



# Full wwPDB X-ray Structure Validation Report ⓘ

May 26, 2020 – 03:23 pm BST

PDB ID : 1VF5  
Title : Crystal Structure of Cytochrome b6f Complex from M.laminosus  
Authors : Kurisu, G.; Zhang, H.; Smith, J.L.; Cramer, W.A.  
Deposited on : 2004-04-08  
Resolution : 3.00 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto: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.

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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

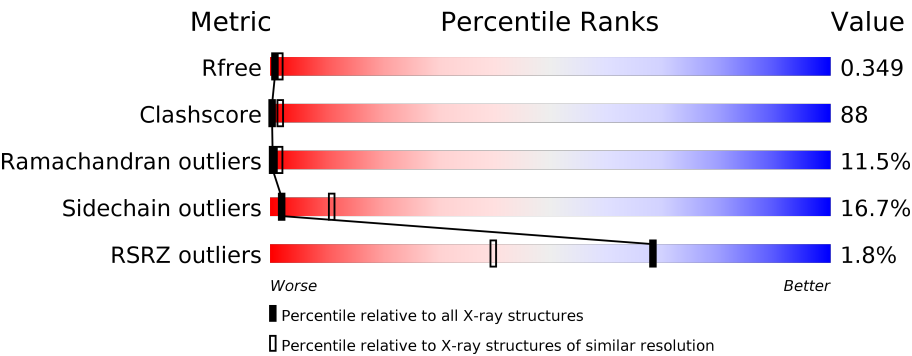
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	215	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>34%47%9%•6%</div></div>
1	N	215	<div><div></div><div></div><div></div><div></div><div></div></div> <div>34%47%12%•6%</div>
2	B	160	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>17%46%18%6%14%</div></div>
2	O	160	<div><div>2%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>16%45%19%6%14%</div></div>
3	C	289	<div><div>%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>27%56%14%••</div></div>
3	P	289	<div><div>3%</div><div><div></div><div></div><div></div><div></div><div></div></div><div>28%54%15%••</div></div>

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*Continued from previous page...*

Mol	Chain	Length	Quality of chain
4	D	179	
4	Q	179	
5	E	32	
5	R	32	
6	F	35	
6	S	35	
7	G	37	
7	T	37	
8	H	29	
8	U	29	

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	PL9	Q	1305	-	-	X	-
12	OPC	D	306	-	-	X	-
12	OPC	Q	1307	-	-	X	-
13	CLA	B	201	X	-	-	-
13	CLA	O	1201	X	-	-	-

## 2 Entry composition

There are 16 unique types of molecules in this entry. The entry contains 15091 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 SUBUNIT IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	138	Total	C	N	O	S	0	0	0
			1075	727	165	178	5			
2	O	138	Total	C	N	O	S	0	0	0
			1075	727	165	178	5			

- Molecule 3 is a protein called CYTOCHROME 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 RIESKE IRON-SULFUR PROTEIN.

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			

- Molecule 5 is a protein called PROTEIN PET L.

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 PROTEIN PET M.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	F	33	Total	C	N	O	S	0	0	0
			251	170	36	43	2			
6	S	35	Total	C	N	O	S	0	0	0
			270	181	39	48	2			

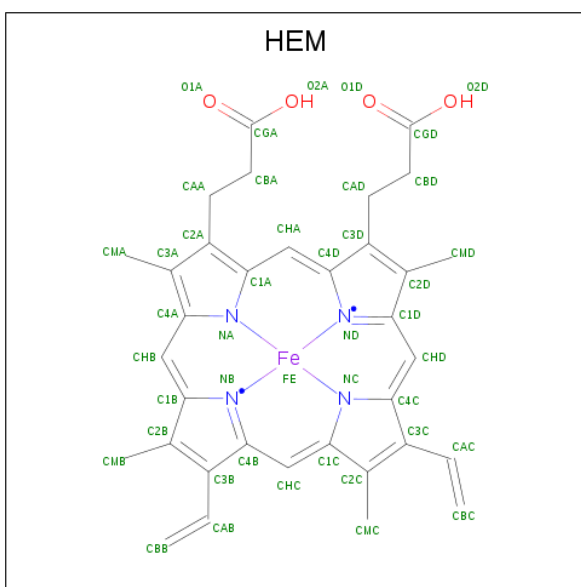
- Molecule 7 is a protein called PROTEIN PET G.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	G	23	Total	C	N	O	0	0	0
			184	126	29	29			
7	T	27	Total	C	N	O	0	0	0
			216	146	34	36			

- Molecule 8 is a protein called PROTEIN PET N.

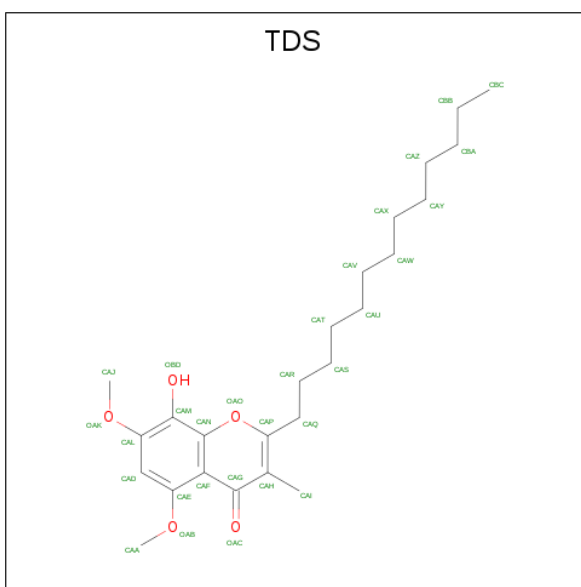
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
8	H	27	Total	C	N	O	S	0	0	0
			214	146	34	33	1			
8	U	27	Total	C	N	O	S	0	0	0
			214	146	34	33	1			

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



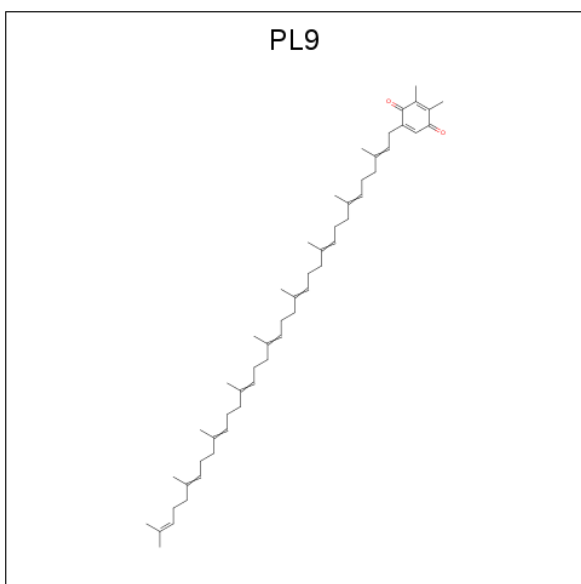
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	C	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	N	1	Total 43	C 34	Fe 1	N 4	O 4	0	0
9	N	1	Total 43	C 34	Fe 1	N 4	O 4	0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

- Molecule 10 is 8-HYDROXY-5,7-DIMETHOXY-3-METHYL-2-TRIDECYL-4H-CHROME N-4-ONE (three-letter code: TDS) (formula:  $C_{25}H_{38}O_5$ ).



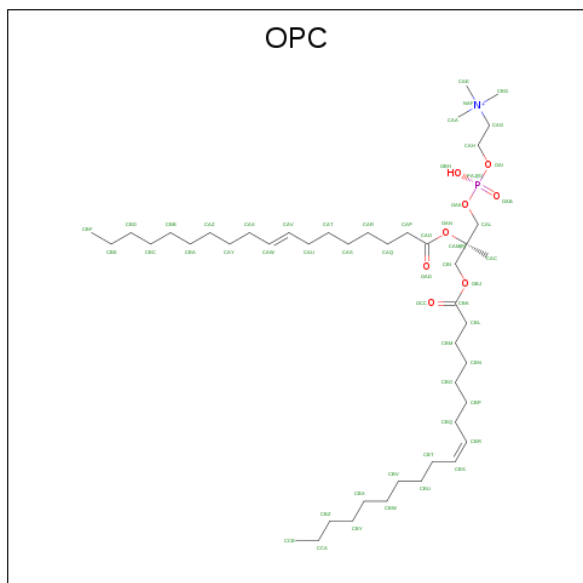
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	A	1	Total 30	C 25	O 5	0	0
10	N	1	Total 30	C 25	O 5	0	0

- Molecule 11 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:  $C_{53}H_{80}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
11	A	1	Total	C	O	0	0
			55	53	2		
11	Q	1	Total	C	O	0	0
			55	53	2		

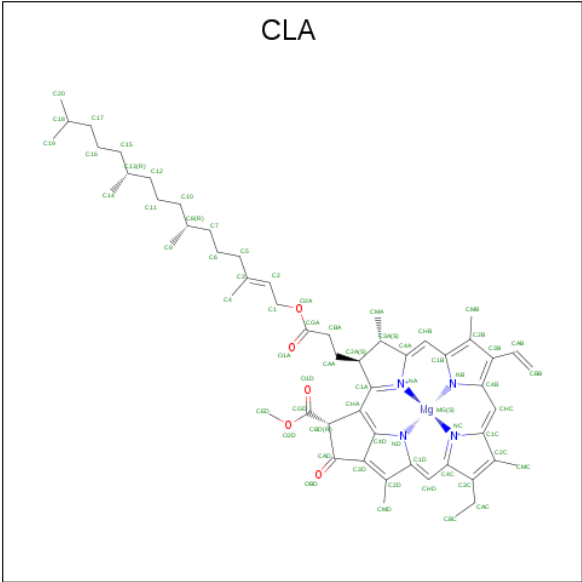
- Molecule 12 is (7R,17E)-4-HYDROXY-N,N,N,7-TETRAMETHYL-7-[(8E)-OCTADEC-8-ENOYLOXY]-10-OXO-3,5,9-TRIOXA-4-PHOSPHAHEPTACOS-17-EN-1-AMINIUM 4-OXIDE (three-letter code: OPC) (formula: C<sub>45</sub>H<sub>87</sub>NO<sub>8</sub>P).



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

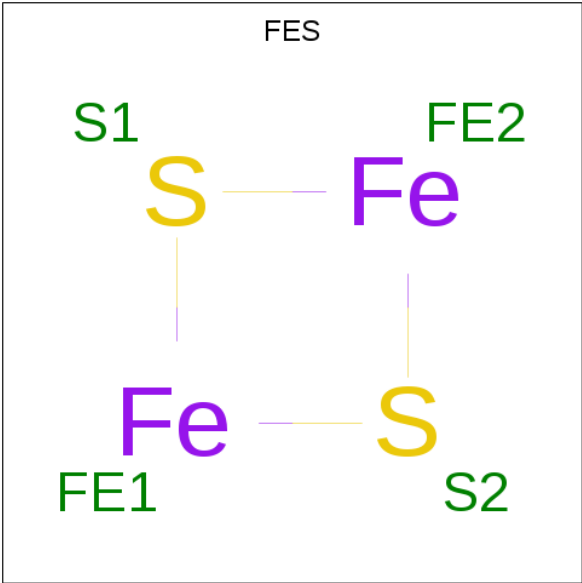
- Molecule 13 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).





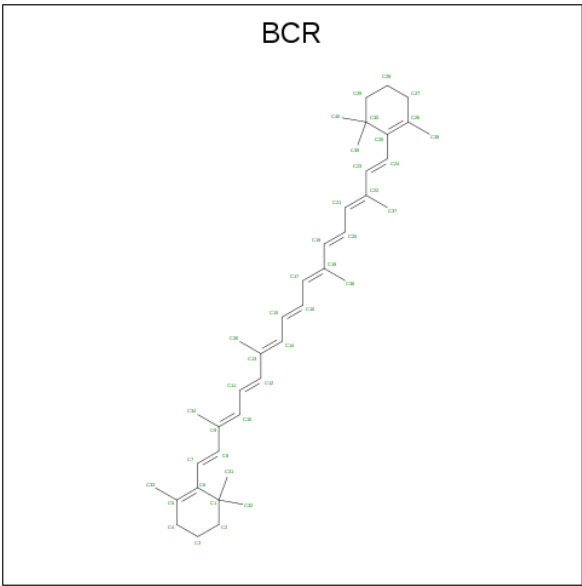
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
13	B	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		
13	O	1	Total	C	Mg	N	O	0	0
			65	55	1	4	5		

- Molecule 14 is FE2/S2 (INORGANIC) CLUSTER (three-letter code: FES) (formula: Fe<sub>2</sub>S<sub>2</sub>).



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<sub>40</sub>H<sub>56</sub>).



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

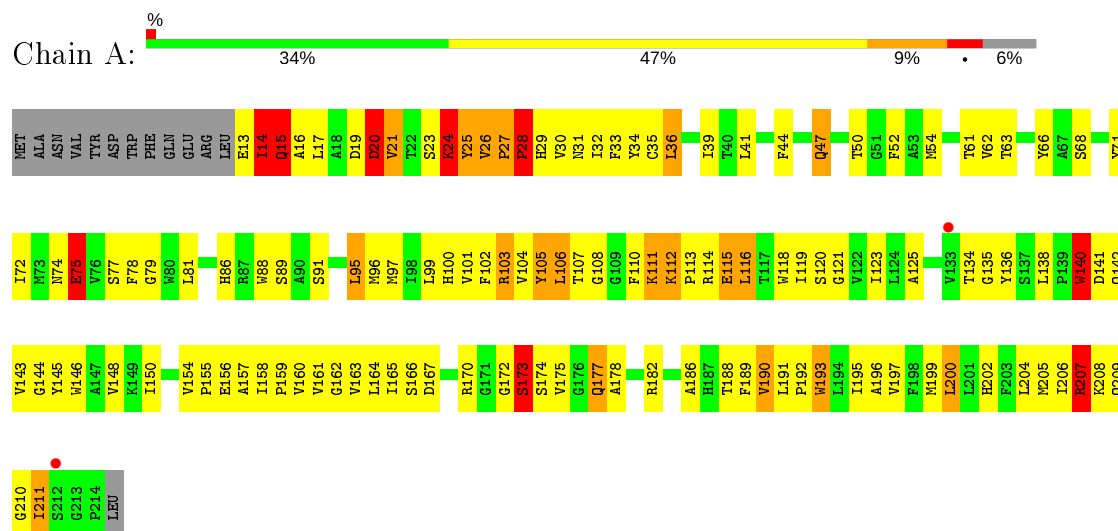
- Molecule 16 is water.

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

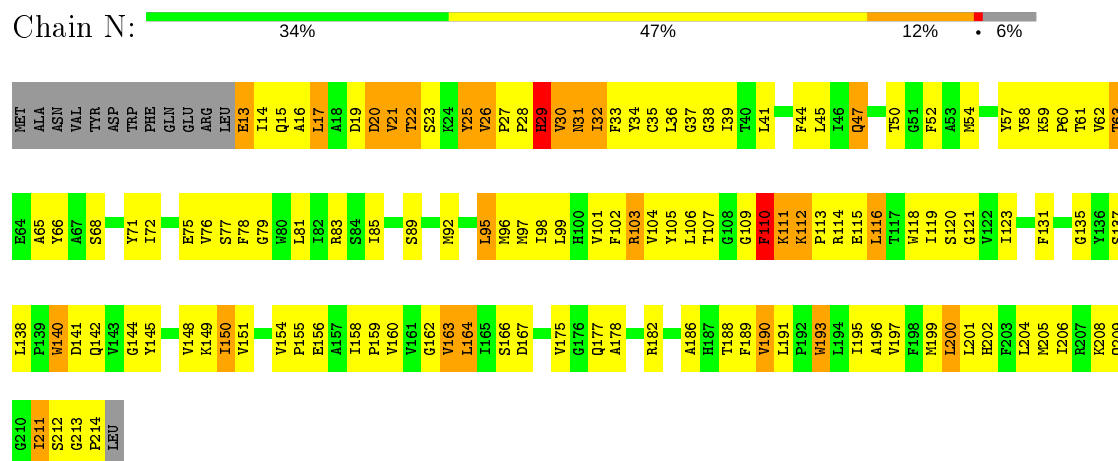
### 3 Residue-property plots [i](#)

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.

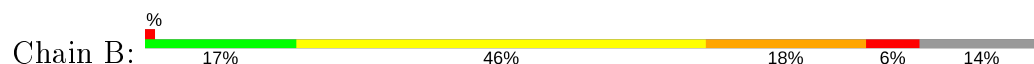
#### • Molecule 1: CYTOCHROME B6

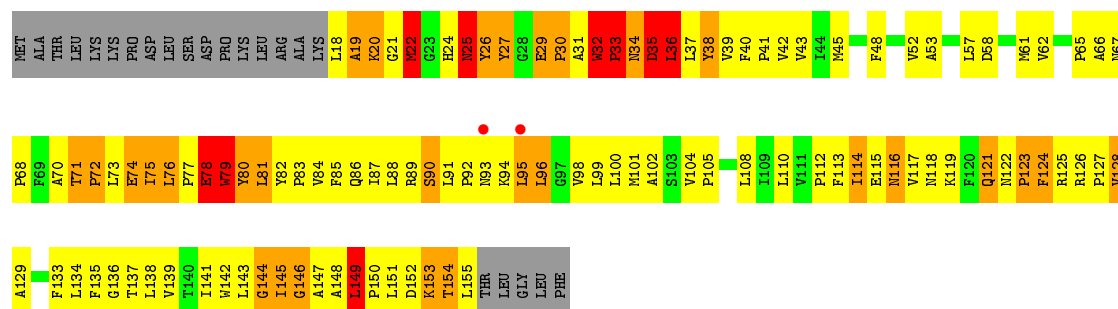


#### • Molecule 1: CYTOCHROME B6

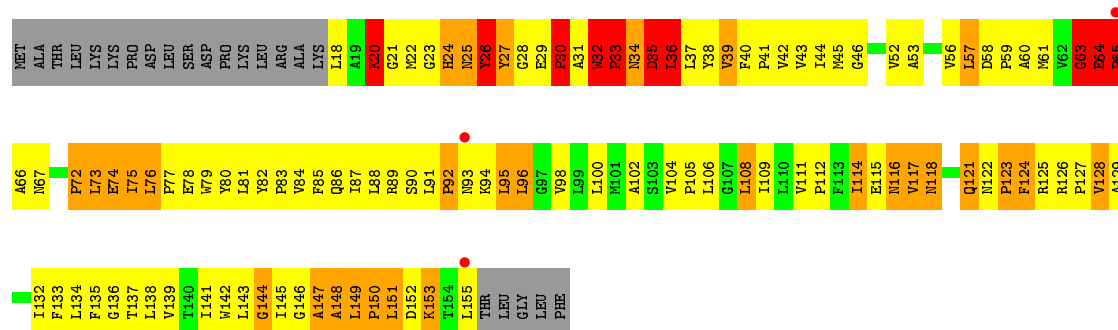
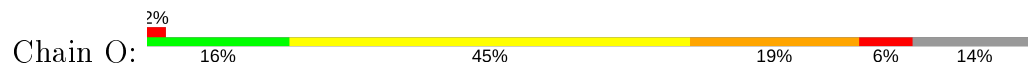


#### • Molecule 2: SUBUNIT IV

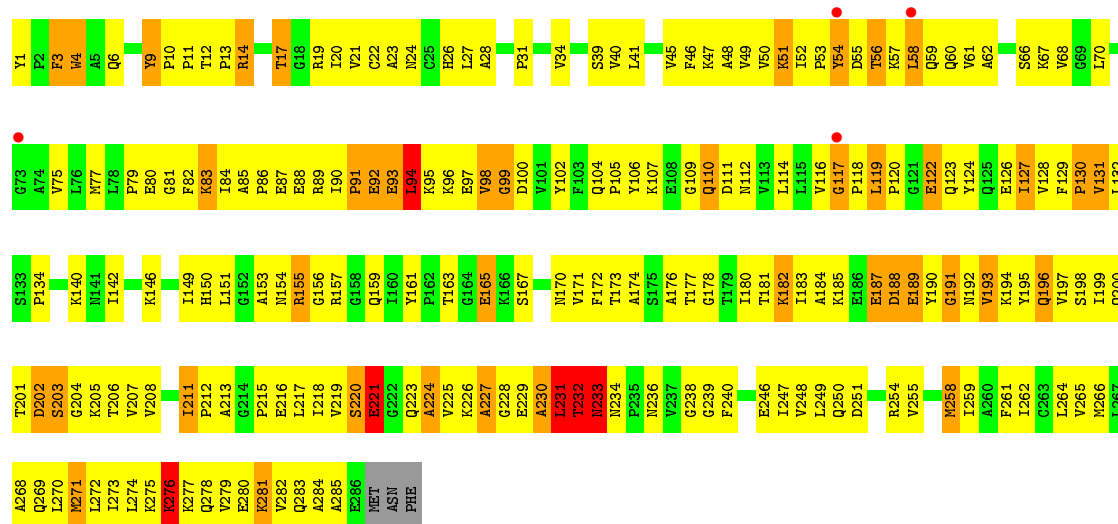




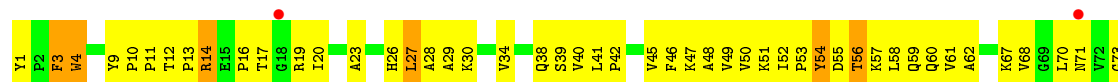
### • Molecule 2: SUBUNIT IV

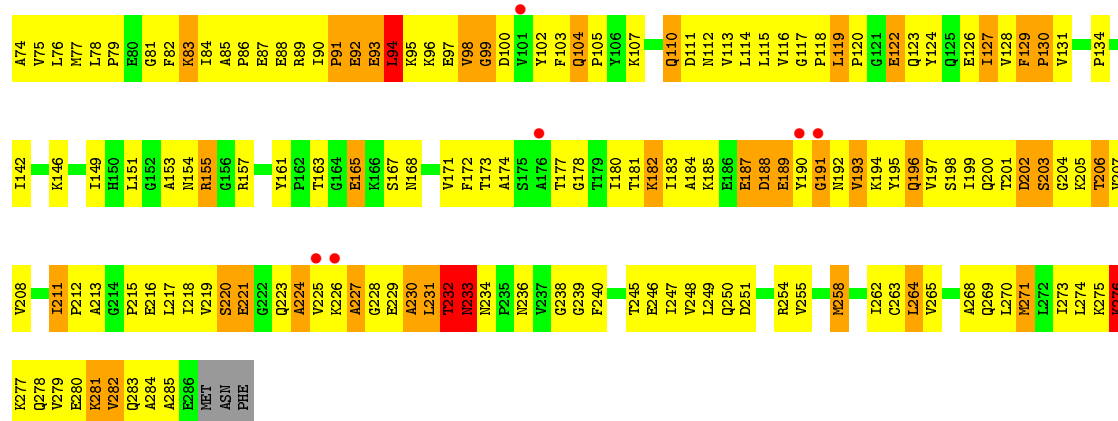


### • Molecule 3: CYTOCHROME F

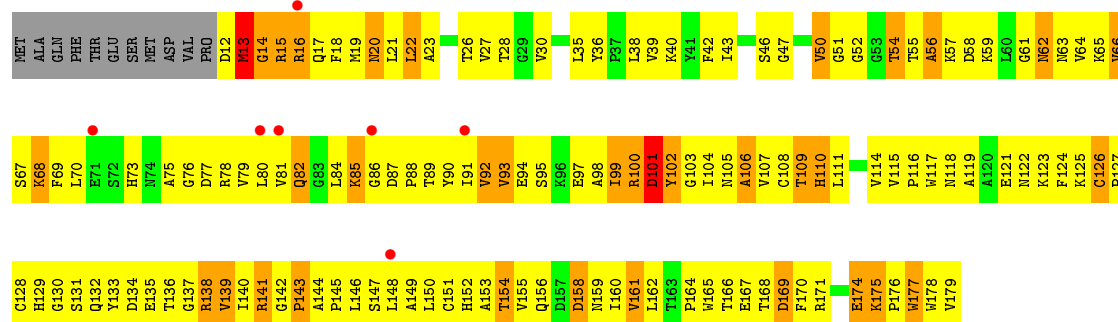
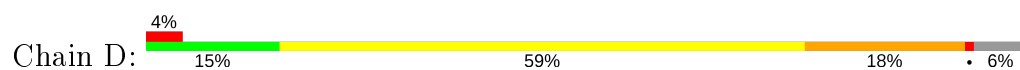


### • Molecule 3: CYTOCHROME F

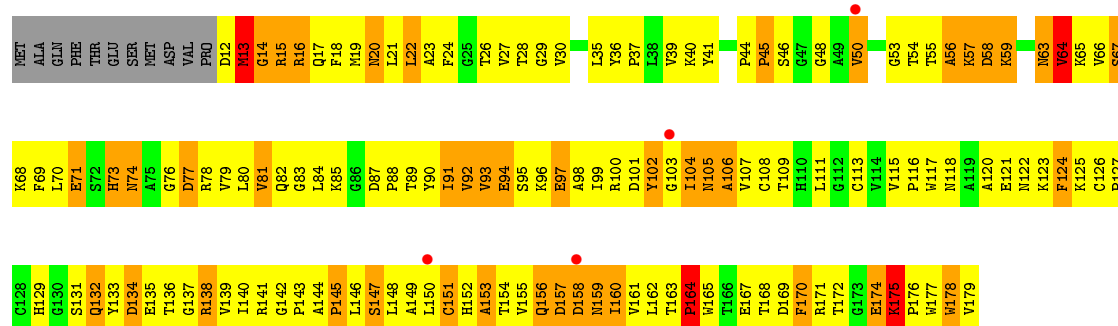
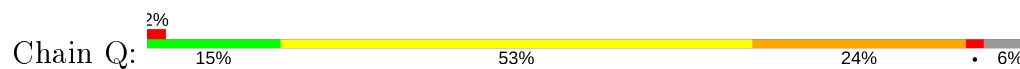




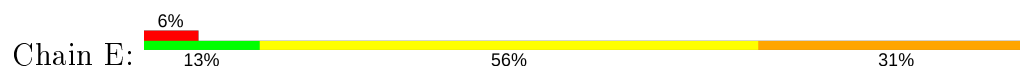
• Molecule 4: RIESKE IRON-SULFUR PROTEIN



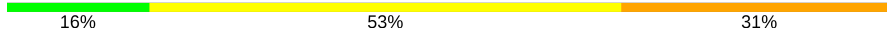
• Molecule 4: RIESKE IRON-SULFUR PROTEIN



• Molecule 5: PROTEIN PET L



• Molecule 5: PROTEIN PET L

Chain R:  16% 53% 31%



- Molecule 6: PROTEIN PET M

Chain F:  34% 51% 9% 6%



- Molecule 6: PROTEIN PET M

Chain S:  23% 66% 9% .



- Molecule 7: PROTEIN PET G

Chain G:  3% 8% 35% 19% 38%

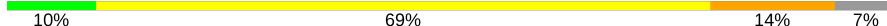


- Molecule 7: PROTEIN PET G

Chain T:  11% 38% 24% 27%



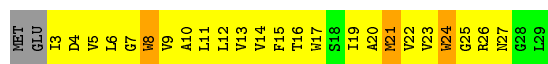
- Molecule 8: PROTEIN PET N

Chain H:  10% 69% 14% 7%



- Molecule 8: PROTEIN PET N

Chain U:  10% 72% 10% 7%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	157.54Å 157.54Å 360.35Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.16 – 3.00 48.16 – 3.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.16-3.00) 99.8 (48.16-3.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.30 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.258 , 0.346 0.259 , 0.349	Depositor DCC
$R_{free}$ test set	2788 reflections (2.77%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	76.0	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 104.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.499 for h,-h-k,-l	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	15091	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.26% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CLA, PL9, FES, OPC, TDS, 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	0.55	0/1641	0.77	2/2239 (0.1%)
1	N	0.56	0/1641	0.81	2/2239 (0.1%)
2	B	0.54	0/1110	0.88	3/1526 (0.2%)
2	O	0.58	0/1110	0.99	8/1526 (0.5%)
3	C	0.44	0/2248	0.73	1/3061 (0.0%)
3	P	0.45	0/2248	0.72	0/3061
4	D	0.47	0/1312	0.86	2/1786 (0.1%)
4	Q	0.47	0/1312	0.76	0/1786
5	E	0.67	0/253	0.80	0/340
5	R	0.64	0/253	0.77	0/340
6	F	0.58	0/255	0.66	0/343
6	S	0.52	0/274	0.61	0/366
7	G	0.64	0/188	0.91	0/253
7	T	0.63	0/221	0.95	0/299
8	H	0.61	0/220	0.83	1/301 (0.3%)
8	U	0.59	0/220	0.81	0/301
All	All	0.52	0/14506	0.80	19/19767 (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	N	0	1

There are no bond length outliers.

All (19) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	63	GLY	N-CA-C	7.67	132.29	113.10
2	B	36	LEU	N-CA-C	-7.09	91.85	111.00
2	O	64	GLU	N-CA-C	6.99	129.88	111.00
2	O	36	LEU	N-CA-C	-6.86	92.47	111.00
1	N	20	ASP	N-CA-C	6.33	128.08	111.00
2	O	117	VAL	N-CA-C	-6.17	94.34	111.00
1	A	207	ARG	N-CA-C	-5.99	94.84	111.00
2	B	144	GLY	N-CA-C	-5.87	98.42	113.10
2	O	144	GLY	N-CA-C	-5.82	98.55	113.10
2	B	35	ASP	N-CA-C	5.52	125.89	111.00
1	A	31	ASN	N-CA-C	5.51	125.89	111.00
2	O	35	ASP	N-CA-C	5.50	125.84	111.00
1	N	29	HIS	N-CA-C	5.40	125.59	111.00
4	D	54	THR	N-CA-C	5.38	125.52	111.00
3	C	231	LEU	CA-CB-CG	5.27	127.43	115.30
4	D	46	SER	N-CA-C	5.27	125.23	111.00
2	O	20	LYS	N-CA-C	5.16	124.94	111.00
2	O	39	VAL	N-CA-C	-5.01	97.47	111.00
8	H	5	VAL	N-CA-C	-5.00	97.49	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	105	TYR	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1593	0	1623	242	0
1	N	1593	0	1623	230	0
2	B	1075	0	1117	258	0
2	O	1075	0	1117	284	0
3	C	2200	0	2216	355	0
3	P	2200	0	2216	338	0
4	D	1280	0	1263	317	0
4	Q	1280	0	1263	380	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
5	E	248	0	284	72	0
5	R	248	0	284	113	0
6	F	251	0	266	39	0
6	S	270	0	285	42	0
7	G	184	0	190	104	0
7	T	216	0	220	70	0
8	H	214	0	221	42	0
8	U	214	0	221	43	0
9	A	129	0	90	18	0
9	C	43	0	30	0	0
9	N	129	0	90	17	0
9	P	43	0	30	1	0
10	A	30	0	37	13	0
10	N	30	0	37	12	0
11	A	55	0	80	18	0
11	Q	55	0	80	23	0
12	B	54	0	83	14	0
12	D	54	0	83	24	0
12	N	54	0	83	10	0
12	Q	54	0	83	30	0
13	B	65	0	70	8	0
13	O	65	0	70	20	0
14	D	4	0	0	1	0
14	Q	4	0	0	1	0
15	E	40	0	56	7	0
15	R	40	0	56	7	0
16	A	1	0	0	0	0
16	N	1	0	0	0	0
All	All	15091	0	15467	2688	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 88.

All (2688) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:38:TYR:HB3	3:P:276:LYS:HG2	1.22	1.20
1:A:14:ILE:HA	1:A:17:LEU:HB2	1.26	1.18
1:N:214:PRO:HB3	5:R:29:ILE:HG22	1.19	1.17
4:D:166:THR:HA	4:D:179:VAL:HG13	1.22	1.17
2:B:71:THR:HB	2:B:72:PRO:HD3	1.28	1.15

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:A:305:PL9:H412	11:A:305:PL9:H462	1.18	1.13
2:B:20:LYS:HG3	2:B:21:GLY:H	1.05	1.13
11:Q:1305:PL9:H212	11:Q:1305:PL9:H262	1.24	1.12
12:D:306:OPC:HBI1	12:D:306:OPC:HAP2	1.31	1.12
5:E:7:PHE:HA	5:E:10:VAL:HG12	1.29	1.11
4:Q:169:ASP:HB2	4:Q:176:PRO:HA	1.32	1.11
12:Q:1307:OPC:HBE1	12:Q:1307:OPC:HBU2	1.11	1.11
4:Q:94:GLU:HB3	4:Q:100:ARG:HD3	1.18	1.10
4:D:136:THR:HB	4:D:138:ARG:HD2	1.25	1.10
4:Q:168:THR:HA	4:Q:176:PRO:HD3	1.19	1.10
4:D:124:PHE:HB2	4:D:133:TYR:HB2	1.32	1.09
2:B:126:ARG:HE	2:B:128:VAL:HG23	0.99	1.08
3:C:255:VAL:HG11	7:G:14:VAL:HG12	1.36	1.08
2:O:118:ASN:HD22	2:O:121:GLN:NE2	1.51	1.08
5:E:5:ALA:HB1	6:F:9:ALA:HB2	1.35	1.08
3:C:273:ILE:HD13	7:G:30:LYS:HD3	1.20	1.07
2:O:132:ILE:HG22	13:O:1201:CLA:HBB2	1.35	1.07
4:Q:156:GLN:HB2	4:Q:161:VAL:HG21	1.37	1.07
3:C:172:PHE:H	3:C:231:LEU:HG	1.17	1.07
5:R:7:PHE:HA	5:R:10:VAL:HG12	1.34	1.06
4:D:66:VAL:HG22	4:D:160:ILE:HG13	1.07	1.06
1:N:27:PRO:HG3	2:O:33:PRO:HG3	1.34	1.06
4:Q:76:GLY:H	4:Q:93:VAL:HG13	1.12	1.06
2:O:64:GLU:HG3	2:O:65:PRO:HD3	1.37	1.05
7:T:25:ALA:HB1	7:T:29:TYR:CZ	1.89	1.05
1:A:209:GLN:HG2	1:A:210:GLY:H	1.19	1.05
11:A:305:PL9:H203	12:D:306:OPC:HBE2	1.37	1.05
5:R:5:ALA:HB1	6:S:9:ALA:HB2	1.30	1.05
5:E:16:PHE:HB3	15:E:101:BCR:H363	1.36	1.05
12:N:1306:OPC:HAP2	12:N:1306:OPC:HBI1	1.39	1.05
3:C:281:LYS:HA	3:C:284:ALA:HB3	1.34	1.04
4:D:70:LEU:HD12	4:D:160:ILE:HD11	1.34	1.04
1:N:29:HIS:O	1:N:30:VAL:HG13	1.56	1.04
4:Q:56:ALA:HA	4:Q:81:VAL:HG13	1.36	1.03
3:P:281:LYS:HA	3:P:284:ALA:HB3	1.37	1.03
3:C:278:GLN:HE21	7:G:30:LYS:HE2	1.20	1.03
4:D:155:VAL:HG22	4:D:160:ILE:HG12	1.39	1.03
3:C:93:GLU:HA	3:C:97:GLU:HB2	1.38	1.02
1:A:207:ARG:HB2	1:A:207:ARG:HH11	1.21	1.02
4:D:51:GLY:HA2	4:D:164:PRO:HG2	1.35	1.02
2:B:18:LEU:HD13	2:B:31:ALA:HB2	1.42	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:25:ALA:HB1	7:G:29:TYR:CZ	1.95	1.01
4:Q:155:VAL:HG12	4:Q:157:ASP:H	1.21	1.01
3:C:172:PHE:O	3:C:231:LEU:HB3	1.60	1.01
5:R:16:PHE:HB3	15:R:1101:BCR:H363	1.38	1.01
2:O:124:PHE:CZ	5:R:26:ILE:HB	1.95	1.01
4:Q:116:PRO:HD2	4:Q:126:CYS:HA	1.41	1.00
3:C:271:MET:HG3	4:D:22:LEU:HD21	1.37	1.00
3:C:28:ALA:HB2	3:C:236:ASN:HD21	1.24	1.00
3:C:262:ILE:HG13	7:G:21:LEU:HG	1.38	1.00
7:G:26:TYR:HA	7:G:29:TYR:CD1	1.97	1.00
5:R:9:ILE:HG21	6:S:9:ALA:O	1.62	1.00
4:D:123:LYS:HB3	4:D:133:TYR:O	1.62	0.99
3:P:94:LEU:HD22	3:P:94:LEU:H	1.28	0.99
2:B:20:LYS:HG3	2:B:21:GLY:N	1.70	0.99
4:D:116:PRO:HG3	4:D:127:PRO:HD3	1.40	0.99
2:B:31:ALA:O	2:B:32:TRP:HB2	1.59	0.98
1:N:61:THR:HG22	1:N:63:THR:H	1.26	0.98
4:Q:57:LYS:HG3	4:Q:82:GLN:HE21	1.27	0.98
7:T:23:TYR:HA	7:T:26:TYR:CG	1.98	0.98
3:P:28:ALA:HB2	3:P:236:ASN:HD21	1.29	0.98
1:A:29:HIS:NE2	1:A:30:VAL:HG22	1.79	0.97
2:B:149:LEU:CD1	2:B:150:PRO:HD2	1.94	0.97
3:P:202:ASP:HA	3:P:206:THR:HB	1.43	0.97
4:D:51:GLY:HA2	4:D:164:PRO:CG	1.95	0.97
3:C:202:ASP:HA	3:C:206:THR:HB	1.45	0.97
3:C:218:ILE:H	3:C:232:THR:HB	1.28	0.97
3:P:146:LYS:HD3	3:P:246:GLU:HG3	1.46	0.97
2:B:61:MET:HB2	3:C:146:LYS:HD2	1.47	0.97
1:A:207:ARG:NH1	1:A:207:ARG:HB2	1.79	0.96
3:C:185:LYS:HG2	3:C:195:TYR:HB3	1.43	0.96
3:P:93:GLU:HA	3:P:97:GLU:HB2	1.43	0.96
4:D:57:LYS:HD2	4:D:82:GLN:HE21	1.27	0.96
5:E:9:ILE:HG21	6:F:9:ALA:O	1.64	0.95
2:B:126:ARG:NE	2:B:128:VAL:HG23	1.82	0.95
3:P:185:LYS:HG2	3:P:195:TYR:HB3	1.47	0.95
1:N:112:LYS:HB2	1:N:113:PRO:HD3	1.49	0.95
4:Q:123:LYS:HD3	4:Q:140:ILE:HD12	1.45	0.94
7:G:23:TYR:HA	7:G:26:TYR:CG	2.02	0.94
1:N:66:TYR:HB2	2:O:65:PRO:HG2	1.49	0.94
4:Q:74:ASN:H	4:Q:93:VAL:HG11	1.30	0.94
12:D:306:OPC:HBL1	12:D:306:OPC:HAR2	1.46	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:154:VAL:HG21	10:N:1304:TDS:HAY2	1.50	0.94
2:O:126:ARG:HG2	2:O:126:ARG:HH11	1.33	0.94
4:D:166:THR:HA	4:D:179:VAL:CG1	1.98	0.93
1:N:95:LEU:HD11	5:R:10:VAL:HG11	1.50	0.93
2:O:118:ASN:HD22	2:O:121:GLN:HE22	1.17	0.93
1:A:161:VAL:O	1:A:165:ILE:HG12	1.68	0.92
2:O:126:ARG:NH1	2:O:128:VAL:HG23	1.83	0.92
3:P:168:ASN:HA	3:P:172:PHE:CZ	2.04	0.92
3:P:172:PHE:H	3:P:231:LEU:HG	1.33	0.92
4:Q:73:HIS:CD2	4:Q:77:ASP:HB2	2.05	0.92
3:C:146:LYS:HD3	3:C:246:GLU:HG3	1.50	0.91
3:C:94:LEU:HD22	3:C:94:LEU:H	1.34	0.91
1:N:142:GLN:HG2	2:O:64:GLU:HG2	1.51	0.91
3:P:218:ILE:H	3:P:232:THR:HB	1.34	0.91
3:C:60:GLN:HE22	3:C:157:ARG:HG3	1.35	0.91
8:U:4:ASP:O	8:U:8:TRP:HB2	1.70	0.91
1:A:209:GLN:CG	1:A:210:GLY:H	1.79	0.90
3:P:172:PHE:O	3:P:231:LEU:HB3	1.71	0.90
1:A:170:ARG:HD3	1:A:174:SER:O	1.68	0.90
2:O:124:PHE:HZ	5:R:26:ILE:HB	1.36	0.90
1:A:114:ARG:HH12	1:A:209:GLN:H	1.06	0.90
2:O:31:ALA:O	2:O:32:TRP:HB2	1.70	0.90
1:A:211:ILE:HD12	1:A:211:ILE:H	1.37	0.90
4:D:99:ILE:HB	4:D:153:ALA:HB1	1.53	0.90
4:D:81:VAL:HG12	4:D:82:GLN:H	1.36	0.90
7:T:26:TYR:HA	7:T:29:TYR:CD1	2.06	0.90
1:A:209:GLN:HG2	1:A:210:GLY:N	1.87	0.90
1:A:24:LYS:HD3	1:A:24:LYS:H	1.35	0.89
4:Q:76:GLY:N	4:Q:93:VAL:HG13	1.86	0.89
2:O:80:TYR:HB3	13:O:1201:CLA:HED1	1.52	0.89
1:A:190:VAL:HG11	10:A:304:TDS:HAA3	1.54	0.89
4:Q:82:GLN:N	4:Q:89:THR:OG1	2.05	0.89
4:D:66:VAL:CG2	4:D:160:ILE:HG13	2.00	0.89
2:O:105:PRO:HG3	13:O:1201:CLA:H112	1.54	0.89
11:A:305:PL9:C46	11:A:305:PL9:H412	2.01	0.89
4:Q:57:LYS:HG3	4:Q:82:GLN:NE2	1.88	0.89
4:Q:91:ILE:HD12	4:Q:160:ILE:HD12	1.54	0.88
1:N:213:GLY:O	5:R:30:LYS:HD2	1.73	0.88
3:P:83:LYS:HB2	3:P:111:ASP:HB3	1.56	0.88
3:P:275:LYS:CE	4:Q:20:ASN:HB3	2.04	0.88
4:Q:146:LEU:HD13	4:Q:177:TRP:HB2	1.56	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:280:GLU:HG2	3:C:281:LYS:HZ3	1.39	0.87
3:P:231:LEU:HD13	3:P:232:THR:H	1.37	0.87
3:C:226:LYS:NZ	3:C:230:ALA:HB3	1.88	0.87
3:C:278:GLN:NE2	7:G:30:LYS:HE2	1.90	0.87
3:P:60:GLN:HE22	3:P:157:ARG:HG3	1.40	0.87
4:Q:78:ARG:HH22	4:Q:100:ARG:NH2	1.71	0.87
4:Q:156:GLN:HB2	4:Q:161:VAL:CG2	2.04	0.87
2:O:79:TRP:CZ2	5:R:1:MET:HB2	2.09	0.87
4:D:102:TYR:HB2	4:D:150:LEU:HG	1.56	0.87
7:T:21:LEU:O	7:T:21:LEU:HD22	1.75	0.87
8:H:4:ASP:O	8:H:8:TRP:HB2	1.74	0.87
1:N:110:PHE:H	1:N:110:PHE:HD2	1.20	0.87
3:P:226:LYS:NZ	3:P:230:ALA:HB3	1.90	0.87
3:C:255:VAL:CG1	7:G:14:VAL:HG12	2.04	0.86
3:P:275:LYS:HE3	4:Q:20:ASN:HB3	1.55	0.86
4:Q:77:ASP:H	4:Q:93:VAL:HG12	1.40	0.86
4:D:117:TRP:HA	4:D:124:PHE:HD1	1.41	0.86
2:O:126:ARG:HG2	2:O:126:ARG:NH1	1.89	0.86
1:N:103:ARG:HE	1:N:107:THR:HG21	1.39	0.86
2:O:64:GLU:HG3	2:O:65:PRO:CD	2.05	0.86
4:Q:163:THR:OG1	4:Q:164:PRO:HD2	1.73	0.86
4:Q:73:HIS:CG	4:Q:77:ASP:HB2	2.10	0.86
1:A:159:PRO:O	1:A:161:VAL:N	2.08	0.86
2:B:38:TYR:HB3	3:C:276:LYS:HG2	1.58	0.86
2:B:149:LEU:HD22	4:Q:129:HIS:HA	1.57	0.86
4:Q:22:LEU:HD23	4:Q:23:ALA:N	1.91	0.86
1:A:101:VAL:HG11	13:B:201:CLA:HMA1	1.58	0.85
12:N:1306:OPC:HBV1	12:N:1306:OPC:HBV2	1.56	0.85
1:A:211:ILE:HG22	5:E:26:ILE:HG12	1.59	0.85
4:Q:133:TYR:HA	4:Q:139:VAL:HA	1.57	0.85
4:D:142:GLY:HA2	4:D:144:ALA:H	1.42	0.85
4:D:22:LEU:HD23	4:D:23:ALA:N	1.92	0.85
1:A:158:ILE:HG23	1:A:159:PRO:HD2	1.59	0.85
1:A:170:ARG:HD2	1:A:172:GLY:O	1.76	0.85
2:B:149:LEU:CD2	4:Q:129:HIS:HA	2.06	0.85
3:C:280:GLU:HG2	3:C:281:LYS:NZ	1.91	0.85
1:A:14:ILE:HD13	1:A:15:GLN:N	1.92	0.85
4:Q:138:ARG:HE	4:Q:171:ARG:HD3	1.43	0.84
5:E:7:PHE:HA	5:E:10:VAL:CG1	2.07	0.84
2:O:149:LEU:O	2:O:151:LEU:N	2.09	0.84
1:A:14:ILE:HA	1:A:17:LEU:CB	2.07	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:38:TYR:CB	3:P:276:LYS:HG2	2.07	0.84
1:N:155:PRO:HG2	1:N:166:SER:OG	1.78	0.84
4:Q:105:ASN:HB3	4:Q:149:ALA:HB3	1.58	0.84
2:B:149:LEU:HD12	2:B:150:PRO:HD2	1.58	0.83
1:A:142:GLN:HE21	2:B:66:ALA:HA	1.42	0.83
4:Q:73:HIS:HB3	4:Q:93:VAL:HG11	1.57	0.83
3:C:83:LYS:HB2	3:C:111:ASP:HB3	1.58	0.83
4:D:142:GLY:HA2	4:D:144:ALA:N	1.94	0.83
4:Q:150:LEU:H	4:Q:178:TRP:HZ2	1.25	0.83
4:Q:64:VAL:HG12	4:Q:91:ILE:CG1	2.08	0.83
3:P:184:ALA:HB2	3:P:198:SER:OG	1.79	0.83
3:C:218:ILE:N	3:C:232:THR:HB	1.94	0.83
3:C:26:HIS:CG	3:C:154:ASN:HD21	1.97	0.83
2:O:122:ASN:HD21	5:R:30:LYS:HD3	1.44	0.83
2:O:79:TRP:HZ2	5:R:1:MET:H3	1.27	0.83
4:D:165:TRP:HD1	4:D:179:VAL:HA	1.44	0.82
3:C:255:VAL:HG11	7:G:14:VAL:CG1	2.08	0.82
4:Q:176:PRO:HG2	4:Q:179:VAL:HB	1.58	0.82
2:O:67:ASN:ND2	3:P:16:PRO:HB3	1.94	0.82
11:Q:1305:PL9:H302	12:Q:1307:OPC:HBC1	1.60	0.82
4:Q:78:ARG:HH22	4:Q:100:ARG:HH22	1.26	0.82
1:A:14:ILE:HD13	1:A:15:GLN:H	1.45	0.82
3:P:275:LYS:NZ	4:Q:20:ASN:HD22	1.77	0.82
12:B:307:OPC:HBI2	12:B:307:OPC:HAP1	1.59	0.82
4:D:154:THR:O	4:D:160:ILE:HG23	1.78	0.82
4:Q:94:GLU:CB	4:Q:100:ARG:HD3	2.05	0.82
3:P:168:ASN:HA	3:P:172:PHE:HZ	1.39	0.82
2:B:137:THR:O	2:B:141:ILE:HG12	1.80	0.82
7:G:27:GLN:O	7:G:31:ARG:NH1	2.13	0.82
3:C:226:LYS:HZ2	3:C:230:ALA:HB3	1.43	0.81
1:A:62:VAL:HG12	1:A:140:TRP:CZ2	2.16	0.81
1:A:44:PHE:HD1	9:A:301:HEM:HBB1	1.45	0.81
12:D:306:OPC:HBI1	12:D:306:OPC:CAP	2.08	0.81
2:O:126:ARG:CZ	2:O:128:VAL:HG23	2.10	0.81
2:O:95:LEU:N	2:O:95:LEU:HD23	1.96	0.81
4:Q:100:ARG:HD2	4:Q:102:TYR:OH	1.80	0.81
3:C:171:VAL:CG1	3:C:234:ASN:HB2	2.10	0.81
12:Q:1307:OPC:HBF2	12:Q:1307:OPC:HBX2	1.63	0.81
3:P:231:LEU:O	3:P:232:THR:HG23	1.80	0.81
3:P:26:HIS:CG	3:P:154:ASN:HD21	1.98	0.81
3:C:183:ILE:HD12	3:C:183:ILE:O	1.81	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112:LYS:HA	1:A:115:GLU:OE1	1.80	0.81
3:C:93:GLU:HA	3:C:97:GLU:CB	2.11	0.81
3:P:217:LEU:HA	3:P:232:THR:HB	1.63	0.81
3:P:90:ILE:HG23	3:P:95:LYS:HB2	1.62	0.81
4:Q:155:VAL:HA	4:Q:161:VAL:H	1.43	0.81
1:A:14:ILE:CA	1:A:17:LEU:HB2	2.11	0.80
1:N:214:PRO:HB3	5:R:29:ILE:CG2	2.09	0.80
2:O:121:GLN:HB2	2:O:125:ARG:HD2	1.63	0.80
12:Q:1307:OPC:HAP1	12:Q:1307:OPC:OBJ	1.80	0.80
11:Q:1305:PL9:H462	11:Q:1305:PL9:H412	1.61	0.80
3:P:161:TYR:HE1	3:P:167:SER:HA	1.47	0.80
4:D:116:PRO:HG3	4:D:127:PRO:CD	2.11	0.80
3:P:183:ILE:O	3:P:183:ILE:HD12	1.80	0.80
11:Q:1305:PL9:H212	11:Q:1305:PL9:C26	2.10	0.80
7:T:11:LEU:HD22	7:T:11:LEU:H	1.44	0.80
3:C:184:ALA:HB2	3:C:198:SER:OG	1.81	0.80
3:C:269:GLN:HE22	7:G:24:ALA:CB	1.94	0.80
3:C:90:ILE:HG23	3:C:95:LYS:HB2	1.64	0.80
3:P:280:GLU:HG2	3:P:281:LYS:NZ	1.96	0.80
1:A:155:PRO:HG2	1:A:166:SER:OG	1.81	0.80
12:N:1306:OPC:HBO1	12:N:1306:OPC:HAT1	1.64	0.80
7:G:30:LYS:HB3	7:G:31:ARG:NH2	1.95	0.80
4:D:138:ARG:HB3	4:D:138:ARG:NH1	1.97	0.80
7:G:30:LYS:O	7:G:31:ARG:NH2	2.15	0.80
4:D:58:ASP:HB2	4:D:62:ASN:O	1.82	0.79
4:Q:139:VAL:HG21	4:Q:144:ALA:HB3	1.64	0.79
3:C:199:ILE:O	3:C:208:VAL:HG12	1.81	0.79
3:C:231:LEU:O	3:C:232:THR:HG23	1.82	0.79
1:A:206:ILE:C	1:A:207:ARG:HD3	2.03	0.79
3:C:91:PRO:HB2	3:C:94:LEU:HB2	1.65	0.79
3:C:161:TYR:HE1	3:C:167:SER:HA	1.48	0.79
7:T:23:TYR:HA	7:T:26:TYR:CD1	2.18	0.79
2:O:122:ASN:HD21	5:R:30:LYS:CD	1.94	0.79
1:A:114:ARG:HH12	1:A:209:GLN:N	1.81	0.79
7:G:11:LEU:H	7:G:11:LEU:HD22	1.44	0.79
4:D:156:GLN:OE1	4:D:161:VAL:HG21	1.83	0.79
4:D:93:VAL:HA	4:D:100:ARG:HB2	1.64	0.79
2:O:122:ASN:ND2	5:R:30:LYS:HD3	1.98	0.79
3:C:102:TYR:H	3:C:118:PRO:HG3	1.46	0.79
11:A:305:PL9:H101	12:D:306:OPC:HBF2	1.65	0.79
12:D:306:OPC:HAP2	12:D:306:OPC:CBI	2.07	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:70:LEU:HD12	4:D:160:ILE:CD1	2.13	0.78
2:O:57:LEU:HD22	7:T:14:VAL:CG2	2.13	0.78
2:B:18:LEU:HD13	2:B:31:ALA:CB	2.14	0.78
5:E:20:VAL:HG12	5:E:21:GLY:N	1.99	0.78
3:P:219:VAL:HG11	3:P:223:GLN:HE21	1.48	0.78
11:Q:1305:PL9:H321	12:Q:1307:OPC:HBW2	1.66	0.78
4:D:64:VAL:HG11	4:D:81:VAL:HG13	1.66	0.78
1:N:71:TYR:HA	1:N:75:GLU:OE1	1.84	0.78
7:T:23:TYR:HA	7:T:26:TYR:CD2	2.17	0.78
1:A:29:HIS:CD2	1:A:30:VAL:HG13	2.19	0.78
2:B:71:THR:HB	2:B:72:PRO:CD	2.11	0.78
1:N:195:ILE:O	1:N:199:MET:HG3	1.84	0.78
2:O:112:PRO:O	2:O:116:ASN:HB2	1.84	0.78
1:N:114:ARG:HH21	1:N:209:GLN:N	1.82	0.77
2:O:149:LEU:HB3	2:O:150:PRO:HD2	1.66	0.77
3:P:134:PRO:HB3	3:P:142:ILE:HD13	1.65	0.77
1:A:28:PRO:HD2	2:B:31:ALA:O	1.85	0.77
3:P:188:ASP:CB	3:P:193:VAL:HA	2.15	0.77
4:Q:154:THR:O	4:Q:160:ILE:HA	1.83	0.77
1:A:112:LYS:H	1:A:113:PRO:HD2	1.50	0.77
1:A:39:ILE:HD11	15:E:101:BCR:H312	1.65	0.77
12:Q:1307:OPC:HAL2	12:Q:1307:OPC:CAP	2.15	0.77
4:Q:169:ASP:HB2	4:Q:176:PRO:CA	2.12	0.77
3:P:255:VAL:HG11	7:T:14:VAL:HG12	1.66	0.77
8:H:19:ILE:O	8:H:23:VAL:HG22	1.84	0.77
4:Q:155:VAL:HG12	4:Q:157:ASP:N	1.98	0.77
7:G:21:LEU:O	7:G:21:LEU:HD22	1.84	0.77
3:C:231:LEU:HD13	3:C:232:THR:H	1.49	0.77
1:N:116:LEU:H	1:N:116:LEU:HD12	1.50	0.77
2:O:149:LEU:HB3	2:O:150:PRO:CD	2.14	0.77
3:C:92:GLU:O	3:C:96:LYS:HB3	1.85	0.77
3:P:102:TYR:H	3:P:118:PRO:HG3	1.49	0.77
4:Q:176:PRO:CG	4:Q:179:VAL:HB	2.14	0.77
5:R:23:ILE:O	5:R:27:LYS:HB2	1.85	0.77
3:C:259:ILE:HA	7:G:17:THR:HG21	1.65	0.77
2:B:34:ASN:HD21	12:B:307:OPC:CBK	1.97	0.77
2:O:38:TYR:CD1	3:P:276:LYS:HD3	2.20	0.77
1:A:47:GLN:HE22	1:A:89:SER:CB	1.97	0.76
12:Q:1307:OPC:HBU2	12:Q:1307:OPC:CBE	2.05	0.76
8:U:19:ILE:O	8:U:23:VAL:HG22	1.85	0.76
2:B:95:LEU:HD23	2:B:95:LEU:N	2.00	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:188:ASP:CB	3:C:193:VAL:HA	2.14	0.76
3:C:28:ALA:HB2	3:C:236:ASN:ND2	1.98	0.76
3:C:281:LYS:CA	3:C:284:ALA:HB3	2.16	0.76
4:D:57:LYS:HB2	4:D:82:GLN:HG2	1.66	0.76
7:G:25:ALA:HB1	7:G:29:TYR:CE2	2.21	0.76
1:N:29:HIS:N	1:N:29:HIS:ND1	2.31	0.76
3:P:199:ILE:O	3:P:208:VAL:HG12	1.85	0.76
2:B:112:PRO:O	2:B:116:ASN:HB2	1.85	0.76
2:O:53:ALA:O	2:O:57:LEU:HG	1.84	0.76
4:Q:150:LEU:HB2	4:Q:178:TRP:HH2	1.51	0.76
5:R:7:PHE:HA	5:R:10:VAL:CG1	2.12	0.76
1:A:158:ILE:HB	1:A:162:GLY:HA3	1.66	0.76
12:D:306:OPC:HBW2	12:D:306:OPC:HCA2	1.67	0.76
3:P:271:MET:HG3	4:Q:22:LEU:HD21	1.67	0.76
2:O:79:TRP:CZ3	5:R:4:GLY:CA	2.69	0.76
2:B:151:LEU:HD12	2:B:153:LYS:HD3	1.67	0.76
3:C:269:GLN:HE22	7:G:24:ALA:HB1	1.50	0.76
4:Q:175:LYS:HB2	4:Q:179:VAL:HG11	1.66	0.76
5:E:23:ILE:O	5:E:27:LYS:HB2	1.86	0.76
3:C:181:THR:O	3:C:221:GLU:HB3	1.86	0.76
3:P:218:ILE:N	3:P:232:THR:HB	1.99	0.76
4:Q:64:VAL:HG12	4:Q:91:ILE:HG12	1.64	0.76
2:B:151:LEU:HA	2:B:153:LYS:HD3	1.67	0.75
1:N:142:GLN:HG2	2:O:64:GLU:CG	2.15	0.75
1:N:141:ASP:HA	2:O:65:PRO:HD3	1.68	0.75
3:P:231:LEU:HD11	3:P:233:ASN:O	1.85	0.75
3:C:218:ILE:H	3:C:232:THR:CB	1.99	0.75
4:D:117:TRP:HA	4:D:124:PHE:CD1	2.21	0.75
2:O:57:LEU:HD22	7:T:14:VAL:HG23	1.67	0.75
1:A:195:ILE:O	1:A:199:MET:HG3	1.87	0.75
4:Q:64:VAL:HB	4:Q:81:VAL:HG22	1.67	0.75
1:A:158:ILE:HB	1:A:162:GLY:CA	2.16	0.75
4:D:123:LYS:HA	4:D:134:ASP:C	2.07	0.75
4:D:84:LEU:HD22	4:D:87:ASP:HB2	1.67	0.75
2:O:122:ASN:HD22	2:O:125:ARG:CZ	1.99	0.75
3:P:91:PRO:HB2	3:P:94:LEU:HB2	1.66	0.75
2:O:79:TRP:HZ2	5:R:1:MET:HB2	1.48	0.75
2:B:122:ASN:ND2	2:B:124:PHE:HB3	2.00	0.75
4:Q:151:CYS:HB3	4:Q:162:LEU:HD23	1.69	0.75
7:T:25:ALA:CB	7:T:29:TYR:CZ	2.69	0.75
12:D:306:OPC:CBL	12:D:306:OPC:HAR2	2.17	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:23:TYR:HA	7:G:26:TYR:CD2	2.20	0.75
2:O:146:GLY:N	2:O:149:LEU:HD12	2.02	0.75
2:O:146:GLY:H	2:O:149:LEU:HD12	1.49	0.75
2:O:122:ASN:OD1	5:R:30:LYS:HD3	1.87	0.75
1:A:24:LYS:CD	1:A:24:LYS:H	2.00	0.75
3:C:39:SER:HB3	3:C:248:VAL:HB	1.66	0.75
4:Q:156:GLN:O	4:Q:157:ASP:HB3	1.86	0.75
3:C:219:VAL:H	3:C:232:THR:HG22	1.52	0.75
4:D:81:VAL:HG21	4:D:91:ILE:HD11	1.68	0.75
4:Q:159:ASN:O	4:Q:161:VAL:HG13	1.85	0.75
4:Q:67:SER:C	4:Q:68:LYS:HD2	2.07	0.75
5:E:16:PHE:HB3	15:E:101:BCR:C36	2.17	0.74
3:P:188:ASP:HB2	3:P:193:VAL:HA	1.69	0.74
1:A:47:GLN:HE22	1:A:89:SER:HB3	1.52	0.74
2:B:122:ASN:HD22	2:B:124:PHE:HD2	1.35	0.74
2:O:117:VAL:HG13	2:O:118:ASN:OD1	1.87	0.74
4:D:134:ASP:CG	4:D:135:GLU:H	1.90	0.74
4:D:65:LYS:HB3	4:D:68:LYS:HD3	1.68	0.74
4:Q:150:LEU:HD11	4:Q:171:ARG:HH21	1.53	0.74
4:Q:87:ASP:HB3	4:Q:88:PRO:HD2	1.67	0.74
4:Q:92:VAL:CG2	4:Q:100:ARG:HB2	2.17	0.74
3:P:52:ILE:HG12	3:P:153:ALA:HB1	1.69	0.74
4:Q:132:GLN:HE22	4:Q:141:ARG:HD3	1.53	0.74
11:A:305:PL9:H252	12:D:306:OPC:HBN1	1.68	0.74
3:P:229:GLU:HG3	3:P:230:ALA:H	1.53	0.74
10:A:304:TDS:HBC1	2:B:85:PHE:HA	1.70	0.73
3:C:182:LYS:HG2	3:C:198:SER:HB2	1.69	0.73
1:N:47:GLN:HE22	1:N:89:SER:HB3	1.53	0.73
2:O:76:LEU:HD12	5:R:1:MET:SD	2.28	0.73
1:A:29:HIS:CD2	1:A:30:VAL:HG22	2.21	0.73
7:G:25:ALA:CB	7:G:29:TYR:CZ	2.70	0.73
2:O:137:THR:O	2:O:141:ILE:HG12	1.89	0.73
3:P:28:ALA:HB2	3:P:236:ASN:ND2	2.03	0.73
2:O:79:TRP:CH2	5:R:4:GLY:HA3	2.24	0.73
1:A:146:TRP:CE3	2:B:71:THR:HG23	2.24	0.73
2:B:79:TRP:HA	2:B:82:TYR:CE2	2.24	0.73
3:P:280:GLU:HG2	3:P:281:LYS:HZ3	1.52	0.73
4:Q:155:VAL:C	4:Q:161:VAL:HG22	2.09	0.73
2:B:133:PHE:O	2:B:137:THR:HG23	1.89	0.73
4:D:78:ARG:HE	4:D:92:VAL:CG1	2.02	0.73
4:Q:20:ASN:C	4:Q:22:LEU:H	1.89	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:A:304:TDS:HBB2	2:B:88:LEU:HD22	1.70	0.73
2:B:144:GLY:O	2:B:145:ILE:HB	1.87	0.73
3:P:93:GLU:HA	3:P:97:GLU:CB	2.19	0.73
8:U:23:VAL:HA	8:U:26:ARG:HD2	1.71	0.73
4:D:133:TYR:HA	4:D:139:VAL:HA	1.71	0.73
4:D:138:ARG:HH21	4:D:171:ARG:CZ	2.02	0.73
4:Q:73:HIS:HB3	4:Q:93:VAL:CG1	2.18	0.73
11:A:305:PL9:H512	11:A:305:PL9:H401	1.71	0.73
3:C:188:ASP:HB2	3:C:193:VAL:HA	1.68	0.73
2:B:149:LEU:HD13	2:B:150:PRO:HD2	1.69	0.72
5:R:23:ILE:HG23	5:R:24:PHE:CD2	2.23	0.72
2:O:122:ASN:HD21	5:R:30:LYS:CG	2.01	0.72
2:O:32:TRP:H	2:O:33:PRO:HD3	1.53	0.72
4:D:165:TRP:CD1	4:D:179:VAL:HA	2.24	0.72
7:T:25:ALA:HB1	7:T:29:TYR:OH	1.89	0.72
2:B:118:ASN:HB3	2:B:121:GLN:O	1.89	0.72
3:C:229:GLU:HG3	3:C:230:ALA:H	1.54	0.72
4:Q:76:GLY:HA2	4:Q:93:VAL:O	1.88	0.72
2:B:32:TRP:HH2	3:C:277:LYS:HD2	1.55	0.72
1:A:116:LEU:H	1:A:116:LEU:HD12	1.53	0.72
3:C:171:VAL:HG13	3:C:234:ASN:HB2	1.71	0.72
3:C:217:LEU:HA	3:C:232:THR:HB	1.72	0.72
3:P:211:ILE:HD11	3:P:231:LEU:HB2	1.71	0.72
12:Q:1307:OPC:HAQ1	12:Q:1307:OPC:HBG3	1.72	0.72
12:Q:1307:OPC:HBX2	12:Q:1307:OPC:CBF	2.19	0.72
4:D:66:VAL:HG21	4:D:155:VAL:HG13	1.71	0.72
4:Q:131:SER:OG	4:Q:144:ALA:HB2	1.89	0.72
4:Q:91:ILE:HG23	4:Q:160:ILE:HD12	1.71	0.72
4:Q:178:TRP:HE3	4:Q:178:TRP:N	1.88	0.72
2:O:79:TRP:CZ3	5:R:4:GLY:HA3	2.25	0.72
6:S:6:LEU:O	6:S:10:LEU:HG	1.88	0.72
4:D:16:ARG:C	4:D:18:PHE:H	1.94	0.72
5:E:23:ILE:HG23	5:E:24:PHE:CD2	2.25	0.72
1:N:200:LEU:O	1:N:204:LEU:HG	1.89	0.72
4:Q:103:GLY:O	4:Q:150:LEU:HA	1.89	0.72
1:A:135:GLY:O	9:A:301:HEM:HAA1	1.90	0.72
1:A:17:LEU:HD23	1:A:17:LEU:O	1.88	0.72
1:A:114:ARG:NH1	1:A:209:GLN:H	1.85	0.72
2:O:133:PHE:O	2:O:137:THR:HG23	1.90	0.72
12:D:306:OPC:HBL1	12:D:306:OPC:HAP2	1.71	0.71
2:O:20:LYS:HD3	2:O:21:GLY:H	1.53	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:278:GLN:NE2	6:F:30:GLN:OE1	2.23	0.71
3:P:219:VAL:H	3:P:232:THR:HG22	1.55	0.71
4:Q:137:GLY:O	4:Q:147:SER:HB3	1.90	0.71
4:Q:66:VAL:HG22	4:Q:160:ILE:CG1	2.20	0.71
1:A:103:ARG:HH11	1:A:103:ARG:HG3	1.54	0.71
6:F:6:LEU:O	6:F:10:LEU:HG	1.90	0.71
8:H:11:LEU:HB3	8:H:15:PHE:CZ	2.24	0.71
3:P:218:ILE:H	3:P:232:THR:CB	2.03	0.71
4:Q:105:ASN:HB3	4:Q:149:ALA:CB	2.20	0.71
1:N:29:HIS:HE2	1:N:209:GLN:HG3	1.56	0.71
1:N:66:TYR:CB	2:O:65:PRO:HG2	2.20	0.71
4:Q:64:VAL:HB	4:Q:81:VAL:CG2	2.20	0.71
2:O:106:LEU:HD21	13:O:1201:CLA:H151	1.72	0.71
3:P:185:LYS:HE2	3:P:195:TYR:HB3	1.71	0.71
3:P:275:LYS:HZ1	4:Q:20:ASN:HD22	1.36	0.71
3:P:275:LYS:HZ3	3:P:276:LYS:NZ	1.89	0.71
2:O:142:TRP:O	2:O:145:ILE:HG12	1.91	0.71
2:O:84:VAL:O	2:O:88:LEU:HD13	1.90	0.71
7:T:14:VAL:O	7:T:17:THR:HB	1.91	0.71
2:B:18:LEU:HD22	2:B:30:PRO:O	1.90	0.71
4:D:57:LYS:CB	4:D:82:GLN:HG2	2.21	0.71
2:B:118:ASN:HB3	2:B:121:GLN:HE21	1.55	0.71
3:P:92:GLU:O	3:P:96:LYS:HB3	1.91	0.71
1:N:212:SER:OG	5:R:26:ILE:HG12	1.90	0.71
2:B:126:ARG:HE	2:B:128:VAL:CG2	1.93	0.71
2:B:151:LEU:C	2:B:153:LYS:H	1.93	0.71
4:Q:117:TRP:HE1	4:Q:135:GLU:HA	1.55	0.71
3:C:218:ILE:HG13	3:C:219:VAL:H	1.56	0.70
4:Q:145:PRO:HG2	4:Q:146:LEU:H	1.55	0.70
1:A:211:ILE:HD11	2:B:122:ASN:OD1	1.91	0.70
4:D:115:VAL:HG21	4:D:148:LEU:HD21	1.73	0.70
4:D:15:ARG:NH2	4:D:17:GLN:HG2	2.05	0.70
6:F:5:MET:HA	6:F:8:ALA:HB3	1.73	0.70
4:Q:56:ALA:O	4:Q:63:ASN:HA	1.91	0.70
7:T:11:LEU:O	7:T:14:VAL:HG22	1.90	0.70
3:C:226:LYS:HG2	3:C:229:GLU:HB3	1.73	0.70
2:O:132:ILE:CG2	13:O:1201:CLA:HBB2	2.18	0.70
3:P:3:PHE:HZ	3:P:119:LEU:HD11	1.56	0.70
3:C:219:VAL:HG11	3:C:223:GLN:HE21	1.54	0.70
4:D:147:SER:HB2	4:D:177:TRP:HH2	1.56	0.70
3:P:172:PHE:CZ	3:P:212:PRO:HG3	2.25	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:1305:PL9:C46	11:Q:1305:PL9:H412	2.21	0.70
4:Q:64:VAL:HA	4:Q:69:PHE:CD1	2.26	0.70
1:A:111:LYS:HG2	1:A:112:LYS:N	2.06	0.70
1:N:189:PHE:O	1:N:193:TRP:HE3	1.74	0.70
1:A:189:PHE:O	1:A:193:TRP:HE3	1.75	0.70
1:A:29:HIS:HD2	1:A:30:VAL:HG13	1.56	0.70
4:D:20:ASN:C	4:D:22:LEU:H	1.91	0.70
1:N:209:GLN:NE2	2:O:28:GLY:H	1.90	0.70
2:B:145:ILE:O	2:B:146:GLY:C	2.29	0.70
4:Q:152:HIS:C	4:Q:162:LEU:HG	2.12	0.70
4:Q:93:VAL:CA	4:Q:100:ARG:HG3	2.21	0.70
2:B:144:GLY:O	2:B:145:ILE:CB	2.39	0.70
2:B:57:LEU:HD21	3:C:258:MET:HE2	1.72	0.70
2:O:117:VAL:O	2:O:118:ASN:HB2	1.92	0.70
2:O:79:TRP:CZ3	5:R:4:GLY:HA2	2.26	0.70
11:Q:1305:PL9:H462	11:Q:1305:PL9:C41	2.21	0.70
6:S:5:MET:HA	6:S:8:ALA:HB3	1.73	0.70
1:A:207:ARG:CB	1:A:207:ARG:HH11	2.00	0.70
4:D:115:VAL:HG11	4:D:148:LEU:HD11	1.74	0.70
2:O:79:TRP:CE3	5:R:4:GLY:HA2	2.26	0.70
3:C:232:THR:O	3:C:233:ASN:HB2	1.91	0.70
3:P:39:SER:HB3	3:P:248:VAL:HB	1.72	0.70
7:T:28:GLN:O	7:T:31:ARG:N	2.24	0.70
2:B:20:LYS:NZ	2:B:21:GLY:O	2.23	0.69
4:D:168:THR:HA	4:D:176:PRO:HD3	1.74	0.69
1:N:34:TYR:OH	1:N:211:ILE:HG22	1.92	0.69
1:N:21:VAL:HG12	1:N:22:THR:H	1.55	0.69
3:P:70:LEU:H	3:P:70:LEU:HD23	1.57	0.69
7:G:23:TYR:HA	7:G:26:TYR:CD1	2.26	0.69
2:B:26:TYR:N	2:B:26:TYR:HD2	1.90	0.69
3:C:171:VAL:HB	3:C:231:LEU:HD12	1.75	0.69
5:E:7:PHE:CA	5:E:10:VAL:HG12	2.17	0.69
1:A:26:VAL:HB	2:B:29:GLU:CB	2.22	0.69
4:D:57:LYS:HD2	4:D:82:GLN:NE2	2.04	0.69
3:P:182:LYS:HG2	3:P:198:SER:HB2	1.74	0.69
2:O:122:ASN:ND2	5:R:26:ILE:HG22	2.08	0.69
1:A:206:ILE:O	1:A:207:ARG:HD3	1.93	0.69
2:B:26:TYR:N	2:B:26:TYR:CD2	2.61	0.69
4:D:78:ARG:HE	4:D:92:VAL:HG11	1.58	0.69
4:D:57:LYS:CD	4:D:82:GLN:HE21	2.04	0.69
10:N:1304:TDS:HBB2	2:O:81:LEU:HD13	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:119:LEU:HD12	3:P:119:LEU:N	2.07	0.69
3:C:126:GLU:OE1	3:C:126:GLU:HA	1.92	0.69
4:Q:138:ARG:HE	4:Q:171:ARG:CD	2.05	0.69
4:Q:69:PHE:O	4:Q:91:ILE:HG21	1.92	0.69
4:Q:68:LYS:N	4:Q:68:LYS:HD2	2.08	0.69
2:B:127:PRO:C	2:B:129:ALA:H	1.94	0.69
3:C:172:PHE:CZ	3:C:212:PRO:HG3	2.28	0.69
4:D:132:GLN:HB2	4:D:140:ILE:HB	1.75	0.69
4:Q:165:TRP:HZ2	4:Q:176:PRO:HB3	1.54	0.69
6:S:25:LEU:HD23	6:S:25:LEU:O	1.92	0.69
2:B:22:MET:CE	2:B:22:MET:HA	2.23	0.69
3:C:119:LEU:HD12	3:C:119:LEU:N	2.08	0.69
3:C:172:PHE:C	3:C:231:LEU:HB3	2.13	0.69
1:N:111:LYS:HB2	1:N:114:ARG:HH11	1.58	0.69
2:O:122:ASN:HD22	2:O:125:ARG:NH2	1.90	0.69
4:Q:123:LYS:HE3	4:Q:125:LYS:NZ	2.08	0.69
5:R:18:ILE:O	5:R:22:ILE:HB	1.91	0.69
4:D:123:LYS:HA	4:D:134:ASP:O	1.91	0.69
7:G:11:LEU:HA	7:G:14:VAL:CG1	2.22	0.69
1:N:102:PHE:HB3	5:R:18:ILE:HD11	1.75	0.69
2:O:132:ILE:HG22	13:O:1201:CLA:CBB	2.19	0.69
3:P:178:GLY:HA2	3:P:225:VAL:HG13	1.75	0.69
4:Q:65:LYS:HE2	4:Q:158:ASP:O	1.90	0.69
2:B:18:LEU:HB3	2:B:30:PRO:O	1.93	0.68
7:G:14:VAL:CG2	7:G:15:PHE:N	2.56	0.68
1:N:110:PHE:N	1:N:110:PHE:HD2	1.90	0.68
5:R:20:VAL:HG12	5:R:21:GLY:N	2.06	0.68
2:O:74:GLU:HG2	2:O:75:ILE:N	2.08	0.68
12:Q:1307:OPC:HAX2	12:Q:1307:OPC:HAT1	1.76	0.68
3:C:277:LYS:HE3	7:G:31:ARG:HG3	1.74	0.68
4:D:103:GLY:O	4:D:151:CYS:HB2	1.92	0.68
4:D:154:THR:HG23	4:D:161:VAL:O	1.94	0.68
3:C:60:GLN:NE2	3:C:157:ARG:HG3	2.08	0.68
2:O:18:LEU:HD13	2:O:31:ALA:CB	2.23	0.68
2:O:52:VAL:O	2:O:56:VAL:HG23	1.93	0.68
4:Q:109:THR:O	4:Q:145:PRO:HG3	1.93	0.68
2:B:32:TRP:HZ3	2:B:36:LEU:HA	1.59	0.68
3:C:134:PRO:HB3	3:C:142:ILE:HD13	1.75	0.68
1:N:110:PHE:N	1:N:110:PHE:CD2	2.61	0.68
2:O:133:PHE:HA	13:O:1201:CLA:HMB1	1.75	0.68
3:P:161:TYR:HE1	3:P:167:SER:CA	2.07	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:180:ILE:HD11	3:C:182:LYS:O	1.93	0.68
3:C:258:MET:O	3:C:262:ILE:HD13	1.93	0.68
4:Q:102:TYR:CE1	4:Q:136:THR:HG23	2.28	0.68
4:Q:24:PHE:CE1	11:Q:1305:PL9:H202	2.28	0.68
4:D:126:CYS:HB3	14:D:200:FES:S1	2.34	0.68
2:O:127:PRO:C	2:O:129:ALA:H	1.95	0.68
3:P:226:LYS:HZ2	3:P:230:ALA:HB3	1.57	0.68
7:T:25:ALA:HB1	7:T:29:TYR:CE2	2.27	0.68
1:A:62:VAL:CG1	1:A:177:GLN:HB3	2.24	0.68
3:P:185:LYS:HD3	3:P:195:TYR:HD2	1.58	0.68
3:P:60:GLN:NE2	3:P:157:ARG:HG3	2.09	0.68
4:Q:92:VAL:HG23	4:Q:100:ARG:HB2	1.75	0.68
2:B:42:VAL:HG12	7:G:28:GLN:HE22	1.59	0.68
2:O:32:TRP:H	2:O:33:PRO:CD	2.06	0.68
4:Q:93:VAL:HA	4:Q:100:ARG:HG3	1.74	0.68
12:B:307:OPC:HBI2	12:B:307:OPC:CAP	2.24	0.68
1:A:142:GLN:NE2	2:B:67:ASN:H	1.92	0.68
3:C:52:ILE:HG12	3:C:153:ALA:HB1	1.75	0.68
3:P:181:THR:O	3:P:221:GLU:HB3	1.92	0.68
4:D:156:GLN:HB2	4:D:161:VAL:HG22	1.75	0.67
3:P:232:THR:O	3:P:233:ASN:HB2	1.92	0.67
7:G:11:LEU:O	7:G:14:VAL:HG22	1.94	0.67
1:N:101:VAL:HG11	13:O:1201:CLA:HMA2	1.76	0.67
4:D:117:TRP:CZ3	4:D:119:ALA:HA	2.30	0.67
6:F:26:LEU:CD2	8:H:17:TRP:HE1	2.07	0.67
1:N:149:LYS:HA	1:N:175:VAL:HG21	1.76	0.67
1:N:188:THR:HG22	9:N:301:HEM:HBC2	1.75	0.67
2:O:89:ARG:HH12	2:O:148:ALA:H	1.43	0.67
4:Q:115:VAL:HG11	4:Q:124:PHE:HB3	1.76	0.67
7:T:14:VAL:CG2	7:T:15:PHE:N	2.56	0.67
8:U:11:LEU:HB3	8:U:15:PHE:CZ	2.29	0.67
3:C:1:TYR:HD2	3:C:119:LEU:HD21	1.59	0.67
1:N:137:SER:O	1:N:140:TRP:HD1	1.78	0.67
3:C:269:GLN:OE1	7:G:24:ALA:HA	1.93	0.67
4:Q:150:LEU:HB2	4:Q:178:TRP:CH2	2.29	0.67
3:P:275:LYS:HE2	4:Q:17:GLN:HB2	1.76	0.67
11:A:305:PL9:H111	12:D:306:OPC:HBF2	1.75	0.67
2:O:79:TRP:HZ2	5:R:1:MET:CB	2.07	0.67
4:Q:16:ARG:C	4:Q:18:PHE:H	1.98	0.67
1:A:114:ARG:CZ	1:A:208:LYS:HG3	2.24	0.67
2:B:153:LYS:O	2:B:154:THR:O	2.12	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:81:VAL:HG12	4:Q:82:GLN:HG3	1.76	0.67
1:N:110:PHE:HD1	2:O:112:PRO:HB3	1.60	0.67
2:O:126:ARG:HH11	2:O:126:ARG:CG	2.04	0.67
4:Q:138:ARG:NE	4:Q:171:ARG:HD3	2.10	0.67
4:D:94:GLU:OE2	4:D:98:ALA:HB3	1.95	0.67
4:Q:77:ASP:C	4:Q:78:ARG:HD3	2.15	0.67
2:B:57:LEU:HD21	3:C:258:MET:CE	2.25	0.66
3:P:226:LYS:HZ1	3:P:230:ALA:HB3	1.60	0.66
5:R:26:ILE:HA	5:R:29:ILE:HG13	1.77	0.66
2:B:38:TYR:OH	12:B:307:OPC:HAU2	1.94	0.66
3:C:226:LYS:HE3	3:C:229:GLU:HB3	1.77	0.66
3:C:211:ILE:HD11	3:C:231:LEU:HB2	1.76	0.66
7:G:9:LEU:N	7:G:9:LEU:HD23	2.10	0.66
3:P:171:VAL:HG13	3:P:234:ASN:HD22	1.61	0.66
9:N:301:HEM:HBD1	9:N:301:HEM:HHA	1.75	0.66
4:Q:108:CYS:HB2	4:Q:113:CYS:O	1.95	0.66
8:U:4:ASP:O	8:U:8:TRP:CB	2.43	0.66
4:Q:134:ASP:CG	4:Q:138:ARG:HB2	2.15	0.66
2:O:149:LEU:C	2:O:151:LEU:H	1.98	0.66
3:P:271:MET:HB3	4:Q:23:ALA:HA	1.77	0.66
4:Q:115:VAL:HG13	4:Q:126:CYS:HB2	1.78	0.66
6:S:34:LYS:HE2	6:S:35:GLU:H	1.60	0.66
1:A:14:ILE:HG23	1:A:15:GLN:H	1.60	0.66
1:A:26:VAL:CG2	2:B:29:GLU:HG3	2.25	0.66
2:B:77:PRO:HG3	2:B:85:PHE:HB2	1.76	0.66
4:D:66:VAL:HG12	4:D:67:SER:N	2.11	0.66
2:O:114:ILE:O	2:O:116:ASN:N	2.28	0.66
2:O:18:LEU:HB2	2:O:31:ALA:HB2	1.77	0.66
4:Q:65:LYS:HD3	4:Q:68:LYS:HG2	1.78	0.66
11:A:305:PL9:H203	12:D:306:OPC:CBE	2.20	0.66
3:C:161:TYR:HE1	3:C:167:SER:CA	2.09	0.66
4:Q:150:LEU:N	4:Q:178:TRP:CZ2	2.63	0.66
1:A:158:ILE:CG2	1:A:159:PRO:HD2	2.25	0.66
3:C:28:ALA:O	3:C:239:GLY:HA3	1.94	0.66
3:C:70:LEU:HD23	3:C:70:LEU:H	1.61	0.66
4:D:105:ASN:O	4:D:107:VAL:N	2.29	0.66
4:D:108:CYS:C	4:D:110:HIS:H	1.99	0.66
4:Q:150:LEU:N	4:Q:178:TRP:HZ2	1.94	0.66
3:P:120:PRO:HB2	3:P:124:TYR:HB2	1.77	0.66
3:P:1:TYR:HD2	3:P:119:LEU:HD21	1.59	0.66
4:Q:66:VAL:HG22	4:Q:160:ILE:HG13	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:73:HIS:NE2	4:D:91:ILE:HG22	2.11	0.65
3:P:180:ILE:HD11	3:P:182:LYS:O	1.96	0.65
4:Q:149:ALA:C	4:Q:150:LEU:HD22	2.17	0.65
1:A:211:ILE:H	1:A:211:ILE:CD1	2.08	0.65
2:B:21:GLY:O	2:B:22:MET:HB2	1.97	0.65
3:C:177:THR:HA	3:C:227:ALA:HA	1.78	0.65
4:Q:104:ILE:HA	4:Q:150:LEU:HD13	1.78	0.65
2:B:80:TYR:HB2	13:B:201:CLA:HED1	1.77	0.65
3:C:120:PRO:HB2	3:C:124:TYR:HB2	1.79	0.65
4:D:124:PHE:O	4:D:133:TYR:N	2.29	0.65
13:O:1201:CLA:HHC	13:O:1201:CLA:HBB1	1.76	0.65
11:Q:1305:PL9:C21	11:Q:1305:PL9:H262	2.12	0.65
4:Q:78:ARG:HH12	4:Q:100:ARG:HH21	1.43	0.65
1:A:209:GLN:CG	1:A:210:GLY:N	2.53	0.65
2:B:118:ASN:HD21	2:B:126:ARG:HD2	1.60	0.65
1:N:114:ARG:HH21	1:N:209:GLN:H	1.41	0.65
1:N:27:PRO:HG3	2:O:33:PRO:CG	2.18	0.65
3:P:188:ASP:HB3	3:P:192:ASN:O	1.95	0.65
6:S:20:TRP:O	6:S:24:VAL:HG23	1.96	0.65
1:A:106:LEU:HD12	5:E:18:ILE:CD1	2.27	0.65
1:A:27:PRO:HG3	2:B:33:PRO:CD	2.27	0.65
4:D:155:VAL:HA	4:D:160:ILE:HA	1.79	0.65
6:F:25:LEU:O	6:F:25:LEU:HD23	1.96	0.65
3:P:218:ILE:HG13	3:P:219:VAL:H	1.60	0.65
3:P:90:ILE:CG2	3:P:95:LYS:HB2	2.26	0.65
4:Q:168:THR:HG23	4:Q:174:GLU:C	2.17	0.65
1:A:26:VAL:HB	2:B:29:GLU:HG3	1.79	0.65
2:B:76:LEU:H	2:B:76:LEU:HD22	1.62	0.65
3:C:188:ASP:HB3	3:C:192:ASN:O	1.97	0.65
3:C:281:LYS:HA	3:C:284:ALA:CB	2.19	0.65
3:C:172:PHE:N	3:C:231:LEU:HG	2.02	0.65
4:D:134:ASP:HB3	4:D:138:ARG:CG	2.27	0.65
5:E:5:ALA:CB	6:F:5:MET:HB2	2.27	0.65
2:O:74:GLU:HG2	2:O:75:ILE:H	1.61	0.65
3:P:277:LYS:HE3	7:T:31:ARG:O	1.96	0.65
6:S:26:LEU:CD2	8:U:17:TRP:HE1	2.09	0.65
1:A:36:LEU:HD23	1:A:100:HIS:HA	1.79	0.65
10:A:304:TDS:CBB	2:B:88:LEU:HD22	2.26	0.65
3:C:231:LEU:HD11	3:C:233:ASN:O	1.96	0.65
4:D:66:VAL:HG23	4:D:158:ASP:C	2.17	0.65
3:P:120:PRO:HB3	3:P:124:TYR:CD1	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Q:1305:PL9:H302	12:Q:1307:OPC:CBC	2.27	0.65
1:A:157:ALA:HB3	2:B:98:VAL:HG21	1.79	0.65
8:H:19:ILE:O	8:H:23:VAL:HG13	1.97	0.65
1:N:103:ARG:HG3	1:N:103:ARG:HH11	1.61	0.65
2:O:146:GLY:O	2:O:149:LEU:HG	1.97	0.65
3:P:226:LYS:HG2	3:P:229:GLU:HB3	1.79	0.65
5:R:16:PHE:HB3	15:R:1101:BCR:C36	2.20	0.65
4:D:65:LYS:HZ2	4:D:158:ASP:HB3	1.61	0.64
4:D:81:VAL:HG12	4:D:82:GLN:N	2.11	0.64
3:P:185:LYS:HE2	3:P:195:TYR:CB	2.28	0.64
7:G:14:VAL:O	7:G:17:THR:HB	1.95	0.64
1:N:47:GLN:HE22	1:N:89:SER:CB	2.11	0.64
2:O:32:TRP:HZ3	2:O:36:LEU:HA	1.62	0.64
3:P:281:LYS:CA	3:P:284:ALA:HB3	2.21	0.64
4:Q:14:GLY:O	4:Q:16:ARG:HG2	1.96	0.64
7:T:26:TYR:H	7:T:26:TYR:HD1	1.44	0.64
4:D:14:GLY:O	4:D:16:ARG:HG2	1.96	0.64
1:A:156:GLU:HA	1:A:162:GLY:O	1.97	0.64
1:A:24:LYS:HD3	1:A:24:LYS:N	2.11	0.64
2:O:27:TYR:HD2	2:O:27:TYR:O	1.80	0.64
3:P:177:THR:HA	3:P:227:ALA:HA	1.78	0.64
4:Q:125:LYS:HD3	4:Q:132:GLN:HG2	1.80	0.64
4:Q:76:GLY:H	4:Q:93:VAL:CG1	2.01	0.64
3:C:273:ILE:HD13	7:G:30:LYS:CD	2.14	0.64
4:D:73:HIS:HE2	4:D:91:ILE:HG22	1.62	0.64
3:C:273:ILE:CD1	7:G:30:LYS:HD3	2.12	0.64
3:P:54:TYR:HD2	3:P:70:LEU:HD13	1.63	0.64
2:B:26:TYR:HD2	2:B:26:TYR:H	1.45	0.64
4:Q:115:VAL:HG22	4:Q:126:CYS:HB2	1.79	0.64
4:Q:153:ALA:N	4:Q:162:LEU:HG	2.12	0.64
1:A:136:TYR:CD1	2:B:78:GLU:HG2	2.33	0.64
3:C:218:ILE:HG12	3:C:232:THR:HA	1.80	0.64
4:D:66:VAL:HB	4:D:158:ASP:HA	1.80	0.64
4:Q:133:TYR:HA	4:Q:139:VAL:CA	2.27	0.64
2:O:122:ASN:CG	5:R:30:LYS:HD3	2.17	0.64
1:A:142:GLN:NE2	2:B:67:ASN:N	2.45	0.64
3:C:216:GLU:O	3:C:233:ASN:HB2	1.96	0.64
4:D:121:GLU:OE2	4:D:125:LYS:HG3	1.98	0.64
6:F:22:LEU:O	6:F:26:LEU:HD23	1.98	0.64
6:F:27:LEU:O	6:F:30:GLN:HG3	1.96	0.64
8:H:4:ASP:O	8:H:8:TRP:CB	2.45	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:107:LYS:HD3	3:P:110:GLN:NE2	2.12	0.64
3:P:126:GLU:HA	3:P:126:GLU:OE1	1.96	0.64
3:P:79:PRO:HG2	3:P:82:PHE:CE1	2.33	0.64
3:C:107:LYS:HD3	3:C:110:GLN:NE2	2.13	0.64
4:D:105:ASN:O	4:D:107:VAL:HG23	1.98	0.64
1:N:111:LYS:CB	1:N:114:ARG:HH11	2.11	0.64
1:N:28:PRO:HG2	2:O:32:TRP:HB2	1.80	0.64
1:N:31:ASN:HB3	1:N:34:TYR:CG	2.32	0.64
4:Q:64:VAL:HG12	4:Q:91:ILE:HG13	1.78	0.64
2:B:26:TYR:C	2:B:27:TYR:CD1	2.72	0.64
2:B:91:LEU:HD22	2:B:96:LEU:HD13	1.80	0.64
3:C:57:LYS:O	3:C:58:LEU:HB2	1.98	0.64
4:D:136:THR:CB	4:D:138:ARG:HD2	2.16	0.64
2:O:22:MET:C	2:O:24:HIS:N	2.50	0.64
3:P:218:ILE:HG12	3:P:232:THR:HA	1.79	0.64
4:Q:15:ARG:NH2	4:Q:17:GLN:HG2	2.12	0.64
4:Q:94:GLU:HG2	4:Q:95:SER:H	1.62	0.64
2:O:24:HIS:O	2:O:25:ASN:ND2	2.31	0.63
3:P:231:LEU:CD1	3:P:232:THR:H	2.11	0.63
2:O:57:LEU:HD21	3:P:258:MET:CE	2.28	0.63
3:P:57:LYS:O	3:P:58:LEU:HB2	1.97	0.63
4:Q:134:ASP:HB2	4:Q:138:ARG:HB2	1.80	0.63
2:B:122:ASN:ND2	2:B:124:PHE:HD2	1.96	0.63
1:A:146:TRP:HB2	2:B:75:ILE:HD11	1.79	0.63
3:C:81:GLY:C	3:C:134:PRO:HG3	2.19	0.63
8:H:10:ALA:O	8:H:14:VAL:HG23	1.97	0.63
1:A:177:GLN:HB2	1:N:59:LYS:HZ3	1.61	0.63
1:A:27:PRO:HG3	2:B:33:PRO:HD3	1.80	0.63
3:C:185:LYS:HD3	3:C:195:TYR:HD2	1.64	0.63
3:C:234:ASN:OD1	3:C:236:ASN:HB3	1.97	0.63
2:O:20:LYS:CG	2:O:21:GLY:N	2.61	0.63
3:P:171:VAL:CG1	3:P:234:ASN:HB2	2.27	0.63
4:Q:176:PRO:HB2	4:Q:178:TRP:CZ3	2.33	0.63
2:B:122:ASN:HD21	2:B:124:PHE:HB3	1.60	0.63
3:C:270:LEU:HA	7:G:27:GLN:OE1	1.98	0.63
4:D:132:GLN:N	4:D:144:ALA:HB2	2.13	0.63
4:D:66:VAL:HG22	4:D:160:ILE:CG1	2.03	0.63
3:P:265:VAL:O	3:P:269:GLN:HG3	1.98	0.63
3:C:218:ILE:HG13	3:C:232:THR:HG22	1.81	0.63
6:S:27:LEU:O	6:S:30:GLN:HG3	1.99	0.63
3:P:38:GLN:OE1	7:T:15:PHE:HE1	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:U:19:ILE:O	8:U:23:VAL:HG13	1.99	0.63
3:C:89:ARG:O	3:C:91:PRO:HD3	1.98	0.63
6:F:26:LEU:HD21	8:H:17:TRP:HE1	1.62	0.63
8:H:23:VAL:HA	8:H:26:ARG:HD2	1.81	0.63
2:O:133:PHE:CD2	13:O:1201:CLA:HMB3	2.32	0.63
4:Q:138:ARG:NH2	4:Q:147:SER:OG	2.31	0.63
2:O:124:PHE:CE2	5:R:26:ILE:HB	2.33	0.63
4:D:134:ASP:OD1	4:D:135:GLU:N	2.32	0.63
4:D:150:LEU:CD1	4:D:171:ARG:HD3	2.28	0.63
4:D:166:THR:CA	4:D:179:VAL:HG13	2.13	0.63
4:Q:121:GLU:OE1	4:Q:125:LYS:HE3	1.99	0.63
4:Q:24:PHE:CD1	11:Q:1305:PL9:H202	2.34	0.63
1:A:177:GLN:HB2	1:N:59:LYS:NZ	2.13	0.63
3:C:262:ILE:HG21	7:G:17:THR:CG2	2.29	0.63
7:G:25:ALA:HB1	7:G:29:TYR:OH	1.99	0.63
2:O:114:ILE:C	2:O:116:ASN:H	2.02	0.63
2:O:67:ASN:HD21	3:P:16:PRO:HB3	1.63	0.63
4:Q:165:TRP:CZ2	4:Q:176:PRO:HB3	2.33	0.63
6:F:26:LEU:HB3	7:G:30:LYS:HE3	1.81	0.62
5:R:3:LEU:HA	5:R:6:VAL:CG2	2.29	0.62
11:A:305:PL9:H462	11:A:305:PL9:C41	2.12	0.62
1:N:13:GLU:OE1	1:N:14:ILE:HG22	1.98	0.62
2:O:117:VAL:O	2:O:118:ASN:CB	2.47	0.62
2:O:146:GLY:C	2:O:149:LEU:HG	2.19	0.62
4:Q:168:THR:HA	4:Q:176:PRO:CD	2.13	0.62
7:T:26:TYR:CD1	7:T:26:TYR:N	2.65	0.62
1:A:62:VAL:HG13	1:A:177:GLN:HB3	1.79	0.62
1:A:26:VAL:HG21	2:B:29:GLU:HG3	1.81	0.62
3:C:226:LYS:HE3	3:C:229:GLU:C	2.19	0.62
4:Q:155:VAL:HG12	4:Q:156:GLN:N	2.14	0.62
5:R:3:LEU:HA	5:R:6:VAL:HG23	1.81	0.62
1:A:118:TRP:HD1	9:A:302:HEM:HMD2	1.64	0.62
3:C:93:GLU:CA	3:C:97:GLU:HB2	2.23	0.62
3:C:271:MET:CG	4:D:22:LEU:HD21	2.23	0.62
1:N:27:PRO:O	2:O:29:GLU:HB3	1.99	0.62
1:N:45:LEU:HB3	11:Q:1305:PL9:H502	1.81	0.62
3:P:94:LEU:H	3:P:94:LEU:CD2	2.06	0.62
4:Q:116:PRO:CD	4:Q:126:CYS:HA	2.24	0.62
4:D:51:GLY:CA	4:D:164:PRO:HG2	2.21	0.62
3:P:83:LYS:HB2	3:P:111:ASP:CB	2.29	0.62
12:B:307:OPC:HBU2	12:B:307:OPC:HBC1	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:117:TRP:HD1	4:D:124:PHE:CE1	2.17	0.62
5:E:23:ILE:HG23	5:E:24:PHE:N	2.14	0.62
3:P:10:PRO:HG2	3:P:11:PRO:HD3	1.80	0.62
12:Q:1307:OPC:HBZ2	12:Q:1307:OPC:HBF1	1.80	0.62
1:A:26:VAL:CB	2:B:29:GLU:HG3	2.29	0.62
2:B:32:TRP:CE3	2:B:36:LEU:HG	2.35	0.62
3:C:10:PRO:HG2	3:C:11:PRO:HD3	1.82	0.62
3:P:89:ARG:O	3:P:91:PRO:HD3	2.00	0.62
4:Q:19:MET:O	4:Q:22:LEU:HB3	1.99	0.62
3:C:185:LYS:HE2	3:C:195:TYR:HB3	1.81	0.62
5:R:5:ALA:CB	6:S:5:MET:HB2	2.30	0.62
2:B:149:LEU:HB2	2:B:150:PRO:CD	2.29	0.62
3:C:218:ILE:HG13	3:C:219:VAL:N	2.14	0.62
4:D:121:GLU:OE1	4:D:125:LYS:HE3	2.00	0.62
5:E:11:PHE:CD1	5:E:11:PHE:C	2.72	0.62
5:E:27:LYS:O	5:E:31:LEU:HD22	1.99	0.62
2:O:20:LYS:CD	2:O:21:GLY:H	2.13	0.62
12:Q:1307:OPC:HAL2	12:Q:1307:OPC:HAP1	1.82	0.62
4:D:90:TYR:CE2	4:D:106:ALA:HB2	2.34	0.62
7:G:26:TYR:CD1	7:G:26:TYR:N	2.67	0.62
1:N:21:VAL:HG12	1:N:22:THR:N	2.15	0.62
1:N:21:VAL:O	1:N:23:SER:N	2.32	0.62
3:P:111:ASP:O	3:P:114:LEU:HD21	2.00	0.62
4:Q:134:ASP:CB	4:Q:138:ARG:HB2	2.30	0.62
2:O:122:ASN:HD21	5:R:30:LYS:HG3	1.64	0.62
7:T:28:GLN:O	7:T:30:LYS:N	2.33	0.62
7:T:9:LEU:HD23	7:T:9:LEU:N	2.15	0.62
2:B:18:LEU:O	2:B:19:ALA:HB3	1.99	0.61
3:P:275:LYS:CD	4:Q:20:ASN:HB3	2.30	0.61
5:R:23:ILE:HG23	5:R:24:PHE:N	2.14	0.61
4:D:121:GLU:HB3	4:D:123:LYS:HG3	1.80	0.61
4:D:73:HIS:ND1	4:D:77:ASP:HB3	2.15	0.61
5:R:11:PHE:C	5:R:11:PHE:CD1	2.73	0.61
4:D:111:LEU:HB3	4:D:129:HIS:CE1	2.36	0.61
12:N:1306:OPC:HAP2	12:N:1306:OPC:CBI	2.23	0.61
2:O:144:GLY:O	2:O:145:ILE:HD13	2.00	0.61
2:O:20:LYS:CG	2:O:21:GLY:H	2.13	0.61
3:P:188:ASP:HB3	3:P:193:VAL:HA	1.82	0.61
1:A:30:VAL:HG21	5:E:26:ILE:HD11	1.82	0.61
4:D:136:THR:HG22	4:D:150:LEU:HD11	1.83	0.61
3:P:117:GLY:O	3:P:119:LEU:HG	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:LEU:HD12	1:A:116:LEU:N	2.14	0.61
1:A:15:GLN:O	1:A:16:ALA:HB3	2.00	0.61
3:C:171:VAL:HB	3:C:231:LEU:CD1	2.30	0.61
3:C:226:LYS:HG2	3:C:229:GLU:CB	2.30	0.61
3:P:81:GLY:C	3:P:134:PRO:HG3	2.20	0.61
1:A:105:TYR:HD2	1:A:106:LEU:HD23	1.65	0.61
10:N:1304:TDS:HAU1	13:O:1201:CLA:H91	1.81	0.61
2:O:134:LEU:O	2:O:138:LEU:HD13	2.01	0.61
7:T:26:TYR:N	7:T:26:TYR:HD1	1.97	0.61
3:C:188:ASP:O	3:C:189:GLU:HB2	2.01	0.61
3:C:188:ASP:HB3	3:C:193:VAL:HA	1.81	0.61
3:P:226:LYS:HE3	3:P:229:GLU:C	2.20	0.61
3:P:231:LEU:HD13	3:P:232:THR:N	2.14	0.61
5:R:21:GLY:O	5:R:25:ALA:HB2	2.00	0.61
1:N:158:ILE:O	1:N:162:GLY:HA3	2.01	0.61
9:N:301:HEM:CHA	9:N:301:HEM:HBD1	2.31	0.61
4:D:65:LYS:HD3	4:D:68:LYS:NZ	2.16	0.61
12:N:1306:OPC:HBQ2	12:N:1306:OPC:HAT1	1.82	0.61
4:Q:104:ILE:CD1	4:Q:136:THR:HA	2.30	0.61
1:N:196:ALA:O	1:N:200:LEU:HB2	2.00	0.61
1:N:98:ILE:HD11	13:O:1201:CLA:HED3	1.81	0.61
2:O:124:PHE:HZ	5:R:26:ILE:CB	2.10	0.61
3:P:226:LYS:HE3	3:P:229:GLU:HB3	1.81	0.61
1:A:200:LEU:O	1:A:204:LEU:HG	2.00	0.60
2:B:75:ILE:O	2:B:76:LEU:O	2.18	0.60
5:E:18:ILE:O	5:E:22:ILE:HB	2.01	0.60
1:N:116:LEU:N	1:N:116:LEU:HD12	2.14	0.60
3:P:91:PRO:HD2	3:P:95:LYS:CG	2.31	0.60
4:Q:123:LYS:HE3	4:Q:125:LYS:HZ3	1.64	0.60
4:Q:172:THR:HB	4:Q:174:GLU:OE2	2.01	0.60
4:Q:65:LYS:HB2	4:Q:68:LYS:HB2	1.82	0.60
2:B:112:PRO:O	2:B:116:ASN:CB	2.49	0.60
3:C:171:VAL:HG12	3:C:233:ASN:O	2.01	0.60
2:O:118:ASN:ND2	2:O:121:GLN:HE22	1.95	0.60
1:N:214:PRO:CB	5:R:29:ILE:HG22	2.13	0.60
3:C:86:PRO:HG2	3:C:89:ARG:HG3	1.83	0.60
1:N:110:PHE:HE1	2:O:111:VAL:HG12	1.67	0.60
2:O:75:ILE:O	2:O:77:PRO:HD2	2.01	0.60
4:Q:58:ASP:OD1	4:Q:64:VAL:HG22	2.01	0.60
4:Q:56:ALA:CA	4:Q:81:VAL:HG13	2.21	0.60
4:D:136:THR:HB	4:D:138:ARG:CD	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:168:THR:CA	4:D:176:PRO:HD3	2.31	0.60
4:D:42:PHE:CD1	12:D:306:OPC:HAG2	2.36	0.60
1:N:37:GLY:HA3	9:N:302:HEM:HBA1	1.82	0.60
3:C:83:LYS:HB2	3:C:111:ASP:CB	2.30	0.60
3:C:275:LYS:CE	4:D:17:GLN:HB2	2.32	0.60
3:C:90:ILE:CG2	3:C:95:LYS:HB2	2.32	0.60
3:P:45:VAL:HG22	3:P:85:ALA:HB2	1.83	0.60
5:R:5:ALA:HA	5:R:8:TYR:HB2	1.84	0.60
3:P:118:PRO:C	3:P:120:PRO:HD3	2.22	0.60
3:C:180:ILE:O	3:C:221:GLU:HA	2.02	0.60
4:D:123:LYS:HD2	4:D:140:ILE:HD11	1.83	0.60
4:D:167:GLU:C	4:D:176:PRO:HG3	2.21	0.60
4:D:19:MET:O	4:D:22:LEU:HB3	2.01	0.60
2:O:106:LEU:HD11	13:O:1201:CLA:H171	1.84	0.60
3:P:275:LYS:HD3	3:P:275:LYS:C	2.21	0.60
4:Q:81:VAL:HB	4:Q:89:THR:OG1	2.01	0.60
1:A:175:VAL:O	1:A:175:VAL:HG12	2.01	0.60
11:A:305:PL9:H252	12:D:306:OPC:CBN	2.31	0.60
3:C:262:ILE:HG21	7:G:17:THR:HG23	1.82	0.60
4:D:51:GLY:C	4:D:85:LYS:HZ1	2.04	0.60
1:N:28:PRO:HG2	2:O:32:TRP:CB	2.31	0.60
2:O:141:ILE:HD11	5:R:11:PHE:CZ	2.36	0.60
1:A:204:LEU:C	1:A:206:ILE:H	2.04	0.60
3:C:218:ILE:HG12	3:C:232:THR:CA	2.31	0.60
6:F:11:LEU:O	6:F:15:LEU:HD23	2.02	0.60
2:O:122:ASN:CG	5:R:26:ILE:HG21	2.21	0.60
3:P:218:ILE:HG13	3:P:219:VAL:N	2.17	0.60
3:P:180:ILE:O	3:P:221:GLU:HA	2.02	0.60
15:R:1101:BCR:H362	6:S:17:PHE:HZ	1.67	0.60
3:C:116:VAL:O	3:C:116:VAL:HG12	2.00	0.60
4:D:101:ASP:HA	4:D:153:ALA:HB2	1.82	0.60
4:D:100:ARG:O	4:D:153:ALA:HB2	2.02	0.60
4:Q:129:HIS:HB2	14:Q:1200:FES:S1	2.42	0.60
2:B:124:PHE:HE1	5:E:23:ILE:HG13	1.67	0.59
2:B:38:TYR:OH	12:B:307:OPC:HAS2	2.01	0.59
2:B:42:VAL:HG23	3:C:272:LEU:HD13	1.82	0.59
3:C:55:ASP:OD1	3:C:57:LYS:HG3	2.02	0.59
4:D:13:MET:SD	4:D:13:MET:N	2.75	0.59
4:D:137:GLY:CA	4:D:148:LEU:HB2	2.32	0.59
4:D:66:VAL:HG11	4:D:155:VAL:HG11	1.83	0.59
1:N:191:LEU:HD21	10:N:1304:TDS:OBD	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:70:ALA:HB1	3:C:17:THR:HA	1.83	0.59
3:C:266:MET:HE3	7:G:20:GLY:O	2.02	0.59
7:G:26:TYR:CA	7:G:29:TYR:CD1	2.82	0.59
2:O:126:ARG:HH12	2:O:128:VAL:C	2.06	0.59
2:O:146:GLY:O	2:O:149:LEU:N	2.31	0.59
3:P:283:GLN:C	3:P:285:ALA:H	2.04	0.59
1:A:95:LEU:HD13	1:A:96:MET:CE	2.32	0.59
4:D:121:GLU:O	4:D:122:ASN:HB2	2.03	0.59
12:D:306:OPC:HBC2	12:D:306:OPC:HAY2	1.83	0.59
1:N:39:ILE:HD11	15:R:1101:BCR:H312	1.83	0.59
3:P:217:LEU:CA	3:P:232:THR:HB	2.32	0.59
4:Q:66:VAL:O	4:Q:70:LEU:HB2	2.02	0.59
4:Q:96:LYS:O	4:Q:97:GLU:HB2	2.01	0.59
2:B:34:ASN:ND2	12:B:307:OPC:CBK	2.64	0.59
3:C:45:VAL:HG22	3:C:85:ALA:HB2	1.84	0.59
4:D:138:ARG:NE	4:D:171:ARG:HD2	2.18	0.59
11:A:305:PL9:H111	12:D:306:OPC:CBF	2.32	0.59
7:G:11:LEU:HA	7:G:14:VAL:HG11	1.84	0.59
3:P:194:LYS:HE3	3:P:212:PRO:HB3	1.83	0.59
4:D:132:GLN:H	4:D:144:ALA:HB2	1.68	0.59
7:G:11:LEU:HA	7:G:14:VAL:HG13	1.85	0.59
3:P:105:PRO:HB3	3:P:110:GLN:O	2.02	0.59
3:P:278:GLN:O	3:P:281:LYS:HE2	2.03	0.59
3:P:28:ALA:O	3:P:239:GLY:HA3	2.03	0.59
4:Q:94:GLU:HG2	4:Q:95:SER:N	2.18	0.59
2:B:71:THR:CB	2:B:72:PRO:HD3	2.11	0.59
3:C:171:VAL:HG13	3:C:234:ASN:HD22	1.68	0.59
3:P:40:VAL:HG13	3:P:247:ILE:HD11	1.85	0.59
4:Q:66:VAL:HG22	4:Q:160:ILE:HG12	1.85	0.59
2:B:32:TRP:CZ3	2:B:36:LEU:HG	2.37	0.59
2:B:86:GLN:HG2	2:B:143:LEU:HA	1.84	0.59
4:D:123:LYS:HZ1	4:D:140:ILE:HG13	1.67	0.59
5:E:3:LEU:HA	5:E:6:VAL:HG23	1.85	0.59
6:F:12:SER:O	6:F:16:ILE:HG12	2.02	0.59
3:C:269:GLN:NE2	7:G:24:ALA:HA	2.17	0.59
1:N:204:LEU:C	1:N:206:ILE:H	2.05	0.59
3:P:195:TYR:O	3:P:196:GLN:O	2.21	0.59
4:Q:91:ILE:HG23	4:Q:160:ILE:CD1	2.32	0.59
4:Q:55:THR:O	4:Q:56:ALA:HB3	2.03	0.59
3:C:49:VAL:HG22	3:C:128:VAL:HG22	1.85	0.59
3:C:54:TYR:HD2	3:C:70:LEU:HD13	1.66	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:65:LYS:O	4:D:68:LYS:HB2	2.03	0.59
4:D:99:ILE:O	4:D:99:ILE:HD12	2.03	0.59
8:H:17:TRP:O	8:H:20:ALA:HB3	2.03	0.59
1:N:81:LEU:HD13	1:N:81:LEU:C	2.23	0.59
3:P:216:GLU:HB2	3:P:233:ASN:OD1	2.03	0.59
3:P:86:PRO:HG2	3:P:89:ARG:HG3	1.84	0.59
4:Q:93:VAL:HG22	4:Q:94:GLU:N	2.17	0.59
7:T:31:ARG:HD3	7:T:32:PRO:HD3	1.85	0.59
10:A:304:TDS:CBC	2:B:85:PHE:HD2	2.15	0.59
5:E:5:ALA:HA	5:E:8:TYR:HB2	1.85	0.59
8:H:11:LEU:HB3	8:H:15:PHE:HZ	1.66	0.59
1:N:154:VAL:HG11	10:N:1304:TDS:HAX1	1.84	0.59
2:O:25:ASN:OD1	2:O:26:TYR:N	2.35	0.59
4:Q:64:VAL:HG21	4:Q:80:LEU:C	2.23	0.59
5:R:16:PHE:O	5:R:20:VAL:HB	2.03	0.59
1:A:35:CYS:O	1:A:39:ILE:HG12	2.02	0.59
4:D:166:THR:C	4:D:179:VAL:HG22	2.23	0.59
5:E:26:ILE:HA	5:E:29:ILE:HG13	1.84	0.59
4:Q:134:ASP:OD1	4:Q:138:ARG:HB2	2.03	0.59
4:Q:138:ARG:HB3	4:Q:138:ARG:NH1	2.18	0.59
4:Q:156:GLN:CB	4:Q:161:VAL:HG21	2.23	0.59
5:R:9:ILE:HG12	6:S:13:PHE:HB2	1.85	0.59
3:P:178:GLY:C	3:P:225:VAL:HA	2.23	0.58
7:T:17:THR:O	7:T:21:LEU:HB2	2.03	0.58
2:B:118:ASN:CB	2:B:121:GLN:O	2.49	0.58
2:B:149:LEU:N	2:B:149:LEU:HD12	2.18	0.58
3:C:194:LYS:HE3	3:C:212:PRO:HB3	1.85	0.58
4:D:131:SER:OG	4:D:144:ALA:HA	2.02	0.58
4:D:80:LEU:HD13	4:D:88:PRO:HB2	1.85	0.58
3:P:116:VAL:HG12	3:P:116:VAL:O	2.03	0.58
3:P:49:VAL:HG22	3:P:128:VAL:HG22	1.85	0.58
1:A:23:SER:HB2	1:A:24:LYS:HD3	1.86	0.58
3:C:59:GLN:CB	3:C:67:LYS:HB3	2.33	0.58
12:Q:1307:OPC:CAX	12:Q:1307:OPC:HAT1	2.33	0.58
4:Q:66:VAL:HG12	4:Q:70:LEU:HD12	1.85	0.58
7:T:27:GLN:HA	7:T:27:GLN:NE2	2.18	0.58
1:A:33:PHE:CE1	5:E:14:LEU:HD22	2.39	0.58
11:A:305:PL9:H162	12:B:307:OPC:HBU1	1.84	0.58
3:C:226:LYS:CD	3:C:229:GLU:HB3	2.33	0.58
3:C:50:VAL:HG13	3:C:151:LEU:HD21	1.85	0.58
4:D:134:ASP:N	4:D:138:ARG:O	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:104:ILE:CG2	4:D:148:LEU:HB3	2.34	0.58
7:G:30:LYS:O	7:G:31:ARG:CZ	2.50	0.58
1:N:23:SER:HA	1:N:25:TYR:CE2	2.39	0.58
2:O:24:HIS:ND1	2:O:24:HIS:N	2.50	0.58
3:P:218:ILE:HG12	3:P:232:THR:CA	2.33	0.58
4:Q:142:GLY:CA	4:Q:144:ALA:H	2.17	0.58
3:P:275:LYS:CE	4:Q:17:GLN:HB2	2.32	0.58
15:R:1101:BCR:H362	6:S:17:PHE:CZ	2.38	0.58
3:C:216:GLU:O	3:C:233:ASN:CB	2.51	0.58
3:C:91:PRO:HD2	3:C:95:LYS:CG	2.33	0.58
4:D:50:VAL:HG12	4:D:164:PRO:HB3	1.84	0.58
1:N:95:LEU:HD13	1:N:96:MET:CE	2.33	0.58
3:P:231:LEU:HD12	3:P:231:LEU:H	1.68	0.58
4:Q:78:ARG:NH2	4:Q:100:ARG:NH2	2.46	0.58
4:Q:133:TYR:HB3	4:Q:137:GLY:C	2.23	0.58
1:A:196:ALA:O	1:A:200:LEU:HB2	2.04	0.58
4:D:136:THR:O	4:D:136:THR:HG22	2.04	0.58
3:C:255:VAL:CG1	7:G:14:VAL:CG1	2.74	0.58
8:H:12:LEU:HA	8:H:15:PHE:CD1	2.38	0.58
3:P:59:GLN:CB	3:P:67:LYS:HB3	2.34	0.58
4:Q:168:THR:HG23	4:Q:175:LYS:N	2.17	0.58
6:F:7:TYR:O	6:F:11:LEU:HD12	2.04	0.58
7:G:26:TYR:HD1	7:G:26:TYR:N	2.00	0.58
8:U:7:GLY:O	8:U:11:LEU:HD11	2.03	0.58
8:U:23:VAL:O	8:U:27:ASN:ND2	2.36	0.58
3:C:120:PRO:HB3	3:C:124:TYR:CD1	2.39	0.58
3:C:261:PHE:CE2	4:D:30:VAL:HG13	2.38	0.58
4:D:129:HIS:O	4:D:143:PRO:HG3	2.03	0.58
4:D:137:GLY:HA3	4:D:148:LEU:HB2	1.85	0.58
7:G:9:LEU:HG	7:G:10:VAL:H	1.69	0.58
1:A:193:TRP:O	1:A:197:VAL:HG23	2.03	0.58
4:Q:152:HIS:H	4:Q:162:LEU:HD23	1.69	0.58
8:U:6:LEU:C	8:U:8:TRP:N	2.57	0.58
2:B:38:TYR:HB3	3:C:276:LYS:CG	2.32	0.58
4:D:116:PRO:CG	4:D:126:CYS:HA	2.34	0.58
4:D:93:VAL:HG13	4:D:94:GLU:O	2.03	0.58
1:N:188:THR:CG2	9:N:301:HEM:HBC2	2.33	0.58
3:P:188:ASP:O	3:P:189:GLU:HB2	2.03	0.58
7:T:21:LEU:C	7:T:23:TYR:H	2.05	0.58
11:A:305:PL9:H513	4:D:28:THR:HG23	1.85	0.57
7:G:26:TYR:HA	7:G:29:TYR:HD1	1.61	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:6:LEU:C	8:H:8:TRP:H	2.05	0.57
2:O:118:ASN:HD22	2:O:121:GLN:CD	2.06	0.57
2:O:122:ASN:CG	5:R:26:ILE:CG2	2.72	0.57
2:B:119:LYS:O	2:B:119:LYS:HD3	2.03	0.57
4:D:134:ASP:HB3	4:D:138:ARG:HG2	1.85	0.57
4:Q:123:LYS:HB2	4:Q:125:LYS:HE2	1.86	0.57
12:Q:1307:OPC:CAQ	12:Q:1307:OPC:HBG3	2.34	0.57
8:U:6:LEU:HA	8:U:9:VAL:HG12	1.86	0.57
3:C:3:PHE:HZ	3:C:119:LEU:HD11	1.69	0.57
2:O:84:VAL:HG22	13:O:1201:CLA:HMD1	1.86	0.57
4:Q:178:TRP:N	4:Q:178:TRP:CE3	2.69	0.57
4:D:84:LEU:O	4:D:86:GLY:N	2.37	0.57
7:G:25:ALA:O	7:G:29:TYR:CD2	2.57	0.57
8:H:6:LEU:C	8:H:8:TRP:N	2.56	0.57
1:N:112:LYS:HB2	1:N:113:PRO:CD	2.27	0.57
1:N:113:PRO:C	1:N:115:GLU:OE1	2.42	0.57
1:N:29:HIS:HE2	1:N:209:GLN:CG	2.16	0.57
3:P:52:ILE:HG12	3:P:153:ALA:CB	2.34	0.57
4:Q:88:PRO:HG3	4:Q:106:ALA:N	2.20	0.57
4:Q:123:LYS:O	4:Q:125:LYS:HG2	2.03	0.57
3:P:255:VAL:CG1	7:T:14:VAL:HG12	2.34	0.57
1:A:27:PRO:HG3	2:B:33:PRO:HG3	1.87	0.57
4:D:150:LEU:HD13	4:D:171:ARG:HD3	1.86	0.57
3:P:217:LEU:HA	3:P:232:THR:CB	2.33	0.57
3:P:84:ILE:HD12	3:P:130:PRO:HD2	1.86	0.57
3:C:278:GLN:O	3:C:281:LYS:HE2	2.04	0.57
4:D:110:HIS:CE1	4:D:129:HIS:HB2	2.39	0.57
3:P:202:ASP:HA	3:P:206:THR:CB	2.25	0.57
4:Q:64:VAL:O	4:Q:91:ILE:HD11	2.04	0.57
1:A:13:GLU:C	1:A:17:LEU:HD12	2.25	0.57
3:C:117:GLY:O	3:C:119:LEU:HG	2.05	0.57
3:C:79:PRO:HG2	3:C:82:PHE:CE1	2.39	0.57
4:D:124:PHE:CB	4:D:133:TYR:HB2	2.22	0.57
4:D:65:LYS:HD3	4:D:68:LYS:HZ1	1.69	0.57
2:O:72:PRO:O	2:O:73:LEU:HB3	2.04	0.57
3:P:216:GLU:O	3:P:233:ASN:HB2	2.03	0.57
3:P:258:MET:O	3:P:262:ILE:HD13	2.04	0.57
1:A:62:VAL:HG13	1:A:177:GLN:CB	2.34	0.57
2:B:114:ILE:C	2:B:116:ASN:H	2.07	0.57
3:C:202:ASP:HA	3:C:206:THR:CB	2.27	0.57
3:C:231:LEU:HD22	3:C:232:THR:N	2.19	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:275:LYS:HD3	3:C:275:LYS:C	2.25	0.57
3:P:61:VAL:O	3:P:157:ARG:NH1	2.37	0.57
1:N:79:GLY:HA2	4:Q:41:TYR:HE1	1.69	0.57
1:A:207:ARG:O	1:A:208:LYS:HD2	2.05	0.57
2:B:134:LEU:O	2:B:138:LEU:HD13	2.05	0.57
3:C:276:LYS:HE3	3:C:276:LYS:HA	1.87	0.57
4:D:128:CYS:HB3	4:D:129:HIS:CE1	2.40	0.57
4:D:166:THR:HG23	4:D:179:VAL:HG11	1.86	0.57
2:O:74:GLU:O	2:O:75:ILE:HB	2.05	0.57
3:P:172:PHE:C	3:P:231:LEU:HB3	2.25	0.57
3:P:91:PRO:HD2	3:P:95:LYS:HG2	1.86	0.57
2:B:32:TRP:H	2:B:33:PRO:HD3	1.70	0.57
3:C:271:MET:HB3	4:D:23:ALA:HA	1.87	0.57
5:E:27:LYS:O	5:E:31:LEU:HB2	2.05	0.57
5:E:3:LEU:HA	5:E:6:VAL:CG2	2.34	0.57
8:H:23:VAL:O	8:H:27:ASN:ND2	2.37	0.57
4:Q:116:PRO:HD2	4:Q:126:CYS:CA	2.26	0.57
2:B:18:LEU:O	2:B:19:ALA:CB	2.51	0.56
2:B:84:VAL:O	2:B:88:LEU:HD13	2.04	0.56
1:N:33:PHE:HB3	1:N:103:ARG:HG2	1.87	0.56
1:N:111:LYS:CB	1:N:114:ARG:NH1	2.68	0.56
1:N:209:GLN:CB	2:O:27:TYR:HB2	2.35	0.56
2:O:80:TYR:CD1	2:O:80:TYR:N	2.73	0.56
1:N:95:LEU:HG	5:R:7:PHE:CB	2.34	0.56
2:B:155:LEU:C	2:B:155:LEU:HD23	2.25	0.56
2:B:155:LEU:O	2:B:155:LEU:HD23	2.04	0.56
1:A:88:TRP:HZ2	2:B:58:ASP:HB3	1.69	0.56
3:C:269:GLN:CD	7:G:24:ALA:HA	2.26	0.56
1:N:149:LYS:HD2	1:N:175:VAL:CG2	2.34	0.56
2:O:79:TRP:CZ2	5:R:1:MET:N	2.66	0.56
11:Q:1305:PL9:C32	12:Q:1307:OPC:HBW2	2.34	0.56
7:T:17:THR:O	7:T:21:LEU:CB	2.52	0.56
1:A:106:LEU:HD12	5:E:18:ILE:HD12	1.85	0.56
5:E:9:ILE:HG23	6:F:12:SER:HB2	1.88	0.56
1:N:213:GLY:O	5:R:30:LYS:CD	2.49	0.56
2:O:141:ILE:O	2:O:144:GLY:N	2.39	0.56
3:P:93:GLU:CA	3:P:97:GLU:HB2	2.28	0.56
4:Q:13:MET:SD	4:Q:13:MET:N	2.78	0.56
1:A:26:VAL:HB	2:B:29:GLU:CG	2.35	0.56
2:B:41:PRO:O	2:B:45:MET:HG3	2.06	0.56
3:C:185:LYS:HE2	3:C:195:TYR:CB	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:5:ALA:HB2	6:F:5:MET:HB2	1.87	0.56
7:G:30:LYS:CB	7:G:31:ARG:NH2	2.66	0.56
2:O:32:TRP:N	2:O:33:PRO:CD	2.67	0.56
3:P:219:VAL:HG11	3:P:223:GLN:NE2	2.19	0.56
4:Q:66:VAL:C	4:Q:68:LYS:H	2.09	0.56
7:T:28:GLN:O	7:T:31:ARG:HB3	2.06	0.56
4:D:65:LYS:NZ	4:D:158:ASP:HB3	2.20	0.56
5:E:6:VAL:O	5:E:10:VAL:HB	2.04	0.56
1:N:109:GLY:C	1:N:111:LYS:H	2.08	0.56
1:N:118:TRP:CZ3	2:O:108:LEU:O	2.58	0.56
3:P:12:THR:OG1	3:P:13:PRO:HD2	2.06	0.56
3:P:38:GLN:OE1	7:T:15:PHE:CE1	2.59	0.56
3:P:54:TYR:OH	3:P:58:LEU:HD22	2.05	0.56
5:R:9:ILE:HG23	6:S:12:SER:HB2	1.88	0.56
1:A:14:ILE:CD1	1:A:15:GLN:N	2.67	0.56
6:F:15:LEU:HD12	7:G:26:TYR:OH	2.05	0.56
3:P:223:GLN:O	3:P:224:ALA:HB3	2.05	0.56
4:Q:73:HIS:O	4:Q:74:ASN:HB2	2.04	0.56
7:T:11:LEU:HA	7:T:14:VAL:CG1	2.36	0.56
7:T:21:LEU:C	7:T:23:TYR:N	2.58	0.56
1:A:13:GLU:O	1:A:17:LEU:HD12	2.06	0.56
3:C:271:MET:HG3	4:D:22:LEU:CD2	2.26	0.56
8:H:6:LEU:HA	8:H:9:VAL:HG12	1.87	0.56
2:O:112:PRO:O	2:O:116:ASN:CB	2.53	0.56
2:O:86:GLN:HG2	2:O:143:LEU:HA	1.87	0.56
5:R:6:VAL:O	5:R:10:VAL:HB	2.05	0.56
1:A:77:SER:O	1:A:78:PHE:HB2	2.05	0.56
2:B:37:LEU:HD23	2:B:40:PHE:CE2	2.41	0.56
3:C:86:PRO:CG	3:C:89:ARG:HG3	2.36	0.56
7:G:25:ALA:O	7:G:29:TYR:CG	2.59	0.56
1:N:15:GLN:O	1:N:17:LEU:N	2.39	0.56
2:O:32:TRP:N	2:O:33:PRO:HD3	2.20	0.56
3:C:94:LEU:CD2	3:C:94:LEU:H	2.12	0.56
7:G:11:LEU:CA	7:G:14:VAL:HG13	2.36	0.56
4:Q:100:ARG:HD2	4:Q:102:TYR:CZ	2.40	0.56
6:S:12:SER:O	6:S:16:ILE:HG12	2.05	0.56
1:A:72:ILE:O	1:A:79:GLY:HA3	2.06	0.56
2:B:36:LEU:O	2:B:39:VAL:HG22	2.06	0.56
3:C:178:GLY:HA2	3:C:225:VAL:HG13	1.86	0.56
4:D:131:SER:CB	4:D:144:ALA:HA	2.36	0.56
2:O:74:GLU:CG	2:O:75:ILE:H	2.18	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:96:LEU:O	2:O:100:LEU:HB2	2.05	0.56
4:Q:152:HIS:O	4:Q:153:ALA:HB2	2.05	0.56
5:R:7:PHE:CA	5:R:10:VAL:HG12	2.23	0.56
12:B:307:OPC:CBI	12:B:307:OPC:HAP1	2.26	0.56
12:N:1306:OPC:HBQ2	12:N:1306:OPC:CAT	2.36	0.56
4:Q:156:GLN:HB2	4:Q:161:VAL:HG11	1.88	0.56
6:S:26:LEU:HD21	8:U:17:TRP:HE1	1.70	0.56
7:G:17:THR:O	7:G:21:LEU:CB	2.54	0.55
7:G:30:LYS:O	7:G:31:ARG:NE	2.39	0.55
2:O:91:LEU:HD22	2:O:96:LEU:HD13	1.88	0.55
3:P:134:PRO:CB	3:P:142:ILE:HD13	2.35	0.55
3:C:269:GLN:HE22	7:G:24:ALA:CA	2.19	0.55
4:D:57:LYS:H	4:D:82:GLN:CG	2.20	0.55
2:O:75:ILE:HD12	2:O:75:ILE:N	2.22	0.55
4:Q:138:ARG:HH11	4:Q:138:ARG:HB3	1.69	0.55
6:S:11:LEU:O	6:S:15:LEU:HD23	2.06	0.55
1:A:166:SER:O	1:A:170:ARG:HG2	2.06	0.55
5:E:26:ILE:N	5:E:26:ILE:HD12	2.22	0.55
1:N:31:ASN:HB3	1:N:34:TYR:CD2	2.41	0.55
2:O:30:PRO:HG2	2:O:31:ALA:H	1.71	0.55
3:P:194:LYS:HD3	3:P:212:PRO:HA	1.89	0.55
3:P:255:VAL:O	3:P:258:MET:HG3	2.07	0.55
3:P:276:LYS:HA	3:P:276:LYS:HE3	1.89	0.55
12:Q:1307:OPC:HBZ2	12:Q:1307:OPC:CBF	2.37	0.55
8:U:3:ILE:HG13	8:U:4:ASP:OD1	2.06	0.55
2:B:150:PRO:HG2	2:B:151:LEU:H	1.72	0.55
3:C:216:GLU:HB2	3:C:233:ASN:OD1	2.06	0.55
3:C:218:ILE:CG1	3:C:232:THR:HG22	2.36	0.55
4:D:73:HIS:HE2	4:D:91:ILE:CG2	2.19	0.55
3:P:168:ASN:HA	3:P:172:PHE:CE1	2.40	0.55
3:P:26:HIS:ND1	3:P:154:ASN:OD1	2.39	0.55
4:Q:155:VAL:HA	4:Q:159:ASN:O	2.05	0.55
7:T:14:VAL:HG23	7:T:15:PHE:N	2.21	0.55
1:A:108:GLY:HA2	1:A:110:PHE:CE2	2.41	0.55
2:B:31:ALA:O	2:B:32:TRP:CB	2.46	0.55
7:G:28:GLN:O	7:G:30:LYS:N	2.39	0.55
12:N:1306:OPC:HBQ2	12:N:1306:OPC:HAU2	1.89	0.55
4:Q:101:ASP:HA	4:Q:153:ALA:CB	2.37	0.55
1:A:105:TYR:CD1	13:B:201:CLA:HMB1	2.41	0.55
1:A:88:TRP:CZ2	2:B:58:ASP:HB3	2.42	0.55
3:C:111:ASP:O	3:C:114:LEU:HD21	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:185:LYS:HE3	3:C:217:LEU:HD11	1.89	0.55
3:C:226:LYS:CG	3:C:229:GLU:HB3	2.36	0.55
4:D:168:THR:HA	4:D:176:PRO:CD	2.36	0.55
1:N:28:PRO:O	2:O:30:PRO:HG2	2.07	0.55
2:O:32:TRP:CZ3	2:O:36:LEU:HG	2.42	0.55
1:N:141:ASP:HA	2:O:65:PRO:CD	2.35	0.55
4:Q:92:VAL:HG21	4:Q:100:ARG:HB2	1.87	0.55
5:R:27:LYS:O	5:R:31:LEU:HD22	2.06	0.55
2:B:149:LEU:N	2:B:149:LEU:CD1	2.66	0.55
1:A:95:LEU:HD11	5:E:10:VAL:HG11	1.88	0.55
1:N:193:TRP:O	1:N:197:VAL:HG23	2.07	0.55
1:N:213:GLY:O	5:R:26:ILE:HG23	2.06	0.55
3:P:82:PHE:O	3:P:112:ASN:HB3	2.07	0.55
3:P:119:LEU:HD12	3:P:119:LEU:H	1.69	0.55
4:Q:115:VAL:CG1	4:Q:124:PHE:HB3	2.35	0.55
1:A:211:ILE:HD12	1:A:211:ILE:N	2.14	0.55
2:B:42:VAL:CG2	3:C:272:LEU:HD13	2.37	0.55
4:D:138:ARG:CZ	4:D:138:ARG:HB3	2.37	0.55
4:D:104:ILE:HG21	4:D:148:LEU:HB3	1.89	0.55
5:R:5:ALA:HB2	6:S:5:MET:HB2	1.89	0.55
2:B:88:LEU:HD11	2:B:101:MET:SD	2.46	0.55
2:O:86:GLN:HG3	2:O:143:LEU:HD22	1.89	0.55
3:P:185:LYS:HD3	3:P:195:TYR:CD2	2.41	0.55
4:Q:104:ILE:HG21	4:Q:124:PHE:HE2	1.71	0.55
3:C:187:GLU:HG3	3:C:188:ASP:N	2.22	0.55
3:C:40:VAL:HG13	3:C:247:ILE:HD11	1.89	0.55
4:D:88:PRO:O	4:D:105:ASN:HA	2.07	0.55
2:O:122:ASN:ND2	2:O:125:ARG:NH1	2.54	0.55
1:A:47:GLN:HG2	9:A:301:HEM:C3B	2.42	0.54
3:C:283:GLN:C	3:C:285:ALA:H	2.10	0.54
4:D:16:ARG:C	4:D:18:PHE:N	2.60	0.54
12:D:306:OPC:CBM	12:D:306:OPC:HAR2	2.38	0.54
8:H:3:ILE:HG13	8:H:4:ASP:OD1	2.06	0.54
3:P:171:VAL:HG12	3:P:233:ASN:O	2.07	0.54
3:P:275:LYS:NZ	3:P:276:LYS:NZ	2.55	0.54
12:Q:1307:OPC:HBP2	12:Q:1307:OPC:HBA1	1.89	0.54
1:A:62:VAL:HG12	1:A:140:TRP:CH2	2.42	0.54
5:R:27:LYS:O	5:R:31:LEU:HB2	2.07	0.54
4:D:87:ASP:HB3	4:D:105:ASN:HB3	1.89	0.54
3:P:174:ALA:HB3	3:P:228:GLY:HA2	1.89	0.54
8:U:3:ILE:HG23	8:U:4:ASP:N	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:106:ALA:HB1	4:D:115:VAL:HB	1.89	0.54
1:N:141:ASP:C	2:O:64:GLU:HG2	2.27	0.54
2:O:106:LEU:CD2	13:O:1201:CLA:H151	2.36	0.54
3:P:199:ILE:HB	3:P:208:VAL:HA	1.90	0.54
3:P:171:VAL:HB	3:P:231:LEU:HD12	1.90	0.54
3:P:231:LEU:HD13	3:P:233:ASN:H	1.71	0.54
12:Q:1307:OPC:HAP2	12:Q:1307:OPC:HAH2	1.88	0.54
4:Q:90:TYR:O	4:Q:91:ILE:HD13	2.08	0.54
2:B:124:PHE:C	2:B:124:PHE:CD1	2.80	0.54
12:B:307:OPC:HAL2	12:B:307:OPC:CAP	2.37	0.54
3:C:273:ILE:O	3:C:278:GLN:HG2	2.08	0.54
3:C:20:ILE:HG21	3:C:75:VAL:HG11	1.88	0.54
4:D:133:TYR:CD2	4:D:148:LEU:HG	2.42	0.54
1:A:33:PHE:HE1	5:E:14:LEU:HD22	1.71	0.54
2:O:79:TRP:HB3	5:R:7:PHE:HZ	1.73	0.54
4:Q:84:LEU:HD21	4:Q:164:PRO:HA	1.89	0.54
4:Q:74:ASN:O	4:Q:94:GLU:O	2.25	0.54
2:B:114:ILE:O	2:B:116:ASN:N	2.40	0.54
3:C:117:GLY:O	3:C:118:PRO:C	2.45	0.54
3:C:118:PRO:C	3:C:120:PRO:HD3	2.28	0.54
3:C:219:VAL:O	3:C:232:THR:HG21	2.07	0.54
3:P:231:LEU:HD22	3:P:232:THR:N	2.21	0.54
3:P:275:LYS:O	3:P:279:VAL:HB	2.08	0.54
4:Q:73:HIS:NE2	4:Q:77:ASP:O	2.40	0.54
8:U:11:LEU:HB3	8:U:15:PHE:HZ	1.72	0.54
8:U:8:TRP:HA	8:U:11:LEU:HG	1.89	0.54
3:C:62:ALA:HB2	3:C:68:VAL:HG11	1.90	0.54
4:D:147:SER:CB	4:D:171:ARG:NH2	2.70	0.54
8:H:3:ILE:HG23	8:H:4:ASP:N	2.21	0.54
1:N:144:GLY:O	1:N:148:VAL:HG12	2.08	0.54
2:O:148:ALA:C	2:O:149:LEU:O	2.44	0.54
4:Q:121:GLU:O	4:Q:123:LYS:HG3	2.08	0.54
4:Q:81:VAL:O	4:Q:82:GLN:HG2	2.08	0.54
3:C:221:GLU:H	3:C:221:GLU:CD	2.12	0.54
3:C:281:LYS:H	3:C:281:LYS:HD2	1.73	0.54
4:D:76:GLY:O	4:D:117:TRP:CH2	2.60	0.54
5:E:9:ILE:HG12	6:F:13:PHE:HB2	1.90	0.54
3:P:79:PRO:HD3	3:P:149:ILE:HG12	1.89	0.54
4:Q:157:ASP:O	4:Q:158:ASP:HB2	2.08	0.54
1:A:14:ILE:CD1	1:A:15:GLN:H	2.18	0.54
3:C:226:LYS:HZ1	3:C:230:ALA:HB3	1.70	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:30:LYS:HB3	7:G:31:ARG:HH22	1.71	0.54
1:N:116:LEU:HD11	1:N:208:LYS:NZ	2.23	0.54
4:Q:73:HIS:HA	4:Q:77:ASP:CG	2.28	0.54
7:T:22:PHE:O	7:T:26:TYR:CE1	2.61	0.54
2:B:96:LEU:HD22	2:B:100:LEU:HG	1.90	0.54
3:C:194:LYS:HD3	3:C:212:PRO:HA	1.89	0.54
5:E:3:LEU:O	5:E:4:GLY:C	2.47	0.54
1:N:118:TRP:HD1	9:N:302:HEM:HMD2	1.72	0.54
3:P:178:GLY:O	3:P:225:VAL:HA	2.07	0.54
3:P:283:GLN:C	3:P:285:ALA:N	2.62	0.54
4:Q:57:LYS:O	4:Q:64:VAL:HG23	2.08	0.54
7:T:9:LEU:HG	7:T:10:VAL:H	1.72	0.54
1:A:166:SER:HB3	1:A:170:ARG:NH2	2.22	0.53
2:B:146:GLY:O	2:B:147:ALA:HB3	2.08	0.53
2:B:40:PHE:N	2:B:41:PRO:HD2	2.22	0.53
3:C:185:LYS:CG	3:C:195:TYR:HB3	2.30	0.53
3:C:273:ILE:HG21	7:G:27:GLN:HB3	1.89	0.53
3:C:55:ASP:OD1	3:C:57:LYS:CG	2.56	0.53
2:O:39:VAL:O	2:O:42:VAL:HB	2.09	0.53
9:N:303:HEM:CBC	2:O:44:ILE:HD11	2.39	0.53
4:Q:132:GLN:NE2	4:Q:141:ARG:HB2	2.23	0.53
8:U:10:ALA:O	8:U:14:VAL:HG23	2.08	0.53
2:B:48:PHE:CE2	2:B:52:VAL:HG21	2.43	0.53
3:C:226:LYS:CE	3:C:229:GLU:HB3	2.37	0.53
3:C:54:TYR:OH	3:C:58:LEU:HD22	2.09	0.53
8:H:5:VAL:O	8:H:9:VAL:HB	2.08	0.53
2:O:96:LEU:HD22	2:O:100:LEU:HG	1.89	0.53
2:O:57:LEU:HD21	3:P:258:MET:HE1	1.89	0.53
4:Q:84:LEU:O	4:Q:85:LYS:HB2	2.07	0.53
6:S:15:LEU:HD12	7:T:26:TYR:OH	2.09	0.53
7:T:10:VAL:O	7:T:14:VAL:HG13	2.08	0.53
1:A:159:PRO:C	1:A:161:VAL:H	2.06	0.53
12:D:306:OPC:HBL1	12:D:306:OPC:CAR	2.28	0.53
3:P:216:GLU:O	3:P:233:ASN:CB	2.56	0.53
4:Q:81:VAL:HB	4:Q:89:THR:CB	2.38	0.53
5:R:18:ILE:HG22	5:R:22:ILE:HD11	1.91	0.53
1:A:207:ARG:C	1:A:208:LYS:HD2	2.28	0.53
1:A:28:PRO:HD2	2:B:32:TRP:HB2	1.91	0.53
2:B:20:LYS:CG	2:B:21:GLY:N	2.55	0.53
5:E:23:ILE:CG2	5:E:24:PHE:N	2.71	0.53
10:A:304:TDS:HBC1	2:B:85:PHE:CD2	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:151:LEU:C	2:B:153:LYS:N	2.62	0.53
3:C:187:GLU:HG3	3:C:188:ASP:H	1.74	0.53
3:C:79:PRO:HD3	3:C:149:ILE:HG12	1.90	0.53
5:R:1:MET:H1	5:R:1:MET:HE2	1.74	0.53
7:T:11:LEU:HA	7:T:14:VAL:HG13	1.91	0.53
4:D:19:MET:O	4:D:21:LEU:N	2.41	0.53
4:D:64:VAL:HG12	4:D:69:PHE:HE2	1.73	0.53
4:D:94:GLU:OE1	4:D:98:ALA:O	2.26	0.53
1:N:200:LEU:HD22	12:N:1306:OPC:HBC1	1.90	0.53
4:Q:109:THR:OG1	4:Q:145:PRO:HG2	2.09	0.53
4:Q:150:LEU:HD23	4:Q:178:TRP:CH2	2.44	0.53
4:Q:64:VAL:CG1	4:Q:91:ILE:HG12	2.36	0.53
3:C:119:LEU:HD12	3:C:119:LEU:H	1.72	0.53
3:C:146:LYS:CD	3:C:246:GLU:HG3	2.32	0.53
3:C:275:LYS:O	3:C:279:VAL:HB	2.07	0.53
3:C:40:VAL:HG11	3:C:46:PHE:CD2	2.44	0.53
4:D:73:HIS:HB3	4:D:93:VAL:HG12	1.90	0.53
1:N:142:GLN:HE21	2:O:64:GLU:CD	2.12	0.53
2:O:21:GLY:C	2:O:24:HIS:CD2	2.82	0.53
3:P:146:LYS:CD	3:P:246:GLU:HG3	2.29	0.53
2:O:38:TYR:CG	3:P:276:LYS:HD3	2.43	0.53
2:B:72:PRO:HB3	4:Q:127:PRO:CG	2.39	0.53
4:Q:178:TRP:H	4:Q:178:TRP:HE3	1.57	0.53
5:R:23:ILE:CG2	5:R:24:PHE:N	2.71	0.53
2:B:136:GLY:HA3	13:B:201:CLA:C2C	2.39	0.53
3:C:219:VAL:HG11	3:C:223:GLN:NE2	2.21	0.53
11:Q:1305:PL9:H301	12:Q:1307:OPC:HBU1	1.89	0.53
4:Q:109:THR:CG2	4:Q:177:TRP:CH2	2.92	0.53
3:C:93:GLU:O	3:C:94:LEU:C	2.48	0.53
1:N:83:ARG:NH1	9:N:301:HEM:O1A	2.41	0.53
4:Q:136:THR:O	4:Q:171:ARG:NH2	2.41	0.53
4:Q:15:ARG:HH12	4:Q:18:PHE:HE2	1.56	0.53
2:B:26:TYR:HB2	2:B:27:TYR:CE1	2.43	0.53
12:D:306:OPC:CAY	12:D:306:OPC:HBC2	2.40	0.53
6:F:20:TRP:O	6:F:24:VAL:HG23	2.09	0.53
6:F:26:LEU:HD21	8:H:17:TRP:NE1	2.24	0.53
2:O:133:PHE:HA	13:O:1201:CLA:CMB	2.39	0.53
3:P:191:GLY:O	3:P:192:ASN:HB2	2.08	0.53
1:A:211:ILE:N	1:A:211:ILE:CD1	2.70	0.52
3:C:194:LYS:HB3	3:C:196:GLN:HE21	1.74	0.52
1:N:28:PRO:CG	2:O:32:TRP:HB3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:79:TRP:HZ2	5:R:1:MET:N	2.03	0.52
3:P:185:LYS:HE3	3:P:217:LEU:HD11	1.90	0.52
1:A:32:ILE:C	1:A:34:TYR:H	2.13	0.52
3:C:202:ASP:O	3:C:204:GLY:N	2.42	0.52
3:C:217:LEU:CA	3:C:232:THR:HB	2.38	0.52
4:D:134:ASP:CG	4:D:135:GLU:N	2.61	0.52
1:N:182:ARG:HB3	10:N:1304:TDS:HAA1	1.92	0.52
1:N:61:THR:HG22	1:N:62:VAL:N	2.23	0.52
2:O:20:LYS:HG3	2:O:21:GLY:N	2.24	0.52
4:Q:142:GLY:HA2	4:Q:144:ALA:H	1.73	0.52
4:Q:20:ASN:C	4:Q:22:LEU:N	2.60	0.52
8:U:6:LEU:O	8:U:8:TRP:N	2.42	0.52
8:U:8:TRP:O	8:U:8:TRP:HE3	1.93	0.52
10:A:304:TDS:HAX2	13:B:201:CLA:H93	1.90	0.52
12:B:307:OPC:HAL2	12:B:307:OPC:HAP1	1.91	0.52
2:B:36:LEU:C	2:B:38:TYR:H	2.11	0.52
7:G:14:VAL:HG23	7:G:15:PHE:N	2.25	0.52
1:N:104:VAL:HA	1:N:107:THR:HG22	1.91	0.52
1:N:142:GLN:HG2	2:O:64:GLU:CB	2.39	0.52
3:P:218:ILE:H	3:P:232:THR:CG2	2.23	0.52
3:P:282:VAL:CG2	4:Q:15:ARG:HE	2.23	0.52
4:Q:153:ALA:HA	4:Q:162:LEU:HD11	1.92	0.52
4:Q:92:VAL:O	4:Q:99:ILE:HA	2.09	0.52
5:R:18:ILE:HB	5:R:22:ILE:HD12	1.92	0.52
7:T:28:GLN:C	7:T:30:LYS:N	2.61	0.52
1:A:189:PHE:CE2	1:N:52:PHE:HB2	2.45	0.52
2:B:125:ARG:O	2:B:127:PRO:HD3	2.09	0.52
3:C:105:PRO:HB3	3:C:110:GLN:O	2.10	0.52
3:C:277:LYS:HB3	3:C:277:LYS:NZ	2.25	0.52
4:D:138:ARG:NH2	4:D:147:SER:HB3	2.24	0.52
3:P:117:GLY:N	3:P:118:PRO:HD2	2.24	0.52
3:P:226:LYS:HG2	3:P:229:GLU:CB	2.39	0.52
3:P:62:ALA:HB2	3:P:68:VAL:HG11	1.92	0.52
3:P:94:LEU:HD22	3:P:94:LEU:N	2.12	0.52
8:U:12:LEU:HA	8:U:15:PHE:CD1	2.44	0.52
9:A:303:HEM:HBC1	11:A:305:PL9:H161	1.92	0.52
2:B:38:TYR:CD1	3:C:276:LYS:HD3	2.44	0.52
3:C:180:ILE:HG13	3:C:199:ILE:HA	1.91	0.52
1:N:23:SER:O	1:N:25:TYR:CE1	2.61	0.52
2:O:78:GLU:HG2	2:O:80:TYR:H	1.74	0.52
3:P:277:LYS:HB3	3:P:277:LYS:NZ	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:79:TRP:HB3	5:R:7:PHE:CZ	2.45	0.52
4:D:19:MET:HG3	4:D:20:ASN:N	2.25	0.52
2:O:24:HIS:O	2:O:25:ASN:CB	2.57	0.52
2:O:32:TRP:CE3	2:O:36:LEU:HG	2.44	0.52
2:O:75:ILE:HG22	2:O:77:PRO:HD3	1.91	0.52
4:Q:104:ILE:HD11	4:Q:136:THR:HA	1.90	0.52
4:Q:152:HIS:HB2	4:Q:162:LEU:HG	1.90	0.52
4:Q:154:THR:O	4:Q:160:ILE:HG23	2.08	0.52
9:A:301:HEM:HHA	9:A:301:HEM:HBD1	1.92	0.52
3:C:231:LEU:HD12	3:C:231:LEU:H	1.75	0.52
8:H:8:TRP:HE3	8:H:8:TRP:O	1.92	0.52
3:P:124:TYR:HB3	3:P:127:ILE:HG12	1.92	0.52
4:Q:100:ARG:HD2	4:Q:102:TYR:HH	1.74	0.52
4:Q:76:GLY:CA	4:Q:93:VAL:HG13	2.40	0.52
5:R:26:ILE:HD12	5:R:26:ILE:N	2.24	0.52
1:A:41:LEU:O	1:A:44:PHE:HB3	2.09	0.52
3:C:11:PRO:HA	3:C:107:LYS:NZ	2.25	0.52
3:C:28:ALA:HB3	3:C:238:GLY:O	2.10	0.52
4:D:73:HIS:CE1	4:D:91:ILE:O	2.63	0.52
8:H:6:LEU:O	8:H:8:TRP:N	2.42	0.52
2:O:127:PRO:C	2:O:129:ALA:N	2.63	0.52
1:N:209:GLN:HB3	2:O:27:TYR:HB2	1.92	0.52
3:P:218:ILE:HG13	3:P:232:THR:HG22	1.90	0.52
3:P:233:ASN:ND2	3:P:234:ASN:H	2.08	0.52
11:Q:1305:PL9:H201	12:Q:1307:OPC:OCC	2.08	0.52
11:Q:1305:PL9:H302	12:Q:1307:OPC:CBB	2.39	0.52
4:Q:64:VAL:HG13	4:Q:69:PHE:CD2	2.45	0.52
4:Q:78:ARG:NH1	4:Q:100:ARG:HH21	2.06	0.52
8:U:22:VAL:O	8:U:26:ARG:HG3	2.10	0.52
8:U:6:LEU:C	8:U:8:TRP:H	2.13	0.52
1:A:44:PHE:HD1	9:A:301:HEM:CBB	2.21	0.52
2:B:72:PRO:HB3	4:Q:127:PRO:HG2	1.90	0.52
3:C:201:THR:O	3:C:203:SER:N	2.43	0.52
3:C:91:PRO:HD2	3:C:95:LYS:HG3	1.92	0.52
4:D:116:PRO:CD	4:D:126:CYS:HA	2.40	0.52
4:D:55:THR:OG1	4:D:57:LYS:NZ	2.36	0.52
5:E:21:GLY:O	5:E:25:ALA:HB2	2.10	0.52
2:O:85:PHE:O	2:O:89:ARG:HG2	2.10	0.52
12:Q:1307:OPC:HBX2	12:Q:1307:OPC:CBE	2.39	0.52
7:T:25:ALA:CB	7:T:29:TYR:OH	2.57	0.52
2:B:79:TRP:CG	2:B:80:TYR:N	2.78	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:84:LEU:H	4:D:89:THR:HG23	1.75	0.52
2:O:24:HIS:O	2:O:25:ASN:HB3	2.10	0.52
2:O:95:LEU:N	2:O:95:LEU:CD2	2.67	0.52
3:P:185:LYS:CD	3:P:195:TYR:HD2	2.23	0.52
3:P:52:ILE:HG21	3:P:154:ASN:O	2.10	0.52
4:Q:84:LEU:HD13	4:Q:164:PRO:HD3	1.91	0.52
2:O:122:ASN:OD1	5:R:26:ILE:HG21	2.10	0.52
6:S:17:PHE:CD1	6:S:17:PHE:N	2.78	0.52
1:A:33:PHE:CZ	5:E:17:GLY:HA3	2.45	0.51
2:B:150:PRO:O	2:B:153:LYS:NZ	2.43	0.51
13:B:201:CLA:HHC	13:B:201:CLA:HBB1	1.93	0.51
3:C:59:GLN:HB2	3:C:67:LYS:HB3	1.93	0.51
5:E:18:ILE:HG22	5:E:22:ILE:HD11	1.92	0.51
7:G:15:PHE:C	7:G:17:THR:N	2.63	0.51
3:P:202:ASP:O	3:P:204:GLY:N	2.44	0.51
3:P:55:ASP:OD1	3:P:57:LYS:HG3	2.10	0.51
4:Q:116:PRO:HD3	4:Q:127:PRO:HD3	1.92	0.51
3:C:218:ILE:H	3:C:232:THR:CG2	2.22	0.51
4:D:78:ARG:HG3	4:D:117:TRP:CG	2.45	0.51
1:N:106:LEU:HD12	5:R:18:ILE:CD1	2.40	0.51
1:N:114:ARG:NH2	1:N:209:GLN:H	2.08	0.51
1:N:29:HIS:O	1:N:30:VAL:CG1	2.45	0.51
3:P:221:GLU:CD	3:P:221:GLU:H	2.14	0.51
1:A:172:GLY:O	1:A:173:SER:C	2.48	0.51
1:N:110:PHE:CD1	2:O:112:PRO:HB3	2.42	0.51
4:Q:150:LEU:HD11	4:Q:171:ARG:NH2	2.22	0.51
1:A:39:ILE:HD11	2:B:43:VAL:CG1	2.40	0.51
1:A:75:GLU:HA	1:A:75:GLU:OE1	2.11	0.51
2:B:39:VAL:O	2:B:42:VAL:HB	2.10	0.51
2:B:79:TRP:HA	2:B:82:TYR:CD2	2.46	0.51
3:C:102:TYR:N	3:C:118:PRO:HG3	2.22	0.51
3:C:134:PRO:CB	3:C:142:ILE:HD13	2.39	0.51
3:C:50:VAL:O	3:C:50:VAL:HG12	2.10	0.51
5:E:20:VAL:CG1	5:E:21:GLY:N	2.69	0.51
15:E:101:BCR:H362	6:F:17:PHE:HZ	1.75	0.51
2:O:143:LEU:O	2:O:145:ILE:N	2.43	0.51
3:P:50:VAL:HG13	3:P:151:LEU:HD21	1.92	0.51
1:A:99:LEU:HD21	5:E:11:PHE:HB2	1.92	0.51
2:B:150:PRO:O	2:B:153:LYS:HD2	2.09	0.51
2:B:96:LEU:O	2:B:100:LEU:HB2	2.11	0.51
4:D:115:VAL:HG21	4:D:148:LEU:CD2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:118:PRO:O	3:P:120:PRO:HD3	2.11	0.51
8:U:17:TRP:O	8:U:20:ALA:HB3	2.10	0.51
4:D:155:VAL:HG12	4:D:156:GLN:N	2.25	0.51
1:N:26:VAL:HG23	1:N:26:VAL:O	2.11	0.51
2:O:118:ASN:ND2	2:O:121:GLN:NE2	2.37	0.51
4:Q:88:PRO:CD	4:Q:107:VAL:HG23	2.41	0.51
4:Q:137:GLY:C	4:Q:171:ARG:HH12	2.14	0.51
4:Q:77:ASP:N	4:Q:93:VAL:HG12	2.18	0.51
2:B:32:TRP:H	2:B:33:PRO:CD	2.24	0.51
3:C:178:GLY:O	3:C:225:VAL:HA	2.11	0.51
5:E:23:ILE:HG23	5:E:24:PHE:HD2	1.75	0.51
4:Q:133:TYR:CD2	4:Q:139:VAL:HB	2.46	0.51
4:Q:152:HIS:CA	4:Q:162:LEU:HG	2.41	0.51
4:Q:35:LEU:O	4:Q:39:VAL:HG23	2.11	0.51
5:R:23:ILE:O	5:R:27:LYS:CB	2.58	0.51
1:A:103:ARG:NH1	1:A:103:ARG:HG3	2.25	0.51
1:A:81:LEU:C	1:A:81:LEU:HD13	2.30	0.51
4:D:35:LEU:HD12	4:D:35:LEU:O	2.11	0.51
3:P:201:THR:O	3:P:203:SER:N	2.43	0.51
3:P:3:PHE:CD1	3:P:3:PHE:N	2.78	0.51
4:Q:109:THR:HG22	4:Q:177:TRP:CH2	2.45	0.51
5:R:3:LEU:O	5:R:4:GLY:C	2.49	0.51
1:A:118:TRP:CZ3	2:B:108:LEU:O	2.64	0.51
3:C:262:ILE:HG12	7:G:17:THR:HG22	1.92	0.51
4:D:100:ARG:C	4:D:153:ALA:HB2	2.31	0.51
4:D:90:TYR:HD2	4:D:104:ILE:O	1.93	0.51
1:N:29:HIS:HE1	2:O:29:GLU:OE2	1.94	0.51
2:O:74:GLU:CG	2:O:75:ILE:N	2.73	0.51
3:P:20:ILE:HG21	3:P:75:VAL:HG11	1.91	0.51
4:Q:152:HIS:HB2	4:Q:162:LEU:CB	2.41	0.51
4:Q:16:ARG:C	4:Q:18:PHE:N	2.64	0.51
4:Q:78:ARG:HD3	4:Q:78:ARG:N	2.25	0.51
2:B:98:VAL:HA	2:B:101:MET:HE2	1.93	0.51
5:E:16:PHE:O	5:E:20:VAL:HB	2.11	0.51
3:C:266:MET:HE3	7:G:23:TYR:CB	2.41	0.51
1:N:14:ILE:O	1:N:14:ILE:HG13	2.11	0.51
3:P:226:LYS:CD	3:P:229:GLU:HB3	2.40	0.51
4:Q:152:HIS:CB	4:Q:162:LEU:HG	2.40	0.51
4:Q:162:LEU:O	4:Q:163:THR:HB	2.11	0.51
8:U:5:VAL:O	8:U:9:VAL:HB	2.11	0.51
2:B:79:TRP:C	2:B:81:LEU:H	2.14	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:61:VAL:O	3:C:157:ARG:NH1	2.42	0.50
4:D:115:VAL:HG12	4:D:124:PHE:HB3	1.92	0.50
4:D:95:SER:C	4:D:97:GLU:H	2.14	0.50
1:N:150:ILE:HD12	2:O:75:ILE:HG12	1.93	0.50
2:O:78:GLU:OE1	2:O:80:TYR:HB2	2.11	0.50
2:O:91:LEU:O	2:O:91:LEU:HD12	2.11	0.50
3:P:187:GLU:HG3	3:P:188:ASP:N	2.26	0.50
1:N:95:LEU:HG	5:R:7:PHE:HB3	1.94	0.50
2:B:127:PRO:C	2:B:129:ALA:N	2.63	0.50
3:C:34:VAL:HG22	3:C:151:LEU:HD22	1.93	0.50
3:C:53:PRO:O	3:C:54:TYR:HB2	2.10	0.50
4:D:59:LYS:HB3	4:D:80:LEU:O	2.10	0.50
2:O:57:LEU:O	3:P:38:GLN:NE2	2.45	0.50
2:O:73:LEU:C	2:O:73:LEU:HD12	2.31	0.50
3:P:194:LYS:HB3	3:P:196:GLN:HE21	1.75	0.50
3:P:231:LEU:CD1	3:P:231:LEU:H	2.24	0.50
4:Q:123:LYS:O	4:Q:125:LYS:N	2.44	0.50
4:Q:132:GLN:NE2	4:Q:141:ARG:HD3	2.22	0.50
4:Q:149:ALA:O	4:Q:150:LEU:HD13	2.11	0.50
5:R:5:ALA:HB1	6:S:9:ALA:CB	2.21	0.50
8:U:24:TRP:CD2	8:U:25:GLY:N	2.79	0.50
2:B:142:TRP:CD1	2:B:155:LEU:C	2.85	0.50
2:B:142:TRP:NE1	2:B:154:THR:O	2.41	0.50
3:C:134:PRO:HB3	3:C:142:ILE:CD1	2.40	0.50
3:C:3:PHE:CD1	3:C:3:PHE:N	2.78	0.50
4:D:118:ASN:OD1	4:D:123:LYS:C	2.50	0.50
4:D:78:ARG:NE	4:D:92:VAL:HG11	2.23	0.50
7:G:26:TYR:HD1	7:G:26:TYR:H	1.59	0.50
1:N:140:TRP:O	2:O:65:PRO:HG3	2.11	0.50
4:Q:70:LEU:HD22	4:Q:71:GLU:OE1	2.12	0.50
1:N:214:PRO:HA	5:R:29:ILE:O	2.12	0.50
3:C:199:ILE:HG22	3:C:200:GLN:N	2.26	0.50
3:C:231:LEU:CD1	3:C:232:THR:H	2.23	0.50
7:G:21:LEU:C	7:G:23:TYR:H	2.13	0.50
1:N:31:ASN:O	1:N:32:ILE:HB	2.12	0.50
1:N:38:GLY:HA3	9:N:303:HEM:C4C	2.46	0.50
2:O:76:LEU:HD23	2:O:76:LEU:H	1.75	0.50
4:Q:156:GLN:O	4:Q:157:ASP:CB	2.59	0.50
4:Q:94:GLU:HB3	4:Q:100:ARG:CD	2.12	0.50
7:T:22:PHE:C	7:T:26:TYR:CE1	2.85	0.50
8:U:9:VAL:HG22	8:U:13:VAL:CG2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:231:LEU:HD22	3:C:232:THR:H	1.77	0.50
3:C:233:ASN:ND2	3:C:234:ASN:H	2.09	0.50
4:D:106:ALA:HB3	4:D:114:VAL:HG13	1.94	0.50
15:E:101:BCR:H362	6:F:17:PHE:CZ	2.46	0.50
1:N:33:PHE:O	1:N:36:LEU:HD23	2.11	0.50
4:Q:147:SER:HB3	4:Q:171:ARG:NH1	2.26	0.50
2:B:86:GLN:HG3	2:B:143:LEU:HD22	1.94	0.50
2:B:79:TRP:C	2:B:81:LEU:N	2.64	0.50
4:D:68:LYS:H	4:D:68:LYS:HD2	1.75	0.50
2:O:22:MET:O	2:O:24:HIS:N	2.44	0.50
2:O:36:LEU:O	2:O:39:VAL:HG22	2.11	0.50
4:Q:116:PRO:CD	4:Q:127:PRO:HD3	2.41	0.50
4:Q:156:GLN:HB2	4:Q:161:VAL:CG1	2.42	0.50
1:A:158:ILE:HB	1:A:162:GLY:HA2	1.91	0.50
1:A:14:ILE:HA	1:A:17:LEU:HD12	1.94	0.50
3:C:178:GLY:C	3:C:225:VAL:HA	2.32	0.50
4:D:110:HIS:HE1	4:D:129:HIS:HB2	1.77	0.50
12:D:306:OPC:CCA	12:D:306:OPC:HBW2	2.39	0.50
4:Q:123:LYS:HA	4:Q:133:TYR:O	2.11	0.50
1:A:27:PRO:HG3	2:B:33:PRO:CG	2.41	0.50
2:B:79:TRP:CD1	2:B:80:TYR:N	2.80	0.50
3:C:52:ILE:HG12	3:C:153:ALA:CB	2.40	0.50
3:C:199:ILE:HB	3:C:208:VAL:HA	1.94	0.50
3:C:274:LEU:HD11	8:H:23:VAL:HG21	1.92	0.50
3:C:56:THR:HG22	3:C:122:GLU:HB3	1.92	0.50
4:D:167:GLU:O	4:D:176:PRO:CB	2.59	0.50
4:D:167:GLU:O	4:D:176:PRO:HB3	2.11	0.50
4:D:149:ALA:HA	4:D:178:TRP:CE2	2.47	0.50
1:N:95:LEU:HD13	1:N:96:MET:HE3	1.92	0.50
3:P:173:THR:HB	3:P:229:GLU:HA	1.92	0.50
3:P:86:PRO:CG	3:P:89:ARG:HG3	2.41	0.50
4:Q:134:ASP:C	4:Q:136:THR:H	2.14	0.50
4:Q:80:LEU:C	4:Q:80:LEU:HD23	2.32	0.50
4:D:121:GLU:CD	4:D:123:LYS:HE2	2.32	0.50
1:N:41:LEU:O	1:N:44:PHE:HB3	2.12	0.50
4:Q:100:ARG:CD	4:Q:102:TYR:OH	2.57	0.50
9:N:303:HEM:O2D	11:Q:1305:PL9:H532	2.11	0.50
4:Q:56:ALA:HA	4:Q:81:VAL:CG1	2.25	0.50
5:R:1:MET:H1	5:R:1:MET:CE	2.24	0.50
1:A:177:GLN:H	1:A:177:GLN:CD	2.13	0.49
2:B:117:VAL:HG22	2:B:117:VAL:O	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:269:GLN:HE22	7:G:24:ALA:HA	1.75	0.49
2:B:32:TRP:CH2	3:C:277:LYS:HD2	2.43	0.49
3:C:277:LYS:HE3	7:G:31:ARG:CG	2.42	0.49
4:D:99:ILE:HD12	4:D:153:ALA:HB3	1.94	0.49
6:F:17:PHE:N	6:F:17:PHE:CD1	2.80	0.49
1:N:115:GLU:O	1:N:119:ILE:HG13	2.12	0.49
3:P:3:PHE:CZ	3:P:119:LEU:HD11	2.41	0.49
3:P:134:PRO:HB3	3:P:142:ILE:CD1	2.36	0.49
4:Q:120:ALA:C	4:Q:122:ASN:H	2.16	0.49
4:Q:64:VAL:HA	4:Q:69:PHE:CE1	2.47	0.49
1:A:36:LEU:CD2	1:A:103:ARG:HB2	2.43	0.49
2:B:127:PRO:O	2:B:129:ALA:N	2.42	0.49
2:B:58:ASP:OD1	3:C:146:LYS:NZ	2.45	0.49
4:D:165:TRP:HA	4:D:167:GLU:OE2	2.12	0.49
4:D:59:LYS:CD	4:D:79:VAL:HB	2.42	0.49
5:E:30:LYS:CB	5:E:30:LYS:NZ	2.75	0.49
2:O:22:MET:C	2:O:24:HIS:H	2.14	0.49
11:Q:1305:PL9:C30	12:Q:1307:OPC:HBU1	2.42	0.49
4:Q:99:ILE:HD12	4:Q:160:ILE:HD13	1.94	0.49
5:R:9:ILE:HB	6:S:9:ALA:HB1	1.94	0.49
1:A:91:SER:CB	2:B:79:TRP:HZ3	2.25	0.49
3:C:26:HIS:ND1	3:C:154:ASN:OD1	2.46	0.49
3:C:226:LYS:O	3:C:227:ALA:HB2	2.12	0.49
7:G:11:LEU:C	7:G:14:VAL:HG13	2.33	0.49
1:N:106:LEU:HD12	5:R:18:ILE:HD12	1.95	0.49
3:P:93:GLU:O	3:P:94:LEU:C	2.49	0.49
3:P:91:PRO:HD2	3:P:95:LYS:HG3	1.94	0.49
4:Q:141:ARG:HG2	4:Q:141:ARG:HH11	1.77	0.49
4:Q:154:THR:O	4:Q:160:ILE:CA	2.58	0.49
4:Q:170:PHE:H	4:Q:170:PHE:HD1	1.60	0.49
2:B:22:MET:SD	2:B:22:MET:O	2.70	0.49
3:C:124:TYR:HB3	3:C:127:ILE:HG12	1.95	0.49
4:D:102:TYR:CE2	4:D:136:THR:HG23	2.47	0.49
4:D:104:ILE:HG23	4:D:149:ALA:O	2.13	0.49
7:G:15:PHE:C	7:G:17:THR:H	2.15	0.49
1:N:212:SER:HB2	2:O:122:ASN:OD1	2.12	0.49
3:P:59:GLN:HB2	3:P:67:LYS:HB3	1.94	0.49
1:A:66:TYR:CZ	2:B:65:PRO:HD3	2.47	0.49
2:B:147:ALA:HB1	2:B:152:ASP:HA	1.95	0.49
3:C:262:ILE:HG13	7:G:21:LEU:CG	2.27	0.49
1:N:71:TYR:O	1:N:76:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:S:7:TYR:O	6:S:11:LEU:HD12	2.12	0.49
8:U:6:LEU:O	8:U:10:ALA:HB3	2.12	0.49
1:A:114:ARG:NH1	1:A:208:LYS:HB3	2.28	0.49
2:B:32:TRP:N	2:B:33:PRO:CD	2.76	0.49
2:B:82:TYR:N	2:B:83:PRO:HD2	2.28	0.49
3:C:174:ALA:HB3	3:C:228:GLY:HA2	1.93	0.49
4:D:126:CYS:N	4:D:131:SER:O	2.38	0.49
4:D:84:LEU:O	4:D:87:ASP:N	2.46	0.49
12:N:1306:OPC:HBQ2	12:N:1306:OPC:CAU	2.42	0.49
2:O:64:GLU:CG	2:O:65:PRO:N	2.75	0.49
2:O:79:TRP:CH2	5:R:1:MET:N	2.79	0.49
3:P:199:ILE:HG22	3:P:200:GLN:N	2.27	0.49
3:P:171:VAL:HG13	3:P:234:ASN:HB2	1.93	0.49
3:P:270:LEU:HG	3:P:274:LEU:CD1	2.43	0.49
3:P:281:LYS:HA	3:P:284:ALA:CB	2.25	0.49
4:Q:94:GLU:OE2	4:Q:100:ARG:HG2	2.12	0.49
1:A:97:MET:O	1:A:101:VAL:HG23	2.13	0.49
2:B:141:ILE:O	2:B:144:GLY:N	2.45	0.49
3:C:191:GLY:O	3:C:192:ASN:HB2	2.13	0.49
3:C:217:LEU:HA	3:C:232:THR:CB	2.39	0.49
5:E:26:ILE:HG13	5:E:29:ILE:HD12	1.95	0.49
7:G:21:LEU:C	7:G:23:TYR:N	2.63	0.49
1:N:111:LYS:HB2	1:N:114:ARG:NH1	2.26	0.49
4:Q:169:ASP:HB3	4:Q:172:THR:OG1	2.13	0.49
2:B:118:ASN:O	2:B:121:GLN:O	2.30	0.49
1:A:142:GLN:HE22	2:B:67:ASN:H	1.59	0.49
2:O:147:ALA:O	2:O:149:LEU:N	2.45	0.49
3:P:226:LYS:O	3:P:227:ALA:HB2	2.12	0.49
3:P:275:LYS:NZ	3:P:276:LYS:HZ2	2.10	0.49
3:P:275:LYS:HB2	4:Q:19:MET:CE	2.43	0.49
1:A:178:ALA:O	1:A:182:ARG:HG3	2.13	0.49
2:B:102:ALA:O	2:B:105:PRO:HD2	2.12	0.49
2:B:32:TRP:N	2:B:33:PRO:HD3	2.28	0.49
4:D:174:GLU:HG2	4:D:175:LYS:O	2.13	0.49
4:D:19:MET:C	4:D:21:LEU:H	2.14	0.49
2:O:146:GLY:O	2:O:149:LEU:CB	2.61	0.49
3:P:26:HIS:ND1	3:P:154:ASN:ND2	2.61	0.49
4:Q:163:THR:O	4:Q:164:PRO:O	2.31	0.49
1:A:102:PHE:O	1:A:103:ARG:C	2.50	0.49
1:A:114:ARG:HB3	1:A:208:LYS:NZ	2.27	0.49
2:B:79:TRP:C	2:B:79:TRP:CD1	2.86	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:182:LYS:CG	3:C:198:SER:HB2	2.40	0.49
3:C:199:ILE:HB	3:C:207:VAL:O	2.13	0.49
4:D:166:THR:CA	4:D:179:VAL:HG22	2.43	0.49
4:D:19:MET:C	4:D:21:LEU:N	2.65	0.49
4:D:35:LEU:O	4:D:39:VAL:HG23	2.13	0.49
7:G:25:ALA:CB	7:G:29:TYR:OH	2.61	0.49
2:O:153:LYS:O	2:O:155:LEU:N	2.40	0.49
1:A:99:LEU:CD2	5:E:11:PHE:HB2	2.43	0.48
3:C:9:TYR:C	3:C:11:PRO:HD2	2.33	0.48
3:C:98:VAL:O	3:C:99:GLY:O	2.31	0.48
4:D:54:THR:HG23	4:D:82:GLN:HG3	1.95	0.48
5:E:26:ILE:HG22	5:E:26:ILE:O	2.12	0.48
1:N:97:MET:O	1:N:101:VAL:HG23	2.12	0.48
1:N:110:PHE:O	1:N:111:LYS:O	2.31	0.48
2:O:18:LEU:HD13	2:O:31:ALA:HB2	1.93	0.48
2:O:59:PRO:HD2	3:P:248:VAL:HG21	1.95	0.48
3:P:9:TYR:C	3:P:11:PRO:HD2	2.33	0.48
7:G:17:THR:O	7:G:21:LEU:HB2	2.13	0.48
7:G:21:LEU:O	7:G:21:LEU:HD13	2.12	0.48
7:G:27:GLN:HA	7:G:27:GLN:NE2	2.28	0.48
1:N:135:GLY:HA2	1:N:138:LEU:HG	1.96	0.48
2:O:46:GLY:HA3	7:T:24:ALA:HB1	1.95	0.48
2:O:79:TRP:HA	2:O:82:TYR:CZ	2.48	0.48
3:P:219:VAL:O	3:P:232:THR:HG21	2.13	0.48
3:P:226:LYS:CG	3:P:229:GLU:HB3	2.43	0.48
4:Q:102:TYR:H	4:Q:153:ALA:HB2	1.78	0.48
8:U:8:TRP:O	8:U:11:LEU:HB2	2.13	0.48
6:S:26:LEU:HD22	8:U:17:TRP:HE1	1.75	0.48
4:Q:28:THR:OG1	11:Q:1305:PL9:H23	2.13	0.48
1:A:104:VAL:O	1:A:107:THR:HG22	2.14	0.48
2:B:135:PHE:O	2:B:138:LEU:HB2	2.13	0.48
2:B:91:LEU:HD12	2:B:91:LEU:O	2.13	0.48
3:C:12:THR:OG1	3:C:13:PRO:HD2	2.12	0.48
4:D:139:VAL:HG23	4:D:144:ALA:HB3	1.96	0.48
4:D:66:VAL:CG2	4:D:158:ASP:C	2.82	0.48
8:H:7:GLY:O	8:H:11:LEU:HD11	2.13	0.48
3:P:34:VAL:HG22	3:P:151:LEU:HD22	1.95	0.48
4:Q:88:PRO:O	4:Q:89:THR:HG23	2.13	0.48
4:Q:74:ASN:N	4:Q:93:VAL:HG11	2.13	0.48
5:R:9:ILE:CG1	6:S:13:PHE:HB2	2.43	0.48
4:D:107:VAL:HG12	4:D:109:THR:HG23	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:147:SER:HB2	4:D:171:ARG:NH2	2.28	0.48
3:C:266:MET:HG3	7:G:21:LEU:HD23	1.95	0.48
1:N:104:VAL:O	1:N:107:THR:HG22	2.12	0.48
2:O:82:TYR:N	2:O:83:PRO:HD2	2.28	0.48
8:U:21:MET:O	8:U:24:TRP:HE3	1.96	0.48
3:C:91:PRO:HD2	3:C:95:LYS:HG2	1.94	0.48
4:D:130:GLY:C	4:D:143:PRO:HG2	2.34	0.48
1:N:141:ASP:O	1:N:145:TYR:HB3	2.13	0.48
1:N:66:TYR:CG	2:O:65:PRO:HG2	2.48	0.48
3:P:231:LEU:CD1	3:P:231:LEU:N	2.77	0.48
3:P:273:ILE:O	3:P:278:GLN:HG2	2.13	0.48
1:A:35:CYS:HA	9:A:303:HEM:C3B	2.49	0.48
4:D:116:PRO:HD2	4:D:126:CYS:SG	2.54	0.48
1:N:109:GLY:HA3	9:N:302:HEM:HBD2	1.96	0.48
1:N:72:ILE:O	1:N:79:GLY:HA3	2.13	0.48
1:N:118:TRP:CH2	2:O:108:LEU:HB3	2.49	0.48
3:P:104:GLN:HG2	3:P:115:LEU:HB2	1.96	0.48
4:Q:159:ASN:O	4:Q:161:VAL:N	2.46	0.48
4:Q:66:VAL:O	4:Q:70:LEU:N	2.46	0.48
3:C:1:TYR:CD2	3:C:119:LEU:HD21	2.46	0.48
3:C:251:ASP:HB3	3:C:254:ARG:HD2	1.94	0.48
3:C:41:LEU:HD21	7:G:11:LEU:HD21	1.96	0.48
4:D:138:ARG:HH11	4:D:138:ARG:HB3	1.75	0.48
4:D:15:ARG:HH22	4:D:17:GLN:HG2	1.75	0.48
8:H:24:TRP:CD2	8:H:25:GLY:N	2.82	0.48
1:N:107:THR:O	2:O:123:PRO:HG2	2.13	0.48
2:O:18:LEU:CB	2:O:31:ALA:HB2	2.43	0.48
2:O:58:ASP:OD1	5:R:2:ILE:HG21	2.13	0.48
4:Q:115:VAL:HG13	4:Q:126:CYS:CA	2.43	0.48
4:Q:155:VAL:HG12	4:Q:156:GLN:H	1.79	0.48
4:Q:77:ASP:OD1	4:Q:93:VAL:HG11	2.14	0.48
1:N:99:LEU:HD21	5:R:11:PHE:HB2	1.96	0.48
5:R:25:ALA:C	5:R:27:LYS:H	2.17	0.48
3:C:275:LYS:HE2	4:D:17:GLN:HB2	1.95	0.48
4:D:138:ARG:HE	4:D:171:ARG:HD2	1.77	0.48
5:E:5:ALA:HB2	6:F:5:MET:CB	2.43	0.48
7:G:14:VAL:HG22	7:G:15:PHE:H	1.78	0.48
1:N:104:VAL:HG11	9:N:302:HEM:HMD2	1.96	0.48
1:N:58:TYR:HE2	1:N:60:PRO:HB3	1.79	0.48
4:D:61:GLY:HA2	2:O:66:ALA:O	2.14	0.48
3:P:226:LYS:CE	3:P:229:GLU:HB3	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:92:VAL:HG23	4:Q:100:ARG:CB	2.44	0.48
4:Q:94:GLU:CG	4:Q:95:SER:N	2.76	0.48
6:S:22:LEU:O	6:S:26:LEU:HD23	2.14	0.48
1:A:23:SER:O	1:A:25:TYR:HD1	1.97	0.48
1:A:30:VAL:O	1:A:30:VAL:HG23	2.14	0.48
2:B:85:PHE:O	2:B:89:ARG:HG2	2.14	0.48
4:D:118:ASN:HB2	4:D:122:ASN:H	1.78	0.48
4:D:138:ARG:HH21	4:D:147:SER:HB3	1.79	0.48
1:N:191:LEU:HD11	10:N:1304:TDS:OBD	2.14	0.48
2:O:153:LYS:C	2:O:155:LEU:H	2.17	0.48
2:O:36:LEU:C	2:O:38:TYR:H	2.17	0.48
3:P:117:GLY:O	3:P:118:PRO:C	2.51	0.48
3:P:187:GLU:HG3	3:P:188:ASP:H	1.79	0.48
4:D:68:LYS:N	4:D:68:LYS:HD2	2.29	0.47
4:D:70:LEU:HD23	4:D:70:LEU:O	2.14	0.47
4:D:94:GLU:N	4:D:94:GLU:OE1	2.40	0.47
1:N:112:LYS:CB	1:N:113:PRO:HD3	2.31	0.47
1:N:163:VAL:CG1	1:N:164:LEU:N	2.77	0.47
3:P:218:ILE:CG1	3:P:232:THR:HG22	2.43	0.47
3:P:275:LYS:HG3	4:Q:20:ASN:CA	2.43	0.47
5:R:26:ILE:HG22	5:R:26:ILE:O	2.12	0.47
7:T:14:VAL:HG22	7:T:15:PHE:H	1.79	0.47
1:A:158:ILE:CB	1:A:162:GLY:HA3	2.40	0.47
2:B:126:ARG:O	2:B:129:ALA:HB3	2.14	0.47
4:D:66:VAL:CG2	4:D:160:ILE:N	2.77	0.47
4:D:147:SER:HB3	4:D:171:ARG:NH2	2.29	0.47
1:N:20:ASP:O	1:N:21:VAL:O	2.32	0.47
2:O:18:LEU:HD21	7:T:35:LEU:O	2.14	0.47
3:P:47:LYS:HG3	3:P:128:VAL:HG13	1.96	0.47
4:Q:93:VAL:HG22	4:Q:94:GLU:H	1.79	0.47
2:O:79:TRP:CH2	5:R:4:GLY:CA	2.92	0.47
10:A:304:TDS:HBC1	2:B:85:PHE:CA	2.41	0.47
2:B:84:VAL:HG21	13:B:201:CLA:H41	1.96	0.47
2:B:38:TYR:CG	3:C:276:LYS:HD3	2.50	0.47
1:N:34:TYR:CE2	1:N:103:ARG:HD3	2.48	0.47
1:N:79:GLY:HA2	4:Q:41:TYR:CE1	2.49	0.47
3:P:77:MET:HG2	3:P:113:VAL:HG13	1.95	0.47
3:P:177:THR:CA	3:P:227:ALA:HA	2.44	0.47
3:P:275:LYS:HB2	4:Q:19:MET:HE2	1.95	0.47
3:P:279:VAL:O	3:P:279:VAL:HG12	2.14	0.47
1:A:188:THR:HG22	9:A:301:HEM:HBC2	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:122:ASN:ND2	2:B:124:PHE:CD2	2.78	0.47
3:C:198:SER:HA	3:C:208:VAL:HB	1.96	0.47
3:C:223:GLN:O	3:C:224:ALA:HB3	2.14	0.47
3:C:211:ILE:HD11	3:C:231:LEU:HD23	1.95	0.47
1:A:39:ILE:CD1	15:E:101:BCR:H312	2.41	0.47
8:H:22:VAL:C	8:H:24:TRP:N	2.67	0.47
2:O:91:LEU:CD2	2:O:100:LEU:HD12	2.44	0.47
2:O:135:PHE:O	2:O:138:LEU:HB2	2.13	0.47
3:P:56:THR:HG22	3:P:122:GLU:HB3	1.95	0.47
2:B:27:TYR:N	2:B:27:TYR:CD1	2.83	0.47
3:C:185:LYS:CD	3:C:195:TYR:HD2	2.26	0.47
3:C:283:GLN:C	3:C:285:ALA:N	2.67	0.47
4:D:55:THR:O	4:D:57:LYS:HG3	2.14	0.47
7:G:11:LEU:O	7:G:14:VAL:HG13	2.15	0.47
8:H:8:TRP:HA	8:H:11:LEU:HG	1.96	0.47
1:N:21:VAL:CG1	1:N:22:THR:H	2.21	0.47
2:O:41:PRO:O	2:O:45:MET:HG3	2.15	0.47
2:O:95:LEU:HD23	2:O:95:LEU:H	1.77	0.47
3:P:50:VAL:O	3:P:50:VAL:HG12	2.14	0.47
3:P:53:PRO:O	3:P:54:TYR:HB2	2.14	0.47
3:P:54:TYR:OH	3:P:58:LEU:HB2	2.14	0.47
1:A:170:ARG:HG3	1:A:172:GLY:H	1.79	0.47
1:A:62:VAL:HG11	1:A:177:GLN:HB3	1.96	0.47
2:B:118:ASN:HB2	2:B:123:PRO:HG3	1.95	0.47
3:C:26:HIS:ND1	3:C:154:ASN:ND2	2.62	0.47
3:C:41:LEU:HD22	3:C:41:LEU:H	1.79	0.47
4:D:52:GLY:CA	4:D:85:LYS:NZ	2.77	0.47
1:N:47:GLN:HG2	9:N:301:HEM:HBB2	1.95	0.47
2:O:91:LEU:HD21	2:O:100:LEU:HD12	1.97	0.47
2:O:127:PRO:O	2:O:129:ALA:N	2.41	0.47
2:O:144:GLY:O	2:O:145:ILE:CD1	2.62	0.47
3:P:281:LYS:HD2	3:P:281:LYS:H	1.79	0.47
12:Q:1307:OPC:HAP2	12:Q:1307:OPC:HAL2	1.93	0.47
1:A:103:ARG:NH2	9:A:302:HEM:HBD1	2.29	0.47
4:D:78:ARG:HB3	4:D:90:TYR:CE1	2.50	0.47
1:N:186:ALA:HB2	10:N:1304:TDS:HAA3	1.97	0.47
1:N:28:PRO:CG	2:O:32:TRP:CB	2.93	0.47
2:O:37:LEU:HD23	2:O:40:PHE:CE2	2.49	0.47
4:Q:35:LEU:HD12	4:Q:35:LEU:O	2.15	0.47
7:T:26:TYR:CA	7:T:29:TYR:CD1	2.90	0.47
1:A:202:HIS:O	1:A:206:ILE:HG13	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:82:PHE:O	3:C:112:ASN:HB3	2.15	0.47
4:D:105:ASN:C	4:D:107:VAL:HG23	2.34	0.47
5:E:25:ALA:C	5:E:27:LYS:H	2.18	0.47
8:H:5:VAL:O	8:H:9:VAL:CB	2.63	0.47
1:N:102:PHE:O	1:N:103:ARG:C	2.53	0.47
1:N:141:ASP:C	2:O:64:GLU:CG	2.83	0.47
2:O:148:ALA:O	2:O:149:LEU:O	2.32	0.47
9:N:303:HEM:CBB	2:O:43:VAL:HG21	2.44	0.47
12:Q:1307:OPC:HAZ2	12:Q:1307:OPC:HBN2	1.97	0.47
4:Q:134:ASP:HB2	4:Q:138:ARG:CB	2.43	0.47
7:T:25:ALA:O	7:T:29:TYR:CD2	2.68	0.47
1:A:14:ILE:CG1	1:A:15:GLN:N	2.77	0.47
11:A:305:PL9:HC71	11:A:305:PL9:H121	1.96	0.47
2:B:144:GLY:O	2:B:145:ILE:CG1	2.63	0.47
2:B:148:ALA:O	2:B:152:ASP:N	2.48	0.47
3:C:13:PRO:O	3:C:21:VAL:HG22	2.14	0.47
4:D:169:ASP:HB3	4:D:178:TRP:CZ2	2.50	0.47
4:D:150:LEU:HD11	4:D:171:ARG:HD3	1.96	0.47
4:D:65:LYS:HB3	4:D:68:LYS:CD	2.42	0.47
1:N:27:PRO:HB3	2:O:33:PRO:HD3	1.97	0.47
2:O:58:ASP:OD2	3:P:146:LYS:HE2	2.14	0.47
1:A:125:ALA:HB2	9:A:302:HEM:CMC	2.45	0.47
1:A:141:ASP:O	1:A:145:TYR:N	2.42	0.47
1:A:144:GLY:O	1:A:148:VAL:HG12	2.14	0.47
1:A:91:SER:HB3	2:B:79:TRP:CZ3	2.50	0.47
1:A:95:LEU:HD13	1:A:96:MET:HE3	1.96	0.47
2:B:154:THR:HG22	2:B:155:LEU:N	2.30	0.47
2:B:53:ALA:O	2:B:57:LEU:HG	2.14	0.47
3:C:1:TYR:O	3:C:4:TRP:HB2	2.15	0.47
3:C:49:VAL:HG12	3:C:51:LYS:HD2	1.96	0.47
4:D:93:VAL:CA	4:D:100:ARG:HB2	2.39	0.47
4:D:84:LEU:HD23	4:D:84:LEU:C	2.35	0.47
1:N:120:SER:HA	1:N:123:ILE:HD12	1.97	0.47
1:N:204:LEU:C	1:N:206:ILE:N	2.68	0.47
1:N:66:TYR:HE1	2:O:63:GLY:H	1.63	0.47
3:P:41:LEU:HD22	3:P:41:LEU:H	1.79	0.47
1:A:146:TRP:HB2	2:B:75:ILE:CD1	2.43	0.47
1:A:15:GLN:CG	1:N:113:PRO:HA	2.44	0.47
1:A:103:ARG:HH22	9:A:302:HEM:HBD1	1.80	0.47
1:A:91:SER:O	2:B:79:TRP:HH2	1.98	0.47
10:A:304:TDS:CBC	2:B:88:LEU:HD22	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:6:LEU:O	8:H:10:ALA:HB3	2.15	0.47
6:F:26:LEU:HD22	8:H:17:TRP:HE1	1.80	0.47
3:P:11:PRO:HA	3:P:107:LYS:NZ	2.29	0.47
3:P:167:SER:O	3:P:172:PHE:CZ	2.68	0.47
3:P:198:SER:HA	3:P:208:VAL:HB	1.97	0.47
4:Q:133:TYR:HA	4:Q:138:ARG:C	2.35	0.47
6:S:26:LEU:HD21	8:U:17:TRP:NE1	2.29	0.47
1:A:105:TYR:O	1:A:107:THR:N	2.48	0.46
4:D:99:ILE:HD13	4:D:153:ALA:O	2.15	0.46
1:A:95:LEU:HD21	5:E:7:PHE:HB2	1.98	0.46
3:P:275:LYS:HZ3	3:P:276:LYS:HZ1	1.60	0.46
4:Q:147:SER:HB3	4:Q:171:ARG:HH12	1.80	0.46
5:R:23:ILE:HG23	5:R:24:PHE:HD2	1.76	0.46
1:A:15:GLN:HG3	1:N:113:PRO:HA	1.97	0.46
1:A:200:LEU:HD22	1:A:200:LEU:HA	1.76	0.46
1:A:204:LEU:C	1:A:206:ILE:N	2.68	0.46
4:D:133:TYR:HE2	4:D:146:LEU:O	1.99	0.46
4:D:50:VAL:O	4:D:164:PRO:HB2	2.15	0.46
5:E:18:ILE:HG22	5:E:22:ILE:CD1	2.45	0.46
2:O:27:TYR:O	2:O:27:TYR:CD2	2.65	0.46
3:P:231:LEU:CD1	3:P:233:ASN:H	2.28	0.46
3:P:79:PRO:HG2	3:P:82:PHE:CD1	2.50	0.46
1:A:39:ILE:CD1	2:B:43:VAL:CG1	2.93	0.46
2:B:73:LEU:O	2:B:74:GLU:HB2	2.15	0.46
3:C:270:LEU:HG	3:C:274:LEU:CD1	2.45	0.46
4:D:156:GLN:HB2	4:D:161:VAL:CG2	2.45	0.46
1:A:61:THR:HA	1:N:59:LYS:HZ2	1.80	0.46
2:O:145:ILE:HG23	2:O:149:LEU:HB2	1.98	0.46
3:P:199:ILE:HB	3:P:207:VAL:O	2.14	0.46
12:Q:1307:OPC:HB2	12:Q:1307:OPC:CBX	2.38	0.46
4:Q:19:MET:C	4:Q:21:LEU:N	2.68	0.46
4:Q:63:ASN:O	4:Q:69:PHE:CE1	2.68	0.46
11:A:305:PL9:C40	11:A:305:PL9:H512	2.42	0.46
3:C:250:GLN:NE2	3:C:251:ASP:H	2.12	0.46
3:C:277:LYS:HE3	7:G:31:ARG:CD	2.45	0.46
3:C:275:LYS:HE3	4:D:20:ASN:HB3	1.96	0.46
7:G:30:LYS:C	7:G:31:ARG:CZ	2.84	0.46
8:H:9:VAL:CG1	8:H:10:ALA:N	2.79	0.46
2:O:60:ALA:C	2:O:61:MET:HG2	2.36	0.46
3:P:26:HIS:CB	3:P:154:ASN:HD21	2.29	0.46
6:S:26:LEU:HB3	7:T:30:LYS:HE3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:TYR:C	1:A:107:THR:H	2.19	0.46
3:C:195:TYR:O	3:C:196:GLN:O	2.34	0.46
3:C:268:ALA:HA	4:D:26:THR:OG1	2.15	0.46
3:C:93:GLU:CA	3:C:97:GLU:CB	2.87	0.46
4:D:168:THR:HA	4:D:176:PRO:HB3	1.97	0.46
7:G:14:VAL:HG22	7:G:15:PHE:N	2.28	0.46
1:N:95:LEU:HG	5:R:7:PHE:HB2	1.97	0.46
2:O:31:ALA:O	2:O:32:TRP:CB	2.54	0.46
4:Q:53:GLY:O	4:Q:54:THR:OG1	2.27	0.46
4:Q:65:LYS:HB2	4:Q:68:LYS:HD3	1.98	0.46
7:T:15:PHE:C	7:T:17:THR:H	2.18	0.46
3:C:221:GLU:N	3:C:221:GLU:CD	2.68	0.46
3:C:231:LEU:CD1	3:C:231:LEU:H	2.29	0.46
4:D:141:ARG:HG2	4:D:141:ARG:HH11	1.81	0.46
4:D:15:ARG:NE	4:D:15:ARG:HA	2.31	0.46
4:D:151:CYS:SG	4:D:162:LEU:HD23	2.55	0.46
5:E:9:ILE:HG21	6:F:9:ALA:C	2.34	0.46
6:F:3:GLU:HA	6:F:6:LEU:HD12	1.96	0.46
5:E:5:ALA:HB2	6:F:5:MET:CG	2.46	0.46
2:B:42:VAL:CG1	7:G:28:GLN:HE22	2.28	0.46
1:A:14:ILE:O	1:A:15:GLN:C	2.54	0.46
1:A:188:THR:CG2	9:A:301:HEM:HBC2	2.46	0.46
3:C:181:THR:C	3:C:221:GLU:HB3	2.35	0.46
8:H:5:VAL:O	8:H:9:VAL:HG12	2.15	0.46
1:N:178:ALA:O	1:N:182:ARG:HG3	2.16	0.46
2:O:72:PRO:O	2:O:73:LEU:CB	2.62	0.46
3:P:163:THR:OG1	3:P:165:GLU:HG2	2.16	0.46
4:Q:12:ASP:O	4:Q:14:GLY:N	2.48	0.46
8:U:5:VAL:O	8:U:9:VAL:HG12	2.16	0.46
3:C:273:ILE:CG2	7:G:27:GLN:HB3	2.46	0.46
3:C:47:LYS:HG3	3:C:128:VAL:HG13	1.97	0.46
4:D:168:THR:HG22	4:D:169:ASP:N	2.30	0.46
5:E:5:ALA:HB3	6:F:5:MET:HB2	1.98	0.46
1:N:27:PRO:HB3	2:O:31:ALA:HA	1.97	0.46
3:P:180:ILE:HG13	3:P:199:ILE:HA	1.97	0.46
4:Q:125:LYS:CD	4:Q:132:GLN:HG2	2.46	0.46
4:Q:165:TRP:HE1	4:Q:176:PRO:HB2	1.81	0.46
4:Q:64:VAL:HA	4:Q:69:PHE:CG	2.51	0.46
7:T:15:PHE:C	7:T:17:THR:N	2.68	0.46
3:C:265:VAL:O	3:C:269:GLN:HG3	2.14	0.46
3:C:59:GLN:OE1	3:C:67:LYS:HE3	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:99:ILE:CD1	4:D:153:ALA:HB3	2.46	0.46
4:D:36:TYR:O	4:D:40:LYS:HG2	2.16	0.46
7:G:28:GLN:C	7:G:30:LYS:N	2.68	0.46
2:O:21:GLY:C	2:O:24:HIS:HD2	2.19	0.46
3:P:167:SER:O	3:P:172:PHE:HZ	1.98	0.46
3:P:181:THR:C	3:P:221:GLU:HB3	2.36	0.46
4:Q:117:TRP:HE1	4:Q:135:GLU:CB	2.29	0.46
4:Q:133:TYR:CA	4:Q:139:VAL:HA	2.38	0.46
4:Q:91:ILE:HD12	4:Q:160:ILE:CD1	2.38	0.46
5:R:18:ILE:HG22	5:R:22:ILE:CD1	2.46	0.46
5:R:9:ILE:CG2	6:S:12:SER:HB2	2.46	0.46
1:A:33:PHE:CD1	5:E:18:ILE:HG23	2.51	0.46
2:B:91:LEU:HD21	2:B:100:LEU:HD12	1.97	0.46
2:B:45:MET:HE3	4:D:27:VAL:HG13	1.97	0.46
4:D:57:LYS:H	4:D:82:GLN:HG2	1.81	0.46
6:F:7:TYR:CD1	6:F:7:TYR:C	2.89	0.46
1:N:141:ASP:HA	2:O:64:GLU:HG3	1.98	0.46
2:O:57:LEU:HD11	7:T:18:LEU:HB2	1.97	0.46
2:O:87:ILE:HG13	2:O:143:LEU:HD13	1.98	0.46
4:Q:133:TYR:CD2	4:Q:148:LEU:HG	2.51	0.46
11:A:305:PL9:H18	12:B:307:OPC:HBU1	1.97	0.45
2:B:104:VAL:HB	2:B:105:PRO:HD3	1.97	0.45
2:B:149:LEU:H	2:B:149:LEU:HG	1.26	0.45
3:P:93:GLU:HG3	3:P:94:LEU:N	2.31	0.45
12:Q:1307:OPC:HBM1	12:Q:1307:OPC:HAR2	1.97	0.45
5:R:7:PHE:O	5:R:11:PHE:HD2	1.98	0.45
1:A:68:SER:O	1:A:71:TYR:HB3	2.15	0.45
3:C:163:THR:OG1	3:C:165:GLU:HG2	2.16	0.45
3:C:177:THR:CA	3:C:227:ALA:HA	2.45	0.45
4:D:123:LYS:CB	4:D:134:ASP:HA	2.46	0.45
3:C:266:MET:HE3	7:G:23:TYR:HB3	1.97	0.45
8:H:3:ILE:HG23	8:H:4:ASP:H	1.81	0.45
1:N:98:ILE:CD1	13:O:1201:CLA:HED3	2.45	0.45
2:O:102:ALA:O	2:O:105:PRO:HD2	2.16	0.45
2:O:57:LEU:HD21	3:P:258:MET:HE2	1.98	0.45
3:P:1:TYR:HD2	3:P:119:LEU:CD2	2.25	0.45
4:Q:115:VAL:HG13	4:Q:126:CYS:CB	2.44	0.45
4:Q:22:LEU:HD23	4:Q:22:LEU:C	2.36	0.45
6:S:30:GLN:HB2	6:S:30:GLN:HE21	1.55	0.45
1:A:106:LEU:HD12	5:E:18:ILE:HG13	1.99	0.45
1:A:112:LYS:HG3	1:A:113:PRO:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:GLN:HE21	1:A:15:GLN:HB2	1.57	0.45
2:B:149:LEU:HD13	2:B:150:PRO:CD	2.43	0.45
1:A:143:VAL:HA	2:B:75:ILE:CD1	2.46	0.45
4:D:66:VAL:HG23	4:D:159:ASN:N	2.32	0.45
4:D:168:THR:HG23	4:D:174:GLU:O	2.17	0.45
5:E:23:ILE:O	5:E:27:LYS:CB	2.60	0.45
7:G:10:VAL:O	7:G:14:VAL:HG13	2.17	0.45
2:O:79:TRP:CZ2	5:R:1:MET:CB	2.86	0.45
3:P:3:PHE:HE1	3:P:117:GLY:CA	2.29	0.45
3:P:282:VAL:HG22	4:Q:15:ARG:HE	1.82	0.45
4:Q:121:GLU:CD	4:Q:125:LYS:HE3	2.37	0.45
1:A:23:SER:C	1:A:25:TYR:H	2.18	0.45
2:B:26:TYR:O	2:B:27:TYR:HD1	1.98	0.45
1:A:142:GLN:HG2	2:B:65:PRO:O	2.16	0.45
2:B:98:VAL:HA	2:B:101:MET:CE	2.46	0.45
4:D:51:GLY:C	4:D:85:LYS:NZ	2.70	0.45
2:O:40:PHE:N	2:O:41:PRO:HD2	2.31	0.45
4:Q:100:ARG:HB3	4:Q:102:TYR:CE2	2.52	0.45
4:Q:175:LYS:HZ3	4:Q:175:LYS:HB3	1.82	0.45
2:B:83:PRO:O	2:B:87:ILE:HG13	2.15	0.45
3:C:52:ILE:HG21	3:C:154:ASN:O	2.16	0.45
4:D:108:CYS:O	4:D:110:HIS:N	2.50	0.45
4:D:123:LYS:NZ	4:D:140:ILE:CD1	2.80	0.45
2:O:28:GLY:O	2:O:29:GLU:OE2	2.35	0.45
4:Q:81:VAL:HB	4:Q:89:THR:HB	1.97	0.45
7:T:25:ALA:O	7:T:29:TYR:CG	2.70	0.45
8:U:9:VAL:HG22	8:U:13:VAL:HG23	1.97	0.45
2:B:84:VAL:HG13	2:B:101:MET:HB2	1.99	0.45
2:B:77:PRO:HG3	2:B:85:PHE:CB	2.47	0.45
4:D:98:ALA:O	4:D:100:ARG:N	2.50	0.45
4:D:116:PRO:HG3	4:D:126:CYS:HA	1.97	0.45
4:D:55:THR:O	4:D:82:GLN:HG3	2.16	0.45
4:D:58:ASP:HB3	4:D:62:ASN:H	1.82	0.45
1:N:209:GLN:HB2	2:O:27:TYR:HB2	1.98	0.45
3:P:219:VAL:HG12	3:P:220:SER:N	2.32	0.45
3:P:55:ASP:OD1	3:P:57:LYS:CG	2.64	0.45
3:P:98:VAL:O	3:P:99:GLY:O	2.34	0.45
4:Q:118:ASN:O	4:Q:122:ASN:HA	2.17	0.45
4:Q:56:ALA:O	4:Q:57:LYS:O	2.34	0.45
6:S:7:TYR:CD1	6:S:7:TYR:C	2.89	0.45
8:U:8:TRP:CE3	8:U:11:LEU:HB2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:ILE:C	1:A:121:GLY:N	2.67	0.45
1:A:26:VAL:HB	2:B:29:GLU:HB2	1.98	0.45
1:A:106:LEU:HD21	2:B:133:PHE:CZ	2.52	0.45
3:C:3:PHE:CZ	3:C:119:LEU:HD11	2.49	0.45
3:C:197:VAL:HG12	3:C:198:SER:N	2.32	0.45
3:C:229:GLU:O	3:C:230:ALA:C	2.55	0.45
3:C:59:GLN:HB2	3:C:67:LYS:HE3	1.97	0.45
4:D:108:CYS:C	4:D:110:HIS:N	2.67	0.45
4:D:123:LYS:HB3	4:D:134:ASP:HA	1.99	0.45
4:D:38:LEU:HG	12:D:306:OPC:OBH	2.17	0.45
4:D:65:LYS:CB	4:D:68:LYS:HD3	2.41	0.45
1:N:202:HIS:O	1:N:206:ILE:HG13	2.16	0.45
2:O:114:ILE:C	2:O:116:ASN:N	2.70	0.45
2:O:86:GLN:NE2	2:O:145:ILE:HB	2.31	0.45
3:P:190:TYR:HB3	3:P:191:GLY:H	1.44	0.45
3:P:185:LYS:HE3	3:P:217:LEU:HD21	1.98	0.45
3:P:251:ASP:HB3	3:P:254:ARG:HD2	1.98	0.45
3:P:28:ALA:HB3	3:P:238:GLY:O	2.17	0.45
3:P:40:VAL:HG11	3:P:46:PHE:CD2	2.51	0.45
4:Q:12:ASP:HB2	4:Q:13:MET:CE	2.47	0.45
4:Q:105:ASN:O	4:Q:149:ALA:HB3	2.16	0.45
4:Q:16:ARG:HH11	4:Q:16:ARG:HG2	1.80	0.45
8:U:7:GLY:O	8:U:11:LEU:CD1	2.64	0.45
2:B:148:ALA:C	2:B:149:LEU:HD12	2.36	0.45
3:C:171:VAL:HG13	3:C:234:ASN:CB	2.45	0.45
4:D:124:PHE:CD2	4:D:148:LEU:HD12	2.52	0.45
4:D:99:ILE:CB	4:D:153:ALA:HB1	2.36	0.45
4:D:58:ASP:OD1	4:D:69:PHE:CE2	2.70	0.45
4:D:57:LYS:N	4:D:82:GLN:HG2	2.32	0.45
3:P:280:GLU:HG2	3:P:281:LYS:HZ1	1.79	0.45
3:P:4:TRP:CE3	3:P:4:TRP:N	2.85	0.45
11:Q:1305:PL9:H512	11:Q:1305:PL9:H412	1.99	0.45
4:Q:19:MET:O	4:Q:21:LEU:N	2.50	0.45
8:U:24:TRP:CG	8:U:25:GLY:N	2.83	0.45
1:A:17:LEU:HA	1:A:20:ASP:OD1	2.17	0.45
1:A:28:PRO:HD2	2:B:31:ALA:C	2.36	0.45
3:C:1:TYR:HD2	3:C:119:LEU:CD2	2.29	0.45
1:N:154:VAL:CG1	10:N:1304:TDS:HAX1	2.47	0.45
1:N:137:SER:O	1:N:140:TRP:CD1	2.64	0.45
4:Q:156:GLN:CB	4:Q:161:VAL:HG11	2.47	0.45
4:Q:165:TRP:HA	4:Q:167:GLU:OE2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:19:MET:C	4:Q:21:LEU:H	2.19	0.45
5:R:30:LYS:CB	5:R:30:LYS:NZ	2.80	0.45
7:T:14:VAL:HG22	7:T:15:PHE:N	2.32	0.45
1:A:114:ARG:NH1	1:A:209:GLN:N	2.55	0.45
2:B:53:ALA:HB2	3:C:262:ILE:HD11	1.99	0.45
3:C:218:ILE:HG23	3:C:232:THR:O	2.17	0.45
4:D:64:VAL:HG21	4:D:81:VAL:CG1	2.47	0.45
2:O:57:LEU:HD22	7:T:14:VAL:CB	2.47	0.45
2:O:57:LEU:HD22	7:T:14:VAL:HB	1.99	0.45
3:P:14:ARG:HG2	3:P:77:MET:CE	2.47	0.45
3:P:93:GLU:HG3	3:P:94:LEU:H	1.82	0.45
4:Q:16:ARG:NH1	4:Q:16:ARG:HG2	2.32	0.45
8:U:9:VAL:C	8:U:11:LEU:N	2.69	0.45
1:A:114:ARG:HB3	1:A:208:LYS:HZ3	1.82	0.44
1:A:71:TYR:CE1	1:A:75:GLU:HG2	2.52	0.44
3:C:187:GLU:CG	3:C:188:ASP:H	2.28	0.44
3:C:84:ILE:HD12	3:C:130:PRO:HD2	1.99	0.44
8:H:11:LEU:O	8:H:12:LEU:C	2.54	0.44
1:N:111:LYS:HB3	1:N:113:PRO:HD2	1.99	0.44
1:N:116:LEU:HD11	1:N:208:LYS:HZ1	1.82	0.44
4:Q:88:PRO:HD3	4:Q:107:VAL:HG23	1.99	0.44
4:Q:117:TRP:HE1	4:Q:135:GLU:CA	2.25	0.44
4:Q:59:LYS:HG2	4:Q:79:VAL:HG13	1.99	0.44
2:B:145:ILE:O	2:B:147:ALA:N	2.50	0.44
3:C:41:LEU:N	3:C:41:LEU:HD22	2.32	0.44
3:C:60:GLN:OE1	3:C:156:GLY:HA2	2.17	0.44
4:D:147:SER:HB2	4:D:177:TRP:CH2	2.45	0.44
8:H:11:LEU:C	8:H:15:PHE:CE1	2.91	0.44
10:N:1304:TDS:CBC	2:O:81:LEU:HB3	2.47	0.44
2:O:122:ASN:HD22	2:O:125:ARG:NH1	2.14	0.44
2:O:147:ALA:C	2:O:149:LEU:N	2.69	0.44
2:O:32:TRP:CZ3	2:O:36:LEU:HA	2.50	0.44
3:P:86:PRO:HB2	3:P:88:GLU:OE1	2.17	0.44
4:Q:149:ALA:O	4:Q:150:LEU:HD22	2.17	0.44
4:Q:81:VAL:HG12	4:Q:82:GLN:N	2.32	0.44
4:Q:90:TYR:O	4:Q:91:ILE:CD1	2.65	0.44
8:U:5:VAL:O	8:U:9:VAL:CB	2.64	0.44
1:A:29:HIS:CG	1:A:30:VAL:N	2.85	0.44
7:G:30:LYS:C	7:G:31:ARG:NE	2.71	0.44
1:N:115:GLU:N	1:N:115:GLU:OE1	2.46	0.44
1:N:58:TYR:CE2	1:N:60:PRO:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:77:SER:O	1:N:78:PHE:HB2	2.17	0.44
3:P:218:ILE:HG23	3:P:232:THR:O	2.17	0.44
4:Q:15:ARG:NE	4:Q:15:ARG:HA	2.32	0.44
1:A:52:PHE:HB2	1:N:189:PHE:CE2	2.52	0.44
2:B:38:TYR:HB3	3:C:276:LYS:HD3	1.99	0.44
2:B:86:GLN:HG2	2:B:143:LEU:CA	2.47	0.44
3:C:154:ASN:OD1	3:C:155:ARG:N	2.49	0.44
3:C:185:LYS:HD3	3:C:195:TYR:CD2	2.47	0.44
3:C:48:ALA:HB3	3:C:129:PHE:HB2	1.98	0.44
4:D:55:THR:HG1	4:D:57:LYS:HZ2	1.60	0.44
3:C:277:LYS:CE	7:G:31:ARG:NE	2.81	0.44
1:N:29:HIS:HE2	1:N:209:GLN:NE2	2.15	0.44
3:P:41:LEU:HD22	3:P:41:LEU:N	2.32	0.44
4:Q:102:TYR:N	4:Q:153:ALA:HB2	2.32	0.44
2:B:86:GLN:O	2:B:90:SER:HB2	2.18	0.44
5:E:15:PHE:O	5:E:16:PHE:C	2.56	0.44
3:P:120:PRO:CB	3:P:124:TYR:CD1	3.01	0.44
3:P:71:ASN:HB2	9:P:301:HEM:CGA	2.47	0.44
4:Q:161:VAL:C	4:Q:162:LEU:HD12	2.38	0.44
1:N:77:SER:O	4:Q:41:TYR:HA	2.18	0.44
7:T:26:TYR:HA	7:T:29:TYR:HD1	1.71	0.44
1:A:189:PHE:O	1:A:192:PRO:HG2	2.17	0.44
1:A:114:ARG:NH1	1:A:209:GLN:O	2.51	0.44
1:A:32:ILE:C	1:A:34:TYR:N	2.68	0.44
3:C:190:TYR:HB3	3:C:191:GLY:H	1.42	0.44
3:C:45:VAL:HG22	3:C:85:ALA:CB	2.48	0.44
4:D:22:LEU:O	4:D:26:THR:HG23	2.17	0.44
4:D:57:LYS:CG	4:D:82:GLN:HG2	2.48	0.44
12:N:1306:OPC:HBG1	4:Q:39:VAL:HG13	1.99	0.44
1:N:159:PRO:C	1:N:160:VAL:HG23	2.38	0.44
4:Q:109:THR:C	4:Q:145:PRO:HG3	2.37	0.44
4:Q:68:LYS:N	4:Q:68:LYS:CD	2.78	0.44
5:R:23:ILE:O	5:R:27:LYS:HG2	2.17	0.44
1:A:105:TYR:C	1:A:107:THR:N	2.71	0.44
1:A:119:ILE:O	1:A:123:ILE:HG13	2.18	0.44
4:D:16:ARG:O	4:D:18:PHE:N	2.48	0.44
4:D:77:ASP:OD2	4:D:77:ASP:C	2.56	0.44
1:N:28:PRO:C	1:N:29:HIS:ND1	2.71	0.44
2:O:96:LEU:O	2:O:100:LEU:CB	2.66	0.44
2:O:146:GLY:O	2:O:149:LEU:CG	2.65	0.44
2:O:25:ASN:OD1	2:O:26:TYR:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:57:LEU:HD13	7:T:15:PHE:CD2	2.53	0.44
2:O:81:LEU:O	2:O:85:PHE:CB	2.66	0.44
4:Q:103:GLY:O	4:Q:105:ASN:N	2.50	0.44
4:Q:123:LYS:CD	4:Q:140:ILE:HD12	2.33	0.44
4:Q:81:VAL:C	4:Q:82:GLN:HG2	2.38	0.44
7:T:28:GLN:C	7:T:30:LYS:H	2.21	0.44
8:U:22:VAL:HG12	8:U:26:ARG:HE	1.82	0.44
1:A:27:PRO:HB3	2:B:31:ALA:C	2.38	0.44
2:B:74:GLU:O	2:B:75:ILE:HB	2.18	0.44
3:C:173:THR:HB	3:C:229:GLU:HA	1.99	0.44
3:C:54:TYR:OH	3:C:58:LEU:HB2	2.18	0.44
4:D:117:TRP:CG	4:D:118:ASN:N	2.85	0.44
4:D:177:TRP:CE3	4:D:178:TRP:HE3	2.36	0.44
4:D:59:LYS:HD2	4:D:79:VAL:HB	1.99	0.44
1:N:44:PHE:HD1	9:N:301:HEM:HBB1	1.82	0.44
1:N:81:LEU:HD13	1:N:81:LEU:O	2.18	0.44
1:N:92:MET:O	1:N:96:MET:HG2	2.18	0.44
2:O:146:GLY:H	2:O:149:LEU:CD1	2.22	0.44
2:O:146:GLY:O	2:O:147:ALA:C	2.55	0.44
3:P:61:VAL:HG23	3:P:61:VAL:O	2.17	0.44
4:Q:78:ARG:HG2	4:Q:117:TRP:CE3	2.53	0.44
4:Q:124:PHE:HD2	4:Q:133:TYR:HB2	1.82	0.44
4:Q:83:GLY:HA3	4:Q:87:ASP:O	2.17	0.44
5:R:26:ILE:CD1	5:R:26:ILE:N	2.80	0.44
8:U:9:VAL:CG1	8:U:10:ALA:N	2.81	0.44
1:A:159:PRO:C	1:A:161:VAL:N	2.68	0.44
2:B:122:ASN:HA	2:B:123:PRO:HD3	1.69	0.44
2:B:32:TRP:CZ3	2:B:36:LEU:HA	2.47	0.44
4:D:138:ARG:CZ	4:D:138:ARG:CB	2.96	0.44
4:D:152:HIS:N	4:D:152:HIS:CD2	2.86	0.44
7:G:9:LEU:CG	7:G:10:VAL:H	2.31	0.44
1:N:119:ILE:C	1:N:121:GLY:N	2.69	0.44
3:P:233:ASN:HD22	3:P:234:ASN:H	1.66	0.44
7:T:11:LEU:CA	7:T:14:VAL:HG13	2.47	0.44
1:A:28:PRO:CD	2:B:32:TRP:HB2	2.48	0.43
2:B:149:LEU:O	2:B:150:PRO:C	2.56	0.43
2:B:151:LEU:HA	2:B:153:LYS:CD	2.42	0.43
3:C:201:THR:HG22	3:C:201:THR:O	2.18	0.43
3:C:231:LEU:N	3:C:231:LEU:CD1	2.80	0.43
3:C:279:VAL:HG12	3:C:279:VAL:O	2.16	0.43
4:D:100:ARG:HD3	4:D:101:ASP:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:118:ASN:HB3	4:D:121:GLU:H	1.83	0.43
4:D:129:HIS:O	4:D:143:PRO:CG	2.65	0.43
1:N:200:LEU:HA	1:N:200:LEU:HD22	1.76	0.43
2:O:145:ILE:HG22	2:O:146:GLY:N	2.33	0.43
3:P:262:ILE:HG13	7:T:21:LEU:HG	2.00	0.43
3:P:48:ALA:HB3	3:P:129:PHE:HB2	1.99	0.43
4:Q:163:THR:O	4:Q:164:PRO:C	2.57	0.43
4:Q:64:VAL:HB	4:Q:81:VAL:HG23	1.98	0.43
5:R:5:ALA:HB2	6:S:5:MET:CB	2.48	0.43
8:U:11:LEU:O	8:U:12:LEU:C	2.56	0.43
1:A:111:LYS:CG	1:A:112:LYS:N	2.73	0.43
10:A:304:TDS:HBC3	2:B:88:LEU:HD22	2.00	0.43
2:B:99:LEU:HD13	2:B:99:LEU:C	2.39	0.43
3:C:26:HIS:CB	3:C:154:ASN:HD21	2.31	0.43
3:C:231:LEU:HD13	3:C:232:THR:N	2.26	0.43
3:C:275:LYS:O	3:C:276:LYS:O	2.36	0.43
4:D:99:ILE:HD12	4:D:101:ASP:OD1	2.17	0.43
1:N:140:TRP:O	2:O:65:PRO:CG	2.65	0.43
3:P:29:ALA:O	3:P:30:LYS:HG2	2.18	0.43
3:P:45:VAL:HG22	3:P:85:ALA:CB	2.47	0.43
4:Q:115:VAL:CG2	4:Q:126:CYS:HB2	2.47	0.43
4:Q:94:GLU:OE1	4:Q:94:GLU:N	2.52	0.43
5:R:27:LYS:HA	5:R:27:LYS:HD3	1.71	0.43
5:R:2:ILE:HG23	5:R:3:LEU:H	1.83	0.43
2:B:149:LEU:CB	2:B:150:PRO:CD	2.95	0.43
2:B:73:LEU:HD22	2:B:73:LEU:N	2.33	0.43
5:E:9:ILE:HB	6:F:9:ALA:HB1	2.00	0.43
6:F:10:LEU:HD23	6:F:10:LEU:N	2.32	0.43
8:H:21:MET:O	8:H:24:TRP:HE3	2.01	0.43
1:N:103:ARG:NE	1:N:107:THR:HG21	2.19	0.43
1:N:119:ILE:O	1:N:123:ILE:HG13	2.18	0.43
12:D:306:OPC:HBX1	1:N:201:LEU:HD13	1.99	0.43
2:O:67:ASN:HD22	3:P:16:PRO:HB3	1.80	0.43
3:P:180:ILE:HG23	3:P:220:SER:C	2.38	0.43
9:A:301:HEM:CHA	9:A:301:HEM:HBD1	2.47	0.43
1:A:30:VAL:O	1:A:30:VAL:CG2	2.66	0.43
2:B:24:HIS:O	2:B:25:ASN:HB3	2.18	0.43
12:B:307:OPC:CAL	12:B:307:OPC:HAP1	2.45	0.43
2:B:67:ASN:HA	2:B:68:PRO:HD2	1.80	0.43
3:C:220:SER:HB2	3:C:221:GLU:CD	2.39	0.43
4:D:78:ARG:HH21	4:D:92:VAL:HG11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:30:VAL:HG23	1:N:30:VAL:O	2.17	0.43
3:P:1:TYR:CD2	3:P:119:LEU:HD21	2.48	0.43
3:P:213:ALA:C	3:P:215:PRO:HD2	2.38	0.43
4:Q:91:ILE:HG22	4:Q:91:ILE:O	2.18	0.43
4:Q:76:GLY:CA	4:Q:93:VAL:O	2.62	0.43
2:B:148:ALA:O	2:B:149:LEU:C	2.57	0.43
4:D:105:ASN:CB	4:D:107:VAL:HG23	2.49	0.43
4:D:57:LYS:H	4:D:82:GLN:HB2	1.84	0.43
4:D:81:VAL:HG21	4:D:91:ILE:CD1	2.43	0.43
5:E:7:PHE:CD1	5:E:7:PHE:C	2.92	0.43
5:E:9:ILE:CG1	6:F:13:PHE:HB2	2.47	0.43
8:H:8:TRP:O	8:H:11:LEU:HB2	2.17	0.43
1:N:118:TRP:CZ3	2:O:108:LEU:C	2.91	0.43
2:O:136:GLY:HA3	13:O:1201:CLA:C4B	2.48	0.43
2:O:94:LYS:HB3	2:O:95:LEU:H	1.66	0.43
4:Q:120:ALA:C	4:Q:122:ASN:N	2.71	0.43
4:Q:16:ARG:NH2	4:Q:18:PHE:HE1	2.16	0.43
4:Q:19:MET:HG3	4:Q:20:ASN:N	2.34	0.43
4:Q:91:ILE:O	4:Q:92:VAL:O	2.35	0.43
5:R:18:ILE:HA	5:R:22:ILE:HG13	2.01	0.43
2:O:57:LEU:HD12	7:T:18:LEU:HD12	2.00	0.43
1:A:142:GLN:HE21	2:B:66:ALA:CA	2.22	0.43
2:B:25:ASN:ND2	2:B:25:ASN:N	2.66	0.43
3:C:14:ARG:HB3	3:C:20:ILE:HD13	2.01	0.43
3:C:255:VAL:O	3:C:258:MET:HG3	2.18	0.43
4:D:68:LYS:H	4:D:68:LYS:CD	2.32	0.43
4:D:73:HIS:ND1	4:D:77:ASP:OD1	2.52	0.43
5:E:27:LYS:HD3	5:E:27:LYS:HA	1.75	0.43
1:N:22:THR:O	1:N:25:TYR:CE2	2.71	0.43
3:P:231:LEU:O	3:P:232:THR:CG2	2.58	0.43
3:P:41:LEU:HB3	3:P:42:PRO:HD2	2.00	0.43
12:Q:1307:OPC:HBX2	12:Q:1307:OPC:HBE1	2.01	0.43
4:Q:152:HIS:HB2	4:Q:162:LEU:HB3	2.01	0.43
4:Q:82:GLN:O	4:Q:87:ASP:O	2.37	0.43
1:A:25:TYR:O	1:A:26:VAL:HG13	2.19	0.43
2:B:24:HIS:O	2:B:25:ASN:CB	2.66	0.43
4:D:118:ASN:CB	4:D:122:ASN:H	2.31	0.43
4:D:118:ASN:HB2	4:D:122:ASN:N	2.34	0.43
4:D:16:ARG:NH2	4:D:18:PHE:HE1	2.17	0.43
4:D:78:ARG:HG3	4:D:117:TRP:CD1	2.54	0.43
1:A:106:LEU:HD12	5:E:18:ILE:CG1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:9:ILE:CG2	6:F:12:SER:HB2	2.47	0.43
3:C:262:ILE:HG21	7:G:17:THR:HG22	1.99	0.43
1:N:34:TYR:CD2	1:N:34:TYR:N	2.87	0.43
2:O:22:MET:O	2:O:23:GLY:C	2.56	0.43
3:P:211:ILE:HD11	3:P:231:LEU:HD23	1.99	0.43
3:P:262:ILE:HG22	3:P:263:CYS:N	2.34	0.43
4:Q:115:VAL:CG1	4:Q:126:CYS:HB2	2.46	0.43
4:Q:134:ASP:N	4:Q:138:ARG:O	2.51	0.43
4:Q:155:VAL:HG13	4:Q:159:ASN:O	2.18	0.43
4:Q:92:VAL:HG23	4:Q:100:ARG:H	1.83	0.43
2:O:141:ILE:CD1	5:R:11:PHE:CZ	3.01	0.43
2:B:45:MET:HE1	4:D:27:VAL:HA	2.01	0.43
1:A:91:SER:OG	2:B:79:TRP:HZ3	2.02	0.43
2:B:94:LYS:HE2	2:B:94:LYS:HB2	1.82	0.43
4:D:12:ASP:HB2	4:D:13:MET:CE	2.49	0.43
4:D:165:TRP:CZ2	4:D:178:TRP:NE1	2.87	0.43
1:N:109:GLY:C	1:N:111:LYS:N	2.72	0.43
1:N:35:CYS:O	1:N:39:ILE:HG12	2.18	0.43
2:O:122:ASN:ND2	5:R:26:ILE:CG2	2.81	0.43
4:Q:154:THR:C	4:Q:155:VAL:HG23	2.38	0.43
4:Q:27:VAL:C	4:Q:29:GLY:N	2.71	0.43
4:Q:36:TYR:O	4:Q:40:LYS:HG2	2.18	0.43
1:A:44:PHE:CD1	9:A:301:HEM:HBB1	2.37	0.43
2:B:126:ARG:HG2	2:B:128:VAL:HG23	2.01	0.43
1:A:27:PRO:HD2	2:B:29:GLU:HB2	2.00	0.43
3:C:193:VAL:HG12	3:C:195:TYR:CE1	2.53	0.43
3:C:250:GLN:NE2	3:C:251:ASP:N	2.67	0.43
4:D:117:TRP:CZ2	4:D:122:ASN:HA	2.54	0.43
11:A:305:PL9:C10	12:D:306:OPC:HBF2	2.45	0.43
4:D:50:VAL:O	4:D:164:PRO:CB	2.66	0.43
8:H:22:VAL:O	8:H:26:ARG:HG3	2.19	0.43
1:N:110:PHE:HB3	1:N:118:TRP:CD1	2.54	0.43
1:N:118:TRP:HZ3	2:O:108:LEU:O	2.02	0.43
3:P:275:LYS:O	3:P:276:LYS:O	2.36	0.43
4:Q:78:ARG:HH12	4:Q:100:ARG:NH2	2.12	0.43
7:T:33:ASN:ND2	7:T:34:GLU:H	2.17	0.43
1:A:189:PHE:O	1:A:193:TRP:CE3	2.65	0.43
3:C:176:ALA:HB1	3:C:201:THR:HG21	2.00	0.43
4:D:73:HIS:CE1	4:D:77:ASP:OD1	2.72	0.43
2:O:126:ARG:NH1	2:O:129:ALA:HB2	2.33	0.43
3:P:88:GLU:CD	3:P:88:GLU:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:133:TYR:HA	4:Q:139:VAL:N	2.34	0.43
4:Q:73:HIS:CE1	4:Q:77:ASP:HB2	2.53	0.43
7:T:28:GLN:O	7:T:29:TYR:C	2.57	0.43
1:A:186:ALA:HA	1:A:190:VAL:HB	1.99	0.42
9:A:301:HEM:HMA1	9:A:301:HEM:HAA2	1.87	0.42
1:A:91:SER:CB	2:B:79:TRP:CZ3	3.02	0.42
2:B:142:TRP:HD1	2:B:155:LEU:C	2.20	0.42
2:B:95:LEU:N	2:B:95:LEU:CD2	2.71	0.42
3:C:270:LEU:HG	3:C:274:LEU:HD11	2.00	0.42
4:D:55:THR:O	4:D:55:THR:OG1	2.32	0.42
4:D:66:VAL:O	4:D:70:LEU:HB2	2.18	0.42
4:D:78:ARG:NE	4:D:92:VAL:CG1	2.78	0.42
5:E:16:PHE:CD2	15:E:101:BCR:H361	2.54	0.42
6:F:22:LEU:O	6:F:26:LEU:HB2	2.18	0.42
1:N:131:PHE:CD1	9:N:301:HEM:HAB	2.53	0.42
2:O:116:ASN:HD22	2:O:116:ASN:C	2.21	0.42
2:O:18:LEU:HD22	2:O:31:ALA:CB	2.49	0.42
3:P:161:TYR:C	3:P:163:THR:H	2.21	0.42
4:Q:146:LEU:O	4:Q:147:SER:O	2.37	0.42
4:Q:175:LYS:NZ	4:Q:175:LYS:CB	2.82	0.42
1:A:141:ASP:OD2	1:A:144:GLY:N	2.49	0.42
1:A:14:ILE:HD13	1:A:15:GLN:CA	2.49	0.42
3:C:117:GLY:N	3:C:118:PRO:HD2	2.33	0.42
3:C:54:TYR:CD2	3:C:70:LEU:HD13	2.52	0.42
4:D:123:LYS:HZ2	4:D:140:ILE:CD1	2.32	0.42
4:D:168:THR:OG1	4:D:176:PRO:HD3	2.18	0.42
1:N:112:LYS:HG2	1:N:112:LYS:H	1.43	0.42
1:N:13:GLU:HB3	1:N:14:ILE:H	1.53	0.42
1:N:154:VAL:N	1:N:155:PRO:HD2	2.34	0.42
1:N:186:ALA:HA	1:N:190:VAL:HB	2.00	0.42
1:N:68:SER:O	1:N:71:TYR:HB3	2.19	0.42
1:N:95:LEU:HD21	5:R:7:PHE:HB2	2.01	0.42
3:P:154:ASN:OD1	3:P:155:ARG:N	2.51	0.42
3:P:27:LEU:HG	3:P:27:LEU:H	1.26	0.42
2:B:145:ILE:HG22	2:B:145:ILE:O	2.20	0.42
3:C:14:ARG:HG2	3:C:77:MET:CE	2.49	0.42
4:D:166:THR:HA	4:D:179:VAL:HG22	2.01	0.42
3:P:197:VAL:HG12	3:P:198:SER:N	2.33	0.42
4:Q:138:ARG:CZ	4:Q:138:ARG:HA	2.48	0.42
1:A:135:GLY:HA2	1:A:138:LEU:HG	2.00	0.42
5:E:18:ILE:HB	5:E:22:ILE:HD12	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:F:30:GLN:HE21	6:F:30:GLN:HB2	1.56	0.42
1:N:34:TYR:CD2	1:N:103:ARG:HD3	2.54	0.42
3:P:153:ALA:O	3:P:240:PHE:CD1	2.72	0.42
4:Q:155:VAL:CG1	4:Q:156:GLN:N	2.82	0.42
4:Q:91:ILE:O	4:Q:99:ILE:HB	2.20	0.42
3:P:245:THR:HB	6:S:1:MET:HE1	2.01	0.42
8:U:3:ILE:HG23	8:U:4:ASP:H	1.85	0.42
1:A:21:VAL:O	1:A:21:VAL:HG12	2.18	0.42
3:C:11:PRO:HA	3:C:107:LYS:HZ3	1.83	0.42
4:D:155:VAL:CG1	4:D:156:GLN:N	2.83	0.42
4:D:52:GLY:CA	4:D:85:LYS:HZ3	2.33	0.42
2:O:64:GLU:CG	2:O:65:PRO:CD	2.86	0.42
2:O:86:GLN:HG2	2:O:143:LEU:CA	2.48	0.42
4:Q:73:HIS:HB3	4:Q:93:VAL:CB	2.50	0.42
4:Q:73:HIS:HD2	4:Q:92:VAL:C	2.23	0.42
6:S:18:VAL:O	6:S:22:LEU:HG	2.18	0.42
1:A:182:ARG:HH21	1:N:57:TYR:HE2	1.67	0.42
1:A:189:PHE:CD1	1:A:193:TRP:CZ3	3.08	0.42
3:C:92:GLU:N	3:C:94:LEU:HD23	2.35	0.42
7:G:17:THR:O	7:G:21:LEU:HB3	2.19	0.42
1:N:149:LYS:HD2	1:N:175:VAL:HG21	2.01	0.42
1:N:211:ILE:HB	1:N:212:SER:H	1.62	0.42
1:N:83:ARG:HD2	9:N:301:HEM:O2D	2.19	0.42
3:P:201:THR:C	3:P:203:SER:N	2.73	0.42
3:P:275:LYS:HG3	4:Q:20:ASN:HB3	2.00	0.42
4:Q:36:TYR:N	4:Q:37:PRO:HD2	2.34	0.42
4:Q:65:LYS:HD3	4:Q:68:LYS:CG	2.48	0.42
4:Q:76:GLY:N	4:Q:93:VAL:CG1	2.72	0.42
1:N:95:LEU:CD2	5:R:7:PHE:HB2	2.50	0.42
7:T:33:ASN:ND2	7:T:34:GLU:N	2.68	0.42
1:A:138:LEU:C	1:A:140:TRP:H	2.23	0.42
1:A:141:ASP:O	1:A:145:TYR:HB3	2.20	0.42
1:A:173:SER:HB2	1:A:174:SER:H	1.60	0.42
2:B:135:PHE:O	2:B:139:VAL:HG23	2.20	0.42
3:C:172:PHE:H	3:C:231:LEU:CG	2.08	0.42
3:C:177:THR:CB	3:C:227:ALA:HA	2.49	0.42
3:C:273:ILE:CG2	7:G:31:ARG:HH12	2.32	0.42
5:E:23:ILE:CG2	5:E:24:PHE:H	2.32	0.42
7:G:23:TYR:O	7:G:24:ALA:C	2.58	0.42
1:N:59:LYS:O	1:N:65:ALA:HA	2.19	0.42
1:N:81:LEU:O	1:N:85:ILE:HG13	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:O:80:TYR:HB3	13:O:1201:CLA:CED	2.38	0.42
3:P:161:TYR:C	3:P:163:THR:N	2.73	0.42
4:Q:155:VAL:HG22	4:Q:160:ILE:HA	2.02	0.42
7:T:33:ASN:CG	7:T:34:GLU:H	2.23	0.42
1:A:88:TRP:HZ2	2:B:58:ASP:CB	2.31	0.42
2:B:91:LEU:CD2	2:B:100:LEU:HD12	2.50	0.42
2:B:38:TYR:HD2	2:B:38:TYR:HA	1.62	0.42
3:C:277:LYS:O	3:C:280:GLU:HB3	2.20	0.42
3:C:280:GLU:O	3:C:284:ALA:HB2	2.20	0.42
3:C:88:GLU:CD	3:C:88:GLU:H	2.23	0.42
4:D:138:ARG:H	4:D:138:ARG:HG2	1.45	0.42
7:G:22:PHE:O	7:G:26:TYR:CE1	2.73	0.42
1:N:28:PRO:HD2	2:O:32:TRP:C	2.40	0.42
2:O:122:ASN:ND2	2:O:125:ARG:CZ	2.74	0.42
2:O:87:ILE:O	2:O:88:LEU:C	2.58	0.42
2:O:94:LYS:HE2	2:O:94:LYS:HB2	1.84	0.42
3:P:84:ILE:HG13	3:P:103:PHE:HD1	1.84	0.42
3:P:185:LYS:CG	3:P:195:TYR:HB3	2.32	0.42
3:P:171:VAL:HB	3:P:231:LEU:CD1	2.49	0.42
3:P:275:LYS:HD3	3:P:276:LYS:N	2.34	0.42
3:P:54:TYR:CD2	3:P:70:LEU:HD13	2.48	0.42
3:P:92:GLU:N	3:P:94:LEU:HD23	2.33	0.42
4:Q:165:TRP:HE1	4:Q:176:PRO:CB	2.33	0.42
6:S:34:LYS:HE2	6:S:34:LYS:N	2.35	0.42
7:T:27:GLN:CA	7:T:27:GLN:NE2	2.83	0.42
1:A:191:LEU:N	1:A:192:PRO:HD2	2.35	0.42
1:A:29:HIS:CD2	1:A:30:VAL:CG2	3.00	0.42
2:B:37:LEU:O	2:B:38:TYR:CD2	2.73	0.42
2:B:77:PRO:O	2:B:78:GLU:C	2.57	0.42
3:C:22:CYS:O	3:C:24:ASN:N	2.53	0.42
4:D:147:SER:CB	4:D:171:ARG:HH22	2.33	0.42
7:G:28:GLN:O	7:G:31:ARG:HD2	2.20	0.42
1:N:116:LEU:H	1:N:116:LEU:CD1	2.16	0.42
2:O:29:GLU:OE2	2:O:29:GLU:HA	2.19	0.42
3:P:248:VAL:HG12	3:P:250:GLN:HG2	2.01	0.42
3:P:52:ILE:HD12	3:P:127:ILE:HD12	2.02	0.42
3:P:50:VAL:HG21	3:P:76:LEU:HD22	2.02	0.42
4:Q:88:PRO:HD2	4:Q:107:VAL:HG23	2.02	0.42
11:Q:1305:PL9:H512	11:Q:1305:PL9:C41	2.50	0.42
3:P:268:ALA:HA	4:Q:26:THR:OG1	2.20	0.42
4:Q:55:THR:O	4:Q:56:ALA:CB	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:73:HIS:CD2	4:Q:77:ASP:CB	2.92	0.42
4:Q:87:ASP:HB3	4:Q:88:PRO:CD	2.43	0.42
3:C:248:VAL:HG12	3:C:250:GLN:HG2	2.01	0.42
4:D:131:SER:HB3	4:D:144:ALA:HA	2.01	0.42
4:D:165:TRP:CE2	4:D:167:GLU:O	2.72	0.42
4:D:177:TRP:CZ2	4:D:178:TRP:HZ3	2.38	0.42
1:N:114:ARG:HH21	1:N:209:GLN:CA	2.33	0.42
3:P:59:GLN:HB2	3:P:67:LYS:CE	2.50	0.42
10:A:304:TDS:HBC2	2:B:85:PHE:HD2	1.84	0.41
4:D:108:CYS:HB3	4:D:115:VAL:HG22	2.01	0.41
4:D:16:ARG:HH11	4:D:16:ARG:HG2	1.85	0.41
1:N:110:PHE:HB3	1:N:118:TRP:HB2	2.02	0.41
1:N:95:LEU:HD11	5:R:10:VAL:CG1	2.36	0.41
3:P:154:ASN:O	3:P:155:ARG:HB3	2.19	0.41
3:P:182:LYS:CG	3:P:198:SER:HB2	2.46	0.41
3:P:59:GLN:HB2	3:P:67:LYS:HE3	2.01	0.41
4:Q:64:VAL:O	4:Q:81:VAL:HG22	2.19	0.41
1:A:103:ARG:O	1:A:107:THR:HG22	2.20	0.41
2:B:79:TRP:HA	2:B:82:TYR:CZ	2.54	0.41
3:C:183:ILE:HG13	3:C:183:ILE:H	1.72	0.41
3:C:231:LEU:HD13	3:C:233:ASN:H	1.85	0.41
4:D:118:ASN:N	4:D:123:LYS:O	2.53	0.41
4:D:156:GLN:OE1	4:D:161:VAL:HG11	2.20	0.41
4:D:15:ARG:HH21	4:D:17:GLN:HG2	1.82	0.41
2:O:104:VAL:HB	2:O:105:PRO:HD3	2.02	0.41
3:P:201:THR:O	3:P:201:THR:HG22	2.20	0.41
4:Q:100:ARG:NH2	4:Q:135:GLU:O	2.50	0.41
2:O:124:PHE:HB2	5:R:23:ILE:HA	2.01	0.41
5:R:23:ILE:O	5:R:27:LYS:CG	2.68	0.41
1:A:50:THR:O	1:A:54:MET:HG3	2.21	0.41
1:A:77:SER:O	1:A:78:PHE:CB	2.67	0.41
3:C:59:GLN:HB2	3:C:67:LYS:CE	2.51	0.41
3:C:93:GLU:HG3	3:C:94:LEU:N	2.35	0.41
4:D:55:THR:O	4:D:56:ALA:C	2.58	0.41
5:E:26:ILE:N	5:E:26:ILE:CD1	2.83	0.41
1:N:118:TRP:HZ3	2:O:108:LEU:C	2.23	0.41
3:P:185:LYS:CD	3:P:217:LEU:HD11	2.49	0.41
3:P:231:LEU:HD21	3:P:233:ASN:O	2.20	0.41
4:Q:109:THR:HG21	4:Q:177:TRP:CH2	2.54	0.41
11:Q:1305:PL9:H171	11:Q:1305:PL9:H151	1.68	0.41
11:Q:1305:PL9:H302	12:Q:1307:OPC:HBB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:77:ASP:N	4:Q:77:ASP:OD1	2.53	0.41
1:A:146:TRP:CH2	2:B:71:THR:OG1	2.59	0.41
9:A:303:HEM:HBD2	9:A:303:HEM:HHA	2.02	0.41
1:A:47:GLN:NE2	1:A:89:SER:HB3	2.29	0.41
2:B:150:PRO:O	2:B:153:LYS:CD	2.68	0.41
2:B:22:MET:N	2:B:24:HIS:CE1	2.88	0.41
10:N:1304:TDS:CBB	2:O:81:LEU:HD13	2.47	0.41
3:P:221:GLU:CD	3:P:221:GLU:N	2.74	0.41
3:P:231:LEU:HD22	3:P:232:THR:H	1.82	0.41
3:P:84:ILE:HG23	3:P:130:PRO:HG2	2.01	0.41
5:R:7:PHE:C	5:R:7:PHE:CD1	2.94	0.41
1:A:104:VAL:HG11	9:A:302:HEM:HMD2	2.03	0.41
1:A:14:ILE:HA	1:A:17:LEU:CD1	2.50	0.41
2:B:110:LEU:O	2:B:113:PHE:HB2	2.20	0.41
2:B:71:THR:CB	2:B:72:PRO:CD	2.80	0.41
3:C:118:PRO:O	3:C:120:PRO:HD3	2.20	0.41
3:C:13:PRO:HB3	3:C:106:TYR:CE1	2.54	0.41
4:D:93:VAL:HG22	4:D:98:ALA:O	2.21	0.41
8:H:25:GLY:O	8:H:29:LEU:HG	2.20	0.41
1:N:158:ILE:HD11	2:O:98:VAL:HG11	2.03	0.41
2:O:155:LEU:HG	2:O:155:LEU:O	2.21	0.41
2:O:78:GLU:HG2	2:O:80:TYR:HD1	1.85	0.41
3:P:229:GLU:O	3:P:230:ALA:C	2.58	0.41
3:P:93:GLU:CA	3:P:97:GLU:CB	2.94	0.41
4:Q:15:ARG:HH21	4:Q:17:GLN:HG2	1.84	0.41
4:Q:50:VAL:O	4:Q:50:VAL:HG12	2.21	0.41
6:S:34:LYS:HD2	6:S:35:GLU:N	2.35	0.41
1:A:105:TYR:CE1	13:B:201:CLA:HAB	2.55	0.41
1:A:156:GLU:HG2	1:A:163:VAL:HG22	2.02	0.41
3:C:159:GLN:HG3	3:C:170:ASN:HB3	2.02	0.41
4:D:78:ARG:NH1	4:D:124:PHE:CZ	2.88	0.41
1:N:140:TRP:CZ2	1:N:145:TYR:HD2	2.39	0.41
1:N:34:TYR:N	1:N:34:TYR:HD2	2.19	0.41
1:N:142:GLN:HG2	2:O:64:GLU:HB3	2.03	0.41
2:O:81:LEU:O	2:O:85:PHE:HB2	2.20	0.41
3:P:52:ILE:CG1	3:P:153:ALA:HB1	2.44	0.41
4:Q:139:VAL:O	4:Q:139:VAL:HG13	2.21	0.41
5:R:9:ILE:HG21	6:S:9:ALA:C	2.33	0.41
7:T:11:LEU:H	7:T:11:LEU:CD2	2.24	0.41
1:A:47:GLN:OE1	1:A:86:HIS:O	2.39	0.41
2:B:89:ARG:NH2	2:B:147:ALA:O	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:B:307:OPC:HBS	12:B:307:OPC:HBC1	2.02	0.41
3:C:177:THR:OG1	3:C:227:ALA:HA	2.21	0.41
4:D:167:GLU:N	4:D:167:GLU:OE2	2.53	0.41
4:D:39:VAL:O	4:D:43:ILE:HD13	2.20	0.41
1:A:33:PHE:HZ	5:E:17:GLY:HA3	1.85	0.41
8:H:15:PHE:O	8:H:19:ILE:HG13	2.21	0.41
2:O:34:ASN:OD1	2:O:35:ASP:N	2.54	0.41
3:P:187:GLU:CG	3:P:188:ASP:H	2.32	0.41
3:P:73:GLY:O	3:P:74:ALA:HB2	2.21	0.41
4:Q:78:ARG:HH21	4:Q:135:GLU:HB2	1.85	0.41
7:T:33:ASN:HD22	7:T:33:ASN:H	1.68	0.41
1:A:120:SER:HA	1:A:123:ILE:HD12	2.03	0.41
1:A:29:HIS:CE1	1:A:210:GLY:O	2.74	0.41
2:B:40:PHE:N	2:B:41:PRO:CD	2.84	0.41
3:C:86:PRO:HB2	3:C:88:GLU:OE1	2.21	0.41
4:D:126:CYS:HB2	4:D:131:SER:HB2	2.02	0.41
5:E:30:LYS:HB3	5:E:30:LYS:HZ3	1.86	0.41
7:G:11:LEU:H	7:G:11:LEU:CD2	2.23	0.41
1:N:148:VAL:HA	1:N:151:VAL:HG22	2.03	0.41
3:P:10:PRO:N	3:P:11:PRO:HD2	2.36	0.41
3:P:161:TYR:CE1	3:P:167:SER:CA	2.96	0.41
3:P:180:ILE:HG12	3:P:181:THR:N	2.36	0.41
3:P:183:ILE:HG13	3:P:183:ILE:H	1.72	0.41
3:P:192:ASN:OD1	3:P:193:VAL:N	2.54	0.41
4:Q:137:GLY:C	4:Q:171:ARG:NH1	2.73	0.41
4:Q:168:THR:HG23	4:Q:175:LYS:CA	2.50	0.41
3:P:264:LEU:HD13	4:Q:30:VAL:HA	2.02	0.41
5:R:22:ILE:HA	5:R:25:ALA:HB2	2.02	0.41
1:A:142:GLN:HE21	2:B:67:ASN:N	2.16	0.41
3:C:131:VAL:CG2	3:C:132:LEU:N	2.83	0.41
3:C:140:LYS:HA	3:C:140:LYS:HD3	1.96	0.41
3:C:213:ALA:C	3:C:215:PRO:HD2	2.40	0.41
3:C:281:LYS:O	3:C:284:ALA:HB3	2.21	0.41
4:D:81:VAL:CG1	4:D:82:GLN:H	2.20	0.41
5:E:15:PHE:HA	5:E:15:PHE:HD2	1.65	0.41
5:E:23:ILE:O	5:E:27:LYS:HG2	2.21	0.41
6:F:26:LEU:HA	6:F:26:LEU:HD13	1.77	0.41
3:C:277:LYS:HE3	7:G:31:ARG:NE	2.35	0.41
1:N:156:GLU:HG3	1:N:166:SER:OG	2.21	0.41
2:O:126:ARG:HA	2:O:127:PRO:HD2	1.78	0.41
2:O:75:ILE:O	2:O:77:PRO:CD	2.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:192:ASN:O	3:P:193:VAL:HG23	2.21	0.41
3:P:270:LEU:HG	3:P:274:LEU:HD11	2.03	0.41
3:P:4:TRP:HE3	3:P:4:TRP:N	2.18	0.41
4:Q:44:PRO:HA	4:Q:45:PRO:HD2	1.51	0.41
4:Q:78:ARG:CD	4:Q:78:ARG:N	2.82	0.41
3:C:6:GLN:HG3	3:C:106:TYR:O	2.20	0.41
3:C:10:PRO:HG2	3:C:11:PRO:CD	2.49	0.41
3:C:20:ILE:HB	3:C:240:PHE:CZ	2.56	0.41
3:C:3:PHE:HE1	3:C:117:GLY:CA	2.33	0.41
3:C:66:SER:O	3:C:68:VAL:HG13	2.21	0.41
4:D:138:ARG:NH2	4:D:147:SER:CB	2.83	0.41
3:C:275:LYS:HE3	4:D:17:GLN:HB2	2.02	0.41
12:D:306:OPC:HBL1	12:D:306:OPC:CAP	2.44	0.41
5:E:2:ILE:O	5:E:2:ILE:HD12	2.21	0.41
6:F:25:LEU:C	6:F:25:LEU:HD23	2.41	0.41
8:H:24:TRP:CE3	8:H:25:GLY:N	2.89	0.41
1:N:17:LEU:C	1:N:17:LEU:HD13	2.41	0.41
2:O:106:LEU:HD21	13:O:1201:CLA:C15	2.48	0.41
4:Q:104:ILE:O	4:Q:106:ALA:N	2.54	0.41
4:Q:80:LEU:HA	4:Q:89:THR:O	2.21	0.41
1:N:39:ILE:CD1	15:R:1101:BCR:H312	2.50	0.41
5:R:23:ILE:CG2	5:R:24:PHE:H	2.34	0.41
6:S:25:LEU:HD23	6:S:25:LEU:C	2.40	0.41
7:T:11:LEU:HA	7:T:14:VAL:HG11	2.03	0.41
1:A:14:ILE:HG23	1:A:15:GLN:N	2.31	0.41
1:A:154:VAL:N	1:A:155:PRO:HD2	2.36	0.41
2:B:152:ASP:OD2	2:B:152:ASP:C	2.58	0.41
2:B:36:LEU:C	2:B:38:TYR:N	2.74	0.41
3:C:231:LEU:HD21	3:C:233:ASN:O	2.20	0.41
3:C:52:ILE:HD12	3:C:127:ILE:HD12	2.03	0.41
4:D:92:VAL:O	4:D:100:ARG:HB2	2.21	0.41
2:B:42:VAL:CG1	7:G:28:GLN:NE2	2.83	0.41
1:N:190:VAL:HG11	10:N:1304:TDS:OAK	2.21	0.41
1:N:23:SER:O	1:N:25:TYR:CZ	2.74	0.41
3:P:130:PRO:O	3:P:130:PRO:HG2	2.21	0.41
3:P:4:TRP:CA	3:P:4:TRP:CE3	3.03	0.41
4:Q:123:LYS:HE3	4:Q:125:LYS:CE	2.51	0.41
15:R:1101:BCR:C14	6:S:16:ILE:HG21	2.51	0.41
2:B:84:VAL:CG1	2:B:101:MET:HB2	2.50	0.40
2:B:118:ASN:HB3	2:B:121:GLN:HG3	2.02	0.40
3:C:127:ILE:HG22	3:C:129:PHE:CE1	2.57	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:161:TYR:C	3:C:163:THR:N	2.74	0.40
3:C:188:ASP:O	3:C:189:GLU:CB	2.68	0.40
4:D:160:ILE:HG22	4:D:162:LEU:HD13	2.04	0.40
8:H:22:VAL:HG12	8:H:26:ARG:HE	1.85	0.40
1:N:112:LYS:CB	1:N:113:PRO:CD	2.95	0.40
1:N:25:TYR:HB2	1:N:26:VAL:H	1.51	0.40
1:N:50:THR:O	1:N:54:MET:HG3	2.20	0.40
1:N:28:PRO:HD2	2:O:32:TRP:CA	2.51	0.40
4:Q:15:ARG:HH22	4:Q:17:GLN:HG2	1.86	0.40
4:Q:64:VAL:HG13	4:Q:69:PHE:CE2	2.56	0.40
4:Q:84:LEU:O	4:Q:87:ASP:OD1	2.38	0.40
1:A:34:TYR:CD2	1:A:34:TYR:N	2.87	0.40
2:B:149:LEU:HD23	4:Q:129:HIS:CD2	2.56	0.40
10:A:304:TDS:HBC1	2:B:85:PHE:CB	2.51	0.40
3:C:161:TYR:C	3:C:163:THR:H	2.25	0.40
3:C:192:ASN:O	3:C:193:VAL:HG23	2.21	0.40
3:C:275:LYS:HG3	4:D:20:ASN:HB3	2.02	0.40
3:C:79:PRO:O	3:C:80:GLU:C	2.60	0.40
4:D:59:LYS:HD3	4:D:79:VAL:HB	2.03	0.40
4:D:95:SER:C	4:D:97:GLU:N	2.75	0.40
1:N:102:PHE:HB3	5:R:18:ILE:CD1	2.49	0.40
3:P:275:LYS:CE	4:Q:20:ASN:HD22	2.34	0.40
6:S:3:GLU:HA	6:S:6:LEU:HD12	2.02	0.40
1:A:116:LEU:CD1	1:A:116:LEU:H	2.18	0.40
1:A:134:THR:HG23	10:A:304:TDS:HAQ2	2.03	0.40
2:B:126:ARG:HG2	2:B:128:VAL:CG2	2.51	0.40
2:B:22:MET:HE2	2:B:22:MET:HA	2.03	0.40
2:B:57:LEU:HD13	7:G:15:PHE:CD2	2.56	0.40
3:C:14:ARG:NH2	3:C:150:HIS:CD2	2.89	0.40
3:C:185:LYS:CD	3:C:217:LEU:HD11	2.51	0.40
3:C:226:LYS:HB3	3:C:227:ALA:H	1.69	0.40
3:C:93:GLU:HG3	3:C:94:LEU:H	1.86	0.40
4:D:50:VAL:HG12	4:D:164:PRO:CB	2.49	0.40
7:G:9:LEU:HG	7:G:10:VAL:N	2.36	0.40
1:N:189:PHE:CD1	1:N:193:TRP:CZ3	3.09	0.40
2:O:135:PHE:O	2:O:139:VAL:HG23	2.22	0.40
1:N:83:ARG:NH2	2:O:61:MET:O	2.54	0.40
3:P:59:GLN:OE1	3:P:67:LYS:HE3	2.21	0.40
4:Q:111:LEU:HD23	4:Q:129:HIS:CE1	2.57	0.40
4:Q:131:SER:CB	4:Q:144:ALA:HB2	2.51	0.40
4:Q:66:VAL:CG2	4:Q:160:ILE:HG13	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:Q:165:TRP:CE2	4:Q:178:TRP:CH2	3.10	0.40
4:Q:138:ARG:CD	4:Q:171:ARG:HD3	2.51	0.40
4:Q:83:GLY:CA	4:Q:87:ASP:O	2.69	0.40
3:C:61:VAL:O	3:C:61:VAL:HG23	2.21	0.40
1:N:163:VAL:HG12	1:N:164:LEU:N	2.36	0.40
3:P:76:LEU:HG	3:P:78:LEU:HD21	2.03	0.40
4:Q:96:LYS:O	4:Q:96:LYS:HD2	2.22	0.40
5:R:5:ALA:HB3	6:S:5:MET:HB2	2.01	0.40
8:U:17:TRP:O	8:U:21:MET:HG3	2.22	0.40
3:C:109:GLY:O	3:C:111:ASP:N	2.55	0.40
4:D:102:TYR:OH	4:D:135:GLU:HG3	2.21	0.40
4:D:149:ALA:HB1	4:D:178:TRP:CD1	2.57	0.40
7:G:21:LEU:HD13	7:G:21:LEU:C	2.41	0.40
7:G:25:ALA:HA	7:G:28:GLN:OE1	2.22	0.40
3:P:188:ASP:O	3:P:189:GLU:CB	2.69	0.40
3:P:193:VAL:HG12	3:P:195:TYR:CE1	2.57	0.40
4:Q:155:VAL:HA	4:Q:161:VAL:N	2.24	0.40
6:S:32:ALA:O	6:S:34:LYS:N	2.55	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%)	152 (76%)	29 (14%)	19 (10%)	0	3
1	N	200/215 (93%)	155 (78%)	32 (16%)	13 (6%)	1	7
2	B	136/160 (85%)	80 (59%)	31 (23%)	25 (18%)	0	0
2	O	136/160 (85%)	67 (49%)	38 (28%)	31 (23%)	0	0
3	C	284/289 (98%)	206 (72%)	47 (16%)	31 (11%)	0	2
3	P	284/289 (98%)	213 (75%)	44 (16%)	27 (10%)	0	3

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	D	166/179 (93%)	123 (74%)	25 (15%)	18 (11%)	0	2
4	Q	166/179 (93%)	85 (51%)	49 (30%)	32 (19%)	0	0
5	E	30/32 (94%)	22 (73%)	6 (20%)	2 (7%)	1	6
5	R	30/32 (94%)	23 (77%)	5 (17%)	2 (7%)	1	6
6	F	31/35 (89%)	25 (81%)	5 (16%)	1 (3%)	4	22
6	S	33/35 (94%)	25 (76%)	5 (15%)	3 (9%)	1	3
7	G	21/37 (57%)	15 (71%)	5 (24%)	1 (5%)	2	13
7	T	25/37 (68%)	18 (72%)	6 (24%)	1 (4%)	3	17
8	H	25/29 (86%)	18 (72%)	7 (28%)	0	100	100
8	U	25/29 (86%)	19 (76%)	6 (24%)	0	100	100
All	All	1792/1952 (92%)	1246 (70%)	340 (19%)	206 (12%)	0	2

All (206) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	25	TYR
1	A	28	PRO
1	A	111	LYS
1	A	160	VAL
1	A	173	SER
1	A	211	ILE
2	B	22	MET
2	B	25	ASN
2	B	32	TRP
2	B	33	PRO
2	B	34	ASN
2	B	35	ASP
2	B	72	PRO
2	B	75	ILE
2	B	76	LEU
2	B	149	LEU
2	B	154	THR
3	C	54	TYR
3	C	92	GLU
3	C	99	GLY
3	C	110	GLN
3	C	189	GLU
3	C	196	GLN

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Mol	Chain	Res	Type
3	C	203	SER
3	C	227	ALA
3	C	232	THR
3	C	276	LYS
4	D	66	VAL
4	D	85	LYS
4	D	110	HIS
1	N	19	ASP
1	N	21	VAL
1	N	22	THR
1	N	30	VAL
1	N	32	ILE
1	N	111	LYS
2	O	25	ASN
2	O	26	TYR
2	O	30	PRO
2	O	32	TRP
2	O	33	PRO
2	O	34	ASN
2	O	35	ASP
2	O	65	PRO
2	O	72	PRO
2	O	73	LEU
2	O	115	GLU
2	O	121	GLN
2	O	123	PRO
2	O	124	PHE
2	O	150	PRO
2	O	151	LEU
3	P	54	TYR
3	P	92	GLU
3	P	99	GLY
3	P	110	GLN
3	P	189	GLU
3	P	196	GLN
3	P	203	SER
3	P	227	ALA
3	P	232	THR
3	P	276	LYS
4	Q	46	SER
4	Q	57	LYS
4	Q	73	HIS

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Mol	Chain	Res	Type
4	Q	74	ASN
4	Q	92	VAL
4	Q	106	ALA
4	Q	124	PHE
4	Q	145	PRO
4	Q	153	ALA
4	Q	164	PRO
1	A	14	ILE
1	A	20	ASP
1	A	27	PRO
1	A	75	GLU
1	A	106	LEU
2	B	19	ALA
2	B	71	THR
2	B	78	GLU
2	B	93	ASN
2	B	115	GLU
2	B	128	VAL
2	B	145	ILE
2	B	146	GLY
2	B	153	LYS
3	C	56	THR
3	C	94	LEU
3	C	188	ASP
3	C	202	ASP
3	C	230	ALA
4	D	14	GLY
4	D	20	ASN
4	D	75	ALA
4	D	106	ALA
4	D	109	THR
7	G	29	TYR
1	N	16	ALA
1	N	110	PHE
1	N	177	GLN
1	N	190	VAL
2	O	20	LYS
2	O	93	ASN
2	O	128	VAL
2	O	147	ALA
2	O	148	ALA
2	O	149	LEU

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Mol	Chain	Res	Type
2	O	153	LYS
3	P	56	THR
3	P	188	ASP
3	P	202	ASP
3	P	230	ALA
4	Q	14	GLY
4	Q	56	ALA
4	Q	81	VAL
4	Q	91	ILE
4	Q	93	VAL
4	Q	104	ILE
4	Q	105	ASN
4	Q	147	SER
4	Q	157	ASP
5	R	25	ALA
6	S	33	GLU
7	T	29	TYR
1	A	112	LYS
1	A	140	TRP
1	A	190	VAL
2	B	92	PRO
3	C	23	ALA
3	C	127	ILE
3	C	220	SER
3	C	233	ASN
4	D	68	LYS
4	D	99	ILE
4	D	141	ARG
5	E	25	ALA
1	N	205	MET
2	O	63	GLY
2	O	64	GLU
2	O	92	PRO
2	O	114	ILE
2	O	118	ASN
3	P	94	LEU
3	P	193	VAL
3	P	220	SER
3	P	233	ASN
4	Q	48	GLY
4	Q	175	LYS
1	A	15	GLN

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Mol	Chain	Res	Type
1	A	205	MET
2	B	30	PRO
2	B	79	TRP
3	C	87	GLU
3	C	130	PRO
3	C	187	GLU
3	C	193	VAL
4	D	56	ALA
2	O	75	ILE
3	P	23	ALA
3	P	87	GLU
3	P	91	PRO
3	P	127	ILE
3	P	130	PRO
3	P	187	GLU
4	Q	13	MET
4	Q	20	ASN
4	Q	45	PRO
4	Q	67	SER
4	Q	143	PRO
1	A	24	LYS
1	A	105	TYR
2	B	114	ILE
3	C	221	GLU
4	D	47	GLY
4	D	50	VAL
4	D	101	ASP
4	D	143	PRO
2	O	76	LEU
3	P	224	ALA
4	Q	50	VAL
4	Q	98	ALA
4	Q	151	CYS
4	Q	160	ILE
6	S	30	GLN
1	A	21	VAL
3	C	58	LEU
3	C	191	GLY
3	C	224	ALA
3	C	282	VAL
4	D	13	MET
1	N	26	VAL

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Mol	Chain	Res	Type
4	Q	102	TYR
3	C	31	PRO
5	E	20	VAL
3	P	282	VAL
3	P	191	GLY
6	S	29	ILE
3	C	91	PRO
6	F	29	ILE
2	O	109	ILE
5	R	20	VAL
2	B	123	PRO
3	C	117	GLY
4	D	145	PRO
4	Q	64	VAL
1	N	211	ILE

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	172/184 (94%)	147 (86%)	25 (14%)	3	15
1	N	172/184 (94%)	153 (89%)	19 (11%)	6	25
2	B	117/136 (86%)	93 (80%)	24 (20%)	1	6
2	O	117/136 (86%)	98 (84%)	19 (16%)	2	12
3	C	240/243 (99%)	207 (86%)	33 (14%)	3	17
3	P	240/243 (99%)	206 (86%)	34 (14%)	3	16
4	D	136/146 (93%)	113 (83%)	23 (17%)	2	11
4	Q	136/146 (93%)	113 (83%)	23 (17%)	2	11
5	E	25/25 (100%)	15 (60%)	10 (40%)	0	0
5	R	25/25 (100%)	14 (56%)	11 (44%)	0	0
6	F	25/27 (93%)	22 (88%)	3 (12%)	5	22
6	S	27/27 (100%)	23 (85%)	4 (15%)	3	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	G	17/28 (61%)	9 (53%)	8 (47%)	0	0
7	T	21/28 (75%)	12 (57%)	9 (43%)	0	0
8	H	22/24 (92%)	18 (82%)	4 (18%)	1	9
8	U	22/24 (92%)	18 (82%)	4 (18%)	1	9
All	All	1514/1626 (93%)	1261 (83%)	253 (17%)	2	11

All (253) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	14	ILE
1	A	15	GLN
1	A	19	ASP
1	A	20	ASP
1	A	24	LYS
1	A	26	VAL
1	A	28	PRO
1	A	36	LEU
1	A	47	GLN
1	A	63	THR
1	A	74	ASN
1	A	75	GLU
1	A	95	LEU
1	A	103	ARG
1	A	115	GLU
1	A	116	LEU
1	A	140	TRP
1	A	150	ILE
1	A	164	LEU
1	A	167	ASP
1	A	173	SER
1	A	177	GLN
1	A	193	TRP
1	A	200	LEU
1	A	207	ARG
2	B	20	LYS
2	B	22	MET
2	B	25	ASN
2	B	26	TYR
2	B	27	TYR
2	B	29	GLU
2	B	32	TRP

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Mol	Chain	Res	Type
2	B	33	PRO
2	B	35	ASP
2	B	36	LEU
2	B	38	TYR
2	B	62	VAL
2	B	74	GLU
2	B	78	GLU
2	B	79	TRP
2	B	80	TYR
2	B	81	LEU
2	B	90	SER
2	B	95	LEU
2	B	96	LEU
2	B	116	ASN
2	B	121	GLN
2	B	124	PHE
2	B	149	LEU
3	C	3	PHE
3	C	4	TRP
3	C	9	TYR
3	C	14	ARG
3	C	17	THR
3	C	19	ARG
3	C	27	LEU
3	C	51	LYS
3	C	83	LYS
3	C	93	GLU
3	C	94	LEU
3	C	98	VAL
3	C	100	ASP
3	C	104	GLN
3	C	119	LEU
3	C	122	GLU
3	C	123	GLN
3	C	131	VAL
3	C	155	ARG
3	C	165	GLU
3	C	182	LYS
3	C	205	LYS
3	C	211	ILE
3	C	221	GLU
3	C	231	LEU

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Mol	Chain	Res	Type
3	C	232	THR
3	C	233	ASN
3	C	249	LEU
3	C	258	MET
3	C	264	LEU
3	C	271	MET
3	C	276	LYS
3	C	281	LYS
4	D	13	MET
4	D	15	ARG
4	D	16	ARG
4	D	22	LEU
4	D	62	ASN
4	D	63	ASN
4	D	82	GLN
4	D	92	VAL
4	D	93	VAL
4	D	100	ARG
4	D	101	ASP
4	D	102	TYR
4	D	126	CYS
4	D	138	ARG
4	D	139	VAL
4	D	154	THR
4	D	158	ASP
4	D	161	VAL
4	D	169	ASP
4	D	170	PHE
4	D	174	GLU
4	D	175	LYS
4	D	177	TRP
5	E	1	MET
5	E	2	ILE
5	E	8	TYR
5	E	11	PHE
5	E	12	ILE
5	E	14	LEU
5	E	15	PHE
5	E	16	PHE
5	E	29	ILE
5	E	30	LYS
6	F	7	TYR

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Mol	Chain	Res	Type
6	F	26	LEU
6	F	30	GLN
7	G	9	LEU
7	G	11	LEU
7	G	13	LEU
7	G	14	VAL
7	G	18	LEU
7	G	22	PHE
7	G	26	TYR
7	G	31	ARG
8	H	8	TRP
8	H	16	THR
8	H	21	MET
8	H	24	TRP
1	N	13	GLU
1	N	17	LEU
1	N	25	TYR
1	N	29	HIS
1	N	31	ASN
1	N	47	GLN
1	N	63	THR
1	N	95	LEU
1	N	103	ARG
1	N	110	PHE
1	N	112	LYS
1	N	116	LEU
1	N	140	TRP
1	N	150	ILE
1	N	163	VAL
1	N	164	LEU
1	N	167	ASP
1	N	193	TRP
1	N	200	LEU
2	O	24	HIS
2	O	26	TYR
2	O	27	TYR
2	O	30	PRO
2	O	32	TRP
2	O	33	PRO
2	O	35	ASP
2	O	36	LEU
2	O	57	LEU

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Mol	Chain	Res	Type
2	O	64	GLU
2	O	65	PRO
2	O	74	GLU
2	O	90	SER
2	O	92	PRO
2	O	95	LEU
2	O	96	LEU
2	O	108	LEU
2	O	116	ASN
2	O	152	ASP
3	P	3	PHE
3	P	4	TRP
3	P	14	ARG
3	P	17	THR
3	P	19	ARG
3	P	27	LEU
3	P	51	LYS
3	P	83	LYS
3	P	93	GLU
3	P	94	LEU
3	P	98	VAL
3	P	100	ASP
3	P	104	GLN
3	P	119	LEU
3	P	122	GLU
3	P	123	GLN
3	P	129	PHE
3	P	131	VAL
3	P	155	ARG
3	P	165	GLU
3	P	182	LYS
3	P	205	LYS
3	P	206	THR
3	P	211	ILE
3	P	221	GLU
3	P	231	LEU
3	P	232	THR
3	P	233	ASN
3	P	249	LEU
3	P	258	MET
3	P	264	LEU
3	P	271	MET

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Mol	Chain	Res	Type
3	P	276	LYS
3	P	281	LYS
4	Q	13	MET
4	Q	15	ARG
4	Q	16	ARG
4	Q	22	LEU
4	Q	58	ASP
4	Q	59	LYS
4	Q	63	ASN
4	Q	64	VAL
4	Q	71	GLU
4	Q	77	ASP
4	Q	94	GLU
4	Q	97	GLU
4	Q	132	GLN
4	Q	134	ASP
4	Q	138	ARG
4	Q	156	GLN
4	Q	158	ASP
4	Q	159	ASN
4	Q	164	PRO
4	Q	170	PHE
4	Q	174	GLU
4	Q	175	LYS
4	Q	178	TRP
5	R	1	MET
5	R	2	ILE
5	R	8	TYR
5	R	11	PHE
5	R	12	ILE
5	R	14	LEU
5	R	15	PHE
5	R	16	PHE
5	R	27	LYS
5	R	29	ILE
5	R	30	LYS
6	S	7	TYR
6	S	26	LEU
6	S	30	GLN
6	S	34	LYS
7	T	9	LEU
7	T	11	LEU

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Mol	Chain	Res	Type
7	T	13	LEU
7	T	14	VAL
7	T	18	LEU
7	T	22	PHE
7	T	26	TYR
7	T	31	ARG
7	T	33	ASN
8	U	8	TRP
8	U	16	THR
8	U	21	MET
8	U	24	TRP

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

Mol	Chain	Res	Type
1	A	15	GLN
1	A	29	HIS
1	A	47	GLN
1	A	142	GLN
2	B	25	ASN
2	B	86	GLN
2	B	116	ASN
2	B	118	ASN
2	B	121	GLN
3	C	7	GLN
3	C	60	GLN
3	C	125	GLN
3	C	150	HIS
3	C	159	GLN
3	C	223	GLN
3	C	236	ASN
3	C	250	GLN
3	C	269	GLN
3	C	278	GLN
4	D	82	GLN
4	D	132	GLN
4	D	152	HIS
7	G	28	GLN
8	H	27	ASN
1	N	47	GLN
1	N	142	GLN
1	N	209	GLN

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Mol	Chain	Res	Type
2	O	86	GLN
2	O	116	ASN
2	O	121	GLN
2	O	122	ASN
3	P	7	GLN
3	P	60	GLN
3	P	125	GLN
3	P	159	GLN
3	P	223	GLN
3	P	234	ASN
3	P	236	ASN
3	P	250	GLN
4	Q	20	ASN
4	Q	63	ASN
4	Q	82	GLN
4	Q	105	ASN
4	Q	122	ASN
4	Q	132	GLN
7	T	27	GLN
8	U	27	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

22 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
15	BCR	E	101	-	41,41,41	2.12	8 (19%)	56,56,56	2.46	23 (41%)
9	HEM	P	301	3	27,50,50	1.58	4 (14%)	17,82,82	1.42	3 (17%)
12	OPC	N	1306	-	53,53,54	1.36	9 (16%)	59,61,64	1.36	6 (10%)
13	CLA	B	201	-	59,73,73	1.60	9 (15%)	67,113,113	2.94	18 (26%)
14	FES	Q	1200	4	0,4,4	0.00	-	-	-	-
12	OPC	Q	1307	-	53,53,54	1.37	9 (16%)	59,61,64	1.18	3 (5%)
10	TDS	N	1304	-	28,31,31	2.16	4 (14%)	35,40,40	2.45	12 (34%)
12	OPC	B	307	-	53,53,54	1.37	9 (16%)	59,61,64	1.06	4 (6%)
11	PL9	A	305	-	55,55,55	3.35	21 (38%)	68,69,69	2.27	19 (27%)
12	OPC	D	306	-	53,53,54	1.37	9 (16%)	59,61,64	1.17	5 (8%)
9	HEM	A	302	1	27,50,50	1.29	3 (11%)	17,82,82	4.76	5 (29%)
14	FES	D	200	4	0,4,4	0.00	-	-	-	-
9	HEM	C	301	3	27,50,50	1.52	4 (14%)	17,82,82	1.39	3 (17%)
15	BCR	R	1101	-	41,41,41	2.06	9 (21%)	56,56,56	2.47	23 (41%)
9	HEM	A	303	1,16	27,50,50	2.00	8 (29%)	17,82,82	3.74	7 (41%)
11	PL9	Q	1305	-	55,55,55	3.34	21 (38%)	68,69,69	2.36	17 (25%)
10	TDS	A	304	-	28,31,31	2.17	4 (14%)	35,40,40	2.45	13 (37%)
9	HEM	A	301	1	27,50,50	1.37	5 (18%)	17,82,82	1.73	6 (35%)
9	HEM	N	301	1	27,50,50	1.48	5 (18%)	17,82,82	2.03	6 (35%)
9	HEM	N	303	1,16	27,50,50	2.07	10 (37%)	17,82,82	2.62	7 (41%)
9	HEM	N	302	1	27,50,50	1.46	5 (18%)	17,82,82	4.71	5 (29%)
13	CLA	O	1201	-	59,73,73	1.58	9 (15%)	67,113,113	3.07	16 (23%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
15	BCR	E	101	-	-	5/29/63/63	0/2/2/2
10	TDS	N	1304	-	-	5/16/17/17	0/2/2/2
12	OPC	N	1306	-	-	12/57/57/60	-
13	CLA	B	201	-	5/5/20/25	18/37/135/135	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
14	FES	Q	1200	4	-	-	0/1/1/1
12	OPC	Q	1307	-	-	9/57/57/60	-
9	HEM	P	301	3	-	0/6/54/54	-
12	OPC	B	307	-	-	14/57/57/60	-
11	PL9	A	305	-	-	28/53/73/73	0/1/1/1
12	OPC	D	306	-	-	11/57/57/60	-
9	HEM	A	302	1	-	0/6/54/54	-
14	FES	D	200	4	-	-	0/1/1/1
9	HEM	C	301	3	-	0/6/54/54	-
15	BCR	R	1101	-	-	5/29/63/63	0/2/2/2
9	HEM	A	303	1,16	-	2/6/54/54	-
11	PL9	Q	1305	-	-	29/53/73/73	0/1/1/1
10	TDS	A	304	-	-	6/16/17/17	0/2/2/2
9	HEM	A	301	1	-	0/6/54/54	-
9	HEM	N	301	1	-	0/6/54/54	-
9	HEM	N	303	1,16	-	2/6/54/54	-
9	HEM	N	302	1	-	0/6/54/54	-
13	CLA	O	1201	-	6/6/20/25	10/37/135/135	-

All (165) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	N	1304	TDS	CAL-CAM	9.80	1.53	1.40
10	A	304	TDS	CAL-CAM	9.79	1.53	1.40
11	A	305	PL9	C13-C14	8.65	1.53	1.33
11	A	305	PL9	C33-C34	8.60	1.53	1.33
11	A	305	PL9	C18-C19	8.59	1.53	1.33
11	Q	1305	PL9	C13-C14	8.58	1.53	1.33
11	Q	1305	PL9	C33-C34	8.55	1.53	1.33
11	Q	1305	PL9	C18-C19	8.54	1.53	1.33
11	A	305	PL9	C7-C8	-7.65	1.39	1.50
11	Q	1305	PL9	C7-C8	-7.62	1.39	1.50
11	Q	1305	PL9	C48-C49	7.42	1.53	1.32
11	A	305	PL9	C48-C49	7.39	1.53	1.32
15	E	101	BCR	C30-C25	6.54	1.62	1.53
13	B	201	CLA	C3A-C2A	-6.29	1.36	1.54
11	Q	1305	PL9	C3-C4	-6.05	1.39	1.49
15	E	101	BCR	C26-C25	5.98	1.44	1.34
11	A	305	PL9	C3-C4	-5.95	1.39	1.49
15	R	1101	BCR	C26-C25	5.70	1.44	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	A	305	PL9	C11-C9	-5.59	1.39	1.51
11	A	305	PL9	C41-C39	-5.58	1.39	1.51
11	Q	1305	PL9	C11-C9	-5.58	1.39	1.51
11	Q	1305	PL9	C41-C39	-5.55	1.39	1.51
13	O	1201	CLA	C3A-C2A	-5.43	1.39	1.54
15	R	1101	BCR	C30-C25	5.38	1.61	1.53
11	Q	1305	PL9	C6-C1	-4.97	1.39	1.48
15	R	1101	BCR	C1-C6	4.83	1.60	1.53
11	A	305	PL9	C6-C1	-4.81	1.40	1.48
15	E	101	BCR	C1-C6	4.72	1.60	1.53
13	O	1201	CLA	O2D-CGD	4.42	1.44	1.33
13	B	201	CLA	O2D-CGD	4.35	1.43	1.33
9	A	303	HEM	CBB-CAB	4.25	1.57	1.29
9	C	301	HEM	C3C-CAC	4.24	1.56	1.47
9	N	303	HEM	CBB-CAB	4.21	1.57	1.29
11	Q	1305	PL9	C41-C42	-4.20	1.39	1.53
11	A	305	PL9	C41-C42	-4.20	1.39	1.53
9	P	301	HEM	C3C-CAC	4.13	1.56	1.47
11	Q	1305	PL9	C51-C49	-4.01	1.39	1.50
9	A	303	HEM	C3B-C2B	-3.98	1.34	1.40
11	A	305	PL9	C51-C49	-3.96	1.39	1.50
9	N	302	HEM	C3C-CAC	3.94	1.55	1.47
10	A	304	TDS	OAK-CAL	3.92	1.43	1.37
9	N	301	HEM	C3B-C2B	-3.92	1.34	1.40
9	P	301	HEM	CBC-CAC	3.92	1.55	1.29
9	A	303	HEM	CBC-CAC	3.91	1.55	1.29
9	C	301	HEM	CBC-CAC	3.91	1.55	1.29
10	N	1304	TDS	OAK-CAL	3.86	1.43	1.37
15	R	1101	BCR	C38-C26	3.84	1.57	1.50
12	Q	1307	OPC	CAV-CAW	3.80	1.53	1.31
12	D	306	OPC	CAV-CAW	3.76	1.53	1.31
12	N	1306	OPC	CAV-CAW	3.75	1.53	1.31
9	N	302	HEM	CBC-CAC	3.75	1.54	1.29
12	B	307	OPC	CAV-CAW	3.73	1.53	1.31
12	D	306	OPC	CAG-CAH	-3.72	1.39	1.51
12	Q	1307	OPC	CAG-CAH	-3.69	1.39	1.51
12	B	307	OPC	CAG-CAH	-3.66	1.39	1.51
15	E	101	BCR	C29-C30	3.65	1.62	1.54
9	N	303	HEM	CBC-CAC	3.63	1.53	1.29
12	N	1306	OPC	CAG-CAH	-3.63	1.39	1.51
9	A	302	HEM	CBC-CAC	3.61	1.53	1.29
15	R	1101	BCR	C29-C30	3.59	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	E	101	BCR	C38-C26	3.54	1.56	1.50
9	A	301	HEM	CBC-CAC	3.48	1.52	1.29
15	R	1101	BCR	C2-C1	3.48	1.62	1.54
12	D	306	OPC	CAQ-CAP	-3.46	1.39	1.52
12	B	307	OPC	CAQ-CAP	-3.46	1.39	1.52
12	N	1306	OPC	CAQ-CAP	-3.43	1.39	1.52
12	Q	1307	OPC	CAQ-CAP	-3.42	1.39	1.52
9	N	303	HEM	C3B-C2B	-3.41	1.35	1.40
9	A	303	HEM	C3C-CAC	3.38	1.54	1.47
9	N	303	HEM	C3B-CAB	3.38	1.54	1.47
9	N	301	HEM	CBC-CAC	3.38	1.51	1.29
9	A	303	HEM	C3B-CAB	3.37	1.54	1.47
13	O	1201	CLA	C2-C3	3.34	1.41	1.33
11	A	305	PL9	C47-C48	-3.34	1.39	1.50
11	A	305	PL9	C27-C28	-3.33	1.39	1.50
11	Q	1305	PL9	C47-C48	-3.33	1.39	1.50
11	A	305	PL9	C22-C23	-3.33	1.39	1.50
11	Q	1305	PL9	C27-C28	-3.32	1.39	1.50
11	Q	1305	PL9	C22-C23	-3.32	1.39	1.50
13	B	201	CLA	O1D-CGD	3.31	1.29	1.21
11	A	305	PL9	C42-C43	-3.27	1.39	1.50
15	E	101	BCR	C2-C1	3.25	1.61	1.54
11	Q	1305	PL9	C42-C43	-3.24	1.39	1.50
13	O	1201	CLA	O1D-CGD	3.21	1.29	1.21
12	D	306	OPC	CBP-CBQ	-3.21	1.39	1.52
12	Q	1307	OPC	CBP-CBQ	-3.21	1.39	1.52
12	B	307	OPC	CBP-CBQ	-3.20	1.39	1.52
12	N	1306	OPC	CBP-CBQ	-3.16	1.39	1.52
9	P	301	HEM	C3B-C2B	-2.91	1.36	1.40
9	N	303	HEM	CAA-C2A	2.89	1.56	1.52
9	N	303	HEM	C3C-CAC	2.86	1.53	1.47
9	A	302	HEM	C3C-CAC	2.86	1.53	1.47
15	R	1101	BCR	C5-C6	2.85	1.39	1.34
9	N	301	HEM	C3C-CAC	2.85	1.53	1.47
11	A	305	PL9	C43-C44	2.84	1.39	1.33
9	N	303	HEM	C3C-C2C	-2.84	1.36	1.40
13	O	1201	CLA	MG-NC	2.83	2.13	2.06
13	B	201	CLA	C2-C3	2.81	1.39	1.33
11	Q	1305	PL9	C43-C44	2.80	1.39	1.33
11	Q	1305	PL9	C38-C39	2.79	1.39	1.33
13	B	201	CLA	C1D-C2D	2.79	1.48	1.42
11	A	305	PL9	C23-C24	2.79	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Q	1305	PL9	C23-C24	2.78	1.39	1.33
11	A	305	PL9	C38-C39	2.78	1.39	1.33
13	O	1201	CLA	C1B-NB	2.77	1.37	1.35
13	O	1201	CLA	C1D-C2D	2.77	1.48	1.42
11	A	305	PL9	C28-C29	2.77	1.39	1.33
11	A	305	PL9	C8-C9	2.74	1.39	1.33
11	Q	1305	PL9	C8-C9	2.73	1.39	1.33
11	Q	1305	PL9	C28-C29	2.73	1.39	1.33
9	N	303	HEM	CMD-C2D	2.68	1.57	1.51
13	B	201	CLA	MG-NC	2.66	2.12	2.06
10	N	1304	TDS	CAR-CAQ	-2.64	1.39	1.52
10	A	304	TDS	CAR-CAQ	-2.61	1.39	1.52
9	N	303	HEM	C4D-C3D	2.60	1.48	1.42
9	A	303	HEM	C4D-C3D	2.57	1.48	1.42
9	N	302	HEM	C3B-C2B	-2.55	1.36	1.40
13	B	201	CLA	CHC-C1C	2.55	1.41	1.35
9	N	302	HEM	CAA-C2A	-2.49	1.48	1.52
9	A	301	HEM	C3B-C2B	-2.49	1.36	1.40
11	A	305	PL9	C7-C3	2.46	1.53	1.51
9	A	301	HEM	C3C-CAC	2.45	1.52	1.47
15	E	101	BCR	C5-C6	2.45	1.38	1.34
13	B	201	CLA	OBD-CAD	2.41	1.25	1.22
9	A	303	HEM	C3C-C2C	-2.39	1.37	1.40
9	A	303	HEM	CAA-C2A	2.37	1.55	1.52
9	N	302	HEM	CMA-C3A	2.35	1.56	1.51
13	O	1201	CLA	CBD-CHA	2.26	1.63	1.52
11	Q	1305	PL9	C7-C3	2.25	1.53	1.51
9	N	303	HEM	C4A-NA	2.24	1.40	1.36
15	E	101	BCR	C8-C9	2.23	1.50	1.45
13	O	1201	CLA	CAC-C3C	2.22	1.56	1.51
9	A	301	HEM	CAA-C2A	2.22	1.55	1.52
9	A	302	HEM	CMA-C3A	2.21	1.56	1.51
12	D	306	OPC	CBC-CBD	-2.19	1.39	1.51
12	B	307	OPC	CBC-CBD	-2.18	1.39	1.51
12	B	307	OPC	CAR-CAS	-2.17	1.39	1.51
10	A	304	TDS	CAR-CAS	-2.17	1.39	1.51
12	N	1306	OPC	CAQ-CAR	-2.16	1.39	1.51
12	Q	1307	OPC	CBP-CBO	-2.16	1.39	1.51
12	N	1306	OPC	CBB-CBC	-2.16	1.39	1.51
12	D	306	OPC	CBB-CBC	-2.16	1.39	1.51
12	D	306	OPC	CAR-CAS	-2.16	1.39	1.51
12	D	306	OPC	CBP-CBO	-2.16	1.39	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	B	307	OPC	CAQ-CAR	-2.16	1.39	1.51
12	N	1306	OPC	CAR-CAS	-2.15	1.39	1.51
12	Q	1307	OPC	CBB-CBC	-2.15	1.39	1.51
12	Q	1307	OPC	CBC-CBD	-2.15	1.39	1.51
12	Q	1307	OPC	CAQ-CAR	-2.15	1.39	1.51
12	N	1306	OPC	CBP-CBO	-2.15	1.39	1.51
10	N	1304	TDS	CAR-CAS	-2.15	1.39	1.51
12	D	306	OPC	CAQ-CAR	-2.14	1.39	1.51
12	N	1306	OPC	CBC-CBD	-2.14	1.39	1.51
12	B	307	OPC	CBB-CBC	-2.14	1.39	1.51
9	N	301	HEM	CMA-C3A	2.14	1.56	1.51
12	Q	1307	OPC	CAR-CAS	-2.13	1.39	1.51
12	B	307	OPC	CBP-CBO	-2.13	1.39	1.51
13	B	201	CLA	CBA-CGA	2.13	1.56	1.50
9	A	301	HEM	CMA-C3A	2.11	1.56	1.51
9	C	301	HEM	C1A-NA	2.08	1.40	1.36
9	P	301	HEM	C1A-NA	2.08	1.40	1.36
9	N	301	HEM	C1A-CHA	-2.06	1.35	1.41
9	C	301	HEM	C3B-C2B	-2.03	1.37	1.40
15	R	1101	BCR	C14-C13	2.01	1.38	1.35
15	R	1101	BCR	C23-C22	-2.01	1.41	1.45

All (201) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	1201	CLA	C4D-C3D-CAD	15.47	117.10	108.47
9	N	302	HEM	CBA-CAA-C2A	-14.41	85.90	112.49
13	B	201	CLA	C4D-C3D-CAD	14.15	116.36	108.47
9	A	302	HEM	CBA-CAA-C2A	-14.13	86.43	112.49
9	A	302	HEM	CAA-CBA-CGA	12.28	133.27	112.67
9	N	302	HEM	CAA-CBA-CGA	11.49	131.95	112.67
13	O	1201	CLA	C4A-NA-C1A	10.57	111.46	106.71
9	A	303	HEM	C1D-C2D-C3D	9.02	113.27	107.00
13	B	201	CLA	C4A-NA-C1A	8.96	110.73	106.71
10	A	304	TDS	CAL-CAM-CAN	-8.27	112.94	120.18
11	A	305	PL9	C7-C8-C9	-8.15	113.23	126.79
10	N	1304	TDS	CAL-CAM-CAN	-8.11	113.07	120.18
11	Q	1305	PL9	C7-C8-C9	-8.08	113.34	126.79
13	B	201	CLA	CMA-C3A-C4A	7.44	131.78	111.77
15	R	1101	BCR	C38-C26-C25	6.99	132.37	124.53
13	O	1201	CLA	CMA-C3A-C4A	6.96	130.49	111.77
11	Q	1305	PL9	C17-C18-C19	-6.68	111.57	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
15	E	101	BCR	C38-C26-C25	6.60	131.94	124.53
11	A	305	PL9	C22-C23-C24	-6.46	112.11	127.66
9	A	303	HEM	CAD-CBD-CGD	6.43	123.46	112.67
11	Q	1305	PL9	C12-C13-C14	-6.41	112.24	127.66
12	N	1306	OPC	OAN-CAO-CAP	6.37	125.24	111.50
11	Q	1305	PL9	C37-C38-C39	-6.25	112.62	127.66
11	A	305	PL9	C17-C18-C19	-6.22	112.69	127.66
9	A	303	HEM	CMD-C2D-C1D	-6.17	118.98	128.46
11	A	305	PL9	C37-C38-C39	-6.16	112.84	127.66
13	O	1201	CLA	CAA-C2A-C1A	6.06	131.82	111.97
11	A	305	PL9	C12-C13-C14	-6.03	113.15	127.66
9	A	303	HEM	CAA-CBA-CGA	6.01	122.75	112.67
11	Q	1305	PL9	C22-C23-C24	-5.96	113.31	127.66
13	B	201	CLA	CAA-C2A-C1A	5.84	131.10	111.97
12	Q	1307	OPC	OAN-CAO-CAP	5.60	123.56	111.50
13	B	201	CLA	C3D-CAD-CBD	-5.50	100.36	107.61
15	R	1101	BCR	C24-C23-C22	5.50	134.54	126.23
12	D	306	OPC	OAN-CAO-CAP	5.32	122.96	111.50
13	B	201	CLA	CBC-CAC-C3C	5.29	127.01	112.43
11	Q	1305	PL9	C25-C24-C26	5.28	124.16	115.27
10	A	304	TDS	CAJ-OAK-CAL	-5.21	109.67	117.53
13	O	1201	CLA	C3D-CAD-CBD	-5.16	100.81	107.61
15	E	101	BCR	C24-C23-C22	5.13	133.98	126.23
10	N	1304	TDS	CAJ-OAK-CAL	-5.05	109.90	117.53
15	E	101	BCR	C20-C21-C22	4.96	134.39	127.31
9	N	303	HEM	C1D-C2D-C3D	4.90	110.41	107.00
15	E	101	BCR	C33-C5-C6	4.89	130.01	124.53
12	B	307	OPC	OAN-CAO-CAP	4.88	122.02	111.50
15	R	1101	BCR	C33-C5-C6	4.86	129.98	124.53
15	R	1101	BCR	C20-C21-C22	4.82	134.20	127.31
9	N	303	HEM	CMD-C2D-C1D	-4.75	121.16	128.46
10	A	304	TDS	CAA-OAB-CAE	-4.67	111.22	117.75
9	N	303	HEM	CAD-CBD-CGD	4.63	120.43	112.67
13	O	1201	CLA	CBC-CAC-C3C	4.62	125.17	112.43
10	N	1304	TDS	OAO-CAP-CAQ	4.44	117.17	111.91
9	N	301	HEM	CAA-CBA-CGA	4.41	120.07	112.67
11	A	305	PL9	C25-C24-C26	4.25	122.42	115.27
13	O	1201	CLA	C3A-C2A-C1A	4.19	107.61	101.34
10	N	1304	TDS	CAA-OAB-CAE	-4.16	111.93	117.75
13	B	201	CLA	OBD-CAD-C3D	4.11	134.81	127.98
15	R	1101	BCR	C38-C26-C27	-4.09	105.77	113.62
15	E	101	BCR	C7-C8-C9	4.00	132.28	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	N	303	HEM	CAA-CBA-CGA	3.97	119.34	112.67
15	E	101	BCR	C38-C26-C27	-3.92	106.08	113.62
15	R	1101	BCR	C23-C22-C21	-3.92	112.93	118.94
9	A	303	HEM	CBA-CAA-C2A	-3.87	105.35	112.49
15	R	1101	BCR	C30-C25-C26	-3.86	117.18	122.61
15	E	101	BCR	C30-C25-C26	-3.84	117.20	122.61
15	R	1101	BCR	C29-C30-C25	3.82	116.35	110.48
13	B	201	CLA	C3A-C2A-C1A	3.80	107.03	101.34
15	R	1101	BCR	C33-C5-C4	-3.77	106.37	113.62
15	E	101	BCR	C29-C30-C25	3.76	116.28	110.48
13	O	1201	CLA	C2A-C1A-CHA	3.75	130.41	123.86
15	R	1101	BCR	C7-C8-C9	3.74	131.89	126.23
15	E	101	BCR	C33-C5-C4	-3.74	106.43	113.62
15	E	101	BCR	C23-C22-C21	-3.71	113.24	118.94
12	N	1306	OPC	OBJ-CBK-CBL	3.71	123.55	111.91
13	B	201	CLA	C1-C2-C3	3.71	132.46	126.04
10	A	304	TDS	OAO-CAP-CAQ	3.69	116.29	111.91
13	O	1201	CLA	OBD-CAD-C3D	3.65	134.03	127.98
13	B	201	CLA	C2A-C3A-C4A	3.64	107.75	101.87
11	Q	1305	PL9	C26-C24-C23	-3.57	113.89	121.12
13	O	1201	CLA	C1-C2-C3	3.53	132.14	126.04
11	Q	1305	PL9	C15-C14-C16	3.51	121.18	115.27
13	O	1201	CLA	C2A-C3A-C4A	3.48	107.48	101.87
10	N	1304	TDS	CAE-CAF-CAN	3.46	122.41	115.15
15	E	101	BCR	C2-C1-C6	3.39	115.70	110.48
11	Q	1305	PL9	C30-C29-C31	3.34	120.90	115.27
9	N	301	HEM	CBA-CAA-C2A	-3.33	106.35	112.49
15	R	1101	BCR	C2-C1-C6	3.32	115.59	110.48
9	A	301	HEM	C1D-C2D-C3D	-3.32	104.69	107.00
15	E	101	BCR	C1-C6-C5	-3.31	117.96	122.61
10	A	304	TDS	CAQ-CAP-CAH	3.26	125.01	120.39
15	R	1101	BCR	C1-C6-C5	-3.24	118.05	122.61
10	A	304	TDS	CAE-CAF-CAN	3.23	121.94	115.15
10	N	1304	TDS	OAB-CAE-CAF	3.22	120.63	115.89
15	E	101	BCR	C23-C24-C25	3.20	136.18	127.20
12	D	306	OPC	OBJ-CBK-CBL	3.20	121.94	111.91
10	N	1304	TDS	OAB-CAE-CAD	-3.12	117.78	123.34
11	A	305	PL9	C30-C29-C31	3.11	120.50	115.27
15	R	1101	BCR	C11-C10-C9	3.10	131.73	127.31
9	N	303	HEM	CBD-CAD-C3D	-3.09	106.78	112.48
15	R	1101	BCR	C23-C24-C25	3.09	135.88	127.20
10	A	304	TDS	CAG-CAF-CAE	-3.05	120.42	124.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	201	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
13	B	201	CLA	O2D-CGD-CBD	2.98	116.57	111.27
9	N	301	HEM	CBD-CAD-C3D	-2.95	107.05	112.48
13	B	201	CLA	C2A-C1A-CHA	2.94	129.00	123.86
10	N	1304	TDS	CAG-CAF-CAE	-2.92	120.61	124.96
11	A	305	PL9	C26-C24-C23	-2.92	115.21	121.12
10	N	1304	TDS	CAQ-CAP-CAH	2.87	124.45	120.39
11	Q	1305	PL9	C35-C34-C36	2.87	120.09	115.27
13	O	1201	CLA	CMB-C2B-C1B	-2.86	124.07	128.46
13	B	201	CLA	CMD-C2D-C3D	2.84	129.98	124.68
12	B	307	OPC	CBM-CBL-CBK	2.75	123.62	113.62
12	N	1306	OPC	OAN-CAO-OAD	-2.75	117.06	123.70
15	E	101	BCR	C15-C14-C13	2.73	131.20	127.31
12	Q	1307	OPC	OAN-CAO-OAD	-2.72	117.13	123.70
9	A	303	HEM	CMB-C2B-C3B	2.71	129.75	124.68
15	E	101	BCR	C11-C10-C9	2.70	131.17	127.31
15	E	101	BCR	C35-C13-C12	2.70	122.32	118.08
9	A	301	HEM	CAA-CBA-CGA	2.68	117.16	112.67
15	E	101	BCR	C1-C6-C7	2.66	123.32	115.78
15	R	1101	BCR	C1-C6-C7	2.64	123.24	115.78
13	B	201	CLA	O2A-CGA-CBA	2.63	120.15	111.91
15	R	1101	BCR	C35-C13-C12	2.63	122.21	118.08
15	E	101	BCR	C37-C22-C23	2.61	122.20	118.08
15	R	1101	BCR	C37-C22-C23	2.61	122.19	118.08
15	R	1101	BCR	C15-C14-C13	2.60	131.01	127.31
13	O	1201	CLA	CAA-C2A-C3A	2.59	119.88	112.78
9	N	303	HEM	CMB-C2B-C3B	2.59	129.53	124.68
12	Q	1307	OPC	OBJ-CBK-CBL	2.58	120.02	111.91
9	A	302	HEM	CMA-C3A-C4A	2.58	132.43	128.46
15	R	1101	BCR	C8-C7-C6	2.56	134.41	127.20
9	N	301	HEM	C1D-C2D-C3D	-2.56	105.22	107.00
15	E	101	BCR	C32-C1-C6	2.54	114.42	110.30
11	A	305	PL9	C35-C34-C36	2.53	119.53	115.27
13	O	1201	CLA	O2A-CGA-CBA	2.53	119.85	111.91
9	P	301	HEM	CAA-C2A-C3A	-2.51	120.03	127.25
15	E	101	BCR	C12-C13-C14	-2.49	115.12	118.94
15	E	101	BCR	C8-C7-C6	2.48	134.18	127.20
15	E	101	BCR	C34-C9-C10	-2.48	119.44	122.92
15	R	1101	BCR	C12-C13-C14	-2.48	115.14	118.94
11	Q	1305	PL9	C10-C9-C11	2.47	119.43	115.27
12	D	306	OPC	OAN-CAO-OAD	-2.46	117.75	123.70
11	Q	1305	PL9	C42-C43-C44	2.46	133.57	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	O	1201	CLA	CED-O2D-CGD	2.44	121.46	115.94
11	Q	1305	PL9	C20-C19-C21	2.44	119.37	115.27
11	A	305	PL9	C20-C19-C21	2.43	119.36	115.27
12	N	1306	OPC	CAM-OAN-CAO	2.43	123.76	117.79
9	C	301	HEM	CAA-C2A-C3A	-2.41	120.31	127.25
10	A	304	TDS	OAB-CAE-CAD	-2.41	119.06	123.34
13	B	201	CLA	CAA-C2A-C3A	2.39	119.33	112.78
11	A	305	PL9	C42-C43-C44	2.38	133.39	127.66
13	O	1201	CLA	CMD-C2D-C3D	2.38	129.12	124.68
9	N	302	HEM	CAA-C2A-C3A	-2.37	120.43	127.25
15	R	1101	BCR	C32-C1-C6	2.36	114.12	110.30
12	N	1306	OPC	OBJ-CBK-OCC	-2.35	117.65	123.59
11	A	305	PL9	C7-C3-C4	-2.35	114.96	116.88
11	Q	1305	PL9	C40-C39-C41	2.35	119.22	115.27
11	A	305	PL9	C40-C39-C41	2.34	119.22	115.27
10	A	304	TDS	CAG-CAH-CAP	2.29	119.14	116.63
11	A	305	PL9	C10-C9-C8	-2.28	117.84	123.68
9	N	301	HEM	CAA-C2A-C3A	-2.26	120.74	127.25
12	N	1306	OPC	CBM-CBL-CBK	2.25	121.80	113.62
11	A	305	PL9	C53-C6-C1	2.24	119.58	114.99
11	A	305	PL9	C51-C49-C50	2.23	119.52	114.60
10	A	304	TDS	CAH-CAG-CAF	-2.23	118.34	120.58
15	E	101	BCR	C34-C9-C8	2.22	121.58	118.08
10	N	1304	TDS	CAG-CAH-CAP	2.22	119.06	116.63
12	B	307	OPC	OAN-CAO-OAD	-2.22	118.34	123.70
11	A	305	PL9	C10-C9-C11	2.22	119.00	115.27
9	N	303	HEM	CMA-C3A-C4A	-2.21	125.06	128.46
10	A	304	TDS	OBD-CAM-CAN	2.21	123.67	119.62
9	A	301	HEM	CAA-C2A-C3A	-2.20	120.92	127.25
10	A	304	TDS	CAS-CAR-CAQ	2.20	122.31	113.76
10	N	1304	TDS	OAO-CAN-CAM	2.20	118.88	116.12
11	Q	1305	PL9	C53-C6-C1	2.19	119.46	114.99
9	N	302	HEM	CMA-C3A-C4A	2.19	131.82	128.46
10	A	304	TDS	OAB-CAE-CAF	2.19	119.10	115.89
9	A	301	HEM	CMA-C3A-C4A	2.16	131.78	128.46
9	C	301	HEM	CMD-C2D-C1D	-2.15	125.15	128.46
10	N	1304	TDS	OBD-CAM-CAN	2.15	123.57	119.62
9	N	302	HEM	CMB-C2B-C3B	2.15	128.69	124.68
9	A	301	HEM	CMA-C3A-C2A	-2.14	120.91	124.94
15	R	1101	BCR	C34-C9-C8	2.12	121.42	118.08
9	A	301	HEM	CMD-C2D-C3D	2.12	128.94	124.94
12	D	306	OPC	CBM-CBL-CBK	2.12	121.32	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	B	201	CLA	CED-O2D-CGD	2.11	120.71	115.94
9	P	301	HEM	CMA-C3A-C2A	-2.11	120.97	124.94
9	P	301	HEM	CMD-C2D-C1D	-2.10	125.23	128.46
9	A	302	HEM	CMB-C2B-C3B	2.09	128.59	124.68
13	B	201	CLA	C12-C11-C10	-2.08	103.66	113.24
9	A	303	HEM	CMC-C2C-C3C	2.08	128.57	124.68
9	C	301	HEM	CMD-C2D-C3D	2.08	128.87	124.94
9	N	301	HEM	CMD-C2D-C3D	2.07	128.84	124.94
11	A	305	PL9	C45-C44-C43	-2.07	118.38	123.68
12	D	306	OPC	OBJ-CBK-OCC	-2.05	118.41	123.59
9	A	302	HEM	C1D-C2D-C3D	-2.04	105.58	107.00
11	Q	1305	PL9	C51-C49-C50	2.03	119.08	114.60
11	A	305	PL9	C45-C44-C46	2.02	118.66	115.27
11	Q	1305	PL9	C45-C44-C46	2.02	118.66	115.27
12	B	307	OPC	CBQ-CBR-CBS	-2.01	109.28	124.73
15	R	1101	BCR	C34-C9-C10	-2.01	120.10	122.92

All (11) chirality outliers are listed below:

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

All (156) 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
15	E	101	BCR	C22-C23-C24-C25
12	N	1306	OPC	CAP-CAO-OAN-CAM
12	N	1306	OPC	OAD-CAO-OAN-CAM

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Mol	Chain	Res	Type	Atoms
12	N	1306	OPC	OCC-CBK-OBJ-CBI
12	N	1306	OPC	CBL-CBK-OBJ-CBI
13	B	201	CLA	C1A-C2A-CAA-CBA
13	B	201	CLA	O2A-C1-C2-C3
12	Q	1307	OPC	CAP-CAO-OAN-CAM
12	Q	1307	OPC	OAD-CAO-OAN-CAM
12	Q	1307	OPC	CAH-OAI-PAJ-OAB
12	B	307	OPC	CAP-CAO-OAN-CAM
12	B	307	OPC	OAD-CAO-OAN-CAM
12	B	307	OPC	CAL-OAK-PAJ-OAB
12	B	307	OPC	CAH-OAI-PAJ-OAB
11	A	305	PL9	C7-C8-C9-C10
11	A	305	PL9	C7-C8-C9-C11
11	A	305	PL9	C12-C13-C14-C15
11	A	305	PL9	C12-C13-C14-C16
11	A	305	PL9	C17-C18-C19-C20
11	A	305	PL9	C17-C18-C19-C21
11	A	305	PL9	C22-C23-C24-C25
11	A	305	PL9	C22-C23-C24-C26
11	A	305	PL9	C32-C33-C34-C35
11	A	305	PL9	C32-C33-C34-C36
11	A	305	PL9	C37-C38-C39-C40
11	A	305	PL9	C37-C38-C39-C41
11	A	305	PL9	C41-C42-C43-C44
12	D	306	OPC	CAP-CAO-OAN-CAM
12	D	306	OPC	OAD-CAO-OAN-CAM
12	D	306	OPC	CAH-OAI-PAJ-OBH
12	D	306	OPC	OCC-CBK-OBJ-CBI
12	D	306	OPC	CBL-CBK-OBJ-CBI
15	R	1101	BCR	C1-C6-C7-C8
15	R	1101	BCR	C5-C6-C7-C8
15	R	1101	BCR	C11-C10-C9-C8
15	R	1101	BCR	C11-C10-C9-C34
15	R	1101	BCR	C22-C23-C24-C25
9	A	303	HEM	C2D-C3D-CAD-CBD
9	A	303	HEM	C4D-C3D-CAD-CBD
11	Q	1305	PL9	C7-C8-C9-C10
11	Q	1305	PL9	C7-C8-C9-C11
11	Q	1305	PL9	C12-C13-C14-C16
11	Q	1305	PL9	C17-C18-C19-C20
11	Q	1305	PL9	C17-C18-C19-C21
11	Q	1305	PL9	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
11	Q	1305	PL9	C22-C23-C24-C26
11	Q	1305	PL9	C30-C29-C31-C32
11	Q	1305	PL9	C32-C33-C34-C35
11	Q	1305	PL9	C32-C33-C34-C36
11	Q	1305	PL9	C37-C38-C39-C40
11	Q	1305	PL9	C37-C38-C39-C41
11	Q	1305	PL9	C41-C42-C43-C44
13	O	1201	CLA	C1A-C2A-CAA-CBA
13	O	1201	CLA	C3-C5-C6-C7
10	N	1304	TDS	CAD-CAE-OAB-CAA
11	Q	1305	PL9	C28-C29-C31-C32
13	O	1201	CLA	C2A-CAA-CBA-CGA
11	Q	1305	PL9	C12-C13-C14-C15
10	A	304	TDS	CAD-CAE-OAB-CAA
10	N	1304	TDS	CAF-CAE-OAB-CAA
10	A	304	TDS	CAF-CAE-OAB-CAA
11	Q	1305	PL9	C15-C14-C16-C17
11	Q	1305	PL9	C25-C24-C26-C27
11	Q	1305	PL9	C13-C14-C16-C17
11	Q	1305	PL9	C23-C24-C26-C27
10	N	1304	TDS	CAD-CAL-OAK-CAJ
11	A	305	PL9	C39-C41-C42-C43
13	B	201	CLA	C3-C5-C6-C7
13	O	1201	CLA	C11-C12-C13-C14
10	A	304	TDS	CAD-CAL-OAK-CAJ
13	B	201	CLA	C10-C11-C12-C13
10	N	1304	TDS	CAM-CAL-OAK-CAJ
11	A	305	PL9	C14-C16-C17-C18
11	Q	1305	PL9	C14-C16-C17-C18
12	B	307	OPC	CAL-OAK-PAJ-OAI
12	B	307	OPC	CAH-OAI-PAJ-OAK
12	D	306	OPC	CAH-OAI-PAJ-OAK
10	A	304	TDS	CAV-CAW-CAX-CAY
10	A	304	TDS	CAM-CAL-OAK-CAJ
11	Q	1305	PL9	C39-C41-C42-C43
10	N	1304	TDS	CAT-CAU-CAV-CAW
12	N	1306	OPC	CAS-CAT-CAU-CAV
13	B	201	CLA	C2C-C3C-CAC-CBC
11	A	305	PL9	C31-C32-C33-C34
12	Q	1307	OPC	CAT-CAU-CAV-CAW
11	Q	1305	PL9	C31-C32-C33-C34
13	B	201	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
10	A	304	TDS	CAT-CAU-CAV-CAW
12	Q	1307	OPC	CAH-OAI-PAJ-OAK
13	B	201	CLA	C6-C7-C8-C9
13	B	201	CLA	C6-C7-C8-C10
13	O	1201	CLA	C12-C13-C15-C16
13	O	1201	CLA	CAD-CBD-CGD-O2D
13	B	201	CLA	C13-C15-C16-C17
13	B	201	CLA	O1A-CGA-O2A-C1
12	Q	1307	OPC	CAH-OAI-PAJ-OBH
12	B	307	OPC	CAL-OAK-PAJ-OBH
12	B	307	OPC	CAH-OAI-PAJ-OBH
13	B	201	CLA	C11-C12-C13-C15
12	N	1306	OPC	NAF-CAG-CAH-OAI
12	Q	1307	OPC	NAF-CAG-CAH-OAI
12	B	307	OPC	NAF-CAG-CAH-OAI
12	D	306	OPC	NAF-CAG-CAH-OAI
9	N	303	HEM	C1A-C2A-CAA-CBA
9	N	303	HEM	C3A-C2A-CAA-CBA
13	B	201	CLA	C4C-C3C-CAC-CBC
12	N	1306	OPC	CBI-CAM-OAN-CAO
12	Q	1307	OPC	CAL-CAM-OAN-CAO
12	D	306	OPC	CAL-OAK-PAJ-OAI
13	B	201	CLA	C4-C3-C5-C6
13	O	1201	CLA	C14-C13-C15-C16
12	B	307	OPC	CAM-CAL-OAK-PAJ
11	A	305	PL9	C12-C11-C9-C10
13	B	201	CLA	C11-C12-C13-C14
12	B	307	OPC	CBI-CAM-OAN-CAO
12	D	306	OPC	CBI-CAM-OAN-CAO
13	O	1201	CLA	C11-C12-C13-C15
12	N	1306	OPC	CAH-OAI-PAJ-OAK
11	A	305	PL9	C24-C26-C27-C28
11	Q	1305	PL9	C20-C19-C21-C22
13	B	201	CLA	C2-C3-C5-C6
11	A	305	PL9	C35-C34-C36-C37
11	A	305	PL9	C40-C39-C41-C42
11	A	305	PL9	C25-C24-C26-C27
11	Q	1305	PL9	C35-C34-C36-C37
11	A	305	PL9	C12-C11-C9-C8
11	A	305	PL9	C20-C19-C21-C22
11	Q	1305	PL9	C18-C19-C21-C22
12	N	1306	OPC	OBJ-CBK-CBL-CBM

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Mol	Chain	Res	Type	Atoms
12	N	1306	OPC	CAT-CAU-CAV-CAW
12	B	307	OPC	CBP-CBQ-CBR-CBS
12	D	306	OPC	CBR-CBS-CBT-CBU
13	B	201	CLA	C2A-CAA-CBA-CGA
11	Q	1305	PL9	C12-C11-C9-C10
11	A	305	PL9	C33-C34-C36-C37
12	Q	1307	OPC	CAV-CAW-CAX-CAY
13	B	201	CLA	CAA-CBA-CGA-O2A
11	A	305	PL9	C38-C39-C41-C42
13	O	1201	CLA	CAA-CBA-CGA-O2A
12	D	306	OPC	CBW-CBX-CBY-CBZ
12	B	307	OPC	CBR-CBS-CBT-CBU
11	Q	1305	PL9	C36-C37-C38-C39
11	Q	1305	PL9	C46-C47-C48-C49
12	N	1306	OPC	OCC-CBK-CBL-CBM
11	A	305	PL9	C18-C19-C21-C22
13	B	201	CLA	CAA-CBA-CGA-O1A
13	O	1201	CLA	CAA-CBA-CGA-O1A
12	N	1306	OPC	CAL-OAK-PAJ-OAB
11	A	305	PL9	C36-C37-C38-C39
11	Q	1305	PL9	C21-C22-C23-C24
12	B	307	OPC	CAL-CAM-OAN-CAO
11	A	305	PL9	C23-C24-C26-C27

There are no ring outliers.

21 monomers are involved in 201 short contacts:

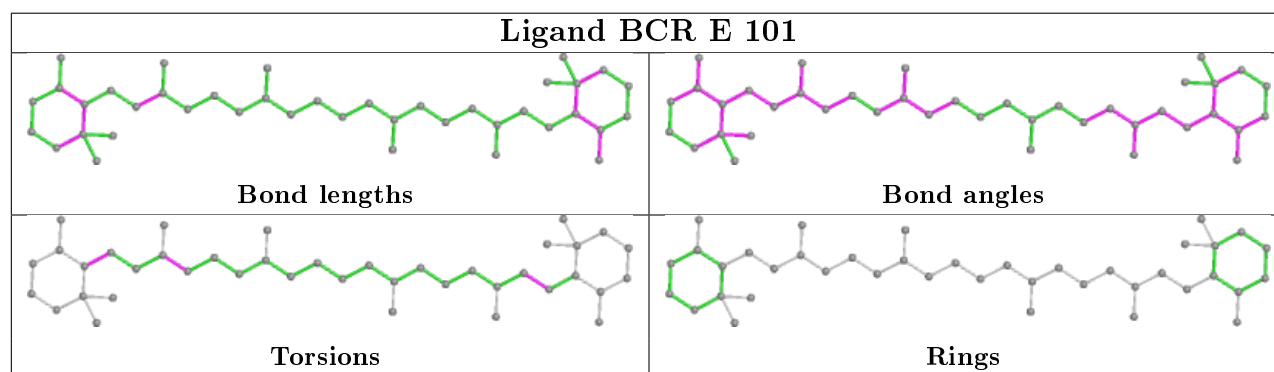
Mol	Chain	Res	Type	Clashes	Symm-Clashes
15	E	101	BCR	7	0
9	P	301	HEM	1	0
12	N	1306	OPC	10	0
13	B	201	CLA	8	0
14	Q	1200	FES	1	0
12	Q	1307	OPC	30	0
10	N	1304	TDS	12	0
12	B	307	OPC	14	0
11	A	305	PL9	18	0
12	D	306	OPC	24	0
9	A	302	HEM	5	0
14	D	200	FES	1	0
15	R	1101	BCR	7	0
9	A	303	HEM	3	0

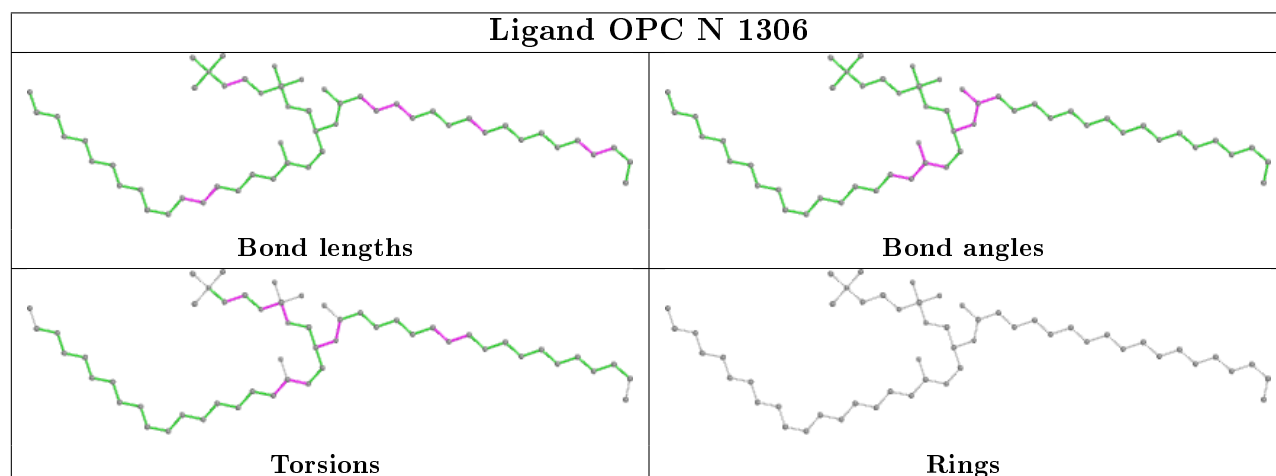
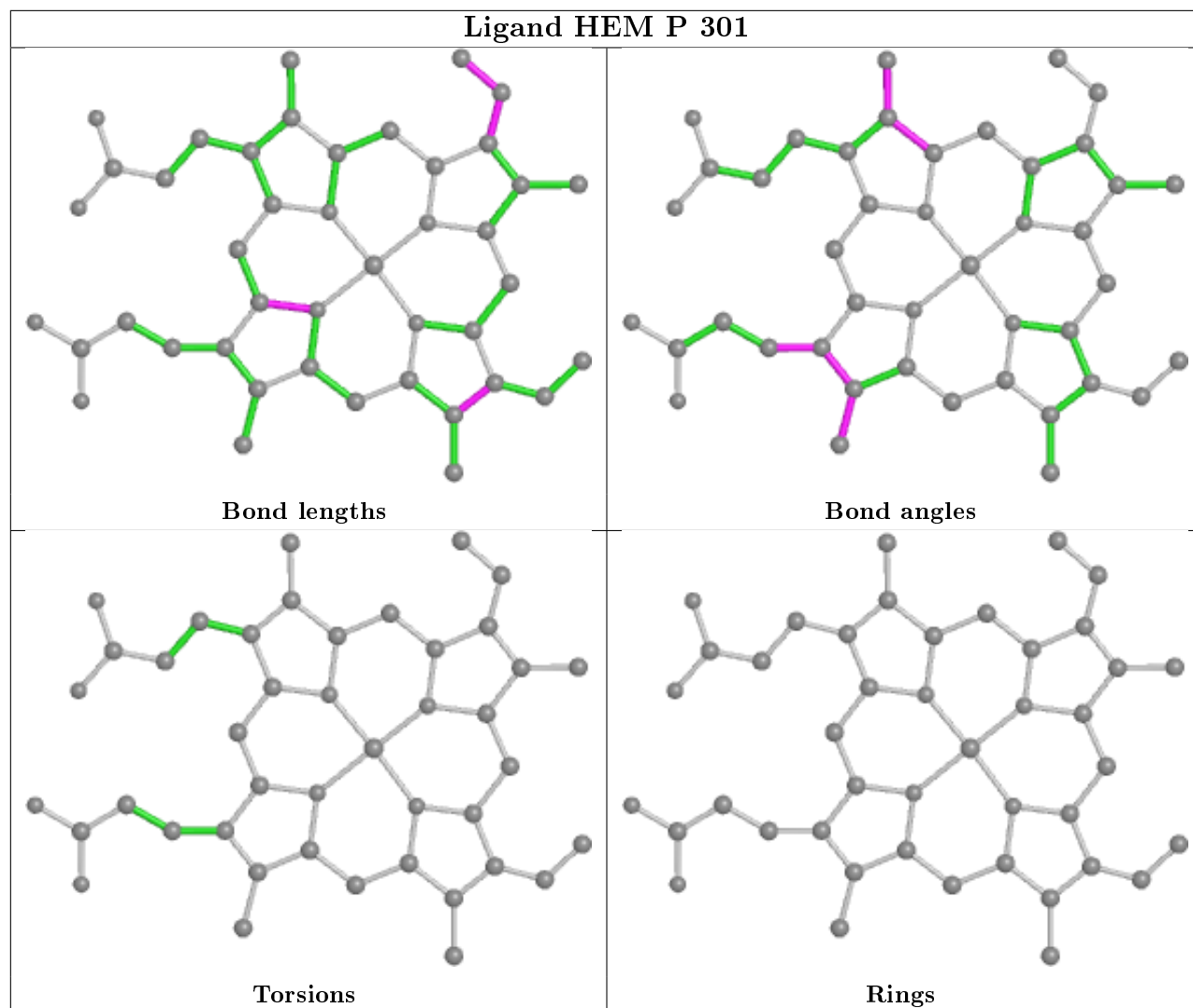
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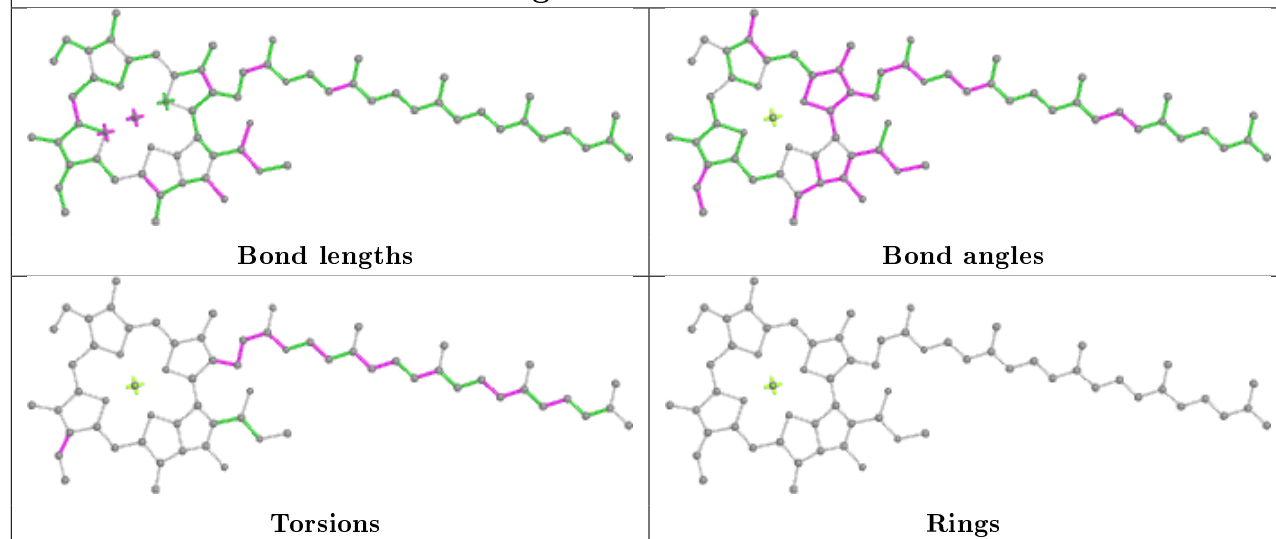
Mol	Chain	Res	Type	Clashes	Symm-Clashes
11	Q	1305	PL9	23	0
10	A	304	TDS	13	0
9	A	301	HEM	10	0
9	N	301	HEM	9	0
9	N	303	HEM	4	0
9	N	302	HEM	4	0
13	O	1201	CLA	20	0

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

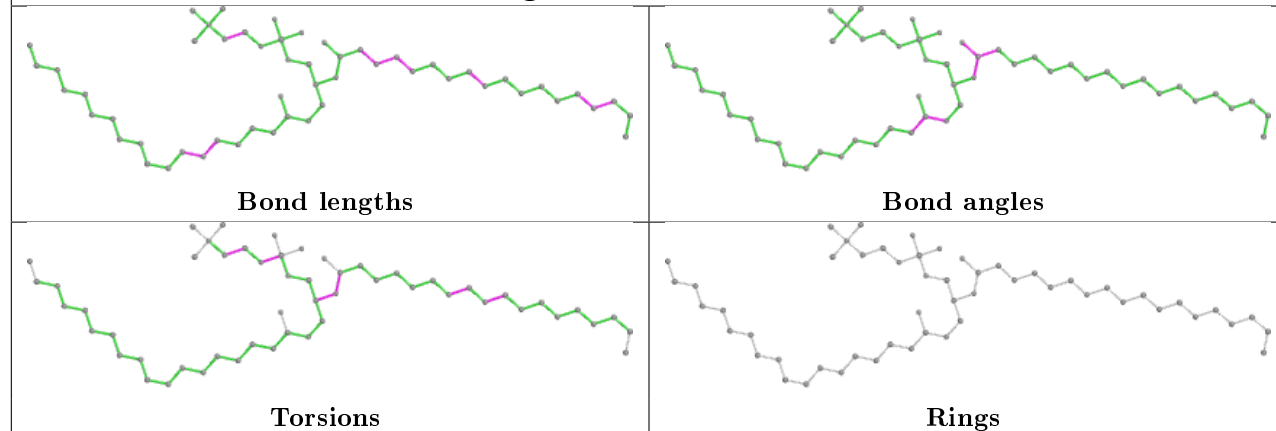




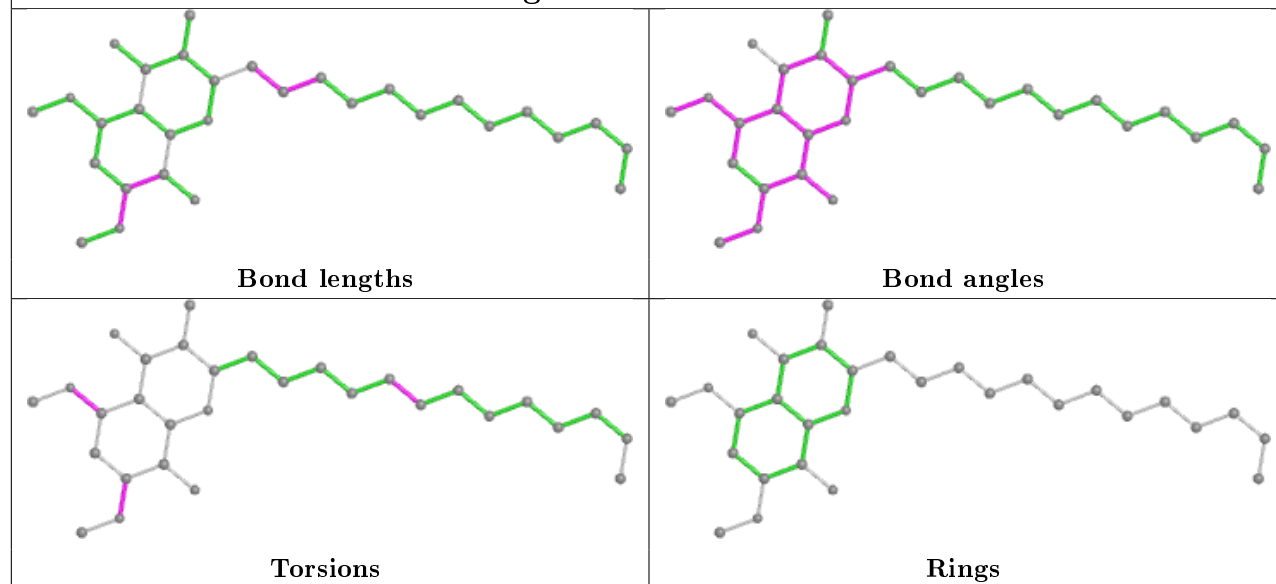
## Ligand CLA B 201

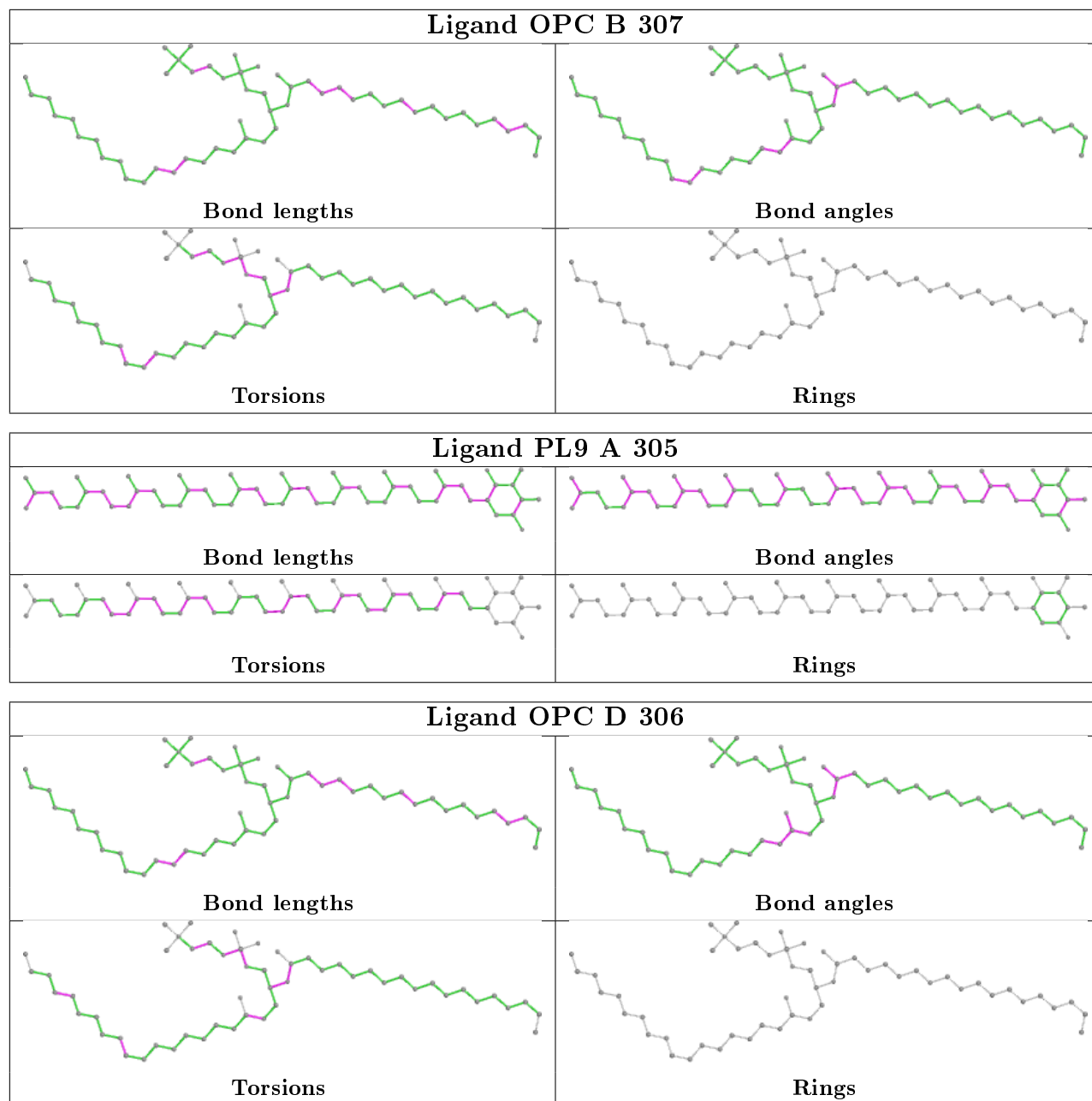


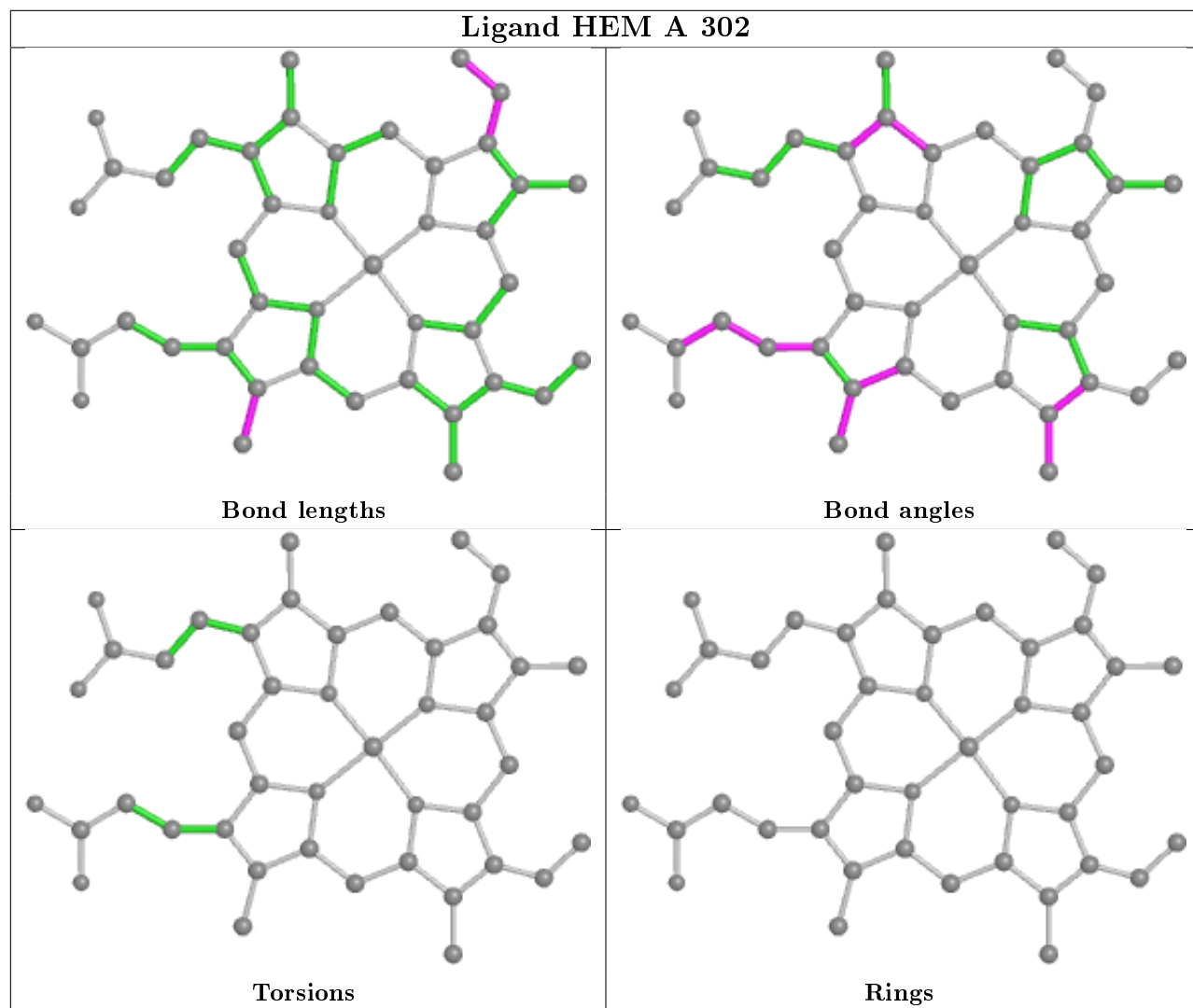
## Ligand OPC Q 1307



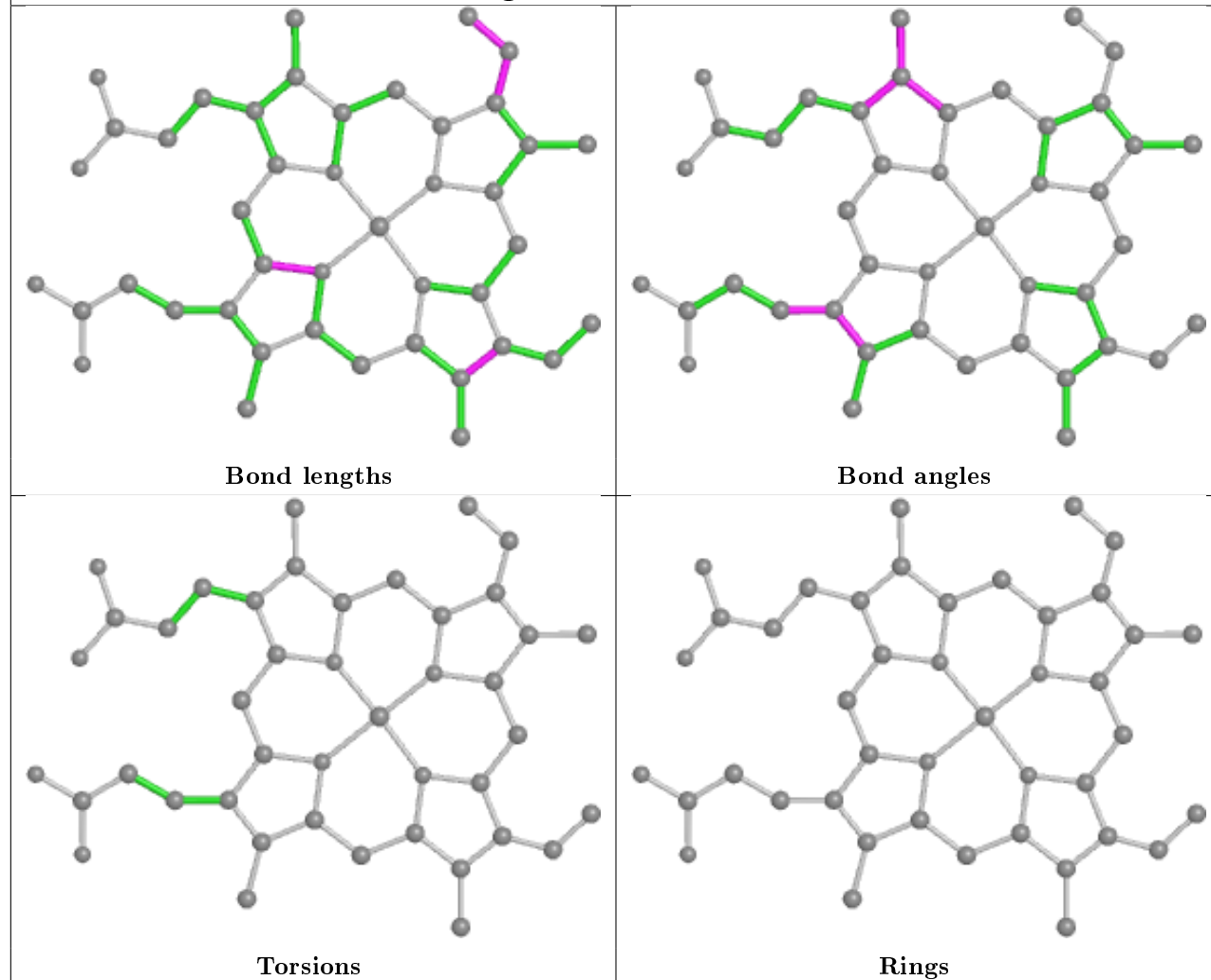
## Ligand TDS N 1304



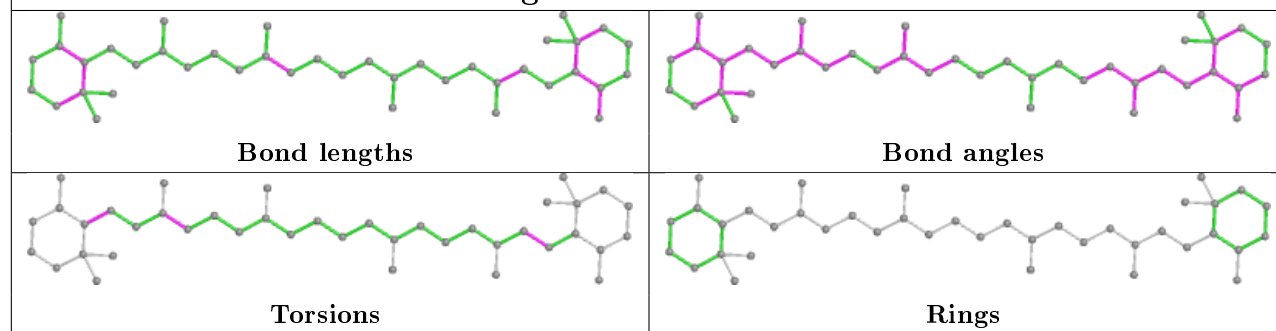


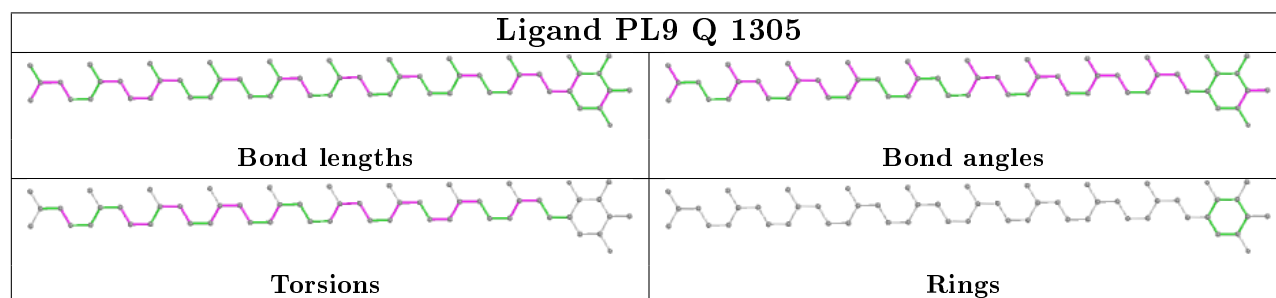
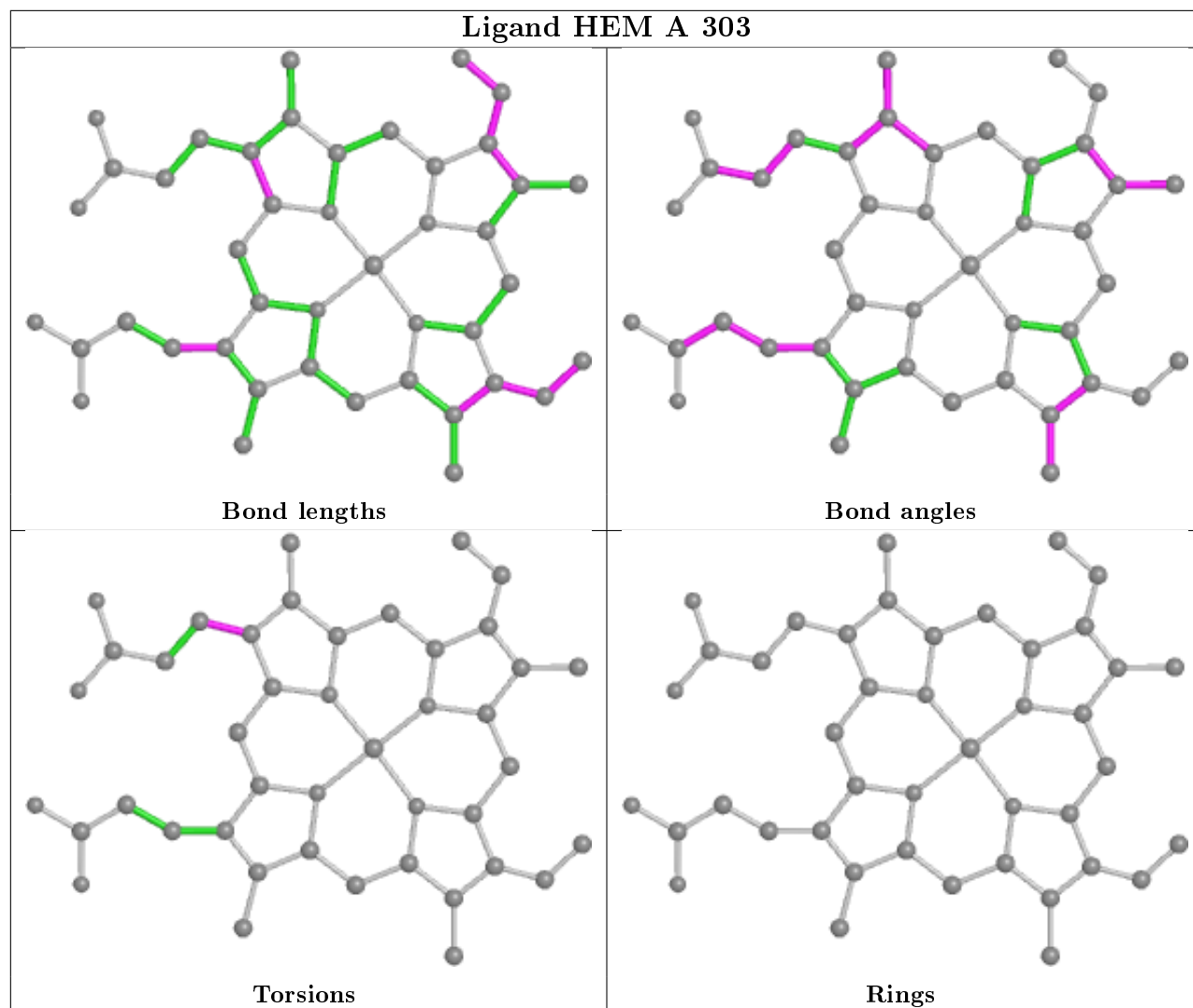


## Ligand HEM C 301



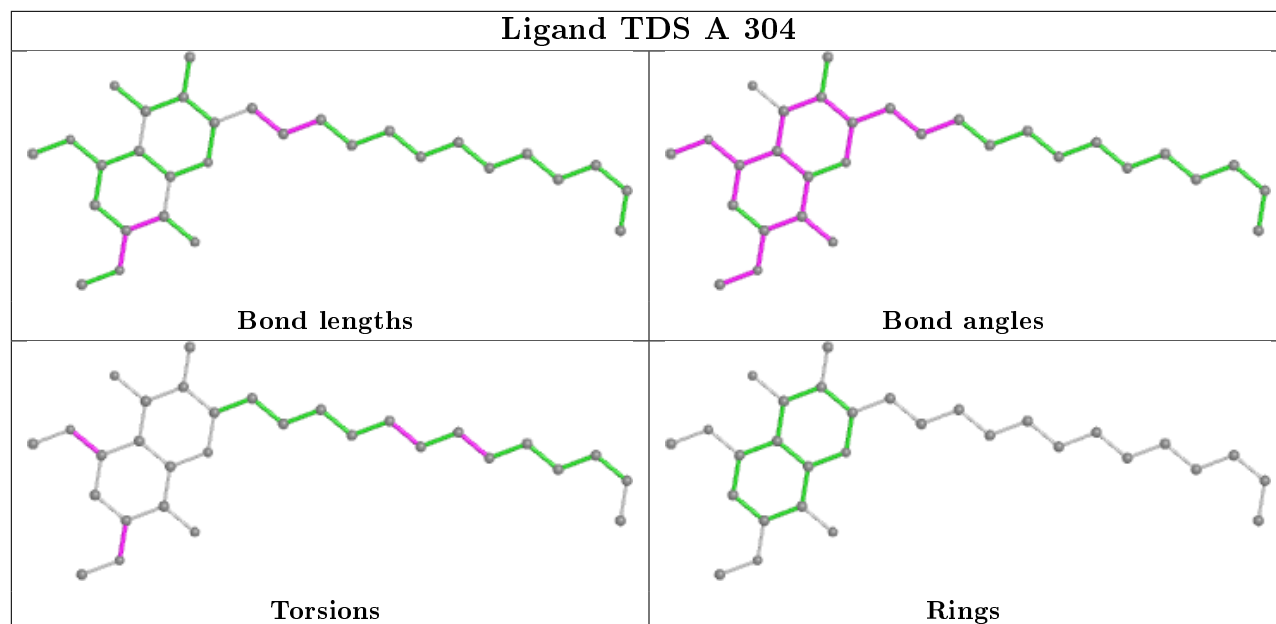
## Ligand BCR R 1101



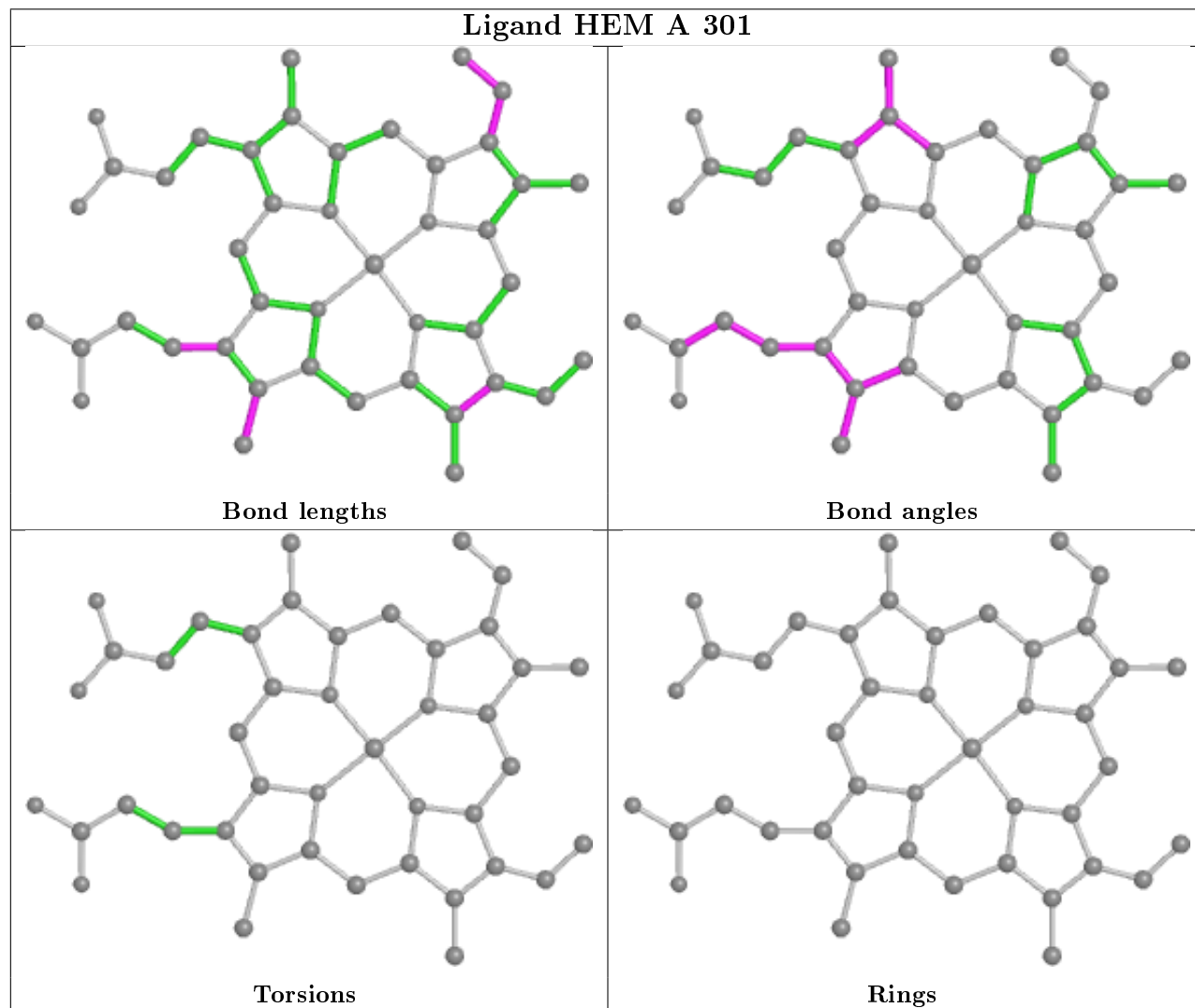


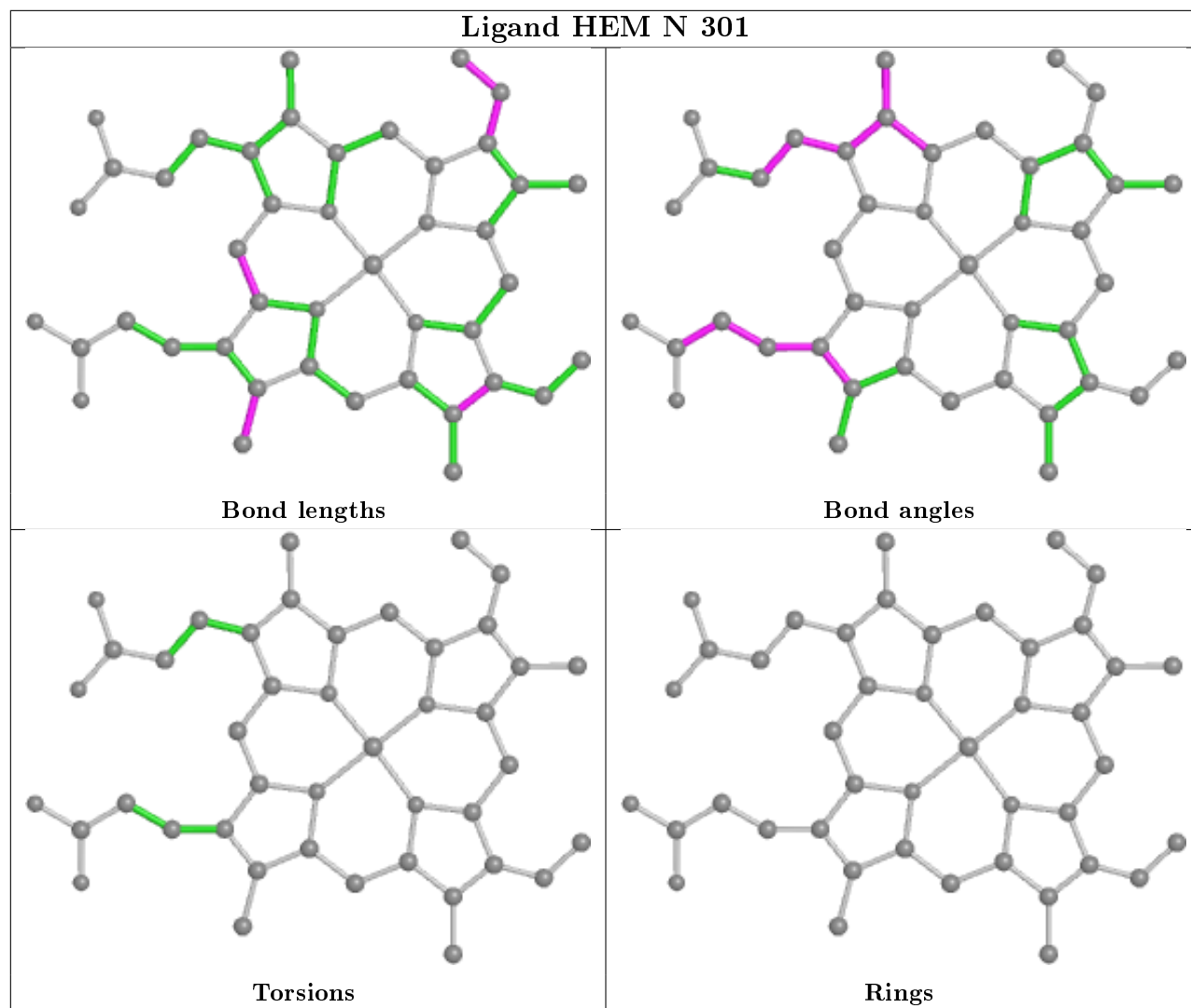


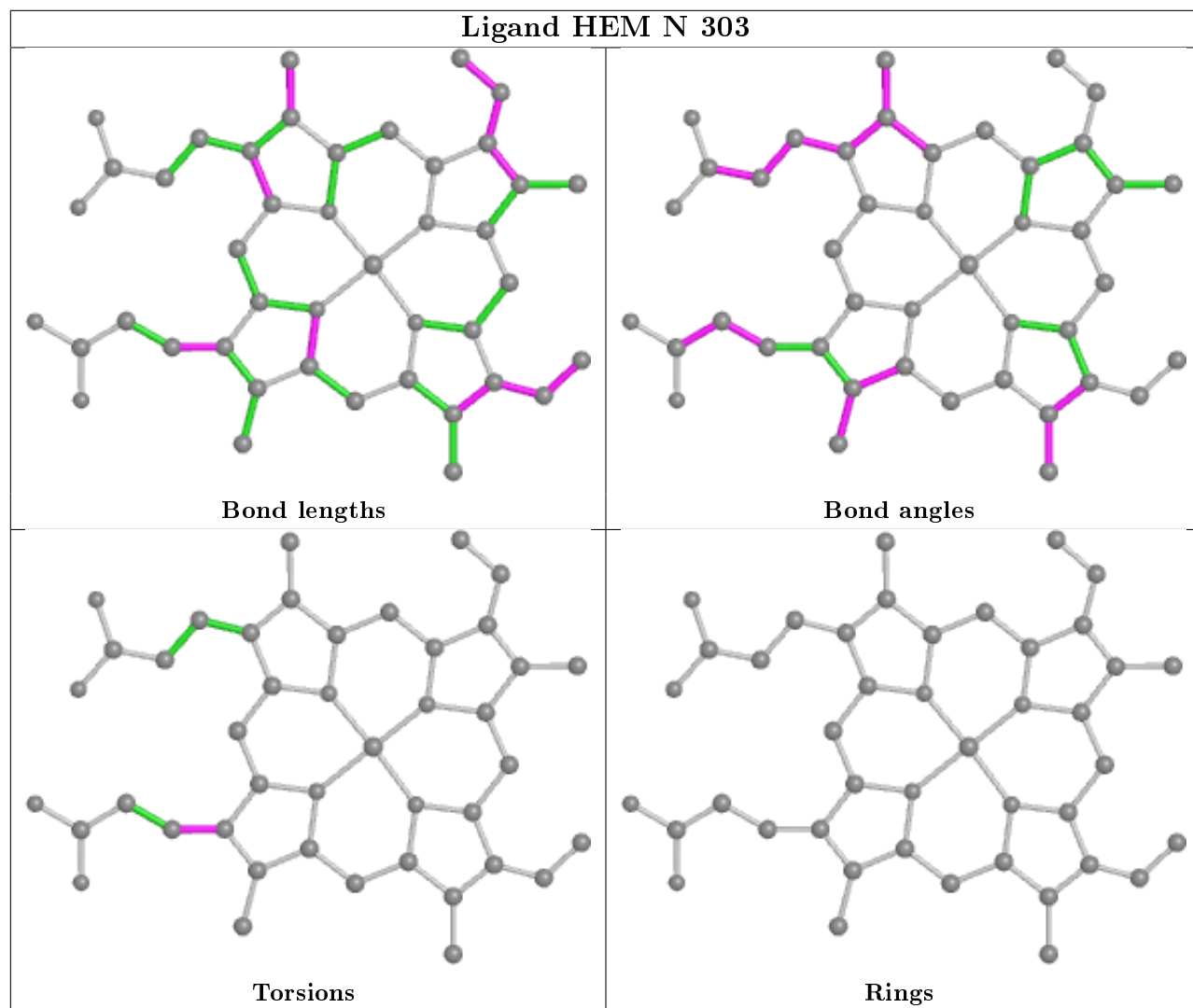
## Ligand TDS A 304



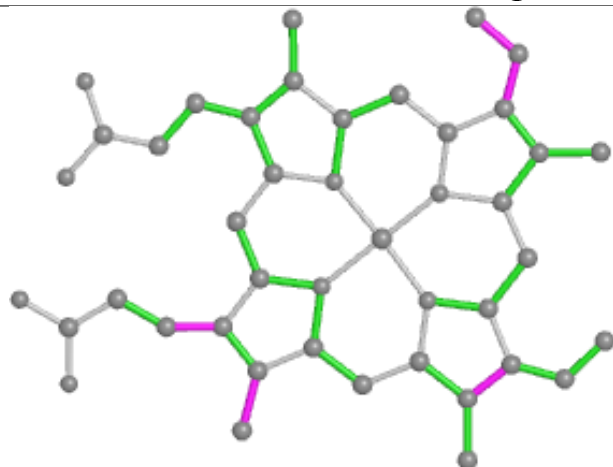
## Ligand HEM A 301



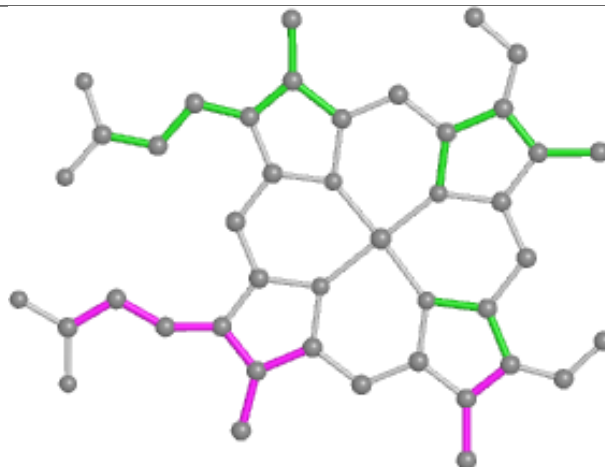




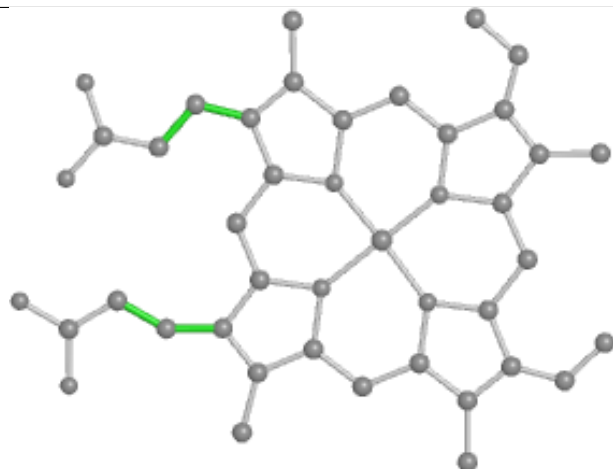
## Ligand HEM N 302



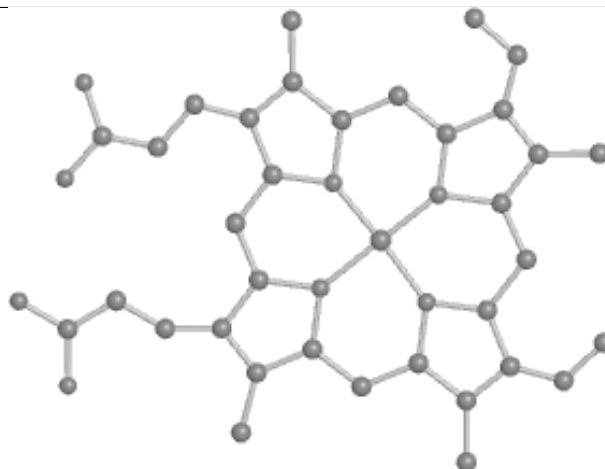
Bond lengths



Bond angles

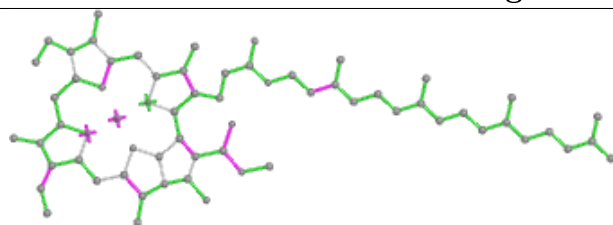


Torsions

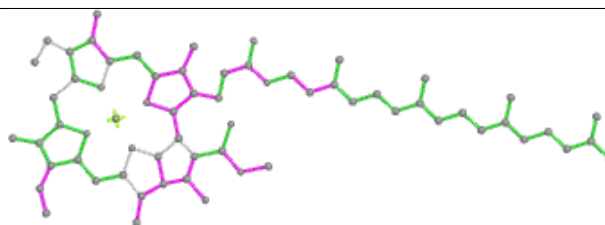


Rings

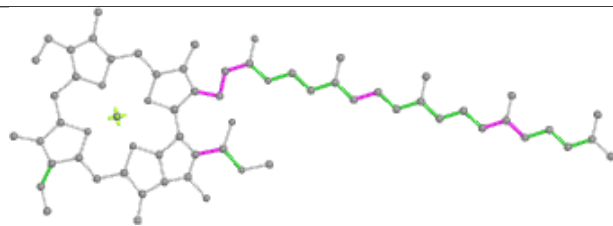
## Ligand CLA O 1201



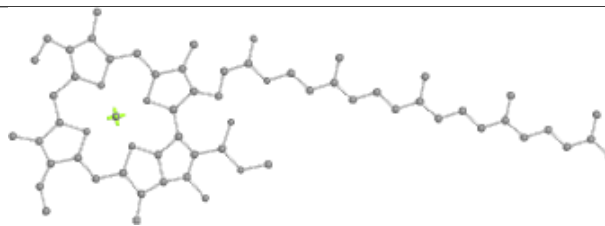
Bond lengths



Bond angles



Torsions



Rings

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	202/215 (93%)	-0.24	2 (0%) 82 59	22, 55, 101, 174	0
1	N	202/215 (93%)	-0.26	0 100 100	19, 53, 86, 121	0
2	B	138/160 (86%)	-0.26	2 (1%) 75 49	24, 65, 122, 194	0
2	O	138/160 (86%)	-0.20	3 (2%) 62 33	28, 62, 139, 184	0
3	C	286/289 (98%)	-0.16	4 (1%) 75 49	5, 82, 153, 200	1 (0%)
3	P	286/289 (98%)	-0.06	8 (2%) 53 25	14, 85, 154, 200	1 (0%)
4	D	168/179 (93%)	-0.09	7 (4%) 36 14	36, 117, 179, 200	0
4	Q	168/179 (93%)	-0.13	4 (2%) 59 30	33, 109, 165, 192	0
5	E	32/32 (100%)	0.15	2 (6%) 20 6	30, 76, 149, 177	0
5	R	32/32 (100%)	0.21	0 100 100	37, 81, 149, 171	0
6	F	33/35 (94%)	-0.13	0 100 100	39, 63, 140, 177	0
6	S	35/35 (100%)	-0.20	0 100 100	41, 78, 152, 167	0
7	G	23/37 (62%)	0.01	1 (4%) 35 13	33, 71, 128, 171	0
7	T	27/37 (72%)	-0.13	0 100 100	37, 65, 100, 152	0
8	H	27/29 (93%)	-0.19	0 100 100	33, 71, 130, 165	0
8	U	27/29 (93%)	-0.15	0 100 100	46, 81, 152, 157	0
All	All	1824/1952 (93%)	-0.15	33 (1%) 68 40	5, 74, 155, 200	2 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	117	GLY	5.5
2	B	93	ASN	5.2
3	P	71	ASN	4.5
3	P	101	VAL	4.1
3	C	73	GLY	3.6

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
4	D	91	ILE	3.4
4	D	16	ARG	3.3
4	D	81	VAL	3.2
2	B	95	LEU	3.1
3	P	191	GLY	3.0
4	D	148	LEU	3.0
5	E	32	ILE	3.0
2	O	93	ASN	2.8
4	D	80	LEU	2.7
4	Q	158	ASP	2.7
2	O	155	LEU	2.5
4	D	86	GLY	2.5
3	P	190	TYR	2.5
1	A	212	SER	2.5
3	P	176	ALA	2.5
4	Q	103	GLY	2.4
7	G	24	ALA	2.4
3	P	18	GLY	2.4
1	A	133	VAL	2.3
4	D	71	GLU	2.3
2	O	65	PRO	2.3
5	E	8	TYR	2.2
3	P	226	LYS	2.2
3	C	54	TYR	2.2
3	P	225	VAL	2.2
4	Q	150	LEU	2.1
4	Q	50	VAL	2.0
3	C	58	LEU	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<sup>th</sup> 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.

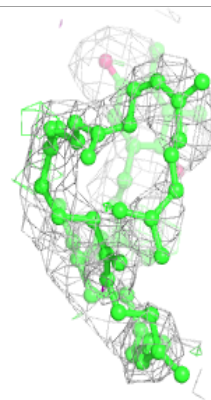
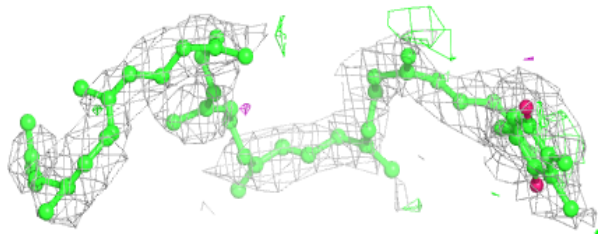
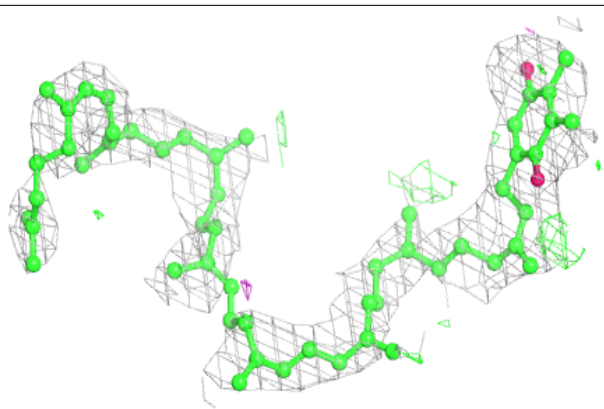
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
11	PL9	A	305	55/55	0.77	0.39	98,98,98,98	0
15	BCR	R	1101	40/40	0.83	0.55	91,91,91,91	0
12	OPC	B	307	54/55	0.84	0.23	84,84,84,84	0
11	PL9	Q	1305	55/55	0.84	0.28	85,85,85,85	0
12	OPC	N	1306	54/55	0.86	0.31	87,87,87,87	0
10	TDS	N	1304	30/30	0.87	0.44	80,80,80,80	0
15	BCR	E	101	40/40	0.88	0.47	77,77,77,77	0
12	OPC	D	306	54/55	0.88	0.28	86,86,86,86	0
12	OPC	Q	1307	54/55	0.91	0.20	72,72,72,72	0
10	TDS	A	304	30/30	0.91	0.33	52,52,52,52	0
14	FES	D	200	4/4	0.93	0.10	144,144,170,170	0
13	CLA	O	1201	65/65	0.93	0.26	22,72,72,72	0
13	CLA	B	201	65/65	0.94	0.27	45,56,56,56	0
9	HEM	A	302	43/43	0.96	0.28	62,62,62,62	0
9	HEM	C	301	43/43	0.97	0.25	62,83,83,83	0
9	HEM	P	301	43/43	0.97	0.23	47,56,56,56	0
9	HEM	A	301	43/43	0.97	0.27	45,45,45,45	0
9	HEM	N	301	43/43	0.97	0.27	41,50,50,50	0
9	HEM	N	303	43/43	0.97	0.21	61,61,61,64	0
9	HEM	N	302	43/43	0.97	0.26	48,56,56,56	0
9	HEM	A	303	43/43	0.97	0.24	55,81,81,81	0
14	FES	Q	1200	4/4	0.98	0.14	94,94,98,98	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.

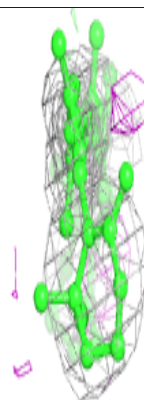
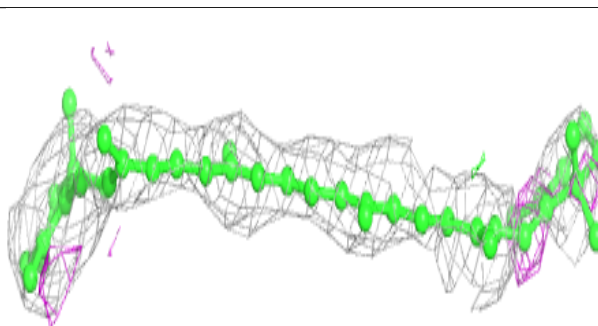
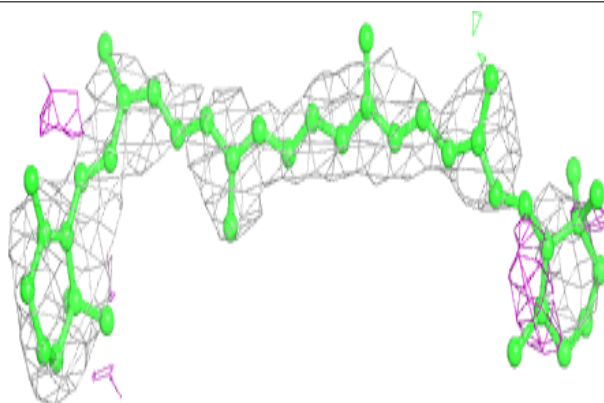


**Electron density around PL9 A 305:**

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

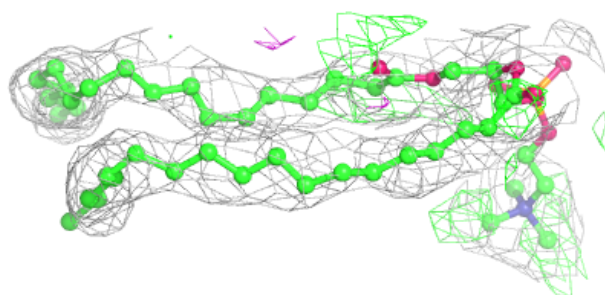
**Electron density around BCR R 1101:**

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

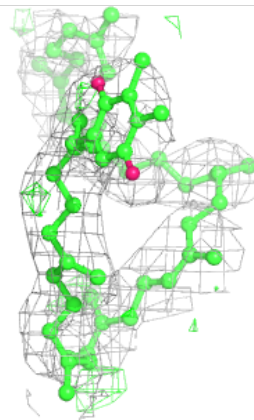
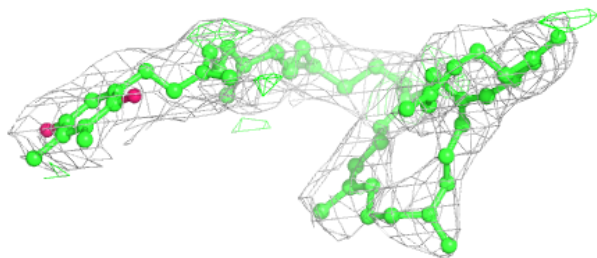
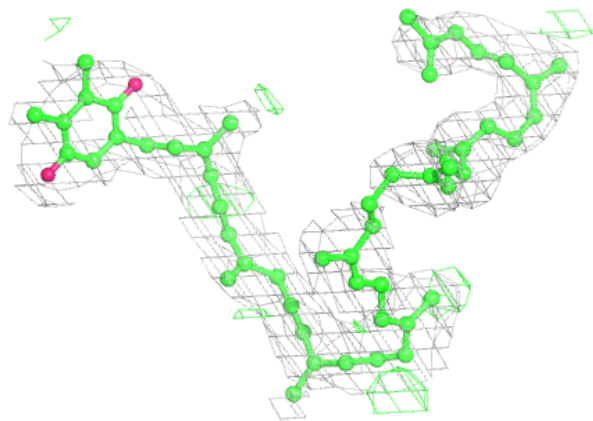


**Electron density around OPC B 307:**

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

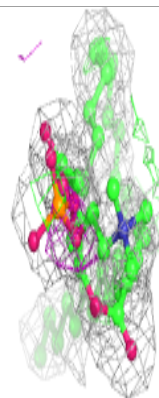
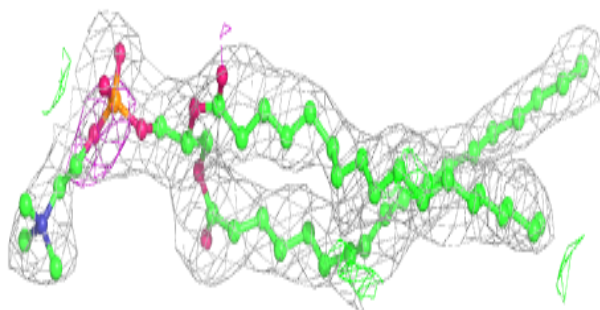
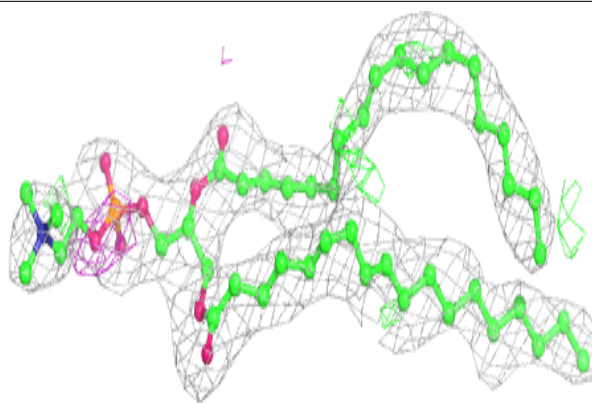
**Electron density around PL9 Q 1305:**

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

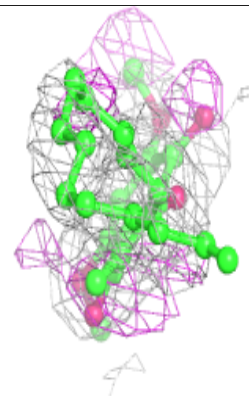
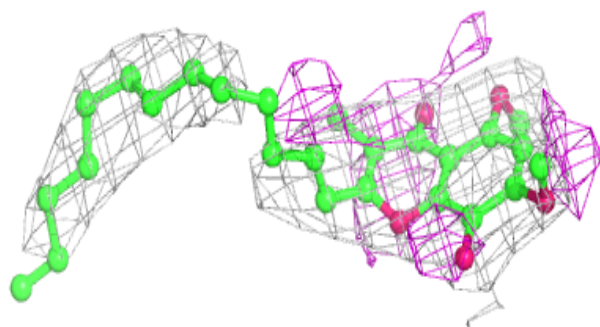
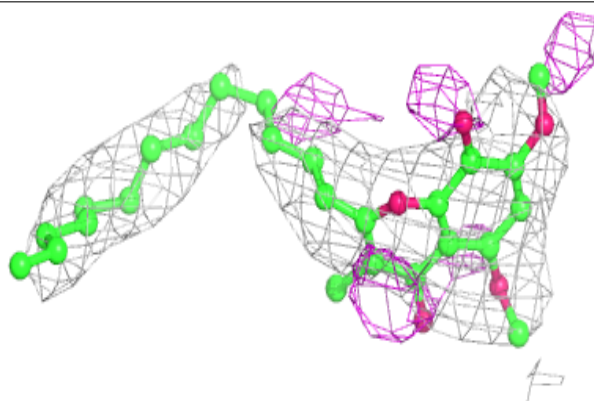


**Electron density around OPC N 1306:**

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and green (positive)

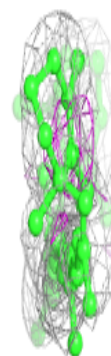
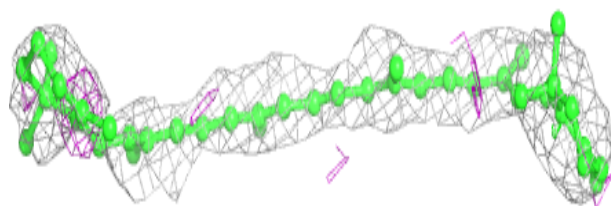
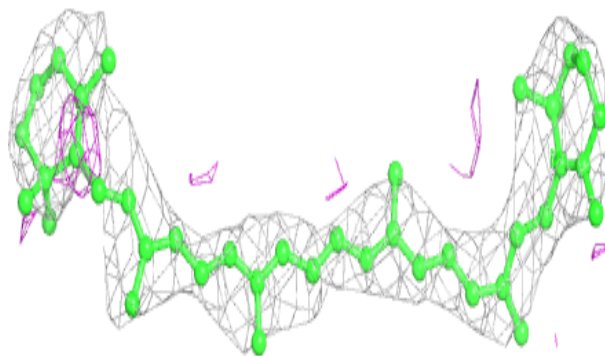
**Electron density around TDS N 1304:**

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and green (positive)

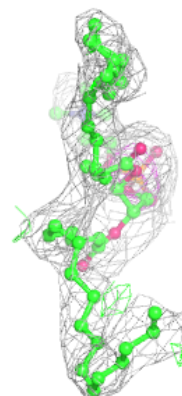
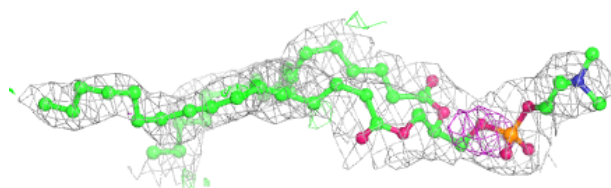
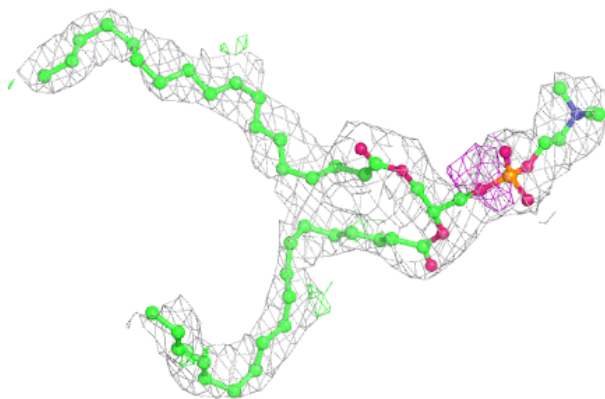


**Electron density around BCR E 101:**

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

**Electron density around OPC D 306:**

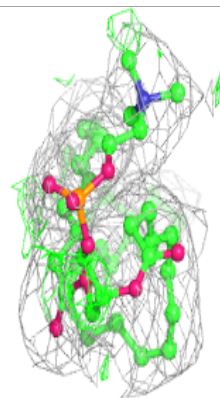
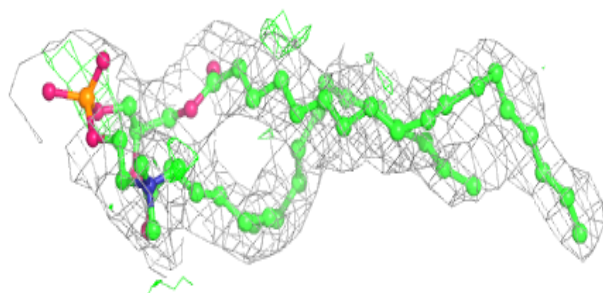
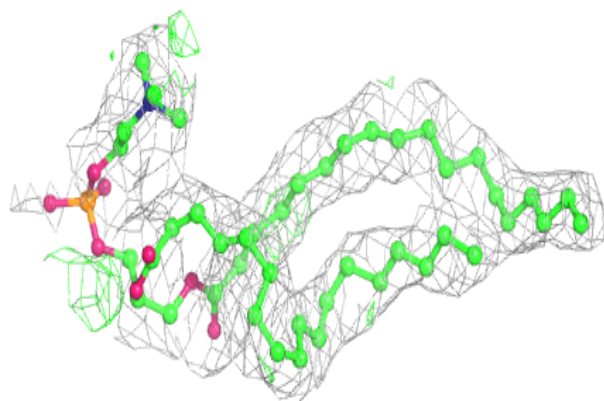
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
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and green (positive)



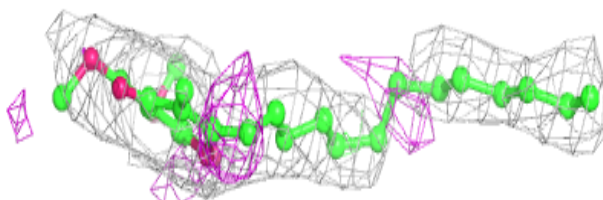
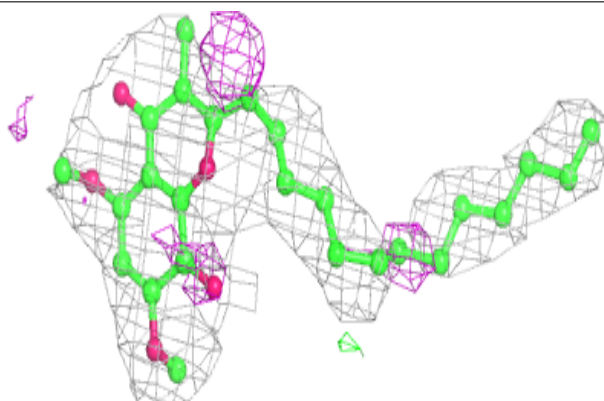


**Electron density around OPC Q 1307:**

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and green (positive)

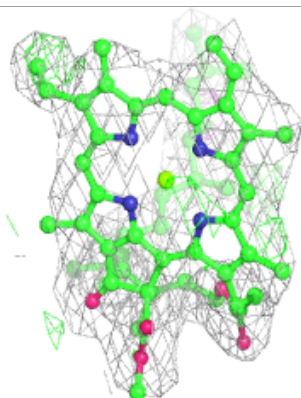
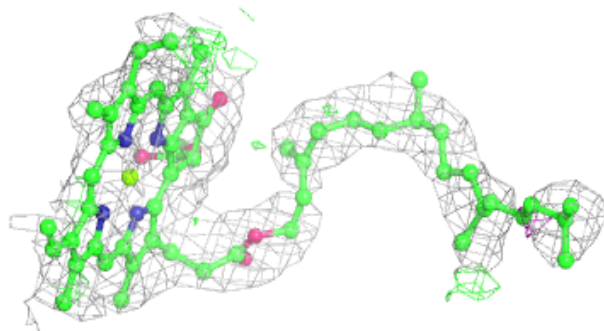
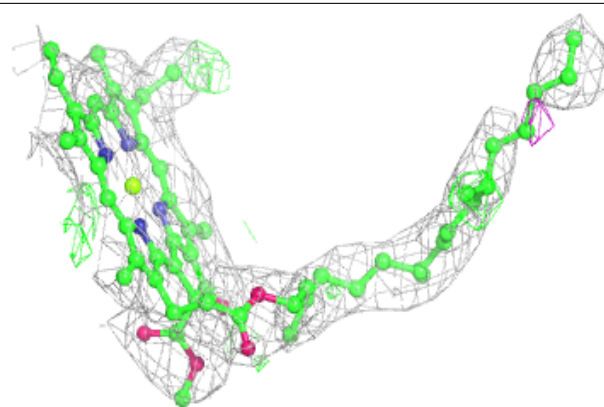
**Electron density around TDS A 304:**

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

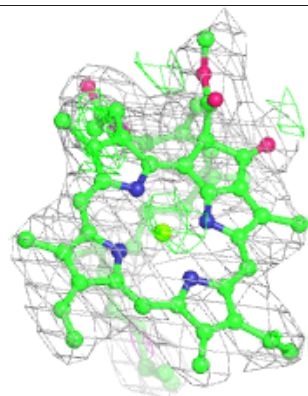
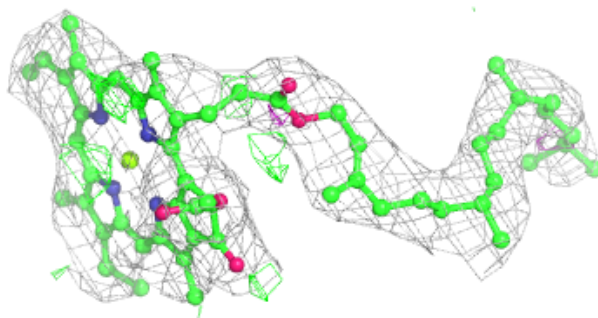
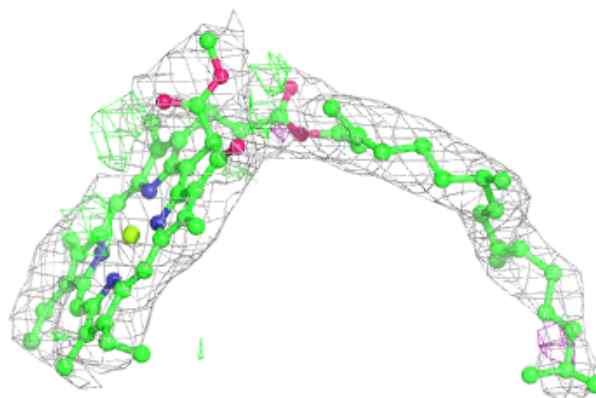


**Electron density around CLA O 1201:**

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and green (positive)

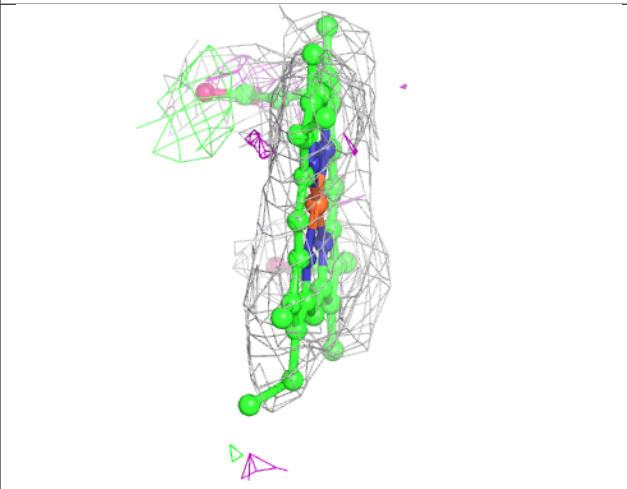
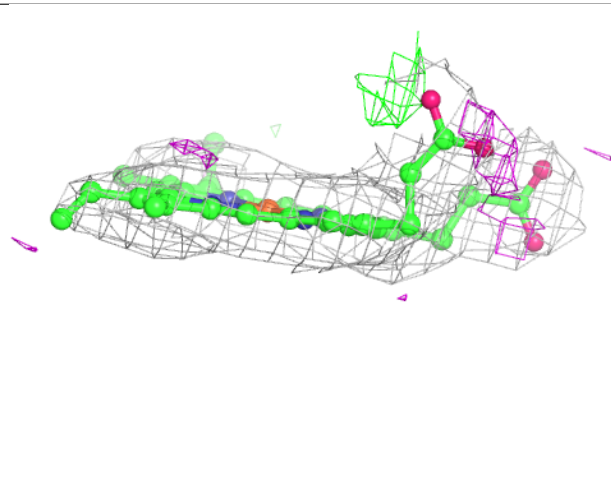
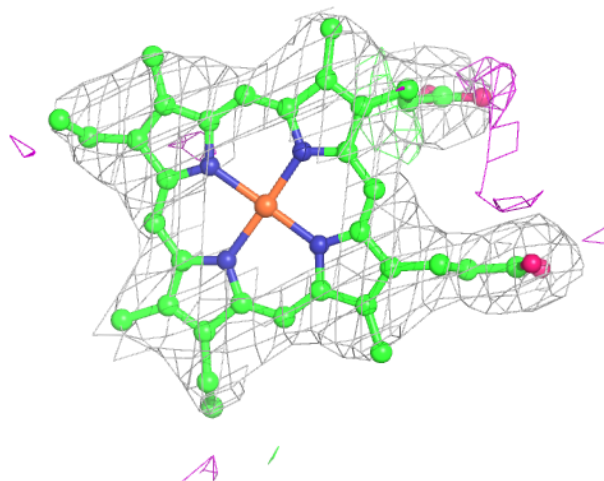
**Electron density around CLA B 201:**

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and green (positive)



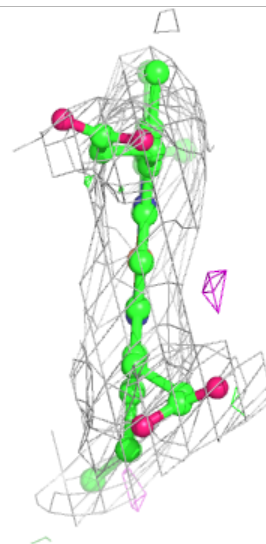
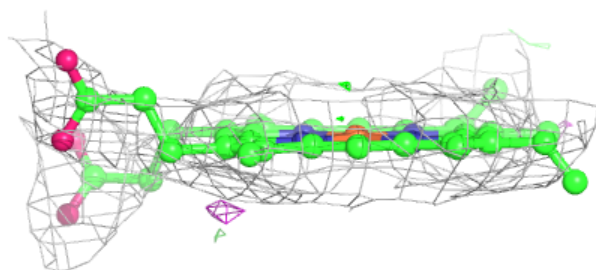
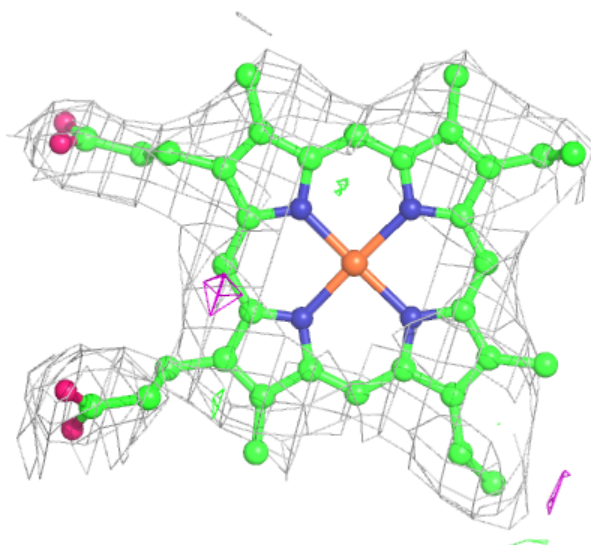
**Electron density around HEM A 302:**

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



**Electron density around HEM C 301:**

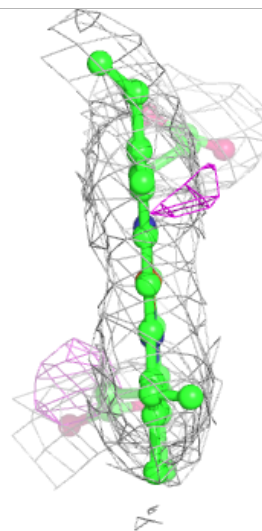
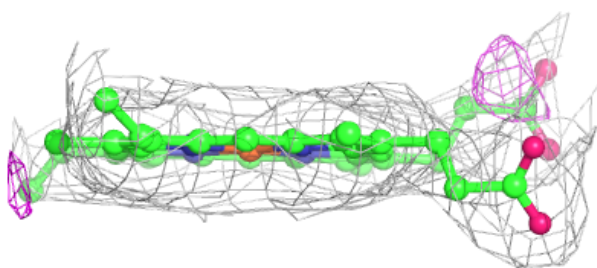
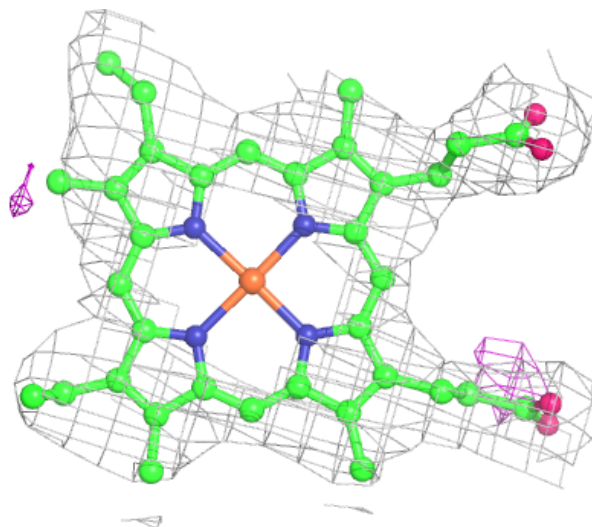
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





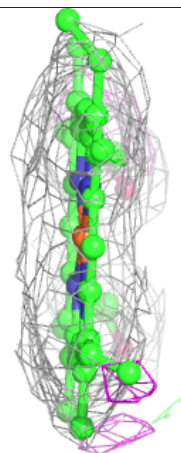
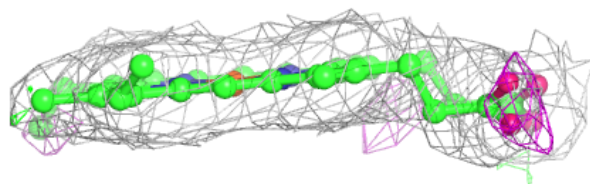
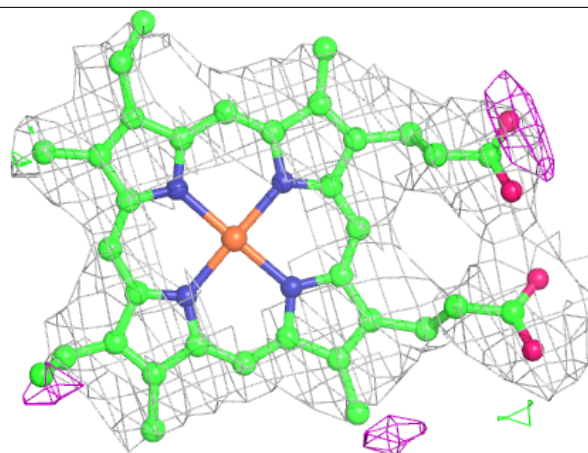
**Electron density around HEM P 301:**

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



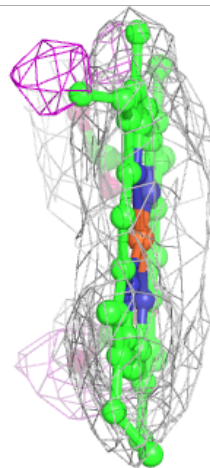
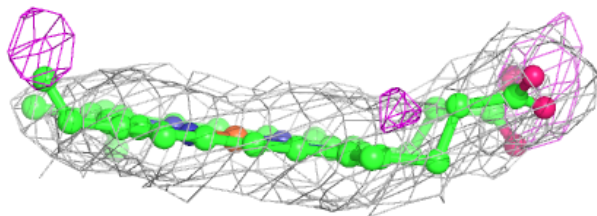
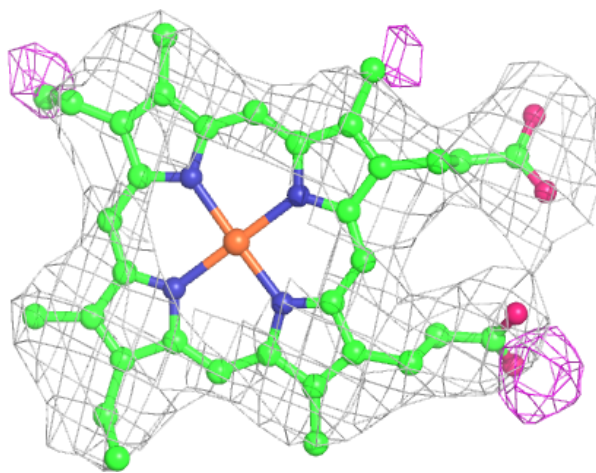
**Electron density around HEM A 301:**

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



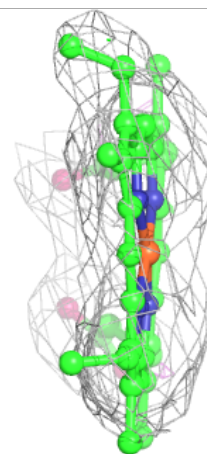
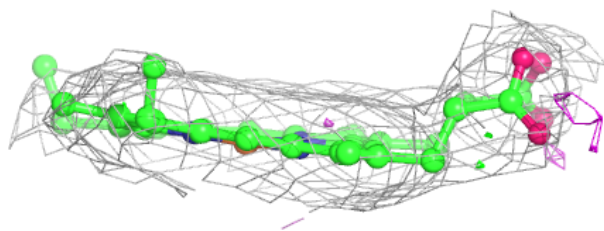
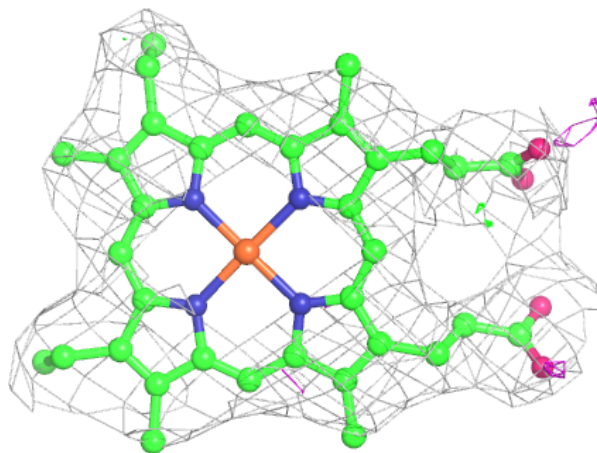
**Electron density around HEM N 301:**

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



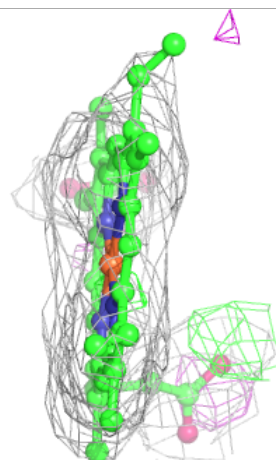
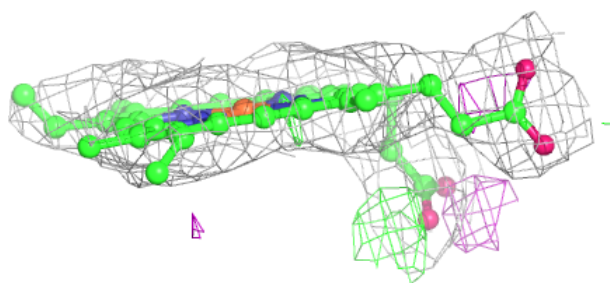
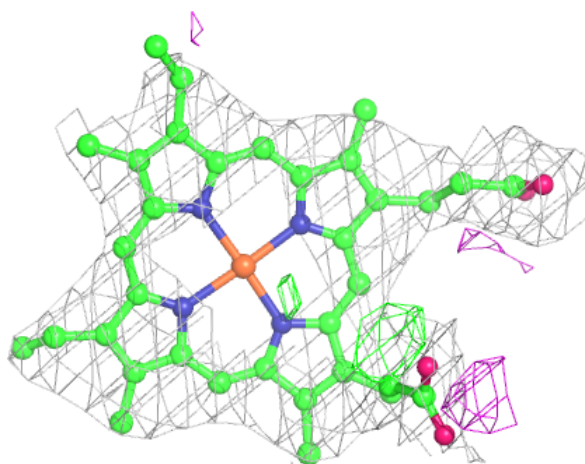
**Electron density around HEM N 303:**

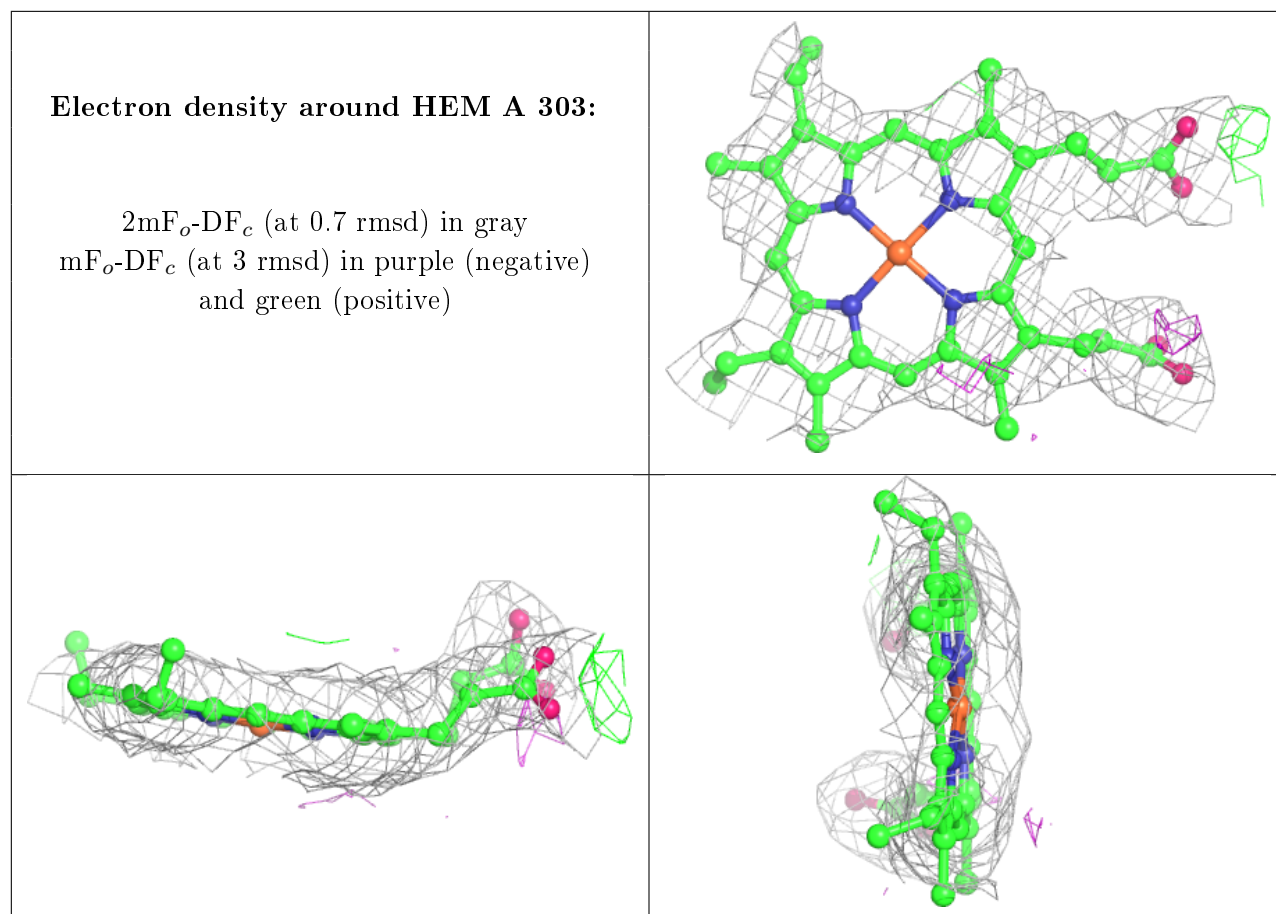
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around HEM 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 ⓘ

There are no such residues in this entry.