:10:PHE:H	1.45	0.81
2:B:39:VAL:HA	2:B:42:VAL:HG23	1.62	0.81
3:C:10:PRO:HA	3:C:106:TYR:HE2	1.46	0.81
2:O:125:ARG:CZ	2:O:125:ARG:HB3	2.07	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:28:LEU:HA	6:S:31:GLN:NE2	1.96	0.81
1:A:114:ARG:C	1:A:116:LEU:H	1.83	0.81
4:Q:118:ASN:OD1	4:Q:121:GLU:HG2	1.80	0.81
7:T:5:VAL:HG13	7:T:8:LEU:HB3	1.63	0.81
2:B:135:PHE:C	2:B:137:THR:H	1.82	0.81
2:B:79:TRP:CH2	5:E:1:MET:HA	2.15	0.81
3:C:86:PRO:HD3	3:C:132:LEU:HD22	1.63	0.81
1:N:66:TYR:CG	2:O:65:PRO:HG2	2.16	0.81
3:C:188:ASP:HB3	3:C:192:ASN:C	2.02	0.80
1:N:202:HIS:O	1:N:206:ILE:HG13	1.81	0.80
1:N:72:ILE:O	1:N:76:VAL:HG12	1.80	0.80
1:A:89:SER:HB2	2:B:51:ILE:HG21	1.63	0.80
2:B:51:ILE:H	2:B:51:ILE:HD12	1.46	0.80
1:N:31:ASN:HB3	1:N:34:TYR:CE2	2.15	0.80
1:N:30:VAL:O	1:N:30:VAL:HG12	1.81	0.80
2:O:105:PRO:HG2	2:O:106:LEU:H	1.46	0.80
3:P:149:ILE:HB	3:P:245:THR:HG23	1.61	0.80
1:A:113:PRO:HG2	1:A:114:ARG:HD3	1.63	0.80
2:B:61:MET:HG3	3:C:146:LYS:O	1.82	0.80
3:C:176:ALA:HB1	3:C:201:THR:OG1	1.80	0.80
3:P:91:PRO:O	3:P:92:GLU:HG2	1.81	0.80
5:R:15:PHE:HB3	5:R:19:ALA:HB3	1.63	0.80
4:Q:113:CYS:HG	4:Q:128:CYS:HG	0.82	0.80
7:T:16:LEU:HD22	7:T:16:LEU:O	1.82	0.80
2:O:32:TRP:H	2:O:33:PRO:HD2	1.47	0.80
2:O:117:VAL:HG13	2:O:118:ASN:N	1.96	0.80
1:A:142:GLN:HE21	2:B:68:PRO:CB	1.95	0.80
3:C:55:ASP:OD1	3:C:57:LYS:HD2	1.82	0.80
1:N:14:ILE:HB	1:N:17:LEU:CD1	2.11	0.80
2:O:122:ASN:HD22	5:R:27:LYS:N	1.79	0.80
7:T:6:LEU:H	7:T:6:LEU:HD22	1.46	0.80
3:P:188:ASP:HB3	3:P:192:ASN:C	2.01	0.80
3:P:55:ASP:O	3:P:58:LEU:HD13	1.82	0.79
4:Q:115:VAL:HG13	4:Q:126:CYS:HA	1.63	0.79
2:B:105:PRO:HG2	2:B:106:LEU:H	1.45	0.79
12:B:309:BNT:HAM2	3:C:148:ALA:N	1.98	0.79
3:C:98:VAL:HB	3:C:128:VAL:HG21	1.64	0.79
2:B:72:PRO:HG2	2:B:75:ILE:HG13	1.64	0.79
4:D:56:ALA:HB1	4:D:81:VAL:HG11	1.64	0.79
3:P:101:VAL:HB	3:P:118:PRO:CB	2.11	0.79
3:P:196:GLN:HE22	3:P:210:THR:CB	1.95	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:84:VAL:HG13	13:B:201:CLA:OBD	1.82	0.79
1:N:17:LEU:HG	1:N:20:ASP:HB2	1.63	0.79
3:P:180:ILE:HD11	3:P:182:LYS:O	1.82	0.79
4:Q:139:VAL:HG21	4:Q:144:ALA:O	1.83	0.79
2:O:135:PHE:C	2:O:137:THR:H	1.80	0.79
4:D:63:ASN:H	4:D:63:ASN:ND2	1.81	0.79
1:N:155:PRO:HG2	1:N:166:SER:HB3	1.65	0.79
1:A:209:GLN:CD	2:B:28:GLY:O	2.21	0.78
3:C:10:PRO:HA	3:C:106:TYR:CE2	2.18	0.78
3:C:91:PRO:O	3:C:92:GLU:HG2	1.83	0.78
2:B:34:ASN:HD22	2:B:35:ASP:H	1.31	0.78
3:C:91:PRO:O	3:C:95:LYS:HG2	1.82	0.78
2:O:32:TRP:H	2:O:33:PRO:CD	1.95	0.78
4:D:19:MET:SD	4:D:20:ASN:N	2.57	0.78
4:Q:111:LEU:HB3	14:Q:201:FES:S2	2.23	0.78
4:Q:70:LEU:CD1	4:Q:71:GLU:H	1.97	0.78
3:C:180:ILE:HD11	3:C:182:LYS:O	1.82	0.78
3:P:176:ALA:HB1	3:P:201:THR:OG1	1.82	0.78
3:C:101:VAL:HB	3:C:118:PRO:CB	2.14	0.78
1:A:69:VAL:HA	1:A:72:ILE:HD13	1.65	0.78
2:B:79:TRP:HZ3	5:E:1:MET:HA	1.43	0.78
1:N:27:PRO:HA	2:O:33:PRO:HD3	1.64	0.78
1:A:77:SER:HB2	4:D:41:TYR:HA	1.66	0.78
3:C:171:VAL:HG13	3:C:234:ASN:CB	2.08	0.78
3:P:79:PRO:HG2	3:P:82:PHE:CD1	2.19	0.78
11:B:305:OPC:OAI	11:B:305:OPC:HAV	1.84	0.78
6:S:27:LEU:HD13	6:S:27:LEU:N	1.99	0.78
2:B:18:LEU:N	2:B:31:ALA:HB2	1.98	0.78
2:B:117:VAL:HG23	2:B:118:ASN:N	1.99	0.78
2:B:129:ALA:O	2:B:132:ILE:HG13	1.81	0.78
5:E:15:PHE:HB3	5:E:19:ALA:HB3	1.66	0.78
11:B:305:OPC:HAS2	11:B:305:OPC:CAO	2.13	0.77
3:C:275:LYS:NZ	11:C:306:OPC:HBG3	1.98	0.77
5:E:9:ILE:HG21	6:F:10:ALA:O	1.84	0.77
1:N:209:GLN:NE2	2:O:28:GLY:N	2.31	0.77
5:R:11:PHE:CA	5:R:14:LEU:HD23	2.13	0.77
1:A:156:GLU:O	1:A:163:VAL:HG22	1.84	0.77
3:C:78:LEU:HD21	3:C:131:VAL:HG21	1.66	0.77
3:C:60:GLN:OE1	3:C:156:GLY:HA2	1.84	0.77
4:D:115:VAL:HG13	4:D:126:CYS:HA	1.63	0.77
1:A:47:GLN:NE2	1:A:90:ALA:N	2.31	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:192:ASN:O	3:C:193:VAL:HG23	1.84	0.77
4:Q:56:ALA:HB1	4:Q:81:VAL:HG11	1.66	0.77
3:C:267:LEU:O	3:C:270:LEU:HB3	1.84	0.77
2:B:79:TRP:CH2	5:E:1:MET:SD	2.78	0.77
4:D:154:THR:HB	4:D:161:VAL:CG2	2.14	0.77
2:O:89:ARG:CG	2:O:90:SER:H	1.96	0.77
4:Q:94:GLU:CD	4:Q:100:ARG:HG2	2.05	0.77
1:A:41:LEU:HD23	1:A:42:THR:N	2.00	0.77
1:A:141:ASP:HA	2:B:65:PRO:HG2	1.65	0.77
8:H:18:ALA:O	8:H:21:VAL:HG22	1.84	0.77
1:N:15:GLN:NE2	1:N:15:GLN:N	2.33	0.77
3:P:267:LEU:O	3:P:270:LEU:HB3	1.84	0.77
4:D:50:VAL:HG21	4:D:164:PRO:HG2	1.67	0.77
6:S:28:LEU:C	6:S:30:ILE:H	1.87	0.77
1:A:29:HIS:CD2	1:A:211:ILE:HB	2.20	0.76
5:E:9:ILE:O	5:E:12:ILE:HG22	1.85	0.76
2:O:40:PHE:HA	2:O:43:VAL:HG23	1.66	0.76
7:T:18:TYR:HA	7:T:21:TYR:CD2	2.20	0.76
8:U:18:ALA:O	8:U:21:VAL:HG22	1.85	0.76
1:A:28:PRO:CG	2:B:32:TRP:HB3	2.15	0.76
4:D:93:VAL:HA	4:D:99:ILE:HG22	1.66	0.76
6:F:26:LEU:O	6:F:26:LEU:HD23	1.85	0.76
1:N:20:ASP:O	1:N:21:VAL:HG13	1.82	0.76
2:B:108:LEU:O	2:B:111:VAL:HG23	1.85	0.76
1:N:63:THR:C	1:N:65:ALA:H	1.84	0.76
2:B:91:LEU:CD2	2:B:96:LEU:HD12	2.14	0.76
3:P:154:ASN:O	3:P:155:ARG:HB3	1.86	0.76
1:A:121:GLY:O	1:A:124:LEU:HB2	1.85	0.76
4:D:51:GLY:CA	4:D:54:THR:HB	2.15	0.76
4:D:70:LEU:CD1	4:D:71:GLU:H	1.97	0.76
6:F:26:LEU:HD22	8:H:15:TRP:HZ2	1.51	0.76
3:P:233:ASN:ND2	3:P:234:ASN:H	1.82	0.76
8:U:1:ILE:HG23	8:U:2:ASP:H	1.50	0.76
2:O:32:TRP:N	2:O:33:PRO:CD	2.48	0.76
2:O:38:TYR:CD1	3:P:276:LYS:NZ	2.51	0.76
2:B:32:TRP:N	2:B:33:PRO:CD	2.48	0.76
1:N:123:ILE:CD1	1:N:123:ILE:H	1.99	0.76
1:N:135:GLY:HA2	1:N:138:LEU:CD1	2.16	0.76
6:S:26:LEU:HD22	8:U:15:TRP:HZ2	1.50	0.76
7:G:16:LEU:O	7:G:16:LEU:HD22	1.85	0.76
3:C:196:GLN:HE22	3:C:210:THR:CB	1.97	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:205:LYS:HZ3	3:C:207:VAL:HG12	1.51	0.76
3:P:63:ALA:HA	3:P:157:ARG:NH1	2.01	0.76
1:N:121:GLY:O	1:N:124:LEU:HB2	1.86	0.75
4:D:139:VAL:HG21	4:D:144:ALA:O	1.85	0.75
1:A:52:PHE:HB2	1:N:189:PHE:CE2	2.21	0.75
11:N:1305:OPC:HBZ1	11:N:1305:OPC:HAY2	1.68	0.75
2:O:91:LEU:HD22	2:O:96:LEU:HD12	1.68	0.75
5:E:18:ILE:HA	5:E:22:ILE:CG2	2.14	0.75
11:B:305:OPC:HBT1	11:C:306:OPC:HBR	1.68	0.75
1:N:63:THR:O	1:N:65:ALA:N	2.18	0.75
1:N:28:PRO:HD2	2:O:33:PRO:CD	2.17	0.75
3:C:280:GLU:C	3:C:282:VAL:H	1.89	0.75
4:D:40:LYS:O	4:D:43:ILE:HB	1.87	0.75
7:G:18:TYR:HA	7:G:21:TYR:CD2	2.21	0.75
3:P:171:VAL:HG13	3:P:234:ASN:CB	2.12	0.75
2:B:112:PRO:O	2:B:116:ASN:HB2	1.87	0.75
2:B:39:VAL:HA	2:B:42:VAL:CG2	2.17	0.75
3:P:10:PRO:HA	3:P:106:TYR:CE2	2.22	0.75
2:B:122:ASN:HB2	2:B:123:PRO:HD2	1.68	0.75
1:N:185:SER:O	1:N:189:PHE:HB3	1.87	0.75
3:C:249:LEU:HD12	3:C:249:LEU:H	1.52	0.75
3:P:86:PRO:HD3	3:P:132:LEU:HD22	1.69	0.75
3:C:188:ASP:OD2	3:C:192:ASN:HB3	1.87	0.74
3:C:79:PRO:HG2	3:C:82:PHE:CD1	2.22	0.74
5:E:22:ILE:CG2	5:E:23:ILE:N	2.50	0.74
1:A:138:LEU:N	1:A:139:PRO:HD2	2.01	0.74
2:O:39:VAL:HA	2:O:42:VAL:HG23	1.67	0.74
3:P:78:LEU:HD21	3:P:131:VAL:HG21	1.67	0.74
4:Q:125:LYS:HA	4:Q:131:SER:O	1.86	0.74
3:C:219:VAL:HG12	3:C:220:SER:H	1.52	0.74
6:F:28:LEU:C	6:F:30:ILE:H	1.90	0.74
2:O:81:LEU:O	2:O:85:PHE:HB2	1.88	0.74
3:P:60:GLN:OE1	3:P:156:GLY:HA2	1.86	0.74
3:P:271:MET:HA	3:P:274:LEU:HD12	1.68	0.74
1:A:158:ILE:O	1:A:163:VAL:HG23	1.87	0.74
3:P:219:VAL:HG12	3:P:220:SER:H	1.52	0.74
4:D:50:VAL:HB	4:D:84:LEU:HD13	1.67	0.74
2:O:29:GLU:N	2:O:30:PRO:HD3	2.01	0.74
1:A:111:LYS:CB	1:A:114:ARG:HH22	2.00	0.74
7:G:8:LEU:O	7:G:8:LEU:HD23	1.88	0.74
11:O:1306:OPC:HBX2	11:O:1306:OPC:HBT2	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:51:ILE:HD12	2:O:51:ILE:N	2.03	0.74
2:B:79:TRP:O	2:B:80:TYR:CD1	2.41	0.74
2:B:91:LEU:HD22	2:B:96:LEU:HD12	1.67	0.74
1:N:47:GLN:NE2	1:N:90:ALA:N	2.36	0.74
4:Q:19:MET:SD	4:Q:20:ASN:N	2.61	0.74
5:R:9:ILE:O	5:R:12:ILE:HG22	1.87	0.74
1:A:102:PHE:O	1:A:106:LEU:HB2	1.88	0.74
2:B:133:PHE:CE2	2:B:137:THR:HG21	2.23	0.74
2:B:57:LEU:HD13	7:G:10:PHE:CD2	2.23	0.74
1:N:41:LEU:HD23	1:N:42:THR:N	2.02	0.74
5:E:10:VAL:O	5:E:11:PHE:HB3	1.87	0.73
6:F:28:LEU:HA	6:F:31:GLN:NE2	2.01	0.73
1:N:15:GLN:C	1:N:15:GLN:HE21	1.91	0.73
3:P:280:GLU:C	3:P:282:VAL:H	1.90	0.73
3:P:2:PRO:HB3	3:P:115:LEU:HD22	1.70	0.73
1:A:111:LYS:HB3	1:A:114:ARG:HH22	1.53	0.73
1:A:147:ALA:HB2	2:B:75:ILE:HG23	1.69	0.73
3:C:2:PRO:HB3	3:C:115:LEU:HD22	1.68	0.73
2:B:57:LEU:HD11	7:G:10:PHE:HA	1.68	0.73
6:S:8:TYR:HA	6:S:11:LEU:HD11	1.70	0.73
1:N:87:ARG:HD2	2:O:61:MET:CE	2.14	0.73
3:P:10:PRO:HA	3:P:106:TYR:HE2	1.52	0.73
4:Q:22:LEU:HD23	4:Q:23:ALA:N	2.03	0.73
1:A:135:GLY:HA2	1:A:138:LEU:CD1	2.18	0.73
1:A:28:PRO:HG3	2:B:32:TRP:HB3	1.70	0.73
2:O:93:ASN:OD1	2:O:94:LYS:N	2.18	0.73
1:A:114:ARG:HG3	1:A:208:LYS:CD	2.19	0.73
3:C:185:LYS:CD	3:C:195:TYR:HB3	2.19	0.73
4:D:73:HIS:HB3	4:D:93:VAL:HG21	1.71	0.73
5:E:5:ALA:HB1	6:F:10:ALA:CB	2.19	0.73
6:F:8:TYR:HA	6:F:11:LEU:HD11	1.68	0.73
3:P:70:LEU:HD11	3:P:122:GLU:HB2	1.71	0.73
3:P:231:LEU:HD13	3:P:233:ASN:N	2.02	0.73
3:P:176:ALA:CB	3:P:199:ILE:HG21	2.19	0.73
4:Q:73:HIS:CB	4:Q:93:VAL:HG21	2.18	0.73
2:B:89:ARG:CG	2:B:90:SER:H	2.01	0.73
5:E:11:PHE:CA	5:E:14:LEU:HD23	2.19	0.73
11:N:1305:OPC:HAT1	11:N:1305:OPC:CAX	2.18	0.73
3:P:282:VAL:O	3:P:285:ALA:HB3	1.89	0.73
2:B:122:ASN:HD21	2:B:124:PHE:HB3	1.51	0.72
3:C:185:LYS:HD2	3:C:195:TYR:CD2	2.24	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:45:LEU:HB2	11:N:1305:OPC:OBH	1.89	0.72
1:N:21:VAL:HG23	1:N:22:THR:H	1.53	0.72
1:N:29:HIS:NE2	1:N:31:ASN:ND2	2.35	0.72
4:Q:171:ARG:HH11	4:Q:171:ARG:HB2	1.53	0.72
1:A:103:ARG:HH11	1:A:103:ARG:HG3	1.53	0.72
1:A:21:VAL:O	1:A:23:SER:N	2.21	0.72
3:C:154:ASN:O	3:C:155:ARG:HB3	1.88	0.72
3:C:63:ALA:HA	3:C:157:ARG:NH1	2.03	0.72
1:N:149:LYS:O	1:N:149:LYS:HD3	1.89	0.72
1:N:15:GLN:C	1:N:17:LEU:H	1.92	0.72
2:O:39:VAL:HA	2:O:42:VAL:CG2	2.18	0.72
4:Q:60:LEU:HB2	4:Q:62:ASN:HD22	1.48	0.72
2:B:62:VAL:HG23	2:B:63:GLY:N	2.04	0.72
3:C:23:ALA:C	3:C:25:CYS:H	1.93	0.72
4:D:105:ASN:O	4:D:148:LEU:HD22	1.90	0.72
4:D:22:LEU:HD23	4:D:23:ALA:N	2.04	0.72
7:G:5:VAL:O	7:G:5:VAL:HG12	1.89	0.72
2:O:52:VAL:O	2:O:56:VAL:HG22	1.88	0.72
4:D:88:PRO:HB3	2:O:69:PHE:HD2	1.55	0.72
3:P:215:PRO:HB3	3:P:235:PRO:HD3	1.72	0.72
2:B:93:ASN:OD1	2:B:94:LYS:N	2.22	0.72
2:O:119:LYS:O	2:O:123:PRO:HB3	1.89	0.72
3:P:249:LEU:H	3:P:249:LEU:HD12	1.53	0.72
4:Q:51:GLY:O	4:Q:54:THR:HG22	1.88	0.72
5:R:10:VAL:O	5:R:10:VAL:HG13	1.90	0.72
1:A:148:VAL:HA	1:A:151:VAL:CG2	2.18	0.72
3:C:185:LYS:HD2	3:C:195:TYR:HB3	1.71	0.72
2:O:74:GLU:O	2:O:75:ILE:O	2.06	0.72
1:A:114:ARG:HH11	1:A:114:ARG:H	0.84	0.72
1:A:123:ILE:CD1	1:A:123:ILE:H	2.01	0.72
3:C:170:ASN:O	3:C:235:PRO:HD2	1.89	0.72
3:C:282:VAL:O	3:C:285:ALA:HB3	1.90	0.72
3:C:70:LEU:HD11	3:C:122:GLU:HB2	1.72	0.72
4:D:104:ILE:HD12	4:D:104:ILE:O	1.90	0.72
1:N:196:ALA:O	1:N:200:LEU:HD23	1.89	0.72
2:O:108:LEU:O	2:O:111:VAL:HG23	1.88	0.72
7:T:8:LEU:HD23	7:T:8:LEU:O	1.88	0.72
1:A:99:LEU:N	1:A:99:LEU:HD23	2.05	0.72
2:B:65:PRO:HB3	2:B:68:PRO:CB	2.19	0.72
2:B:65:PRO:C	2:B:68:PRO:HD3	2.10	0.72
5:E:10:VAL:HG13	5:E:10:VAL:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:19:ASP:O	1:N:21:VAL:N	2.22	0.72
11:O:1306:OPC:HCB3	11:O:1306:OPC:HBB2	1.70	0.72
2:B:18:LEU:N	2:B:31:ALA:CB	2.53	0.72
3:C:271:MET:HG3	3:C:274:LEU:HD12	1.70	0.72
4:D:94:GLU:CD	4:D:100:ARG:HG2	2.10	0.72
1:N:58:TYR:HD2	1:N:184:TYR:HE1	1.38	0.72
2:O:106:LEU:O	2:O:109:ILE:HG22	1.90	0.71
3:P:9:TYR:C	3:P:11:PRO:HD2	2.10	0.71
3:P:185:LYS:HD2	3:P:195:TYR:HB3	1.69	0.71
4:Q:67:SER:HA	4:Q:70:LEU:CD2	2.20	0.71
1:A:158:ILE:CG2	1:A:159:PRO:HD2	2.20	0.71
11:C:306:OPC:CAP	11:C:306:OPC:HAL2	2.20	0.71
3:C:233:ASN:ND2	3:C:234:ASN:N	2.38	0.71
3:P:34:VAL:CG1	3:P:151:LEU:HD13	2.21	0.71
1:A:171:GLY:HA3	1:A:178:ALA:HB1	1.71	0.71
1:A:21:VAL:HG12	1:A:22:THR:N	2.04	0.71
1:A:25:TYR:O	1:A:26:VAL:HG22	1.91	0.71
2:B:122:ASN:HD22	2:B:124:PHE:HB3	1.52	0.71
3:C:231:LEU:HD13	3:C:233:ASN:N	2.04	0.71
2:O:133:PHE:CE2	2:O:137:THR:HG21	2.25	0.71
1:N:208:LYS:HG2	2:O:27:TYR:CZ	2.25	0.71
4:D:88:PRO:HB3	2:O:69:PHE:CD2	2.26	0.71
2:B:74:GLU:O	2:B:75:ILE:HB	1.90	0.71
3:C:271:MET:HA	3:C:274:LEU:HD12	1.72	0.71
7:G:26:ARG:HD3	7:G:27:PRO:CD	2.15	0.71
4:Q:21:LEU:O	4:Q:25:GLY:HA3	1.90	0.71
5:R:10:VAL:O	5:R:11:PHE:HB3	1.89	0.71
3:C:34:VAL:CG1	3:C:151:LEU:HD13	2.20	0.71
3:P:188:ASP:OD2	3:P:192:ASN:HB3	1.89	0.71
3:P:271:MET:HG3	3:P:274:LEU:HD12	1.72	0.71
3:C:233:ASN:HD22	3:C:234:ASN:N	1.89	0.71
5:E:7:PHE:HA	5:E:10:VAL:CG1	2.20	0.71
1:N:111:LYS:HB3	1:N:113:PRO:HD2	1.72	0.71
1:N:127:ILE:HD13	1:N:194:LEU:HB2	1.71	0.71
3:P:192:ASN:O	3:P:193:VAL:HG23	1.90	0.71
3:P:91:PRO:O	3:P:95:LYS:HG2	1.90	0.71
1:A:149:LYS:HD3	1:A:149:LYS:O	1.88	0.71
3:C:159:GLN:HG3	3:C:169:ASN:O	1.90	0.71
1:N:16:ALA:O	1:N:17:LEU:O	2.08	0.71
3:C:282:VAL:HG23	3:C:283:GLN:H	1.55	0.71
6:F:27:LEU:HD11	8:H:15:TRP:NE1	2.06	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:SER:O	1:A:189:PHE:HB3	1.91	0.70
8:H:4:LEU:C	8:H:6:TRP:N	2.44	0.70
3:P:83:LYS:NZ	3:P:132:LEU:O	2.24	0.70
6:S:26:LEU:HD23	6:S:26:LEU:O	1.90	0.70
11:C:306:OPC:HAP1	11:C:306:OPC:OBJ	1.91	0.70
4:D:154:THR:HG22	4:D:155:VAL:N	2.04	0.70
4:D:84:LEU:O	4:D:85:LYS:HB2	1.90	0.70
5:R:15:PHE:HB3	5:R:19:ALA:CB	2.21	0.70
3:C:9:TYR:C	3:C:11:PRO:HD2	2.11	0.70
1:N:123:ILE:N	1:N:123:ILE:HD12	2.05	0.70
3:P:25:CYS:HA	3:P:160:ILE:HD12	1.73	0.70
2:O:38:TYR:HB2	3:P:276:LYS:CE	2.21	0.70
8:U:4:LEU:C	8:U:6:TRP:N	2.43	0.70
1:A:176:GLY:O	1:A:177:GLN:C	2.30	0.70
6:F:23:LEU:O	6:F:27:LEU:HD13	1.90	0.70
1:N:80:TRP:CZ3	1:N:81:LEU:HD23	2.27	0.70
1:A:52:PHE:O	1:A:54:MET:N	2.25	0.70
2:B:43:VAL:HA	7:G:23:GLN:OE1	1.91	0.70
3:C:25:CYS:HA	3:C:160:ILE:HD12	1.74	0.70
6:F:27:LEU:HD13	6:F:27:LEU:N	2.05	0.70
1:N:15:GLN:O	1:N:17:LEU:N	2.20	0.70
2:O:62:VAL:HG22	12:O:1309:BNT:CAM	2.21	0.70
3:P:185:LYS:CD	3:P:195:TYR:HB3	2.21	0.70
4:Q:154:THR:HB	4:Q:161:VAL:HG23	1.72	0.70
5:R:24:PHE:C	5:R:26:ILE:H	1.93	0.70
6:S:26:LEU:HD22	8:U:15:TRP:CZ2	2.27	0.70
6:F:16:LEU:HD13	6:F:19:VAL:HG21	1.73	0.70
1:A:47:GLN:HE22	1:A:89:SER:CB	2.04	0.70
3:C:266:MET:HA	3:C:269:GLN:NE2	2.07	0.70
4:D:50:VAL:C	4:D:84:LEU:HD21	2.12	0.70
3:P:169:ASN:ND2	3:P:237:VAL:H	1.90	0.70
4:Q:65:LYS:O	4:Q:68:LYS:HG2	1.91	0.70
5:R:22:ILE:CG2	5:R:23:ILE:N	2.54	0.70
7:T:5:VAL:O	7:T:5:VAL:HG12	1.91	0.70
1:N:47:GLN:CB	9:N:301:HEM:HBB2	2.22	0.70
2:O:104:VAL:N	2:O:105:PRO:HD2	2.07	0.70
2:O:122:ASN:ND2	5:R:27:LYS:N	2.40	0.70
2:B:124:PHE:CZ	5:E:27:LYS:HB2	2.27	0.70
5:E:5:ALA:O	6:F:10:ALA:HA	1.92	0.70
1:N:56:PHE:O	1:N:57:TYR:HD2	1.75	0.70
1:N:85:ILE:HA	2:O:51:ILE:HG22	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:104:VAL:H	2:O:105:PRO:HD2	1.56	0.69
2:B:32:TRP:O	2:B:32:TRP:CE3	2.44	0.69
1:A:142:GLN:N	2:B:65:PRO:HG2	2.06	0.69
3:C:28:ALA:HB1	3:C:238:GLY:O	1.91	0.69
7:G:20:ALA:CB	7:G:24:TYR:OH	2.40	0.69
1:N:188:THR:C	1:N:192:PRO:HG3	2.12	0.69
4:Q:27:VAL:C	4:Q:29:GLY:H	1.96	0.69
2:O:57:LEU:HD21	7:T:9:VAL:O	1.91	0.69
5:E:22:ILE:HG22	5:E:23:ILE:H	1.58	0.69
8:H:22:TRP:NE1	8:H:26:GLY:HA3	2.06	0.69
2:O:117:VAL:CG1	2:O:118:ASN:H	2.00	0.69
4:Q:116:PRO:HD2	4:Q:127:PRO:HD3	1.74	0.69
1:N:139:PRO:HG3	9:N:301:HEM:O1A	1.92	0.69
2:O:42:VAL:HG13	3:P:269:GLN:CB	2.20	0.69
7:T:28:ASN:OD1	7:T:30:LEU:HD21	1.92	0.69
2:B:125:ARG:CA	2:B:125:ARG:HH11	1.98	0.69
7:G:8:LEU:O	7:G:12:THR:HG23	1.92	0.69
1:N:15:GLN:N	1:N:15:GLN:CD	2.43	0.69
3:P:233:ASN:HD22	3:P:234:ASN:N	1.91	0.69
3:P:89:ARG:HG3	3:P:89:ARG:HH11	1.57	0.69
4:Q:126:CYS:SG	4:Q:127:PRO:HD2	2.32	0.69
4:Q:18:PHE:O	4:Q:21:LEU:HG	1.92	0.69
1:A:152:SER:HB2	1:A:170:ARG:HD2	1.74	0.69
2:B:106:LEU:O	2:B:109:ILE:HG22	1.92	0.69
2:O:51:ILE:CD1	2:O:51:ILE:H	2.05	0.69
6:S:23:LEU:O	6:S:27:LEU:HD13	1.91	0.69
1:A:160:VAL:HG12	1:A:161:VAL:H	1.58	0.69
2:B:49:ALA:O	2:B:52:VAL:HB	1.93	0.69
8:U:1:ILE:HG23	8:U:2:ASP:N	2.08	0.69
1:A:158:ILE:CG2	1:A:162:GLY:HA3	2.23	0.69
1:A:188:THR:C	1:A:192:PRO:HG3	2.13	0.69
1:N:105:TYR:HH	2:O:129:ALA:HB1	1.56	0.69
12:O:1309:BNT:HAM2	3:P:148:ALA:H	1.56	0.69
5:R:9:ILE:HG13	6:S:14:PHE:HB2	1.73	0.69
6:S:27:LEU:HD23	7:T:25:LYS:HD2	1.73	0.69
1:A:60:PRO:C	1:A:180:LEU:HD21	2.12	0.69
4:D:53:GLY:CA	4:D:57:LYS:HD3	2.20	0.69
5:E:24:PHE:C	5:E:26:ILE:H	1.96	0.69
3:P:179:THR:HB	3:P:225:VAL:HG22	1.74	0.69
7:T:10:PHE:O	7:T:12:THR:N	2.26	0.69
11:B:305:OPC:HAG2	11:B:305:OPC:HBX1	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:59:LYS:HB2	4:D:59:LYS:NZ	2.08	0.69
1:N:211:ILE:CD1	1:N:212:SER:H	2.06	0.69
1:A:155:PRO:HG2	1:A:166:SER:CB	2.22	0.69
1:A:66:TYR:CB	1:A:140:TRP:HE3	2.06	0.69
3:C:84:ILE:HD12	3:C:130:PRO:O	1.93	0.69
5:E:15:PHE:HB3	5:E:19:ALA:CB	2.23	0.69
1:N:103:ARG:HG3	1:N:103:ARG:HH11	1.56	0.69
3:P:263:CYS:O	3:P:267:LEU:HD13	1.93	0.69
3:C:219:VAL:HG12	3:C:220:SER:N	2.08	0.68
3:C:36:VAL:HB	3:C:37:PRO:HD2	1.75	0.68
3:C:45:VAL:HG13	3:C:85:ALA:HB2	1.75	0.68
5:R:13:ALA:HA	6:S:14:PHE:HE1	1.58	0.68
5:R:11:PHE:O	5:R:14:LEU:HB2	1.91	0.68
3:C:263:CYS:O	3:C:267:LEU:HD13	1.93	0.68
1:N:104:VAL:HG12	1:N:105:TYR:N	2.07	0.68
3:P:188:ASP:N	3:P:193:VAL:HA	2.08	0.68
3:P:23:ALA:C	3:P:25:CYS:H	1.94	0.68
1:A:214:PRO:HD3	5:E:29:ILE:HG21	1.76	0.68
5:E:16:PHE:HE2	15:E:101:BCR:H373	1.56	0.68
5:R:5:ALA:HB1	6:S:10:ALA:CB	2.20	0.68
1:A:61:THR:HG21	1:A:64:GLU:OE1	1.91	0.68
3:C:241:GLY:O	3:C:242:GLN:HB2	1.93	0.68
4:D:67:SER:HA	4:D:70:LEU:CD2	2.23	0.68
1:N:118:TRP:CZ3	2:O:109:ILE:HA	2.29	0.68
2:O:42:VAL:CG2	3:P:272:LEU:HB3	2.23	0.68
11:C:306:OPC:OBH	11:C:306:OPC:HAP2	1.94	0.68
5:E:13:ALA:HA	6:F:14:PHE:HE1	1.59	0.68
1:N:139:PRO:HG2	1:N:141:ASP:OD1	1.94	0.68
2:O:40:PHE:HA	2:O:43:VAL:CG2	2.23	0.68
4:Q:104:ILE:HD12	4:Q:104:ILE:O	1.94	0.68
1:A:33:PHE:HB3	1:A:103:ARG:HG2	1.76	0.68
3:C:176:ALA:CB	3:C:199:ILE:HG21	2.22	0.68
7:T:20:ALA:CB	7:T:24:TYR:OH	2.41	0.68
2:B:123:PRO:HB2	2:B:129:ALA:CB	2.23	0.68
4:D:154:THR:HB	4:D:161:VAL:HG23	1.76	0.68
5:E:5:ALA:CB	6:F:10:ALA:HB2	2.22	0.68
1:N:111:LYS:NZ	1:N:112:LYS:HG3	2.09	0.68
1:N:52:PHE:O	1:N:54:MET:N	2.27	0.68
3:P:185:LYS:HD2	3:P:195:TYR:CD2	2.29	0.68
3:P:282:VAL:HG23	3:P:283:GLN:H	1.57	0.68
6:S:8:TYR:CD2	6:S:9:ALA:N	2.62	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:VAL:HG12	1:A:105:TYR:N	2.06	0.68
3:C:89:ARG:HH11	3:C:89:ARG:HG3	1.58	0.68
11:N:1305:OPC:HBN2	11:N:1305:OPC:CBR	2.24	0.68
2:O:81:LEU:O	2:O:85:PHE:CB	2.42	0.68
4:Q:40:LYS:O	4:Q:43:ILE:HB	1.94	0.68
4:Q:67:SER:O	4:Q:70:LEU:HD11	1.94	0.68
4:D:63:ASN:HD22	4:D:63:ASN:N	1.92	0.68
1:N:167:ASP:CA	1:N:170:ARG:HE	1.97	0.68
1:N:51:GLY:HA2	1:N:54:MET:HE3	1.73	0.68
1:N:111:LYS:HE2	2:O:118:ASN:O	1.93	0.68
3:P:82:PHE:HA	3:P:83:LYS:HZ2	1.59	0.68
6:S:16:LEU:HD13	6:S:19:VAL:HG21	1.75	0.68
7:T:8:LEU:O	7:T:12:THR:HG23	1.94	0.68
2:B:18:LEU:HD12	2:B:18:LEU:O	1.94	0.67
2:B:38:TYR:HB2	3:C:276:LYS:NZ	2.08	0.67
1:A:127:ILE:HD13	1:A:194:LEU:HB2	1.75	0.67
2:B:133:PHE:O	2:B:135:PHE:N	2.26	0.67
2:B:132:ILE:HA	2:B:135:PHE:HD2	1.59	0.67
1:A:141:ASP:CA	2:B:65:PRO:HG2	2.23	0.67
3:C:154:ASN:OD1	3:C:155:ARG:N	2.26	0.67
4:D:18:PHE:O	4:D:21:LEU:HG	1.95	0.67
5:E:9:ILE:HG13	6:F:14:PHE:HB2	1.76	0.67
2:O:40:PHE:CA	2:O:43:VAL:HG23	2.24	0.67
5:R:18:ILE:HA	5:R:22:ILE:CG2	2.18	0.67
4:D:53:GLY:HA2	4:D:57:LYS:CD	2.22	0.67
1:N:188:THR:O	1:N:192:PRO:HG3	1.94	0.67
5:E:26:ILE:HG23	5:E:30:LYS:HE2	1.76	0.67
1:N:159:PRO:C	1:N:161:VAL:H	1.97	0.67
1:N:165:ILE:CG2	1:N:166:SER:N	2.57	0.67
1:A:140:TRP:CH2	2:B:67:ASN:HA	2.29	0.67
1:A:77:SER:O	1:A:78:PHE:HB2	1.94	0.67
2:B:77:PRO:O	2:B:78:GLU:O	2.12	0.67
3:C:78:LEU:HG	3:C:79:PRO:HD2	1.76	0.67
6:F:26:LEU:HD22	8:H:15:TRP:CZ2	2.29	0.67
1:N:170:ARG:HA	1:N:179:THR:HA	1.75	0.67
2:O:32:TRP:O	2:O:32:TRP:CE3	2.44	0.67
5:R:7:PHE:HA	5:R:10:VAL:CG1	2.24	0.67
7:T:10:PHE:C	7:T:12:THR:N	2.47	0.67
2:B:75:ILE:O	2:B:77:PRO:CD	2.42	0.67
7:G:16:LEU:O	7:G:16:LEU:HD13	1.95	0.67
7:T:26:ARG:N	7:T:27:PRO:HD3	2.08	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ILE:CG2	1:A:166:SER:N	2.57	0.67
1:N:111:LYS:HZ2	1:N:112:LYS:HG3	1.60	0.67
1:N:162:GLY:HA2	1:N:165:ILE:HG21	1.76	0.67
2:O:132:ILE:HA	2:O:135:PHE:HD2	1.59	0.67
3:P:233:ASN:ND2	3:P:234:ASN:N	2.43	0.67
2:O:38:TYR:CB	3:P:276:LYS:HD3	2.25	0.67
4:Q:154:THR:HG22	4:Q:155:VAL:N	2.06	0.67
2:B:150:PRO:HB2	2:B:153:LYS:O	1.94	0.67
2:B:40:PHE:HA	2:B:43:VAL:HG23	1.75	0.67
7:G:16:LEU:HD13	7:G:16:LEU:C	2.15	0.67
1:N:114:ARG:HG3	1:N:117:THR:CG2	2.24	0.67
1:N:99:LEU:N	1:N:99:LEU:HD23	2.09	0.67
2:O:105:PRO:HG3	13:O:1201:CLA:H112	1.77	0.67
2:O:78:GLU:HB3	2:O:80:TYR:CE1	2.29	0.67
3:P:45:VAL:HG13	3:P:85:ALA:HB2	1.76	0.67
3:P:91:PRO:O	3:P:95:LYS:HE2	1.94	0.67
7:T:17:PHE:HB3	7:T:21:TYR:CE1	2.29	0.67
8:U:3:VAL:O	8:U:6:TRP:HB2	1.95	0.67
1:A:114:ARG:HG3	1:A:208:LYS:HD2	1.74	0.67
8:H:1:ILE:HG23	8:H:2:ASP:H	1.60	0.67
1:N:25:TYR:O	1:N:26:VAL:HG22	1.95	0.67
1:N:80:TRP:HZ3	2:O:56:VAL:HG12	1.59	0.67
3:P:6:GLN:O	3:P:10:PRO:HB3	1.95	0.67
5:R:16:PHE:HE2	15:R:1101:BCR:H373	1.58	0.67
8:H:3:VAL:O	8:H:6:TRP:HB2	1.94	0.66
1:N:85:ILE:HG23	2:O:51:ILE:HG21	1.78	0.66
1:N:101:VAL:CG1	13:O:1201:CLA:HMA2	2.25	0.66
4:Q:92:VAL:HG12	4:Q:93:VAL:H	1.59	0.66
5:E:22:ILE:HG22	5:E:23:ILE:N	2.10	0.66
11:N:1305:OPC:HBU1	11:O:1306:OPC:HBE2	1.76	0.66
11:B:305:OPC:CAG	11:B:305:OPC:HAV	2.25	0.66
4:D:116:PRO:HD2	4:D:127:PRO:HD3	1.77	0.66
8:H:7:VAL:HG12	8:H:11:VAL:HG21	1.76	0.66
1:N:158:ILE:HG23	1:N:159:PRO:HD2	1.78	0.66
1:N:17:LEU:HA	1:N:20:ASP:OD1	1.95	0.66
2:O:118:ASN:OD1	2:O:123:PRO:HA	1.96	0.66
3:P:148:ALA:HB1	3:P:150:HIS:NE2	2.10	0.66
4:Q:63:ASN:ND2	4:Q:63:ASN:H	1.91	0.66
5:R:5:ALA:O	6:S:10:ALA:HA	1.94	0.66
6:S:27:LEU:HD11	8:U:15:TRP:NE1	2.09	0.66
1:A:121:GLY:HA2	1:A:124:LEU:HD12	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:56:VAL:O	2:B:59:PRO:HD3	1.95	0.66
2:B:79:TRP:O	2:B:80:TYR:HD1	1.79	0.66
4:D:50:VAL:HG21	4:D:164:PRO:CG	2.25	0.66
4:D:22:LEU:HD23	4:D:23:ALA:H	1.61	0.66
1:A:189:PHE:CE2	1:N:52:PHE:HB2	2.31	0.66
3:C:179:THR:HB	3:C:225:VAL:HG22	1.77	0.66
1:N:114:ARG:HG3	1:N:117:THR:HG23	1.77	0.66
2:B:102:ALA:C	2:B:105:PRO:HD2	2.15	0.66
3:C:271:MET:HA	3:C:274:LEU:CG	2.26	0.66
4:D:60:LEU:HB2	4:D:62:ASN:HD22	1.60	0.66
4:Q:149:ALA:HB2	4:Q:178:TRP:CH2	2.31	0.66
5:R:9:ILE:HB	6:S:10:ALA:HB1	1.77	0.66
3:C:27:LEU:HD12	3:C:27:LEU:O	1.96	0.66
5:R:9:ILE:HG21	6:S:10:ALA:C	2.16	0.66
7:T:16:LEU:C	7:T:16:LEU:HD13	2.16	0.66
2:O:123:PRO:HG2	2:O:124:PHE:CE2	2.30	0.66
3:P:52:ILE:HG23	3:P:155:ARG:NH2	2.11	0.66
4:Q:90:TYR:HB2	4:Q:104:ILE:CD1	2.26	0.66
1:A:41:LEU:O	1:A:44:PHE:HB3	1.96	0.66
3:C:273:ILE:HG21	7:G:22:GLN:HB3	1.78	0.66
1:A:213:GLY:HA2	5:E:30:LYS:NZ	2.10	0.66
7:G:17:PHE:HB3	7:G:21:TYR:CE1	2.31	0.66
3:P:154:ASN:OD1	3:P:155:ARG:N	2.27	0.66
3:P:241:GLY:O	3:P:242:GLN:HB2	1.96	0.66
2:O:46:GLY:HA3	7:T:19:ALA:CB	2.26	0.66
2:B:77:PRO:O	2:B:78:GLU:C	2.33	0.66
1:N:41:LEU:O	1:N:44:PHE:HB3	1.96	0.66
2:O:133:PHE:O	2:O:135:PHE:N	2.22	0.66
4:Q:171:ARG:HB2	4:Q:171:ARG:NH1	2.10	0.66
4:Q:94:GLU:OE1	4:Q:100:ARG:NE	2.28	0.66
3:P:78:LEU:HG	3:P:79:PRO:HD2	1.78	0.65
5:E:3:LEU:HD12	5:E:6:VAL:HB	1.79	0.65
1:A:32:ILE:HD11	7:G:26:ARG:NE	2.11	0.65
2:O:135:PHE:C	2:O:137:THR:N	2.50	0.65
1:N:146:TRP:HZ2	2:O:69:PHE:HA	1.61	0.65
3:P:28:ALA:HB1	3:P:238:GLY:O	1.95	0.65
7:T:16:LEU:C	7:T:18:TYR:H	2.00	0.65
8:U:22:TRP:NE1	8:U:26:GLY:HA3	2.12	0.65
1:A:188:THR:O	1:A:192:PRO:HG3	1.96	0.65
1:A:36:LEU:HA	1:A:39:ILE:HB	1.78	0.65
4:D:21:LEU:O	4:D:25:GLY:HA3	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:27:VAL:C	4:D:29:GLY:H	1.99	0.65
4:D:51:GLY:C	4:D:54:THR:HB	2.17	0.65
1:N:33:PHE:CE1	1:N:34:TYR:HE1	2.15	0.65
3:P:219:VAL:HG12	3:P:220:SER:N	2.10	0.65
4:Q:145:PRO:O	4:Q:146:LEU:HB2	1.97	0.65
2:B:104:VAL:N	2:B:105:PRO:HD2	2.10	0.65
2:B:149:LEU:HB3	2:B:150:PRO:CD	2.26	0.65
2:B:55:SER:O	2:B:58:ASP:C	2.35	0.65
3:C:154:ASN:CG	3:C:155:ARG:H	1.98	0.65
3:C:159:GLN:N	3:C:159:GLN:OE1	2.29	0.65
4:D:23:ALA:O	4:D:27:VAL:HG23	1.97	0.65
8:H:7:VAL:CG1	8:H:11:VAL:HG21	2.26	0.65
1:N:141:ASP:HB2	1:N:144:GLY:H	1.61	0.65
1:N:159:PRO:O	1:N:161:VAL:N	2.29	0.65
2:O:102:ALA:C	2:O:105:PRO:HD2	2.15	0.65
2:O:41:PRO:HG2	3:P:272:LEU:HD13	1.78	0.65
3:P:78:LEU:HD23	3:P:82:PHE:HB3	1.77	0.65
3:P:84:ILE:HD12	3:P:130:PRO:O	1.97	0.65
4:Q:36:TYR:N	4:Q:37:PRO:CD	2.58	0.65
2:B:98:VAL:O	2:B:101:MET:HG2	1.97	0.65
3:C:82:PHE:HA	3:C:83:LYS:HZ2	1.59	0.65
1:N:142:GLN:HG2	2:O:64:GLU:CD	2.16	0.65
1:A:46:ILE:O	1:A:50:THR:HG23	1.97	0.65
2:B:144:GLY:O	2:B:145:ILE:HD13	1.97	0.65
2:B:42:VAL:HG22	3:C:272:LEU:CB	2.24	0.65
2:B:64:GLU:HG2	12:B:309:BNT:BRAI	2.52	0.65
6:F:4:GLU:HG3	6:F:5:GLU:OE1	1.97	0.65
1:N:119:ILE:O	1:N:122:VAL:HB	1.96	0.65
1:N:155:PRO:HG2	1:N:166:SER:CB	2.26	0.65
1:N:167:ASP:C	1:N:169:LEU:H	1.99	0.65
3:P:278:GLN:O	3:P:279:VAL:HG23	1.95	0.65
1:N:52:PHE:HA	9:N:301:HEM:HAC	1.77	0.65
1:N:47:GLN:HE22	1:N:89:SER:CB	2.08	0.65
2:O:24:HIS:O	2:O:24:HIS:ND1	2.26	0.65
5:R:17:GLY:O	5:R:18:ILE:HG23	1.97	0.65
1:A:104:VAL:O	1:A:107:THR:N	2.22	0.65
1:A:214:PRO:CG	5:E:29:ILE:HD13	2.27	0.65
2:B:91:LEU:HD12	2:B:91:LEU:O	1.97	0.65
7:G:10:PHE:C	7:G:12:THR:H	2.00	0.65
1:N:165:ILE:O	1:N:168:LEU:HG	1.96	0.65
1:A:28:PRO:HD2	2:B:33:PRO:CD	2.25	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:149:ALA:HB2	4:D:178:TRP:CH2	2.31	0.65
4:D:65:LYS:O	4:D:68:LYS:HG2	1.96	0.65
7:G:21:TYR:CD1	7:G:21:TYR:N	2.62	0.65
1:N:125:ALA:O	1:N:129:VAL:HG23	1.96	0.65
2:O:75:ILE:O	2:O:76:LEU:HB2	1.95	0.65
7:T:10:PHE:C	7:T:12:THR:H	1.97	0.65
6:F:35:LYS:O	6:F:36:GLU:HG2	1.97	0.65
8:H:9:LEU:HB3	8:H:13:PHE:CE1	2.32	0.65
2:O:31:ALA:HB3	7:T:30:LEU:C	2.18	0.65
3:P:91:PRO:HB2	3:P:95:LYS:HE3	1.79	0.65
3:C:139:ASP:HB3	3:C:142:ILE:HD12	1.79	0.64
3:C:52:ILE:HG23	3:C:155:ARG:NH2	2.12	0.64
4:D:94:GLU:OE1	4:D:100:ARG:NE	2.30	0.64
1:N:141:ASP:O	1:N:145:TYR:N	2.27	0.64
3:P:157:ARG:HB2	3:P:169:ASN:HB2	1.78	0.64
3:P:26:HIS:CG	3:P:154:ASN:HD21	2.15	0.64
7:T:26:ARG:H	7:T:27:PRO:HD3	1.62	0.64
2:B:40:PHE:N	2:B:41:PRO:HD2	2.12	0.64
3:C:188:ASP:N	3:C:193:VAL:HA	2.12	0.64
2:B:79:TRP:HH2	5:E:1:MET:SD	2.19	0.64
7:G:10:PHE:C	7:G:12:THR:N	2.47	0.64
2:O:122:ASN:OD1	2:O:124:PHE:HB2	1.96	0.64
2:O:64:GLU:N	2:O:65:PRO:HD2	2.11	0.64
1:A:58:TYR:HD2	1:A:184:TYR:HE1	1.44	0.64
3:C:185:LYS:HD2	3:C:195:TYR:HD2	1.62	0.64
7:G:29:GLU:HG3	7:G:30:LEU:H	1.62	0.64
1:N:209:GLN:HE22	2:O:28:GLY:H	1.44	0.64
2:O:131:THR:O	2:O:135:PHE:HB3	1.96	0.64
3:P:154:ASN:CG	3:P:155:ARG:H	2.00	0.64
3:P:1:TYR:O	3:P:4:TRP:HB2	1.98	0.64
3:P:54:TYR:HB2	3:P:58:LEU:HD22	1.79	0.64
1:A:51:GLY:HA2	1:A:54:MET:HE3	1.79	0.64
2:B:61:MET:HE2	12:B:309:BNT:HAM3	1.80	0.64
3:C:91:PRO:O	3:C:95:LYS:HE2	1.98	0.64
4:D:108:CYS:HB2	4:D:115:VAL:HG23	1.79	0.64
5:E:15:PHE:C	5:E:17:GLY:H	1.99	0.64
1:N:211:ILE:HG23	1:N:212:SER:N	2.12	0.64
4:Q:23:ALA:O	4:Q:27:VAL:HG23	1.98	0.64
3:P:277:LYS:CE	7:T:27:PRO:HD2	2.28	0.64
1:A:123:ILE:HD12	1:A:123:ILE:N	2.07	0.64
1:A:15:GLN:O	1:A:17:LEU:HD12	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:R:22:ILE:HG22	5:R:23:ILE:H	1.62	0.64
7:T:16:LEU:O	7:T:16:LEU:HD13	1.98	0.64
3:C:278:GLN:O	3:C:279:VAL:HG23	1.97	0.64
7:G:24:TYR:O	7:G:26:ARG:HG3	1.97	0.64
1:N:121:GLY:HA2	1:N:124:LEU:HD12	1.79	0.64
3:P:159:GLN:HG3	3:P:169:ASN:O	1.97	0.64
4:Q:84:LEU:O	4:Q:85:LYS:HB2	1.97	0.64
1:A:106:LEU:CG	5:E:18:ILE:HD12	2.15	0.64
3:P:36:VAL:HB	3:P:37:PRO:HD2	1.78	0.64
4:D:36:TYR:N	4:D:37:PRO:CD	2.59	0.64
1:N:137:SER:HB2	1:N:144:GLY:O	1.98	0.64
2:O:112:PRO:O	2:O:116:ASN:HB2	1.98	0.64
2:O:130:THR:O	2:O:133:PHE:HB3	1.98	0.64
5:R:26:ILE:HG23	5:R:30:LYS:HE2	1.80	0.64
3:C:103:PHE:HB3	3:C:114:LEU:HD22	1.79	0.64
3:C:172:PHE:HB2	3:C:211:ILE:HG13	1.79	0.64
3:C:61:VAL:HG23	3:C:62:ALA:H	1.63	0.64
3:C:6:GLN:O	3:C:10:PRO:HB3	1.97	0.64
6:F:16:LEU:HA	6:F:19:VAL:CG2	2.27	0.64
1:N:28:PRO:HD2	2:O:33:PRO:N	2.12	0.64
3:P:187:GLU:HA	3:P:193:VAL:HG13	1.80	0.64
3:P:205:LYS:HZ3	3:P:207:VAL:HG12	1.63	0.64
4:Q:175:LYS:HD3	4:Q:176:PRO:CD	2.28	0.64
5:R:5:ALA:CB	6:S:10:ALA:HB2	2.24	0.64
2:B:131:THR:O	2:B:135:PHE:HB3	1.98	0.64
4:D:90:TYR:HB2	4:D:104:ILE:CD1	2.27	0.64
6:F:27:LEU:HD23	7:G:25:LYS:HD2	1.80	0.64
4:Q:118:ASN:ND2	4:Q:120:ALA:H	1.95	0.64
7:T:21:TYR:CD1	7:T:21:TYR:N	2.62	0.64
2:B:117:VAL:HG23	2:B:118:ASN:H	1.62	0.63
2:B:117:VAL:CG2	2:B:118:ASN:N	2.61	0.63
7:G:5:VAL:O	7:G:9:VAL:HG13	1.99	0.63
3:P:110:GLN:OE1	3:P:113:VAL:HG21	1.97	0.63
3:P:281:LYS:HA	3:P:284:ALA:HB3	1.80	0.63
7:T:8:LEU:HA	7:T:11:ALA:HB3	1.80	0.63
3:C:148:ALA:HB1	3:C:150:HIS:NE2	2.13	0.63
1:N:111:LYS:NZ	1:N:112:LYS:HE3	2.13	0.63
1:N:38:GLY:N	16:N:1306:HOH:O	2.29	0.63
1:A:49:ALA:O	1:A:50:THR:C	2.37	0.63
5:R:27:LYS:O	5:R:27:LYS:HD3	1.98	0.63
1:A:148:VAL:HG12	1:A:148:VAL:O	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:135:PHE:C	2:B:137:THR:N	2.52	0.63
5:E:27:LYS:HD3	5:E:27:LYS:O	1.99	0.63
5:E:9:ILE:HG21	6:F:10:ALA:C	2.19	0.63
1:N:71:TYR:HD2	1:N:71:TYR:O	1.80	0.63
4:Q:22:LEU:HD23	4:Q:23:ALA:H	1.62	0.63
4:Q:53:GLY:HA2	4:Q:57:LYS:CD	2.23	0.63
4:D:88:PRO:HG3	4:D:114:VAL:HG22	1.80	0.63
1:A:102:PHE:CE1	5:E:15:PHE:HZ	2.17	0.63
5:E:22:ILE:O	5:E:24:PHE:N	2.31	0.63
5:E:9:ILE:HB	6:F:10:ALA:HB1	1.80	0.63
1:N:95:LEU:HD11	5:R:7:PHE:HB2	1.81	0.63
2:O:39:VAL:H	2:O:41:PRO:HD2	1.64	0.63
2:O:68:PRO:HG2	2:O:69:PHE:H	1.64	0.63
6:S:27:LEU:N	6:S:27:LEU:CD1	2.62	0.63
1:A:80:TRP:CZ3	1:A:81:LEU:HD23	2.34	0.63
3:C:182:LYS:HG2	3:C:198:SER:HB3	1.79	0.63
4:D:63:ASN:HD22	4:D:63:ASN:H	1.42	0.63
2:O:39:VAL:O	2:O:42:VAL:HB	1.98	0.63
2:O:91:LEU:HD21	2:O:96:LEU:HD12	1.79	0.63
1:A:117:THR:HG22	1:A:205:MET:CB	2.29	0.63
3:C:83:LYS:NZ	3:C:132:LEU:O	2.31	0.63
4:D:165:TRP:O	4:D:166:THR:HG23	1.99	0.63
4:D:63:ASN:N	4:D:63:ASN:ND2	2.46	0.63
15:E:101:BCR:HC21	7:G:23:GLN:HE22	1.64	0.63
5:E:17:GLY:O	5:E:18:ILE:HG23	1.99	0.63
1:N:97:MET:O	1:N:100:HIS:HB3	1.99	0.63
2:O:98:VAL:O	2:O:101:MET:HG2	1.97	0.63
2:O:82:TYR:HB2	2:O:83:PRO:CD	2.29	0.63
1:N:95:LEU:HD11	5:R:7:PHE:CB	2.29	0.63
3:C:26:HIS:CG	3:C:154:ASN:HD21	2.17	0.63
2:B:149:LEU:HD11	6:F:2:MET:HB2	1.80	0.63
8:H:4:LEU:O	8:H:6:TRP:N	2.31	0.63
1:N:190:VAL:C	1:N:192:PRO:HD2	2.19	0.63
2:O:41:PRO:O	2:O:45:MET:HE2	1.98	0.63
3:P:271:MET:HA	3:P:274:LEU:CD1	2.29	0.63
1:A:66:TYR:HB2	1:A:140:TRP:HE3	1.62	0.62
3:C:157:ARG:HB2	3:C:169:ASN:HB2	1.80	0.62
4:D:57:LYS:HG2	4:D:62:ASN:O	1.99	0.62
7:G:8:LEU:HA	7:G:11:ALA:HB3	1.81	0.62
7:G:10:PHE:O	7:G:12:THR:N	2.31	0.62
7:G:16:LEU:C	7:G:18:TYR:H	2.02	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:27:PRO:CA	2:O:33:PRO:HD3	2.28	0.62
3:P:28:ALA:HB3	3:P:240:PHE:N	2.14	0.62
3:P:104:GLN:NE2	3:P:104:GLN:H	1.97	0.62
3:P:182:LYS:HG2	3:P:198:SER:HB3	1.81	0.62
3:P:34:VAL:O	3:P:34:VAL:HG23	1.99	0.62
4:Q:108:CYS:HB2	4:Q:113:CYS:O	1.98	0.62
4:Q:80:LEU:HB2	4:Q:90:TYR:HA	1.80	0.62
6:S:14:PHE:O	6:S:17:ILE:HG12	2.00	0.62
6:S:16:LEU:HA	6:S:19:VAL:CG2	2.29	0.62
1:A:165:ILE:O	1:A:168:LEU:HG	2.00	0.62
1:A:183:TYR:O	1:A:186:ALA:HB3	1.98	0.62
1:A:196:ALA:O	1:A:200:LEU:HD23	1.99	0.62
1:A:29:HIS:HD2	1:A:211:ILE:HB	1.65	0.62
4:D:145:PRO:O	4:D:146:LEU:HB2	1.98	0.62
4:D:129:HIS:HB2	14:D:201:FES:S1	2.39	0.62
5:E:6:VAL:O	5:E:6:VAL:HG12	1.98	0.62
6:F:14:PHE:O	6:F:17:ILE:HG12	1.99	0.62
2:O:22:MET:O	2:O:24:HIS:N	2.32	0.62
5:R:22:ILE:HG22	5:R:23:ILE:N	2.14	0.62
3:C:34:VAL:HG12	3:C:151:LEU:HD13	1.81	0.62
3:C:251:ASP:O	3:C:254:ARG:HB3	1.99	0.62
1:N:117:THR:HG22	1:N:205:MET:CB	2.30	0.62
2:O:40:PHE:N	2:O:41:PRO:HD2	2.14	0.62
5:R:6:VAL:HG12	5:R:6:VAL:O	1.99	0.62
2:B:82:TYR:HB2	2:B:83:PRO:CD	2.29	0.62
3:C:54:TYR:HB2	3:C:58:LEU:HD22	1.81	0.62
1:N:162:GLY:HA2	1:N:165:ILE:CG2	2.30	0.62
1:N:31:ASN:CB	1:N:34:TYR:HE2	2.12	0.62
11:O:1306:OPC:CCB	11:O:1306:OPC:HBB2	2.28	0.62
1:A:39:ILE:HD11	2:B:43:VAL:CG1	2.29	0.62
2:B:104:VAL:H	2:B:105:PRO:HD2	1.63	0.62
3:C:121:GLY:C	3:C:123:GLN:H	2.02	0.62
3:C:187:GLU:HA	3:C:193:VAL:HG13	1.80	0.62
4:D:67:SER:O	4:D:70:LEU:HD11	2.00	0.62
3:P:48:ALA:HB3	3:P:129:PHE:HB2	1.81	0.62
3:P:271:MET:HG2	4:Q:22:LEU:HG	1.81	0.62
4:Q:70:LEU:HD12	4:Q:71:GLU:H	1.64	0.62
8:U:4:LEU:O	8:U:6:TRP:N	2.32	0.62
3:C:28:ALA:HB3	3:C:240:PHE:N	2.15	0.62
1:N:46:ILE:O	1:N:50:THR:HG23	1.99	0.62
2:O:24:HIS:C	2:O:24:HIS:HD1	2.03	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:10:PRO:N	3:P:11:PRO:HD2	2.14	0.62
3:P:34:VAL:HG12	3:P:151:LEU:HD13	1.82	0.62
1:A:29:HIS:CE1	2:B:30:PRO:HG3	2.35	0.62
3:C:191:GLY:O	3:C:192:ASN:HB2	1.99	0.62
3:C:172:PHE:H	3:C:231:LEU:HG	1.63	0.62
4:D:175:LYS:HD3	4:D:176:PRO:CD	2.30	0.62
1:N:105:TYR:OH	2:O:129:ALA:CB	2.42	0.62
1:N:148:VAL:O	1:N:148:VAL:HG12	1.98	0.62
2:O:78:GLU:O	2:O:80:TYR:N	2.32	0.62
4:D:50:VAL:HB	4:D:84:LEU:CD1	2.29	0.62
5:E:11:PHE:O	5:E:14:LEU:HB2	1.99	0.62
3:P:251:ASP:O	3:P:254:ARG:HB3	1.99	0.62
3:P:266:MET:HA	3:P:269:GLN:NE2	2.14	0.62
3:P:271:MET:HA	3:P:274:LEU:CG	2.30	0.62
4:Q:92:VAL:HG12	4:Q:93:VAL:N	2.15	0.62
8:U:7:VAL:HG12	8:U:11:VAL:HG21	1.82	0.62
1:A:116:LEU:HD12	1:A:116:LEU:H	1.65	0.62
1:A:78:PHE:CE1	4:D:37:PRO:HA	2.35	0.62
2:B:124:PHE:HZ	5:E:27:LYS:HB2	1.62	0.62
2:B:129:ALA:HA	2:B:132:ILE:HD11	1.82	0.62
3:C:45:VAL:HG13	3:C:85:ALA:CB	2.29	0.62
1:N:148:VAL:HA	1:N:151:VAL:CG2	2.22	0.62
1:N:110:PHE:CD1	2:O:112:PRO:HB3	2.35	0.62
2:O:34:ASN:ND2	2:O:35:ASP:N	2.42	0.62
1:A:136:TYR:HA	9:A:301:HEM:HAA2	1.80	0.61
1:A:44:PHE:O	1:A:47:GLN:N	2.33	0.61
1:A:27:PRO:HB3	2:B:33:PRO:HD3	1.82	0.61
3:C:193:VAL:O	3:C:193:VAL:HG12	2.00	0.61
1:N:44:PHE:O	1:N:47:GLN:N	2.33	0.61
2:O:149:LEU:C	2:O:151:LEU:H	2.03	0.61
3:P:117:GLY:N	3:P:118:PRO:HD2	2.13	0.61
3:P:172:PHE:H	3:P:231:LEU:HG	1.63	0.61
6:S:4:GLU:HG3	6:S:5:GLU:OE1	2.00	0.61
2:B:82:TYR:H	2:B:83:PRO:HD2	1.64	0.61
3:C:104:GLN:NE2	3:C:104:GLN:H	1.98	0.61
3:C:10:PRO:N	3:C:11:PRO:HD2	2.15	0.61
1:N:114:ARG:HB2	1:N:116:LEU:CD1	2.30	0.61
11:O:1306:OPC:CBT	11:O:1306:OPC:HBX2	2.30	0.61
3:P:44:THR:C	3:P:132:LEU:HD12	2.20	0.61
1:A:47:GLN:HE22	1:A:90:ALA:N	1.97	0.61
1:A:28:PRO:CD	2:B:33:PRO:HD3	2.24	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:104:VAL:N	2:O:105:PRO:CD	2.63	0.61
3:P:136:PRO:HB3	3:P:142:ILE:HG22	1.81	0.61
3:P:139:ASP:OD2	3:P:142:ILE:HG13	2.00	0.61
3:P:191:GLY:O	3:P:192:ASN:HB2	1.99	0.61
1:A:33:PHE:O	1:A:34:TYR:C	2.38	0.61
2:B:39:VAL:O	2:B:43:VAL:HG23	2.00	0.61
2:B:86:GLN:HG3	2:B:90:SER:OG	2.01	0.61
1:N:112:LYS:HE2	2:O:116:ASN:HD21	1.64	0.61
1:N:191:LEU:O	1:N:195:ILE:HG22	2.00	0.61
2:O:123:PRO:HD2	2:O:124:PHE:CE1	2.36	0.61
2:O:37:LEU:HB2	2:O:38:TYR:CE1	2.35	0.61
3:P:79:PRO:HG2	3:P:82:PHE:CG	2.35	0.61
1:A:106:LEU:HG	5:E:18:ILE:CD1	2.14	0.61
1:A:158:ILE:HG21	1:A:162:GLY:HA3	1.82	0.61
3:C:78:LEU:HD23	3:C:82:PHE:HB3	1.82	0.61
4:D:22:LEU:O	4:D:26:THR:HG23	2.00	0.61
4:D:70:LEU:HD13	4:D:71:GLU:H	1.65	0.61
5:E:15:PHE:C	5:E:17:GLY:N	2.50	0.61
4:Q:108:CYS:HB2	4:Q:115:VAL:HG23	1.83	0.61
15:R:1101:BCR:H362	6:S:18:PHE:CE2	2.36	0.61
5:R:21:GLY:O	5:R:22:ILE:HD12	2.00	0.61
2:B:117:VAL:CG2	2:B:118:ASN:H	2.13	0.61
2:B:39:VAL:O	2:B:42:VAL:HB	2.01	0.61
3:C:172:PHE:H	3:C:231:LEU:CD2	2.12	0.61
4:D:171:ARG:HH11	4:D:171:ARG:HB2	1.64	0.61
2:O:118:ASN:HD21	2:O:123:PRO:HB2	1.65	0.61
2:O:86:GLN:HG3	2:O:90:SER:OG	2.00	0.61
4:D:92:VAL:HG12	4:D:93:VAL:H	1.65	0.61
5:E:9:ILE:HG23	5:E:10:VAL:N	2.16	0.61
1:N:59:LYS:O	1:N:64:GLU:O	2.17	0.61
2:O:78:GLU:HB3	2:O:80:TYR:CD1	2.35	0.61
3:P:252:PRO:C	3:P:254:ARG:H	2.04	0.61
4:Q:126:CYS:O	4:Q:130:GLY:HA2	2.01	0.61
5:R:9:ILE:CG2	5:R:10:VAL:N	2.64	0.61
8:U:9:LEU:HB3	8:U:13:PHE:CE1	2.35	0.61
1:A:104:VAL:HG13	1:A:108:GLY:O	2.01	0.61
1:A:167:ASP:C	1:A:169:LEU:H	2.03	0.61
1:A:66:TYR:HB3	1:A:140:TRP:CE3	2.35	0.61
2:B:39:VAL:H	2:B:41:PRO:HD2	1.65	0.61
3:C:271:MET:HA	3:C:274:LEU:CD1	2.30	0.61
2:O:95:LEU:O	2:O:99:LEU:N	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:102:TYR:O	3:P:118:PRO:HD2	2.01	0.61
3:P:281:LYS:N	3:P:281:LYS:HD3	2.16	0.61
5:R:2:ILE:O	5:R:4:GLY:N	2.34	0.61
8:U:7:VAL:CG1	8:U:11:VAL:HG21	2.31	0.61
1:A:76:VAL:O	1:A:78:PHE:N	2.34	0.61
2:B:61:MET:SD	2:B:62:VAL:HG22	2.41	0.61
3:C:257:TRP:HA	3:C:257:TRP:HE3	1.66	0.61
2:O:20:LYS:NZ	2:O:20:LYS:HB2	2.15	0.61
4:Q:73:HIS:HB3	4:Q:93:VAL:HG21	1.82	0.61
5:R:22:ILE:O	5:R:24:PHE:N	2.34	0.61
11:B:305:OPC:HBY1	11:C:306:OPC:HBX1	1.82	0.61
2:B:65:PRO:HD3	12:B:309:BNT:BRAI	2.56	0.61
5:E:9:ILE:CG2	5:E:10:VAL:N	2.64	0.61
15:E:101:BCR:HC21	7:G:23:GLN:NE2	2.15	0.61
2:O:86:GLN:HG2	2:O:143:LEU:HD22	1.83	0.61
2:O:25:ASN:O	2:O:26:TYR:HB3	2.01	0.61
2:O:73:LEU:HD11	3:P:244:ASP:OD2	2.01	0.61
4:Q:116:PRO:CD	4:Q:127:PRO:HD3	2.31	0.61
1:A:30:VAL:H	1:A:211:ILE:CD1	2.13	0.60
1:A:142:GLN:NE2	2:B:68:PRO:HB2	2.10	0.60
6:F:8:TYR:CD2	6:F:9:ALA:N	2.69	0.60
4:Q:132:GLN:O	4:Q:133:TYR:HD2	1.84	0.60
4:Q:22:LEU:O	4:Q:26:THR:HG23	2.00	0.60
6:S:27:LEU:HD13	6:S:27:LEU:H	1.63	0.60
3:C:91:PRO:HB2	3:C:95:LYS:HE3	1.82	0.60
4:D:111:LEU:HB3	14:D:201:FES:S2	2.40	0.60
5:E:21:GLY:O	5:E:22:ILE:HD12	2.02	0.60
2:O:83:PRO:HA	2:O:143:LEU:HB3	1.82	0.60
2:O:94:LYS:C	2:O:96:LEU:H	2.04	0.60
5:R:23:ILE:C	5:R:23:ILE:HD12	2.21	0.60
1:N:159:PRO:HG2	1:N:161:VAL:CG2	2.31	0.60
2:O:57:LEU:HD21	7:T:9:VAL:C	2.20	0.60
3:P:61:VAL:HG23	3:P:62:ALA:H	1.66	0.60
1:A:191:LEU:O	1:A:195:ILE:HG22	2.01	0.60
1:A:195:ILE:HG23	1:A:196:ALA:N	2.16	0.60
2:B:65:PRO:HB3	2:B:68:PRO:CG	2.32	0.60
11:B:305:OPC:HBW1	11:C:306:OPC:HBW2	1.82	0.60
3:P:45:VAL:HG13	3:P:85:ALA:CB	2.31	0.60
1:A:116:LEU:N	1:A:116:LEU:HD12	2.16	0.60
1:A:16:ALA:O	1:A:17:LEU:HB2	2.02	0.60
1:A:193:TRP:O	1:A:196:ALA:HB3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:57:LEU:CD1	7:G:10:PHE:HA	2.31	0.60
5:E:2:ILE:O	5:E:4:GLY:N	2.34	0.60
2:O:78:GLU:C	2:O:80:TYR:H	2.05	0.60
3:P:159:GLN:OE1	3:P:159:GLN:N	2.34	0.60
3:P:171:VAL:HG12	3:P:231:LEU:CD1	2.28	0.60
3:C:281:LYS:HA	3:C:284:ALA:HB3	1.84	0.60
1:N:135:GLY:HA2	1:N:138:LEU:HG	1.83	0.60
2:O:147:ALA:O	2:O:149:LEU:HD23	2.01	0.60
3:P:121:GLY:C	3:P:123:GLN:H	2.05	0.60
3:P:122:GLU:O	3:P:122:GLU:HG2	2.01	0.60
3:P:185:LYS:HD2	3:P:195:TYR:HD2	1.65	0.60
7:T:5:VAL:O	7:T:9:VAL:HG13	2.01	0.60
3:C:117:GLY:N	3:C:118:PRO:HD2	2.16	0.60
4:D:126:CYS:SG	4:D:127:PRO:HD2	2.41	0.60
4:D:126:CYS:O	4:D:130:GLY:HA2	2.00	0.60
4:D:146:LEU:HD13	4:D:177:TRP:CE3	2.37	0.60
7:G:18:TYR:HA	7:G:21:TYR:CG	2.36	0.60
7:G:26:ARG:H	7:G:27:PRO:HD2	1.65	0.60
1:N:114:ARG:HB2	1:N:116:LEU:HD11	1.84	0.60
2:O:70:ALA:O	2:O:71:THR:CB	2.49	0.60
3:P:139:ASP:HB3	3:P:142:ILE:HD12	1.84	0.60
2:O:57:LEU:HD13	7:T:10:PHE:CD2	2.37	0.60
2:B:63:GLY:HA2	12:B:309:BNT:CAK	2.32	0.60
2:B:86:GLN:HG2	2:B:143:LEU:HD22	1.83	0.60
4:D:107:VAL:HG12	4:D:107:VAL:O	2.02	0.60
5:R:9:ILE:HG23	5:R:10:VAL:N	2.17	0.60
1:A:125:ALA:O	1:A:129:VAL:HG23	2.02	0.60
1:A:190:VAL:C	1:A:192:PRO:HD2	2.21	0.60
1:A:66:TYR:CB	1:A:140:TRP:CE3	2.84	0.60
2:B:95:LEU:O	2:B:99:LEU:N	2.35	0.60
2:B:73:LEU:HD23	3:C:18:GLY:HA3	1.84	0.60
3:C:217:LEU:HA	3:C:232:THR:HB	1.83	0.60
4:D:35:LEU:H	4:D:37:PRO:CD	2.15	0.60
4:Q:88:PRO:HG3	4:Q:114:VAL:HG22	1.83	0.60
1:A:135:GLY:H	1:A:187:HIS:HD1	1.49	0.60
1:A:127:ILE:HG21	1:A:195:ILE:HB	1.83	0.60
2:B:114:ILE:HG22	2:B:115:GLU:N	2.16	0.60
4:D:155:VAL:O	4:D:155:VAL:HG12	2.02	0.60
1:N:52:PHE:N	9:N:301:HEM:HAC	2.17	0.60
1:N:58:TYR:O	1:N:60:PRO:HD3	2.00	0.60
2:O:39:VAL:O	2:O:43:VAL:HG23	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:271:MET:CE	4:Q:26:THR:HG21	2.32	0.60
3:P:280:GLU:HG2	3:P:280:GLU:O	2.02	0.60
3:P:55:ASP:N	3:P:55:ASP:OD2	2.31	0.60
5:R:15:PHE:C	5:R:17:GLY:H	2.05	0.60
1:A:132:GLY:O	1:A:134:THR:N	2.35	0.59
2:B:94:LYS:C	2:B:96:LEU:H	2.05	0.59
3:C:268:ALA:C	3:C:270:LEU:H	2.05	0.59
4:D:108:CYS:HB2	4:D:113:CYS:O	2.02	0.59
5:E:18:ILE:HG13	5:E:19:ALA:H	1.67	0.59
2:O:81:LEU:HA	2:O:84:VAL:CG2	2.32	0.59
3:P:257:TRP:HA	3:P:257:TRP:CE3	2.35	0.59
3:C:251:ASP:HB3	3:C:254:ARG:HB2	1.83	0.59
2:B:38:TYR:HB2	3:C:276:LYS:CE	2.30	0.59
1:N:137:SER:HB3	1:N:148:VAL:HG21	1.83	0.59
1:N:52:PHE:CA	9:N:301:HEM:HAC	2.31	0.59
11:O:1306:OPC:CAP	11:O:1306:OPC:CAL	2.78	0.59
2:O:39:VAL:O	2:O:43:VAL:N	2.35	0.59
4:Q:70:LEU:HD13	4:Q:71:GLU:HG2	1.83	0.59
1:A:119:ILE:O	1:A:122:VAL:HB	2.01	0.59
1:A:191:LEU:H	1:A:191:LEU:CD1	2.10	0.59
2:B:34:ASN:ND2	2:B:35:ASP:N	2.45	0.59
3:C:281:LYS:HD3	3:C:281:LYS:N	2.17	0.59
4:D:38:LEU:HD11	4:D:42:PHE:CE1	2.37	0.59
5:E:15:PHE:HA	5:E:18:ILE:HG13	1.84	0.59
8:H:1:ILE:HG23	8:H:2:ASP:N	2.15	0.59
2:O:59:PRO:HG2	3:P:146:LYS:HG3	1.84	0.59
6:S:28:LEU:O	6:S:30:ILE:N	2.35	0.59
1:N:29:HIS:CE1	1:N:31:ASN:HD21	2.20	0.59
3:P:40:VAL:CG1	3:P:247:ILE:HD11	2.28	0.59
3:P:26:HIS:CE1	3:P:154:ASN:HD21	2.19	0.59
1:A:113:PRO:HD2	1:A:114:ARG:NH1	2.16	0.59
1:A:47:GLN:NE2	1:A:89:SER:HB3	2.15	0.59
2:B:125:ARG:CA	2:B:125:ARG:NH1	2.62	0.59
2:B:32:TRP:H	2:B:33:PRO:HD2	1.64	0.59
3:P:257:TRP:HE3	3:P:257:TRP:HA	1.67	0.59
4:Q:35:LEU:H	4:Q:37:PRO:CD	2.14	0.59
1:A:105:TYR:HA	1:A:110:PHE:CE2	2.37	0.59
3:C:34:VAL:HG23	3:C:34:VAL:O	2.02	0.59
8:U:18:ALA:O	8:U:21:VAL:CG2	2.49	0.59
3:C:188:ASP:H	3:C:193:VAL:CG2	2.12	0.59
3:C:2:PRO:HA	9:C:301:HEM:HBB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:27:PRO:O	2:O:29:GLU:HA	2.02	0.59
2:O:57:LEU:HD11	7:T:10:PHE:HA	1.84	0.59
7:G:21:TYR:N	7:G:21:TYR:HD1	2.00	0.59
4:Q:65:LYS:HB2	4:Q:68:LYS:NZ	2.17	0.59
5:R:9:ILE:CG1	6:S:14:PHE:HB2	2.32	0.59
7:T:20:ALA:O	7:T:24:TYR:CE2	2.56	0.59
1:A:114:ARG:C	1:A:116:LEU:N	2.51	0.59
1:A:39:ILE:HD11	2:B:43:VAL:HG12	1.85	0.59
3:C:139:ASP:OD2	3:C:142:ILE:HG13	2.03	0.59
3:C:79:PRO:HG2	3:C:82:PHE:CG	2.37	0.59
4:D:80:LEU:HB2	4:D:90:TYR:HA	1.85	0.59
15:E:101:BCR:H362	6:F:18:PHE:CE2	2.38	0.59
1:N:160:VAL:HG13	1:N:164:LEU:HB2	1.83	0.59
2:O:122:ASN:C	2:O:124:PHE:N	2.53	0.59
2:O:127:PRO:O	2:O:129:ALA:N	2.35	0.59
3:P:172:PHE:HB2	3:P:211:ILE:HG13	1.85	0.59
5:R:3:LEU:HD12	5:R:6:VAL:HB	1.84	0.59
1:A:25:TYR:C	1:A:26:VAL:HG22	2.23	0.59
1:A:47:GLN:HG3	1:A:86:HIS:CE1	2.38	0.59
1:A:110:PHE:HB2	2:B:112:PRO:HB3	1.84	0.59
2:B:79:TRP:HA	2:B:82:TYR:CE2	2.38	0.59
3:C:122:GLU:O	3:C:122:GLU:HG2	2.03	0.59
3:C:26:HIS:CE1	3:C:154:ASN:HD21	2.21	0.59
4:D:123:LYS:O	4:D:125:LYS:HG3	2.03	0.59
1:N:114:ARG:HD3	1:N:208:LYS:HB3	1.85	0.59
2:O:129:ALA:HA	2:O:132:ILE:HD11	1.84	0.59
2:O:147:ALA:O	2:O:149:LEU:N	2.34	0.59
1:N:157:ALA:HB1	2:O:95:LEU:HD22	1.84	0.59
3:P:251:ASP:HB3	3:P:254:ARG:HB2	1.84	0.59
3:P:83:LYS:H	3:P:83:LYS:NZ	2.01	0.59
4:Q:165:TRP:O	4:Q:166:THR:HG23	2.03	0.59
4:Q:70:LEU:HD13	4:Q:71:GLU:H	1.67	0.59
1:A:24:LYS:HG3	1:A:24:LYS:O	2.02	0.58
1:A:39:ILE:HD12	2:B:47:THR:CG2	2.28	0.58
4:D:132:GLN:O	4:D:133:TYR:HD2	1.85	0.58
4:D:38:LEU:O	4:D:38:LEU:HD12	2.02	0.58
7:G:8:LEU:HD23	7:G:12:THR:CG2	2.33	0.58
1:N:183:TYR:O	1:N:186:ALA:HB3	2.02	0.58
2:O:122:ASN:O	2:O:124:PHE:N	2.35	0.58
3:P:103:PHE:HB3	3:P:114:LEU:HD22	1.85	0.58
3:P:116:VAL:HG13	3:P:118:PRO:HG2	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:36:TYR:O	4:Q:40:LYS:HB2	2.03	0.58
5:R:15:PHE:C	5:R:17:GLY:N	2.56	0.58
1:A:21:VAL:CG1	1:A:22:THR:H	2.14	0.58
1:A:57:TYR:HE1	1:A:76:VAL:HG13	1.67	0.58
2:B:111:VAL:N	2:B:112:PRO:HD2	2.18	0.58
3:C:252:PRO:C	3:C:254:ARG:H	2.07	0.58
4:D:171:ARG:HB2	4:D:171:ARG:NH1	2.18	0.58
1:N:47:GLN:HG3	1:N:86:HIS:CE1	2.37	0.58
2:O:45:MET:HE3	3:P:269:GLN:HB3	1.85	0.58
8:U:9:LEU:O	8:U:11:VAL:N	2.36	0.58
1:A:33:PHE:HE1	5:E:18:ILE:CD1	2.12	0.58
3:C:257:TRP:HA	3:C:257:TRP:CE3	2.35	0.58
5:E:23:ILE:HD12	5:E:23:ILE:C	2.24	0.58
2:B:40:PHE:HA	2:B:43:VAL:CG2	2.31	0.58
3:C:187:GLU:HG3	3:C:188:ASP:N	2.19	0.58
4:D:113:CYS:HG	4:D:128:CYS:HG	0.75	0.58
4:D:65:LYS:HB2	4:D:68:LYS:NZ	2.18	0.58
1:N:83:ARG:HH12	2:O:60:ALA:HB1	1.67	0.58
7:T:10:PHE:O	7:T:13:LEU:N	2.35	0.58
1:A:137:SER:HB2	1:A:144:GLY:O	2.02	0.58
1:A:70:GLN:O	1:A:74:ASN:HB2	2.03	0.58
3:C:28:ALA:HB1	3:C:238:GLY:C	2.24	0.58
1:N:115:GLU:O	1:N:118:TRP:HB3	2.03	0.58
1:N:17:LEU:HG	1:N:20:ASP:CB	2.30	0.58
1:N:49:ALA:O	1:N:50:THR:C	2.41	0.58
1:N:63:THR:C	1:N:65:ALA:N	2.54	0.58
1:N:94:VAL:O	1:N:98:ILE:HG13	2.03	0.58
2:O:145:ILE:O	2:O:145:ILE:HG22	2.04	0.58
2:O:82:TYR:O	2:O:86:GLN:N	2.34	0.58
3:P:127:ILE:HD12	3:P:127:ILE:N	2.18	0.58
3:P:50:VAL:HG21	3:P:129:PHE:CE1	2.38	0.58
2:B:126:ARG:CZ	2:B:128:VAL:HB	2.34	0.58
2:O:116:ASN:HD22	2:O:116:ASN:C	2.07	0.58
5:R:18:ILE:HG13	5:R:19:ALA:H	1.68	0.58
1:A:154:VAL:HB	1:A:155:PRO:HD3	1.86	0.58
11:B:305:OPC:HAE2	11:B:305:OPC:HBX1	1.84	0.58
3:C:217:LEU:O	3:C:218:ILE:HG23	2.04	0.58
1:N:38:GLY:HA3	10:N:303:HEC:NC	2.19	0.58
1:N:90:ALA:C	1:N:92:MET:H	2.07	0.58
1:A:97:MET:O	1:A:100:HIS:HB3	2.03	0.58
1:A:162:GLY:O	1:A:165:ILE:HG22	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:LEU:CD2	1:A:99:LEU:HD21	2.34	0.58
3:C:110:GLN:OE1	3:C:113:VAL:HG21	2.04	0.58
3:C:25:CYS:O	3:C:26:HIS:C	2.42	0.58
7:G:20:ALA:O	7:G:24:TYR:CE2	2.56	0.58
2:O:111:VAL:N	2:O:112:PRO:HD2	2.18	0.58
12:O:1309:BNT:CAM	3:P:148:ALA:H	2.15	0.58
3:P:169:ASN:HD21	3:P:237:VAL:HG22	1.67	0.58
4:Q:38:LEU:HD11	4:Q:42:PHE:CE1	2.39	0.58
4:Q:63:ASN:N	4:Q:63:ASN:HD22	2.02	0.58
5:R:13:ALA:HA	6:S:14:PHE:CE1	2.39	0.58
7:T:18:TYR:HA	7:T:21:TYR:CG	2.38	0.58
1:A:71:TYR:HD2	1:A:71:TYR:O	1.87	0.58
4:D:146:LEU:HD13	4:D:177:TRP:CZ3	2.38	0.58
4:D:70:LEU:HD12	4:D:71:GLU:H	1.67	0.58
1:N:191:LEU:N	1:N:192:PRO:HD2	2.19	0.58
1:N:209:GLN:OE1	2:O:28:GLY:O	2.22	0.58
1:N:27:PRO:HA	2:O:33:PRO:CD	2.32	0.58
2:O:49:ALA:O	2:O:52:VAL:HB	2.03	0.58
2:O:94:LYS:C	2:O:96:LEU:N	2.57	0.58
2:O:122:ASN:HD22	5:R:26:ILE:C	2.08	0.58
3:C:188:ASP:HB3	3:C:192:ASN:O	2.04	0.58
3:C:280:GLU:C	3:C:282:VAL:N	2.56	0.58
1:N:162:GLY:C	1:N:165:ILE:HG22	2.22	0.58
3:P:102:TYR:H	3:P:118:PRO:CG	2.11	0.58
4:Q:154:THR:CG2	4:Q:155:VAL:H	2.08	0.58
15:R:1101:BCR:HC21	7:T:23:GLN:HE22	1.68	0.58
7:T:16:LEU:C	7:T:18:TYR:N	2.56	0.58
2:B:130:THR:O	2:B:133:PHE:HB3	2.03	0.57
1:A:27:PRO:HG2	2:B:20:LYS:NZ	2.19	0.57
2:B:31:ALA:O	2:B:32:TRP:HB2	2.03	0.57
4:D:125:LYS:HG2	4:D:132:GLN:HG2	1.86	0.57
5:E:26:ILE:HG23	5:E:30:LYS:CE	2.34	0.57
10:N:303:HEC:HBD2	10:N:303:HEC:HHA	1.85	0.57
3:P:3:PHE:N	3:P:3:PHE:CD1	2.72	0.57
3:P:60:GLN:NE2	3:P:157:ARG:HG3	2.19	0.57
6:S:28:LEU:C	6:S:30:ILE:N	2.57	0.57
1:A:165:ILE:HG23	1:A:166:SER:N	2.19	0.57
3:C:40:VAL:CG1	3:C:247:ILE:HD11	2.31	0.57
3:C:282:VAL:HG23	3:C:283:GLN:N	2.19	0.57
4:D:35:LEU:HD23	4:D:36:TYR:N	2.19	0.57
1:N:158:ILE:CG2	1:N:159:PRO:HD2	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:195:ILE:HG23	1:N:196:ALA:N	2.19	0.57
1:N:205:MET:O	1:N:207:ARG:N	2.37	0.57
11:O:1306:OPC:HAP2	11:O:1306:OPC:CAT	2.31	0.57
3:P:14:ARG:HG3	3:P:14:ARG:NH1	2.19	0.57
3:P:14:ARG:HG3	3:P:14:ARG:HH11	1.69	0.57
1:A:34:TYR:CD1	1:A:103:ARG:HD3	2.40	0.57
7:G:10:PHE:O	7:G:13:LEU:N	2.37	0.57
1:N:190:VAL:HG12	1:N:191:LEU:N	2.17	0.57
2:O:75:ILE:HG22	2:O:76:LEU:N	2.14	0.57
2:O:91:LEU:O	2:O:91:LEU:HD12	2.04	0.57
3:P:34:VAL:HG11	3:P:151:LEU:HD13	1.86	0.57
4:Q:146:LEU:HD13	4:Q:177:TRP:CE3	2.39	0.57
1:A:189:PHE:O	1:A:193:TRP:HE3	1.87	0.57
2:B:104:VAL:N	2:B:105:PRO:CD	2.67	0.57
2:O:63:GLY:O	2:O:64:GLU:CB	2.52	0.57
3:P:280:GLU:C	3:P:282:VAL:N	2.58	0.57
3:P:2:PRO:HA	9:P:301:HEM:HBB2	1.85	0.57
4:Q:123:LYS:O	4:Q:125:LYS:HG3	2.04	0.57
4:Q:57:LYS:HG2	4:Q:62:ASN:O	2.04	0.57
1:A:117:THR:HG22	1:A:205:MET:HB2	1.86	0.57
1:A:205:MET:O	1:A:207:ARG:HG2	2.05	0.57
3:C:180:ILE:HG13	3:C:198:SER:O	2.05	0.57
3:C:275:LYS:HZ2	11:C:306:OPC:HBG3	1.69	0.57
1:N:119:ILE:HG23	2:O:109:ILE:CD1	2.31	0.57
3:P:28:ALA:HB1	3:P:238:GLY:C	2.24	0.57
4:Q:155:VAL:HG12	4:Q:155:VAL:O	2.03	0.57
3:C:136:PRO:HB3	3:C:142:ILE:HG22	1.85	0.57
3:C:136:PRO:HA	3:C:142:ILE:HB	1.87	0.57
4:D:35:LEU:C	4:D:35:LEU:HD23	2.24	0.57
4:D:45:PRO:O	4:D:46:SER:HB2	2.05	0.57
1:N:159:PRO:O	1:N:161:VAL:HG22	2.04	0.57
1:N:32:ILE:CG2	1:N:33:PHE:N	2.57	0.57
3:P:217:LEU:HA	3:P:232:THR:HB	1.87	0.57
5:R:24:PHE:C	5:R:26:ILE:N	2.58	0.57
1:A:62:VAL:HG23	1:A:63:THR:N	2.14	0.57
2:B:79:TRP:CH2	5:E:1:MET:CA	2.87	0.57
1:N:174:SER:O	1:N:175:VAL:HG23	2.05	0.57
1:N:83:ARG:HG3	1:N:84:SER:N	2.18	0.57
4:Q:146:LEU:HD13	4:Q:177:TRP:CZ3	2.40	0.57
6:S:29:LYS:HG2	6:S:29:LYS:O	2.05	0.57
7:T:29:GLU:C	7:T:30:LEU:HD13	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:VAL:HG12	1:A:22:THR:HG22	1.86	0.57
11:B:305:OPC:HBP2	11:B:305:OPC:HAH1	1.86	0.57
2:B:40:PHE:CA	2:B:43:VAL:HG23	2.34	0.57
4:D:116:PRO:CD	4:D:127:PRO:HD3	2.35	0.57
1:N:85:ILE:HG23	2:O:51:ILE:CG2	2.35	0.57
2:O:114:ILE:HG22	2:O:115:GLU:N	2.19	0.57
2:O:64:GLU:CG	2:O:65:PRO:CD	2.81	0.57
8:U:2:ASP:O	8:U:4:LEU:N	2.37	0.57
1:N:33:PHE:CE1	1:N:34:TYR:CE1	2.92	0.57
2:O:43:VAL:HA	7:T:23:GLN:OE1	2.04	0.57
5:R:26:ILE:HG23	5:R:30:LYS:CE	2.35	0.57
2:B:96:LEU:HD11	2:B:100:LEU:HD12	1.86	0.57
3:C:176:ALA:H	3:C:228:GLY:HA3	1.70	0.57
4:D:36:TYR:O	4:D:40:LYS:HB2	2.05	0.57
4:D:92:VAL:HG12	4:D:93:VAL:N	2.18	0.57
2:O:125:ARG:HB3	2:O:125:ARG:HH11	1.67	0.57
2:O:127:PRO:C	2:O:129:ALA:H	2.08	0.57
2:O:77:PRO:CG	2:O:81:LEU:HB3	2.34	0.57
3:P:188:ASP:HB3	3:P:192:ASN:O	2.04	0.57
4:Q:107:VAL:HG12	4:Q:107:VAL:O	2.04	0.57
4:Q:175:LYS:HD3	4:Q:176:PRO:HD2	1.86	0.57
2:B:84:VAL:HG11	13:B:201:CLA:H42	1.86	0.56
3:C:279:VAL:HG12	3:C:279:VAL:O	2.04	0.56
5:E:13:ALA:HA	6:F:14:PHE:CE1	2.40	0.56
6:F:28:LEU:C	6:F:30:ILE:N	2.58	0.56
6:F:28:LEU:O	6:F:30:ILE:N	2.37	0.56
7:G:29:GLU:HG3	7:G:30:LEU:N	2.19	0.56
1:N:132:GLY:O	1:N:134:THR:N	2.38	0.56
1:N:154:VAL:HB	1:N:155:PRO:HD3	1.87	0.56
3:P:25:CYS:O	3:P:26:HIS:C	2.42	0.56
3:P:283:GLN:C	3:P:285:ALA:H	2.08	0.56
2:B:38:TYR:HB2	3:C:276:LYS:HZ3	1.70	0.56
2:B:56:VAL:HG12	2:B:57:LEU:N	2.19	0.56
3:C:157:ARG:O	3:C:159:GLN:NE2	2.38	0.56
2:B:124:PHE:CZ	5:E:23:ILE:HD11	2.40	0.56
6:F:25:VAL:O	6:F:28:LEU:HB2	2.04	0.56
1:A:190:VAL:HG12	1:A:191:LEU:N	2.19	0.56
11:B:305:OPC:HCB3	11:B:305:OPC:HAU1	1.87	0.56
3:C:60:GLN:NE2	3:C:157:ARG:HG3	2.19	0.56
6:F:35:LYS:H	6:F:35:LYS:HD2	1.70	0.56
9:N:302:HEM:HBD2	9:N:302:HEM:HMD1	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:268:ALA:C	3:P:270:LEU:H	2.08	0.56
3:C:120:PRO:CB	3:C:124:TYR:HB2	2.35	0.56
3:C:34:VAL:HG11	3:C:151:LEU:HD13	1.86	0.56
3:C:1:TYR:O	3:C:4:TRP:HB2	2.05	0.56
6:F:35:LYS:N	6:F:35:LYS:HD2	2.20	0.56
3:P:187:GLU:HG3	3:P:188:ASP:N	2.20	0.56
5:R:26:ILE:HG23	5:R:30:LYS:NZ	2.20	0.56
1:A:94:VAL:O	1:A:98:ILE:HG13	2.05	0.56
2:B:109:ILE:HG23	2:B:110:LEU:HD23	1.88	0.56
2:B:91:LEU:HD21	2:B:96:LEU:HD12	1.86	0.56
3:C:66:SER:O	3:C:68:VAL:HG22	2.06	0.56
4:D:123:LYS:O	4:D:125:LYS:N	2.38	0.56
4:D:132:GLN:NE2	4:D:141:ARG:HB2	2.21	0.56
1:A:78:PHE:HD1	4:D:37:PRO:O	1.89	0.56
8:H:18:ALA:O	8:H:21:VAL:CG2	2.52	0.56
2:B:39:VAL:O	2:B:43:VAL:N	2.36	0.56
8:H:9:LEU:HD22	8:H:13:PHE:HZ	1.69	0.56
1:N:117:THR:HG22	1:N:205:MET:HB2	1.87	0.56
2:O:127:PRO:HA	2:O:130:THR:HB	1.87	0.56
3:P:272:LEU:HD21	4:Q:24:PHE:CZ	2.41	0.56
4:Q:123:LYS:O	4:Q:125:LYS:N	2.39	0.56
6:S:8:TYR:HD2	6:S:9:ALA:N	2.03	0.56
3:C:169:ASN:ND2	3:C:237:VAL:H	2.03	0.56
6:F:27:LEU:N	6:F:27:LEU:CD1	2.68	0.56
7:G:8:LEU:HD23	7:G:12:THR:HG23	1.88	0.56
1:N:114:ARG:CD	1:N:208:LYS:HE2	2.35	0.56
1:N:25:TYR:O	1:N:26:VAL:CG2	2.54	0.56
3:P:205:LYS:HE2	3:P:206:THR:N	2.20	0.56
1:A:30:VAL:O	1:A:211:ILE:HD13	2.05	0.56
1:A:52:PHE:O	1:A:55:THR:N	2.32	0.56
2:B:34:ASN:ND2	2:B:35:ASP:OD1	2.37	0.56
3:C:102:TYR:O	3:C:118:PRO:HD2	2.05	0.56
5:E:17:GLY:O	5:E:22:ILE:HG21	2.06	0.56
8:H:2:ASP:O	8:H:4:LEU:N	2.38	0.56
1:N:189:PHE:O	1:N:193:TRP:HE3	1.88	0.56
2:O:133:PHE:HB2	13:O:1201:CLA:CAB	2.36	0.56
4:Q:35:LEU:C	4:Q:35:LEU:HD23	2.25	0.56
11:B:305:OPC:CAO	11:B:305:OPC:CAS	2.84	0.56
4:D:81:VAL:HG12	4:D:82:GLN:N	2.15	0.56
5:E:9:ILE:CG1	6:F:14:PHE:HB2	2.36	0.56
1:N:47:GLN:HE22	1:N:90:ALA:N	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:35:ASP:HB3	3:P:276:LYS:HE3	1.86	0.56
2:O:39:VAL:C	2:O:42:VAL:H	2.09	0.56
1:A:14:ILE:O	1:A:15:GLN:O	2.24	0.56
1:A:122:VAL:HA	9:A:302:HEM:HMC2	1.86	0.56
2:B:40:PHE:N	2:B:41:PRO:CD	2.69	0.56
2:B:89:ARG:O	2:B:91:LEU:N	2.39	0.56
3:C:146:LYS:HG2	3:C:248:VAL:CG2	2.32	0.56
4:D:154:THR:CG2	4:D:155:VAL:H	2.07	0.56
4:D:175:LYS:HD3	4:D:176:PRO:HD2	1.88	0.56
2:O:42:VAL:HG23	3:P:272:LEU:HB3	1.87	0.56
1:N:66:TYR:CB	2:O:65:PRO:HG2	2.35	0.56
2:O:89:ARG:O	2:O:91:LEU:N	2.38	0.56
3:P:93:GLU:O	3:P:95:LYS:N	2.39	0.56
2:O:122:ASN:ND2	5:R:27:LYS:HB2	2.21	0.56
1:A:43:CYS:HA	1:A:46:ILE:HD12	1.88	0.56
3:C:127:ILE:N	3:C:127:ILE:HD12	2.21	0.56
1:N:117:THR:HA	1:N:205:MET:HE1	1.88	0.56
1:N:61:THR:O	1:N:62:VAL:C	2.43	0.56
1:A:170:ARG:HA	1:A:179:THR:HG23	1.87	0.55
3:C:241:GLY:O	3:C:242:GLN:CB	2.54	0.55
1:N:113:PRO:HB3	2:O:27:TYR:HE1	1.70	0.55
1:N:157:ALA:O	1:N:158:ILE:HB	2.06	0.55
1:N:15:GLN:NE2	1:N:15:GLN:CA	2.67	0.55
1:N:90:ALA:O	1:N:92:MET:N	2.39	0.55
3:P:120:PRO:CB	3:P:124:TYR:HB2	2.36	0.55
1:A:74:ASN:HB3	1:A:75:GLU:OE2	2.06	0.55
1:N:167:ASP:O	1:N:169:LEU:N	2.38	0.55
1:N:61:THR:HG22	1:N:64:GLU:HB3	1.89	0.55
2:O:63:GLY:O	2:O:64:GLU:HB3	2.06	0.55
3:P:180:ILE:HG13	3:P:198:SER:O	2.05	0.55
3:P:271:MET:CG	4:Q:23:ALA:HA	2.36	0.55
1:A:214:PRO:CG	5:E:29:ILE:HG21	2.36	0.55
2:B:85:PHE:O	2:B:86:GLN:C	2.44	0.55
3:C:177:THR:HA	3:C:227:ALA:HA	1.88	0.55
3:C:55:ASP:N	3:C:55:ASP:OD2	2.32	0.55
3:P:27:LEU:HD12	3:P:27:LEU:O	2.06	0.55
2:B:79:TRP:C	2:B:80:TYR:HD1	2.08	0.55
3:C:161:TYR:CE1	3:C:167:SER:HA	2.42	0.55
3:C:249:LEU:N	3:C:249:LEU:HD12	2.20	0.55
11:B:305:OPC:HBT1	11:C:306:OPC:CBR	2.35	0.55
7:G:30:LEU:H	7:G:30:LEU:CD1	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:165:ILE:O	1:N:165:ILE:HD13	2.06	0.55
1:N:191:LEU:H	1:N:191:LEU:CD1	2.10	0.55
2:B:65:PRO:O	2:B:68:PRO:HD3	2.06	0.55
3:C:14:ARG:HH11	3:C:14:ARG:HG3	1.69	0.55
3:C:172:PHE:H	3:C:231:LEU:CG	2.19	0.55
7:G:16:LEU:C	7:G:18:TYR:N	2.58	0.55
8:H:3:VAL:O	8:H:6:TRP:N	2.39	0.55
1:N:33:PHE:O	1:N:35:CYS:SG	2.64	0.55
1:N:61:THR:O	1:N:63:THR:N	2.39	0.55
1:N:47:GLN:NE2	1:N:89:SER:HB3	2.16	0.55
1:N:119:ILE:CG2	2:O:109:ILE:HD11	2.31	0.55
3:P:197:VAL:HG13	3:P:211:ILE:HG22	1.87	0.55
6:S:9:ALA:HA	6:S:12:LEU:HD12	1.87	0.55
3:C:169:ASN:HD21	3:C:237:VAL:HG22	1.72	0.55
1:N:116:LEU:H	1:N:116:LEU:HD12	1.71	0.55
3:P:161:TYR:CE1	3:P:167:SER:HA	2.42	0.55
4:Q:59:LYS:HB2	4:Q:59:LYS:NZ	2.21	0.55
7:T:21:TYR:N	7:T:21:TYR:HD1	2.02	0.55
2:B:63:GLY:C	2:B:65:PRO:CD	2.75	0.55
3:C:34:VAL:CG1	3:C:151:LEU:HD22	2.36	0.55
4:D:58:ASP:O	4:D:59:LYS:HB2	2.07	0.55
3:P:241:GLY:O	3:P:242:GLN:CB	2.54	0.55
3:P:93:GLU:C	3:P:95:LYS:N	2.60	0.55
6:S:24:GLY:CA	6:S:27:LEU:HD22	2.37	0.55
8:U:2:ASP:OD1	8:U:3:VAL:N	2.39	0.55
3:C:10:PRO:CA	3:C:106:TYR:HE2	2.18	0.55
3:C:44:THR:C	3:C:132:LEU:HD12	2.28	0.55
3:C:48:ALA:HB3	3:C:129:PHE:HB2	1.87	0.55
6:F:29:LYS:HG2	6:F:29:LYS:O	2.07	0.55
2:O:38:TYR:HB2	3:P:276:LYS:HE2	1.88	0.55
2:B:96:LEU:HD13	2:B:96:LEU:O	2.07	0.55
3:C:102:TYR:H	3:C:118:PRO:CG	2.09	0.55
3:C:171:VAL:HG12	3:C:231:LEU:CD1	2.31	0.55
1:N:170:ARG:HB3	1:N:179:THR:HG23	1.88	0.55
2:O:40:PHE:N	2:O:41:PRO:CD	2.70	0.55
3:P:85:ALA:HA	3:P:132:LEU:HB2	1.89	0.55
3:P:180:ILE:HA	3:P:200:GLN:HB2	1.89	0.55
3:P:200:GLN:O	3:P:206:THR:HA	2.07	0.55
4:Q:143:PRO:O	4:Q:145:PRO:HD3	2.07	0.55
1:A:114:ARG:HG3	1:A:208:LYS:HD3	1.86	0.55
1:A:191:LEU:N	1:A:192:PRO:HD2	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:9:LEU:HD22	8:H:13:PHE:CZ	2.41	0.55
3:P:249:LEU:HD12	3:P:249:LEU:N	2.20	0.55
4:Q:63:ASN:H	4:Q:63:ASN:HD22	1.53	0.55
1:A:214:PRO:CD	5:E:29:ILE:HG21	2.36	0.54
2:B:141:ILE:C	2:B:143:LEU:H	2.09	0.54
3:C:22:CYS:HB2	3:C:240:PHE:CZ	2.42	0.54
3:C:280:GLU:HA	3:C:282:VAL:HG22	1.89	0.54
4:D:51:GLY:CA	4:D:84:LEU:HD21	2.36	0.54
1:N:113:PRO:HB3	2:O:27:TYR:CE1	2.42	0.54
3:P:23:ALA:C	3:P:25:CYS:N	2.60	0.54
6:S:25:VAL:O	6:S:28:LEU:HB2	2.07	0.54
8:U:9:LEU:O	8:U:10:LEU:C	2.46	0.54
1:A:60:PRO:HB3	1:A:184:TYR:CD1	2.42	0.54
3:C:120:PRO:HB2	3:C:124:TYR:HB2	1.89	0.54
3:C:217:LEU:HD23	3:C:232:THR:OG1	2.07	0.54
1:N:108:GLY:O	1:N:111:LYS:HB2	2.06	0.54
1:N:165:ILE:HG23	1:N:166:SER:N	2.21	0.54
2:O:20:LYS:HZ2	2:O:20:LYS:HB2	1.72	0.54
2:O:53:ALA:O	2:O:57:LEU:CB	2.52	0.54
3:P:199:ILE:HG22	3:P:200:GLN:N	2.15	0.54
1:A:103:ARG:NH1	1:A:103:ARG:HG3	2.21	0.54
1:A:202:HIS:O	1:A:206:ILE:CG1	2.53	0.54
1:A:52:PHE:HA	1:A:55:THR:HG23	1.89	0.54
1:A:62:VAL:HG13	1:A:177:GLN:CG	2.25	0.54
11:B:305:OPC:HAG1	11:B:305:OPC:HAV	1.89	0.54
2:B:85:PHE:C	2:B:85:PHE:CD1	2.79	0.54
3:C:23:ALA:C	3:C:25:CYS:N	2.60	0.54
6:F:27:LEU:HD13	6:F:27:LEU:H	1.71	0.54
1:N:88:TRP:O	1:N:89:SER:C	2.46	0.54
3:P:280:GLU:HA	3:P:282:VAL:HG22	1.89	0.54
4:Q:115:VAL:HG11	4:Q:124:PHE:O	2.07	0.54
4:Q:145:PRO:O	4:Q:146:LEU:CB	2.55	0.54
4:Q:165:TRP:HE3	4:Q:167:GLU:OE2	1.89	0.54
4:Q:64:VAL:HG13	4:Q:68:LYS:HG3	1.88	0.54
1:A:137:SER:HB3	1:A:148:VAL:HG21	1.88	0.54
2:B:96:LEU:HD13	2:B:100:LEU:HB2	1.88	0.54
2:B:115:GLU:OE2	2:B:126:ARG:NH2	2.41	0.54
4:D:50:VAL:O	4:D:84:LEU:HD11	2.06	0.54
5:E:25:ALA:O	5:E:29:ILE:HD12	2.07	0.54
1:N:103:ARG:HG3	1:N:103:ARG:NH1	2.23	0.54
2:O:62:VAL:HG22	12:O:1309:BNT:CAL	2.36	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:10:PRO:C	3:P:106:TYR:HE2	2.11	0.54
3:P:140:LYS:HD2	3:P:140:LYS:H	1.73	0.54
15:R:1101:BCR:HC21	7:T:23:GLN:NE2	2.23	0.54
3:C:26:HIS:CD2	3:C:158:GLY:HA2	2.43	0.54
3:C:54:TYR:CD1	3:C:58:LEU:HD22	2.42	0.54
3:C:61:VAL:HG23	3:C:62:ALA:N	2.23	0.54
6:F:9:ALA:HA	6:F:12:LEU:HD12	1.87	0.54
6:F:16:LEU:HA	6:F:19:VAL:HB	1.90	0.54
2:O:133:PHE:C	2:O:135:PHE:N	2.60	0.54
1:A:35:CYS:HA	10:A:303:HEC:C3B	2.36	0.54
2:B:100:LEU:HD23	2:B:100:LEU:O	2.08	0.54
2:B:125:ARG:O	2:B:127:PRO:CD	2.52	0.54
2:B:93:ASN:CG	2:B:94:LYS:H	2.03	0.54
3:C:116:VAL:HG13	3:C:118:PRO:HG2	1.90	0.54
3:C:262:ILE:O	3:C:265:VAL:N	2.40	0.54
6:F:26:LEU:C	6:F:26:LEU:HD23	2.28	0.54
1:N:28:PRO:O	2:O:30:PRO:HB2	2.08	0.54
2:O:85:PHE:C	2:O:85:PHE:CD1	2.81	0.54
5:R:15:PHE:HA	5:R:18:ILE:HG13	1.89	0.54
1:A:135:GLY:HA2	1:A:138:LEU:HG	1.89	0.54
4:D:143:PRO:O	4:D:145:PRO:HD3	2.08	0.54
7:G:20:ALA:C	7:G:24:TYR:CE2	2.81	0.54
5:R:24:PHE:O	5:R:26:ILE:N	2.41	0.54
1:A:119:ILE:O	1:A:120:SER:C	2.46	0.54
1:A:90:ALA:O	1:A:92:MET:N	2.41	0.54
3:C:14:ARG:HG3	3:C:14:ARG:NH1	2.21	0.54
1:N:43:CYS:HA	1:N:46:ILE:HD12	1.90	0.54
2:O:135:PHE:HA	2:O:138:LEU:HB2	1.90	0.54
3:P:120:PRO:HB2	3:P:124:TYR:HB2	1.89	0.54
1:A:173:SER:HB2	4:Q:85:LYS:O	2.07	0.54
2:O:43:VAL:CG2	7:T:23:GLN:OE1	2.50	0.54
1:A:141:ASP:C	2:B:65:PRO:HG2	2.28	0.54
2:B:83:PRO:HB2	13:B:201:CLA:CMD	2.38	0.54
2:B:39:VAL:C	2:B:42:VAL:H	2.10	0.54
3:C:205:LYS:HZ3	3:C:207:VAL:CG1	2.20	0.54
3:C:31:PRO:O	3:C:32:ALA:HB2	2.08	0.54
3:C:54:TYR:HD2	3:C:155:ARG:HH11	1.56	0.54
7:G:28:ASN:ND2	7:G:30:LEU:HD22	2.18	0.54
8:H:9:LEU:O	8:H:11:VAL:N	2.41	0.54
3:P:188:ASP:H	3:P:193:VAL:CG2	2.17	0.54
3:P:282:VAL:HG23	3:P:283:GLN:N	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:46:PHE:CE1	3:P:131:VAL:HG13	2.43	0.54
3:P:61:VAL:HG23	3:P:62:ALA:N	2.23	0.54
4:Q:106:ALA:HB1	4:Q:114:VAL:HG13	1.90	0.54
5:R:5:ALA:C	5:R:7:PHE:H	2.12	0.54
6:S:24:GLY:HA2	6:S:27:LEU:HD22	1.89	0.54
2:B:18:LEU:C	2:B:18:LEU:HD12	2.29	0.54
3:C:205:LYS:HE2	3:C:206:THR:N	2.23	0.54
3:C:83:LYS:NZ	3:C:83:LYS:H	2.06	0.54
8:H:6:TRP:O	8:H:9:LEU:HB2	2.07	0.54
1:N:106:LEU:HD21	2:O:133:PHE:CE1	2.43	0.54
1:N:88:TRP:HB2	2:O:51:ILE:HG23	1.90	0.54
2:O:100:LEU:HD23	2:O:100:LEU:O	2.07	0.54
2:O:38:TYR:N	2:O:38:TYR:CD1	2.75	0.54
5:R:16:PHE:CE2	15:R:1101:BCR:H373	2.41	0.54
5:E:16:PHE:CE2	15:E:101:BCR:H373	2.41	0.53
1:N:135:GLY:HA2	1:N:138:LEU:CG	2.37	0.53
1:N:58:TYR:CE2	1:N:60:PRO:HB3	2.42	0.53
2:O:116:ASN:ND2	2:O:116:ASN:C	2.61	0.53
5:E:24:PHE:C	5:E:26:ILE:N	2.61	0.53
1:N:127:ILE:HG21	1:N:195:ILE:HB	1.90	0.53
3:P:17:THR:OG1	3:P:18:GLY:N	2.41	0.53
3:P:277:LYS:HE3	7:T:27:PRO:HD2	1.90	0.53
1:A:24:LYS:NZ	1:A:26:VAL:H	2.06	0.53
1:A:90:ALA:C	1:A:92:MET:H	2.11	0.53
2:B:41:PRO:HB3	11:B:305:OPC:HBI2	1.90	0.53
3:C:85:ALA:HA	3:C:132:LEU:HB2	1.89	0.53
4:D:90:TYR:HD2	4:D:104:ILE:HD11	1.73	0.53
7:G:9:VAL:HG23	7:G:10:PHE:N	2.20	0.53
2:O:85:PHE:O	2:O:86:GLN:C	2.45	0.53
3:P:104:GLN:N	3:P:104:GLN:NE2	2.57	0.53
3:P:231:LEU:HD21	3:P:233:ASN:O	2.09	0.53
4:Q:90:TYR:CD2	4:Q:104:ILE:HD11	2.44	0.53
1:A:146:TRP:CB	2:B:75:ILE:HD11	2.39	0.53
1:A:176:GLY:O	1:A:178:ALA:N	2.41	0.53
1:A:205:MET:O	1:A:207:ARG:N	2.41	0.53
11:B:305:OPC:HBA1	11:C:306:OPC:CBX	2.36	0.53
3:C:283:GLN:C	3:C:285:ALA:H	2.09	0.53
3:C:53:PRO:O	3:C:54:TYR:CD2	2.60	0.53
6:F:14:PHE:C	6:F:17:ILE:HG12	2.29	0.53
11:N:1305:OPC:CAY	11:N:1305:OPC:HCB2	2.39	0.53
1:N:170:ARG:NH1	1:N:173:SER:O	2.41	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:193:TRP:O	1:N:197:VAL:HG23	2.08	0.53
2:O:26:TYR:O	2:O:26:TYR:CD1	2.60	0.53
2:O:45:MET:HE3	3:P:269:GLN:CB	2.39	0.53
3:P:101:VAL:HB	3:P:118:PRO:HB2	1.87	0.53
3:P:44:THR:O	3:P:132:LEU:HA	2.08	0.53
3:P:54:TYR:CD1	3:P:58:LEU:HD22	2.44	0.53
4:Q:115:VAL:HG22	4:Q:126:CYS:CB	2.37	0.53
8:U:6:TRP:O	8:U:9:LEU:HB2	2.07	0.53
1:A:194:LEU:N	1:A:194:LEU:HD23	2.22	0.53
9:A:302:HEM:HMA2	16:A:304:HOH:O	2.07	0.53
10:A:303:HEC:HBC2	2:B:44:ILE:HD11	1.91	0.53
1:A:39:ILE:HG23	2:B:47:THR:CG2	2.35	0.53
4:D:94:GLU:C	4:D:96:LYS:H	2.11	0.53
1:N:211:ILE:O	1:N:212:SER:OG	2.23	0.53
2:O:130:THR:O	2:O:133:PHE:N	2.39	0.53
2:O:64:GLU:CD	2:O:65:PRO:HD3	2.29	0.53
2:O:93:ASN:O	2:O:94:LYS:HB2	2.08	0.53
3:P:120:PRO:HG2	3:P:124:TYR:CD1	2.44	0.53
4:Q:58:ASP:O	4:Q:59:LYS:HB2	2.08	0.53
1:A:194:LEU:O	1:A:195:ILE:C	2.47	0.53
2:B:115:GLU:OE2	2:B:126:ARG:CZ	2.57	0.53
2:B:133:PHE:C	2:B:135:PHE:N	2.62	0.53
2:B:82:TYR:O	2:B:86:GLN:N	2.35	0.53
1:N:118:TRP:HZ3	2:O:109:ILE:HA	1.70	0.53
1:N:17:LEU:CG	1:N:20:ASP:HB2	2.35	0.53
1:N:27:PRO:HA	2:O:33:PRO:HG3	1.91	0.53
1:N:52:PHE:HA	1:N:55:THR:HG23	1.90	0.53
2:O:87:ILE:O	2:O:88:LEU:C	2.46	0.53
2:O:95:LEU:N	2:O:95:LEU:HD23	2.24	0.53
5:R:25:ALA:C	5:R:26:ILE:HD12	2.28	0.53
7:T:7:GLY:C	7:T:9:VAL:H	2.10	0.53
1:A:113:PRO:HA	1:N:16:ALA:HB1	1.86	0.53
1:A:165:ILE:O	1:A:165:ILE:HD13	2.09	0.53
1:A:34:TYR:OH	1:A:107:THR:HG21	2.09	0.53
2:B:124:PHE:HZ	5:E:27:LYS:CB	2.21	0.53
2:B:94:LYS:C	2:B:96:LEU:N	2.59	0.53
3:C:118:PRO:C	3:C:120:PRO:HD3	2.29	0.53
3:C:213:ALA:O	3:C:215:PRO:HD2	2.08	0.53
3:C:280:GLU:O	3:C:280:GLU:HG2	2.08	0.53
11:C:306:OPC:HAL2	11:C:306:OPC:HAP2	1.90	0.53
3:C:89:ARG:NH1	3:C:89:ARG:HG3	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:3:LEU:O	5:E:4:GLY:C	2.47	0.53
1:N:166:SER:OG	1:N:170:ARG:NH2	2.42	0.53
2:O:99:LEU:O	2:O:102:ALA:N	2.42	0.53
3:P:151:LEU:HG	3:P:152:GLY:N	2.23	0.53
3:P:277:LYS:NZ	7:T:27:PRO:HD2	2.24	0.53
2:O:57:LEU:CD1	7:T:10:PHE:HA	2.39	0.53
7:T:9:VAL:HG23	7:T:10:PHE:N	2.18	0.53
1:A:42:THR:O	1:A:44:PHE:N	2.42	0.53
3:C:118:PRO:O	3:C:120:PRO:HD3	2.09	0.53
3:C:93:GLU:C	3:C:95:LYS:N	2.61	0.53
4:D:115:VAL:HG13	4:D:126:CYS:CA	2.36	0.53
5:E:2:ILE:HG23	5:E:3:LEU:N	2.19	0.53
1:N:170:ARG:HD2	1:N:171:GLY:N	2.23	0.53
1:N:32:ILE:HD11	7:T:26:ARG:HH22	1.74	0.53
1:N:41:LEU:HD21	1:N:45:LEU:HD11	1.90	0.53
2:O:125:ARG:O	2:O:126:ARG:HB3	2.07	0.53
1:N:27:PRO:HD2	2:O:29:GLU:HB3	1.90	0.53
2:O:75:ILE:CG2	2:O:76:LEU:H	2.11	0.53
3:P:22:CYS:HB2	3:P:240:PHE:CZ	2.44	0.53
3:P:91:PRO:HB2	3:P:95:LYS:CE	2.39	0.53
3:P:271:MET:HE2	4:Q:26:THR:HG21	1.90	0.53
1:A:146:TRP:HB3	2:B:75:ILE:HD11	1.90	0.53
2:B:37:LEU:HB2	2:B:38:TYR:CE1	2.44	0.53
3:C:10:PRO:C	3:C:106:TYR:HE2	2.11	0.53
3:C:277:LYS:C	3:C:279:VAL:H	2.11	0.53
1:N:160:VAL:C	1:N:162:GLY:N	2.60	0.53
3:P:126:GLU:C	3:P:127:ILE:HD12	2.29	0.53
3:P:61:VAL:O	3:P:62:ALA:HB2	2.07	0.53
4:Q:102:TYR:CG	4:Q:150:LEU:HD23	2.43	0.53
2:O:79:TRP:CZ3	5:R:4:GLY:HA3	2.43	0.53
1:A:25:TYR:O	1:A:26:VAL:HG13	2.09	0.53
2:B:105:PRO:HG2	2:B:106:LEU:N	2.21	0.53
3:C:76:LEU:HD23	3:C:77:MET:N	2.23	0.53
3:C:90:ILE:O	3:C:90:ILE:HG22	2.07	0.53
3:C:91:PRO:HB2	3:C:95:LYS:CE	2.39	0.53
4:D:145:PRO:O	4:D:146:LEU:CB	2.57	0.53
1:A:33:PHE:CE1	5:E:14:LEU:HD12	2.44	0.53
1:N:116:LEU:HD12	1:N:117:THR:H	1.74	0.53
1:N:17:LEU:HG	1:N:20:ASP:OD1	2.08	0.53
1:N:41:LEU:HD13	10:N:303:HEC:HMD2	1.91	0.53
2:O:127:PRO:C	2:O:129:ALA:N	2.62	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:277:LYS:C	3:P:279:VAL:H	2.11	0.53
3:P:53:PRO:O	3:P:54:TYR:CD2	2.62	0.53
4:Q:38:LEU:HD12	4:Q:38:LEU:O	2.08	0.53
3:C:101:VAL:HB	3:C:118:PRO:HB2	1.88	0.52
3:C:219:VAL:CG1	3:C:220:SER:H	2.21	0.52
1:N:34:TYR:N	1:N:34:TYR:CD1	2.76	0.52
2:O:96:LEU:HD11	2:O:100:LEU:HD12	1.91	0.52
3:P:89:ARG:NH1	3:P:89:ARG:HG3	2.24	0.52
4:Q:90:TYR:HD2	4:Q:104:ILE:HD11	1.75	0.52
3:C:3:PHE:N	3:C:3:PHE:CD1	2.72	0.52
4:D:90:TYR:CD2	4:D:104:ILE:HD11	2.44	0.52
4:D:118:ASN:ND2	4:D:120:ALA:H	2.07	0.52
1:A:212:SER:O	5:E:26:ILE:HG12	2.08	0.52
1:N:158:ILE:HG22	1:N:161:VAL:CG2	2.32	0.52
2:O:139:VAL:O	2:O:142:TRP:HB3	2.09	0.52
2:O:39:VAL:O	2:O:42:VAL:N	2.43	0.52
5:R:3:LEU:O	5:R:4:GLY:C	2.45	0.52
1:A:114:ARG:NH1	1:A:114:ARG:HB2	2.24	0.52
2:B:135:PHE:HA	2:B:138:LEU:HB2	1.91	0.52
11:B:305:OPC:CAV	11:B:305:OPC:CAG	2.86	0.52
1:N:58:TYR:CD2	1:N:184:TYR:HE1	2.22	0.52
1:N:194:LEU:HD23	1:N:194:LEU:N	2.23	0.52
12:B:309:BNT:HAM2	3:C:148:ALA:H	1.71	0.52
5:E:5:ALA:HB1	6:F:10:ALA:CA	2.38	0.52
7:G:7:GLY:C	7:G:9:VAL:H	2.10	0.52
1:A:52:PHE:HB2	1:N:189:PHE:CZ	2.44	0.52
1:N:114:ARG:HD3	1:N:208:LYS:CB	2.39	0.52
1:N:90:ALA:C	1:N:92:MET:N	2.63	0.52
2:O:71:THR:O	2:O:71:THR:HG22	2.08	0.52
1:A:112:LYS:HZ3	2:B:27:TYR:HE1	1.56	0.52
1:A:155:PRO:O	1:A:158:ILE:HD12	2.08	0.52
1:A:30:VAL:H	1:A:211:ILE:HD12	1.75	0.52
1:A:77:SER:O	1:A:78:PHE:CB	2.57	0.52
3:C:153:ALA:O	3:C:240:PHE:HA	2.10	0.52
3:C:180:ILE:HA	3:C:200:GLN:HB2	1.90	0.52
3:C:268:ALA:O	3:C:270:LEU:N	2.43	0.52
3:C:97:GLU:HG2	3:C:97:GLU:O	2.08	0.52
4:D:55:THR:O	4:D:64:VAL:HB	2.10	0.52
1:N:210:GLY:O	1:N:211:ILE:HB	2.09	0.52
1:N:102:PHE:CE2	13:O:1201:CLA:HMA3	2.45	0.52
2:O:133:PHE:HE2	2:O:137:THR:HG21	1.71	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:136:PRO:HA	3:P:142:ILE:HB	1.91	0.52
1:A:88:TRP:O	1:A:89:SER:C	2.47	0.52
3:C:172:PHE:N	3:C:231:LEU:HG	2.25	0.52
3:C:61:VAL:O	3:C:62:ALA:HB2	2.08	0.52
4:D:137:GLY:O	4:D:138:ARG:C	2.48	0.52
7:G:6:LEU:H	7:G:6:LEU:CD2	2.13	0.52
8:H:9:LEU:O	8:H:10:LEU:C	2.47	0.52
3:P:255:VAL:O	3:P:258:MET:HG3	2.08	0.52
3:P:26:HIS:HA	3:P:159:GLN:OE1	2.09	0.52
3:P:34:VAL:CG1	3:P:151:LEU:HD22	2.40	0.52
6:S:26:LEU:HD23	6:S:26:LEU:C	2.30	0.52
8:U:3:VAL:O	8:U:6:TRP:N	2.42	0.52
2:B:82:TYR:N	2:B:83:PRO:HD2	2.23	0.52
2:B:99:LEU:O	2:B:102:ALA:N	2.43	0.52
3:C:157:ARG:NH2	3:C:161:TYR:OH	2.43	0.52
4:D:126:CYS:HB3	4:D:131:SER:H	1.75	0.52
4:D:102:TYR:CG	4:D:150:LEU:HD23	2.45	0.52
4:D:165:TRP:HE3	4:D:167:GLU:OE2	1.91	0.52
8:H:7:VAL:O	8:H:9:LEU:N	2.43	0.52
1:N:160:VAL:HA	1:N:163:VAL:HB	1.91	0.52
7:T:20:ALA:C	7:T:24:TYR:CE2	2.83	0.52
2:B:127:PRO:HA	2:B:130:THR:HB	1.92	0.52
2:B:69:PHE:O	2:B:69:PHE:CD2	2.63	0.52
3:C:245:THR:OG1	3:C:246:GLU:N	2.41	0.52
6:F:18:PHE:N	6:F:18:PHE:CD2	2.78	0.52
2:O:150:PRO:O	2:O:151:LEU:HB3	2.10	0.52
3:P:219:VAL:CG1	3:P:220:SER:H	2.22	0.52
8:U:9:LEU:HD22	8:U:13:PHE:CZ	2.44	0.52
2:B:45:MET:CE	3:C:272:LEU:HD12	2.40	0.52
1:A:78:PHE:HE1	4:D:37:PRO:HA	1.74	0.52
4:D:55:THR:OG1	4:D:63:ASN:HA	2.09	0.52
6:F:10:ALA:O	6:F:12:LEU:N	2.43	0.52
7:G:28:ASN:HD21	7:G:30:LEU:CD2	2.18	0.52
1:N:15:GLN:H	1:N:15:GLN:NE2	2.06	0.52
2:O:36:LEU:HA	2:O:39:VAL:CG1	2.40	0.52
6:S:16:LEU:HA	6:S:19:VAL:HB	1.92	0.52
7:T:8:LEU:HD23	7:T:12:THR:CG2	2.39	0.52
3:C:226:LYS:NZ	3:C:226:LYS:CB	2.73	0.52
1:N:104:VAL:O	1:N:105:TYR:C	2.48	0.52
11:N:1305:OPC:CBR	11:N:1305:OPC:CBN	2.86	0.52
9:N:302:HEM:HAA2	10:N:303:HEC:CHA	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:36:LEU:HA	2:O:39:VAL:HG13	1.92	0.52
3:P:157:ARG:NH2	3:P:161:TYR:OH	2.43	0.52
3:P:245:THR:OG1	3:P:246:GLU:N	2.43	0.52
4:Q:152:HIS:HB2	4:Q:163:THR:OG1	2.09	0.52
5:R:10:VAL:O	5:R:10:VAL:CG1	2.58	0.52
5:R:11:PHE:CG	5:R:12:ILE:N	2.77	0.52
6:S:23:LEU:O	6:S:27:LEU:HD22	2.10	0.52
1:A:116:LEU:HD12	1:A:117:THR:H	1.74	0.51
1:A:175:VAL:O	1:A:176:GLY:O	2.28	0.51
1:A:134:THR:HB	1:A:187:HIS:HB2	1.92	0.51
1:A:28:PRO:HG2	1:A:29:HIS:H	1.74	0.51
1:A:70:GLN:O	1:A:74:ASN:CB	2.58	0.51
2:B:49:ALA:O	2:B:52:VAL:CB	2.59	0.51
4:D:90:TYR:O	4:D:103:GLY:HA3	2.10	0.51
7:G:30:LEU:H	7:G:30:LEU:HD12	1.75	0.51
1:N:184:TYR:CE2	1:N:188:THR:HG21	2.44	0.51
2:O:42:VAL:HG22	3:P:269:GLN:HA	1.92	0.51
3:P:161:TYR:HA	9:P:301:HEM:HMD2	1.91	0.51
3:P:177:THR:HA	3:P:227:ALA:HA	1.91	0.51
4:Q:27:VAL:C	4:Q:29:GLY:N	2.62	0.51
4:Q:94:GLU:HA	4:Q:94:GLU:OE1	2.10	0.51
8:U:7:VAL:O	8:U:8:ALA:C	2.49	0.51
1:A:31:ASN:CG	1:A:211:ILE:HD11	2.31	0.51
3:C:271:MET:HA	3:C:274:LEU:HG	1.92	0.51
1:N:157:ALA:O	1:N:158:ILE:CB	2.57	0.51
1:N:95:LEU:CD2	1:N:99:LEU:HD21	2.41	0.51
3:P:66:SER:O	3:P:68:VAL:HG22	2.10	0.51
1:A:141:ASP:O	1:A:145:TYR:HB2	2.10	0.51
1:A:85:ILE:O	1:A:89:SER:N	2.44	0.51
2:B:127:PRO:C	2:B:129:ALA:H	2.13	0.51
11:B:305:OPC:HBZ2	11:B:305:OPC:CAX	2.40	0.51
2:B:51:ILE:HD12	2:B:51:ILE:N	2.22	0.51
3:C:117:GLY:O	3:C:119:LEU:HG	2.11	0.51
3:C:54:TYR:OH	3:C:125:GLN:NE2	2.43	0.51
3:C:188:ASP:CG	3:C:192:ASN:HB3	2.30	0.51
3:C:255:VAL:O	3:C:258:MET:HG3	2.10	0.51
5:E:10:VAL:O	5:E:10:VAL:CG1	2.59	0.51
1:N:15:GLN:CA	1:N:15:GLN:HE21	2.20	0.51
2:O:118:ASN:ND2	2:O:123:PRO:HB2	2.24	0.51
2:O:141:ILE:C	2:O:143:LEU:H	2.12	0.51
2:O:64:GLU:N	2:O:65:PRO:CD	2.72	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:53:ALA:HA	3:P:258:MET:CE	2.40	0.51
7:T:29:GLU:O	7:T:30:LEU:HD13	2.09	0.51
2:B:133:PHE:C	2:B:135:PHE:H	2.11	0.51
5:E:5:ALA:CB	6:F:6:MET:O	2.59	0.51
1:N:41:LEU:O	1:N:42:THR:C	2.49	0.51
1:N:90:ALA:O	1:N:94:VAL:HG23	2.10	0.51
3:P:81:GLY:O	3:P:83:LYS:HD3	2.10	0.51
4:Q:110:HIS:CD2	4:Q:143:PRO:HB2	2.46	0.51
6:S:28:LEU:HB3	6:S:33:ALA:HB2	1.92	0.51
1:A:116:LEU:C	1:A:118:TRP:N	2.63	0.51
1:A:142:GLN:N	2:B:65:PRO:CG	2.73	0.51
1:A:31:ASN:ND2	1:A:211:ILE:HD11	2.26	0.51
2:B:41:PRO:O	2:B:45:MET:HG3	2.11	0.51
2:B:39:VAL:O	2:B:42:VAL:N	2.44	0.51
3:C:102:TYR:HB3	3:C:118:PRO:HD3	1.91	0.51
3:C:120:PRO:HG2	3:C:124:TYR:CD1	2.46	0.51
4:D:19:MET:O	4:D:22:LEU:HD22	2.11	0.51
4:D:80:LEU:HD23	4:D:80:LEU:H	1.74	0.51
7:G:18:TYR:O	7:G:21:TYR:N	2.43	0.51
2:O:36:LEU:CA	2:O:39:VAL:HG13	2.41	0.51
3:P:118:PRO:C	3:P:120:PRO:HD3	2.31	0.51
4:Q:115:VAL:HG22	4:Q:126:CYS:HB2	1.91	0.51
4:Q:35:LEU:HD23	4:Q:36:TYR:N	2.26	0.51
8:U:9:LEU:HD22	8:U:13:PHE:HZ	1.75	0.51
3:C:110:GLN:HB3	3:C:113:VAL:CG2	2.40	0.51
3:C:168:ASN:O	3:C:170:ASN:N	2.44	0.51
3:P:83:LYS:HZ1	3:P:133:SER:CA	2.23	0.51
1:N:87:ARG:HH12	3:P:146:LYS:NZ	2.08	0.51
4:Q:132:GLN:NE2	4:Q:141:ARG:HB2	2.25	0.51
5:R:13:ALA:HB2	6:S:14:PHE:HD1	1.75	0.51
1:A:158:ILE:HG22	1:A:162:GLY:HA3	1.92	0.51
1:A:117:THR:HA	1:A:205:MET:CE	2.41	0.51
1:A:41:LEU:HD21	1:A:45:LEU:HD11	1.93	0.51
1:A:52:PHE:C	1:A:54:MET:N	2.62	0.51
2:B:127:PRO:O	2:B:129:ALA:N	2.44	0.51
2:B:130:THR:O	2:B:133:PHE:N	2.42	0.51
2:B:80:TYR:O	2:B:82:TYR:N	2.35	0.51
2:B:82:TYR:O	2:B:83:PRO:C	2.48	0.51
3:C:158:GLY:HA3	9:C:301:HEM:C2D	2.46	0.51
3:C:41:LEU:O	3:C:133:SER:HB3	2.11	0.51
5:E:32:ILE:HG22	5:E:32:ILE:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:135:GLY:H	1:N:187:HIS:HD1	1.56	0.51
2:O:38:TYR:C	3:P:272:LEU:HD22	2.30	0.51
1:A:104:VAL:O	1:A:105:TYR:C	2.49	0.51
1:A:193:TRP:O	1:A:197:VAL:HG23	2.11	0.51
2:B:36:LEU:CA	2:B:39:VAL:HG13	2.40	0.51
3:C:181:THR:OG1	3:C:200:GLN:HG2	2.11	0.51
3:C:44:THR:O	3:C:132:LEU:HA	2.11	0.51
1:N:23:SER:HA	1:N:25:TYR:CE1	2.42	0.51
4:Q:113:CYS:CB	4:Q:128:CYS:HG	2.20	0.51
1:N:32:ILE:HD11	7:T:26:ARG:NH2	2.26	0.51
1:A:167:ASP:O	1:A:169:LEU:N	2.44	0.51
1:A:117:THR:HA	1:A:205:MET:HE1	1.92	0.51
2:B:83:PRO:HA	2:B:143:LEU:HB3	1.92	0.51
3:C:26:HIS:HA	3:C:159:GLN:OE1	2.11	0.51
1:A:82:ILE:HD13	4:D:41:TYR:CD1	2.46	0.51
1:A:33:PHE:CE2	15:E:101:BCR:H352	2.46	0.51
5:E:28:SER:C	5:E:30:LYS:N	2.63	0.51
6:F:10:ALA:C	6:F:12:LEU:N	2.63	0.51
7:G:14:GLY:C	7:G:16:LEU:H	2.14	0.51
1:N:32:ILE:HG22	1:N:33:PHE:HD1	1.75	0.51
2:O:20:LYS:CB	2:O:20:LYS:NZ	2.72	0.51
3:P:117:GLY:O	3:P:119:LEU:HG	2.11	0.51
3:P:193:VAL:HG12	3:P:193:VAL:O	2.10	0.51
3:P:76:LEU:HD23	3:P:77:MET:N	2.26	0.51
4:Q:38:LEU:HD11	4:Q:42:PHE:HE1	1.75	0.51
1:A:102:PHE:HE1	5:E:11:PHE:HD1	1.59	0.51
3:C:265:VAL:O	3:C:269:GLN:HG3	2.11	0.51
3:C:81:GLY:O	3:C:83:LYS:HD3	2.11	0.51
1:N:146:TRP:CZ2	2:O:69:PHE:HA	2.43	0.51
1:N:202:HIS:O	1:N:206:ILE:CG1	2.57	0.51
2:O:96:LEU:HD13	2:O:100:LEU:HB2	1.92	0.51
3:P:172:PHE:N	3:P:231:LEU:HG	2.26	0.51
5:R:14:LEU:O	5:R:17:GLY:C	2.49	0.51
5:R:2:ILE:HG23	5:R:3:LEU:N	2.19	0.51
6:S:24:GLY:HA2	6:S:27:LEU:CD2	2.41	0.51
8:U:7:VAL:O	8:U:9:LEU:N	2.44	0.51
1:A:140:TRP:CE3	2:B:68:PRO:HD2	2.46	0.50
1:A:52:PHE:N	9:A:301:HEM:HAC	2.26	0.50
1:A:77:SER:O	4:D:41:TYR:HA	2.10	0.50
3:P:144:PHE:O	3:P:147:TYR:HE1	1.94	0.50
3:P:172:PHE:H	3:P:231:LEU:CD2	2.24	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:172:PHE:H	3:P:231:LEU:CG	2.23	0.50
3:P:189:GLU:O	3:P:190:TYR:HB2	2.10	0.50
3:P:199:ILE:HB	3:P:207:VAL:O	2.11	0.50
3:P:158:GLY:HA3	9:P:301:HEM:C2D	2.46	0.50
3:P:54:TYR:OH	3:P:125:GLN:NE2	2.43	0.50
3:P:61:VAL:CG2	3:P:62:ALA:H	2.23	0.50
3:P:90:ILE:HG22	3:P:90:ILE:O	2.12	0.50
3:P:92:GLU:HG3	3:P:94:LEU:H	1.76	0.50
5:R:5:ALA:HB1	6:S:10:ALA:CA	2.40	0.50
1:A:148:VAL:CG1	1:A:183:TYR:CE2	2.94	0.50
1:A:47:GLN:HA	1:A:47:GLN:OE1	2.11	0.50
3:C:17:THR:OG1	3:C:18:GLY:N	2.44	0.50
3:C:87:GLU:HA	3:C:90:ILE:HD12	1.93	0.50
4:D:132:GLN:HB2	4:D:141:ARG:HB3	1.94	0.50
2:O:125:ARG:CB	2:O:125:ARG:CZ	2.85	0.50
6:S:9:ALA:HA	6:S:12:LEU:CD1	2.40	0.50
3:P:269:GLN:HE22	7:T:18:TYR:HD2	1.57	0.50
7:T:8:LEU:HD23	7:T:12:THR:HG23	1.94	0.50
1:A:110:PHE:HB3	1:A:118:TRP:CD1	2.46	0.50
1:A:124:LEU:CB	9:A:302:HEM:HBB2	2.14	0.50
2:B:81:LEU:HD12	2:B:81:LEU:N	2.26	0.50
3:C:70:LEU:O	3:C:70:LEU:HD12	2.11	0.50
4:D:132:GLN:NE2	4:D:141:ARG:CB	2.73	0.50
4:D:70:LEU:HD13	4:D:71:GLU:HG2	1.92	0.50
1:N:123:ILE:HG21	1:N:198:PHE:CE2	2.47	0.50
3:P:10:PRO:N	3:P:11:PRO:CD	2.74	0.50
3:P:118:PRO:O	3:P:120:PRO:HD3	2.11	0.50
2:O:38:TYR:O	3:P:272:LEU:HD22	2.11	0.50
3:P:46:PHE:HE2	3:P:133:SER:HB2	1.76	0.50
6:S:14:PHE:C	6:S:17:ILE:HG12	2.32	0.50
1:A:152:SER:HB2	1:A:170:ARG:CG	2.41	0.50
1:A:152:SER:HB2	1:A:170:ARG:CD	2.40	0.50
2:B:31:ALA:O	2:B:32:TRP:CB	2.60	0.50
3:C:185:LYS:HD2	3:C:195:TYR:CB	2.40	0.50
4:D:115:VAL:HG11	4:D:124:PHE:O	2.12	0.50
5:E:2:ILE:HD11	6:F:9:ALA:CB	2.42	0.50
8:H:3:VAL:O	8:H:6:TRP:CB	2.59	0.50
1:N:197:VAL:O	1:N:200:LEU:HB2	2.11	0.50
2:O:130:THR:HG22	2:O:131:THR:N	2.24	0.50
2:O:24:HIS:ND1	2:O:24:HIS:C	2.61	0.50
5:R:32:ILE:HG22	5:R:32:ILE:O	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:16:LEU:O	7:T:18:TYR:N	2.44	0.50
7:T:28:ASN:O	7:T:29:GLU:HB2	2.11	0.50
3:C:140:LYS:HD2	3:C:140:LYS:H	1.76	0.50
5:E:26:ILE:HG23	5:E:30:LYS:NZ	2.25	0.50
6:F:11:LEU:N	6:F:11:LEU:HD12	2.26	0.50
8:H:2:ASP:OD1	8:H:3:VAL:N	2.44	0.50
1:N:114:ARG:HD3	1:N:208:LYS:HE2	1.94	0.50
2:O:50:CYS:O	2:O:54:LEU:HG	2.12	0.50
2:O:73:LEU:N	2:O:73:LEU:HD23	2.26	0.50
5:R:3:LEU:O	5:R:7:PHE:CD2	2.64	0.50
6:S:10:ALA:C	6:S:12:LEU:N	2.64	0.50
1:A:157:ALA:C	1:A:158:ILE:HG13	2.32	0.50
2:B:82:TYR:O	2:B:85:PHE:N	2.45	0.50
3:C:277:LYS:NZ	3:C:278:GLN:OE1	2.40	0.50
3:C:50:VAL:HG21	3:C:129:PHE:CE1	2.46	0.50
1:N:51:GLY:HA2	1:N:54:MET:CE	2.41	0.50
2:O:105:PRO:HG2	2:O:106:LEU:N	2.23	0.50
2:O:105:PRO:CG	2:O:106:LEU:H	2.21	0.50
3:P:170:ASN:HA	3:P:236:ASN:HB2	1.93	0.50
3:P:262:ILE:O	3:P:265:VAL:N	2.45	0.50
2:B:71:THR:OG1	4:Q:114:VAL:HB	2.11	0.50
4:Q:126:CYS:SG	4:Q:127:PRO:CD	3.00	0.50
5:R:11:PHE:HA	5:R:14:LEU:CD2	2.37	0.50
5:R:2:ILE:HD11	6:S:9:ALA:CB	2.41	0.50
1:A:41:LEU:O	1:A:42:THR:C	2.50	0.50
1:A:68:SER:O	1:A:71:TYR:HB3	2.11	0.50
2:B:66:ALA:O	2:B:67:ASN:ND2	2.45	0.50
4:D:41:TYR:HD2	4:D:42:PHE:N	2.09	0.50
1:N:52:PHE:C	1:N:54:MET:N	2.63	0.50
2:O:41:PRO:HB2	3:P:272:LEU:CD1	2.42	0.50
3:P:188:ASP:CG	3:P:192:ASN:HB3	2.32	0.50
3:P:31:PRO:O	3:P:32:ALA:HB2	2.11	0.50
3:P:55:ASP:HB2	3:P:57:LYS:HD2	1.92	0.50
4:Q:51:GLY:C	4:Q:54:THR:HG22	2.32	0.50
5:R:11:PHE:CD2	5:R:12:ILE:N	2.79	0.50
8:U:1:ILE:CG2	8:U:2:ASP:H	2.21	0.50
1:A:102:PHE:CE1	5:E:15:PHE:CZ	2.97	0.50
1:A:184:TYR:CE2	1:A:188:THR:HG21	2.47	0.50
1:A:83:ARG:HG3	1:A:84:SER:N	2.26	0.50
2:B:135:PHE:CD1	2:B:135:PHE:C	2.83	0.50
2:B:31:ALA:HB1	7:G:30:LEU:O	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:83:LYS:HZ1	3:C:133:SER:CA	2.25	0.50
3:C:189:GLU:O	3:C:190:TYR:HB2	2.12	0.50
1:N:114:ARG:O	1:N:114:ARG:HG2	2.10	0.50
1:N:167:ASP:C	1:N:169:LEU:N	2.63	0.50
1:N:17:LEU:CD2	1:N:20:ASP:HB2	2.42	0.50
2:O:59:PRO:HD2	3:P:248:VAL:HG21	1.93	0.50
3:P:252:PRO:C	3:P:254:ARG:N	2.64	0.50
5:R:12:ILE:HA	5:R:15:PHE:CE1	2.46	0.50
2:B:63:GLY:HA2	12:B:309:BNT:OAN	2.12	0.50
3:C:268:ALA:C	3:C:270:LEU:N	2.65	0.50
7:G:19:ALA:O	7:G:20:ALA:C	2.50	0.50
7:G:18:TYR:O	7:G:21:TYR:HB2	2.12	0.50
2:O:38:TYR:HA	2:O:41:PRO:CG	2.42	0.50
2:O:98:VAL:O	2:O:99:LEU:C	2.50	0.50
3:P:102:TYR:HB3	3:P:118:PRO:HD3	1.93	0.50
7:T:26:ARG:N	7:T:27:PRO:CD	2.73	0.50
2:B:36:LEU:C	2:B:39:VAL:HG13	2.32	0.49
2:B:36:LEU:HA	2:B:39:VAL:CG1	2.41	0.49
3:C:151:LEU:HG	3:C:152:GLY:N	2.27	0.49
3:C:205:LYS:C	3:C:205:LYS:HE2	2.32	0.49
4:D:51:GLY:HA2	4:D:54:THR:CB	2.33	0.49
5:E:2:ILE:HG13	5:E:6:VAL:CG2	2.42	0.49
7:G:24:TYR:N	7:G:24:TYR:CD2	2.80	0.49
1:N:111:LYS:HZ1	1:N:112:LYS:HE3	1.76	0.49
2:O:38:TYR:HA	2:O:41:PRO:HG3	1.94	0.49
3:P:263:CYS:HA	3:P:266:MET:HB2	1.94	0.49
3:P:86:PRO:HG2	3:P:89:ARG:HB2	1.94	0.49
6:S:11:LEU:HD12	6:S:11:LEU:N	2.27	0.49
1:A:154:VAL:N	1:A:155:PRO:HD2	2.26	0.49
1:A:87:ARG:HD3	2:B:60:ALA:HB2	1.93	0.49
3:C:76:LEU:C	3:C:76:LEU:HD23	2.33	0.49
3:C:93:GLU:O	3:C:95:LYS:N	2.45	0.49
4:D:155:VAL:HG13	4:D:158:ASP:HA	1.94	0.49
4:D:113:CYS:SG	14:D:201:FES:S2	3.09	0.49
5:E:11:PHE:CD2	5:E:12:ILE:N	2.79	0.49
6:F:9:ALA:HA	6:F:12:LEU:CD1	2.41	0.49
7:G:29:GLU:O	7:G:30:LEU:O	2.30	0.49
2:O:36:LEU:O	2:O:40:PHE:N	2.44	0.49
2:O:82:TYR:O	2:O:83:PRO:C	2.48	0.49
3:P:146:LYS:HG2	3:P:248:VAL:CG2	2.34	0.49
3:P:217:LEU:HD23	3:P:232:THR:OG1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:271:MET:CG	3:P:274:LEU:HD12	2.41	0.49
6:S:21:TRP:O	6:S:25:VAL:HG23	2.11	0.49
3:P:278:GLN:NE2	7:T:25:LYS:HE3	2.27	0.49
1:A:59:LYS:HD2	1:A:68:SER:HB2	1.93	0.49
1:A:88:TRP:HZ2	2:B:58:ASP:OD1	1.95	0.49
2:B:130:THR:HG22	2:B:131:THR:N	2.25	0.49
1:A:85:ILE:HG23	2:B:51:ILE:HG22	1.93	0.49
3:C:34:VAL:HG22	3:C:243:ASP:HB3	1.95	0.49
5:E:5:ALA:C	5:E:7:PHE:H	2.15	0.49
1:N:104:VAL:O	1:N:107:THR:N	2.45	0.49
1:N:116:LEU:CD1	1:N:117:THR:H	2.25	0.49
3:P:110:GLN:HB3	3:P:113:VAL:CG2	2.41	0.49
3:P:89:ARG:O	3:P:90:ILE:C	2.50	0.49
5:R:2:ILE:O	5:R:3:LEU:C	2.49	0.49
2:O:79:TRP:CZ3	5:R:4:GLY:CA	2.95	0.49
7:T:28:ASN:CG	7:T:30:LEU:HD21	2.31	0.49
3:C:11:PRO:HA	3:C:107:LYS:HD2	1.93	0.49
4:D:106:ALA:HB1	4:D:114:VAL:HG13	1.95	0.49
4:D:118:ASN:C	4:D:120:ALA:N	2.66	0.49
4:D:94:GLU:HA	4:D:94:GLU:OE1	2.12	0.49
5:E:14:LEU:O	5:E:17:GLY:C	2.50	0.49
1:N:119:ILE:O	1:N:120:SER:C	2.51	0.49
3:P:10:PRO:O	3:P:106:TYR:CE2	2.65	0.49
3:P:176:ALA:H	3:P:228:GLY:HA3	1.77	0.49
1:A:135:GLY:HA2	1:A:138:LEU:CG	2.43	0.49
2:B:127:PRO:C	2:B:129:ALA:N	2.66	0.49
2:B:133:PHE:HE2	2:B:137:THR:HG21	1.72	0.49
1:A:209:GLN:OE1	2:B:28:GLY:O	2.30	0.49
2:B:87:ILE:O	2:B:88:LEU:C	2.51	0.49
3:C:161:TYR:HA	9:C:301:HEM:HMD2	1.95	0.49
3:C:175:SER:O	3:C:176:ALA:HB2	2.13	0.49
3:C:223:GLN:O	3:C:224:ALA:HB3	2.13	0.49
2:B:45:MET:HE2	3:C:272:LEU:HD12	1.93	0.49
1:N:103:ARG:O	1:N:103:ARG:HD2	2.12	0.49
1:N:116:LEU:C	1:N:118:TRP:N	2.65	0.49
1:N:193:TRP:O	1:N:196:ALA:HB3	2.12	0.49
1:N:52:PHE:O	1:N:55:THR:N	2.36	0.49
11:O:1306:OPC:HCB3	11:O:1306:OPC:CBB	2.42	0.49
3:P:26:HIS:CD2	3:P:158:GLY:HA2	2.48	0.49
4:Q:125:LYS:HG2	4:Q:132:GLN:HG2	1.93	0.49
5:R:2:ILE:HG13	5:R:6:VAL:CG2	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:T:18:TYR:O	7:T:21:TYR:N	2.45	0.49
1:A:114:ARG:C	1:A:116:LEU:HD12	2.33	0.49
1:A:116:LEU:CD1	1:A:117:THR:H	2.25	0.49
1:A:158:ILE:CG2	1:A:159:PRO:CD	2.91	0.49
4:D:27:VAL:C	4:D:29:GLY:N	2.64	0.49
5:E:7:PHE:C	5:E:9:ILE:N	2.66	0.49
1:N:118:TRP:CH2	2:O:108:LEU:HD23	2.48	0.49
3:P:272:LEU:O	3:P:276:LYS:HG2	2.12	0.49
3:P:61:VAL:HA	3:P:67:LYS:HA	1.95	0.49
4:Q:55:THR:OG1	4:Q:63:ASN:HA	2.12	0.49
4:Q:81:VAL:HG12	4:Q:82:GLN:N	2.17	0.49
4:Q:83:GLY:HA3	4:Q:89:THR:OG1	2.13	0.49
5:R:17:GLY:O	5:R:22:ILE:HG21	2.12	0.49
6:S:22:GLY:O	6:S:25:VAL:N	2.44	0.49
1:A:105:TYR:HA	1:A:110:PHE:HE2	1.74	0.49
1:A:52:PHE:HA	1:A:55:THR:CG2	2.43	0.49
11:B:305:OPC:HBM1	11:B:305:OPC:OAB	2.12	0.49
3:C:83:LYS:O	3:C:131:VAL:HG23	2.12	0.49
3:C:153:ALA:O	3:C:240:PHE:HD1	1.96	0.49
3:C:270:LEU:O	3:C:273:ILE:HG12	2.13	0.49
3:C:34:VAL:HG11	3:C:151:LEU:HB3	1.94	0.49
5:E:18:ILE:O	5:E:19:ALA:O	2.31	0.49
1:N:175:VAL:HA	1:N:179:THR:OG1	2.12	0.49
1:N:27:PRO:CA	2:O:33:PRO:HG3	2.43	0.49
1:N:38:GLY:HA3	10:N:303:HEC:C4C	2.43	0.49
1:N:42:THR:O	1:N:44:PHE:N	2.46	0.49
3:P:217:LEU:O	3:P:218:ILE:HG23	2.12	0.49
3:P:155:ARG:HG2	3:P:239:GLY:CA	2.42	0.49
3:P:86:PRO:O	3:P:90:ILE:HG13	2.12	0.49
4:Q:115:VAL:HG13	4:Q:126:CYS:CA	2.37	0.49
5:R:7:PHE:O	5:R:11:PHE:HD2	1.96	0.49
1:A:77:SER:HB2	4:D:41:TYR:CA	2.41	0.49
2:B:93:ASN:O	2:B:94:LYS:HB2	2.13	0.49
3:C:10:PRO:N	3:C:11:PRO:CD	2.75	0.49
3:C:25:CYS:O	3:C:27:LEU:N	2.45	0.49
5:E:3:LEU:O	5:E:7:PHE:CD2	2.65	0.49
5:E:5:ALA:O	5:E:9:ILE:HG22	2.11	0.49
1:N:116:LEU:N	1:N:116:LEU:HD12	2.28	0.49
1:N:194:LEU:O	1:N:195:ILE:C	2.51	0.49
10:N:303:HEC:HBC3	11:N:1305:OPC:HAS1	1.94	0.49
1:N:62:VAL:HG23	1:N:63:THR:H	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:64:GLU:OE1	2:O:65:PRO:N	2.45	0.49
1:A:178:ALA:O	1:A:179:THR:C	2.52	0.49
1:A:34:TYR:O	1:A:35:CYS:HB2	2.12	0.49
2:B:65:PRO:CB	2:B:68:PRO:HB3	2.35	0.49
3:C:91:PRO:C	3:C:92:GLU:HG2	2.33	0.49
1:N:50:THR:OG1	1:N:51:GLY:N	2.46	0.49
2:O:34:ASN:CG	2:O:35:ASP:H	2.03	0.49
1:N:39:ILE:HD11	2:O:43:VAL:HG11	1.95	0.49
3:P:10:PRO:O	3:P:106:TYR:HE2	1.94	0.49
3:P:157:ARG:O	3:P:159:GLN:NE2	2.46	0.49
8:U:10:LEU:O	8:U:13:PHE:HB2	2.13	0.49
1:A:117:THR:O	1:A:202:HIS:CE1	2.66	0.49
1:A:135:GLY:HA2	1:A:138:LEU:HD12	1.94	0.49
1:A:158:ILE:O	1:A:163:VAL:CG2	2.60	0.49
1:A:52:PHE:C	1:A:54:MET:H	2.17	0.49
2:B:141:ILE:C	2:B:143:LEU:N	2.66	0.49
2:B:139:VAL:O	2:B:142:TRP:HB3	2.12	0.49
3:C:79:PRO:HB3	3:C:147:TYR:HB3	1.94	0.49
4:D:38:LEU:HD11	4:D:42:PHE:HE1	1.78	0.49
5:E:11:PHE:CG	5:E:12:ILE:N	2.81	0.49
6:F:24:GLY:HA2	6:F:27:LEU:HD22	1.94	0.49
7:G:16:LEU:O	7:G:18:TYR:N	2.46	0.49
2:O:152:ASP:OD2	2:O:152:ASP:N	2.46	0.49
3:P:55:ASP:CB	3:P:57:LYS:HD2	2.43	0.49
1:A:14:ILE:C	1:A:14:ILE:HD12	2.33	0.48
1:A:90:ALA:C	1:A:92:MET:N	2.66	0.48
2:B:34:ASN:HD22	2:B:35:ASP:CG	2.17	0.48
1:A:85:ILE:HG23	2:B:51:ILE:CG2	2.43	0.48
3:C:168:ASN:ND2	3:C:168:ASN:C	2.67	0.48
3:C:200:GLN:O	3:C:206:THR:HA	2.13	0.48
3:C:263:CYS:HA	3:C:266:MET:HB2	1.96	0.48
1:N:104:VAL:O	1:N:106:LEU:N	2.46	0.48
1:N:47:GLN:HB2	9:N:301:HEM:HBB2	1.95	0.48
1:N:29:HIS:CE1	1:N:31:ASN:ND2	2.81	0.48
2:O:109:ILE:HG23	2:O:110:LEU:HD23	1.94	0.48
2:O:82:TYR:O	2:O:85:PHE:N	2.46	0.48
3:P:28:ALA:HB3	3:P:240:PHE:HB3	1.94	0.48
7:T:19:ALA:O	7:T:20:ALA:C	2.51	0.48
1:A:170:ARG:O	1:A:179:THR:N	2.45	0.48
3:C:126:GLU:C	3:C:127:ILE:HD12	2.34	0.48
5:E:2:ILE:O	5:E:3:LEU:C	2.51	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:13:ALA:HB2	6:F:14:PHE:HD1	1.78	0.48
6:F:24:GLY:CA	6:F:27:LEU:HD22	2.42	0.48
1:N:159:PRO:C	1:N:161:VAL:N	2.64	0.48
1:N:142:GLN:HG2	2:O:64:GLU:OE1	2.13	0.48
5:R:7:PHE:C	5:R:9:ILE:N	2.66	0.48
1:A:140:TRP:CZ3	2:B:68:PRO:HD2	2.47	0.48
1:A:112:LYS:NZ	2:B:27:TYR:CE1	2.80	0.48
1:A:112:LYS:NZ	2:B:27:TYR:HE1	2.11	0.48
1:A:87:ARG:HD3	2:B:60:ALA:CB	2.43	0.48
3:C:205:LYS:NZ	3:C:207:VAL:HA	2.28	0.48
5:E:14:LEU:O	5:E:17:GLY:CA	2.61	0.48
5:E:7:PHE:C	5:E:9:ILE:H	2.17	0.48
1:N:116:LEU:C	1:N:118:TRP:H	2.17	0.48
1:N:54:MET:C	1:N:56:PHE:N	2.64	0.48
1:N:68:SER:O	1:N:71:TYR:HB3	2.13	0.48
1:N:78:PHE:O	1:N:79:GLY:C	2.51	0.48
2:O:34:ASN:ND2	2:O:35:ASP:OD1	2.45	0.48
3:P:11:PRO:HA	3:P:107:LYS:HD2	1.95	0.48
3:P:270:LEU:O	3:P:273:ILE:HG12	2.13	0.48
4:Q:90:TYR:HB2	4:Q:104:ILE:HD11	1.94	0.48
4:Q:69:PHE:HA	4:Q:73:HIS:CE1	2.48	0.48
1:A:165:ILE:O	1:A:167:ASP:N	2.46	0.48
1:A:34:TYR:CD1	1:A:103:ARG:NE	2.81	0.48
1:A:33:PHE:O	1:A:35:CYS:HB2	2.13	0.48
2:B:153:LYS:O	2:B:154:THR:O	2.31	0.48
11:B:305:OPC:OCC	11:B:305:OPC:CAO	2.62	0.48
2:B:64:GLU:N	2:B:65:PRO:CD	2.77	0.48
3:C:270:LEU:O	3:C:274:LEU:HG	2.14	0.48
3:C:277:LYS:HZ3	3:C:278:GLN:CD	2.17	0.48
3:C:61:VAL:CG2	3:C:62:ALA:H	2.23	0.48
3:C:91:PRO:O	3:C:92:GLU:O	2.32	0.48
1:N:117:THR:HA	1:N:205:MET:CE	2.43	0.48
2:O:18:LEU:O	2:O:19:ALA:HB2	2.13	0.48
3:P:278:GLN:O	3:P:279:VAL:CG2	2.59	0.48
4:Q:163:THR:HB	4:Q:164:PRO:HD2	1.96	0.48
2:B:45:MET:HE3	2:B:45:MET:HB2	1.67	0.48
2:B:59:PRO:O	3:C:146:LYS:NZ	2.46	0.48
3:C:219:VAL:CG1	3:C:220:SER:N	2.76	0.48
11:B:305:OPC:HBW1	11:C:306:OPC:HBU2	1.96	0.48
4:D:27:VAL:O	4:D:29:GLY:N	2.38	0.48
6:F:23:LEU:O	6:F:27:LEU:HD22	2.12	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:148:VAL:O	1:N:148:VAL:CG1	2.62	0.48
3:P:10:PRO:CA	3:P:106:TYR:HE2	2.22	0.48
3:P:15:GLU:HB2	3:P:19:ARG:O	2.12	0.48
3:P:196:GLN:HE22	3:P:210:THR:HB	1.78	0.48
4:Q:90:TYR:HB2	4:Q:104:ILE:HD12	1.95	0.48
6:S:23:LEU:O	6:S:24:GLY:C	2.52	0.48
1:A:129:VAL:HG13	2:B:81:LEU:HD11	1.94	0.48
3:C:168:ASN:HD22	3:C:168:ASN:C	2.16	0.48
3:C:252:PRO:C	3:C:254:ARG:N	2.67	0.48
3:C:83:LYS:HZ1	3:C:133:SER:C	2.17	0.48
4:D:152:HIS:HB2	4:D:163:THR:OG1	2.13	0.48
5:E:28:SER:C	5:E:30:LYS:H	2.16	0.48
1:N:85:ILE:O	1:N:89:SER:N	2.45	0.48
3:P:199:ILE:CG1	3:P:208:VAL:HA	2.44	0.48
3:P:41:LEU:O	3:P:133:SER:HB3	2.14	0.48
3:P:4:TRP:NE1	3:P:162:PRO:HG3	2.28	0.48
6:S:10:ALA:O	6:S:12:LEU:N	2.46	0.48
8:U:3:VAL:O	8:U:6:TRP:CB	2.60	0.48
1:A:151:VAL:HA	1:A:154:VAL:HG23	1.96	0.48
1:A:167:ASP:C	1:A:169:LEU:N	2.66	0.48
2:B:41:PRO:HA	2:B:44:ILE:HD12	1.95	0.48
3:C:144:PHE:O	3:C:147:TYR:HE1	1.96	0.48
3:C:75:VAL:HG12	3:C:152:GLY:O	2.14	0.48
4:D:88:PRO:O	4:D:106:ALA:HB3	2.13	0.48
4:D:118:ASN:O	4:D:120:ALA:N	2.46	0.48
4:D:120:ALA:O	4:D:122:ASN:ND2	2.47	0.48
4:D:88:PRO:HD2	4:D:107:VAL:HG23	1.96	0.48
1:N:200:LEU:O	1:N:204:LEU:HG	2.14	0.48
1:N:82:ILE:CD1	1:N:82:ILE:H	2.27	0.48
1:N:85:ILE:HA	2:O:51:ILE:CG2	2.42	0.48
2:O:122:ASN:HA	2:O:124:PHE:CD1	2.48	0.48
3:P:25:CYS:O	3:P:27:LEU:N	2.46	0.48
11:B:305:OPC:HBY1	11:C:306:OPC:CBX	2.44	0.48
2:B:87:ILE:HA	2:B:90:SER:HB2	1.96	0.48
6:F:11:LEU:HD12	6:F:12:LEU:H	1.78	0.48
6:F:12:LEU:O	6:F:16:LEU:HD23	2.14	0.48
7:G:26:ARG:N	7:G:27:PRO:CD	2.73	0.48
1:N:111:LYS:HZ2	1:N:112:LYS:CG	2.26	0.48
1:N:28:PRO:HG2	2:O:32:TRP:CB	2.31	0.48
1:N:82:ILE:HD12	1:N:82:ILE:N	2.27	0.48
3:P:170:ASN:O	3:P:235:PRO:HD2	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:256:LYS:O	3:P:259:ILE:N	2.47	0.48
3:P:268:ALA:O	3:P:270:LEU:N	2.46	0.48
1:A:82:ILE:HD12	1:A:82:ILE:N	2.29	0.48
3:C:86:PRO:O	3:C:90:ILE:HG13	2.14	0.48
4:D:67:SER:HA	4:D:70:LEU:CG	2.44	0.48
5:E:25:ALA:C	5:E:26:ILE:HD12	2.34	0.48
6:F:20:GLY:HA3	7:G:21:TYR:CE1	2.49	0.48
1:N:151:VAL:HA	1:N:154:VAL:HG23	1.95	0.48
2:O:52:VAL:O	2:O:53:ALA:C	2.52	0.48
3:P:79:PRO:HB3	3:P:147:TYR:HB3	1.95	0.48
4:Q:80:LEU:CB	4:Q:90:TYR:HA	2.43	0.48
2:O:124:PHE:HB2	5:R:23:ILE:HD13	1.96	0.48
7:T:9:VAL:HG23	7:T:10:PHE:HD1	1.77	0.48
7:T:4:LEU:N	7:T:6:LEU:HD11	2.29	0.48
1:A:148:VAL:HG11	1:A:183:TYR:CE2	2.49	0.48
2:B:98:VAL:O	2:B:99:LEU:C	2.51	0.48
4:D:115:VAL:HG22	4:D:126:CYS:CB	2.44	0.48
4:D:131:SER:O	4:D:132:GLN:HG3	2.13	0.48
1:N:39:ILE:HD11	2:O:43:VAL:CG1	2.43	0.48
2:O:127:PRO:O	2:O:130:THR:N	2.47	0.48
2:O:72:PRO:C	2:O:74:GLU:N	2.68	0.48
3:P:205:LYS:HZ3	3:P:207:VAL:CG1	2.27	0.48
3:P:256:LYS:HE2	3:P:257:TRP:CZ3	2.49	0.48
3:P:268:ALA:C	3:P:270:LEU:N	2.67	0.48
3:P:41:LEU:HB3	3:P:42:PRO:HD2	1.95	0.48
3:P:97:GLU:HG2	3:P:97:GLU:O	2.14	0.48
4:Q:131:SER:O	4:Q:132:GLN:HG3	2.14	0.48
4:Q:155:VAL:HG13	4:Q:158:ASP:HA	1.96	0.48
4:Q:27:VAL:O	4:Q:29:GLY:N	2.36	0.48
1:N:77:SER:HG	4:Q:41:TYR:HA	1.75	0.48
4:Q:83:GLY:N	4:Q:87:ASP:O	2.42	0.48
5:R:5:ALA:O	5:R:9:ILE:HG22	2.14	0.48
7:T:14:GLY:C	7:T:16:LEU:H	2.17	0.48
7:T:17:PHE:HB3	7:T:21:TYR:HE1	1.79	0.48
1:A:102:PHE:O	1:A:103:ARG:C	2.51	0.47
2:B:36:LEU:O	2:B:40:PHE:N	2.47	0.47
1:A:83:ARG:NH1	2:B:60:ALA:HB1	2.29	0.47
2:B:81:LEU:CD1	2:B:81:LEU:N	2.77	0.47
3:C:158:GLY:H	9:C:301:HEM:CAD	2.27	0.47
3:C:251:ASP:O	3:C:254:ARG:CB	2.62	0.47
3:C:262:ILE:O	3:C:264:LEU:N	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:55:ASP:HB2	3:C:57:LYS:HD2	1.95	0.47
7:G:9:VAL:HG23	7:G:10:PHE:HD1	1.78	0.47
1:N:165:ILE:HD11	1:N:168:LEU:HD12	1.96	0.47
1:N:188:THR:HB	9:N:301:HEM:HBC2	1.96	0.47
2:O:78:GLU:C	2:O:82:TYR:CE2	2.87	0.47
3:P:168:ASN:HD22	3:P:168:ASN:C	2.18	0.47
3:P:187:GLU:HB2	3:P:193:VAL:HG13	1.96	0.47
3:P:205:LYS:C	3:P:205:LYS:HE2	2.35	0.47
3:P:28:ALA:HB3	3:P:240:PHE:CB	2.44	0.47
3:P:259:ILE:HD11	7:T:12:THR:CG2	2.44	0.47
3:P:273:ILE:O	3:P:278:GLN:CG	2.61	0.47
4:Q:110:HIS:HB2	4:Q:144:ALA:CA	2.34	0.47
4:Q:132:GLN:NE2	4:Q:141:ARG:CB	2.77	0.47
1:A:138:LEU:N	1:A:139:PRO:CD	2.74	0.47
1:A:62:VAL:CG2	1:A:63:THR:H	2.17	0.47
11:B:305:OPC:HAS2	11:B:305:OPC:OAD	2.12	0.47
2:B:38:TYR:N	2:B:38:TYR:CD1	2.82	0.47
10:A:303:HEC:HMC1	2:B:44:ILE:HG12	1.96	0.47
2:B:80:TYR:O	2:B:83:PRO:HD2	2.14	0.47
3:C:199:ILE:HG22	3:C:200:GLN:N	2.20	0.47
3:C:176:ALA:N	3:C:228:GLY:HA3	2.28	0.47
3:C:278:GLN:O	3:C:279:VAL:CG2	2.62	0.47
4:D:82:GLN:HE21	4:D:82:GLN:HA	1.78	0.47
1:N:47:GLN:HA	1:N:47:GLN:OE1	2.14	0.47
1:N:87:ARG:CD	2:O:61:MET:HE1	2.22	0.47
2:O:67:ASN:HD22	3:P:16:PRO:HB3	1.79	0.47
3:P:168:ASN:O	3:P:170:ASN:N	2.47	0.47
3:P:153:ALA:O	3:P:240:PHE:HA	2.13	0.47
3:P:279:VAL:O	3:P:279:VAL:HG12	2.14	0.47
4:Q:132:GLN:HB2	4:Q:141:ARG:HB3	1.96	0.47
4:Q:154:THR:HB	4:Q:161:VAL:HG22	1.90	0.47
1:A:197:VAL:O	1:A:200:LEU:HB2	2.13	0.47
1:A:29:HIS:CB	1:A:211:ILE:HD12	2.38	0.47
2:B:37:LEU:O	11:B:305:OPC:HBL1	2.15	0.47
2:B:65:PRO:CA	2:B:68:PRO:HD3	2.44	0.47
2:B:91:LEU:HD12	2:B:91:LEU:C	2.34	0.47
5:E:5:ALA:HB3	6:F:6:MET:O	2.14	0.47
1:N:134:THR:HB	1:N:187:HIS:HB2	1.96	0.47
2:O:104:VAL:H	2:O:105:PRO:CD	2.24	0.47
2:O:141:ILE:C	2:O:143:LEU:N	2.68	0.47
2:O:79:TRP:HA	2:O:82:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:70:LEU:O	3:P:70:LEU:HD12	2.14	0.47
7:T:20:ALA:O	7:T:24:TYR:CD2	2.67	0.47
1:A:116:LEU:HD13	1:A:205:MET:SD	2.55	0.47
1:A:66:TYR:HB2	1:A:140:TRP:CE3	2.45	0.47
1:A:29:HIS:ND1	2:B:30:PRO:HG3	2.29	0.47
3:C:54:TYR:HD2	3:C:155:ARG:NH1	2.12	0.47
4:D:67:SER:CA	4:D:70:LEU:HD21	2.36	0.47
8:H:7:VAL:O	8:H:8:ALA:C	2.50	0.47
1:N:154:VAL:N	1:N:155:PRO:HD2	2.30	0.47
1:N:47:GLN:HB3	9:N:301:HEM:HBB2	1.94	0.47
1:N:54:MET:C	1:N:56:PHE:H	2.17	0.47
1:N:66:TYR:CE1	2:O:65:PRO:HD2	2.49	0.47
2:O:76:LEU:N	2:O:76:LEU:HD22	2.29	0.47
3:P:168:ASN:ND2	3:P:168:ASN:C	2.67	0.47
3:P:205:LYS:NZ	3:P:207:VAL:HA	2.29	0.47
3:P:223:GLN:O	3:P:224:ALA:HB3	2.14	0.47
3:P:169:ASN:ND2	3:P:236:ASN:HA	2.29	0.47
3:P:274:LEU:O	3:P:275:LYS:O	2.31	0.47
4:Q:118:ASN:C	4:Q:120:ALA:N	2.64	0.47
4:Q:19:MET:O	4:Q:22:LEU:HD22	2.13	0.47
4:Q:67:SER:HA	4:Q:70:LEU:CG	2.45	0.47
8:U:3:VAL:HA	8:U:6:TRP:HD1	1.79	0.47
1:A:118:TRP:HA	9:A:302:HEM:CHD	2.44	0.47
1:A:122:VAL:O	1:A:125:ALA:N	2.44	0.47
13:B:201:CLA:HHC	13:B:201:CLA:HBB1	1.95	0.47
2:B:36:LEU:HA	2:B:39:VAL:HG13	1.95	0.47
3:C:6:GLN:HB3	3:C:106:TYR:CE2	2.49	0.47
6:F:23:LEU:O	6:F:24:GLY:C	2.51	0.47
1:A:189:PHE:CZ	1:N:52:PHE:HB2	2.50	0.47
2:O:82:TYR:O	2:O:85:PHE:HB3	2.15	0.47
7:T:18:TYR:O	7:T:21:TYR:HB2	2.15	0.47
1:A:140:TRP:HH2	2:B:67:ASN:OD1	1.98	0.47
2:B:82:TYR:O	2:B:85:PHE:HB3	2.15	0.47
3:C:92:GLU:HG3	3:C:94:LEU:H	1.79	0.47
6:F:27:LEU:CD1	8:H:15:TRP:NE1	2.68	0.47
7:G:20:ALA:O	7:G:24:TYR:CD2	2.67	0.47
2:O:72:PRO:C	2:O:74:GLU:H	2.18	0.47
3:P:91:PRO:O	3:P:95:LYS:CG	2.61	0.47
3:P:92:GLU:HG3	3:P:94:LEU:CB	2.44	0.47
6:S:18:PHE:CD2	6:S:18:PHE:N	2.81	0.47
1:A:116:LEU:C	1:A:118:TRP:H	2.16	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:54:TYR:HB2	3:C:58:LEU:CD2	2.45	0.47
3:C:91:PRO:O	3:C:95:LYS:CG	2.57	0.47
6:F:22:GLY:O	6:F:25:VAL:N	2.45	0.47
1:N:114:ARG:NH1	1:N:114:ARG:HG2	2.30	0.47
11:N:1305:OPC:HAY1	11:N:1305:OPC:HCB2	1.97	0.47
1:N:15:GLN:C	1:N:17:LEU:N	2.64	0.47
2:O:133:PHE:C	2:O:135:PHE:H	2.10	0.47
3:P:271:MET:CE	4:Q:22:LEU:HG	2.44	0.47
3:P:83:LYS:HZ1	3:P:133:SER:C	2.18	0.47
4:Q:118:ASN:O	4:Q:120:ALA:N	2.48	0.47
5:R:18:ILE:O	5:R:19:ALA:O	2.32	0.47
1:A:34:TYR:CG	1:A:103:ARG:HD3	2.49	0.47
2:B:64:GLU:N	2:B:65:PRO:HD3	2.30	0.47
3:C:197:VAL:HG13	3:C:211:ILE:HG22	1.96	0.47
4:D:90:TYR:HB2	4:D:104:ILE:HD12	1.96	0.47
4:D:35:LEU:C	4:D:37:PRO:HD2	2.35	0.47
4:D:73:HIS:HB2	4:D:93:VAL:HG21	1.94	0.47
3:C:259:ILE:HD11	7:G:12:THR:HG21	1.97	0.47
1:N:178:ALA:O	1:N:179:THR:C	2.52	0.47
1:N:28:PRO:CD	2:O:33:PRO:HD3	2.37	0.47
2:O:64:GLU:HG3	2:O:65:PRO:CD	2.30	0.47
2:O:70:ALA:O	2:O:71:THR:HB	2.14	0.47
3:P:153:ALA:O	3:P:240:PHE:HD1	1.96	0.47
6:S:8:TYR:C	6:S:8:TYR:CD2	2.87	0.47
1:A:15:GLN:O	1:A:16:ALA:C	2.53	0.47
3:C:159:GLN:N	3:C:159:GLN:CD	2.68	0.47
3:C:216:GLU:C	3:C:217:LEU:HG	2.36	0.47
3:C:4:TRP:NE1	3:C:162:PRO:HG3	2.29	0.47
4:D:24:PHE:HA	4:D:27:VAL:HB	1.97	0.47
4:D:64:VAL:HG13	4:D:68:LYS:HG3	1.97	0.47
1:N:105:TYR:HD2	1:N:106:LEU:HD23	1.80	0.47
3:P:4:TRP:HE3	3:P:4:TRP:N	2.13	0.47
4:Q:113:CYS:HG	4:Q:128:CYS:CB	2.27	0.47
5:R:7:PHE:O	5:R:11:PHE:CD2	2.68	0.47
5:R:12:ILE:HA	5:R:15:PHE:HE1	1.78	0.47
1:N:95:LEU:HD11	5:R:7:PHE:HB3	1.97	0.47
13:B:201:CLA:CGD	13:B:201:CLA:HAA1	2.45	0.47
3:C:136:PRO:HB2	3:C:142:ILE:O	2.15	0.47
15:E:101:BCR:H322	7:G:23:GLN:HE22	1.80	0.47
1:N:148:VAL:CG1	1:N:183:TYR:CE2	2.97	0.47
2:O:151:LEU:O	2:O:151:LEU:HD12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:90:ILE:HG21	3:P:96:LYS:HG2	1.97	0.47
6:S:11:LEU:HD12	6:S:12:LEU:H	1.79	0.47
11:B:305:OPC:CBN	11:B:305:OPC:OAB	2.62	0.47
3:C:10:PRO:O	3:C:106:TYR:CE2	2.68	0.47
3:C:34:VAL:HG11	3:C:151:LEU:CB	2.45	0.47
3:C:81:GLY:O	3:C:134:PRO:HG3	2.14	0.47
6:F:20:GLY:HA3	7:G:21:TYR:CD1	2.50	0.47
8:H:7:VAL:C	8:H:9:LEU:N	2.67	0.47
1:N:140:TRP:O	1:N:141:ASP:C	2.52	0.47
1:N:41:LEU:HD23	1:N:41:LEU:C	2.35	0.47
12:O:1309:BNT:CAM	3:P:148:ALA:HB2	2.45	0.47
3:P:251:ASP:O	3:P:254:ARG:CB	2.60	0.47
2:B:36:LEU:O	2:B:39:VAL:HG22	2.14	0.46
3:C:92:GLU:HG3	3:C:94:LEU:CB	2.45	0.46
1:N:31:ASN:C	1:N:34:TYR:CE2	2.89	0.46
4:Q:43:ILE:O	4:Q:44:PRO:O	2.33	0.46
8:U:7:VAL:C	8:U:9:LEU:N	2.66	0.46
1:A:128:THR:OG1	9:A:302:HEM:HBB1	2.15	0.46
1:A:19:ASP:O	1:A:20:ASP:CB	2.63	0.46
1:A:57:TYR:CE1	1:A:76:VAL:HG13	2.47	0.46
1:A:83:ARG:O	1:A:84:SER:C	2.53	0.46
2:B:50:CYS:C	2:B:52:VAL:N	2.66	0.46
11:N:1305:OPC:HAY2	11:N:1305:OPC:HCB2	1.97	0.46
3:P:52:ILE:CG2	3:P:155:ARG:NH2	2.77	0.46
3:P:158:GLY:H	9:P:301:HEM:CAD	2.27	0.46
3:P:269:GLN:NE2	7:T:18:TYR:HD2	2.13	0.46
1:N:32:ILE:HG12	7:T:26:ARG:NH2	2.30	0.46
7:T:30:LEU:HD22	7:T:30:LEU:N	2.30	0.46
1:A:29:HIS:CD2	1:A:211:ILE:HD12	2.50	0.46
2:B:48:PHE:CE1	2:B:52:VAL:HG22	2.51	0.46
2:B:76:LEU:HD13	2:B:79:TRP:HZ2	1.81	0.46
2:B:81:LEU:O	2:B:85:PHE:HB2	2.15	0.46
1:A:87:ARG:HH12	3:C:146:LYS:NZ	2.13	0.46
1:N:122:VAL:O	1:N:125:ALA:N	2.45	0.46
1:N:160:VAL:C	1:N:162:GLY:H	2.17	0.46
1:N:163:VAL:C	1:N:165:ILE:H	2.18	0.46
1:N:185:SER:O	1:N:189:PHE:CB	2.61	0.46
1:N:25:TYR:C	1:N:26:VAL:HG22	2.35	0.46
2:O:101:MET:CG	2:O:102:ALA:N	2.78	0.46
2:O:136:GLY:HA3	13:O:1201:CLA:C1C	2.45	0.46
2:O:40:PHE:O	2:O:43:VAL:N	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:46:GLY:HA3	7:T:19:ALA:HB2	1.97	0.46
3:P:34:VAL:HG11	3:P:151:LEU:HB3	1.97	0.46
4:Q:80:LEU:H	4:Q:80:LEU:HD23	1.79	0.46
5:R:28:SER:C	5:R:30:LYS:N	2.68	0.46
1:A:154:VAL:HB	1:A:155:PRO:CD	2.45	0.46
1:A:58:TYR:HD2	1:A:184:TYR:CE1	2.30	0.46
2:B:50:CYS:C	2:B:54:LEU:HG	2.34	0.46
4:D:80:LEU:CB	4:D:90:TYR:HA	2.45	0.46
5:E:24:PHE:O	5:E:26:ILE:N	2.48	0.46
1:N:105:TYR:CD2	1:N:106:LEU:HD23	2.50	0.46
1:N:110:PHE:N	1:N:110:PHE:CD2	2.81	0.46
1:N:61:THR:CG2	1:N:64:GLU:HB3	2.46	0.46
3:P:9:TYR:CE1	3:P:21:VAL:HG11	2.51	0.46
6:S:12:LEU:O	6:S:16:LEU:HD23	2.15	0.46
1:A:41:LEU:C	1:A:41:LEU:HD23	2.35	0.46
11:B:305:OPC:CAH	11:B:305:OPC:HBP2	2.46	0.46
12:B:309:BNT:CAM	3:C:148:ALA:HB2	2.46	0.46
2:B:38:TYR:HA	2:B:41:PRO:HG3	1.98	0.46
3:C:104:GLN:NE2	3:C:104:GLN:N	2.62	0.46
3:C:90:ILE:HG21	3:C:96:LYS:HG2	1.96	0.46
4:D:59:LYS:HZ2	4:D:59:LYS:HB2	1.79	0.46
2:B:57:LEU:HD22	7:G:10:PHE:CE1	2.50	0.46
7:G:4:LEU:N	7:G:6:LEU:HD11	2.30	0.46
1:N:111:LYS:HG3	1:N:112:LYS:N	2.30	0.46
1:N:191:LEU:C	1:N:193:TRP:H	2.19	0.46
3:P:169:ASN:C	3:P:236:ASN:HB2	2.36	0.46
3:P:92:GLU:HG3	3:P:94:LEU:HB2	1.97	0.46
4:Q:90:TYR:O	4:Q:103:GLY:HA3	2.15	0.46
1:A:114:ARG:CD	1:A:208:LYS:HD3	2.46	0.46
1:A:72:ILE:HD12	1:A:72:ILE:N	2.31	0.46
3:C:46:PHE:HE2	3:C:133:SER:HB2	1.80	0.46
4:D:90:TYR:HB2	4:D:104:ILE:HD11	1.96	0.46
11:N:1305:OPC:HAY2	11:N:1305:OPC:CBZ	2.42	0.46
1:N:140:TRP:C	1:N:141:ASP:O	2.51	0.46
3:P:251:ASP:HB3	3:P:254:ARG:CB	2.46	0.46
3:P:81:GLY:C	3:P:134:PRO:HG2	2.36	0.46
4:Q:126:CYS:HB3	4:Q:131:SER:H	1.80	0.46
4:Q:82:GLN:CA	4:Q:82:GLN:HE21	2.28	0.46
1:A:148:VAL:CG1	1:A:148:VAL:O	2.61	0.46
2:B:144:GLY:O	2:B:145:ILE:CD1	2.63	0.46
3:C:10:PRO:O	3:C:106:TYR:HE2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:4:TRP:HE3	3:C:4:TRP:N	2.13	0.46
4:D:69:PHE:HA	4:D:73:HIS:CE1	2.50	0.46
5:E:3:LEU:HG	5:E:7:PHE:CE2	2.51	0.46
8:H:3:VAL:HA	8:H:6:TRP:HD1	1.80	0.46
1:N:14:ILE:C	1:N:15:GLN:CG	2.83	0.46
1:N:72:ILE:N	1:N:72:ILE:HD12	2.30	0.46
2:O:18:LEU:HG	2:O:30:PRO:O	2.16	0.46
2:O:96:LEU:HD13	2:O:96:LEU:O	2.15	0.46
3:P:101:VAL:CG2	3:P:103:PHE:HE2	2.22	0.46
3:P:272:LEU:HG	4:Q:27:VAL:HG21	1.97	0.46
3:P:54:TYR:HB2	3:P:58:LEU:CD2	2.44	0.46
4:Q:121:GLU:OE2	4:Q:125:LYS:HE3	2.15	0.46
4:Q:137:GLY:O	4:Q:138:ARG:C	2.53	0.46
5:R:14:LEU:O	5:R:17:GLY:CA	2.64	0.46
1:A:179:THR:O	1:A:183:TYR:CD1	2.68	0.46
1:A:191:LEU:C	1:A:193:TRP:H	2.18	0.46
2:B:118:ASN:HB3	2:B:121:GLN:O	2.15	0.46
2:B:85:PHE:HD1	2:B:86:GLN:N	2.14	0.46
3:C:171:VAL:HG13	3:C:234:ASN:HD22	1.81	0.46
4:D:41:TYR:C	4:D:41:TYR:CD2	2.89	0.46
6:F:16:LEU:HA	6:F:19:VAL:CB	2.46	0.46
6:F:21:TRP:O	6:F:25:VAL:HG23	2.16	0.46
1:N:165:ILE:CD1	1:N:168:LEU:HD12	2.46	0.46
1:N:52:PHE:HA	1:N:55:THR:CG2	2.45	0.46
1:N:68:SER:O	1:N:72:ILE:HD12	2.16	0.46
1:N:118:TRP:HH2	2:O:108:LEU:O	1.99	0.46
2:O:41:PRO:O	2:O:45:MET:HG3	2.15	0.46
3:P:75:VAL:HG12	3:P:152:GLY:O	2.15	0.46
3:P:280:GLU:O	3:P:280:GLU:CG	2.63	0.46
4:Q:24:PHE:HA	4:Q:27:VAL:HB	1.98	0.46
2:O:124:PHE:O	5:R:23:ILE:HD13	2.16	0.46
1:A:29:HIS:HB3	1:A:30:VAL:H	1.55	0.46
11:B:305:OPC:PAJ	11:B:305:OPC:OAN	2.74	0.46
3:C:266:MET:HA	3:C:269:GLN:HE22	1.80	0.46
3:C:278:GLN:NE2	7:G:25:LYS:HE3	2.31	0.46
3:C:28:ALA:HB3	3:C:240:PHE:HB3	1.97	0.46
11:B:305:OPC:OBH	11:C:306:OPC:HAU1	2.16	0.46
4:D:113:CYS:CB	4:D:128:CYS:HG	2.27	0.46
1:N:145:TYR:C	1:N:145:TYR:CD2	2.89	0.46
1:N:13:GLU:OE2	1:N:14:ILE:HG12	2.15	0.46
2:O:135:PHE:O	2:O:137:THR:N	2.49	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:36:LEU:C	2:O:39:VAL:HG13	2.35	0.46
3:P:269:GLN:O	3:P:273:ILE:HG23	2.16	0.46
3:P:270:LEU:O	3:P:274:LEU:HG	2.15	0.46
3:P:54:TYR:HD2	3:P:155:ARG:HH11	1.63	0.46
4:Q:94:GLU:C	4:Q:96:LYS:H	2.19	0.46
1:A:123:ILE:HG21	1:A:198:PHE:CE2	2.50	0.46
4:D:121:GLU:OE2	4:D:125:LYS:HE3	2.16	0.46
2:B:57:LEU:HD13	7:G:10:PHE:CG	2.51	0.46
1:N:148:VAL:HG11	1:N:183:TYR:CE2	2.51	0.46
1:N:87:ARG:HH12	3:P:146:LYS:HZ2	1.64	0.46
2:O:151:LEU:O	2:O:152:ASP:CB	2.62	0.46
2:O:34:ASN:CG	2:O:35:ASP:N	2.68	0.46
3:P:180:ILE:HG13	3:P:199:ILE:HA	1.98	0.46
3:P:277:LYS:NZ	3:P:278:GLN:OE1	2.43	0.46
3:P:65:GLY:O	3:P:66:SER:C	2.54	0.46
1:A:30:VAL:C	1:A:211:ILE:HD13	2.37	0.45
2:B:65:PRO:HB3	2:B:68:PRO:HG3	1.98	0.45
2:B:73:LEU:HD23	3:C:18:GLY:CA	2.46	0.45
3:C:155:ARG:HG2	3:C:239:GLY:CA	2.45	0.45
3:C:271:MET:CG	3:C:274:LEU:HD12	2.42	0.45
4:D:82:GLN:HE21	4:D:82:GLN:CA	2.29	0.45
1:N:135:GLY:HA2	1:N:138:LEU:HD12	1.94	0.45
2:O:64:GLU:CD	2:O:65:PRO:N	2.69	0.45
3:P:169:ASN:CG	3:P:236:ASN:HA	2.36	0.45
1:A:72:ILE:HD12	1:A:72:ILE:H	1.81	0.45
1:A:81:LEU:C	1:A:81:LEU:HD13	2.35	0.45
11:B:305:OPC:CAV	11:B:305:OPC:HAG1	2.46	0.45
2:B:40:PHE:H	2:B:41:PRO:HD2	1.79	0.45
3:C:121:GLY:C	3:C:123:GLN:N	2.69	0.45
4:D:83:GLY:N	4:D:87:ASP:O	2.47	0.45
1:N:56:PHE:C	1:N:57:TYR:CD2	2.89	0.45
1:N:78:PHE:CE1	4:Q:37:PRO:HA	2.51	0.45
5:R:14:LEU:O	5:R:18:ILE:N	2.50	0.45
1:A:142:GLN:H	2:B:65:PRO:HG2	1.79	0.45
1:A:50:THR:OG1	1:A:51:GLY:N	2.48	0.45
1:A:78:PHE:O	1:A:79:GLY:C	2.53	0.45
3:C:277:LYS:HA	3:C:280:GLU:HB3	1.97	0.45
3:C:82:PHE:CE1	3:C:134:PRO:HD2	2.52	0.45
8:H:1:ILE:CG2	8:H:2:ASP:H	2.29	0.45
2:O:85:PHE:HD1	2:O:86:GLN:N	2.14	0.45
3:P:199:ILE:HG13	3:P:208:VAL:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:265:VAL:O	3:P:269:GLN:HG3	2.17	0.45
2:O:45:MET:CE	3:P:269:GLN:HB3	2.46	0.45
3:P:54:TYR:CE1	3:P:70:LEU:HD22	2.52	0.45
4:Q:56:ALA:O	4:Q:57:LYS:C	2.55	0.45
15:R:1101:BCR:H361	15:R:1101:BCR:H20C	1.79	0.45
5:R:11:PHE:C	5:R:14:LEU:HD23	2.36	0.45
2:O:31:ALA:CB	7:T:30:LEU:C	2.85	0.45
2:B:79:TRP:HH2	5:E:1:MET:CG	2.30	0.45
3:C:225:VAL:O	3:C:226:LYS:HB3	2.16	0.45
3:C:256:LYS:O	3:C:259:ILE:N	2.50	0.45
3:C:41:LEU:HB3	3:C:42:PRO:HD2	1.99	0.45
3:C:52:ILE:CG2	3:C:155:ARG:NH2	2.77	0.45
3:C:55:ASP:CB	3:C:57:LYS:HD2	2.46	0.45
4:D:83:GLY:HA3	4:D:89:THR:OG1	2.16	0.45
6:F:28:LEU:HB3	6:F:33:ALA:CB	2.46	0.45
1:N:165:ILE:O	1:N:167:ASP:N	2.50	0.45
1:N:39:ILE:O	1:N:40:THR:C	2.55	0.45
1:N:52:PHE:C	1:N:54:MET:H	2.18	0.45
1:N:83:ARG:NH1	2:O:60:ALA:CB	2.75	0.45
2:O:42:VAL:HA	2:O:45:MET:HE2	1.99	0.45
3:P:226:LYS:NZ	3:P:226:LYS:CB	2.79	0.45
3:P:3:PHE:O	3:P:5:ALA:N	2.50	0.45
5:R:7:PHE:C	5:R:9:ILE:H	2.17	0.45
6:S:27:LEU:CD1	8:U:15:TRP:NE1	2.71	0.45
6:S:20:GLY:HA3	7:T:21:TYR:CD1	2.52	0.45
1:A:118:TRP:HB2	9:A:302:HEM:HMD1	1.97	0.45
1:A:51:GLY:HA2	1:A:54:MET:CE	2.46	0.45
1:N:208:LYS:HG2	2:O:27:TYR:OH	2.16	0.45
3:P:205:LYS:HZ3	3:P:207:VAL:HA	1.82	0.45
1:A:120:SER:O	1:A:121:GLY:C	2.54	0.45
1:A:41:LEU:O	1:A:44:PHE:N	2.45	0.45
1:A:68:SER:O	1:A:72:ILE:HD12	2.15	0.45
2:B:124:PHE:CE2	5:E:27:LYS:HB2	2.52	0.45
11:B:305:OPC:HBN2	11:B:305:OPC:OAB	2.17	0.45
2:B:34:ASN:CG	2:B:35:ASP:N	2.70	0.45
3:C:161:TYR:HB2	3:C:165:GLU:O	2.16	0.45
3:C:269:GLN:O	3:C:273:ILE:HG23	2.17	0.45
3:C:273:ILE:O	3:C:278:GLN:CG	2.65	0.45
3:C:89:ARG:O	3:C:90:ILE:C	2.55	0.45
4:D:122:ASN:HD22	4:D:122:ASN:N	2.14	0.45
4:D:170:PHE:CD1	4:D:170:PHE:N	2.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:19:MET:C	4:D:21:LEU:H	2.20	0.45
4:D:38:LEU:C	4:D:38:LEU:HD12	2.36	0.45
5:E:2:ILE:CG2	5:E:3:LEU:H	2.22	0.45
6:F:35:LYS:C	6:F:36:GLU:HG2	2.37	0.45
1:N:56:PHE:C	1:N:57:TYR:HD2	2.20	0.45
2:O:123:PRO:HG2	2:O:124:PHE:CZ	2.51	0.45
4:Q:93:VAL:HA	4:Q:99:ILE:CG2	2.39	0.45
1:A:103:ARG:O	1:A:103:ARG:HD2	2.17	0.45
1:A:109:GLY:HA3	9:A:302:HEM:HBD2	1.98	0.45
1:A:28:PRO:HG2	1:A:29:HIS:N	2.32	0.45
1:A:79:GLY:O	1:A:80:TRP:C	2.55	0.45
5:E:7:PHE:O	5:E:11:PHE:HD2	2.00	0.45
2:O:135:PHE:C	2:O:135:PHE:CD1	2.88	0.45
2:O:91:LEU:C	2:O:91:LEU:HD12	2.37	0.45
3:P:273:ILE:HD12	7:T:25:LYS:HD3	1.98	0.45
3:C:101:VAL:CG1	3:C:118:PRO:HB2	2.47	0.45
3:C:121:GLY:O	3:C:123:GLN:N	2.49	0.45
3:C:199:ILE:HB	3:C:207:VAL:O	2.17	0.45
3:C:169:ASN:ND2	3:C:236:ASN:HA	2.32	0.45
1:N:57:TYR:HE1	1:N:76:VAL:HG21	1.82	0.45
3:P:159:GLN:CD	3:P:159:GLN:N	2.70	0.45
3:P:185:LYS:HD2	3:P:195:TYR:CB	2.42	0.45
3:P:34:VAL:HG22	3:P:243:ASP:HB3	1.99	0.45
3:P:25:CYS:HB3	3:P:26:HIS:H	1.56	0.45
4:Q:82:GLN:HA	4:Q:82:GLN:HE21	1.82	0.45
1:A:157:ALA:O	1:A:158:ILE:HG13	2.17	0.45
4:D:88:PRO:HG3	4:D:114:VAL:CG2	2.45	0.45
8:H:10:LEU:O	8:H:13:PHE:HB2	2.17	0.45
1:N:117:THR:HG22	1:N:205:MET:HB3	1.98	0.45
1:N:120:SER:O	1:N:121:GLY:C	2.55	0.45
1:N:209:GLN:NE2	2:O:27:TYR:C	2.70	0.45
1:N:51:GLY:CA	1:N:54:MET:HE3	2.44	0.45
2:O:64:GLU:CD	2:O:65:PRO:CD	2.86	0.45
2:O:82:TYR:N	2:O:83:PRO:HD2	2.32	0.45
4:Q:118:ASN:C	4:Q:120:ALA:H	2.21	0.45
6:S:33:ALA:O	6:S:34:GLU:HG3	2.17	0.45
1:A:90:ALA:O	1:A:94:VAL:HG23	2.17	0.45
2:B:146:GLY:O	2:B:147:ALA:CB	2.64	0.45
1:A:27:PRO:O	2:B:29:GLU:CD	2.55	0.45
3:C:180:ILE:HB	3:C:199:ILE:HA	1.99	0.45
3:C:251:ASP:HB3	3:C:254:ARG:CB	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:56:ALA:O	4:D:57:LYS:C	2.55	0.45
1:A:33:PHE:CE2	15:E:101:BCR:C35	3.00	0.45
7:G:4:LEU:O	7:G:6:LEU:HD22	2.16	0.45
1:N:19:ASP:OD1	1:N:22:THR:O	2.35	0.45
1:N:27:PRO:HA	2:O:33:PRO:CG	2.47	0.45
1:N:32:ILE:CD1	7:T:26:ARG:NH2	2.80	0.45
3:P:101:VAL:CG1	3:P:118:PRO:HB2	2.47	0.45
3:P:28:ALA:CB	3:P:240:PHE:N	2.80	0.45
3:P:44:THR:O	3:P:133:SER:N	2.50	0.45
1:A:174:SER:OG	4:Q:86:GLY:HA3	2.17	0.45
5:R:2:ILE:HG13	5:R:3:LEU:N	2.32	0.45
1:A:101:VAL:O	1:A:104:VAL:HB	2.17	0.44
1:A:142:GLN:HG2	2:B:65:PRO:HG3	1.98	0.44
1:A:145:TYR:C	1:A:145:TYR:CD2	2.89	0.44
2:B:105:PRO:CG	2:B:106:LEU:H	2.21	0.44
1:A:29:HIS:ND1	2:B:30:PRO:CG	2.80	0.44
3:C:182:LYS:HD2	3:C:182:LYS:N	2.33	0.44
5:E:23:ILE:O	5:E:25:ALA:N	2.50	0.44
8:H:3:VAL:CA	8:H:6:TRP:HD1	2.29	0.44
1:N:154:VAL:HB	1:N:155:PRO:CD	2.46	0.44
1:N:178:ALA:O	1:N:180:LEU:N	2.50	0.44
1:N:179:THR:O	1:N:183:TYR:CD1	2.70	0.44
1:N:191:LEU:HD12	1:N:191:LEU:N	2.14	0.44
2:O:43:VAL:HB	2:O:44:ILE:H	1.58	0.44
2:O:73:LEU:N	2:O:73:LEU:CD2	2.80	0.44
3:P:280:GLU:OE2	7:T:28:ASN:ND2	2.50	0.44
2:O:43:VAL:CA	7:T:23:GLN:OE1	2.64	0.44
7:T:24:TYR:CD2	7:T:24:TYR:N	2.83	0.44
2:B:124:PHE:CZ	5:E:27:LYS:HG3	2.52	0.44
2:B:125:ARG:HA	2:B:125:ARG:HD3	1.89	0.44
2:B:81:LEU:CD1	2:B:81:LEU:H	2.30	0.44
3:C:60:GLN:HE22	3:C:157:ARG:HG3	1.82	0.44
3:C:78:LEU:HD21	3:C:131:VAL:CG2	2.42	0.44
1:N:114:ARG:HD2	1:N:208:LYS:HE2	1.99	0.44
1:N:158:ILE:O	1:N:160:VAL:N	2.50	0.44
4:Q:19:MET:C	4:Q:21:LEU:H	2.20	0.44
4:Q:55:THR:O	4:Q:64:VAL:HB	2.17	0.44
7:T:4:LEU:O	7:T:6:LEU:HD22	2.17	0.44
1:A:28:PRO:HG2	2:B:31:ALA:O	2.17	0.44
1:A:82:ILE:CD1	1:A:82:ILE:H	2.30	0.44
11:B:305:OPC:CAH	11:B:305:OPC:HAV	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:256:LYS:HE2	3:C:257:TRP:CZ3	2.52	0.44
3:C:3:PHE:O	3:C:5:ALA:N	2.51	0.44
3:C:61:VAL:HA	3:C:67:LYS:HA	1.98	0.44
4:D:137:GLY:O	4:D:138:ARG:O	2.35	0.44
1:N:101:VAL:O	1:N:104:VAL:HB	2.17	0.44
1:N:44:PHE:C	1:N:46:ILE:N	2.70	0.44
2:O:128:VAL:O	2:O:132:ILE:HD11	2.18	0.44
2:O:40:PHE:H	2:O:41:PRO:HD2	1.81	0.44
3:P:175:SER:O	3:P:176:ALA:HB2	2.16	0.44
4:Q:67:SER:CA	4:Q:70:LEU:HD21	2.35	0.44
5:R:6:VAL:O	5:R:10:VAL:HG12	2.18	0.44
1:A:33:PHE:CE1	5:E:18:ILE:CD1	2.88	0.44
6:F:28:LEU:HD22	6:F:31:GLN:HE22	1.83	0.44
10:N:303:HEC:HBC1	11:N:1305:OPC:HAQ1	1.99	0.44
2:O:85:PHE:CD1	2:O:86:GLN:N	2.86	0.44
3:P:161:TYR:HB2	3:P:165:GLU:O	2.18	0.44
3:P:181:THR:OG1	3:P:200:GLN:HG2	2.17	0.44
4:Q:173:GLY:O	4:Q:174:GLU:OE2	2.35	0.44
5:R:29:ILE:CG2	5:R:29:ILE:O	2.65	0.44
6:S:18:PHE:O	6:S:19:VAL:C	2.55	0.44
7:T:18:TYR:O	7:T:19:ALA:C	2.55	0.44
1:A:178:ALA:O	1:A:180:LEU:N	2.51	0.44
1:A:127:ILE:CD1	1:A:194:LEU:HB2	2.47	0.44
2:B:101:MET:CG	2:B:102:ALA:N	2.80	0.44
2:B:132:ILE:HA	2:B:135:PHE:CD2	2.46	0.44
2:B:144:GLY:C	2:B:145:ILE:HG12	2.38	0.44
3:C:172:PHE:CD1	3:C:215:PRO:HG3	2.52	0.44
3:C:274:LEU:O	3:C:275:LYS:O	2.35	0.44
3:C:50:VAL:O	3:C:52:ILE:HG13	2.17	0.44
1:N:14:ILE:CB	1:N:17:LEU:HD11	2.38	0.44
1:N:52:PHE:C	1:N:52:PHE:CD1	2.89	0.44
3:P:82:PHE:CE1	3:P:134:PRO:HD2	2.53	0.44
3:P:91:PRO:C	3:P:92:GLU:HG2	2.35	0.44
4:Q:94:GLU:CG	4:Q:100:ARG:HG2	2.47	0.44
4:Q:88:PRO:HD2	4:Q:107:VAL:HG23	1.99	0.44
4:Q:73:HIS:HB2	4:Q:93:VAL:HG21	1.99	0.44
3:P:277:LYS:HE3	7:T:27:PRO:CD	2.47	0.44
1:A:121:GLY:O	1:A:122:VAL:C	2.56	0.44
2:B:51:ILE:CD1	2:B:51:ILE:H	2.20	0.44
3:C:14:ARG:CZ	3:C:150:HIS:ND1	2.80	0.44
3:C:154:ASN:CG	3:C:155:ARG:N	2.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:91:PRO:O	3:C:92:GLU:CG	2.61	0.44
4:D:65:LYS:HD2	4:D:65:LYS:N	2.32	0.44
6:F:8:TYR:HD2	6:F:9:ALA:N	2.15	0.44
1:N:33:PHE:O	1:N:35:CYS:N	2.51	0.44
3:P:46:PHE:CD1	3:P:131:VAL:HG13	2.52	0.44
3:P:231:LEU:HD11	3:P:233:ASN:O	2.18	0.44
4:Q:41:TYR:CD2	4:Q:41:TYR:C	2.91	0.44
5:R:6:VAL:O	5:R:10:VAL:CG1	2.65	0.44
3:P:259:ILE:HD11	7:T:12:THR:HG21	2.00	0.44
2:B:55:SER:O	2:B:56:VAL:C	2.56	0.44
2:O:29:GLU:N	2:O:30:PRO:CD	2.77	0.44
2:O:42:VAL:HA	2:O:45:MET:CE	2.47	0.44
3:P:3:PHE:HD2	3:P:4:TRP:CZ3	2.36	0.44
3:P:60:GLN:HE22	3:P:157:ARG:HG3	1.82	0.44
4:Q:70:LEU:CD1	4:Q:71:GLU:HG2	2.47	0.44
1:A:62:VAL:HG23	1:A:63:THR:HG23	1.99	0.44
3:C:144:PHE:O	3:C:147:TYR:CE1	2.71	0.44
3:C:15:GLU:HB2	3:C:19:ARG:O	2.17	0.44
3:C:167:SER:OG	3:C:168:ASN:N	2.49	0.44
4:D:118:ASN:C	4:D:120:ALA:H	2.21	0.44
1:N:120:SER:HA	1:N:123:ILE:HD13	2.00	0.44
2:O:72:PRO:O	2:O:74:GLU:N	2.51	0.44
3:P:237:VAL:O	3:P:238:GLY:C	2.56	0.44
3:P:277:LYS:HA	3:P:280:GLU:HB3	2.00	0.44
3:P:55:ASP:HB2	3:P:57:LYS:CD	2.48	0.44
4:Q:117:TRP:CZ3	4:Q:119:ALA:HA	2.53	0.44
5:R:15:PHE:O	5:R:19:ALA:N	2.50	0.44
8:U:3:VAL:CA	8:U:6:TRP:HD1	2.31	0.44
1:A:139:PRO:O	1:A:140:TRP:CB	2.66	0.44
2:B:120:PHE:O	2:B:121:GLN:C	2.56	0.44
2:B:42:VAL:HA	2:B:45:MET:CE	2.48	0.44
3:C:196:GLN:HE22	3:C:210:THR:HB	1.79	0.44
3:C:184:ALA:HB3	3:C:197:VAL:N	2.33	0.44
3:C:221:GLU:C	3:C:223:GLN:H	2.22	0.44
3:C:46:PHE:CE1	3:C:131:VAL:HG13	2.52	0.44
4:D:173:GLY:O	4:D:174:GLU:OE2	2.36	0.44
4:D:35:LEU:N	4:D:37:PRO:HD2	2.22	0.44
6:F:4:GLU:HG3	6:F:5:GLU:H	1.82	0.44
1:N:105:TYR:HD2	1:N:106:LEU:CD2	2.31	0.44
1:N:121:GLY:O	1:N:122:VAL:C	2.56	0.44
1:N:132:GLY:O	1:N:133:VAL:C	2.56	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:57:LEU:HA	2:O:57:LEU:HD23	1.87	0.44
2:O:62:VAL:HG22	12:O:1309:BNT:CAK	2.48	0.44
3:P:120:PRO:HG2	3:P:124:TYR:HB2	1.99	0.44
3:P:144:PHE:O	3:P:147:TYR:CE1	2.70	0.44
3:P:199:ILE:HD12	3:P:208:VAL:HA	2.00	0.44
1:N:78:PHE:HE1	4:Q:37:PRO:HA	1.82	0.44
6:S:16:LEU:HA	6:S:19:VAL:CB	2.48	0.44
1:A:160:VAL:HG12	1:A:161:VAL:N	2.30	0.43
1:A:48:PHE:O	1:A:52:PHE:HB3	2.18	0.43
4:D:19:MET:O	4:D:21:LEU:N	2.50	0.43
4:D:73:HIS:CG	4:D:93:VAL:HG21	2.53	0.43
5:E:12:ILE:HA	5:E:15:PHE:CE1	2.53	0.43
5:E:15:PHE:O	5:E:19:ALA:N	2.51	0.43
13:O:1201:CLA:HMA1	13:O:1201:CLA:HHB	1.80	0.43
3:P:6:GLN:HB3	3:P:106:TYR:CE2	2.53	0.43
2:O:122:ASN:ND2	5:R:26:ILE:C	2.71	0.43
11:B:305:OPC:HAU1	11:B:305:OPC:HAX2	1.67	0.43
11:B:305:OPC:HAX2	11:B:305:OPC:HBZ2	1.99	0.43
2:B:34:ASN:CG	2:B:35:ASP:H	2.03	0.43
3:C:151:LEU:HD23	3:C:151:LEU:O	2.18	0.43
4:D:80:LEU:H	4:D:80:LEU:CD2	2.29	0.43
8:H:6:TRP:O	8:H:7:VAL:C	2.55	0.43
1:N:122:VAL:O	1:N:123:ILE:C	2.56	0.43
1:N:82:ILE:HD12	1:N:82:ILE:H	1.84	0.43
1:N:43:CYS:HB2	1:N:93:MET:HB2	2.00	0.43
3:P:126:GLU:O	3:P:127:ILE:C	2.55	0.43
1:A:34:TYR:CD1	1:A:103:ARG:CD	3.01	0.43
1:A:117:THR:HG22	1:A:205:MET:HB3	1.98	0.43
1:A:42:THR:C	1:A:44:PHE:N	2.70	0.43
2:B:38:TYR:HA	2:B:41:PRO:CG	2.48	0.43
4:D:108:CYS:SG	4:D:110:HIS:HB3	2.58	0.43
4:D:115:VAL:HG22	4:D:126:CYS:HB2	1.99	0.43
4:D:71:GLU:HG3	4:D:72:SER:N	2.33	0.43
5:E:9:ILE:CG2	5:E:10:VAL:H	2.31	0.43
5:E:23:ILE:C	5:E:25:ALA:H	2.21	0.43
1:N:110:PHE:HA	1:N:114:ARG:O	2.18	0.43
1:N:211:ILE:CG2	1:N:212:SER:N	2.81	0.43
1:N:83:ARG:O	1:N:84:SER:C	2.56	0.43
2:O:125:ARG:HH11	2:O:126:ARG:N	1.88	0.43
2:O:79:TRP:HA	2:O:82:TYR:CZ	2.53	0.43
3:P:6:GLN:HB3	3:P:106:TYR:CZ	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:177:THR:O	3:P:177:THR:HG22	2.18	0.43
3:P:199:ILE:N	3:P:208:VAL:HG12	2.33	0.43
3:P:76:LEU:C	3:P:76:LEU:HD23	2.38	0.43
3:P:87:GLU:HA	3:P:90:ILE:HD12	2.00	0.43
4:Q:102:TYR:HB2	4:Q:150:LEU:HB3	2.00	0.43
3:P:261:PHE:HE2	4:Q:34:ALA:N	2.16	0.43
1:A:119:ILE:O	1:A:122:VAL:N	2.52	0.43
1:A:122:VAL:O	1:A:123:ILE:C	2.55	0.43
1:A:15:GLN:O	1:A:17:LEU:CD1	2.67	0.43
1:A:165:ILE:O	1:A:168:LEU:N	2.49	0.43
1:A:170:ARG:HA	1:A:179:THR:HA	2.00	0.43
1:A:195:ILE:CG2	1:A:196:ALA:N	2.81	0.43
2:B:146:GLY:O	2:B:147:ALA:HB3	2.18	0.43
2:B:96:LEU:CD1	2:B:100:LEU:HD12	2.48	0.43
3:C:177:THR:HG22	3:C:177:THR:O	2.19	0.43
3:C:81:GLY:C	3:C:134:PRO:HG2	2.38	0.43
3:C:83:LYS:HE3	3:C:134:PRO:CA	2.48	0.43
3:C:9:TYR:CE1	3:C:21:VAL:HG11	2.54	0.43
11:C:306:OPC:CAA	4:D:17:GLN:HG2	2.49	0.43
1:N:200:LEU:N	1:N:200:LEU:HD22	2.33	0.43
2:O:37:LEU:C	2:O:41:PRO:HD2	2.38	0.43
2:O:43:VAL:O	2:O:44:ILE:C	2.56	0.43
3:P:110:GLN:HB3	3:P:113:VAL:HG23	2.00	0.43
3:P:91:PRO:O	3:P:92:GLU:CG	2.60	0.43
5:R:14:LEU:N	5:R:14:LEU:HD22	2.32	0.43
5:R:22:ILE:HG23	5:R:23:ILE:N	2.33	0.43
2:B:122:ASN:HB2	2:B:123:PRO:CD	2.43	0.43
2:B:67:ASN:N	2:B:68:PRO:CD	2.81	0.43
2:B:95:LEU:N	2:B:95:LEU:HD23	2.32	0.43
3:C:6:GLN:HB3	3:C:106:TYR:CZ	2.53	0.43
3:C:126:GLU:O	3:C:127:ILE:C	2.57	0.43
3:C:275:LYS:HZ1	11:C:306:OPC:HBG3	1.77	0.43
4:D:117:TRP:CZ3	4:D:119:ALA:HA	2.53	0.43
4:D:163:THR:HB	4:D:164:PRO:HD2	2.00	0.43
4:D:65:LYS:HB2	4:D:68:LYS:HZ3	1.83	0.43
5:E:26:ILE:HG23	5:E:30:LYS:HZ1	1.84	0.43
6:F:25:VAL:O	6:F:28:LEU:N	2.41	0.43
1:N:117:THR:O	1:N:202:HIS:CE1	2.71	0.43
1:N:14:ILE:C	1:N:15:GLN:CD	2.77	0.43
1:N:167:ASP:OD2	1:N:172:GLY:O	2.36	0.43
1:N:79:GLY:O	1:N:80:TRP:C	2.56	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:28:PRO:CG	2:O:32:TRP:HB3	2.29	0.43
4:D:88:PRO:CB	2:O:69:PHE:CD2	2.99	0.43
3:P:55:ASP:C	3:P:57:LYS:N	2.71	0.43
3:P:81:GLY:O	3:P:134:PRO:HG3	2.19	0.43
4:Q:66:VAL:HG13	4:Q:159:ASN:O	2.18	0.43
4:Q:88:PRO:O	4:Q:106:ALA:HB3	2.18	0.43
2:O:79:TRP:HZ2	5:R:1:MET:HA	1.82	0.43
3:P:273:ILE:CG2	7:T:22:GLN:HB3	2.34	0.43
1:A:201:LEU:C	1:A:205:MET:HE2	2.39	0.43
2:B:79:TRP:C	2:B:80:TYR:CD1	2.88	0.43
3:C:28:ALA:CB	3:C:238:GLY:C	2.87	0.43
3:C:28:ALA:HB3	3:C:240:PHE:CB	2.48	0.43
5:E:18:ILE:C	5:E:23:ILE:HG23	2.39	0.43
1:N:15:GLN:H	1:N:17:LEU:HD12	1.83	0.43
1:N:142:GLN:HG2	2:O:64:GLU:CG	2.49	0.43
3:P:140:LYS:N	3:P:140:LYS:HD2	2.33	0.43
3:P:180:ILE:HB	3:P:199:ILE:HA	2.00	0.43
3:P:271:MET:HA	3:P:274:LEU:HG	1.98	0.43
3:P:54:TYR:CD1	3:P:54:TYR:C	2.91	0.43
4:Q:173:GLY:O	4:Q:174:GLU:CD	2.57	0.43
5:R:18:ILE:C	5:R:23:ILE:HG23	2.39	0.43
5:R:18:ILE:O	5:R:23:ILE:HG23	2.19	0.43
5:R:25:ALA:O	5:R:29:ILE:HD12	2.18	0.43
5:R:5:ALA:C	5:R:7:PHE:N	2.72	0.43
7:T:16:LEU:CD2	7:T:16:LEU:O	2.61	0.43
1:A:112:LYS:HG3	1:A:113:PRO:HD3	2.00	0.43
2:B:124:PHE:CE1	5:E:23:ILE:HD11	2.53	0.43
3:C:180:ILE:HG13	3:C:199:ILE:HA	2.01	0.43
1:N:114:ARG:HH11	1:N:114:ARG:HG2	1.83	0.43
1:N:201:LEU:C	1:N:205:MET:HE2	2.39	0.43
1:N:25:TYR:HB2	1:N:26:VAL:H	1.73	0.43
2:O:147:ALA:O	2:O:149:LEU:CD2	2.64	0.43
3:P:225:VAL:O	3:P:226:LYS:HB3	2.18	0.43
4:Q:163:THR:HB	4:Q:164:PRO:CD	2.48	0.43
15:R:1101:BCR:H322	7:T:23:GLN:HE22	1.83	0.43
5:R:28:SER:C	5:R:30:LYS:H	2.21	0.43
6:S:8:TYR:HD2	6:S:9:ALA:H	1.67	0.43
1:A:108:GLY:O	1:A:110:PHE:CD2	2.72	0.43
1:A:26:VAL:HB	2:B:29:GLU:CG	2.27	0.43
1:A:54:MET:C	1:A:56:PHE:N	2.72	0.43
2:B:127:PRO:O	2:B:130:THR:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:ARG:NH1	2:B:60:ALA:HA	2.33	0.43
3:C:34:VAL:HG11	3:C:151:LEU:HD22	2.00	0.43
3:C:161:TYR:HE1	3:C:167:SER:HA	1.82	0.43
4:D:110:HIS:CD2	4:D:143:PRO:HB2	2.53	0.43
4:D:41:TYR:CD2	4:D:42:PHE:N	2.86	0.43
4:D:63:ASN:O	4:D:65:LYS:HD2	2.19	0.43
7:G:22:GLN:C	7:G:24:TYR:H	2.22	0.43
1:N:111:LYS:CB	1:N:113:PRO:HD2	2.44	0.43
1:N:205:MET:O	1:N:207:ARG:HG3	2.18	0.43
2:O:53:ALA:HA	3:P:258:MET:HE2	2.01	0.43
3:P:117:GLY:O	3:P:119:LEU:CD2	2.66	0.43
4:Q:33:GLY:O	4:Q:37:PRO:CD	2.67	0.43
1:A:65:ALA:O	1:A:69:VAL:HG23	2.18	0.43
1:A:99:LEU:HA	1:A:102:PHE:CD1	2.54	0.43
2:B:121:GLN:O	2:B:121:GLN:CD	2.57	0.43
2:B:141:ILE:O	2:B:144:GLY:N	2.42	0.43
3:C:83:LYS:HE3	3:C:134:PRO:HA	2.01	0.43
4:D:69:PHE:HA	4:D:73:HIS:ND1	2.34	0.43
5:E:5:ALA:HB1	6:F:10:ALA:N	2.34	0.43
7:G:18:TYR:O	7:G:19:ALA:C	2.57	0.43
7:G:29:GLU:O	7:G:30:LEU:C	2.57	0.43
1:N:43:CYS:O	1:N:46:ILE:HB	2.18	0.43
1:N:81:LEU:O	1:N:82:ILE:C	2.56	0.43
3:P:34:VAL:HG11	3:P:151:LEU:CB	2.49	0.43
3:P:76:LEU:HD21	3:P:78:LEU:HD12	2.01	0.43
4:Q:157:ASP:O	4:Q:158:ASP:CB	2.67	0.43
4:Q:19:MET:O	4:Q:21:LEU:N	2.51	0.43
4:Q:41:TYR:HD2	4:Q:42:PHE:N	2.16	0.43
1:A:210:GLY:O	1:A:211:ILE:HB	2.18	0.43
1:A:48:PHE:HA	9:A:301:HEM:CMC	2.49	0.43
3:C:258:MET:SD	3:C:258:MET:C	2.97	0.43
3:C:54:TYR:CE1	3:C:70:LEU:HD22	2.54	0.43
3:C:55:ASP:C	3:C:57:LYS:H	2.22	0.43
1:N:165:ILE:HG22	1:N:166:SER:H	1.84	0.43
1:N:116:LEU:HD13	1:N:205:MET:SD	2.59	0.43
3:P:6:GLN:HA	3:P:106:TYR:OH	2.19	0.43
3:P:216:GLU:O	3:P:217:LEU:HD23	2.19	0.43
5:R:3:LEU:O	5:R:3:LEU:HD12	2.19	0.43
2:B:79:TRP:HA	2:B:82:TYR:HE2	1.80	0.42
4:D:102:TYR:HB2	4:D:150:LEU:HB3	2.00	0.42
11:C:306:OPC:HAA1	4:D:17:GLN:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:36:LEU:HB3	1:N:100:HIS:HB2	2.00	0.42
1:N:110:PHE:CB	1:N:115:GLU:HA	2.48	0.42
1:N:15:GLN:HE21	1:N:16:ALA:N	2.16	0.42
1:N:165:ILE:O	1:N:168:LEU:N	2.48	0.42
1:N:57:TYR:CE1	1:N:76:VAL:HG21	2.53	0.42
2:O:150:PRO:O	2:O:151:LEU:CB	2.67	0.42
2:O:48:PHE:C	2:O:48:PHE:CD1	2.92	0.42
2:O:81:LEU:O	2:O:81:LEU:HD23	2.19	0.42
3:P:78:LEU:HD21	3:P:131:VAL:CG2	2.43	0.42
4:Q:14:GLY:O	4:Q:15:ARG:HB2	2.19	0.42
1:A:171:GLY:HA3	1:A:178:ALA:CB	2.46	0.42
3:C:110:GLN:HB3	3:C:113:VAL:HG23	2.01	0.42
3:C:226:LYS:HZ3	3:C:226:LYS:HB3	1.84	0.42
3:C:280:GLU:O	3:C:282:VAL:N	2.52	0.42
3:C:65:GLY:O	3:C:66:SER:C	2.58	0.42
4:D:128:CYS:HB2	4:D:129:HIS:ND1	2.34	0.42
4:D:178:TRP:O	4:D:179:VAL:C	2.58	0.42
15:E:101:BCR:H20C	15:E:101:BCR:H361	1.76	0.42
5:E:6:VAL:O	5:E:10:VAL:CG1	2.67	0.42
2:B:32:TRP:CE2	7:G:28:ASN:HB3	2.54	0.42
1:N:114:ARG:NH2	9:N:302:HEM:O1D	2.52	0.42
1:N:80:TRP:CD2	3:P:254:ARG:NH2	2.86	0.42
11:O:1306:OPC:HBR	11:O:1306:OPC:HBF2	2.01	0.42
2:O:99:LEU:O	2:O:100:LEU:C	2.57	0.42
3:P:136:PRO:HB2	3:P:142:ILE:O	2.19	0.42
3:P:161:TYR:HE1	3:P:167:SER:HA	1.82	0.42
7:T:20:ALA:C	7:T:24:TYR:CZ	2.93	0.42
7:T:6:LEU:CD2	7:T:6:LEU:H	2.23	0.42
1:A:165:ILE:HD11	1:A:168:LEU:HD12	2.00	0.42
1:A:39:ILE:O	1:A:40:THR:C	2.57	0.42
1:A:44:PHE:HD1	9:A:301:HEM:HBB1	1.84	0.42
1:A:43:CYS:O	1:A:46:ILE:HB	2.18	0.42
2:B:48:PHE:O	2:B:49:ALA:C	2.58	0.42
3:C:55:ASP:C	3:C:57:LYS:N	2.72	0.42
6:F:20:GLY:O	6:F:21:TRP:C	2.57	0.42
6:F:28:LEU:HD23	6:F:31:GLN:NE2	2.34	0.42
7:G:20:ALA:C	7:G:24:TYR:CZ	2.93	0.42
1:N:102:PHE:O	1:N:103:ARG:C	2.58	0.42
1:N:204:LEU:O	1:N:207:ARG:HG3	2.19	0.42
2:O:122:ASN:HD22	5:R:27:LYS:CA	2.31	0.42
2:O:149:LEU:HA	2:O:150:PRO:HD3	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:62:VAL:HG23	2:O:63:GLY:N	2.35	0.42
2:O:64:GLU:H	2:O:65:PRO:HD2	1.83	0.42
3:P:13:PRO:HB2	3:P:20:ILE:HG22	2.00	0.42
6:S:20:GLY:HA3	7:T:21:TYR:CE1	2.54	0.42
7:T:22:GLN:C	7:T:24:TYR:H	2.22	0.42
1:A:146:TRP:HB3	2:B:75:ILE:CD1	2.50	0.42
1:A:163:VAL:C	1:A:165:ILE:H	2.21	0.42
1:A:175:VAL:O	1:A:176:GLY:C	2.58	0.42
2:B:105:PRO:CG	2:B:106:LEU:N	2.82	0.42
1:A:142:GLN:NE2	2:B:68:PRO:CB	2.75	0.42
2:B:96:LEU:HD13	2:B:96:LEU:C	2.39	0.42
3:C:216:GLU:O	3:C:217:LEU:HD23	2.18	0.42
3:C:54:TYR:CD1	3:C:54:TYR:C	2.91	0.42
3:C:86:PRO:HG2	3:C:89:ARG:HB2	2.00	0.42
4:D:173:GLY:O	4:D:174:GLU:CD	2.57	0.42
5:E:14:LEU:HD22	5:E:14:LEU:N	2.34	0.42
1:N:33:PHE:CD1	1:N:34:TYR:CE1	3.08	0.42
3:P:225:VAL:HB	3:P:226:LYS:H	1.49	0.42
1:A:165:ILE:C	1:A:167:ASP:N	2.72	0.42
1:A:27:PRO:HG2	2:B:20:LYS:HZ2	1.84	0.42
1:A:55:THR:OG1	1:N:185:SER:CB	2.68	0.42
2:B:108:LEU:C	2:B:110:LEU:N	2.73	0.42
2:B:116:ASN:O	2:B:116:ASN:ND2	2.52	0.42
2:B:72:PRO:HG2	2:B:75:ILE:CG1	2.40	0.42
3:C:275:LYS:O	3:C:276:LYS:C	2.57	0.42
3:C:34:VAL:HG13	3:C:151:LEU:HD22	2.00	0.42
5:E:14:LEU:O	5:E:18:ILE:N	2.52	0.42
8:H:6:TRP:O	8:H:9:LEU:N	2.53	0.42
1:N:170:ARG:O	1:N:179:THR:N	2.53	0.42
1:N:24:LYS:HG2	1:N:24:LYS:H	1.49	0.42
1:N:81:LEU:HD13	1:N:81:LEU:C	2.40	0.42
2:O:34:ASN:HD22	2:O:35:ASP:CG	2.22	0.42
2:O:48:PHE:O	2:O:49:ALA:C	2.56	0.42
1:N:84:SER:HB2	2:O:55:SER:HB3	2.02	0.42
3:P:83:LYS:O	3:P:131:VAL:HG23	2.20	0.42
4:Q:105:ASN:ND2	4:Q:107:VAL:HB	2.33	0.42
4:Q:115:VAL:CG2	4:Q:126:CYS:HB2	2.50	0.42
1:A:191:LEU:O	1:A:193:TRP:N	2.53	0.42
1:A:40:THR:O	1:A:93:MET:HG3	2.20	0.42
2:B:85:PHE:CD1	2:B:86:GLN:N	2.87	0.42
4:D:110:HIS:HB2	4:D:144:ALA:CA	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:124:PHE:CZ	5:E:27:LYS:CB	2.98	0.42
1:N:127:ILE:CD1	1:N:194:LEU:HB2	2.45	0.42
2:O:48:PHE:O	2:O:50:CYS:N	2.53	0.42
3:P:54:TYR:HD2	3:P:155:ARG:NH1	2.17	0.42
4:Q:150:LEU:C	4:Q:151:CYS:SG	2.98	0.42
5:R:5:ALA:CB	6:S:6:MET:O	2.67	0.42
1:A:95:LEU:HD23	1:A:99:LEU:HD21	2.00	0.42
2:B:126:ARG:HA	2:B:127:PRO:HD2	1.73	0.42
2:B:126:ARG:HG2	2:B:128:VAL:HG23	2.00	0.42
11:B:305:OPC:HBV2	11:C:306:OPC:HBT1	2.01	0.42
3:C:263:CYS:HA	3:C:266:MET:CB	2.50	0.42
4:D:82:GLN:NE2	4:D:82:GLN:HA	2.35	0.42
6:F:8:TYR:O	6:F:11:LEU:CD1	2.68	0.42
7:G:26:ARG:CD	7:G:27:PRO:HD3	2.27	0.42
1:N:15:GLN:NE2	1:N:15:GLN:C	2.67	0.42
2:O:68:PRO:HG2	2:O:69:PHE:N	2.32	0.42
3:P:55:ASP:C	3:P:57:LYS:H	2.23	0.42
4:Q:132:GLN:C	4:Q:133:TYR:HD2	2.23	0.42
4:Q:81:VAL:CG1	4:Q:82:GLN:H	2.16	0.42
1:A:120:SER:OG	1:A:121:GLY:N	2.53	0.42
1:A:174:SER:HB3	4:Q:86:GLY:HA3	2.02	0.42
5:E:7:PHE:O	5:E:11:PHE:CD2	2.72	0.42
6:F:18:PHE:O	6:F:19:VAL:C	2.58	0.42
1:N:186:ALA:HA	1:N:190:VAL:HB	2.02	0.42
1:N:74:ASN:HB3	3:P:143:HIS:CG	2.54	0.42
1:N:66:TYR:HB2	2:O:65:PRO:HG2	2.01	0.42
2:O:70:ALA:O	2:O:71:THR:OG1	2.36	0.42
4:Q:110:HIS:ND1	4:Q:111:LEU:HB2	2.34	0.42
4:Q:65:LYS:HB2	4:Q:68:LYS:HZ2	1.84	0.42
4:Q:82:GLN:NE2	4:Q:82:GLN:HA	2.35	0.42
1:A:52:PHE:O	1:A:53:ALA:C	2.58	0.42
2:B:100:LEU:O	2:B:103:SER:HB2	2.20	0.42
2:B:108:LEU:O	2:B:110:LEU:N	2.53	0.42
4:D:63:ASN:O	4:D:159:ASN:ND2	2.52	0.42
4:D:35:LEU:O	4:D:36:TYR:C	2.58	0.42
4:D:69:PHE:O	4:D:99:ILE:HD13	2.20	0.42
1:N:41:LEU:O	1:N:44:PHE:CB	2.66	0.42
1:N:72:ILE:HD12	1:N:72:ILE:H	1.85	0.42
3:P:265:VAL:O	3:P:266:MET:C	2.59	0.42
3:P:52:ILE:HA	3:P:53:PRO:HD2	1.66	0.42
5:R:3:LEU:HG	5:R:7:PHE:CE2	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:16:LEU:HD22	6:S:16:LEU:N	2.34	0.42
1:A:105:TYR:CD2	1:A:105:TYR:C	2.93	0.42
1:A:22:THR:HG23	1:A:22:THR:O	2.19	0.42
2:B:149:LEU:HB3	2:B:150:PRO:HD2	2.02	0.42
1:A:39:ILE:CD1	2:B:43:VAL:HG12	2.49	0.42
2:B:57:LEU:HD22	7:G:10:PHE:CD1	2.55	0.42
3:C:20:ILE:HG13	3:C:152:GLY:HA3	2.02	0.42
3:C:185:LYS:NZ	3:C:195:TYR:HB3	2.35	0.42
3:C:19:ARG:NH1	3:C:23:ALA:HB3	2.35	0.42
4:D:163:THR:HB	4:D:164:PRO:CD	2.50	0.42
1:A:53:ALA:CA	4:D:42:PHE:CZ	2.97	0.42
5:E:22:ILE:HG23	5:E:23:ILE:N	2.30	0.42
6:F:8:TYR:C	6:F:8:TYR:CD2	2.94	0.42
7:G:17:PHE:HB3	7:G:21:TYR:HE1	1.82	0.42
1:N:58:TYR:CD2	1:N:184:TYR:CE1	3.05	0.42
1:N:38:GLY:CA	16:N:1306:HOH:O	2.67	0.42
2:O:18:LEU:N	2:O:18:LEU:HD23	2.34	0.42
3:P:193:VAL:O	3:P:213:ALA:HB2	2.20	0.42
3:P:272:LEU:HA	3:P:272:LEU:HD23	1.82	0.42
6:S:6:MET:O	6:S:9:ALA:N	2.53	0.42
1:A:116:LEU:O	1:A:118:TRP:N	2.53	0.41
1:A:19:ASP:O	1:A:20:ASP:CG	2.59	0.41
1:A:31:ASN:ND2	1:A:34:TYR:CE2	2.87	0.41
1:A:36:LEU:HD13	1:A:36:LEU:N	2.35	0.41
3:C:181:THR:O	3:C:181:THR:HG22	2.20	0.41
3:C:272:LEU:HA	3:C:272:LEU:HD23	1.83	0.41
3:C:281:LYS:HD3	3:C:281:LYS:H	1.85	0.41
5:E:7:PHE:CA	5:E:10:VAL:HG12	2.38	0.41
6:F:8:TYR:O	6:F:11:LEU:HD12	2.20	0.41
6:F:5:GLU:O	6:F:8:TYR:CD2	2.73	0.41
1:N:167:ASP:N	1:N:167:ASP:OD1	2.53	0.41
1:N:206:ILE:HB	10:N:303:HEC:O1D	2.20	0.41
10:N:303:HEC:HBD2	10:N:303:HEC:CHA	2.50	0.41
1:N:42:THR:C	1:N:44:PHE:N	2.73	0.41
1:N:64:GLU:OE1	1:N:64:GLU:HA	2.20	0.41
11:O:1306:OPC:HBX2	11:O:1306:OPC:CBS	2.49	0.41
2:O:36:LEU:O	2:O:39:VAL:HG22	2.19	0.41
3:P:93:GLU:O	3:P:94:LEU:C	2.57	0.41
4:Q:63:ASN:O	4:Q:159:ASN:ND2	2.53	0.41
5:R:9:ILE:HG12	6:S:11:LEU:HA	2.01	0.41
8:U:7:VAL:O	8:U:11:VAL:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:120:PRO:HG2	3:C:124:TYR:HB2	2.01	0.41
4:D:110:HIS:ND1	4:D:111:LEU:HB2	2.35	0.41
5:E:2:ILE:HG13	5:E:3:LEU:N	2.34	0.41
6:F:22:GLY:O	6:F:23:LEU:C	2.59	0.41
6:F:24:GLY:HA2	6:F:27:LEU:CD2	2.50	0.41
1:N:110:PHE:HB2	1:N:115:GLU:HA	2.02	0.41
1:N:116:LEU:O	1:N:118:TRP:N	2.53	0.41
1:N:62:VAL:H	1:N:177:GLN:HE22	1.68	0.41
11:O:1306:OPC:HAU1	11:O:1306:OPC:OBH	2.19	0.41
2:O:133:PHE:HB2	13:O:1201:CLA:HAB	2.02	0.41
1:A:165:ILE:CD1	1:A:168:LEU:HD12	2.50	0.41
1:A:190:VAL:HB	1:A:191:LEU:HD12	2.02	0.41
1:A:203:PHE:O	1:A:206:ILE:HB	2.19	0.41
1:A:22:THR:O	1:A:23:SER:C	2.59	0.41
2:B:102:ALA:O	2:B:105:PRO:HD2	2.19	0.41
2:B:37:LEU:C	2:B:41:PRO:HD2	2.41	0.41
2:B:42:VAL:CG2	3:C:272:LEU:HD13	2.50	0.41
2:B:86:GLN:HB2	2:B:86:GLN:HE21	1.61	0.41
3:C:78:LEU:HB2	3:C:112:ASN:O	2.20	0.41
3:C:200:GLN:O	3:C:201:THR:C	2.58	0.41
3:C:90:ILE:O	3:C:91:PRO:C	2.59	0.41
4:D:110:HIS:CE1	4:D:111:LEU:HB2	2.55	0.41
5:E:6:VAL:O	5:E:6:VAL:CG1	2.68	0.41
1:N:135:GLY:CA	1:N:138:LEU:HG	2.50	0.41
1:N:44:PHE:C	1:N:46:ILE:H	2.23	0.41
1:N:74:ASN:O	1:N:75:GLU:CB	2.45	0.41
2:O:86:GLN:HB2	2:O:86:GLN:HE21	1.60	0.41
3:P:41:LEU:CD2	7:T:6:LEU:HD12	2.50	0.41
3:P:50:VAL:O	3:P:52:ILE:HG13	2.20	0.41
3:P:78:LEU:HB2	3:P:112:ASN:O	2.20	0.41
2:B:71:THR:HG1	4:Q:114:VAL:HB	1.85	0.41
6:S:20:GLY:O	6:S:21:TRP:C	2.58	0.41
1:A:36:LEU:H	1:A:36:LEU:CD2	2.07	0.41
1:A:82:ILE:HG12	4:D:41:TYR:CE1	2.55	0.41
2:B:89:ARG:CG	2:B:90:SER:N	2.65	0.41
3:C:216:GLU:HB2	3:C:233:ASN:OD1	2.20	0.41
3:C:170:ASN:HA	3:C:236:ASN:HB2	2.02	0.41
3:C:38:GLN:O	3:C:247:ILE:HG13	2.21	0.41
3:C:3:PHE:HD2	3:C:4:TRP:CZ3	2.39	0.41
3:C:84:ILE:HG23	3:C:84:ILE:O	2.21	0.41
3:C:92:GLU:HG3	3:C:94:LEU:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:9:TYR:N	3:C:9:TYR:CD1	2.88	0.41
1:N:123:ILE:CD1	1:N:123:ILE:N	2.72	0.41
1:N:40:THR:O	1:N:93:MET:HG3	2.20	0.41
1:N:82:ILE:CD1	1:N:82:ILE:N	2.84	0.41
2:O:78:GLU:C	2:O:80:TYR:N	2.65	0.41
2:O:80:TYR:N	2:O:80:TYR:CD2	2.80	0.41
3:P:216:GLU:C	3:P:217:LEU:HG	2.40	0.41
3:P:75:VAL:HG22	3:P:76:LEU:N	2.36	0.41
3:P:271:MET:HG2	4:Q:23:ALA:HA	2.03	0.41
4:Q:88:PRO:HG3	4:Q:114:VAL:CG2	2.47	0.41
2:O:79:TRP:CZ2	5:R:1:MET:HA	2.55	0.41
3:C:265:VAL:O	3:C:266:MET:C	2.58	0.41
6:F:28:LEU:CD2	6:F:31:GLN:HE22	2.34	0.41
7:G:18:TYR:O	7:G:21:TYR:CB	2.68	0.41
1:N:195:ILE:HG23	1:N:196:ALA:H	1.84	0.41
1:N:64:GLU:O	1:N:68:SER:HB3	2.19	0.41
3:P:121:GLY:C	3:P:123:GLN:N	2.71	0.41
3:P:176:ALA:N	3:P:228:GLY:HA3	2.35	0.41
3:P:53:PRO:O	3:P:54:TYR:O	2.38	0.41
5:R:23:ILE:O	5:R:25:ALA:N	2.54	0.41
1:A:132:GLY:O	1:A:133:VAL:C	2.58	0.41
1:A:24:LYS:HB2	1:A:24:LYS:HZ2	1.85	0.41
3:C:237:VAL:O	3:C:238:GLY:C	2.59	0.41
3:C:95:LYS:O	3:C:98:VAL:HG23	2.21	0.41
8:H:1:ILE:CG2	8:H:2:ASP:N	2.83	0.41
1:N:203:PHE:O	1:N:204:LEU:C	2.58	0.41
1:N:33:PHE:CG	1:N:34:TYR:N	2.89	0.41
1:N:52:PHE:O	1:N:53:ALA:C	2.58	0.41
2:O:43:VAL:O	2:O:46:GLY:N	2.53	0.41
3:P:281:LYS:HD3	3:P:281:LYS:H	1.85	0.41
3:P:83:LYS:HE3	3:P:134:PRO:CA	2.50	0.41
4:Q:121:GLU:O	4:Q:122:ASN:HB2	2.19	0.41
1:A:174:SER:CB	4:Q:86:GLY:HA3	2.50	0.41
1:A:111:LYS:HB2	1:A:114:ARG:HH22	1.78	0.41
1:A:24:LYS:HZ3	1:A:26:VAL:H	1.68	0.41
1:A:54:MET:C	1:A:56:PHE:H	2.23	0.41
4:D:141:ARG:C	4:D:142:GLY:O	2.57	0.41
1:N:118:TRP:CH2	2:O:109:ILE:HA	2.55	0.41
3:P:155:ARG:HG2	3:P:239:GLY:N	2.36	0.41
3:P:26:HIS:CE1	3:P:154:ASN:ND2	2.88	0.41
4:Q:178:TRP:HB2	4:Q:179:VAL:H	1.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:35:LEU:O	4:Q:36:TYR:C	2.58	0.41
2:B:135:PHE:O	2:B:137:THR:N	2.52	0.41
13:B:201:CLA:H41	13:B:201:CLA:H61	1.91	0.41
2:B:26:TYR:HD1	2:B:26:TYR:C	2.24	0.41
2:B:55:SER:O	2:B:59:PRO:N	2.54	0.41
3:C:272:LEU:O	3:C:276:LYS:HG2	2.21	0.41
15:E:101:BCR:H322	7:G:23:GLN:NE2	2.35	0.41
2:O:144:GLY:O	2:O:145:ILE:HD12	2.21	0.41
2:O:31:ALA:HB1	7:T:30:LEU:CB	2.40	0.41
3:P:277:LYS:NZ	3:P:278:GLN:HE22	2.19	0.41
4:Q:106:ALA:CB	4:Q:114:VAL:HG13	2.50	0.41
4:Q:20:ASN:O	4:Q:23:ALA:HB3	2.21	0.41
5:R:9:ILE:HG21	6:S:10:ALA:CA	2.51	0.41
1:A:191:LEU:C	1:A:193:TRP:N	2.74	0.41
10:A:303:HEC:HMC1	2:B:44:ILE:CG1	2.51	0.41
1:A:44:PHE:C	1:A:46:ILE:N	2.73	0.41
2:B:48:PHE:O	2:B:50:CYS:N	2.53	0.41
3:C:194:LYS:HE3	3:C:212:PRO:HB3	2.03	0.41
4:D:105:ASN:ND2	4:D:107:VAL:HB	2.36	0.41
4:D:139:VAL:HG11	4:D:144:ALA:O	2.20	0.41
5:E:9:ILE:HG21	6:F:10:ALA:CA	2.50	0.41
1:N:19:ASP:OD1	1:N:19:ASP:O	2.38	0.41
1:N:200:LEU:N	1:N:200:LEU:CD2	2.84	0.41
11:O:1306:OPC:HBR	11:O:1306:OPC:CBF	2.51	0.41
10:N:303:HEC:HMC1	2:O:44:ILE:HG12	2.02	0.41
2:O:68:PRO:CG	2:O:69:PHE:H	2.32	0.41
2:O:87:ILE:HA	2:O:90:SER:HB2	2.01	0.41
3:P:266:MET:CE	7:T:15:GLY:O	2.69	0.41
4:Q:137:GLY:O	4:Q:138:ARG:O	2.39	0.41
4:Q:141:ARG:C	4:Q:142:GLY:O	2.59	0.41
4:Q:79:VAL:O	4:Q:79:VAL:HG23	2.21	0.41
2:O:43:VAL:HG13	15:R:1101:BCR:HC22	2.03	0.41
7:T:7:GLY:C	7:T:9:VAL:N	2.74	0.41
2:B:104:VAL:H	2:B:105:PRO:CD	2.32	0.41
2:B:43:VAL:O	2:B:46:GLY:N	2.54	0.41
4:D:157:ASP:O	4:D:158:ASP:CB	2.69	0.41
4:D:66:VAL:HG13	4:D:159:ASN:O	2.21	0.41
5:E:3:LEU:HG	5:E:7:PHE:HE2	1.86	0.41
1:N:69:VAL:HA	1:N:72:ILE:CD1	2.42	0.41
2:O:101:MET:C	2:O:103:SER:H	2.24	0.41
2:O:61:MET:N	2:O:61:MET:SD	2.93	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:76:LEU:HD13	2:O:76:LEU:HA	1.89	0.41
3:P:181:THR:HG22	3:P:181:THR:O	2.21	0.41
3:P:262:ILE:O	3:P:264:LEU:N	2.54	0.41
3:P:281:LYS:N	3:P:281:LYS:CD	2.81	0.41
4:Q:70:LEU:HD12	4:Q:71:GLU:N	2.34	0.41
5:R:11:PHE:O	5:R:14:LEU:HD23	2.20	0.41
1:A:137:SER:C	1:A:139:PRO:HD2	2.42	0.41
1:A:165:ILE:HG22	1:A:166:SER:H	1.86	0.41
1:A:200:LEU:O	1:A:204:LEU:HG	2.21	0.41
1:A:51:GLY:O	1:A:52:PHE:C	2.59	0.41
1:A:81:LEU:HD11	1:A:85:ILE:HD11	2.02	0.41
1:A:82:ILE:CD1	1:A:82:ILE:N	2.84	0.41
2:B:26:TYR:CD1	2:B:26:TYR:C	2.94	0.41
3:C:25:CYS:HB3	3:C:26:HIS:H	1.56	0.41
6:F:9:ALA:O	6:F:12:LEU:HB3	2.21	0.41
1:N:115:GLU:N	1:N:115:GLU:OE1	2.54	0.41
1:N:155:PRO:C	1:N:157:ALA:H	2.23	0.41
1:N:165:ILE:C	1:N:167:ASP:N	2.75	0.41
1:A:18:ALA:CB	1:N:208:LYS:HZ1	2.34	0.41
1:N:85:ILE:O	1:N:86:HIS:C	2.60	0.41
11:O:1306:OPC:CCA	11:O:1306:OPC:HBB2	2.51	0.41
2:O:81:LEU:HA	2:O:84:VAL:HG22	2.03	0.41
3:P:101:VAL:CB	3:P:118:PRO:HB2	2.51	0.41
3:P:213:ALA:O	3:P:215:PRO:HD2	2.21	0.41
3:P:28:ALA:CB	3:P:238:GLY:C	2.88	0.41
3:P:278:GLN:C	3:P:279:VAL:HG23	2.41	0.41
3:P:160:ILE:O	9:P:301:HEM:HMD3	2.21	0.41
4:Q:130:GLY:C	4:Q:131:SER:O	2.60	0.41
4:Q:69:PHE:HA	4:Q:73:HIS:ND1	2.36	0.41
7:T:13:LEU:C	7:T:13:LEU:HD13	2.41	0.41
2:B:58:ASP:C	2:B:58:ASP:OD2	2.59	0.40
3:C:218:ILE:HD11	3:C:232:THR:HA	2.03	0.40
11:C:306:OPC:HAP1	11:C:306:OPC:HAL2	1.97	0.40
3:C:93:GLU:O	3:C:94:LEU:C	2.59	0.40
4:D:35:LEU:O	4:D:38:LEU:N	2.54	0.40
1:N:36:LEU:HD22	1:N:36:LEU:H	1.85	0.40
1:N:58:TYR:HD2	1:N:184:TYR:CE1	2.27	0.40
2:O:108:LEU:C	2:O:110:LEU:N	2.74	0.40
2:O:130:THR:O	2:O:131:THR:C	2.59	0.40
3:P:25:CYS:CA	3:P:160:ILE:HD12	2.46	0.40
3:P:172:PHE:CD1	3:P:215:PRO:HG3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:171:VAL:HG13	3:P:234:ASN:HD22	1.85	0.40
3:P:73:GLY:O	3:P:74:ALA:HB2	2.21	0.40
4:Q:35:LEU:HD21	4:Q:39:VAL:HG21	2.03	0.40
1:A:110:PHE:HB3	1:A:118:TRP:CG	2.56	0.40
1:A:120:SER:HA	1:A:123:ILE:HD13	2.04	0.40
1:A:81:LEU:O	1:A:82:ILE:C	2.57	0.40
3:C:28:ALA:CB	3:C:240:PHE:N	2.83	0.40
3:C:58:LEU:HD12	3:C:58:LEU:N	2.36	0.40
4:D:113:CYS:HG	4:D:128:CYS:CB	2.27	0.40
4:D:131:SER:OG	4:D:143:PRO:HD2	2.21	0.40
4:D:44:PRO:HA	4:D:45:PRO:HD3	1.77	0.40
4:D:73:HIS:ND1	4:D:93:VAL:CG2	2.84	0.40
5:E:23:ILE:C	5:E:25:ALA:N	2.75	0.40
7:G:16:LEU:O	7:G:16:LEU:CD2	2.63	0.40
1:N:157:ALA:O	1:N:158:ILE:HG13	2.21	0.40
1:N:174:SER:O	1:N:175:VAL:CG2	2.68	0.40
2:O:146:GLY:O	2:O:147:ALA:HB3	2.21	0.40
3:P:184:ALA:HB3	3:P:197:VAL:N	2.36	0.40
3:P:202:ASP:O	3:P:204:GLY:N	2.53	0.40
3:P:60:GLN:O	3:P:68:VAL:N	2.51	0.40
3:P:261:PHE:CZ	4:Q:34:ALA:HB2	2.57	0.40
5:R:23:ILE:C	5:R:23:ILE:CD1	2.87	0.40
1:A:81:LEU:CD1	1:A:85:ILE:HD11	2.51	0.40
2:B:133:PHE:CD2	2:B:137:THR:HG21	2.56	0.40
2:B:149:LEU:HD11	6:F:2:MET:CB	2.50	0.40
2:B:56:VAL:O	2:B:57:LEU:C	2.59	0.40
2:B:78:GLU:O	2:B:82:TYR:HE2	2.04	0.40
2:B:86:GLN:O	2:B:87:ILE:C	2.59	0.40
2:B:61:MET:CG	3:C:146:LYS:O	2.60	0.40
3:C:188:ASP:N	3:C:193:VAL:HG22	2.20	0.40
3:C:83:LYS:HZ2	3:C:83:LYS:H	1.68	0.40
1:A:82:ILE:CD1	4:D:41:TYR:CD1	3.03	0.40
6:F:21:TRP:HA	7:G:24:TYR:CD1	2.57	0.40
6:F:35:LYS:CD	6:F:35:LYS:H	2.35	0.40
7:G:17:PHE:O	7:G:20:ALA:HB3	2.20	0.40
2:O:96:LEU:CD1	2:O:100:LEU:HD12	2.51	0.40
1:N:66:TYR:CE1	2:O:63:GLY:HA3	2.57	0.40
2:O:69:PHE:HD1	2:O:69:PHE:O	2.04	0.40
3:P:194:LYS:HE3	3:P:212:PRO:HB3	2.03	0.40
3:P:231:LEU:HD13	3:P:232:THR:N	2.36	0.40
4:Q:134:ASP:HB2	4:Q:135:GLU:H	1.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:139:VAL:CG2	4:Q:144:ALA:O	2.63	0.40
4:Q:147:SER:O	4:Q:148:LEU:HG	2.22	0.40
4:Q:80:LEU:H	4:Q:80:LEU:CD2	2.34	0.40
4:Q:92:VAL:CG1	4:Q:93:VAL:N	2.84	0.40
1:A:117:THR:HG22	1:A:205:MET:SD	2.61	0.40
3:C:271:MET:HA	3:C:274:LEU:HB2	2.04	0.40
3:C:44:THR:O	3:C:133:SER:N	2.54	0.40
4:D:41:TYR:C	4:D:43:ILE:H	2.24	0.40
15:E:101:BCR:H362	6:F:18:PHE:CZ	2.57	0.40
5:E:12:ILE:HA	5:E:15:PHE:HE1	1.86	0.40
1:A:33:PHE:CZ	5:E:14:LEU:HD13	2.57	0.40
7:G:16:LEU:CD1	7:G:16:LEU:C	2.87	0.40
3:P:83:LYS:HE3	3:P:134:PRO:HG3	2.04	0.40
3:P:34:VAL:HG13	3:P:151:LEU:HD22	2.02	0.40
3:P:155:ARG:HG2	3:P:239:GLY:H	1.85	0.40
3:P:258:MET:SD	3:P:258:MET:C	2.99	0.40
3:P:54:TYR:CZ	3:P:70:LEU:HD22	2.57	0.40
4:Q:38:LEU:HD12	4:Q:38:LEU:C	2.40	0.40
5:R:23:ILE:C	5:R:25:ALA:N	2.75	0.40
1:A:162:GLY:O	1:A:165:ILE:CG2	2.69	0.40
2:B:61:MET:CE	12:B:309:BNT:HAM3	2.49	0.40
2:B:29:GLU:HA	2:B:30:PRO:HD2	1.98	0.40
2:B:40:PHE:O	2:B:44:ILE:N	2.54	0.40
3:C:144:PHE:HB3	3:C:145:GLY:H	1.41	0.40
3:C:265:VAL:HG12	3:C:269:GLN:CG	2.51	0.40
7:G:10:PHE:O	7:G:11:ALA:C	2.60	0.40
1:N:165:ILE:HG22	1:N:166:SER:N	2.33	0.40
1:N:200:LEU:O	1:N:204:LEU:N	2.45	0.40
1:N:32:ILE:O	1:N:34:TYR:CD2	2.75	0.40
3:P:2:PRO:CB	3:P:115:LEU:HD22	2.47	0.40
3:P:55:ASP:CG	3:P:57:LYS:HD2	2.41	0.40
3:P:93:GLU:HA	3:P:96:LYS:HD2	2.03	0.40
5:R:4:GLY:HA2	5:R:7:PHE:CE2	2.57	0.40
5:R:9:ILE:CG2	5:R:10:VAL:H	2.33	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	200/215 (93%)	90 (45%)	64 (32%)	46 (23%)	0	1
1	N	200/215 (93%)	92 (46%)	58 (29%)	50 (25%)	0	1
2	B	135/160 (84%)	56 (42%)	45 (33%)	34 (25%)	0	1
2	O	135/160 (84%)	52 (38%)	39 (29%)	44 (33%)	0	0
3	C	284/289 (98%)	153 (54%)	83 (29%)	48 (17%)	0	3
3	P	284/289 (98%)	153 (54%)	81 (28%)	50 (18%)	0	2
4	D	166/179 (93%)	85 (51%)	50 (30%)	31 (19%)	0	2
4	Q	166/179 (93%)	86 (52%)	49 (30%)	31 (19%)	0	2
5	E	30/32 (94%)	13 (43%)	6 (20%)	11 (37%)	0	0
5	R	30/32 (94%)	13 (43%)	6 (20%)	11 (37%)	0	0
6	F	33/35 (94%)	15 (46%)	11 (33%)	7 (21%)	0	1
6	S	33/35 (94%)	15 (46%)	12 (36%)	6 (18%)	0	2
7	G	25/37 (68%)	11 (44%)	10 (40%)	4 (16%)	0	3
7	T	25/37 (68%)	11 (44%)	10 (40%)	4 (16%)	0	3
8	H	25/29 (86%)	12 (48%)	6 (24%)	7 (28%)	0	0
8	U	25/29 (86%)	12 (48%)	6 (24%)	7 (28%)	0	0
All	All	1796/1952 (92%)	869 (48%)	536 (30%)	391 (22%)	0	1

All (391) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	20	ASP
1	A	21	VAL
1	A	22	THR
1	A	26	VAL
1	A	28	PRO

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Mol	Chain	Res	Type
1	A	29	HIS
1	A	53	ALA
1	A	65	ALA
1	A	77	SER
1	A	115	GLU
1	A	133	VAL
1	A	176	GLY
1	A	190	VAL
1	A	206	ILE
2	B	32	TRP
2	B	33	PRO
2	B	35	ASP
2	B	44	ILE
2	B	49	ALA
2	B	56	VAL
2	B	67	ASN
2	B	76	LEU
2	B	78	GLU
2	B	90	SER
2	B	93	ASN
2	B	98	VAL
2	B	126	ARG
2	B	147	ALA
3	C	53	PRO
3	C	61	VAL
3	C	89	ARG
3	C	92	GLU
3	C	193	VAL
3	C	218	ILE
3	C	225	VAL
3	C	227	ALA
3	C	242	GLN
3	C	275	LYS
3	C	276	LYS
3	C	279	VAL
4	D	49	ALA
4	D	70	LEU
4	D	98	ALA
4	D	107	VAL
4	D	124	PHE
4	D	146	LEU
4	D	161	VAL

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Mol	Chain	Res	Type
4	D	164	PRO
4	D	166	THR
5	E	3	LEU
5	E	18	ILE
5	E	19	ALA
5	E	22	ILE
5	E	23	ILE
6	F	35	LYS
8	H	3	VAL
8	H	10	LEU
1	N	16	ALA
1	N	17	LEU
1	N	20	ASP
1	N	21	VAL
1	N	30	VAL
1	N	32	ILE
1	N	33	PHE
1	N	34	TYR
1	N	53	ALA
1	N	62	VAL
1	N	75	GLU
1	N	77	SER
1	N	133	VAL
1	N	160	VAL
1	N	163	VAL
1	N	174	SER
1	N	190	VAL
1	N	206	ILE
1	N	209	GLN
1	N	211	ILE
2	O	26	TYR
2	O	30	PRO
2	O	33	PRO
2	O	35	ASP
2	O	44	ILE
2	O	49	ALA
2	O	64	GLU
2	O	65	PRO
2	O	71	THR
2	O	75	ILE
2	O	77	PRO
2	O	79	TRP

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Mol	Chain	Res	Type
2	O	90	SER
2	O	93	ASN
2	O	98	VAL
2	O	117	VAL
2	O	118	ASN
2	O	125	ARG
2	O	127	PRO
2	O	153	LYS
3	P	53	PRO
3	P	61	VAL
3	P	89	ARG
3	P	193	VAL
3	P	218	ILE
3	P	225	VAL
3	P	227	ALA
3	P	242	GLN
3	P	275	LYS
3	P	276	LYS
3	P	279	VAL
4	Q	44	PRO
4	Q	70	LEU
4	Q	98	ALA
4	Q	107	VAL
4	Q	124	PHE
4	Q	138	ARG
4	Q	146	LEU
4	Q	161	VAL
4	Q	164	PRO
4	Q	166	THR
5	R	3	LEU
5	R	18	ILE
5	R	19	ALA
5	R	22	ILE
5	R	23	ILE
8	U	3	VAL
8	U	10	LEU
1	A	17	LEU
1	A	35	CYS
1	A	43	CYS
1	A	64	GLU
1	A	90	ALA
1	A	104	VAL

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Mol	Chain	Res	Type
1	A	145	TYR
1	A	160	VAL
1	A	168	LEU
2	B	30	PRO
2	B	39	VAL
2	B	43	VAL
2	B	62	VAL
2	B	75	ILE
2	B	105	PRO
2	B	128	VAL
2	B	135	PHE
3	C	4	TRP
3	C	26	HIS
3	C	54	TYR
3	C	62	ALA
3	C	91	PRO
3	C	97	GLU
3	C	110	GLN
3	C	122	GLU
3	C	155	ARG
3	C	169	ASN
3	C	184	ALA
3	C	216	GLU
3	C	263	CYS
4	D	20	ASN
4	D	35	LEU
4	D	45	PRO
4	D	46	SER
4	D	138	ARG
4	D	159	ASN
4	D	176	PRO
5	E	11	PHE
6	F	10	ALA
6	F	29	LYS
7	G	11	ALA
8	H	9	LEU
1	N	15	GLN
1	N	28	PRO
1	N	36	LEU
1	N	43	CYS
1	N	64	GLU
1	N	73	MET

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Mol	Chain	Res	Type
1	N	90	ALA
1	N	91	SER
1	N	104	VAL
1	N	112	LYS
1	N	145	TYR
1	N	159	PRO
1	N	168	LEU
2	O	19	ALA
2	O	23	GLY
2	O	39	VAL
2	O	43	VAL
2	O	105	PRO
2	O	121	GLN
2	O	128	VAL
2	O	135	PHE
2	O	146	GLY
2	O	151	LEU
3	P	4	TRP
3	P	26	HIS
3	P	54	TYR
3	P	66	SER
3	P	91	PRO
3	P	92	GLU
3	P	97	GLU
3	P	110	GLN
3	P	155	ARG
3	P	184	ALA
3	P	190	TYR
3	P	196	GLN
3	P	216	GLU
4	Q	20	ASN
4	Q	35	LEU
4	Q	52	GLY
4	Q	159	ASN
4	Q	176	PRO
5	R	11	PHE
5	R	25	ALA
6	S	10	ALA
6	S	29	LYS
7	T	11	ALA
7	T	27	PRO
7	T	29	GLU

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Mol	Chain	Res	Type
8	U	9	LEU
8	U	11	VAL
1	A	74	ASN
1	A	78	PHE
1	A	91	SER
1	A	166	SER
2	B	69	PHE
2	B	81	LEU
2	B	99	LEU
3	C	29	ALA
3	C	32	ALA
3	C	48	ALA
3	C	66	SER
3	C	170	ASN
3	C	190	TYR
3	C	223	GLN
3	C	269	GLN
4	D	85	LYS
4	D	145	PRO
4	D	147	SER
5	E	24	PHE
5	E	25	ALA
6	F	4	GLU
6	F	11	LEU
6	F	12	LEU
7	G	28	ASN
8	H	5	GLY
8	H	11	VAL
1	N	25	TYR
1	N	83	ARG
1	N	111	LYS
1	N	158	ILE
2	O	20	LYS
2	O	73	LEU
2	O	99	LEU
2	O	152	ASP
3	P	29	ALA
3	P	32	ALA
3	P	48	ALA
3	P	62	ALA
3	P	69	GLY
3	P	122	GLU

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Mol	Chain	Res	Type
3	P	127	ILE
3	P	169	ASN
3	P	176	ALA
3	P	192	ASN
3	P	223	GLN
3	P	263	CYS
3	P	269	GLN
4	Q	19	MET
4	Q	57	LYS
4	Q	64	VAL
4	Q	106	ALA
4	Q	145	PRO
4	Q	147	SER
5	R	24	PHE
6	S	4	GLU
6	S	12	LEU
8	U	2	ASP
8	U	5	GLY
1	A	34	TYR
1	A	42	THR
1	A	49	ALA
1	A	76	VAL
1	A	83	ARG
1	A	177	GLN
1	A	211	ILE
2	B	52	VAL
2	B	86	GLN
3	C	69	GLY
3	C	127	ILE
3	C	173	THR
3	C	176	ALA
3	C	186	GLU
3	C	192	ASN
3	C	196	GLN
4	D	19	MET
4	D	51	GLY
4	D	57	LYS
4	D	64	VAL
4	D	97	GLU
4	D	106	ALA
4	D	119	ALA
5	E	7	PHE

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Mol	Chain	Res	Type
7	G	27	PRO
8	H	2	ASP
1	N	42	THR
1	N	49	ALA
1	N	105	TYR
1	N	166	SER
1	N	173	SER
1	N	179	THR
2	O	86	GLN
2	O	149	LEU
3	P	94	LEU
3	P	173	THR
3	P	186	GLU
3	P	199	ILE
4	Q	85	LYS
5	R	7	PHE
6	S	11	LEU
1	A	19	ASP
1	A	80	TRP
1	A	178	ALA
1	A	179	THR
2	B	64	GLU
2	B	68	PRO
2	B	87	ILE
2	B	114	ILE
3	C	68	VAL
3	C	199	ILE
4	D	87	ASP
4	D	112	GLY
1	N	18	ALA
1	N	23	SER
1	N	147	ALA
2	O	32	TRP
2	O	76	LEU
2	O	114	ILE
3	P	34	VAL
4	Q	15	ARG
4	Q	45	PRO
4	Q	87	ASP
4	Q	112	GLY
4	Q	131	SER
4	Q	158	ASP

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Mol	Chain	Res	Type
6	S	19	VAL
8	U	16	SER
1	A	30	VAL
1	A	147	ALA
2	B	71	THR
3	C	18	GLY
3	C	34	VAL
3	C	144	PHE
4	D	158	ASP
4	D	173	GLY
6	F	19	VAL
8	H	16	SER
1	N	26	VAL
2	O	68	PRO
2	O	87	ILE
2	O	134	LEU
3	P	25	CYS
3	P	68	VAL
3	P	144	PHE
3	P	226	LYS
3	P	266	MET
4	Q	28	THR
4	Q	173	GLY
1	A	112	LYS
2	B	122	ASN
1	N	14	ILE
3	P	18	GLY
3	P	238	GLY
2	B	149	LEU
2	O	21	GLY
1	A	122	VAL
5	E	4	GLY
7	G	9	VAL
1	N	122	VAL
2	O	123	PRO
5	R	4	GLY
1	A	132	GLY
1	A	197	VAL
3	C	120	PRO
3	C	238	GLY
4	D	29	GLY
1	N	197	VAL

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Mol	Chain	Res	Type
4	Q	29	GLY
5	R	20	VAL
7	T	9	VAL
1	A	161	VAL
3	C	191	GLY
5	E	20	VAL
3	P	21	VAL

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	172/184 (94%)	145 (84%)	27 (16%)	2 17
1	N	172/184 (94%)	141 (82%)	31 (18%)	1 12
2	B	116/136 (85%)	99 (85%)	17 (15%)	3 19
2	O	116/136 (85%)	92 (79%)	24 (21%)	1 8
3	C	240/243 (99%)	198 (82%)	42 (18%)	2 13
3	P	240/243 (99%)	199 (83%)	41 (17%)	2 14
4	D	136/146 (93%)	110 (81%)	26 (19%)	1 10
4	Q	136/146 (93%)	110 (81%)	26 (19%)	1 10
5	E	25/25 (100%)	22 (88%)	3 (12%)	5 25
5	R	25/25 (100%)	22 (88%)	3 (12%)	5 25
6	F	27/27 (100%)	23 (85%)	4 (15%)	3 19
6	S	27/27 (100%)	22 (82%)	5 (18%)	1 11
7	G	21/28 (75%)	15 (71%)	6 (29%)	0 2
7	T	21/28 (75%)	14 (67%)	7 (33%)	0 1
8	H	22/24 (92%)	20 (91%)	2 (9%)	9 36
8	U	22/24 (92%)	20 (91%)	2 (9%)	9 36
All	All	1518/1626 (93%)	1252 (82%)	266 (18%)	2 13

All (266) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	GLU
1	A	24	LYS
1	A	26	VAL
1	A	29	HIS
1	A	33	PHE
1	A	35	CYS
1	A	36	LEU
1	A	52	PHE
1	A	71	TYR
1	A	83	ARG
1	A	95	LEU
1	A	99	LEU
1	A	103	ARG
1	A	112	LYS
1	A	114	ARG
1	A	116	LEU
1	A	134	THR
1	A	140	TRP
1	A	145	TYR
1	A	149	LYS
1	A	150	ILE
1	A	165	ILE
1	A	167	ASP
1	A	170	ARG
1	A	177	GLN
1	A	185	SER
1	A	193	TRP
2	B	26	TYR
2	B	27	TYR
2	B	32	TRP
2	B	33	PRO
2	B	47	THR
2	B	48	PHE
2	B	61	MET
2	B	76	LEU
2	B	86	GLN
2	B	106	LEU
2	B	115	GLU
2	B	116	ASN
2	B	120	PHE
2	B	124	PHE
2	B	125	ARG
2	B	132	ILE

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Mol	Chain	Res	Type
2	B	135	PHE
3	C	3	PHE
3	C	4	TRP
3	C	6	GLN
3	C	9	TYR
3	C	20	ILE
3	C	25	CYS
3	C	35	GLU
3	C	51	LYS
3	C	54	TYR
3	C	55	ASP
3	C	70	LEU
3	C	80	GLU
3	C	83	LYS
3	C	91	PRO
3	C	93	GLU
3	C	97	GLU
3	C	104	GLN
3	C	123	GLN
3	C	126	GLU
3	C	151	LEU
3	C	168	ASN
3	C	169	ASN
3	C	171	VAL
3	C	180	ILE
3	C	182	LYS
3	C	187	GLU
3	C	202	ASP
3	C	205	LYS
3	C	206	THR
3	C	216	GLU
3	C	221	GLU
3	C	231	LEU
3	C	233	ASN
3	C	249	LEU
3	C	253	ASN
3	C	257	TRP
3	C	258	MET
3	C	266	MET
3	C	269	GLN
3	C	271	MET
3	C	280	GLU

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Mol	Chain	Res	Type
3	C	283	GLN
4	D	12	ASP
4	D	13	MET
4	D	15	ARG
4	D	17	GLN
4	D	22	LEU
4	D	41	TYR
4	D	63	ASN
4	D	69	PHE
4	D	70	LEU
4	D	72	SER
4	D	82	GLN
4	D	84	LEU
4	D	90	TYR
4	D	99	ILE
4	D	101	ASP
4	D	102	TYR
4	D	105	ASN
4	D	118	ASN
4	D	134	ASP
4	D	152	HIS
4	D	165	TRP
4	D	166	THR
4	D	170	PHE
4	D	171	ARG
4	D	172	THR
4	D	178	TRP
5	E	2	ILE
5	E	11	PHE
5	E	22	ILE
6	F	6	MET
6	F	8	TYR
6	F	11	LEU
6	F	27	LEU
7	G	6	LEU
7	G	16	LEU
7	G	17	PHE
7	G	21	TYR
7	G	26	ARG
7	G	29	GLU
8	H	19	MET
8	H	25	ASN

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Mol	Chain	Res	Type
1	N	15	GLN
1	N	17	LEU
1	N	21	VAL
1	N	24	LYS
1	N	25	TYR
1	N	29	HIS
1	N	34	TYR
1	N	62	VAL
1	N	71	TYR
1	N	75	GLU
1	N	83	ARG
1	N	95	LEU
1	N	99	LEU
1	N	103	ARG
1	N	110	PHE
1	N	114	ARG
1	N	115	GLU
1	N	116	LEU
1	N	134	THR
1	N	141	ASP
1	N	145	TYR
1	N	149	LYS
1	N	150	ILE
1	N	161	VAL
1	N	165	ILE
1	N	167	ASP
1	N	170	ARG
1	N	185	SER
1	N	193	TRP
1	N	208	LYS
1	N	211	ILE
2	O	20	LYS
2	O	24	HIS
2	O	32	TRP
2	O	33	PRO
2	O	47	THR
2	O	48	PHE
2	O	61	MET
2	O	65	PRO
2	O	69	PHE
2	O	73	LEU
2	O	77	PRO

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Mol	Chain	Res	Type
2	O	80	TYR
2	O	86	GLN
2	O	106	LEU
2	O	115	GLU
2	O	116	ASN
2	O	120	PHE
2	O	125	ARG
2	O	127	PRO
2	O	132	ILE
2	O	135	PHE
2	O	145	ILE
2	O	152	ASP
2	O	154	THR
3	P	3	PHE
3	P	4	TRP
3	P	6	GLN
3	P	9	TYR
3	P	20	ILE
3	P	25	CYS
3	P	35	GLU
3	P	51	LYS
3	P	54	TYR
3	P	55	ASP
3	P	70	LEU
3	P	80	GLU
3	P	83	LYS
3	P	91	PRO
3	P	93	GLU
3	P	97	GLU
3	P	104	GLN
3	P	123	GLN
3	P	126	GLU
3	P	151	LEU
3	P	168	ASN
3	P	169	ASN
3	P	171	VAL
3	P	180	ILE
3	P	182	LYS
3	P	202	ASP
3	P	205	LYS
3	P	206	THR
3	P	216	GLU

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Mol	Chain	Res	Type
3	P	221	GLU
3	P	231	LEU
3	P	233	ASN
3	P	249	LEU
3	P	253	ASN
3	P	257	TRP
3	P	258	MET
3	P	266	MET
3	P	269	GLN
3	P	271	MET
3	P	280	GLU
3	P	283	GLN
4	Q	12	ASP
4	Q	13	MET
4	Q	17	GLN
4	Q	22	LEU
4	Q	41	TYR
4	Q	50	VAL
4	Q	63	ASN
4	Q	69	PHE
4	Q	70	LEU
4	Q	72	SER
4	Q	82	GLN
4	Q	84	LEU
4	Q	90	TYR
4	Q	99	ILE
4	Q	101	ASP
4	Q	102	TYR
4	Q	105	ASN
4	Q	118	ASN
4	Q	134	ASP
4	Q	152	HIS
4	Q	165	TRP
4	Q	166	THR
4	Q	170	PHE
4	Q	171	ARG
4	Q	172	THR
4	Q	178	TRP
5	R	2	ILE
5	R	11	PHE
5	R	22	ILE
6	S	6	MET

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Mol	Chain	Res	Type
6	S	8	TYR
6	S	11	LEU
6	S	27	LEU
6	S	36	GLU
7	T	6	LEU
7	T	16	LEU
7	T	17	PHE
7	T	21	TYR
7	T	26	ARG
7	T	28	ASN
7	T	30	LEU
8	U	19	MET
8	U	25	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (60) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	31	ASN
1	A	47	GLN
1	A	74	ASN
1	A	142	GLN
1	A	209	GLN
2	B	25	ASN
2	B	34	ASN
2	B	86	GLN
2	B	116	ASN
2	B	122	ASN
3	C	6	GLN
3	C	7	GLN
3	C	24	ASN
3	C	104	GLN
3	C	125	GLN
3	C	154	ASN
3	C	168	ASN
3	C	169	ASN
3	C	196	GLN
3	C	233	ASN
3	C	234	ASN
3	C	242	GLN
4	D	17	GLN
4	D	63	ASN

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Mol	Chain	Res	Type
4	D	82	GLN
4	D	105	ASN
4	D	118	ASN
4	D	122	ASN
4	D	132	GLN
4	D	159	ASN
6	F	31	GLN
7	G	23	GLN
1	N	15	GLN
1	N	31	ASN
1	N	47	GLN
1	N	209	GLN
2	O	34	ASN
2	O	116	ASN
3	P	6	GLN
3	P	7	GLN
3	P	104	GLN
3	P	125	GLN
3	P	154	ASN
3	P	168	ASN
3	P	169	ASN
3	P	196	GLN
3	P	233	ASN
3	P	234	ASN
3	P	242	GLN
4	Q	17	GLN
4	Q	63	ASN
4	Q	82	GLN
4	Q	105	ASN
4	Q	118	ASN
4	Q	122	ASN
4	Q	132	GLN
4	Q	159	ASN
6	S	31	GLN
7	T	28	ASN

5.3.3 RNA

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 carbohydrates in this entry.

5.6 Ligand geometry (i)

20 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	$\#\|Z\| > 2$
14	FES	Q	201	4	0,4,4	0.00	-	-		
15	BCR	E	101	-	41,41,41	2.54	16 (39%)	56,56,56	2.38	21 (37%)
11	OPC	B	305	-	53,53,54	1.32	8 (15%)	59,61,64	1.08	3 (5%)
13	CLA	O	1201	-	59,73,73	2.17	20 (33%)	67,113,113	2.24	18 (26%)
13	CLA	B	201	-	59,73,73	2.19	15 (25%)	67,113,113	2.25	19 (28%)
11	OPC	C	306	-	53,53,54	1.33	8 (15%)	59,61,64	1.19	4 (6%)
9	HEM	N	302	1	27,50,50	2.04	8 (29%)	17,82,82	4.84	8 (47%)
9	HEM	P	301	3	27,50,50	1.81	6 (22%)	17,82,82	2.86	9 (52%)
9	HEM	C	301	3	27,50,50	1.80	4 (14%)	17,82,82	2.79	7 (41%)
9	HEM	N	301	1	27,50,50	1.86	8 (29%)	17,82,82	3.18	9 (52%)
10	HEC	A	303	1,16	26,50,50	2.29	10 (38%)	18,82,82	2.58	9 (50%)
12	BNT	B	309	-	13,14,14	3.22	6 (46%)	15,21,21	1.61	3 (20%)
9	HEM	A	302	1	27,50,50	1.94	9 (33%)	17,82,82	4.48	8 (47%)
12	BNT	O	1309	-	13,14,14	3.38	6 (46%)	15,21,21	1.51	2 (13%)
11	OPC	N	1305	-	53,53,54	1.33	8 (15%)	59,61,64	1.16	5 (8%)
10	HEC	N	303	1,16	26,50,50	2.19	10 (38%)	18,82,82	3.36	9 (50%)
15	BCR	R	1101	-	41,41,41	2.61	16 (39%)	56,56,56	2.38	22 (39%)
14	FES	D	201	4	0,4,4	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
11	OPC	O	1306	-	53,53,54	1.33	8 (15%)	59,61,64	1.11	4 (6%)
9	HEM	A	301	1	27,50,50	1.99	7 (25%)	17,82,82	2.93	8 (47%)

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
14	FES	Q	201	4	-	-	0/1/1/1
15	BCR	E	101	-	-	7/29/63/63	0/2/2/2
11	OPC	B	305	-	-	11/57/57/60	-
14	FES	D	201	4	-	-	0/1/1/1
13	CLA	O	1201	-	6/6/20/25	14/37/135/135	-
13	CLA	B	201	-	6/6/20/25	10/37/135/135	-
11	OPC	C	306	-	-	11/57/57/60	-
9	HEM	N	302	1	-	2/6/54/54	-
9	HEM	P	301	3	-	0/6/54/54	-
9	HEM	C	301	3	-	0/6/54/54	-
9	HEM	N	301	1	-	0/6/54/54	-
10	HEC	A	303	1,16	-	4/6/54/54	-
12	BNT	B	309	-	-	0/4/28/28	0/1/1/1
9	HEM	A	302	1	-	2/6/54/54	-
11	OPC	N	1305	-	-	17/57/57/60	-
10	HEC	N	303	1,16	-	2/6/54/54	-
15	BCR	R	1101	-	-	7/29/63/63	0/2/2/2
12	BNT	O	1309	-	-	0/4/28/28	0/1/1/1
11	OPC	O	1306	-	-	15/57/57/60	-
9	HEM	A	301	1	-	0/6/54/54	-

All (173) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	O	1309	BNT	CAD-CAE	-9.68	1.39	1.52
12	B	309	BNT	CAD-CAE	-8.92	1.40	1.52
15	R	1101	BCR	C30-C25	7.70	1.64	1.53
13	O	1201	CLA	C3A-C2A	-6.94	1.35	1.54
13	B	201	CLA	C3A-C2A	-6.50	1.36	1.54
15	E	101	BCR	C30-C25	6.41	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	B	201	CLA	C1C-C2C	6.34	1.56	1.44
10	A	303	HEC	C3B-C2B	-6.27	1.34	1.40
15	E	101	BCR	C26-C25	6.21	1.45	1.34
15	R	1101	BCR	C1-C6	6.10	1.62	1.53
9	A	301	HEM	C1C-C2C	6.08	1.56	1.42
13	B	201	CLA	C4C-C3C	6.08	1.55	1.45
13	O	1201	CLA	C1C-C2C	5.93	1.56	1.44
10	N	303	HEC	C3B-C2B	-5.87	1.34	1.40
15	E	101	BCR	C1-C6	5.84	1.61	1.53
15	R	1101	BCR	C26-C25	5.82	1.44	1.34
9	N	302	HEM	C1C-C2C	5.47	1.55	1.42
9	N	301	HEM	C1C-C2C	5.46	1.54	1.42
9	C	301	HEM	C1C-C2C	5.43	1.54	1.42
12	O	1309	BNT	CAM-CAL	-5.33	1.39	1.50
12	B	309	BNT	CAM-CAL	-5.29	1.39	1.50
13	O	1201	CLA	O2D-CGD	5.14	1.45	1.33
13	B	201	CLA	O2D-CGD	5.13	1.45	1.33
9	P	301	HEM	C1C-C2C	5.07	1.54	1.42
13	O	1201	CLA	C4C-C3C	5.00	1.53	1.45
9	A	302	HEM	C1C-C2C	4.78	1.53	1.42
9	C	301	HEM	C3C-CAC	4.65	1.57	1.47
15	R	1101	BCR	C2-C1	4.21	1.63	1.54
15	E	101	BCR	C10-C9	4.20	1.41	1.35
9	A	302	HEM	C3C-C2C	-4.15	1.34	1.40
10	N	303	HEC	C3C-C2C	-4.10	1.36	1.40
13	O	1201	CLA	MG-NA	-4.08	1.96	2.06
9	A	301	HEM	CAD-C3D	-4.05	1.45	1.52
15	R	1101	BCR	C10-C9	4.03	1.41	1.35
15	E	101	BCR	C29-C30	3.99	1.63	1.54
15	R	1101	BCR	C29-C30	3.95	1.63	1.54
15	R	1101	BCR	C5-C6	3.88	1.41	1.34
13	O	1201	CLA	C4B-NB	3.86	1.38	1.35
11	N	1305	OPC	CAV-CAW	3.79	1.53	1.31
13	B	201	CLA	O2A-CGA	3.78	1.44	1.33
11	C	306	OPC	CAV-CAW	3.77	1.53	1.31
9	N	301	HEM	CAD-C3D	-3.76	1.45	1.52
11	O	1306	OPC	CAV-CAW	3.75	1.53	1.31
11	B	305	OPC	CAV-CAW	3.74	1.53	1.31
9	P	301	HEM	C3C-CAC	3.71	1.55	1.47
15	E	101	BCR	C2-C1	3.68	1.62	1.54
11	O	1306	OPC	CAL-CAM	-3.65	1.39	1.50
11	B	305	OPC	CAL-CAM	-3.65	1.39	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	E	101	BCR	C38-C26	3.63	1.56	1.50
11	C	306	OPC	CAL-CAM	-3.57	1.39	1.50
10	A	303	HEC	C4A-C3A	3.57	1.50	1.42
10	A	303	HEC	C3C-C2C	-3.57	1.37	1.40
9	N	302	HEM	C3C-CAC	3.56	1.55	1.47
11	N	1305	OPC	CAL-CAM	-3.56	1.39	1.50
13	B	201	CLA	CBC-CAC	-3.53	1.35	1.51
10	N	303	HEC	C3B-C4B	3.53	1.49	1.43
9	N	302	HEM	CAA-C2A	-3.52	1.46	1.52
11	N	1305	OPC	CAQ-CAP	-3.49	1.39	1.52
13	O	1201	CLA	CBC-CAC	-3.45	1.36	1.51
9	A	301	HEM	C3C-CAC	3.44	1.54	1.47
15	E	101	BCR	C5-C6	3.43	1.40	1.34
11	B	305	OPC	CAQ-CAP	-3.42	1.39	1.52
11	C	306	OPC	CAQ-CAP	-3.41	1.39	1.52
11	O	1306	OPC	CAQ-CAP	-3.40	1.39	1.52
15	E	101	BCR	C17-C18	3.38	1.40	1.35
10	A	303	HEC	CMD-C2D	3.34	1.58	1.51
15	E	101	BCR	C14-C13	3.34	1.40	1.35
13	B	201	CLA	C2-C3	3.33	1.41	1.33
13	B	201	CLA	O1D-CGD	3.32	1.29	1.21
15	R	1101	BCR	C38-C26	3.31	1.56	1.50
9	A	302	HEM	CAD-C3D	-3.31	1.46	1.52
10	A	303	HEC	C3B-C4B	3.29	1.49	1.43
9	N	302	HEM	C3C-C2C	-3.27	1.35	1.40
10	N	303	HEC	C4A-C3A	3.26	1.50	1.42
13	O	1201	CLA	C3B-C2B	-3.25	1.35	1.40
11	O	1306	OPC	CAY-CAX	-3.22	1.39	1.52
11	N	1305	OPC	CAY-CAX	-3.22	1.39	1.52
11	B	305	OPC	CAY-CAX	-3.22	1.39	1.52
11	C	306	OPC	CAY-CAX	-3.20	1.39	1.52
9	N	302	HEM	C4D-C3D	3.19	1.49	1.42
9	A	302	HEM	CAA-C2A	-3.16	1.47	1.52
9	N	302	HEM	C3B-C2B	-3.15	1.36	1.40
13	B	201	CLA	MG-NC	3.06	2.13	2.06
10	A	303	HEC	C1B-NB	2.98	1.42	1.36
13	B	201	CLA	C4B-NB	2.93	1.37	1.35
13	B	201	CLA	C1B-NB	2.93	1.37	1.35
9	P	301	HEM	CAA-C2A	2.91	1.56	1.52
10	A	303	HEC	CAA-C2A	2.88	1.57	1.52
13	O	1201	CLA	O2A-CGA	2.87	1.41	1.33
12	O	1309	BNT	CAL-CAG	2.87	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	O	1201	CLA	C2-C3	2.84	1.39	1.33
9	N	301	HEM	C1A-CHA	-2.84	1.33	1.41
13	B	201	CLA	CAC-C3C	2.79	1.58	1.51
9	A	301	HEM	C3B-C2B	-2.75	1.36	1.40
15	E	101	BCR	C8-C9	2.75	1.51	1.45
15	R	1101	BCR	C21-C22	2.73	1.39	1.35
9	A	302	HEM	C4D-C3D	2.71	1.48	1.42
9	A	302	HEM	C3B-C2B	-2.71	1.36	1.40
15	R	1101	BCR	C14-C13	2.70	1.39	1.35
10	N	303	HEC	CMD-C2D	2.69	1.57	1.51
9	P	301	HEM	C3B-C2B	-2.65	1.36	1.40
12	B	309	BNT	CAL-CAG	2.65	1.39	1.35
9	A	301	HEM	C3C-C2C	-2.65	1.36	1.40
15	R	1101	BCR	C8-C9	2.64	1.51	1.45
13	O	1201	CLA	C3D-C2D	-2.63	1.34	1.39
12	B	309	BNT	CAE-CAF	-2.60	1.39	1.47
15	R	1101	BCR	C17-C18	2.60	1.39	1.35
10	N	303	HEC	C1B-NB	2.59	1.41	1.36
13	B	201	CLA	CBA-CGA	2.58	1.58	1.50
13	O	1201	CLA	MG-NC	2.57	2.12	2.06
13	O	1201	CLA	O1D-CGD	2.56	1.27	1.21
15	R	1101	BCR	C24-C23	2.52	1.40	1.33
9	A	302	HEM	C3C-CAC	2.52	1.53	1.47
9	A	301	HEM	C1A-CHA	-2.51	1.34	1.41
15	R	1101	BCR	C7-C6	2.50	1.54	1.45
9	N	301	HEM	C3C-C2C	-2.50	1.36	1.40
9	N	302	HEM	CAD-C3D	-2.50	1.47	1.52
9	N	301	HEM	C3C-CAC	2.49	1.52	1.47
13	O	1201	CLA	CHC-C1C	2.48	1.41	1.35
15	E	101	BCR	C24-C23	2.43	1.40	1.33
10	A	303	HEC	CAD-C3D	-2.42	1.48	1.52
10	N	303	HEC	CAA-C2A	2.42	1.56	1.52
10	A	303	HEC	C1D-ND	2.40	1.41	1.36
9	P	301	HEM	C3C-C2C	-2.39	1.37	1.40
15	E	101	BCR	C7-C6	2.39	1.53	1.45
12	O	1309	BNT	CAE-CAF	-2.39	1.40	1.47
10	N	303	HEC	CBB-CAB	2.38	1.58	1.49
15	R	1101	BCR	C33-C5	2.34	1.54	1.50
9	N	301	HEM	CMA-C3A	2.32	1.56	1.51
15	E	101	BCR	C21-C22	2.31	1.38	1.35
13	B	201	CLA	C5-C3	2.29	1.56	1.51
9	N	302	HEM	C4A-CHB	-2.28	1.34	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	309	BNT	CAK-CAJ	2.28	1.54	1.46
9	C	301	HEM	C3B-C2B	-2.25	1.37	1.40
9	P	301	HEM	C4D-C3D	2.25	1.47	1.42
13	B	201	CLA	MG-NA	2.24	2.11	2.06
13	O	1201	CLA	C4-C3	2.22	1.56	1.50
15	R	1101	BCR	C8-C7	2.21	1.39	1.33
9	N	301	HEM	CAA-C2A	2.21	1.55	1.52
10	A	303	HEC	CBB-CAB	2.21	1.57	1.49
10	N	303	HEC	C1D-ND	2.21	1.40	1.36
13	O	1201	CLA	C3D-CAD	-2.18	1.40	1.46
11	N	1305	OPC	CAQ-CAR	-2.18	1.39	1.51
9	N	301	HEM	C3B-C2B	-2.18	1.37	1.40
10	N	303	HEC	C1B-CHB	-2.17	1.35	1.41
11	O	1306	OPC	OAK-CAL	-2.17	1.36	1.44
11	B	305	OPC	CBP-CBO	-2.17	1.39	1.51
13	O	1201	CLA	C5-C3	2.16	1.55	1.51
11	B	305	OPC	CBO-CBN	-2.16	1.39	1.51
9	C	301	HEM	C4D-C3D	2.15	1.47	1.42
11	O	1306	OPC	CBP-CBO	-2.15	1.39	1.51
11	C	306	OPC	CBO-CBN	-2.15	1.39	1.51
9	A	302	HEM	C4A-CHB	-2.15	1.35	1.41
11	O	1306	OPC	CBO-CBN	-2.14	1.39	1.51
12	O	1309	BNT	CAK-CAJ	2.14	1.53	1.46
11	N	1305	OPC	CBO-CBN	-2.13	1.39	1.51
11	C	306	OPC	CBP-CBO	-2.13	1.39	1.51
11	O	1306	OPC	CAQ-CAR	-2.13	1.39	1.51
11	C	306	OPC	OAK-CAL	-2.13	1.36	1.44
13	O	1201	CLA	CAC-C3C	2.13	1.56	1.51
11	N	1305	OPC	CBP-CBO	-2.13	1.39	1.51
9	A	302	HEM	CMA-C3A	2.13	1.56	1.51
11	B	305	OPC	CAQ-CAR	-2.13	1.39	1.51
11	B	305	OPC	OAK-CAL	-2.12	1.36	1.44
11	C	306	OPC	CAQ-CAR	-2.12	1.39	1.51
15	E	101	BCR	C8-C7	2.08	1.39	1.33
11	N	1305	OPC	OAK-CAL	-2.07	1.36	1.44
13	O	1201	CLA	CBD-CHA	2.06	1.62	1.52
12	O	1309	BNT	CAL-CAK	-2.06	1.39	1.47
13	O	1201	CLA	C1C-NC	2.05	1.40	1.37
15	E	101	BCR	C33-C5	2.01	1.54	1.50
12	B	309	BNT	CAL-CAK	-2.01	1.40	1.47
9	A	301	HEM	CMA-C3A	2.01	1.55	1.51

All (168) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	N	302	HEM	CBA-CAA-C2A	-12.78	88.92	112.49
9	A	302	HEM	CBA-CAA-C2A	-12.01	90.33	112.49
9	N	302	HEM	CAA-CBA-CGA	10.63	130.51	112.67
10	N	303	HEC	CAA-CBA-CGA	8.63	127.15	112.67
9	A	302	HEM	CAA-CBA-CGA	8.47	126.88	112.67
9	A	301	HEM	CMA-C3A-C4A	-7.93	116.28	128.46
9	A	302	HEM	CMA-C3A-C4A	-7.62	116.75	128.46
9	P	301	HEM	CMA-C3A-C4A	-7.58	116.82	128.46
9	N	302	HEM	CMA-C3A-C4A	-7.57	116.83	128.46
9	C	301	HEM	CMA-C3A-C4A	-7.49	116.96	128.46
9	N	301	HEM	CMA-C3A-C4A	-7.45	117.02	128.46
13	B	201	CLA	C4A-NA-C1A	7.42	110.04	106.71
13	B	201	CLA	CAA-C2A-C3A	7.23	132.57	112.78
15	R	1101	BCR	C38-C26-C25	6.98	132.36	124.53
15	E	101	BCR	C38-C26-C25	6.92	132.29	124.53
13	O	1201	CLA	C4D-C3D-CAD	6.65	112.18	108.47
13	O	1201	CLA	CAA-C2A-C3A	6.61	130.87	112.78
11	C	306	OPC	OAN-CAO-CAP	5.94	124.31	111.50
10	A	303	HEC	CAA-CBA-CGA	5.92	122.60	112.67
13	O	1201	CLA	C4A-NA-C1A	5.87	109.34	106.71
11	O	1306	OPC	OAN-CAO-CAP	5.69	123.76	111.50
11	N	1305	OPC	OAN-CAO-CAP	5.68	123.75	111.50
9	N	302	HEM	CMA-C3A-C2A	5.58	135.47	124.94
9	A	301	HEM	CMA-C3A-C2A	5.57	135.44	124.94
9	A	302	HEM	CMA-C3A-C2A	5.51	135.34	124.94
9	N	301	HEM	CAA-CBA-CGA	5.39	121.72	112.67
13	B	201	CLA	CBC-CAC-C3C	5.28	127.00	112.43
13	O	1201	CLA	CMA-C3A-C2A	5.25	135.01	113.83
11	B	305	OPC	OAN-CAO-CAP	5.25	122.81	111.50
9	C	301	HEM	CMA-C3A-C2A	5.23	134.81	124.94
9	P	301	HEM	CMA-C3A-C2A	5.19	134.72	124.94
9	N	301	HEM	CMA-C3A-C2A	5.15	134.66	124.94
10	A	303	HEC	CMD-C2D-C1D	-5.14	120.57	128.46
10	N	303	HEC	C1D-C2D-C3D	5.09	110.54	107.00
13	B	201	CLA	C4D-C3D-CAD	5.03	111.28	108.47
13	O	1201	CLA	CBC-CAC-C3C	5.01	126.24	112.43
13	B	201	CLA	CMA-C3A-C2A	4.97	133.88	113.83
15	E	101	BCR	C33-C5-C6	4.85	129.97	124.53
15	E	101	BCR	C30-C25-C26	-4.78	115.89	122.61
13	O	1201	CLA	C2A-C3A-C4A	4.72	109.49	101.87
15	R	1101	BCR	C33-C5-C6	4.71	129.81	124.53
10	N	303	HEC	CMC-C2C-C3C	4.53	131.14	125.82
15	R	1101	BCR	C30-C25-C26	-4.52	116.25	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	B	201	CLA	C2A-C3A-C4A	4.47	109.09	101.87
15	E	101	BCR	C38-C26-C27	-4.42	105.12	113.62
15	R	1101	BCR	C38-C26-C27	-4.34	105.28	113.62
10	N	303	HEC	CAD-CBD-CGD	4.13	119.60	112.67
15	E	101	BCR	C29-C30-C25	3.98	116.61	110.48
9	N	301	HEM	CAD-C3D-C2D	3.89	138.43	127.25
15	R	1101	BCR	C11-C10-C9	3.79	132.72	127.31
15	E	101	BCR	C11-C10-C9	3.76	132.68	127.31
15	E	101	BCR	C2-C1-C6	3.75	116.26	110.48
10	N	303	HEC	CMC-C2C-C1C	-3.75	122.70	128.46
15	R	1101	BCR	C7-C8-C9	3.74	131.88	126.23
13	O	1201	CLA	C2A-C1A-CHA	3.73	130.39	123.86
15	R	1101	BCR	C29-C30-C25	3.73	116.23	110.48
15	R	1101	BCR	C21-C20-C19	3.69	134.75	123.22
15	E	101	BCR	C33-C5-C4	-3.66	106.59	113.62
15	E	101	BCR	C21-C20-C19	3.63	134.53	123.22
15	R	1101	BCR	C24-C23-C22	3.61	131.69	126.23
15	E	101	BCR	C1-C6-C5	-3.59	117.55	122.61
9	A	301	HEM	CAD-C3D-C2D	3.59	137.56	127.25
15	R	1101	BCR	C33-C5-C4	-3.57	106.75	113.62
15	R	1101	BCR	C2-C1-C6	3.55	115.94	110.48
10	N	303	HEC	CMB-C2B-C3B	3.51	129.95	125.82
10	N	303	HEC	CMB-C2B-C1B	-3.48	123.11	128.46
15	E	101	BCR	C7-C8-C9	3.46	131.47	126.23
9	P	301	HEM	CAD-C3D-C2D	3.46	137.20	127.25
15	R	1101	BCR	C1-C6-C5	-3.45	117.75	122.61
13	B	201	CLA	C2A-C1A-CHA	3.42	129.84	123.86
9	C	301	HEM	CAD-C3D-C2D	3.40	137.01	127.25
15	E	101	BCR	C24-C23-C22	3.27	131.17	126.23
13	O	1201	CLA	CED-O2D-CGD	3.23	123.25	115.94
13	O	1201	CLA	C3A-C2A-C1A	3.20	106.13	101.34
13	B	201	CLA	CED-O2D-CGD	3.12	122.99	115.94
10	A	303	HEC	CMD-C2D-C3D	3.10	130.79	124.94
13	O	1201	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
15	R	1101	BCR	C23-C24-C25	3.07	135.81	127.20
13	B	201	CLA	C1-C2-C3	3.05	131.31	126.04
10	N	303	HEC	CBA-CAA-C2A	-3.03	106.89	112.48
13	B	201	CLA	OBD-CAD-C3D	3.02	133.00	127.98
12	B	309	BNT	CAC-CAD-CAE	3.02	119.57	112.91
11	C	306	OPC	CAM-OAN-CAO	3.01	125.21	117.79
15	E	101	BCR	C23-C24-C25	2.98	135.58	127.20
9	N	301	HEM	CAD-CBD-CGD	-2.94	107.73	112.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	O	1201	CLA	C3D-CAD-CBD	-2.94	103.74	107.61
10	A	303	HEC	CMC-C2C-C1C	-2.93	123.96	128.46
10	A	303	HEC	CMB-C2B-C1B	-2.91	123.99	128.46
13	O	1201	CLA	CAA-C2A-C1A	2.90	121.49	111.97
9	A	301	HEM	CAA-CBA-CGA	2.88	117.51	112.67
9	A	302	HEM	CMD-C2D-C1D	-2.88	124.04	128.46
13	B	201	CLA	CMB-C2B-C1B	-2.87	124.06	128.46
13	B	201	CLA	CAA-C2A-C1A	2.85	121.33	111.97
12	O	1309	BNT	CAC-CAD-CAE	2.85	119.19	112.91
15	E	101	BCR	C8-C7-C6	2.83	135.14	127.20
13	B	201	CLA	C3A-C2A-C1A	2.82	105.56	101.34
15	E	101	BCR	C1-C6-C7	2.78	123.66	115.78
9	N	301	HEM	CBA-CAA-C2A	-2.78	107.36	112.49
9	P	301	HEM	CMC-C2C-C3C	2.78	129.88	124.68
10	A	303	HEC	CMC-C2C-C3C	2.78	129.09	125.82
9	N	301	HEM	CMC-C2C-C3C	2.75	129.82	124.68
9	C	301	HEM	CMC-C2C-C3C	2.72	129.77	124.68
11	O	1306	OPC	OAN-CAO-OAD	-2.70	117.19	123.70
15	R	1101	BCR	C8-C7-C6	2.69	134.76	127.20
9	N	302	HEM	CAD-C3D-C2D	2.68	134.96	127.25
15	R	1101	BCR	C1-C6-C7	2.68	123.36	115.78
9	N	301	HEM	CMB-C2B-C3B	2.65	129.63	124.68
10	N	303	HEC	CMD-C2D-C1D	-2.63	124.42	128.46
13	O	1201	CLA	OBD-CAD-C3D	2.58	132.27	127.98
11	N	1305	OPC	OAN-CAO-OAD	-2.58	117.48	123.70
15	R	1101	BCR	C36-C18-C17	-2.57	119.32	122.92
9	A	301	HEM	CMB-C2B-C3B	2.57	129.49	124.68
12	B	309	BNT	BRAH-CAG-CAL	-2.57	120.36	122.47
9	A	302	HEM	CMC-C2C-C3C	2.57	129.48	124.68
9	A	302	HEM	CAD-C3D-C2D	2.56	134.60	127.25
9	A	302	HEM	CMB-C2B-C3B	2.55	129.45	124.68
11	C	306	OPC	OAN-CAO-OAD	-2.55	117.54	123.70
15	E	101	BCR	C15-C16-C17	2.49	128.58	123.47
15	E	101	BCR	C34-C9-C10	-2.48	119.45	122.92
9	N	302	HEM	CMD-C2D-C1D	-2.47	124.67	128.46
13	B	201	CLA	OBD-CAD-CBD	-2.46	122.39	125.89
13	O	1201	CLA	O2A-CGA-CBA	2.44	119.56	111.91
13	O	1201	CLA	C1D-CHD-C4C	2.43	125.76	122.56
11	B	305	OPC	OAN-CAO-OAD	-2.40	117.89	123.70
9	A	301	HEM	CMC-C2C-C3C	2.36	129.09	124.68
10	A	303	HEC	C1D-C2D-C3D	2.36	108.64	107.00
12	O	1309	BNT	BRAI-CAJ-CAK	2.35	120.55	116.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	R	1101	BCR	C32-C1-C6	2.34	114.10	110.30
10	A	303	HEC	CMB-C2B-C3B	2.34	128.57	125.82
11	N	1305	OPC	OBJ-CBK-CBL	2.34	119.25	111.91
15	R	1101	BCR	C15-C16-C17	2.34	128.26	123.47
15	E	101	BCR	C32-C1-C6	2.33	114.09	110.30
9	N	302	HEM	CMB-C2B-C3B	2.33	129.03	124.68
13	B	201	CLA	C1D-CHD-C4C	2.32	125.62	122.56
15	E	101	BCR	C36-C18-C17	-2.31	119.68	122.92
10	A	303	HEC	CMA-C3A-C2A	2.31	129.29	124.94
13	B	201	CLA	CMB-C2B-C3B	2.31	128.99	124.68
13	O	1201	CLA	CBA-CAA-C2A	-2.31	107.06	113.86
9	N	302	HEM	CMC-C2C-C3C	2.30	128.99	124.68
11	O	1306	OPC	OBJ-CBK-CBL	2.30	119.13	111.91
9	C	301	HEM	CAA-C2A-C3A	2.29	133.82	127.25
9	P	301	HEM	CAA-C2A-C3A	2.28	133.80	127.25
13	O	1201	CLA	CMB-C2B-C3B	2.28	128.94	124.68
11	B	305	OPC	OBJ-CBK-CBL	2.27	119.05	111.91
13	B	201	CLA	C3D-CAD-CBD	-2.27	104.61	107.61
15	R	1101	BCR	C34-C9-C10	-2.26	119.76	122.92
11	O	1306	OPC	CAM-OAN-CAO	2.23	123.27	117.79
12	B	309	BNT	OAB-CAF-CAG	-2.22	118.60	123.15
9	C	301	HEM	CMB-C2B-C3B	2.21	128.81	124.68
11	N	1305	OPC	OBJ-CBI-CAM	2.19	114.81	108.43
9	P	301	HEM	CMB-C2B-C3B	2.19	128.77	124.68
9	A	301	HEM	CAA-C2A-C3A	2.18	133.50	127.25
13	B	201	CLA	O2D-CGD-CBD	2.16	115.11	111.27
15	R	1101	BCR	C30-C25-C24	2.15	121.86	115.78
11	C	306	OPC	OBJ-CBK-CBL	2.12	118.58	111.91
13	B	201	CLA	O2A-CGA-CBA	2.12	118.56	111.91
15	E	101	BCR	C30-C25-C24	2.11	121.76	115.78
9	P	301	HEM	C4A-C3A-C2A	2.10	108.46	107.00
9	N	301	HEM	CAA-C2A-C3A	2.06	133.18	127.25
15	R	1101	BCR	C40-C30-C29	-2.06	100.66	108.91
9	P	301	HEM	CMD-C2D-C1D	-2.05	125.31	128.46
11	N	1305	OPC	CBO-CBP-CBQ	2.05	122.72	113.79
13	O	1201	CLA	C7-C6-C5	-2.03	107.84	113.36
9	P	301	HEM	CBD-CAD-C3D	2.03	116.21	112.48
15	E	101	BCR	C40-C30-C29	-2.01	100.85	108.91
9	A	301	HEM	CAD-CBD-CGD	-2.01	109.30	112.67
9	C	301	HEM	CAD-CBD-CGD	-2.00	109.31	112.67
15	R	1101	BCR	C20-C21-C22	-2.00	124.45	127.31

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
13	O	1201	CLA	C8
13	O	1201	CLA	C2A
13	O	1201	CLA	NA
13	O	1201	CLA	NC
13	O	1201	CLA	C3A
13	O	1201	CLA	ND
13	B	201	CLA	C8
13	B	201	CLA	C2A
13	B	201	CLA	NA
13	B	201	CLA	NC
13	B	201	CLA	C3A
13	B	201	CLA	ND

All (102) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
15	E	101	BCR	C1-C6-C7-C8
15	E	101	BCR	C5-C6-C7-C8
15	E	101	BCR	C11-C10-C9-C8
15	E	101	BCR	C11-C10-C9-C34
11	B	305	OPC	CAP-CAO-OAN-CAM
11	B	305	OPC	OAD-CAO-OAN-CAM
11	B	305	OPC	CAL-OAK-PAJ-OBH
11	B	305	OPC	CAL-OAK-PAJ-OAB
11	B	305	OPC	CAH-OAI-PAJ-OBH
13	O	1201	CLA	C1A-C2A-CAA-CBA
13	B	201	CLA	C1A-C2A-CAA-CBA
11	C	306	OPC	CAP-CAO-OAN-CAM
11	C	306	OPC	OAD-CAO-OAN-CAM
11	C	306	OPC	CAH-OAI-PAJ-OBH
9	N	302	HEM	C2D-C3D-CAD-CBD
9	N	302	HEM	C4D-C3D-CAD-CBD
10	A	303	HEC	C1A-C2A-CAA-CBA
10	A	303	HEC	C3A-C2A-CAA-CBA
9	A	302	HEM	C2D-C3D-CAD-CBD
9	A	302	HEM	C4D-C3D-CAD-CBD
15	R	1101	BCR	C5-C6-C7-C8
15	R	1101	BCR	C11-C10-C9-C8
15	R	1101	BCR	C11-C10-C9-C34
11	N	1305	OPC	CAP-CAO-OAN-CAM
11	N	1305	OPC	OAD-CAO-OAN-CAM
11	N	1305	OPC	CAL-OAK-PAJ-OBH
11	N	1305	OPC	CAL-OAK-PAJ-OAB

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Mol	Chain	Res	Type	Atoms
11	N	1305	OPC	CAL-OAK-PAJ-OAI
11	N	1305	OPC	CAH-OAI-PAJ-OAB
11	O	1306	OPC	CAP-CAO-OAN-CAM
11	O	1306	OPC	OAD-CAO-OAN-CAM
11	O	1306	OPC	CAL-OAK-PAJ-OBH
11	O	1306	OPC	CAL-OAK-PAJ-OAB
11	O	1306	OPC	CAH-OAI-PAJ-OBH
11	O	1306	OPC	CAG-CAH-OAI-PAJ
13	O	1201	CLA	C2A-CAA-CBA-CGA
13	B	201	CLA	C2A-CAA-CBA-CGA
15	E	101	BCR	C22-C23-C24-C25
15	R	1101	BCR	C22-C23-C24-C25
11	B	305	OPC	CAL-OAK-PAJ-OAI
11	B	305	OPC	CAH-OAI-PAJ-OAK
11	C	306	OPC	CAL-OAK-PAJ-OAI
11	N	1305	OPC	CAH-OAI-PAJ-OAK
11	O	1306	OPC	CAH-OAI-PAJ-OAK
15	E	101	BCR	C35-C13-C14-C15
15	R	1101	BCR	C35-C13-C14-C15
15	E	101	BCR	C12-C13-C14-C15
15	R	1101	BCR	C12-C13-C14-C15
13	O	1201	CLA	C13-C15-C16-C17
15	R	1101	BCR	C1-C6-C7-C8
13	B	201	CLA	CBA-CGA-O2A-C1
11	O	1306	OPC	CAL-OAK-PAJ-OAI
13	B	201	CLA	O1A-CGA-O2A-C1
11	O	1306	OPC	CBS-CBT-CBU-CBV
11	B	305	OPC	CAM-CAL-OAK-PAJ
13	B	201	CLA	C11-C12-C13-C15
13	O	1201	CLA	C3-C5-C6-C7
13	O	1201	CLA	C6-C7-C8-C9
13	B	201	CLA	C14-C13-C15-C16
13	O	1201	CLA	CBA-CGA-O2A-C1
13	O	1201	CLA	C2C-C3C-CAC-CBC
11	N	1305	OPC	CAT-CAU-CAV-CAW
13	O	1201	CLA	O1A-CGA-O2A-C1
13	B	201	CLA	C11-C12-C13-C14
13	O	1201	CLA	C6-C7-C8-C10
13	B	201	CLA	C12-C13-C15-C16
11	C	306	OPC	CAL-CAM-OAN-CAO
11	C	306	OPC	CAH-OAI-PAJ-OAK
11	C	306	OPC	CAL-OAK-PAJ-OAB

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Mol	Chain	Res	Type	Atoms
11	C	306	OPC	CAH-OAI-PAJ-OAB
11	N	1305	OPC	CAH-OAI-PAJ-OBH
11	O	1306	OPC	CAH-OAI-PAJ-OAB
11	N	1305	OPC	CBP-CBQ-CBR-CBS
11	B	305	OPC	NAF-CAG-CAH-OAI
11	C	306	OPC	NAF-CAG-CAH-OAI
10	A	303	HEC	C2D-C3D-CAD-CBD
10	A	303	HEC	C4D-C3D-CAD-CBD
11	N	1305	OPC	NAF-CAG-CAH-OAI
10	N	303	HEC	C2D-C3D-CAD-CBD
10	N	303	HEC	C4D-C3D-CAD-CBD
11	O	1306	OPC	NAF-CAG-CAH-OAI
11	O	1306	OPC	CAL-CAM-OAN-CAO
11	C	306	OPC	CAM-CAL-OAK-PAJ
11	N	1305	OPC	CAL-CAM-OAN-CAO
13	O	1201	CLA	C11-C12-C13-C15
11	N	1305	OPC	CAV-CAW-CAX-CAY
11	B	305	OPC	OAK-CAL-CAM-OAN
13	B	201	CLA	C4-C3-C5-C6
11	O	1306	OPC	CBR-CBS-CBT-CBU
11	N	1305	OPC	CBI-CAM-OAN-CAO
13	O	1201	CLA	C2-C1-O2A-CGA
11	O	1306	OPC	OAK-CAL-CAM-OAN
13	O	1201	CLA	C4C-C3C-CAC-CBC
11	N	1305	OPC	OBJ-CBK-CBL-CBM
13	O	1201	CLA	C11-C12-C13-C14
11	B	305	OPC	CBP-CBQ-CBR-CBS
11	O	1306	OPC	CBU-CBV-CBW-CBX
11	N	1305	OPC	OCC-CBK-CBL-CBM
11	C	306	OPC	OBJ-CBK-CBL-CBM
13	O	1201	CLA	C4-C3-C5-C6
13	B	201	CLA	C13-C15-C16-C17
11	N	1305	OPC	OAN-CAO-CAP-CAQ

There are no ring outliers.

20 monomers are involved in 171 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
14	Q	201	FES	2	0
15	E	101	BCR	11	0
11	B	305	OPC	34	0
13	O	1201	CLA	8	0

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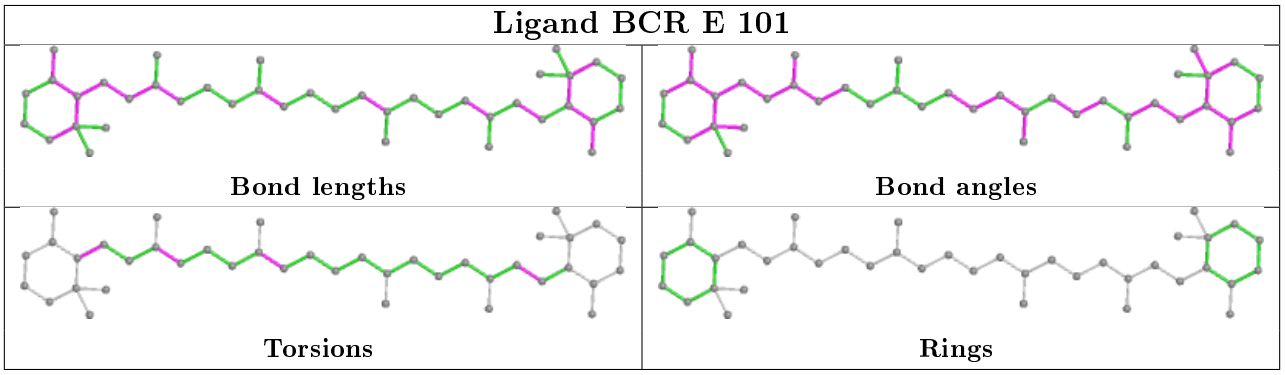
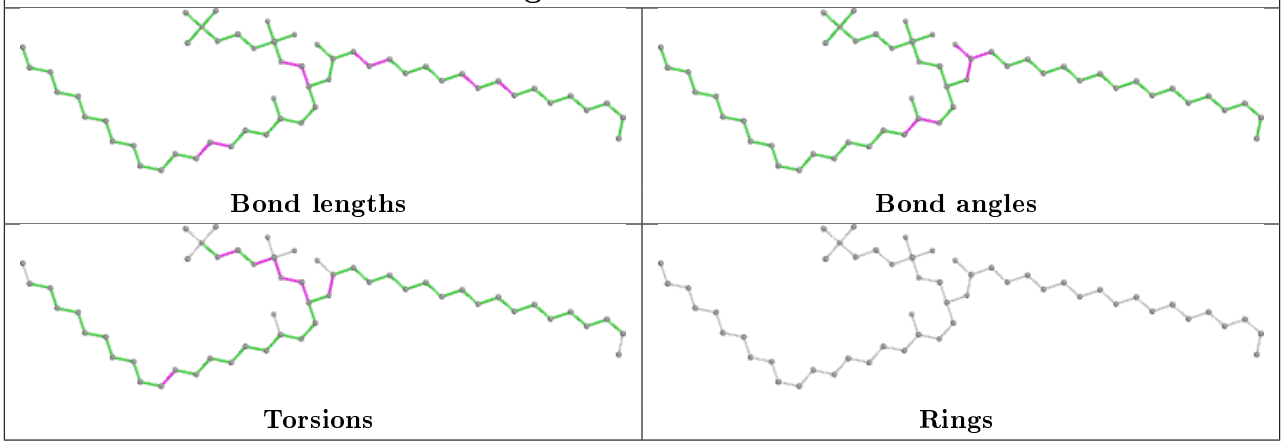
Mol	Chain	Res	Type	Clashes	Symm-Clashes
13	B	201	CLA	6	0
11	C	306	OPC	20	0
9	N	302	HEM	3	0
9	P	301	HEM	5	0
9	C	301	HEM	4	0
9	N	301	HEM	8	0
10	A	303	HEC	4	0
12	B	309	BNT	9	0
9	A	302	HEM	8	0
12	O	1309	BNT	7	0
11	N	1305	OPC	14	0
10	N	303	HEC	10	0
15	R	1101	BCR	8	0
14	D	201	FES	3	0
11	O	1306	OPC	17	0
9	A	301	HEM	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.

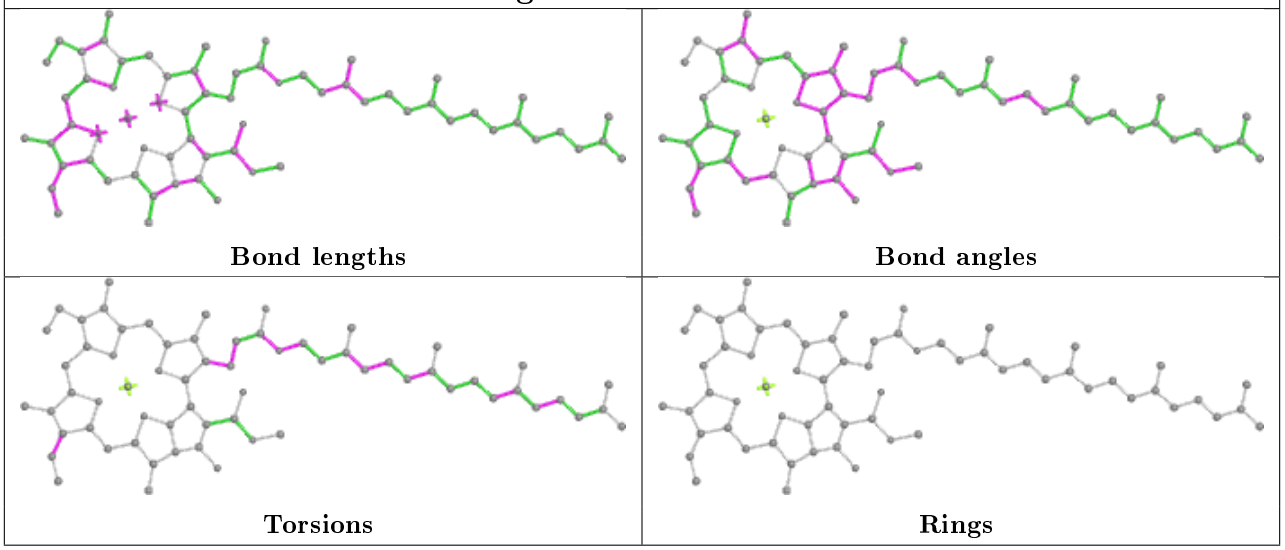
Ligand BCR E 101



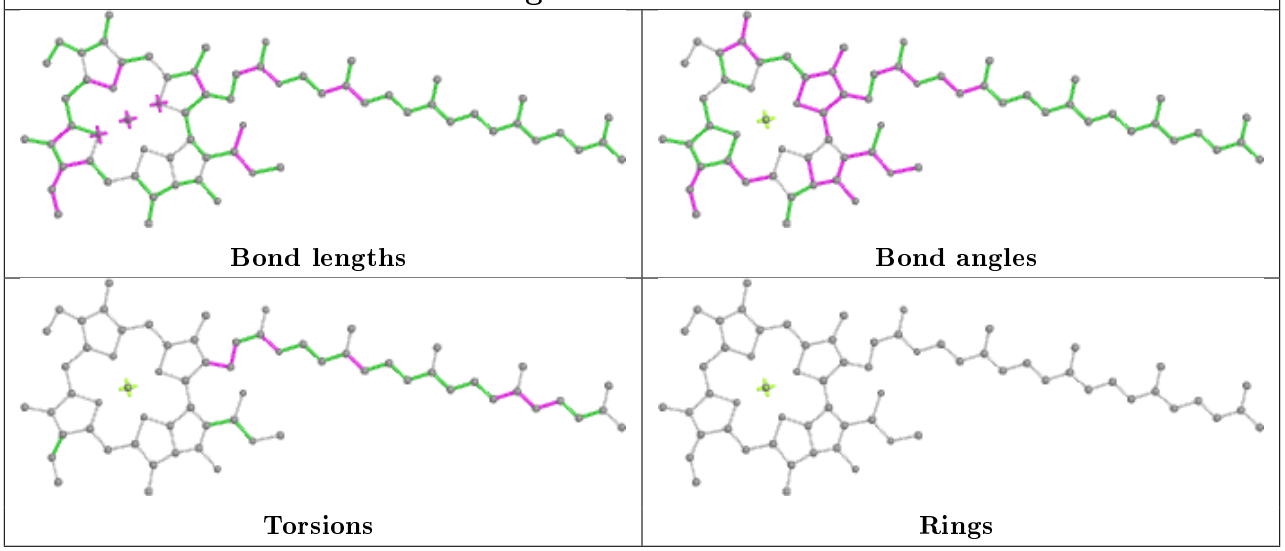
Ligand OPC B 305



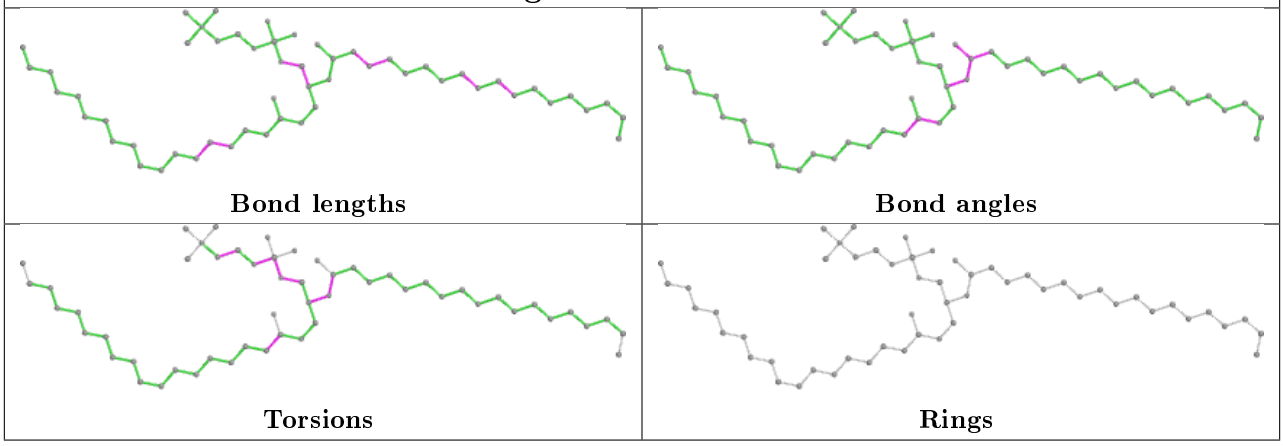
Ligand CLA O 1201



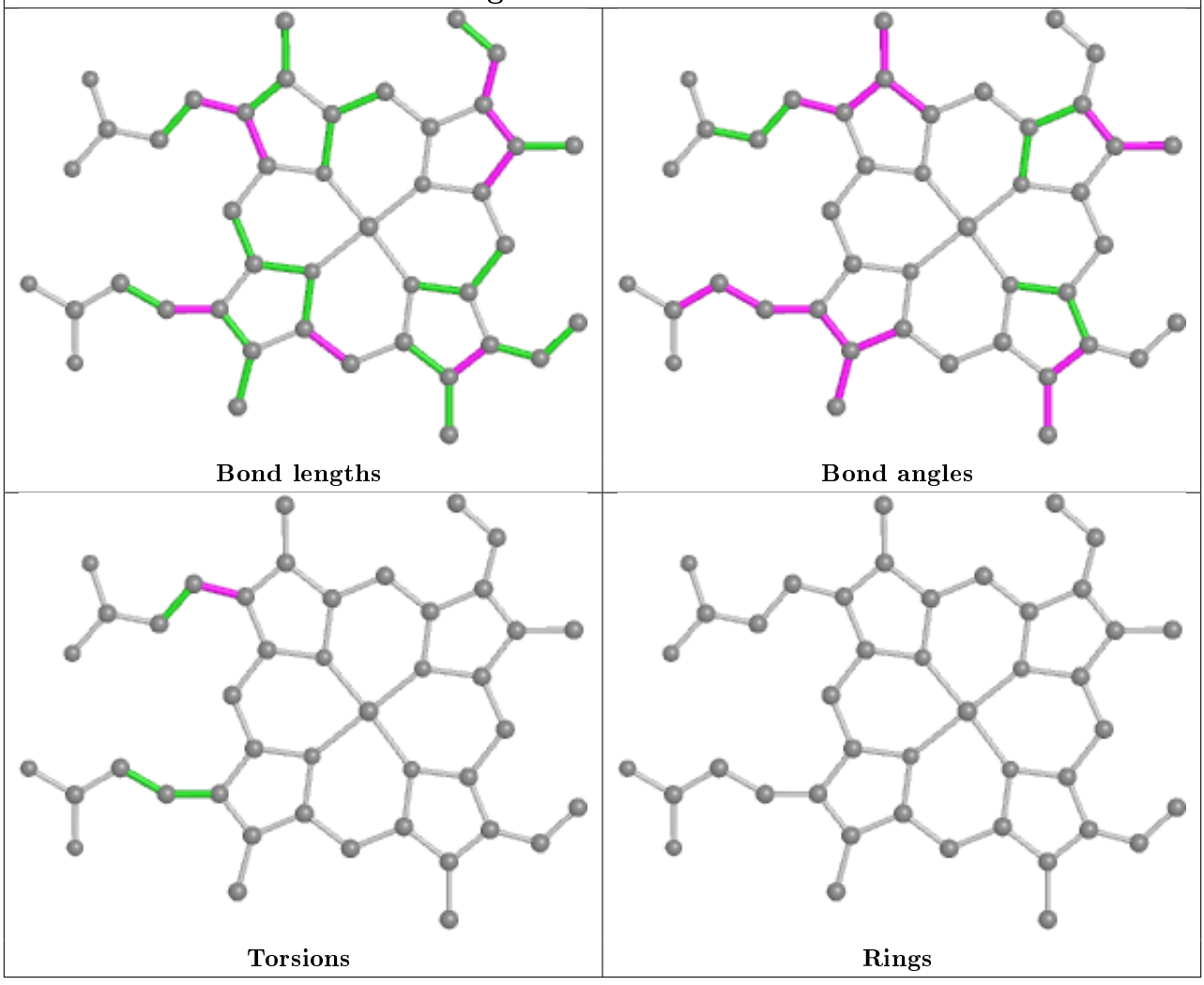
Ligand CLA B 201



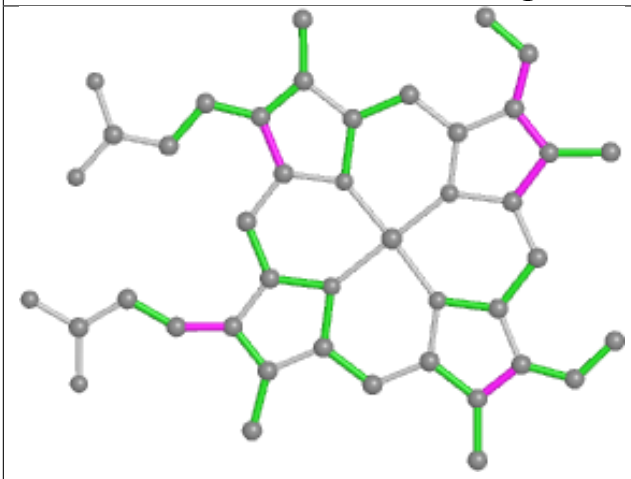
Ligand OPC C 306



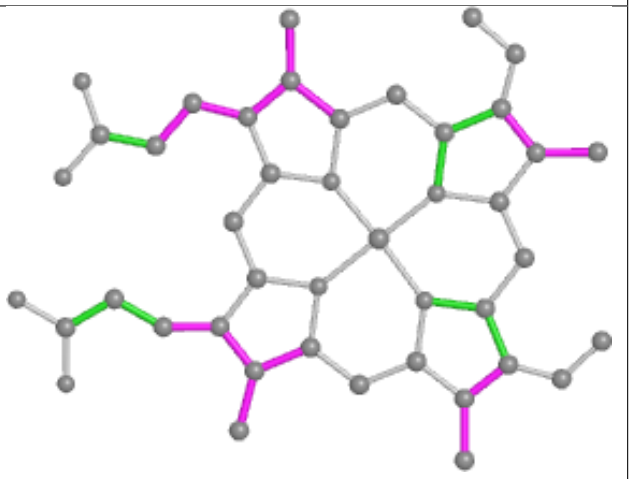
Ligand HEM N 302



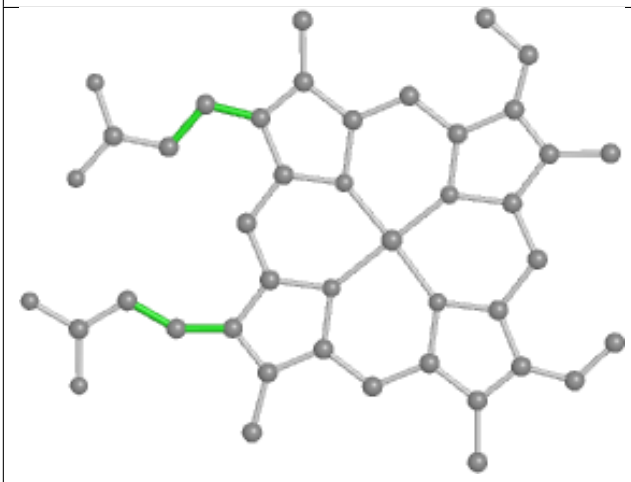
Ligand HEM P 301



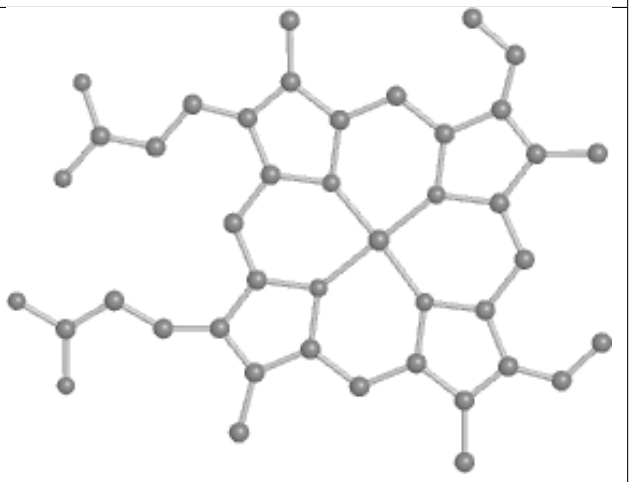
Bond lengths



Bond angles

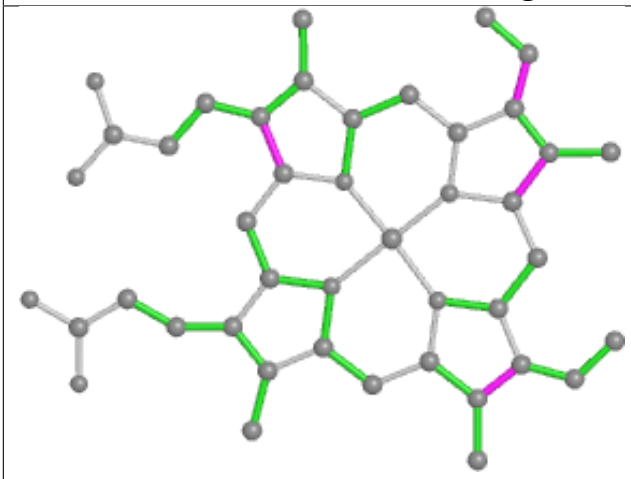


Torsions

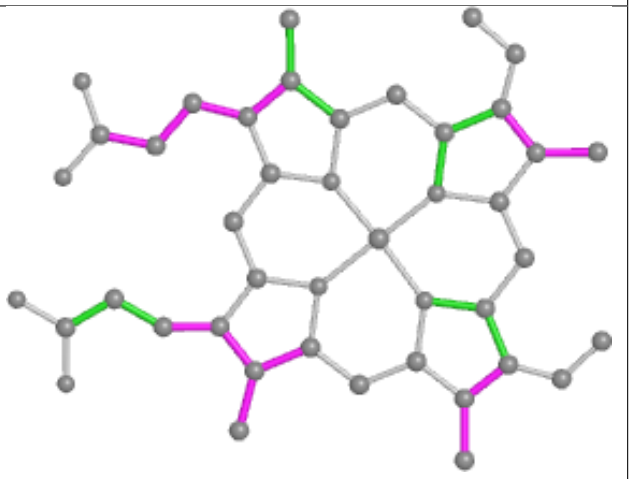


Rings

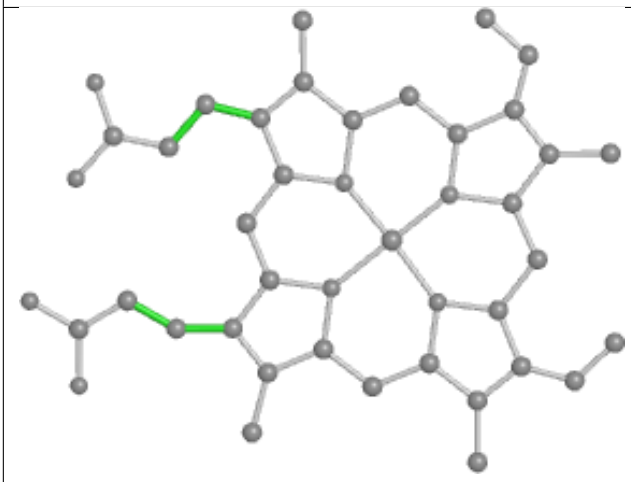
Ligand HEM C 301



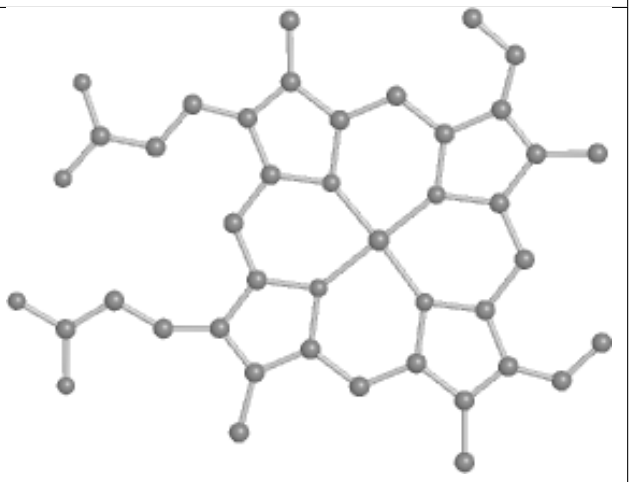
Bond lengths



Bond angles

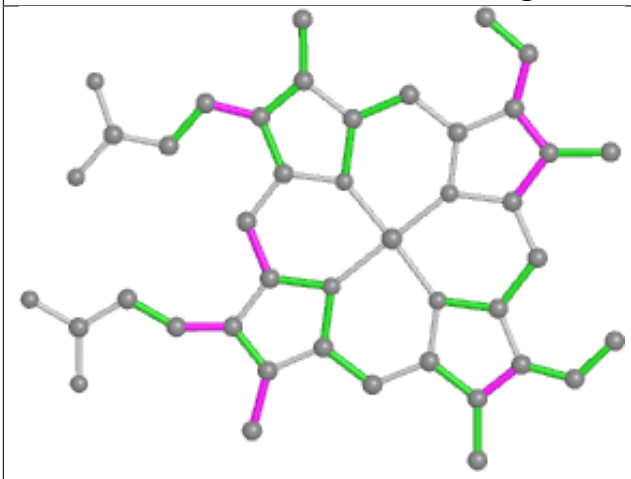


Torsions

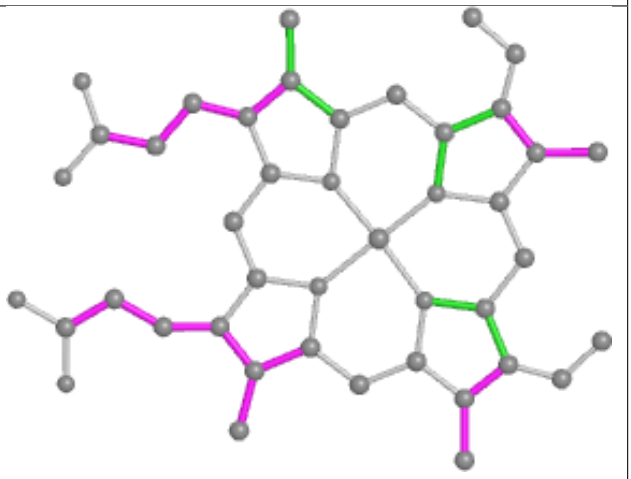


Rings

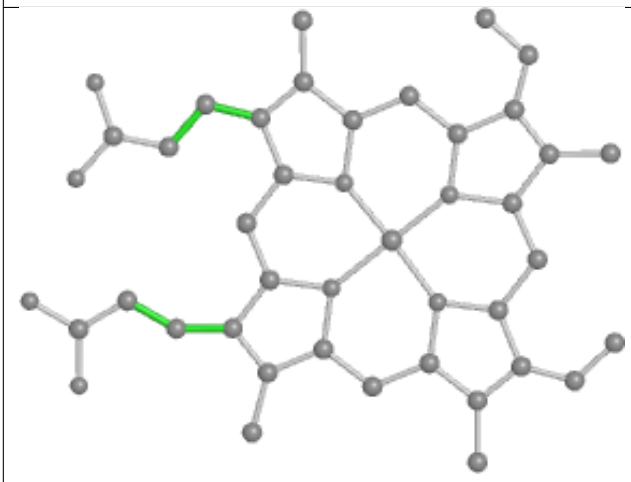
Ligand HEM N 301



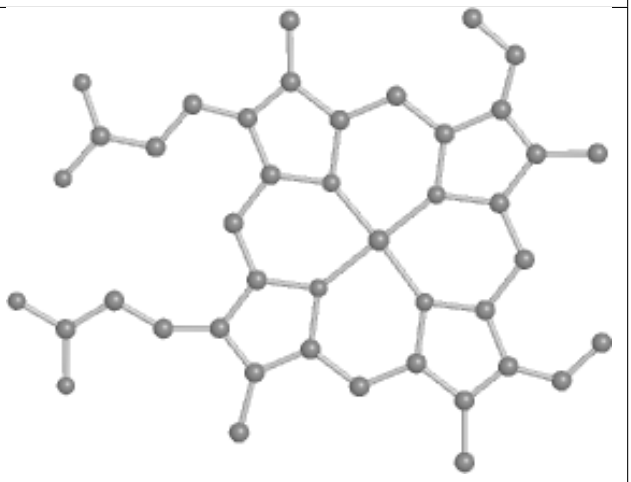
Bond lengths



Bond angles

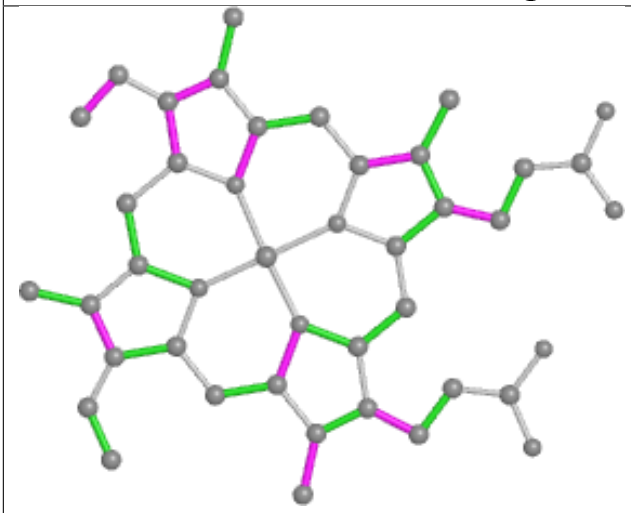


Torsions

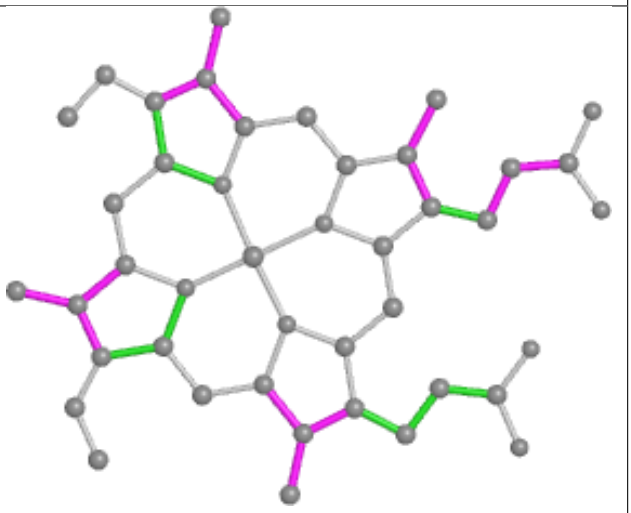


Rings

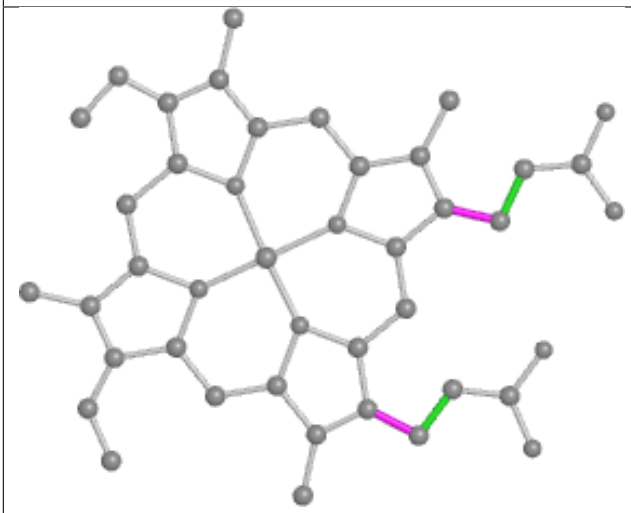
Ligand HEC A 303



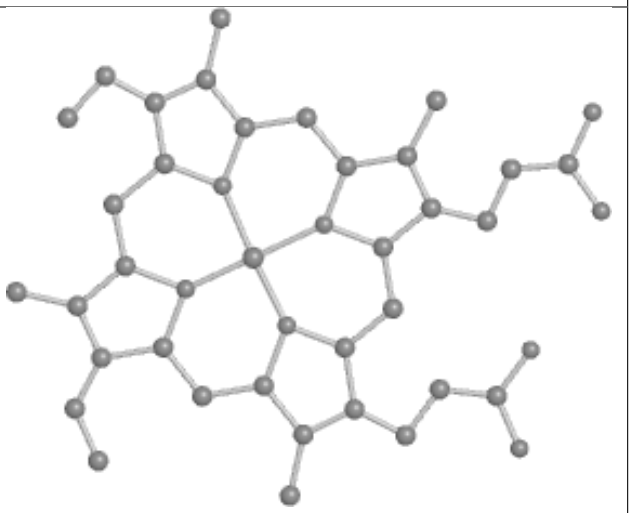
Bond lengths



Bond angles

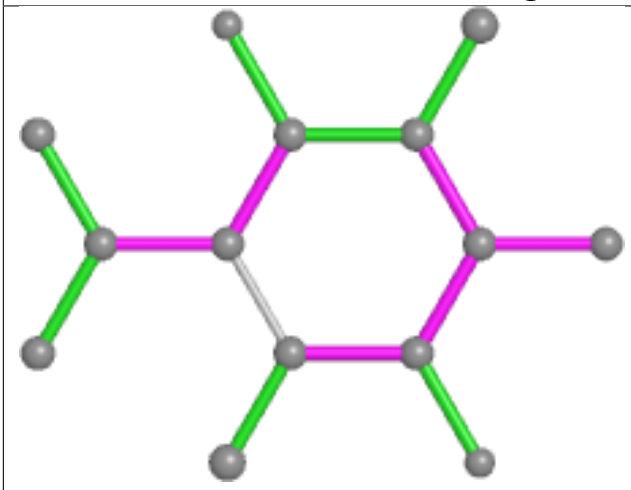


Torsions

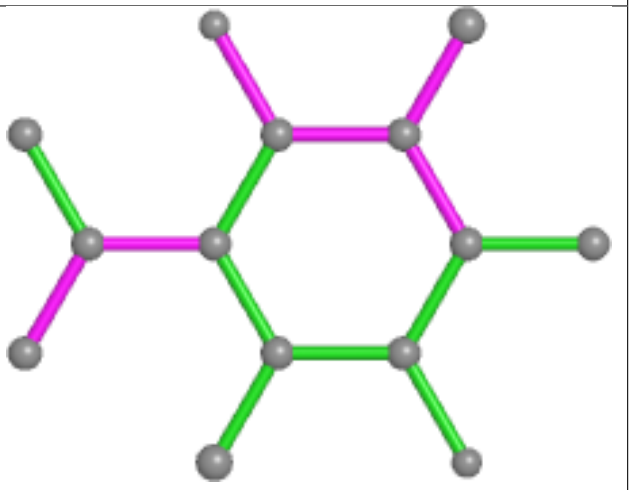


Rings

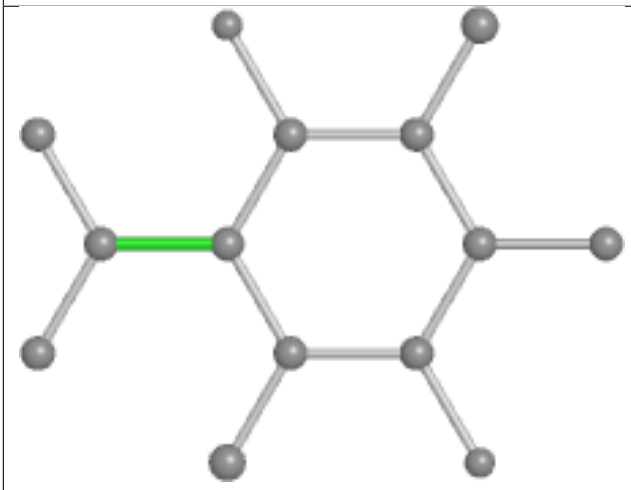
Ligand BNT B 309



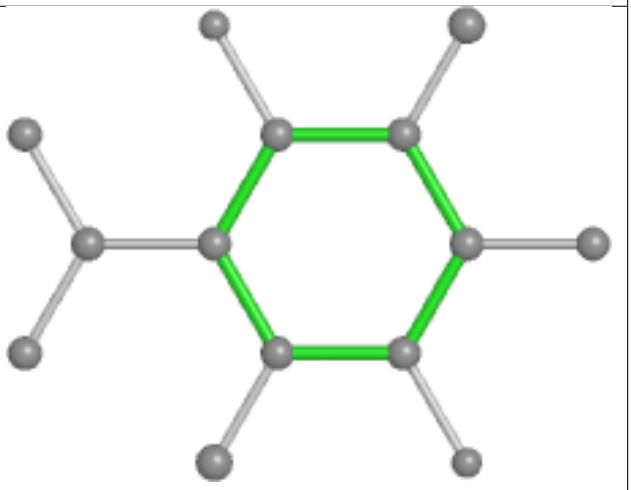
Bond lengths



Bond angles

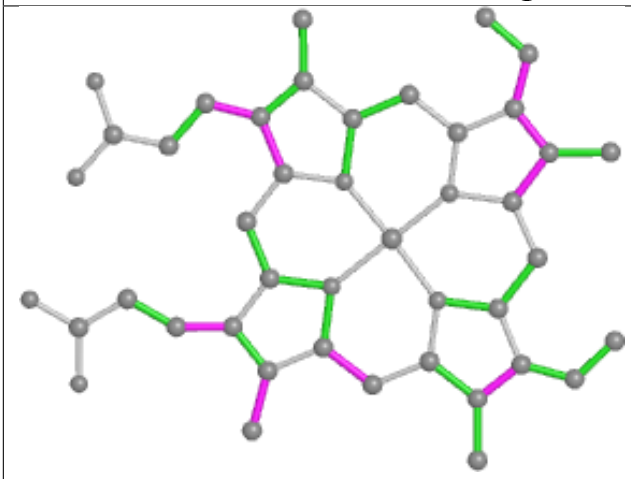


Torsions

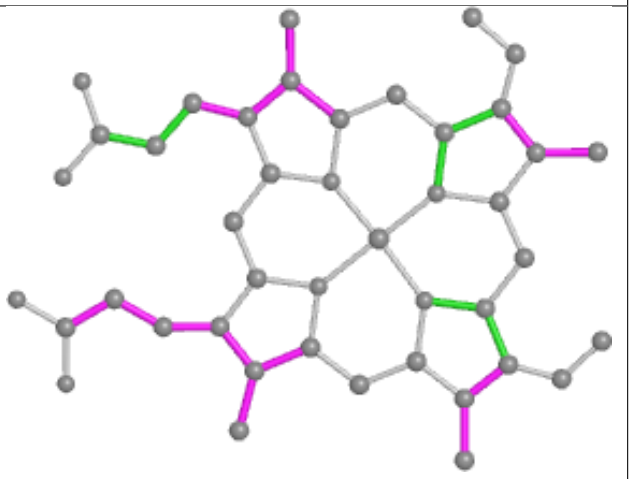


Rings

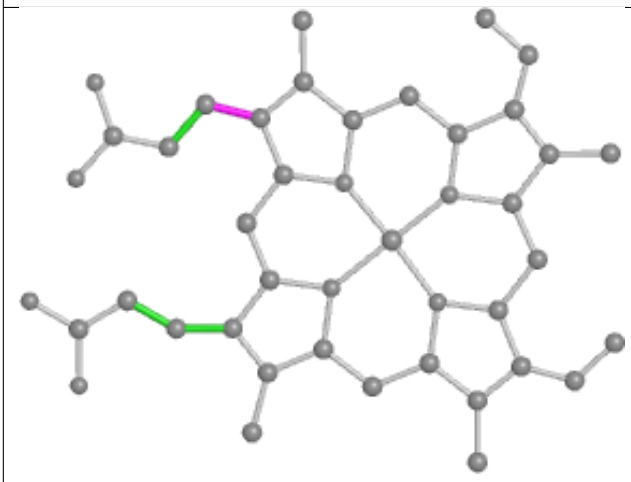
Ligand HEM A 302



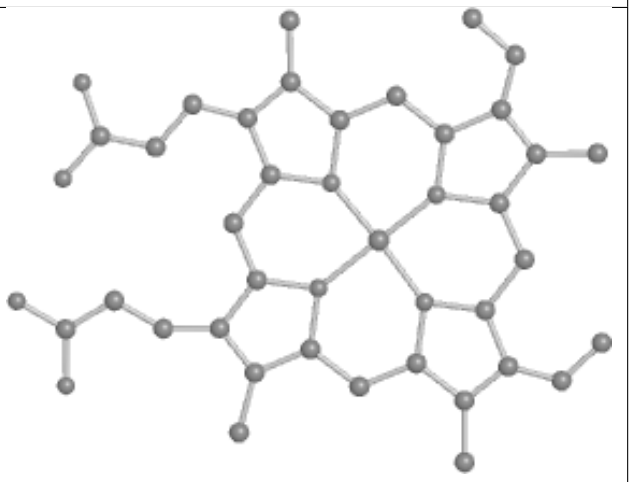
Bond lengths



Bond angles

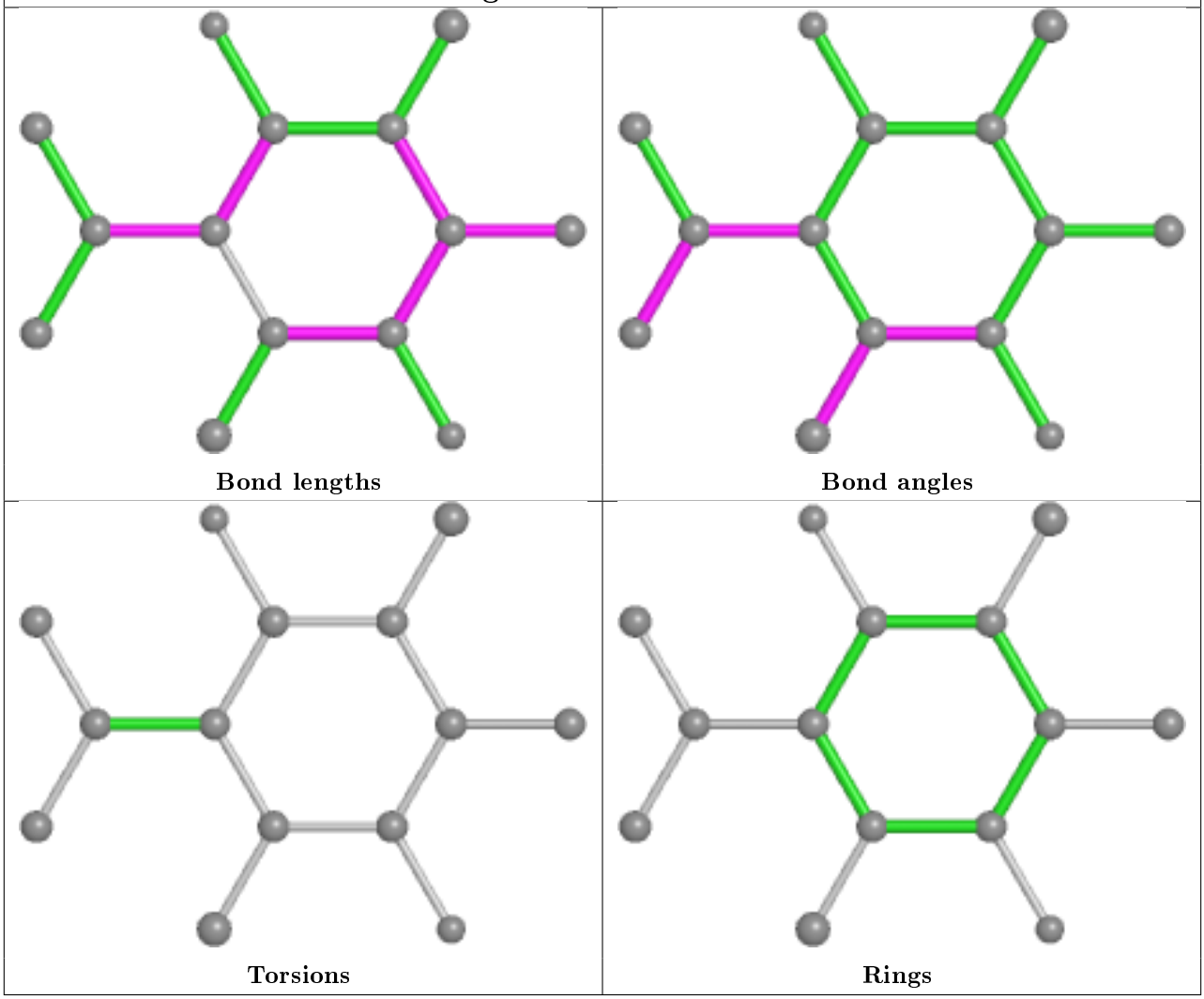


Torsions

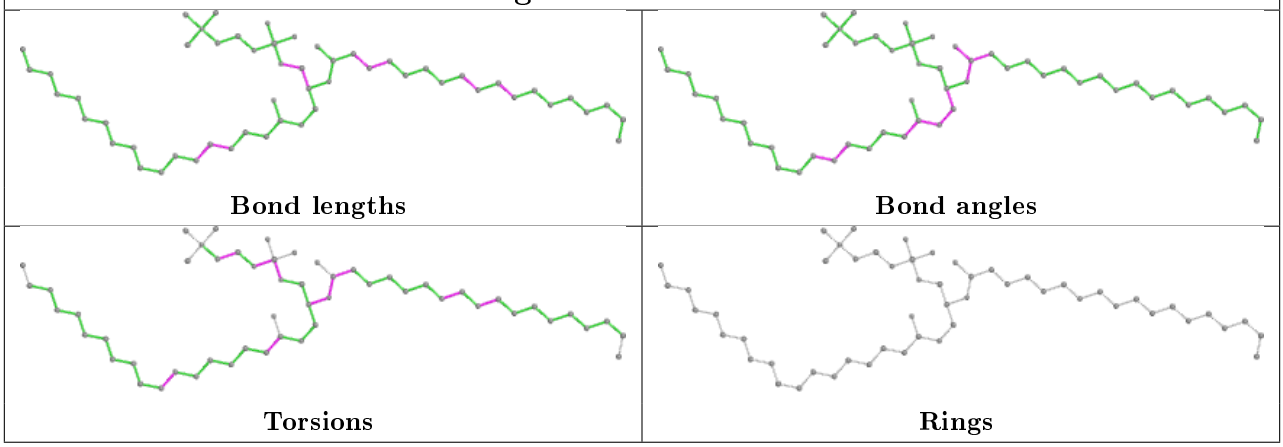


Rings

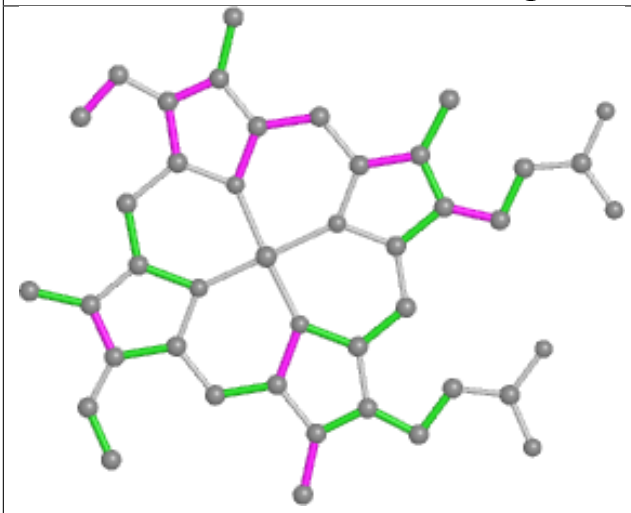
Ligand BNT O 1309



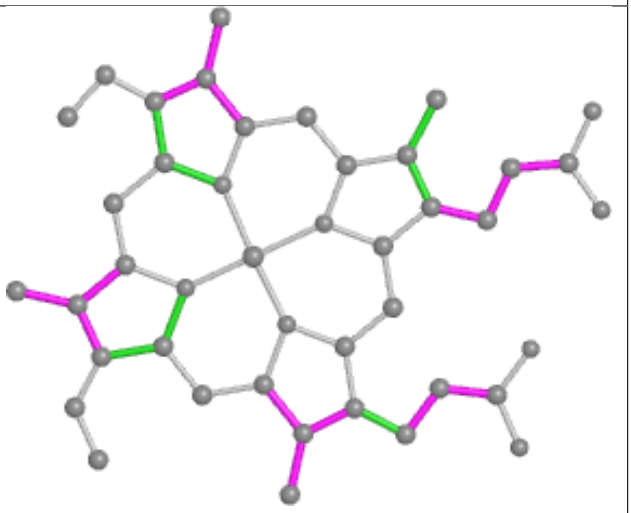
Ligand OPC N 1305



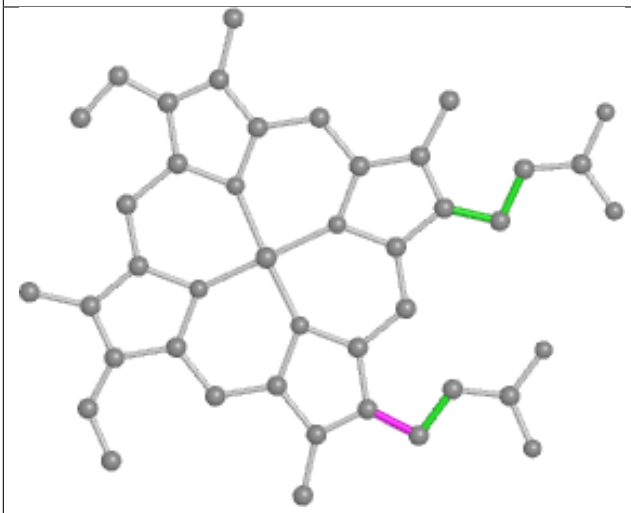
Ligand HEC N 303



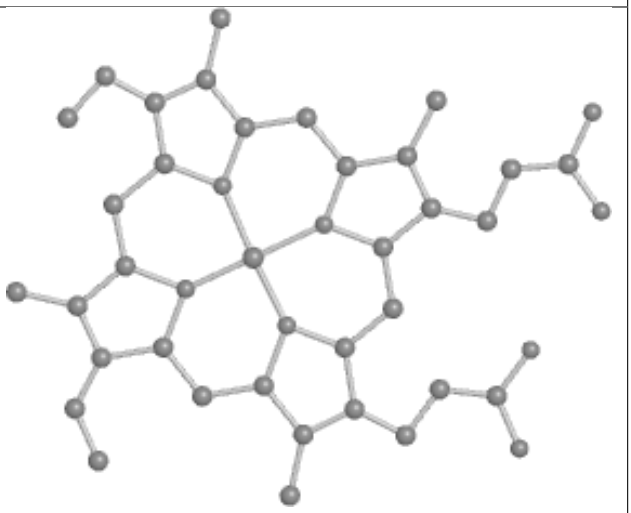
Bond lengths



Bond angles

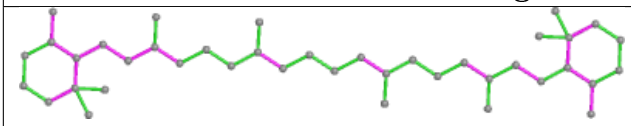


Torsions

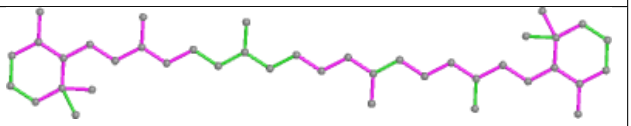


Rings

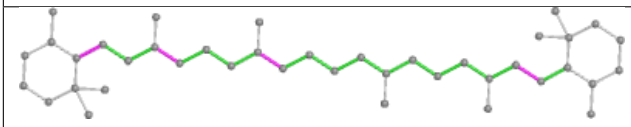
Ligand BCR R 1101



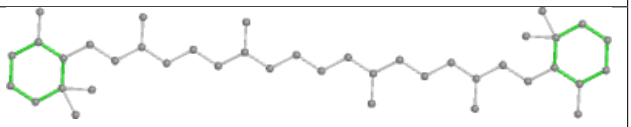
Bond lengths



Bond angles

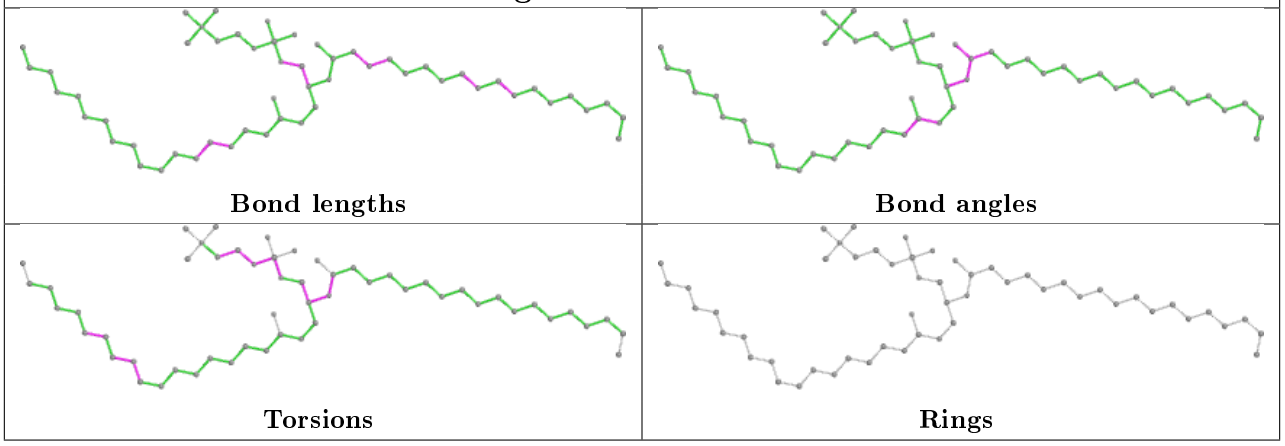


Torsions

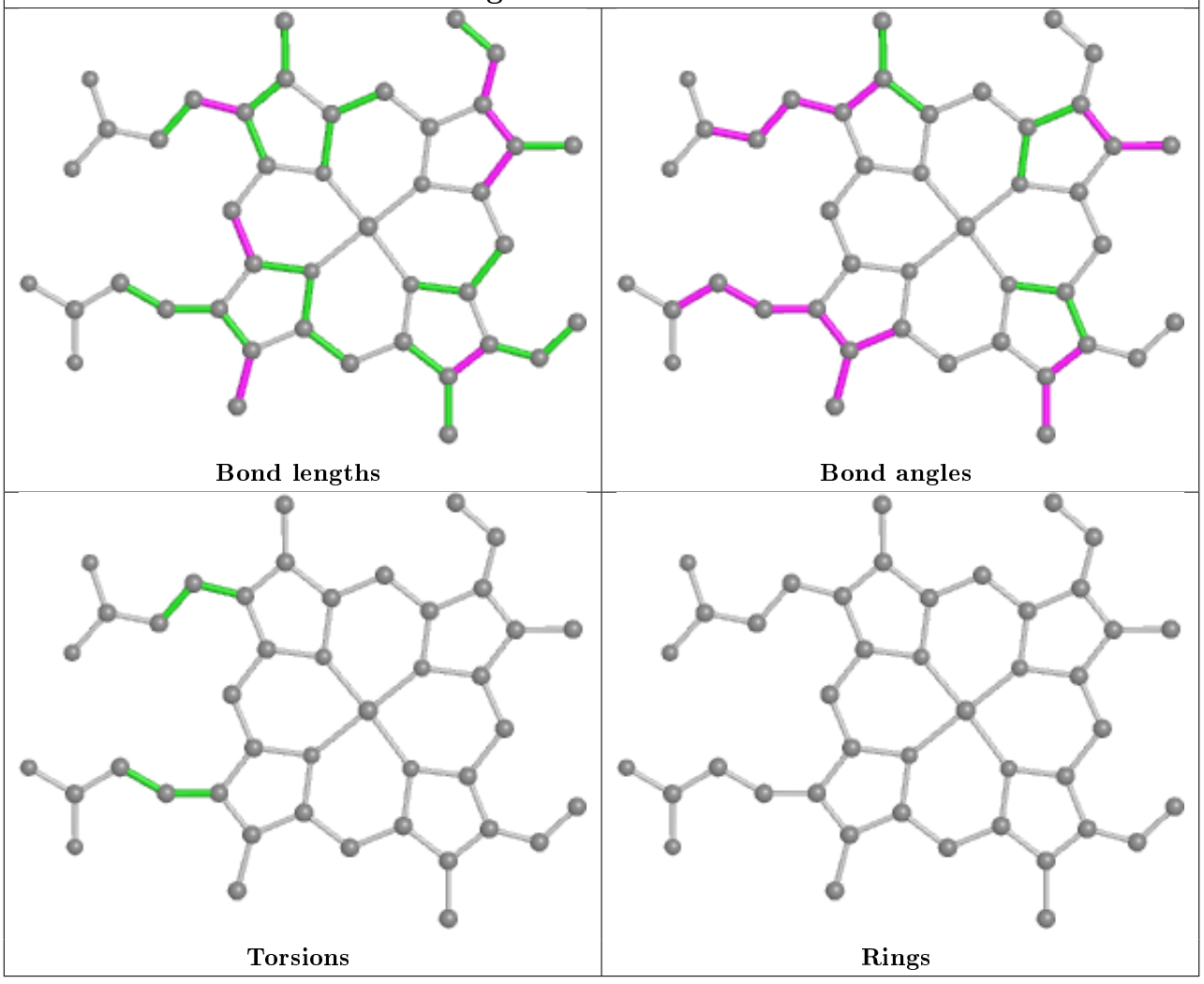


Rings

Ligand OPC O 1306



Ligand HEM A 301



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	202/215 (93%)	-0.41	1 (0%) 91 87	12, 58, 120, 164	0
1	N	202/215 (93%)	-0.46	0 100 100	11, 53, 104, 158	0
2	B	137/160 (85%)	-0.54	0 100 100	16, 67, 137, 177	0
2	O	137/160 (85%)	-0.43	1 (0%) 87 83	13, 63, 130, 183	0
3	C	286/289 (98%)	-0.26	10 (3%) 44 36	9, 85, 150, 200	1 (0%)
3	P	286/289 (98%)	-0.18	6 (2%) 63 55	1, 85, 160, 200	1 (0%)
4	D	168/179 (93%)	-0.20	7 (4%) 36 30	18, 93, 169, 200	0
4	Q	168/179 (93%)	-0.37	2 (1%) 79 72	26, 94, 158, 195	0
5	E	32/32 (100%)	-0.08	2 (6%) 20 15	20, 67, 163, 195	0
5	R	32/32 (100%)	-0.55	0 100 100	21, 59, 111, 162	0
6	F	35/35 (100%)	-0.43	0 100 100	8, 69, 133, 144	0
6	S	35/35 (100%)	-0.48	0 100 100	16, 71, 113, 153	0
7	G	27/37 (72%)	-0.33	0 100 100	34, 66, 133, 147	0
7	T	27/37 (72%)	-0.33	1 (3%) 41 34	30, 76, 136, 178	0
8	H	27/29 (93%)	-0.58	0 100 100	25, 68, 119, 156	0
8	U	27/29 (93%)	-0.46	0 100 100	29, 69, 128, 180	0
All	All	1828/1952 (93%)	-0.34	30 (1%) 72 64	1, 73, 149, 200	2 (0%)

All (30) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
4	D	156	GLN	5.5
4	D	152	HIS	4.9
4	D	103	GLY	4.5
4	D	61	GLY	4.4
3	P	221	GLU	4.4

Continued on next page...

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Mol	Chain	Res	Type	RSRZ
4	D	96	LYS	4.3
3	C	153	ALA	4.2
3	P	16	PRO	4.1
3	C	215	PRO	3.9
4	D	102	TYR	3.4
3	C	221	GLU	3.4
2	O	66	ALA	3.4
3	C	152	GLY	3.4
3	P	15	GLU	3.3
3	P	220	SER	3.3
5	E	21	GLY	3.2
5	E	32	ILE	3.2
3	P	32	ALA	2.8
3	C	222	GLY	2.8
3	P	222	GLY	2.5
3	C	278	GLN	2.5
3	C	115	LEU	2.4
3	C	73	GLY	2.4
3	C	151	LEU	2.4
3	C	30	LYS	2.3
7	T	27	PRO	2.3
4	Q	151	CYS	2.2
4	Q	123	LYS	2.2
4	D	101	ASP	2.0
1	A	111	LYS	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

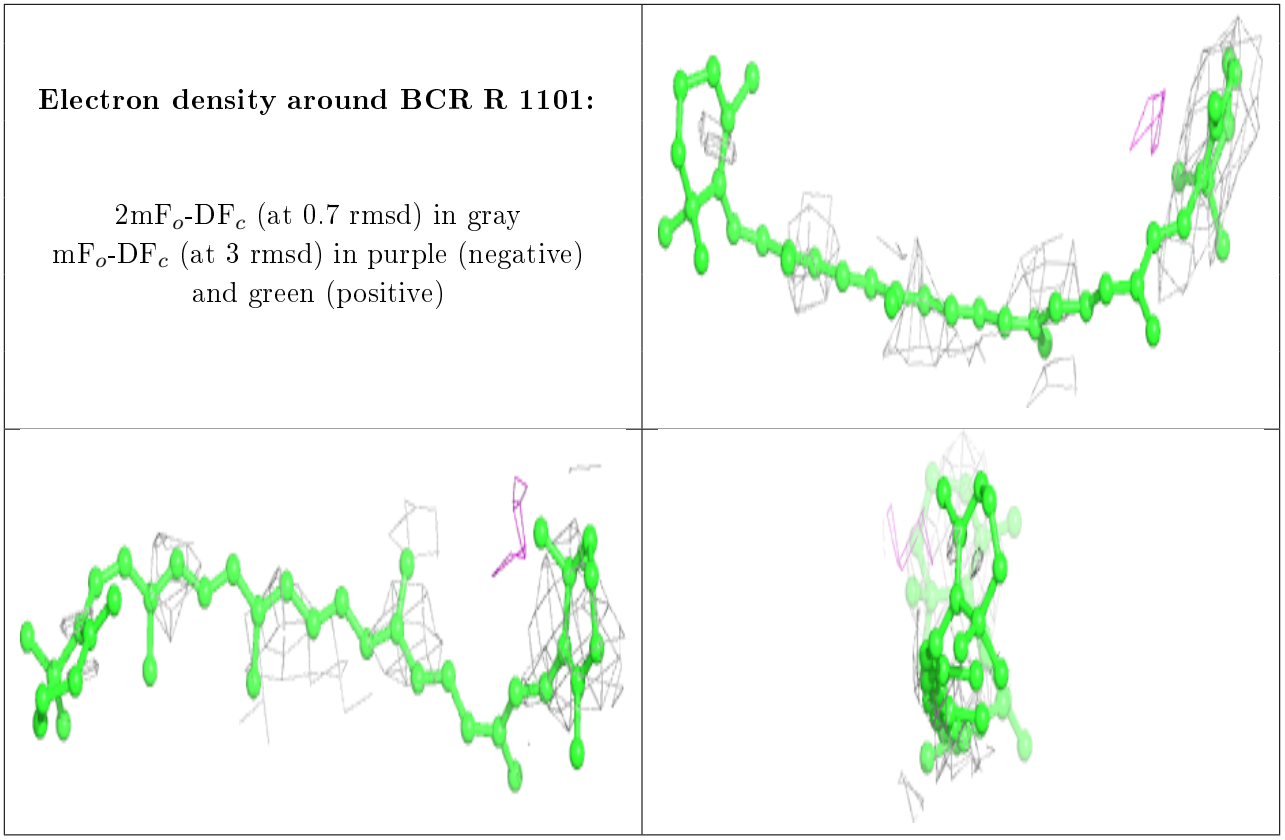
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
15	BCR	R	1101	40/40	0.77	0.99	181,181,181,181	0
11	OPC	N	1305	54/55	0.84	0.44	107,107,107,107	0
15	BCR	E	101	40/40	0.85	0.54	84,84,84,84	0
11	OPC	C	306	54/55	0.86	0.36	84,84,84,84	0
11	OPC	O	1306	54/55	0.86	0.38	73,73,73,73	0
12	BNT	O	1309	14/14	0.92	0.29	64,64,64,64	0
11	OPC	B	305	54/55	0.92	0.23	66,66,66,66	0
13	CLA	O	1201	65/65	0.93	0.39	29,72,72,72	0
12	BNT	B	309	14/14	0.93	0.30	64,64,64,64	0
13	CLA	B	201	65/65	0.93	0.48	20,112,112,112	0
10	HEC	A	303	43/43	0.94	0.27	57,104,104,104	0
10	HEC	N	303	43/43	0.95	0.25	67,74,74,74	0
9	HEM	C	301	43/43	0.96	0.26	36,59,59,59	0
9	HEM	A	302	43/43	0.97	0.29	41,58,58,58	0
9	HEM	P	301	43/43	0.97	0.24	54,76,76,76	0
9	HEM	A	301	43/43	0.97	0.33	31,48,48,48	0
9	HEM	N	301	43/43	0.98	0.36	26,64,64,64	0
9	HEM	N	302	43/43	0.98	0.29	30,61,61,61	0
14	FES	Q	201	4/4	0.99	0.13	28,28,53,53	0
14	FES	D	201	4/4	0.99	0.13	70,70,97,97	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.

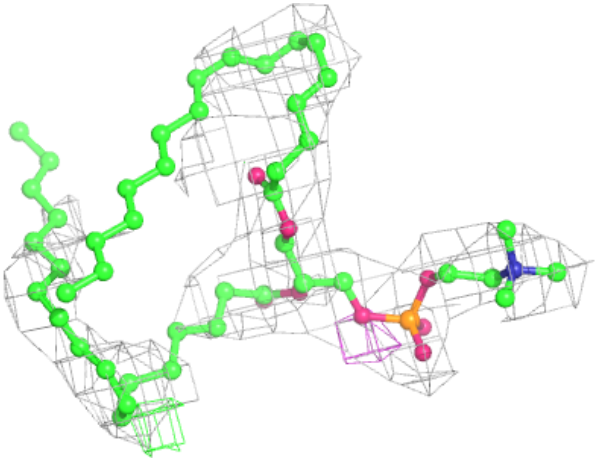
Electron density around BCR R 1101:

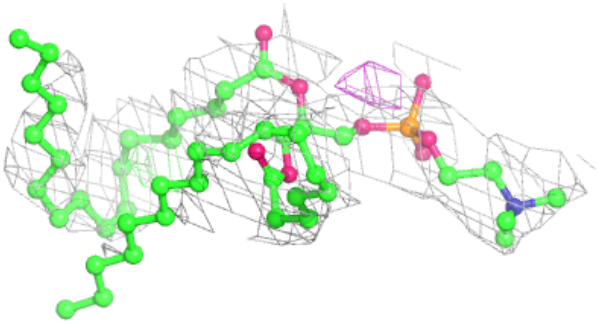
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

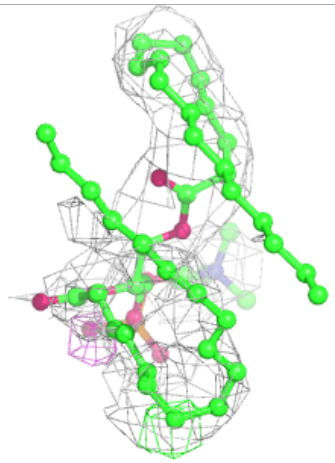


Electron density around OPC N 1305:

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

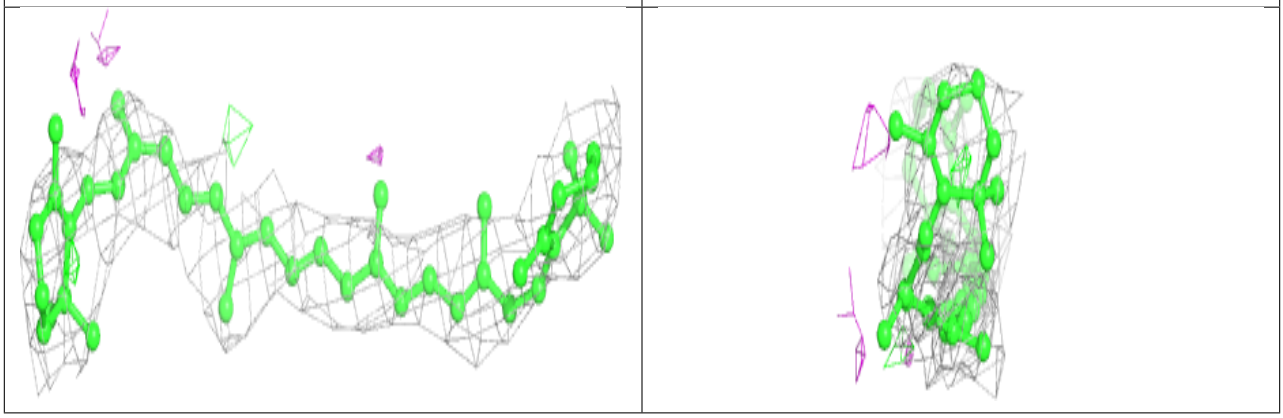






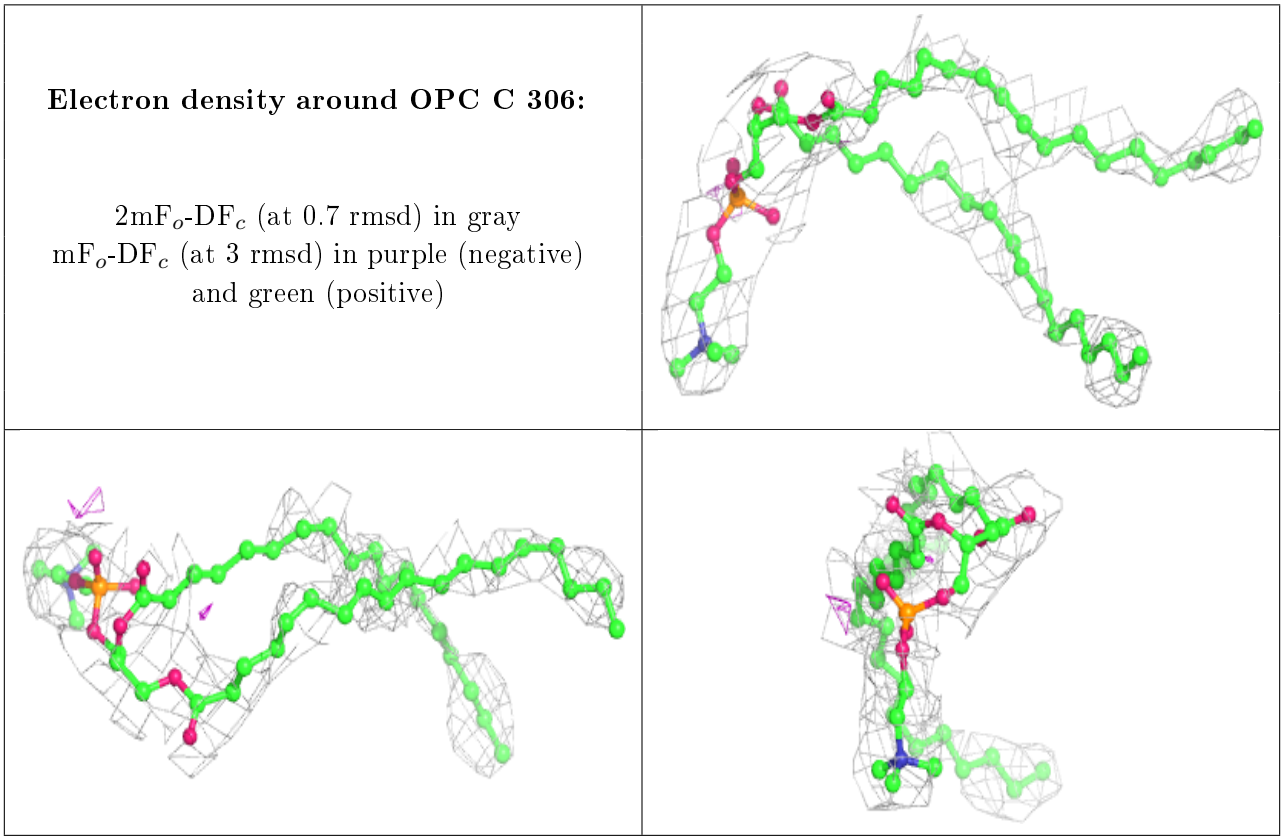
Electron density around BCR E 101:

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



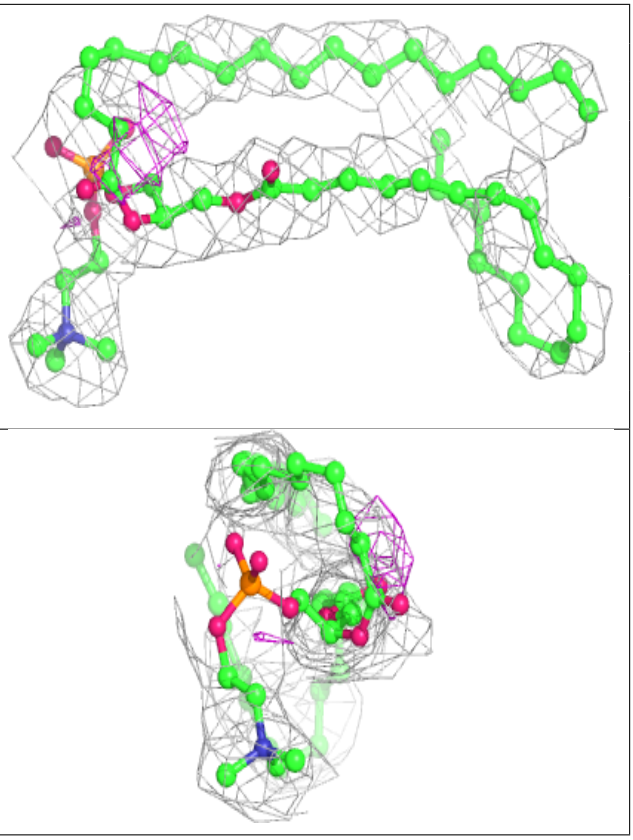
Electron density around OPC C 306:

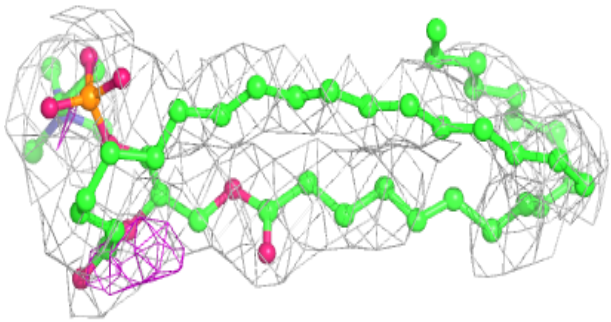
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around OPC O 1306:

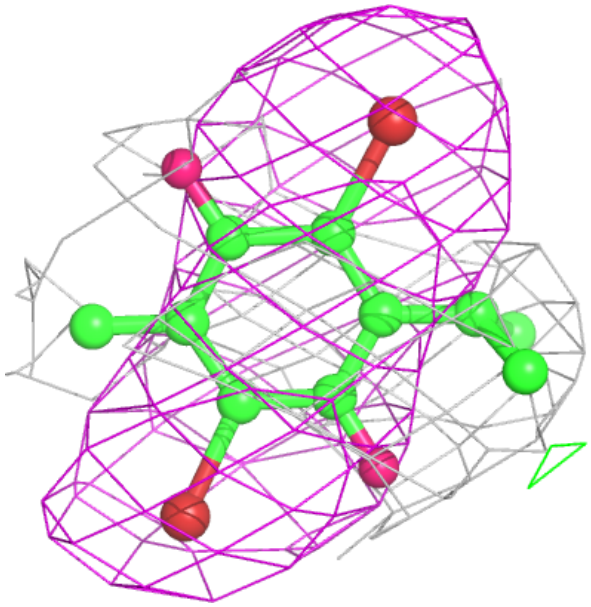
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

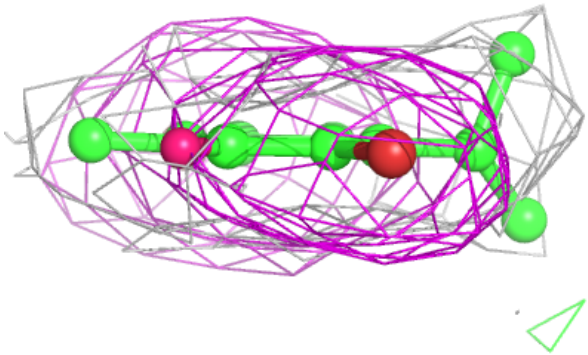


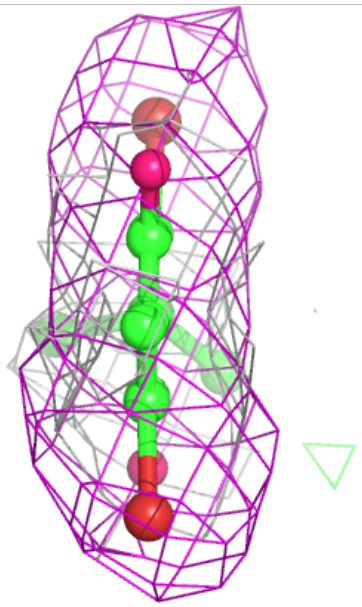


Electron density around BNT O 1309:

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

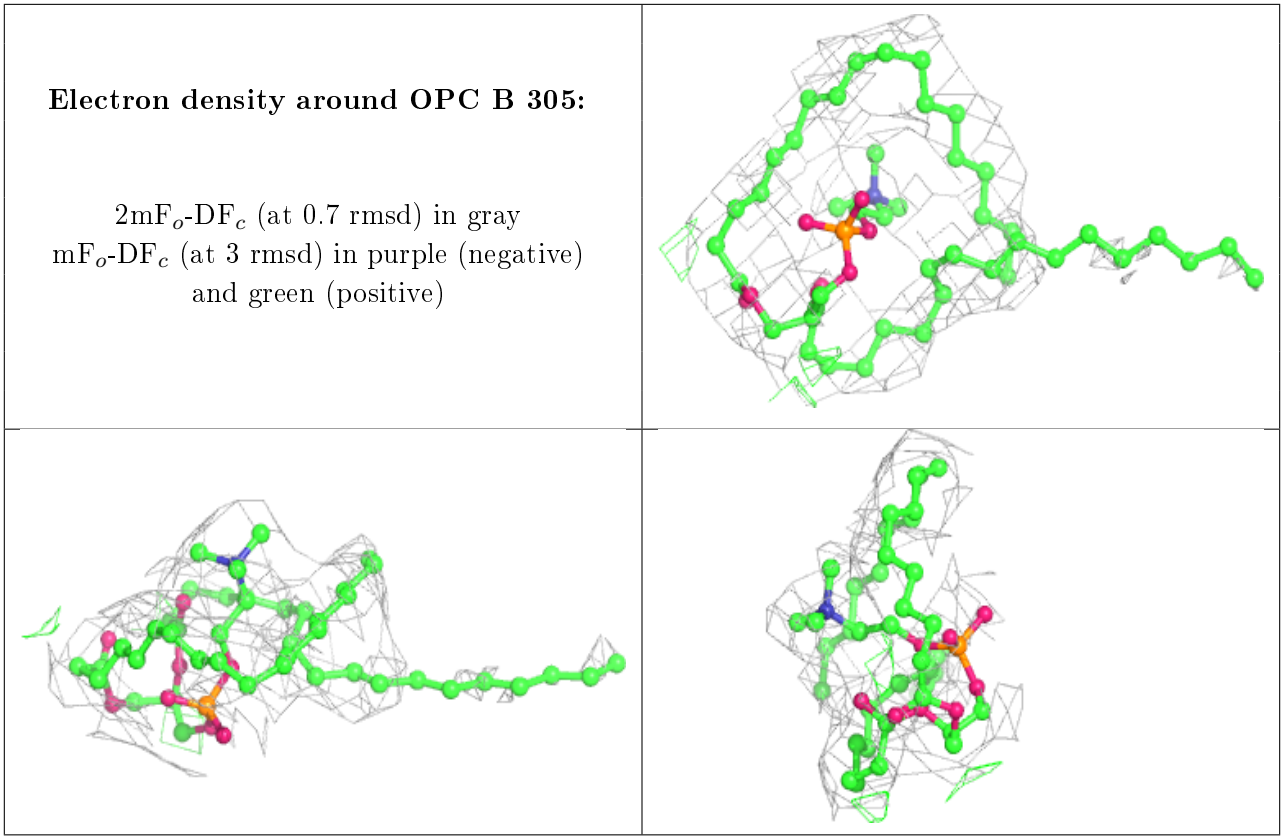






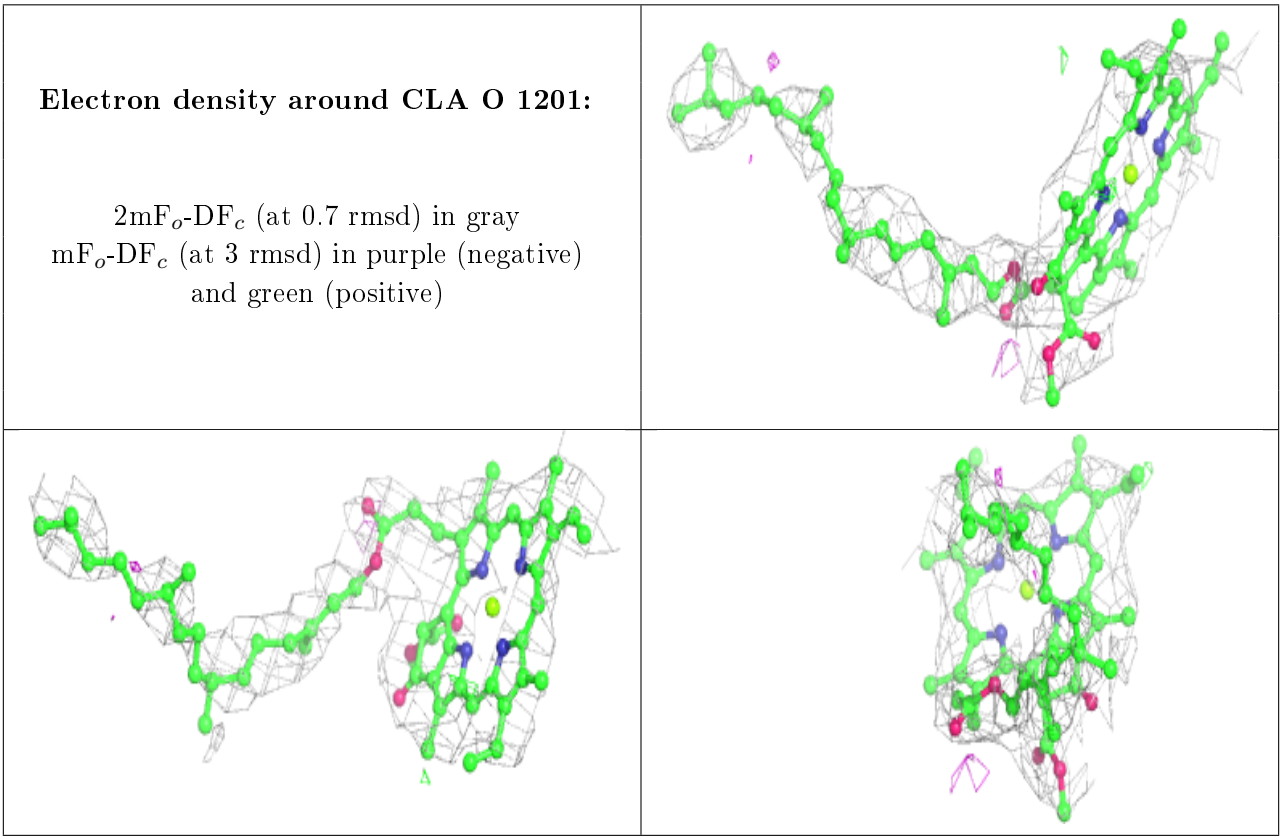
Electron density around OPC B 305:

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



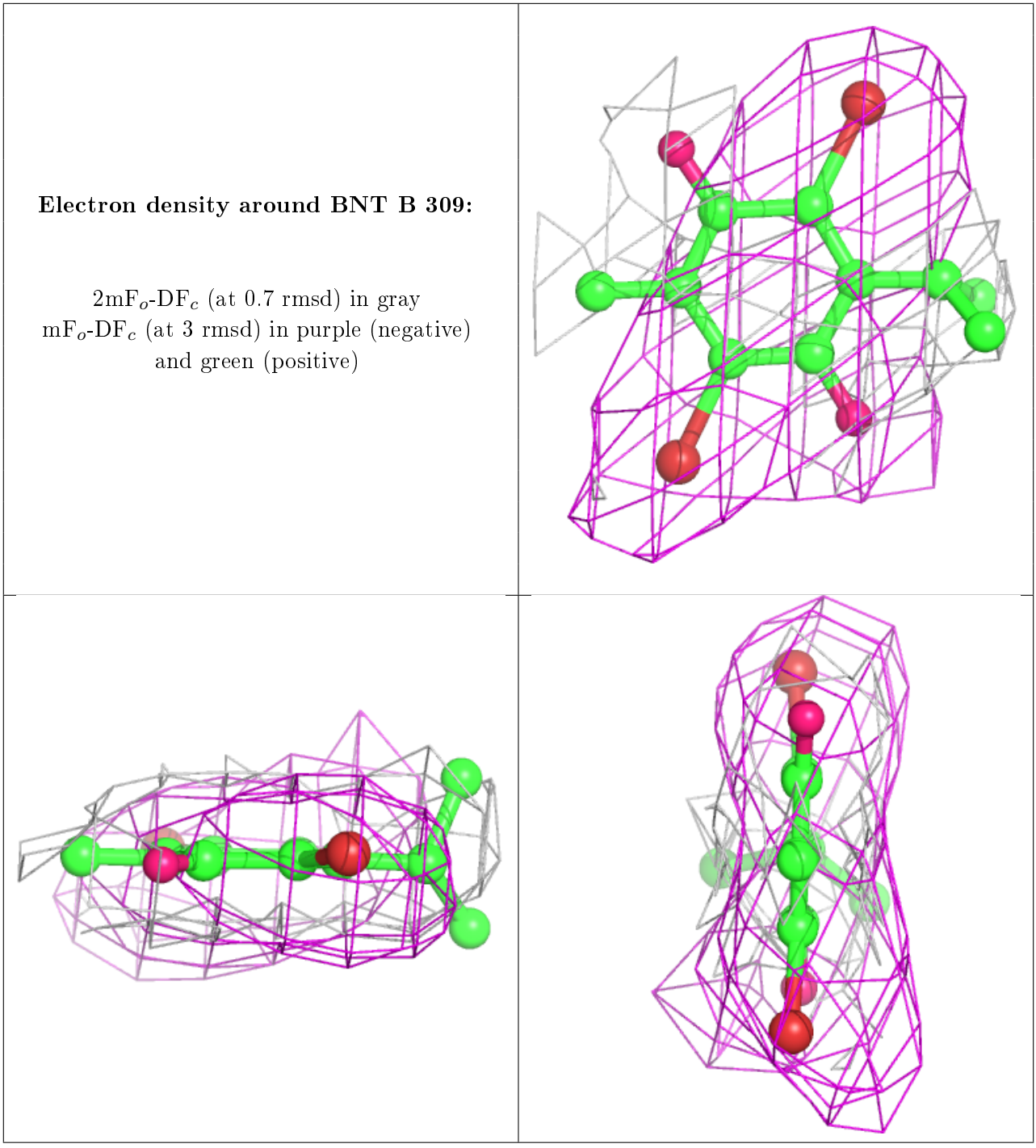
Electron density around CLA O 1201:

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



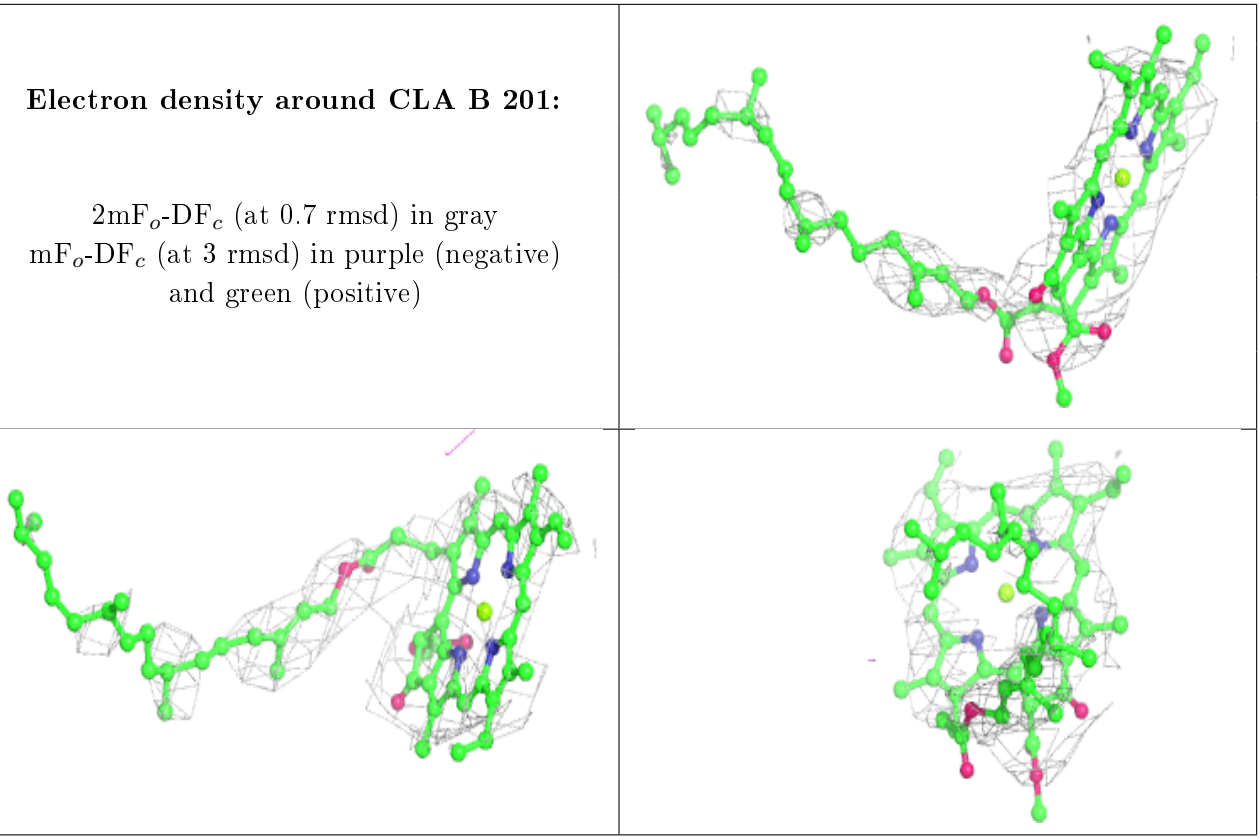
Electron density around BNT B 309:

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



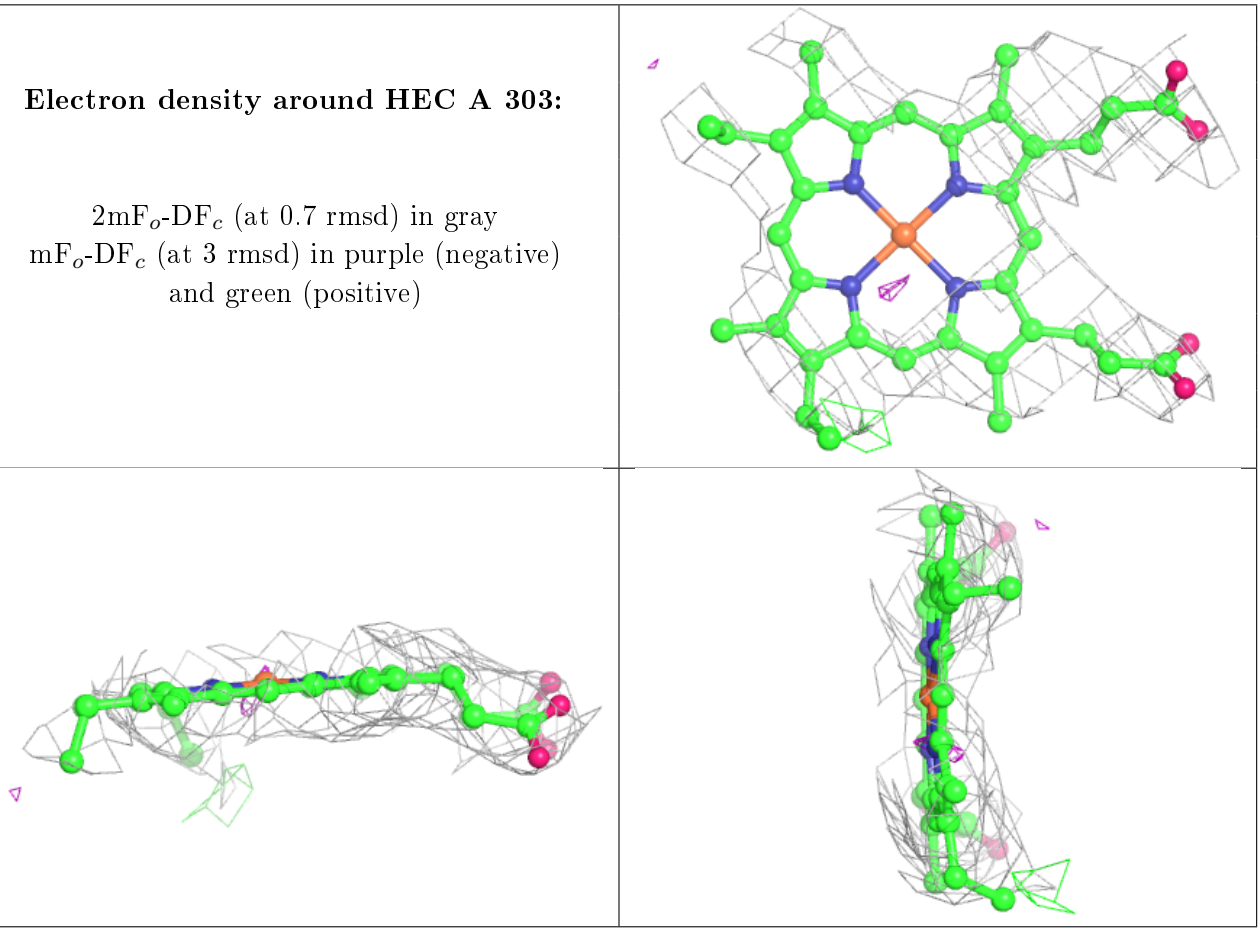
Electron density around CLA B 201:

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



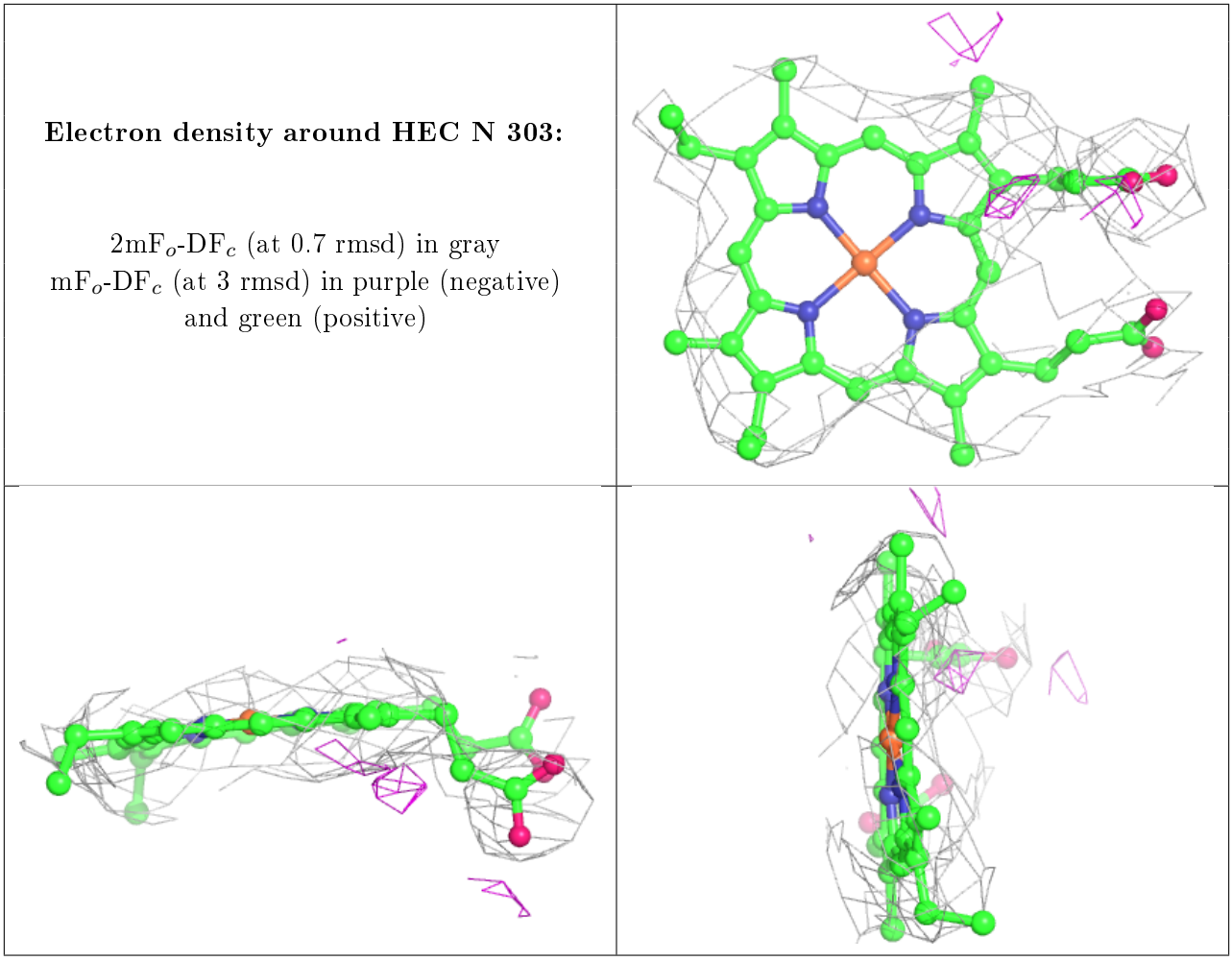
Electron density around HEC A 303:

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



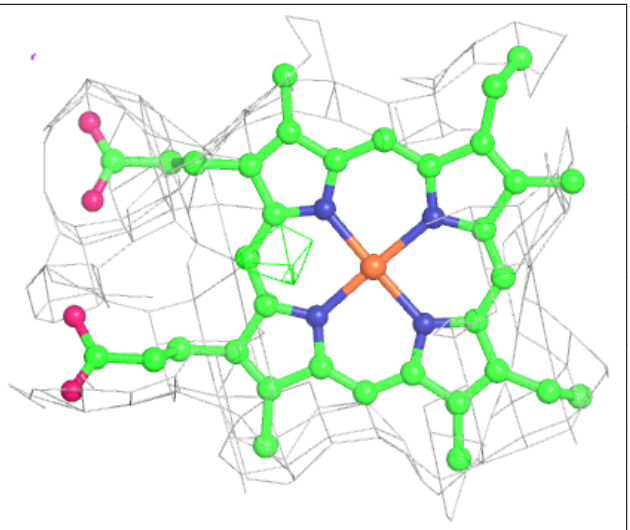
Electron density around HEC N 303:

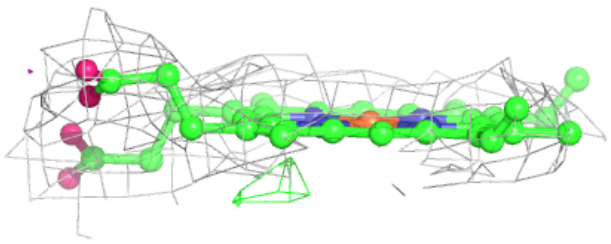
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

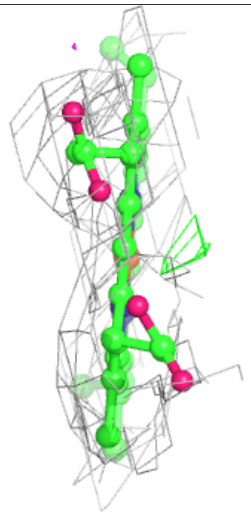


Electron density around HEM C 301:

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

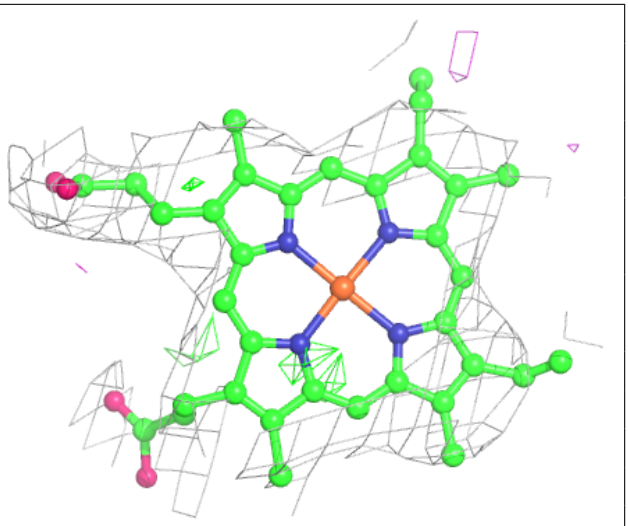


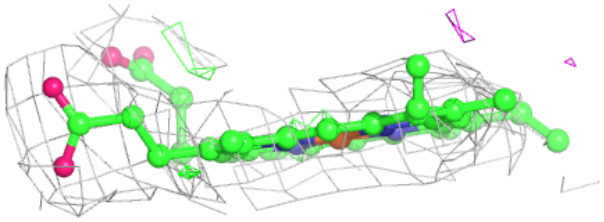


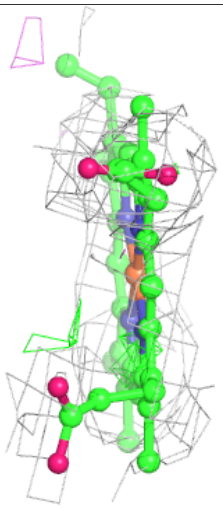


Electron density around HEM A 302:

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

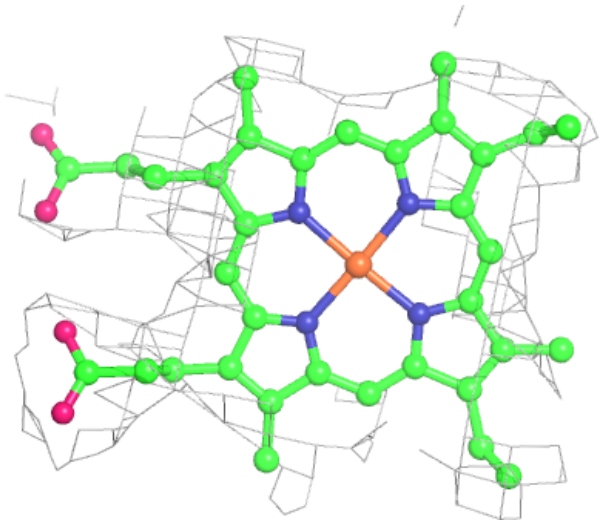


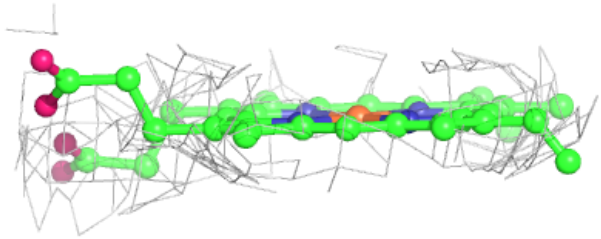


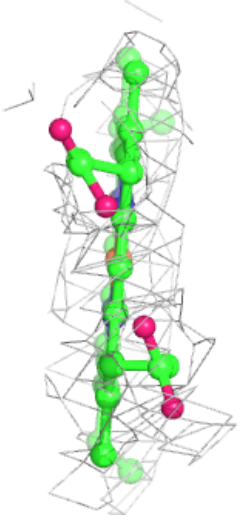


Electron density around HEM P 301:

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

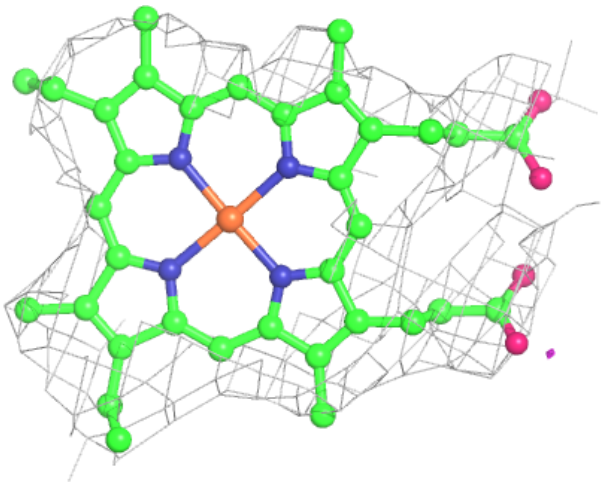


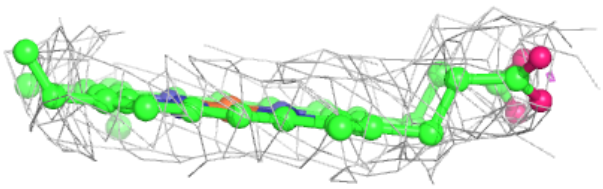


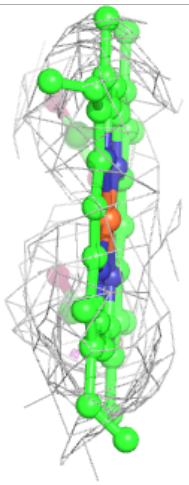


Electron density around HEM A 301:

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

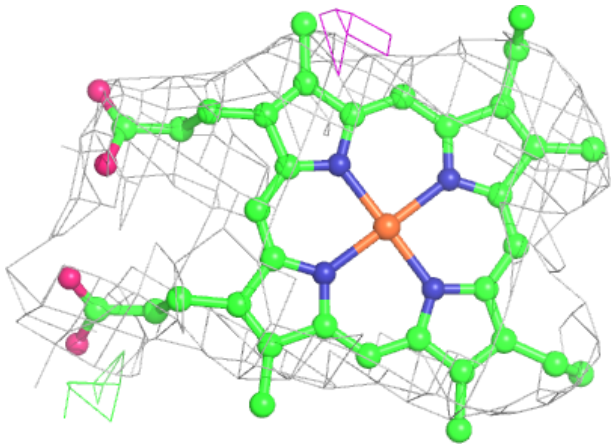


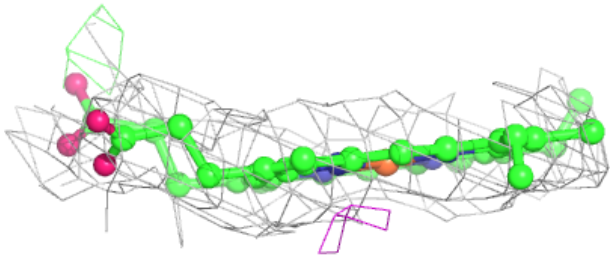


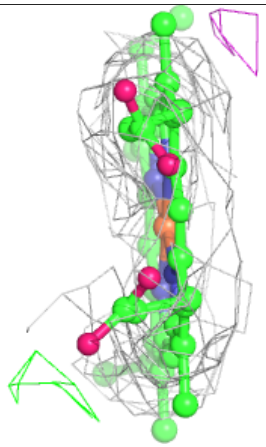


Electron density around HEM N 301:

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

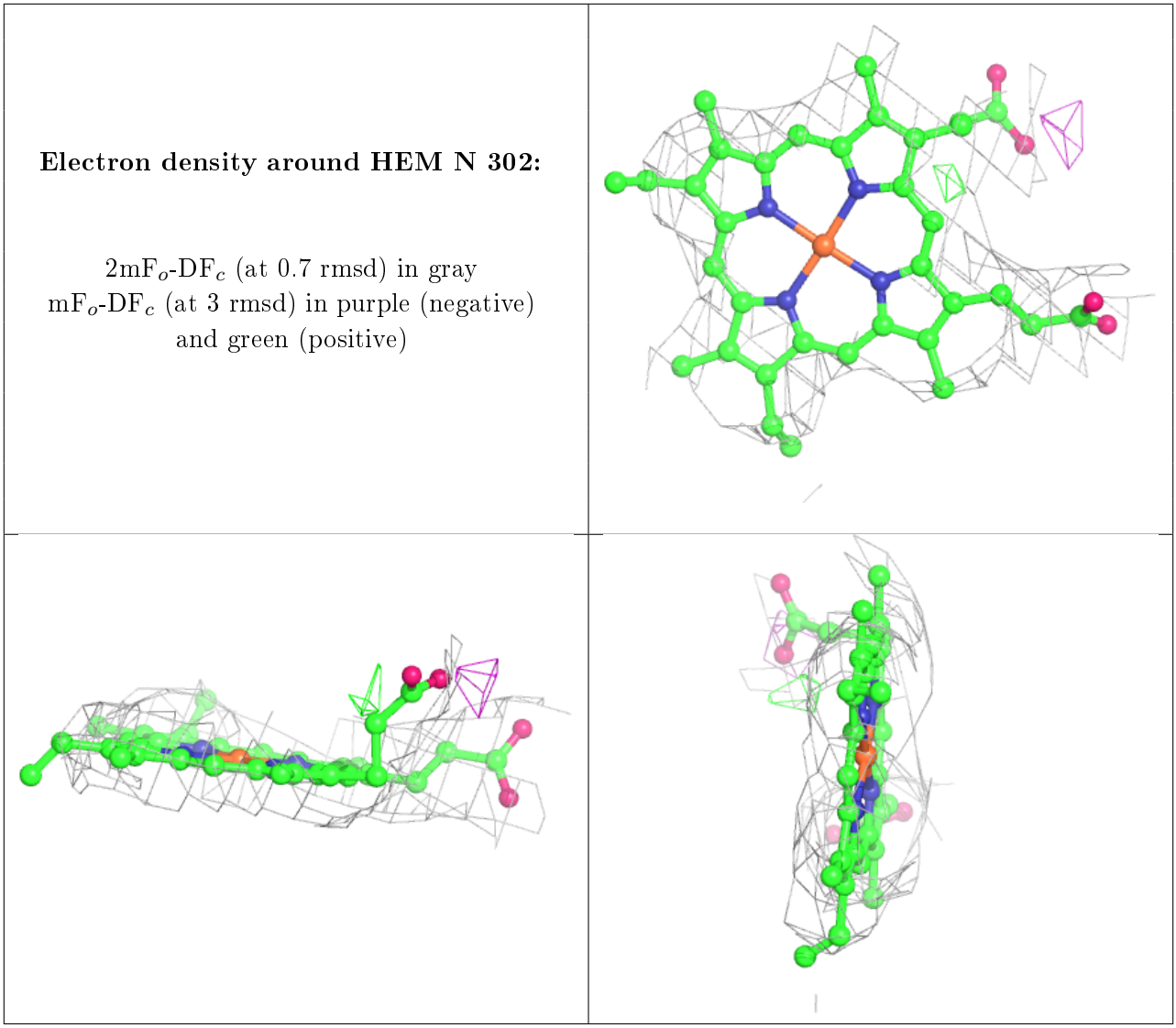






Electron density around HEM N 302:

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



6.5 Other polymers (i)

There are no such residues in this entry.