Full wwPDB X-ray Structure Validation Report (i)

Jun 21, 2021 – 10:02 PM EDT

PDB ID	:	1M56
Title	:	Structure of cytochrome c oxidase from Rhodobactor sphaeroides (Wild Type)
Authors	:	Svensson-Ek, M.; Abramson, J.; Larsson, G.; Tornroth, S.; Brezezinski, P.; Iwata, S.
Deposited on	:	2002-07-08
Resolution	:	2.30 Å(reported)

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

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

The following versions of software and data (see references (1)) were used in the production of this report:

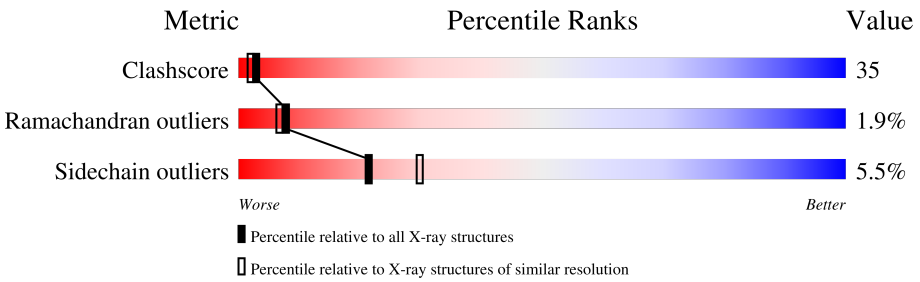
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.20

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 2.30 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	566	41% 43% 11% • •
1	G	566	38% 45% 11% • •
2	B	264	44% 45% 8% • •
2	H	264	45% 44% 8% • •
3	C	266	48% 44% 6% •
3	I	266	44% 49% 6% •
4	D	51	49% 27% • • 18%
4	J	51	39% 33% 8% • 18%

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
8	HEA	A	1001	X	-	-	-
8	HEA	A	1002	X	-	-	-
8	HEA	G	1001	X	-	-	-
8	HEA	G	1002	X	-	-	-
9	3PE	C	2013	-	-	X	-
9	3PE	D	2011	-	-	X	-
9	3PE	I	3010	-	-	X	-
9	3PE	I	3013	-	-	X	-

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 18934 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 C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	547	4322	2892	684	715	31	0	0	0
1	G	547	4322	2892	684	715	31	0	0	0

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	436	ILE	SER	SEE REMARK 999	UNP P33517
A	437	TYR	THR	SEE REMARK 999	UNP P33517
A	438	PHE	SER	SEE REMARK 999	UNP P33517
A	439	TRP	GLY	SEE REMARK 999	UNP P33517
A	518	THR	SER	SEE REMARK 999	UNP P33517
A	520	THR	SER	SEE REMARK 999	UNP P33517
A	521	ARG	-	SEE REMARK 999	UNP P33517
G	436	ILE	SER	SEE REMARK 999	UNP P33517
G	437	TYR	THR	SEE REMARK 999	UNP P33517
G	438	PHE	SER	SEE REMARK 999	UNP P33517
G	439	TRP	GLY	SEE REMARK 999	UNP P33517
G	518	THR	SER	SEE REMARK 999	UNP P33517
G	520	THR	SER	SEE REMARK 999	UNP P33517
G	521	ARG	-	SEE REMARK 999	UNP P33517

- Molecule 2 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	B	260	2046	1334	332	374	6	0	0	0
2	H	260	2046	1334	332	374	6	0	0	0

- Molecule 3 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
3	C	265	2139	1448	342	337	12	0	0	0
3	I	265	2139	1448	342	337	12	0	0	0

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	30	PHE	ASN	SEE REMARK 999	UNP P84153
C	92	MET	ILE	SEE REMARK 999	UNP P84153
C	244	ILE	MET	SEE REMARK 999	UNP P84153
I	30	PHE	ASN	SEE REMARK 999	UNP P84153
I	92	MET	ILE	SEE REMARK 999	UNP P84153
I	244	ILE	MET	SEE REMARK 999	UNP P84153

- Molecule 4 is a protein called CYTOCHROME C OXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
4	D	42	311	203	52	54	2	0	0	0
4	J	42	311	203	52	54	2	0	0	0

- Molecule 5 is COPPER (II) ION (three-letter code: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cu		
5	A	1	1	1	0	0
5	B	2	2	2	0	0
5	G	1	1	1	0	0
5	H	2	2	2	0	0

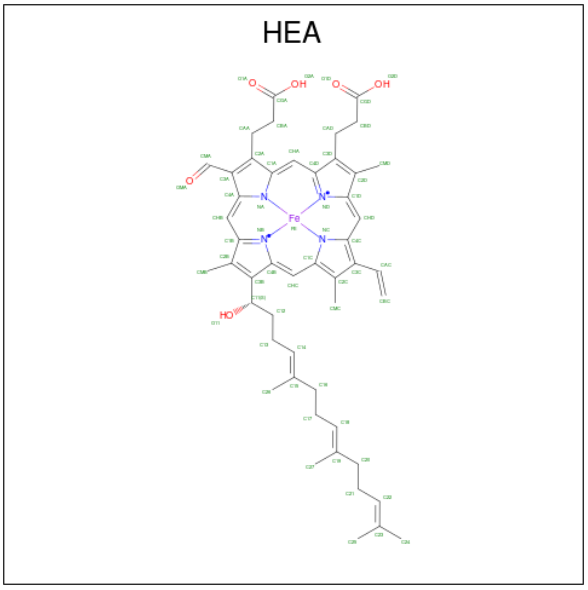
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Mg		
6	A	1	1	1	0	0
6	G	1	1	1	0	0

- Molecule 7 is CALCIUM ION (three-letter code: CA) (formula: Ca).

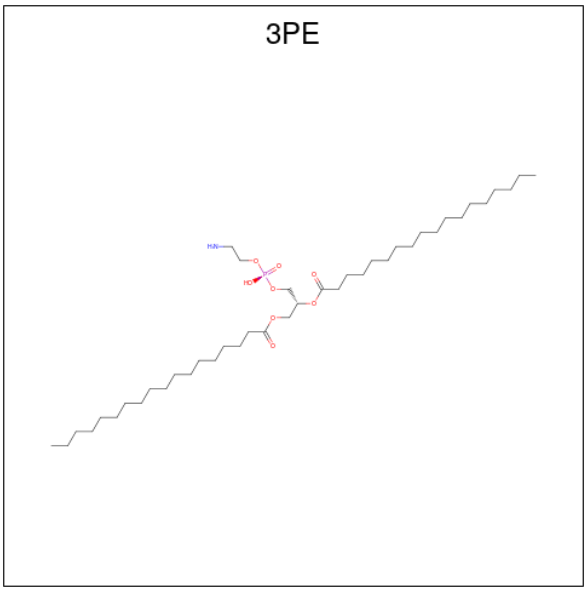
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Ca		
7	A	1	1	1	0	0
7	G	1	1	1	0	0

- Molecule 8 is HEME-A (three-letter code: HEA) (formula: $C_{49}H_{56}FeN_4O_6$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	Fe	N	O		
8	A	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
8	A	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
8	G	1	60	49	1	4	6	0	0
			Total	C	Fe	N	O		
8	G	1	60	49	1	4	6	0	0

- Molecule 9 is 1,2-Distearoyl-sn-glycerophosphoethanolamine (three-letter code: 3PE) (formula: $C_{41}H_{82}NO_8P$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
9	A	1	51	41	1	8	1	0	0
9	A	1	51	41	1	8	1	0	0
9	C	1	51	41	1	8	1	0	0
9	C	1	51	41	1	8	1	0	0
9	C	1	51	41	1	8	1	0	0
9	D	1	51	41	1	8	1	0	0
9	G	1	51	41	1	8	1	0	0
9	G	1	51	41	1	8	1	0	0
9	I	1	51	41	1	8	1	0	0
9	I	1	51	41	1	8	1	0	0
9	I	1	51	41	1	8	1	0	0
9	J	1	51	41	1	8	1	0	0

- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
10	A	101	101	101	0	0
			Total	O		
10	B	68	68	68	0	0
			Total	O		
10	C	39	39	39	0	0
			Total	O		
10	D	12	12	12	0	0
			Total	O		
10	G	106	106	106	0	0
			Total	O		
10	H	64	64	64	0	0
			Total	O		
10	I	38	38	38	0	0
			Total	O		
10	J	8	8	8	0	0

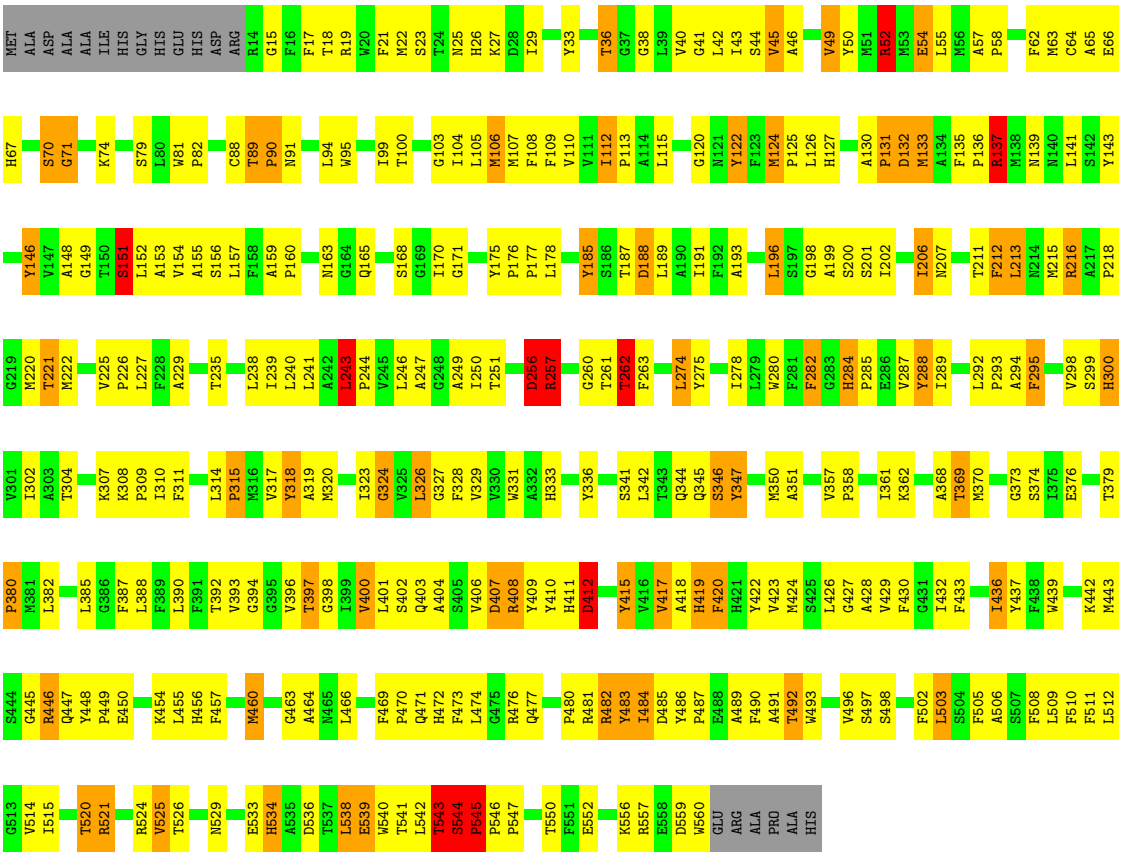
3 Residue-property plots (i)

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

Note EDS was not executed.

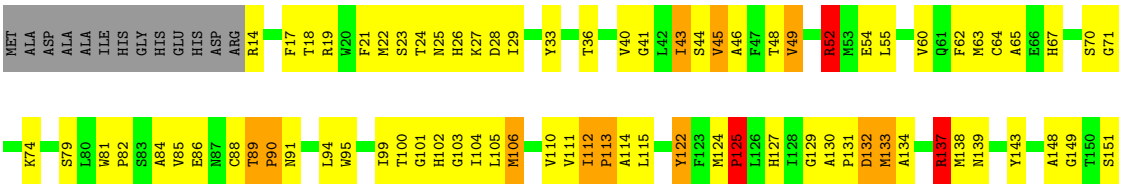
• Molecule 1: CYTOCHROME C OXIDASE

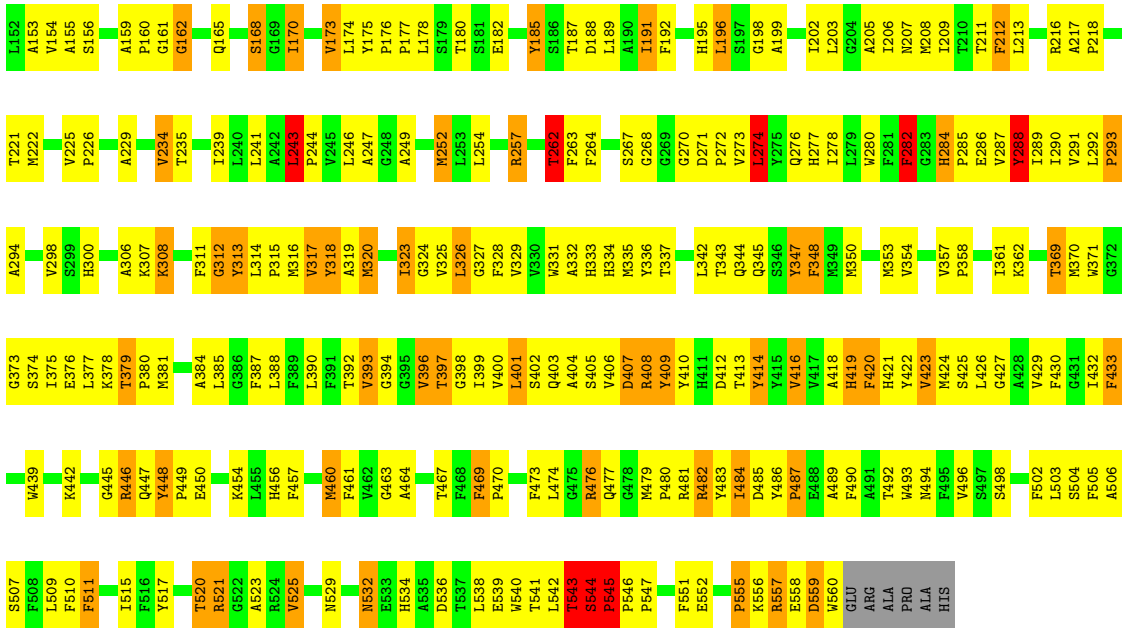
Chain A: 41% 43% 11%



• Molecule 1: CYTOCHROME C OXIDASE

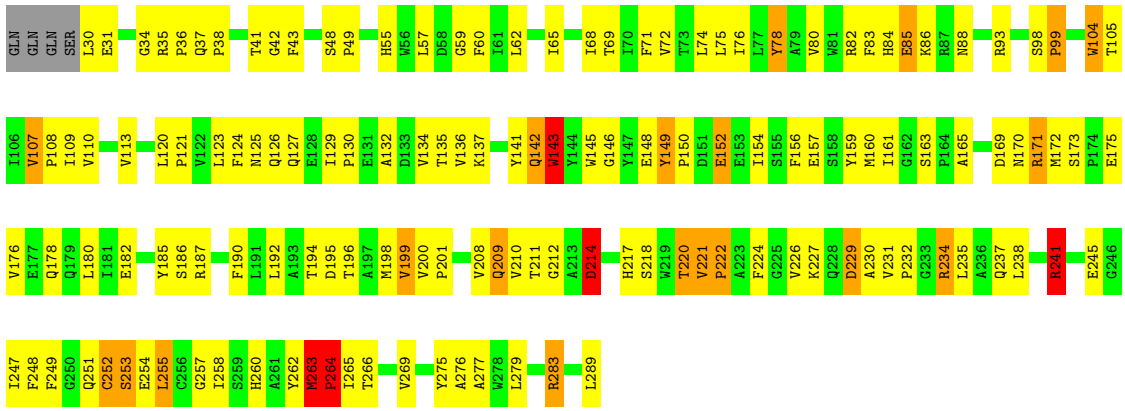
Chain G: 38% 45% 11%





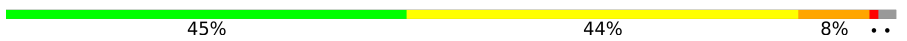
- Molecule 2: CYTOCHROME C OXIDASE

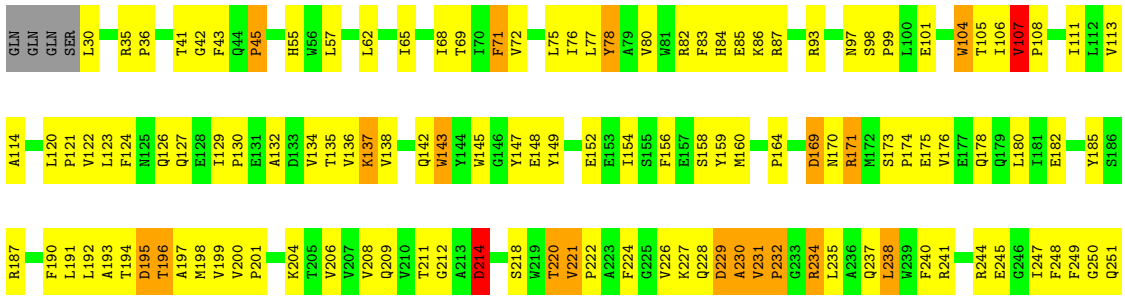
Chain B:



- Molecule 2: CYTOCHROME C OXIDASE

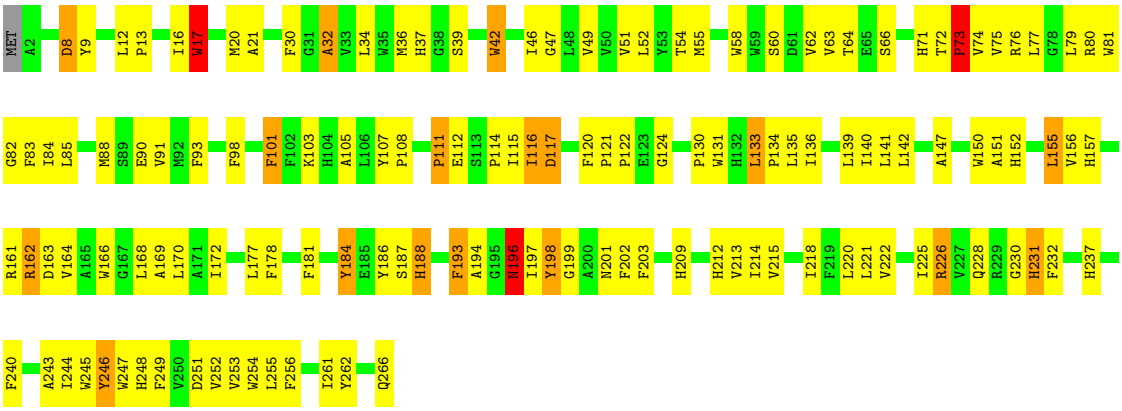
Chain H:





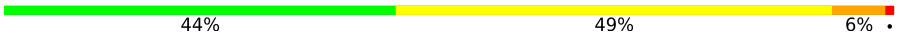
• Molecule 3: CYTOCHROME C OXIDASE

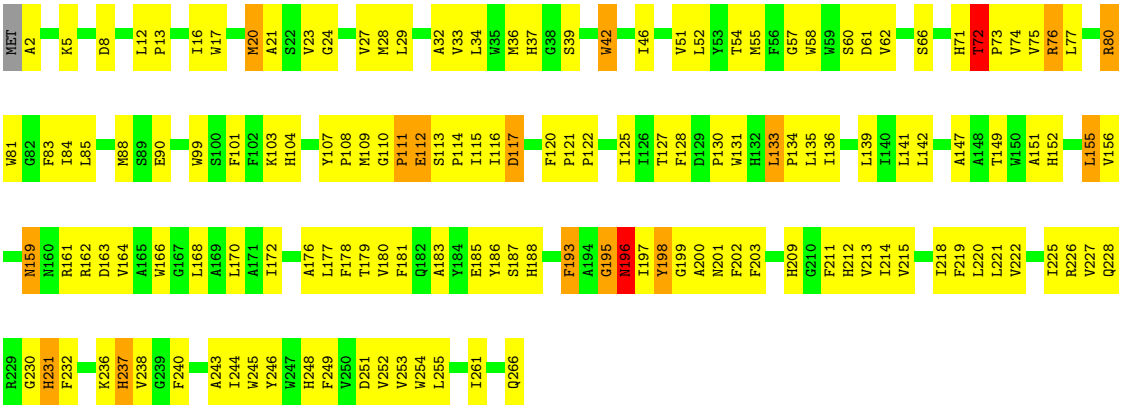
Chain C:



• Molecule 3: CYTOCHROME C OXIDASE

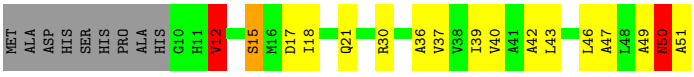
Chain I:





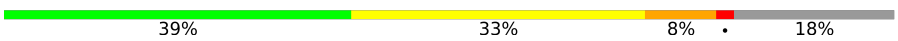
• Molecule 4: CYTOCHROME C OXIDASE

Chain D:



• Molecule 4: CYTOCHROME C OXIDASE

Chain J:



4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α, β, γ	340.36Å 340.36Å 89.67Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	40.00 – 2.30	Depositor
% Data completeness (in resolution range)	(Not available) (40.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC	Depositor
R, R_{free}	0.236 , 0.275	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	18934	wwPDB-VP
Average B, all atoms ($Å^2$)	29.0	wwPDB-VP

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: MG, CU, CA, HEA, 3PE

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	0.70	2/4482 (0.0%)	1.91	106/6114 (1.7%)
1	G	0.71	1/4482 (0.0%)	1.86	97/6114 (1.6%)
2	B	0.57	0/2105	1.73	38/2879 (1.3%)
2	H	0.58	0/2105	1.67	36/2879 (1.3%)
3	C	0.53	0/2232	1.43	22/3054 (0.7%)
3	I	0.55	0/2232	1.49	22/3054 (0.7%)
4	D	0.52	0/316	1.66	6/428 (1.4%)
4	J	0.53	0/316	1.61	6/428 (1.4%)
All	All	0.63	3/18270 (0.0%)	1.74	333/24950 (1.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	12
1	G	0	15
2	B	0	6
2	H	0	5
3	C	0	3
3	I	0	2
4	D	0	1
All	All	0	44

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	543	THR	C-O	5.96	1.34	1.23
1	G	544	SER	N-CA	-5.23	1.35	1.46
1	A	544	SER	N-CA	-5.20	1.35	1.46

All (333) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	543	THR	C-N-CA	21.14	174.56	121.70
1	A	257	ARG	NE-CZ-NH1	-20.04	110.28	120.30
2	B	171	ARG	NE-CZ-NH1	16.88	128.74	120.30
1	A	521	ARG	NE-CZ-NH2	-16.71	111.94	120.30
2	B	234	ARG	NE-CZ-NH2	-16.71	111.95	120.30
2	H	171	ARG	NE-CZ-NH1	15.23	127.92	120.30
1	A	543	THR	C-N-CA	14.88	158.89	121.70
1	G	257	ARG	NE-CZ-NH1	-14.32	113.14	120.30
1	G	485	ASP	CB-CG-OD1	14.01	130.91	118.30
1	G	288	TYR	CZ-CE2-CD2	13.67	132.10	119.80
1	A	544	SER	N-CA-CB	13.30	130.45	110.50
1	A	288	TYR	CZ-CE2-CD2	13.22	131.70	119.80
1	A	545	PRO	N-CA-CB	12.87	118.74	103.30
1	A	216	ARG	NE-CZ-NH2	-12.86	113.87	120.30
1	A	19	ARG	NE-CZ-NH2	-12.40	114.10	120.30
1	A	137	ARG	NE-CZ-NH2	12.35	126.48	120.30
1	G	446	ARG	NE-CZ-NH2	12.22	126.41	120.30
1	G	545	PRO	N-CA-CB	11.72	117.36	103.30
1	G	216	ARG	NE-CZ-NH2	-11.71	114.44	120.30
1	A	376	GLU	OE1-CD-OE2	-11.33	109.70	123.30
1	A	536	ASP	CB-CG-OD2	11.29	128.46	118.30
2	B	171	ARG	NE-CZ-NH2	-11.09	114.76	120.30
1	A	52	ARG	NE-CZ-NH2	-11.00	114.80	120.30
1	A	544	SER	CA-C-O	-10.98	97.05	120.10
2	B	82	ARG	CD-NE-CZ	10.72	138.61	123.60
2	B	143	TRP	CB-CA-C	10.65	131.70	110.40
1	G	137	ARG	NE-CZ-NH1	-10.64	114.98	120.30
1	A	175	TYR	CA-CB-CG	10.56	133.47	113.40
1	G	333	HIS	CA-CB-CG	10.46	131.38	113.60
4	D	30	ARG	NE-CZ-NH2	-10.36	115.12	120.30
1	A	446	ARG	NE-CZ-NH1	-10.34	115.13	120.30
2	H	234	ARG	NE-CZ-NH2	-10.31	115.14	120.30
1	A	485	ASP	CB-CG-OD1	10.17	127.45	118.30
1	A	54	GLU	OE1-CD-OE2	-10.15	111.12	123.30
2	B	283	ARG	NE-CZ-NH1	9.91	125.25	120.30
2	B	93	ARG	NE-CZ-NH1	9.81	125.21	120.30
2	H	171	ARG	CD-NE-CZ	9.73	137.22	123.60
2	H	107	VAL	CA-CB-CG1	9.71	125.46	110.90
1	G	288	TYR	CG-CD2-CE2	-9.70	113.54	121.30
1	G	482	ARG	CD-NE-CZ	9.62	137.07	123.60
1	A	318	TYR	CB-CG-CD2	9.58	126.75	121.00
1	G	376	GLU	OE1-CD-OE2	-9.58	111.81	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	283	ARG	NE-CZ-NH1	9.51	125.06	120.30
1	A	545	PRO	CA-N-CD	-9.47	98.25	111.50
3	I	61	ASP	CB-CG-OD1	9.43	126.79	118.30
1	G	132	ASP	CB-CG-OD1	9.37	126.73	118.30
1	G	476	ARG	NE-CZ-NH2	-9.29	115.66	120.30
1	G	545	PRO	CA-N-CD	-9.12	98.73	111.50
1	G	482	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	A	216	ARG	CD-NE-CZ	9.11	136.35	123.60
3	I	90	GLU	OE1-CD-OE2	8.98	134.08	123.30
2	B	171	ARG	CD-NE-CZ	8.96	136.14	123.60
2	H	283	ARG	CD-NE-CZ	8.86	136.01	123.60
2	H	143	TRP	CB-CA-C	8.76	127.93	110.40
2	B	104	TRP	CA-CB-CG	8.76	130.35	113.70
2	B	195	ASP	CB-CG-OD1	8.74	126.16	118.30
1	A	284	HIS	CA-CB-CG	-8.73	98.75	113.60
3	I	251	ASP	CB-CG-OD1	8.73	126.16	118.30
1	G	284	HIS	CA-CB-CG	-8.63	98.93	113.60
1	A	52	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	G	19	ARG	NE-CZ-NH1	-8.56	116.02	120.30
1	G	544	SER	CA-C-O	-8.53	102.19	120.10
1	A	318	TYR	CB-CG-CD1	-8.43	115.94	121.00
2	B	149	TYR	CB-CG-CD1	8.40	126.04	121.00
2	B	82	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	A	132	ASP	CB-CG-OD2	-8.32	110.81	118.30
1	G	485	ASP	CB-CG-OD2	-8.26	110.87	118.30
1	A	420	PHE	CA-CB-CG	8.24	133.67	113.90
1	G	52	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	A	412	ASP	CB-CG-OD2	8.18	125.66	118.30
1	G	313	TYR	CB-CG-CD1	8.13	125.88	121.00
2	B	283	ARG	CD-NE-CZ	8.13	134.98	123.60
1	A	369	THR	CA-CB-CG2	8.11	123.75	112.40
1	A	188	ASP	CB-CG-OD2	8.10	125.59	118.30
4	J	30	ARG	NE-CZ-NH1	-8.00	116.30	120.30
3	C	17	TRP	CB-CA-C	8.00	126.39	110.40
1	G	420	PHE	CA-CB-CG	7.96	133.01	113.90
1	A	36	THR	CA-CB-CG2	-7.96	101.26	112.40
1	A	482	ARG	CD-NE-CZ	7.94	134.72	123.60
2	B	143	TRP	O-C-N	-7.87	110.10	122.70
1	A	288	TYR	CG-CD2-CE2	-7.83	115.04	121.30
1	G	175	TYR	CB-CG-CD1	7.78	125.67	121.00
3	I	80	ARG	NE-CZ-NH2	-7.62	116.49	120.30
4	D	12	VAL	CG1-CB-CG2	-7.59	98.76	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	261	ALA	O-C-N	-7.57	110.58	122.70
2	B	107	VAL	CA-CB-CG1	7.54	122.20	110.90
4	D	30	ARG	NH1-CZ-NH2	7.52	127.67	119.40
1	G	482	ARG	NE-CZ-NH2	-7.49	116.55	120.30
3	I	198	TYR	CB-CG-CD1	-7.48	116.51	121.00
1	G	175	TYR	CA-CB-CG	7.45	127.55	113.40
1	G	318	TYR	CB-CG-CD1	-7.42	116.55	121.00
1	A	534	HIS	CA-CB-CG	-7.42	100.98	113.60
3	C	90	GLU	OE1-CD-OE2	7.38	132.15	123.30
2	H	234	ARG	NH1-CZ-NH2	7.36	127.49	119.40
1	A	521	ARG	NH1-CZ-NH2	7.35	127.49	119.40
2	H	107	VAL	CB-CA-C	7.34	125.35	111.40
1	G	521	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	G	52	ARG	NE-CZ-NH1	7.30	123.95	120.30
3	C	198	TYR	CB-CG-CD2	7.29	125.37	121.00
2	H	87	ARG	NE-CZ-NH2	-7.27	116.66	120.30
3	I	76	ARG	NE-CZ-NH1	-7.26	116.67	120.30
1	A	146	TYR	CB-CG-CD1	-7.25	116.65	121.00
1	A	320	MET	CA-CB-CG	-7.25	100.97	113.30
1	A	380	PRO	O-C-N	-7.25	111.11	122.70
1	G	318	TYR	CB-CG-CD2	7.24	125.34	121.00
2	H	195	ASP	CB-CG-OD1	7.24	124.81	118.30
1	G	216	ARG	CD-NE-CZ	7.18	133.65	123.60
2	H	104	TRP	CA-CB-CG	7.17	127.33	113.70
1	G	14	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	A	545	PRO	N-CD-CG	7.14	113.91	103.20
1	G	288	TYR	O-C-N	-7.13	111.30	122.70
3	C	251	ASP	CB-CG-OD1	7.12	124.71	118.30
1	A	483	TYR	CB-CG-CD2	-7.11	116.73	121.00
3	I	17	TRP	CB-CA-C	7.10	124.59	110.40
1	A	483	TYR	CB-CG-CD1	7.09	125.25	121.00
1	A	333	HIS	CA-CB-CG	7.02	125.54	113.60
1	A	243	LEU	CB-CG-CD1	-7.01	99.08	111.00
2	B	78	TYR	CB-CG-CD2	-6.94	116.83	121.00
1	G	130	ALA	N-CA-CB	-6.94	100.38	110.10
1	G	461	PHE	CB-CG-CD2	6.94	125.66	120.80
3	C	226	ARG	NE-CZ-NH2	-6.94	116.83	120.30
2	H	159	TYR	CB-CG-CD1	6.93	125.16	121.00
1	G	257	ARG	NE-CZ-NH2	6.87	123.74	120.30
2	B	214	ASP	CB-CG-OD1	6.83	124.45	118.30
1	G	408	ARG	NE-CZ-NH1	-6.83	116.89	120.30
1	A	132	ASP	CB-CG-OD1	6.81	124.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	185	TYR	CA-CB-CG	6.76	126.24	113.40
1	G	408	ARG	CD-NE-CZ	6.68	132.95	123.60
1	G	216	ARG	NH1-CZ-NH2	6.67	126.74	119.40
2	B	241	ARG	NE-CZ-NH2	6.67	123.63	120.30
1	A	319	ALA	N-CA-CB	6.62	119.37	110.10
1	G	545	PRO	N-CD-CG	6.61	113.12	103.20
3	I	198	TYR	CB-CG-CD2	6.60	124.96	121.00
2	H	137	LYS	N-CA-CB	6.58	122.45	110.60
2	B	107	VAL	CB-CA-C	6.57	123.88	111.40
4	J	17	ASP	CB-CG-OD1	6.54	124.19	118.30
2	H	263	MET	N-CA-CB	6.54	122.37	110.60
1	G	313	TYR	CB-CG-CD2	-6.52	117.09	121.00
1	G	407	ASP	CB-CG-OD1	6.48	124.13	118.30
1	A	526	THR	CA-CB-CG2	-6.46	103.35	112.40
1	G	282	PHE	CB-CG-CD1	6.45	125.31	120.80
1	G	354	VAL	O-C-N	-6.42	112.42	122.70
1	A	257	ARG	NH1-CZ-NH2	6.41	126.45	119.40
1	A	304	THR	CA-CB-CG2	-6.41	103.43	112.40
3	C	98	PHE	CB-CG-CD1	-6.39	116.33	120.80
2	B	234	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	G	348	PHE	O-C-N	-6.35	112.53	122.70
3	C	32	ALA	N-CA-CB	6.33	118.97	110.10
3	C	184	TYR	CB-CG-CD2	6.33	124.80	121.00
2	B	159	TYR	CB-CG-CD2	-6.32	117.21	121.00
3	C	42	TRP	CA-CB-CG	-6.29	101.74	113.70
3	I	195	GLY	N-CA-C	6.29	128.83	113.10
1	A	243	LEU	CB-CG-CD2	6.25	121.62	111.00
1	A	146	TYR	CB-CG-CD2	6.25	124.75	121.00
2	B	229	ASP	CB-CG-OD2	-6.24	112.68	118.30
2	B	221	VAL	CA-CB-CG1	-6.24	101.54	110.90
1	A	347	TYR	N-CA-CB	6.23	121.82	110.60
2	H	258	ILE	CB-CA-C	-6.21	99.17	111.60
3	C	117	ASP	CB-CG-OD2	-6.21	112.71	118.30
2	B	262	TYR	O-C-N	-6.20	112.77	122.70
1	A	400	VAL	CA-CB-CG1	-6.20	101.60	110.90
3	C	262	TYR	CB-CG-CD2	6.19	124.72	121.00
4	D	30	ARG	NE-CZ-NH1	-6.19	117.20	120.30
2	H	221	VAL	CA-CB-CG2	6.17	120.15	110.90
1	G	552	GLU	CA-CB-CG	6.17	126.96	113.40
1	G	114	ALA	N-CA-CB	-6.16	101.48	110.10
2	H	220	THR	CA-CB-CG2	-6.14	103.80	112.40
1	A	471	GLN	O-C-N	-6.14	112.88	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	243	LEU	CB-CG-CD1	-6.13	100.58	111.00
1	G	185	TYR	CB-CG-CD2	-6.13	117.32	121.00
1	A	336	TYR	CB-CG-CD1	6.10	124.66	121.00
2	H	87	ARG	NE-CZ-NH1	6.07	123.33	120.30
1	A	485	ASP	CB-CG-OD2	-6.06	112.84	118.30
1	G	125	PRO	O-C-N	-6.06	113.00	122.70
2	B	149	TYR	CB-CG-CD2	-6.04	117.38	121.00
2	B	275	TYR	CB-CG-CD2	-6.04	117.38	121.00
1	A	213	LEU	CA-CB-CG	6.03	129.16	115.30
1	G	511	PHE	CB-CG-CD2	-6.02	116.59	120.80
2	H	159	TYR	CB-CG-CD2	-6.01	117.39	121.00
1	A	552	GLU	CA-CB-CG	6.01	126.61	113.40
1	A	57	ALA	CB-CA-C	-6.00	101.11	110.10
1	A	178	LEU	O-C-N	-5.97	113.15	122.70
3	C	246	TYR	CG-CD2-CE2	-5.97	116.53	121.30
1	G	106	MET	CG-SD-CE	5.97	109.75	100.20
1	A	257	ARG	NE-CZ-NH2	5.94	123.27	120.30
1	G	170	ILE	CB-CA-C	-5.93	99.73	111.60
1	G	252	MET	O-C-N	-5.93	113.22	122.70
1	G	369	THR	CA-CB-OG1	-5.92	96.56	109.00
2	H	199	VAL	CG1-CB-CG2	5.92	120.37	110.90
1	A	196	LEU	CB-CA-C	5.91	121.44	110.20
1	G	19	ARG	NH1-CZ-NH2	5.91	125.91	119.40
4	J	12	VAL	CG1-CB-CG2	-5.91	101.45	110.90
3	I	80	ARG	NH1-CZ-NH2	5.90	125.89	119.40
1	G	234	VAL	CA-CB-CG1	-5.90	102.05	110.90
1	G	487	PRO	CA-C-O	5.90	134.36	120.20
1	G	544	SER	N-CA-C	5.90	126.93	111.00
1	A	326	LEU	O-C-N	-5.88	113.21	123.20
2	H	234	ARG	NE-CZ-NH1	-5.88	117.36	120.30
2	B	199	VAL	CG1-CB-CG2	5.86	120.27	110.90
1	A	539	GLU	OE1-CD-OE2	5.84	130.31	123.30
1	G	401	LEU	O-C-N	-5.82	113.39	122.70
1	G	557	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	G	552	GLU	OE1-CD-OE2	-5.79	116.36	123.30
1	G	154	VAL	CA-CB-CG2	-5.77	102.24	110.90
2	H	196	THR	CA-CB-CG2	-5.77	104.32	112.40
3	C	76	ARG	NE-CZ-NH2	5.77	123.18	120.30
1	A	412	ASP	OD1-CG-OD2	-5.76	112.35	123.30
1	A	175	TYR	CB-CG-CD1	5.76	124.45	121.00
1	A	420	PHE	O-C-N	5.75	131.90	122.70
1	A	397	THR	CA-CB-CG2	-5.75	104.35	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	93	PHE	CB-CG-CD1	5.75	124.82	120.80
1	G	543	THR	N-CA-C	-5.75	95.49	111.00
1	G	461	PHE	CB-CG-CD1	-5.74	116.78	120.80
3	I	20	MET	CA-CB-CG	5.73	123.05	113.30
1	G	423	VAL	CA-CB-CG2	-5.71	102.34	110.90
1	A	309	PRO	O-C-N	-5.70	113.58	122.70
3	I	200	ALA	N-CA-CB	-5.70	102.12	110.10
2	B	220	THR	CA-CB-CG2	-5.68	104.44	112.40
1	G	433	PHE	CB-CG-CD2	-5.68	116.82	120.80
1	G	33	TYR	CA-CB-CG	5.67	124.18	113.40
2	H	71	PHE	CB-CG-CD2	-5.66	116.83	120.80
1	G	14	ARG	NE-CZ-NH2	-5.65	117.47	120.30
1	A	275	TYR	CB-CG-CD2	5.65	124.39	121.00
3	C	101	PHE	CB-CG-CD1	5.65	124.76	120.80
1	G	243	LEU	CB-CG-CD2	5.65	120.61	111.00
1	G	347	TYR	N-CA-CB	5.64	120.76	110.60
1	A	49	VAL	CB-CA-C	5.63	122.10	111.40
1	A	124	MET	CA-CB-CG	5.63	122.86	113.30
2	H	169	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	A	539	GLU	CG-CD-OE1	-5.59	107.12	118.30
3	C	198	TYR	CB-CG-CD1	-5.59	117.65	121.00
1	G	168	SER	O-C-N	-5.58	113.71	123.20
1	A	420	PHE	CA-C-O	-5.57	108.41	120.10
1	A	171	GLY	N-CA-C	-5.57	99.19	113.10
2	H	232	PRO	O-C-N	-5.57	113.74	123.20
3	I	17	TRP	CB-CG-CD2	5.55	133.81	126.60
2	H	113	VAL	CA-CB-CG1	-5.55	102.58	110.90
1	A	436	ILE	CA-C-O	5.54	131.73	120.10
3	I	42	TRP	CA-CB-CG	-5.53	103.19	113.70
1	G	320	MET	CA-CB-CG	-5.53	103.91	113.30
2	B	159	TYR	CB-CG-CD1	5.52	124.31	121.00
1	G	414	TYR	CB-CG-CD1	5.51	124.31	121.00
3	I	76	ARG	NH1-CZ-NH2	5.51	125.46	119.40
1	A	168	SER	CB-CA-C	-5.50	99.64	110.10
1	A	229	ALA	O-C-N	-5.50	113.90	122.70
1	A	415	TYR	CB-CG-CD2	5.50	124.30	121.00
1	G	523	ALA	CB-CA-C	5.50	118.36	110.10
2	B	157	GLU	CG-CD-OE2	-5.50	107.30	118.30
1	G	396	VAL	CA-CB-CG1	-5.50	102.65	110.90
3	I	112	GLU	OE1-CD-OE2	-5.50	116.70	123.30
3	I	72	THR	CA-CB-CG2	-5.50	104.70	112.40
1	A	19	ARG	NH1-CZ-NH2	5.48	125.43	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	312	GLY	O-C-N	-5.48	113.93	122.70
2	H	78	TYR	CB-CG-CD2	-5.47	117.72	121.00
1	A	287	VAL	CG1-CB-CG2	-5.46	102.16	110.90
1	G	439	TRP	CA-CB-CG	5.46	124.07	113.70
3	C	8	ASP	CA-CB-CG	5.45	125.39	113.40
1	G	36	THR	CA-CB-CG2	-5.45	104.77	112.40
1	A	415	TYR	CB-CG-CD1	-5.43	117.74	121.00
2	H	214	ASP	CB-CG-OD1	5.42	123.18	118.30
2	B	263	MET	N-CA-CB	5.41	120.34	110.60
4	D	42	ALA	CB-CA-C	-5.40	102.00	110.10
2	H	221	VAL	CA-CB-CG1	-5.39	102.81	110.90
1	A	503	LEU	O-C-N	5.39	131.33	122.70
1	G	229	ALA	CB-CA-C	5.38	118.18	110.10
3	I	80	ARG	NE-CZ-NH1	-5.37	117.61	120.30
1	G	397	THR	CA-CB-CG2	-5.37	104.89	112.40
1	A	221	THR	CA-CB-CG2	-5.37	104.89	112.40
1	G	60	VAL	CA-CB-CG2	-5.36	102.86	110.90
2	H	230	ALA	CB-CA-C	5.35	118.13	110.10
1	A	292	LEU	CB-CA-C	5.35	120.37	110.20
1	A	256	ASP	O-C-N	-5.35	114.14	122.70
1	G	418	ALA	N-CA-CB	-5.35	102.61	110.10
3	I	72	THR	N-CA-CB	-5.35	100.14	110.30
1	A	120	GLY	O-C-N	-5.35	114.15	122.70
2	H	256	CYS	CA-C-O	-5.33	108.91	120.10
2	H	35	ARG	NE-CZ-NH2	-5.32	117.64	120.30
2	B	31	GLU	OE1-CD-OE2	-5.31	116.92	123.30
4	J	28	PHE	CB-CG-CD2	5.30	124.51	120.80
1	A	408	ARG	CD-NE-CZ	5.30	131.02	123.60
1	G	555	PRO	N-CA-CB	5.29	109.65	103.30
3	C	256	PHE	CB-CA-C	5.29	120.98	110.40
1	A	33	TYR	CB-CG-CD1	5.29	124.17	121.00
2	B	252	CYS	CA-CB-SG	5.28	123.50	114.00
1	A	196	LEU	N-CA-CB	-5.28	99.85	110.40
1	A	376	GLU	CG-CD-OE1	5.27	128.83	118.30
3	C	73	PRO	CA-C-N	5.26	128.78	117.20
1	G	517	TYR	CB-CG-CD1	-5.26	117.84	121.00
1	G	316	MET	CA-CB-CG	-5.25	104.38	113.30
1	A	407	ASP	CB-CG-OD1	5.24	123.02	118.30
3	C	93	PHE	CB-CG-CD2	-5.23	117.14	120.80
1	A	315	PRO	O-C-N	-5.22	114.34	122.70
2	H	82	ARG	CD-NE-CZ	5.22	130.91	123.60
1	A	175	TYR	CA-C-O	5.21	131.05	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	117	ASP	CB-CG-OD1	-5.20	113.62	118.30
4	D	50	ASN	CA-CB-CG	-5.20	101.96	113.40
1	G	143	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	A	52	ARG	CB-CA-C	5.19	120.78	110.40
1	G	196	LEU	O-C-N	-5.18	114.40	122.70
1	A	524	ARG	NE-CZ-NH2	5.18	122.89	120.30
1	A	417	VAL	CA-CB-CG2	-5.17	103.14	110.90
1	G	101	GLY	CA-C-O	5.17	129.91	120.60
1	G	414	TYR	CB-CG-CD2	-5.17	117.90	121.00
1	A	262	THR	CA-CB-CG2	-5.13	105.21	112.40
1	G	203	LEU	CA-C-O	5.12	130.86	120.10
3	I	193	PHE	CB-CG-CD1	5.12	124.39	120.80
1	A	36	THR	O-C-N	-5.11	114.51	123.20
1	A	346	SER	N-CA-CB	-5.11	102.84	110.50
1	G	536	ASP	N-CA-CB	-5.11	101.41	110.60
1	G	28	ASP	CB-CG-OD2	-5.10	113.71	118.30
1	A	295	PHE	CB-CG-CD1	5.08	124.36	120.80
1	A	376	GLU	CA-CB-CG	5.08	124.58	113.40
1	A	300	HIS	CA-CB-CG	-5.08	104.97	113.60
3	C	193	PHE	CB-CG-CD1	5.08	124.35	120.80
1	G	448	TYR	CA-CB-CG	-5.08	103.76	113.40
1	A	256	ASP	CB-CG-OD1	5.07	122.86	118.30
4	J	36	ALA	N-CA-CB	-5.07	103.00	110.10
1	A	227	LEU	N-CA-CB	-5.07	100.27	110.40
2	B	152	GLU	OE1-CD-OE2	-5.06	117.23	123.30
2	B	264	PRO	CA-CB-CG	-5.06	94.38	104.00
1	A	324	GLY	O-C-N	-5.05	114.62	122.70
2	B	110	VAL	CG1-CB-CG2	5.04	118.97	110.90
1	A	15	GLY	N-CA-C	-5.04	100.50	113.10
2	H	93	ARG	NE-CZ-NH1	5.04	122.82	120.30
4	J	17	ASP	OD1-CG-OD2	-5.03	113.74	123.30
1	G	262	THR	CA-CB-CG2	-5.03	105.36	112.40
3	C	116	ILE	CB-CA-C	-5.03	101.55	111.60
1	G	308	LYS	N-CA-CB	-5.03	101.56	110.60
3	I	61	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	G	376	GLU	N-CA-CB	-5.02	101.57	110.60
2	B	60	PHE	CA-CB-CG	5.01	125.93	113.90
2	B	258	ILE	CB-CA-C	-5.01	101.58	111.60
1	A	151	SER	N-CA-CB	-5.00	103.00	110.50

There are no chirality outliers.

All (44) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	108	PHE	Mainchain
1	A	112	ILE	Mainchain
1	A	157	LEU	Mainchain
1	A	202	ILE	Mainchain
1	A	257	ARG	Mainchain
1	A	274	LEU	Mainchain
1	A	538	LEU	Mainchain
1	A	543	THR	Peptide,Mainchain
1	A	544	SER	Peptide,Mainchain
1	A	545	PRO	Mainchain
2	B	142	GLN	Mainchain
2	B	143	TRP	Mainchain
2	B	163	SER	Mainchain
2	B	209	GLN	Mainchain
2	B	253	SER	Mainchain
2	B	263	MET	Mainchain
3	C	162	ARG	Mainchain
3	C	17	TRP	Mainchain
3	C	196	ASN	Mainchain
4	D	49	ALA	Mainchain
1	G	112	ILE	Mainchain
1	G	173	VAL	Mainchain
1	G	234	VAL	Mainchain
1	G	274	LEU	Mainchain
1	G	288	TYR	Mainchain
1	G	317	VAL	Mainchain
1	G	326	LEU	Mainchain
1	G	334	HIS	Mainchain
1	G	343	THR	Mainchain
1	G	416	VAL	Mainchain
1	G	419	HIS	Mainchain
1	G	469	PHE	Mainchain
1	G	543	THR	Peptide
1	G	544	SER	Peptide,Mainchain
2	H	107	VAL	Mainchain
2	H	142	GLN	Mainchain
2	H	229	ASP	Mainchain
2	H	231	VAL	Mainchain
2	H	254	GLU	Mainchain
3	I	196	ASN	Mainchain
3	I	57	GLY	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4322	0	4238	314	0
1	G	4322	0	4238	339	0
2	B	2046	0	2011	126	0
2	H	2046	0	2011	143	0
3	C	2139	0	2056	155	0
3	I	2139	0	2056	153	0
4	D	311	0	319	25	0
4	J	311	0	319	42	0
5	A	1	0	0	0	0
5	B	2	0	0	0	0
5	G	1	0	0	0	0
5	H	2	0	0	0	0
6	A	1	0	0	0	0
6	G	1	0	0	0	0
7	A	1	0	0	0	0
7	G	1	0	0	0	0
8	A	120	0	108	26	0
8	G	120	0	108	18	0
9	A	102	0	164	34	0
9	C	153	0	246	48	0
9	D	51	0	82	21	0
9	G	102	0	164	29	0
9	I	153	0	246	51	0
9	J	51	0	82	16	0
10	A	101	0	0	7	0
10	B	68	0	0	3	0
10	C	39	0	0	5	0
10	D	12	0	0	0	0
10	G	106	0	0	9	0
10	H	64	0	0	6	0
10	I	38	0	0	4	0
10	J	8	0	0	2	0
All	All	18934	0	18448	1291	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 35.

All (1291) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:8:ASP:HB3	3:I:72:THR:HG21	1.27	1.12
1:A:520:THR:HG22	1:A:521:ARG:HG2	1.32	1.12
9:I:3013:3PE:O14	9:I:3013:3PE:H121	1.51	1.11
9:I:3013:3PE:C3H	9:I:3013:3PE:H2D2	1.78	1.11
9:C:2013:3PE:O14	9:C:2013:3PE:H121	1.48	1.06
1:A:284:HIS:NE2	1:A:288:TYR:HE2	1.53	1.04
9:I:3013:3PE:C2D	9:I:3013:3PE:H3H2	1.88	1.04
3:C:8:ASP:HB3	3:C:72:THR:HG21	1.39	1.03
3:I:161:ARG:HH12	3:I:230:GLY:HA2	1.24	1.01
3:C:161:ARG:HH12	3:C:230:GLY:HA2	1.22	1.01
9:C:2013:3PE:C3H	9:C:2013:3PE:H2D2	1.89	1.01
1:G:543:THR:HG22	1:G:547:PRO:HD3	1.40	1.01
1:G:284:HIS:NE2	1:G:288:TYR:HE2	1.58	1.00
1:G:106:MET:HB3	8:G:1001:HEA:HAC	1.43	0.99
1:A:124:MET:HB3	1:A:125:PRO:HD3	1.39	0.98
1:A:127:HIS:HB3	1:A:226:PRO:HG2	1.42	0.98
1:A:390:LEU:HD13	1:A:426:LEU:HB3	1.44	0.98
1:G:345:GLN:HE22	1:G:408:ARG:HH22	1.08	0.98
9:C:2013:3PE:H2D2	9:C:2013:3PE:H3H2	1.41	0.97
1:G:63:MET:HG2	1:G:94:LEU:HD23	1.46	0.97
1:A:543:THR:HG22	1:A:547:PRO:HD3	1.45	0.95
1:A:489:ALA:HB3	2:B:36:PRO:HB2	1.47	0.95
1:G:379:THR:HB	1:G:380:PRO:HD3	1.48	0.94
1:G:63:MET:HE1	1:G:95:TRP:HB2	1.48	0.94
1:A:379:THR:HB	1:A:380:PRO:HD3	1.48	0.93
1:G:284:HIS:HE2	1:G:288:TYR:HE2	1.15	0.93
1:G:520:THR:HG22	1:G:521:ARG:HG2	1.46	0.93
9:I:3013:3PE:H2D2	9:I:3013:3PE:H3H1	1.50	0.92
3:C:21:ALA:HB2	3:C:54:THR:HG21	1.51	0.92
9:I:3013:3PE:H2D2	9:I:3013:3PE:H3H2	1.43	0.91
1:A:18:THR:HA	1:A:22:MET:HE3	1.53	0.91
1:G:432:ILE:HG21	8:G:1001:HEA:H252	1.50	0.91
3:I:21:ALA:HB2	3:I:54:THR:HG21	1.52	0.91
9:A:2012:3PE:H2F1	9:D:2011:3PE:H2I2	1.54	0.90
1:G:342:LEU:HD13	2:H:127:GLN:HB2	1.51	0.90
1:G:99:ILE:HD12	8:G:1001:HEA:HBA2	1.55	0.89
1:G:18:THR:HA	1:G:22:MET:HE3	1.52	0.89
9:C:2013:3PE:H3H2	9:C:2013:3PE:C2D	2.02	0.88
1:A:397:THR:HG21	1:A:419:HIS:HB2	1.55	0.88
9:I:3013:3PE:H261	9:I:3013:3PE:H3B1	1.56	0.88
1:A:239:ILE:HG12	1:A:289:ILE:HD13	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:3010:3PE:H3E2	9:I:3010:3PE:H3I3	1.54	0.87
1:A:106:MET:HB3	8:A:1001:HEA:HAC	1.55	0.86
2:H:245:GLU:HA	2:H:269:VAL:HG13	1.57	0.86
1:A:284:HIS:HE2	1:A:288:TYR:HE2	1.17	0.86
1:G:222:MET:H	9:G:3012:3PE:H111	1.38	0.86
1:A:357:VAL:HB	1:A:358:PRO:HD3	1.57	0.86
8:A:1002:HEA:HBC1	8:A:1002:HEA:HMC1	1.55	0.86
3:C:161:ARG:NH1	3:C:230:GLY:HA2	1.91	0.85
2:H:211:THR:HG22	2:H:212:GLY:H	1.40	0.85
1:G:397:THR:HG21	1:G:419:HIS:HB2	1.58	0.85
3:I:85:LEU:HA	3:I:88:MET:HE2	1.59	0.85
9:C:2013:3PE:O14	9:C:2013:3PE:C12	2.24	0.84
1:A:22:MET:HG2	3:C:16:ILE:HA	1.57	0.84
9:I:3013:3PE:O14	9:I:3013:3PE:C12	2.25	0.84
1:G:489:ALA:HB3	2:H:36:PRO:HB2	1.57	0.84
1:G:390:LEU:HD13	1:G:426:LEU:HB3	1.59	0.83
3:I:8:ASP:CB	3:I:72:THR:HG21	2.08	0.83
1:G:345:GLN:NE2	1:G:408:ARG:HH22	1.75	0.83
1:A:345:GLN:HE22	1:A:408:ARG:HH22	1.25	0.83
1:G:249:ALA:HB2	1:G:278:ILE:HG22	1.60	0.83
9:C:2010:3PE:H3E2	9:C:2010:3PE:H3I3	1.59	0.83
2:H:136:VAL:HG11	2:H:198:MET:HE2	1.61	0.83
2:B:245:GLU:HA	2:B:269:VAL:HG13	1.61	0.82
1:A:63:MET:HE1	1:A:95:TRP:HB2	1.62	0.81
3:I:161:ARG:NH1	3:I:230:GLY:HA2	1.94	0.81
2:H:107:VAL:CG1	2:H:108:PRO:HD3	2.10	0.81
1:A:222:MET:H	9:A:2012:3PE:H111	1.43	0.81
1:A:473:PHE:CD1	2:B:41:THR:HB	2.15	0.81
1:G:25:ASN:HD21	1:G:27:LYS:HZ3	1.26	0.80
3:I:62:VAL:HG11	9:I:3008:3PE:H31	1.63	0.80
3:C:255:LEU:HB3	9:D:2011:3PE:H3I3	1.64	0.79
3:C:8:ASP:CB	3:C:72:THR:HG21	2.12	0.79
1:A:243:LEU:HD22	1:A:282:PHE:CE2	2.18	0.79
2:B:235:LEU:HD21	4:J:11:HIS:HB2	1.66	0.78
1:G:124:MET:HB3	1:G:125:PRO:HD3	1.64	0.78
1:A:432:ILE:CG2	8:A:1001:HEA:H252	2.13	0.78
3:C:133:LEU:H	3:C:134:PRO:HD2	1.48	0.78
1:G:473:PHE:CD1	2:H:41:THR:HB	2.19	0.78
1:A:511:PHE:CZ	1:A:515:ILE:HD11	2.17	0.78
1:G:432:ILE:CG2	8:G:1001:HEA:H252	2.12	0.78
1:A:342:LEU:HD13	2:B:127:GLN:HB2	1.64	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:136:VAL:HG11	2:B:198:MET:HE2	1.65	0.78
1:G:127:HIS:HB3	1:G:226:PRO:HG2	1.66	0.77
1:A:294:ALA:O	1:A:298:VAL:HG23	1.85	0.77
3:I:255:LEU:HB3	9:J:3011:3PE:H3I3	1.65	0.77
3:I:108:PRO:HD2	3:I:117:ASP:HB3	1.66	0.77
1:A:284:HIS:NE2	1:A:288:TYR:CE2	2.46	0.77
3:C:152:HIS:HA	3:C:240:PHE:HE1	1.50	0.77
3:C:111:PRO:HA	4:J:12:VAL:HB	1.67	0.77
9:A:2012:3PE:H2H1	9:C:2010:3PE:H2I3	1.67	0.76
8:G:1002:HEA:HBC1	8:G:1002:HEA:HMC1	1.64	0.76
1:A:63:MET:HG2	1:A:94:LEU:HD23	1.67	0.76
2:H:226:VAL:HA	10:H:1157:HOH:O	1.85	0.76
1:A:284:HIS:HB3	1:A:285:PRO:HD3	1.66	0.76
9:I:3013:3PE:H261	9:I:3013:3PE:C3B	2.15	0.76
9:A:2009:3PE:H2C2	9:A:2009:3PE:H3A1	1.68	0.76
1:A:442:LYS:O	1:A:546:PRO:HD3	1.86	0.76
3:I:197:ILE:HG13	3:I:198:TYR:H	1.50	0.76
1:G:374:SER:HB2	2:H:85:GLU:HA	1.67	0.76
9:I:3010:3PE:H3I3	9:I:3010:3PE:C3E	2.11	0.75
1:A:243:LEU:HD22	1:A:282:PHE:HE2	1.51	0.75
9:A:2009:3PE:C3E	9:A:2009:3PE:H2E1	2.16	0.75
1:G:22:MET:HG2	3:I:16:ILE:HA	1.69	0.75
9:G:3009:3PE:H2C2	9:G:3009:3PE:H3A1	1.68	0.75
1:G:170:ILE:HD11	1:G:187:THR:OG1	1.87	0.75
3:C:108:PRO:HD2	3:C:117:ASP:HB3	1.69	0.75
9:G:3009:3PE:H3E1	9:G:3009:3PE:H2E1	1.69	0.75
1:G:429:VAL:HG13	8:G:1001:HEA:H273	1.68	0.75
1:A:63:MET:HE1	1:A:484:ILE:HG13	1.67	0.74
3:C:152:HIS:HA	3:C:240:PHE:CE1	2.22	0.74
9:G:3009:3PE:H2E1	9:G:3009:3PE:C3E	2.17	0.74
3:C:80:ARG:O	3:C:84:ILE:HG13	1.87	0.74
2:H:107:VAL:HG13	2:H:108:PRO:HD3	1.68	0.74
1:G:520:THR:CG2	1:G:521:ARG:HG2	2.16	0.73
3:I:220:LEU:HD23	3:I:243:ALA:HB1	1.71	0.73
1:A:137:ARG:HH21	9:A:2009:3PE:H112	1.52	0.73
3:I:152:HIS:HA	3:I:240:PHE:HE1	1.53	0.73
9:A:2009:3PE:H2E1	9:A:2009:3PE:H3E1	1.71	0.73
1:G:25:ASN:HD21	1:G:27:LYS:NZ	1.87	0.72
1:A:529:ASN:OD1	1:A:529:ASN:C	2.26	0.72
3:C:130:PRO:HA	3:C:134:PRO:HG2	1.72	0.72
2:H:191:LEU:O	2:H:264:PRO:HG3	1.88	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:42:TRP:O	3:C:46:ILE:HG12	1.90	0.72
3:C:133:LEU:H	3:C:134:PRO:CD	2.03	0.72
9:C:2013:3PE:H261	9:C:2013:3PE:H3B1	1.71	0.71
3:I:197:ILE:HG13	3:I:198:TYR:N	2.04	0.71
3:C:58:TRP:O	3:C:62:VAL:HG23	1.91	0.71
1:A:170:ILE:HD11	1:A:187:THR:OG1	1.91	0.71
1:A:314:LEU:HB3	1:A:315:PRO:HD3	1.71	0.71
1:G:127:HIS:HB3	1:G:226:PRO:CG	2.21	0.71
1:G:511:PHE:CZ	1:G:515:ILE:HD11	2.25	0.70
3:I:152:HIS:HA	3:I:240:PHE:CE1	2.26	0.70
3:I:83:PHE:HE1	9:I:3008:3PE:H262	1.54	0.70
3:I:62:VAL:CG1	9:I:3008:3PE:H31	2.21	0.70
3:C:51:VAL:O	3:C:55:MET:HG3	1.92	0.70
1:G:284:HIS:HB3	1:G:285:PRO:HD3	1.74	0.70
9:G:3009:3PE:H111	3:I:12:LEU:HD11	1.74	0.70
3:I:161:ARG:NH2	3:I:232:PHE:H	1.90	0.70
3:I:122:PRO:HG2	3:I:198:TYR:HB2	1.74	0.69
1:G:241:LEU:HD13	9:J:3011:3PE:H2H2	1.75	0.69
1:A:345:GLN:NE2	1:A:408:ARG:HH22	1.90	0.69
1:G:81:TRP:CD2	1:G:82:PRO:HD2	2.27	0.69
2:B:107:VAL:CG1	2:B:108:PRO:HD3	2.22	0.69
3:C:197:ILE:HG13	3:C:198:TYR:H	1.56	0.69
1:A:373:GLY:O	2:B:83:PHE:HB3	1.92	0.69
9:C:2013:3PE:H2D2	9:C:2013:3PE:H3H1	1.74	0.69
1:G:394:GLY:O	1:G:397:THR:HB	1.93	0.69
3:I:248:HIS:O	3:I:252:VAL:HG23	1.93	0.69
9:I:3010:3PE:C3E	9:I:3010:3PE:C3I	2.71	0.69
1:A:99:ILE:CD1	8:A:1001:HEA:HBA2	2.24	0.69
2:B:72:VAL:O	2:B:76:ILE:HG13	1.93	0.68
3:C:62:VAL:CG1	9:C:2008:3PE:H31	2.22	0.68
3:C:73:PRO:HB2	4:D:18:ILE:CD1	2.23	0.68
3:C:161:ARG:NH2	3:C:232:PHE:H	1.91	0.68
3:C:240:PHE:CE1	3:C:244:ILE:HD11	2.28	0.68
1:G:426:LEU:HD21	1:G:464:ALA:HB1	1.75	0.68
3:I:133:LEU:H	3:I:134:PRO:CD	2.06	0.68
1:G:406:VAL:CG2	2:H:57:LEU:HD23	2.24	0.68
3:C:122:PRO:HG2	3:C:198:TYR:HB2	1.75	0.68
1:G:99:ILE:CD1	8:G:1001:HEA:HBA2	2.24	0.68
1:G:486:TYR:CD2	1:G:490:PHE:HB2	2.28	0.68
1:A:400:VAL:HG11	1:A:410:TYR:HE2	1.57	0.68
1:A:543:THR:CG2	1:A:547:PRO:HD3	2.23	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:194:THR:HG22	2:H:266:THR:OG1	1.94	0.68
3:I:80:ARG:O	3:I:84:ILE:HG13	1.92	0.68
9:C:2010:3PE:H3I3	9:C:2010:3PE:C3E	2.19	0.68
2:H:211:THR:HG23	2:H:234:ARG:O	1.94	0.68
9:I:3013:3PE:H351	9:I:3013:3PE:C31	2.23	0.68
1:A:543:THR:HG23	1:A:545:PRO:O	1.95	0.68
1:A:81:TRP:CD2	1:A:82:PRO:HD2	2.29	0.67
1:G:249:ALA:HB2	1:G:278:ILE:CG2	2.24	0.67
9:G:3012:3PE:H2H1	9:I:3010:3PE:H2I3	1.76	0.67
2:H:175:GLU:O	2:H:178:GLN:HG2	1.94	0.67
4:D:47:ALA:HA	9:D:2011:3PE:H321	1.75	0.67
4:J:47:ALA:HA	9:J:3011:3PE:H321	1.76	0.67
1:G:63:MET:HE1	1:G:484:ILE:HG13	1.76	0.67
9:G:3012:3PE:H261	4:J:31:MET:SD	2.35	0.67
3:I:133:LEU:H	3:I:134:PRO:HD2	1.59	0.66
1:A:213:LEU:HB2	3:C:81:TRP:CH2	2.31	0.66
3:C:162:ARG:HG3	3:C:163:ASP:N	2.10	0.66
1:G:284:HIS:NE2	1:G:288:TYR:CE2	2.51	0.66
1:G:543:THR:HG23	1:G:545:PRO:O	1.95	0.66
2:H:185:TYR:HE1	2:H:247:ILE:HD13	1.60	0.66
1:A:489:ALA:CB	2:B:36:PRO:HB2	2.25	0.66
3:C:73:PRO:HB2	4:D:18:ILE:HD11	1.78	0.66
3:C:62:VAL:HG11	9:C:2008:3PE:H31	1.76	0.66
3:I:130:PRO:HA	3:I:134:PRO:HG2	1.78	0.66
1:G:345:GLN:HE22	1:G:408:ARG:NH2	1.87	0.66
1:G:88:CYS:O	1:G:90:PRO:HD3	1.96	0.65
9:I:3013:3PE:H3H2	9:I:3013:3PE:C2E	2.26	0.65
1:G:373:GLY:O	2:H:83:PHE:HB3	1.96	0.65
1:G:480:PRO:HG2	1:G:483:TYR:CE2	2.32	0.65
2:H:72:VAL:O	2:H:76:ILE:HG13	1.95	0.65
2:H:43:PHE:CD2	2:H:55:HIS:CD2	2.85	0.65
1:A:357:VAL:HB	1:A:358:PRO:CD	2.26	0.65
2:H:145:TRP:NE1	2:H:263:MET:HE2	2.11	0.65
9:A:2009:3PE:H2C2	9:A:2009:3PE:H3B2	1.78	0.65
1:G:543:THR:CG2	1:G:547:PRO:HD3	2.20	0.65
1:G:493:TRP:HA	1:G:493:TRP:CE3	2.32	0.65
2:H:30:LEU:HD22	2:H:247:ILE:HD11	1.79	0.65
3:I:73:PRO:HB2	4:J:18:ILE:HD11	1.77	0.65
2:B:175:GLU:O	2:B:178:GLN:HG2	1.97	0.65
9:C:2013:3PE:H351	9:C:2013:3PE:C31	2.27	0.64
1:G:486:TYR:HD2	1:G:490:PHE:HB2	1.63	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:241:LEU:HD13	9:J:3011:3PE:C2H	2.27	0.64
3:I:74:VAL:HG13	4:J:18:ILE:HG12	1.78	0.64
2:B:238:LEU:HD12	2:B:238:LEU:C	2.18	0.64
1:G:137:ARG:HH21	9:G:3009:3PE:H112	1.61	0.64
3:I:162:ARG:HG3	3:I:163:ASP:N	2.12	0.64
1:A:422:TYR:CD2	1:A:426:LEU:HD12	2.33	0.64
2:B:105:THR:O	2:B:109:ILE:HG13	1.98	0.64
9:C:2010:3PE:C3E	9:C:2010:3PE:C3I	2.76	0.64
1:A:124:MET:HB3	1:A:125:PRO:CD	2.23	0.63
3:C:101:PHE:CE2	3:C:261:ILE:HG12	2.33	0.63
1:G:18:THR:HA	1:G:22:MET:CE	2.26	0.63
1:G:221:THR:HG22	9:G:3012:3PE:H121	1.79	0.63
1:A:486:TYR:CD2	1:A:490:PHE:HB2	2.34	0.63
3:C:85:LEU:HA	3:C:88:MET:HE2	1.79	0.63
2:B:263:MET:N	2:B:264:PRO:HD3	2.13	0.63
1:A:247:ALA:HB2	9:A:2009:3PE:H3I2	1.80	0.63
1:A:374:SER:HB2	2:B:85:GLU:HA	1.79	0.63
1:A:401:LEU:HD13	8:A:1002:HEA:HBA2	1.79	0.63
2:B:200:VAL:HG13	2:B:201:PRO:HD2	1.79	0.63
3:I:8:ASP:HB3	3:I:72:THR:CG2	2.18	0.63
1:A:533:GLU:OE1	10:A:2113:HOH:O	2.16	0.63
2:B:71:PHE:O	2:B:75:LEU:HD12	1.99	0.63
1:G:91:ASN:C	1:G:91:ASN:OD1	2.36	0.63
1:G:63:MET:CG	1:G:94:LEU:HD23	2.27	0.63
2:H:238:LEU:C	2:H:238:LEU:HD12	2.19	0.63
3:C:220:LEU:HD23	3:C:243:ALA:HB1	1.80	0.62
1:G:247:ALA:HB2	9:G:3009:3PE:H3I2	1.79	0.62
1:G:379:THR:HB	1:G:380:PRO:CD	2.26	0.62
1:G:447:GLN:HG3	1:G:448:TYR:N	2.13	0.62
3:C:124:GLY:HA2	1:G:557:ARG:HH12	1.64	0.62
2:H:156:PHE:CD2	2:H:196:THR:HG21	2.34	0.62
1:A:397:THR:CG2	1:A:419:HIS:HB2	2.29	0.62
2:B:160:MET:HG3	2:B:264:PRO:HG2	1.81	0.62
1:G:484:ILE:HG12	1:G:484:ILE:O	2.00	0.62
1:A:221:THR:HG22	9:A:2012:3PE:H121	1.82	0.62
1:G:91:ASN:ND2	1:G:165:GLN:HE22	1.96	0.62
9:G:3012:3PE:H2F1	9:J:3011:3PE:H2I2	1.82	0.62
3:I:252:VAL:HG12	9:I:3010:3PE:H3H2	1.81	0.62
1:G:397:THR:CG2	1:G:419:HIS:HB2	2.30	0.62
1:A:221:THR:HA	9:A:2012:3PE:H121	1.80	0.62
1:A:429:VAL:HG13	8:A:1001:HEA:H273	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:445:GLY:HA2	1:A:525:VAL:HG12	1.82	0.62
2:B:145:TRP:NE1	2:B:263:MET:HE2	2.15	0.62
3:C:231:HIS:O	9:C:2008:3PE:H121	1.99	0.62
2:H:200:VAL:O	2:H:269:VAL:HA	1.99	0.62
3:I:253:VAL:HA	9:I:3010:3PE:H3H1	1.81	0.61
1:A:408:ARG:NE	2:B:126:GLN:OE1	2.27	0.61
1:A:539:GLU:HG2	1:A:540:TRP:N	2.14	0.61
3:I:240:PHE:CE1	3:I:244:ILE:HD11	2.35	0.61
2:H:231:VAL:O	2:H:232:PRO:C	2.37	0.61
1:G:394:GLY:HA3	1:G:423:VAL:HG13	1.83	0.61
1:A:213:LEU:CB	3:C:81:TRP:CH2	2.83	0.61
2:H:211:THR:HG22	2:H:212:GLY:N	2.12	0.61
1:A:135:PHE:HE1	3:C:79:LEU:HD23	1.66	0.61
3:C:13:PRO:HG3	10:C:2036:HOH:O	2.00	0.61
3:C:133:LEU:N	3:C:134:PRO:CD	2.60	0.61
1:G:276:GLN:HB2	1:G:335:MET:HE1	1.83	0.61
3:I:120:PHE:HA	3:I:121:PRO:C	2.20	0.61
1:G:133:MET:HE3	1:G:211:THR:HG21	1.82	0.61
1:G:357:VAL:HB	1:G:358:PRO:HD3	1.82	0.61
3:C:112:GLU:HB2	3:C:116:ILE:HB	1.81	0.61
3:C:162:ARG:HG3	3:C:163:ASP:H	1.66	0.61
3:C:214:ILE:O	3:C:218:ILE:HG12	2.01	0.61
8:G:1002:HEA:HHC	8:G:1002:HEA:O11	2.01	0.61
9:G:3012:3PE:H3E1	9:J:3011:3PE:H2I3	1.83	0.61
9:I:3013:3PE:C3H	9:I:3013:3PE:C2D	2.54	0.61
1:G:221:THR:HA	9:G:3012:3PE:H121	1.83	0.60
1:G:498:SER:O	1:G:502:PHE:HD2	1.84	0.60
2:H:263:MET:N	2:H:264:PRO:CD	2.64	0.60
1:A:46:ALA:O	1:A:49:VAL:HG12	2.01	0.60
1:A:299:SER:O	1:A:300:HIS:C	2.38	0.60
2:H:160:MET:HB2	2:H:264:PRO:HD2	1.83	0.60
3:I:34:LEU:HB3	3:I:39:SER:OG	2.01	0.60
3:I:249:PHE:O	3:I:253:VAL:HG23	2.02	0.60
2:B:30:LEU:HD22	2:B:247:ILE:HD11	1.81	0.60
3:C:133:LEU:N	3:C:134:PRO:HD2	2.16	0.60
1:G:95:TRP:CZ2	1:G:99:ILE:HD11	2.36	0.60
1:G:243:LEU:HD22	1:G:282:PHE:HE2	1.66	0.60
9:A:2009:3PE:H3A1	9:A:2009:3PE:H2A2	1.82	0.60
1:A:480:PRO:HG2	1:A:483:TYR:CE2	2.37	0.60
4:D:18:ILE:O	4:D:18:ILE:HG22	2.02	0.60
1:G:185:TYR:HB3	3:I:37:HIS:CD2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:279:LEU:O	2:H:283:ARG:HG2	2.02	0.60
1:A:241:LEU:HD13	9:D:2011:3PE:H2I1	1.83	0.60
2:B:169:ASP:O	2:B:170:ASN:HB2	2.01	0.60
1:A:206:ILE:HG22	1:A:207:ASN:N	2.16	0.60
1:G:99:ILE:HD12	8:G:1001:HEA:CBA	2.31	0.60
1:A:160:PRO:HG2	1:A:185:TYR:CE1	2.37	0.59
1:G:243:LEU:HD22	1:G:282:PHE:CE2	2.37	0.59
1:G:396:VAL:CG1	2:H:65:ILE:HB	2.32	0.59
1:G:560:TRP:CD1	1:G:560:TRP:C	2.74	0.59
3:I:151:ALA:O	3:I:164:VAL:HG22	2.02	0.59
1:G:306:ALA:O	1:G:307:LYS:HB2	2.02	0.59
2:H:143:TRP:HZ2	2:H:257:GLY:HA3	1.67	0.59
1:A:25:ASN:HD21	1:A:27:LYS:NZ	2.00	0.59
9:A:2009:3PE:H111	3:C:12:LEU:HD11	1.84	0.59
3:I:73:PRO:HB2	4:J:18:ILE:CD1	2.32	0.59
3:I:42:TRP:O	3:I:46:ILE:HG12	2.02	0.59
1:G:63:MET:CE	1:G:484:ILE:HG13	2.31	0.59
3:I:133:LEU:N	3:I:134:PRO:CD	2.65	0.59
1:A:472:HIS:O	1:A:476:ARG:HG3	2.02	0.59
2:H:98:SER:O	2:H:99:PRO:C	2.40	0.59
9:A:2009:3PE:H2E1	9:A:2009:3PE:H3E2	1.84	0.59
3:C:8:ASP:HB3	3:C:72:THR:CG2	2.24	0.59
1:G:374:SER:HA	2:H:83:PHE:O	2.03	0.59
3:I:52:LEU:HD22	9:I:3008:3PE:H3C2	1.85	0.59
3:I:58:TRP:O	3:I:62:VAL:HG23	2.03	0.59
1:A:422:TYR:HH	1:A:469:PHE:HD1	1.50	0.59
9:A:2009:3PE:H2C2	9:A:2009:3PE:C3A	2.32	0.59
1:G:235:THR:OG1	1:G:293:PRO:HD3	2.03	0.59
1:A:198:GLY:HA2	1:A:243:LEU:HD12	1.84	0.59
2:B:194:THR:HG22	2:B:266:THR:OG1	2.02	0.59
1:G:460:MET:O	1:G:460:MET:HG3	2.02	0.59
1:A:185:TYR:HB3	3:C:37:HIS:CD2	2.38	0.58
1:A:247:ALA:HB2	9:A:2009:3PE:C3I	2.32	0.58
2:B:84:HIS:HD2	2:B:86:LYS:H	1.51	0.58
3:C:155:LEU:HB2	3:C:164:VAL:HG21	1.84	0.58
1:G:489:ALA:CB	2:H:36:PRO:HB2	2.28	0.58
1:A:235:THR:OG1	1:A:293:PRO:HD3	2.03	0.58
3:C:107:TYR:OH	4:D:51:ALA:HA	2.03	0.58
1:G:112:ILE:N	1:G:113:PRO:CD	2.65	0.58
9:C:2013:3PE:H3H2	9:C:2013:3PE:C2E	2.33	0.58
1:A:199:ALA:O	1:A:200:SER:C	2.41	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:ILE:HG21	8:A:1001:HEA:H252	1.85	0.58
3:I:131:TRP:HE3	3:I:135:LEU:HD22	1.68	0.58
1:A:127:HIS:CE1	1:A:300:HIS:CE1	2.91	0.58
2:H:84:HIS:HD2	2:H:86:LYS:H	1.49	0.58
1:A:520:THR:CG2	1:A:521:ARG:HG2	2.21	0.58
2:H:134:VAL:HG12	2:H:135:THR:N	2.19	0.58
2:H:220:THR:HB	2:H:227:LYS:HG3	1.84	0.58
1:A:25:ASN:HD21	1:A:27:LYS:HZ3	1.52	0.58
1:A:463:GLY:HA2	1:A:503:LEU:HD23	1.85	0.58
1:A:538:LEU:HD21	1:A:560:TRP:CE3	2.39	0.58
1:A:127:HIS:CE1	1:A:300:HIS:HE1	2.22	0.58
1:A:41:GLY:O	1:A:45:VAL:HB	2.03	0.58
1:A:153:ALA:O	1:A:156:SER:HB3	2.04	0.58
1:A:511:PHE:O	1:A:515:ILE:HG13	2.04	0.58
2:B:279:LEU:O	2:B:283:ARG:HG2	2.03	0.58
3:C:222:VAL:O	3:C:226:ARG:HG3	2.04	0.58
3:I:186:TYR:O	3:I:187:SER:C	2.39	0.58
1:A:439:TRP:O	1:A:443:MET:HG3	2.04	0.57
1:A:63:MET:CE	1:A:484:ILE:HG13	2.34	0.57
2:B:235:LEU:HD11	4:J:11:HIS:N	2.17	0.57
3:C:184:TYR:O	3:C:187:SER:HB3	2.05	0.57
1:G:429:VAL:CG1	8:G:1001:HEA:H273	2.35	0.57
1:A:396:VAL:CG1	2:B:65:ILE:HD12	2.34	0.57
3:C:150:TRP:NE1	3:C:163:ASP:OD1	2.30	0.57
1:G:112:ILE:N	1:G:113:PRO:HD2	2.20	0.57
1:A:539:GLU:HG2	1:A:540:TRP:H	1.67	0.57
2:B:185:TYR:HE1	2:B:247:ILE:HD13	1.69	0.57
1:G:426:LEU:CD2	1:G:464:ALA:HB1	2.34	0.57
9:I:3010:3PE:H2I2	4:J:36:ALA:HB1	1.85	0.57
2:B:48:SER:HB2	2:B:241:ARG:O	2.03	0.57
1:A:538:LEU:HD21	1:A:560:TRP:HE3	1.69	0.57
1:G:326:LEU:O	1:G:328:PHE:N	2.38	0.57
2:H:143:TRP:CZ2	2:H:257:GLY:HA3	2.40	0.57
1:A:18:THR:HA	1:A:22:MET:CE	2.32	0.57
1:A:188:ASP:CG	1:A:257:ARG:HH12	2.08	0.57
1:A:456:HIS:CE1	1:A:511:PHE:HB2	2.40	0.57
1:G:442:LYS:O	1:G:546:PRO:HD3	2.04	0.57
3:C:253:VAL:HA	9:C:2010:3PE:H3H1	1.85	0.57
2:H:197:ALA:HB1	2:H:268:LYS:HG3	1.87	0.57
3:I:199:GLY:O	3:I:203:PHE:HB2	2.05	0.57
1:A:225:VAL:HG12	1:A:226:PRO:O	2.04	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:LEU:N	1:A:244:PRO:CD	2.68	0.56
2:H:201:PRO:HB2	2:H:204:LYS:HG3	1.86	0.56
9:C:2010:3PE:H381	9:C:2010:3PE:H2B1	1.86	0.56
1:G:408:ARG:NE	2:H:126:GLN:OE1	2.28	0.56
1:A:159:ALA:HB1	1:A:160:PRO:HD2	1.87	0.56
3:C:133:LEU:O	3:C:136:ILE:HB	2.06	0.56
3:C:150:TRP:CD1	3:C:150:TRP:C	2.79	0.56
1:G:410:TYR:O	1:G:413:THR:OG1	2.17	0.56
1:G:504:SER:O	1:G:507:SER:HB2	2.05	0.56
3:I:228:GLN:HA	3:I:228:GLN:OE1	2.05	0.56
4:J:36:ALA:O	4:J:40:VAL:HG23	2.05	0.56
2:B:211:THR:HG23	2:B:234:ARG:O	2.05	0.56
1:G:332:ALA:HB3	1:G:348:PHE:CG	2.40	0.56
1:G:396:VAL:HG11	2:H:65:ILE:HB	1.86	0.56
2:H:76:ILE:O	2:H:80:VAL:HG23	2.06	0.56
1:A:148:ALA:HB3	1:A:196:LEU:HD13	1.88	0.56
1:G:127:HIS:NE2	1:G:539:GLU:OE1	2.39	0.56
1:A:95:TRP:HB2	1:A:484:ILE:HG13	1.87	0.56
1:A:241:LEU:HD13	9:D:2011:3PE:C2H	2.35	0.56
1:A:460:MET:O	1:A:460:MET:HG3	2.05	0.56
1:G:270:GLY:O	3:I:109:MET:HG3	2.06	0.56
1:A:387:PHE:CD1	1:A:387:PHE:C	2.78	0.56
2:B:235:LEU:HD11	4:J:11:HIS:H	1.71	0.56
3:I:209:HIS:NE2	3:I:254:TRP:HB2	2.20	0.56
9:G:3012:3PE:H3E1	9:J:3011:3PE:H2F1	1.88	0.56
1:G:225:VAL:HG12	1:G:226:PRO:O	2.06	0.56
2:H:98:SER:HB2	2:H:99:PRO:HD3	1.88	0.56
2:H:132:ALA:HB1	2:H:134:VAL:O	2.06	0.56
1:A:127:HIS:HE1	1:A:300:HIS:CE1	2.24	0.55
1:A:394:GLY:HA3	1:A:423:VAL:HG13	1.88	0.55
2:B:200:VAL:O	2:B:269:VAL:HA	2.06	0.55
3:C:83:PHE:HE1	9:C:2008:3PE:H262	1.71	0.55
3:C:248:HIS:O	3:C:252:VAL:HG23	2.05	0.55
3:C:266:GLN:OXT	3:C:266:GLN:HG2	2.05	0.55
1:G:264:PHE:HA	1:G:271:ASP:H	1.71	0.55
3:I:168:LEU:O	3:I:172:ILE:HG13	2.07	0.55
1:A:212:PHE:O	1:A:216:ARG:HG3	2.06	0.55
1:A:420:PHE:HB2	8:A:1002:HEA:HMD3	1.88	0.55
2:B:221:VAL:HB	2:B:224:PHE:HD2	1.70	0.55
1:G:378:LYS:HE2	10:G:3034:HOH:O	2.05	0.55
1:G:483:TYR:OH	2:H:251:GLN:HB3	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:249:PHE:HE1	2:H:266:THR:HG1	1.54	0.55
3:I:21:ALA:HB2	3:I:54:THR:CG2	2.31	0.55
1:G:315:PRO:HG2	10:H:1132:HOH:O	2.07	0.55
9:I:3010:3PE:H331	9:I:3010:3PE:H231	1.88	0.55
3:C:74:VAL:HG13	4:D:18:ILE:HG12	1.88	0.55
2:H:145:TRP:CD1	2:H:263:MET:HE2	2.41	0.55
3:I:133:LEU:HD23	3:I:185:GLU:HG3	1.86	0.55
1:A:345:GLN:HE22	1:A:408:ARG:NH2	2.01	0.55
1:A:508:PHE:CE2	1:A:512:LEU:HD11	2.42	0.55
1:G:112:ILE:HD12	10:G:3038:HOH:O	2.05	0.55
9:G:3009:3PE:H2E1	9:G:3009:3PE:H3E2	1.88	0.55
1:A:331:TRP:CD1	1:A:331:TRP:C	2.80	0.55
3:C:21:ALA:HB2	3:C:54:THR:CG2	2.30	0.55
3:C:34:LEU:HB3	3:C:39:SER:OG	2.07	0.55
4:J:18:ILE:HG22	4:J:18:ILE:O	2.06	0.55
1:A:396:VAL:CG1	2:B:65:ILE:HB	2.37	0.55
2:H:145:TRP:CE2	2:H:265:ILE:HD11	2.41	0.55
3:I:222:VAL:HA	3:I:225:ILE:HD12	1.88	0.55
1:A:374:SER:HB3	2:B:88:ASN:O	2.07	0.55
1:A:379:THR:HB	1:A:380:PRO:CD	2.29	0.55
8:A:1002:HEA:O11	8:A:1002:HEA:HHC	2.06	0.55
2:B:98:SER:HB2	2:B:99:PRO:CD	2.37	0.55
2:B:98:SER:HB2	2:B:99:PRO:HD3	1.88	0.55
1:G:357:VAL:HB	1:G:358:PRO:CD	2.37	0.55
1:G:532:ASN:OD1	1:G:532:ASN:C	2.43	0.55
3:I:155:LEU:HB2	3:I:164:VAL:HG21	1.87	0.55
1:A:17:PHE:O	1:A:21:PHE:HB2	2.07	0.55
1:A:241:LEU:HD13	9:D:2011:3PE:C2I	2.37	0.55
9:A:2009:3PE:H3E1	9:A:2009:3PE:C2E	2.37	0.55
2:B:145:TRP:CE2	2:B:265:ILE:HD11	2.42	0.54
3:C:141:LEU:O	3:C:142:LEU:C	2.45	0.54
3:C:197:ILE:HG13	3:C:198:TYR:N	2.21	0.54
3:C:228:GLN:OE1	3:C:228:GLN:HA	2.07	0.54
1:G:420:PHE:O	1:G:424:MET:HB2	2.07	0.54
2:H:111:ILE:O	2:H:114:ALA:HB3	2.06	0.54
1:A:143:TYR:O	1:A:146:TYR:HB3	2.07	0.54
1:G:284:HIS:O	1:G:287:VAL:HG22	2.07	0.54
1:G:406:VAL:HG23	2:H:57:LEU:HD23	1.88	0.54
3:I:122:PRO:HB2	3:I:125:ILE:HG13	1.89	0.54
1:A:246:LEU:O	1:A:250:ILE:HG12	2.08	0.54
1:A:308:LYS:HD3	1:A:369:THR:O	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:406:VAL:CG2	2:B:57:LEU:HD23	2.37	0.54
2:B:248:PHE:HE2	2:B:269:VAL:HG12	1.73	0.54
1:G:539:GLU:HG2	1:G:540:TRP:H	1.72	0.54
3:I:220:LEU:CD2	3:I:243:ALA:HB1	2.37	0.54
9:A:2012:3PE:C2H	9:C:2010:3PE:H2I3	2.37	0.54
1:G:342:LEU:HD21	2:H:124:PHE:CD1	2.43	0.54
2:H:218:SER:HA	2:H:229:ASP:HA	1.90	0.54
3:C:151:ALA:O	3:C:164:VAL:HG22	2.07	0.54
2:H:263:MET:N	2:H:264:PRO:HD3	2.23	0.54
3:I:147:ALA:CB	3:I:170:LEU:HD23	2.37	0.54
1:A:406:VAL:HG23	2:B:57:LEU:HD23	1.89	0.54
3:C:226:ARG:HH21	3:C:231:HIS:HB3	1.71	0.54
1:G:105:LEU:O	1:G:110:VAL:HG23	2.07	0.54
2:H:106:ILE:O	2:H:107:VAL:C	2.45	0.54
3:I:152:HIS:CG	3:I:244:ILE:HD13	2.43	0.54
2:H:234:ARG:HD3	10:H:1128:HOH:O	2.07	0.54
1:A:115:LEU:HG	1:A:432:ILE:HG12	1.89	0.54
1:G:64:CYS:HB2	1:G:67:HIS:CD2	2.43	0.54
1:G:127:HIS:CE1	1:G:300:HIS:CE1	2.95	0.54
2:H:252:CYS:HB2	2:H:263:MET:SD	2.46	0.54
1:A:505:PHE:O	1:A:509:LEU:HG	2.07	0.54
1:G:26:HIS:CD2	1:G:26:HIS:C	2.81	0.54
1:G:148:ALA:HB3	1:G:196:LEU:HD13	1.90	0.54
2:H:173:SER:H	2:H:176:VAL:HB	1.73	0.54
1:A:52:ARG:NH1	1:A:498:SER:OG	2.41	0.54
1:A:99:ILE:HD12	8:A:1001:HEA:HBA2	1.90	0.54
1:A:342:LEU:HD21	2:B:124:PHE:CD1	2.43	0.54
1:A:424:MET:HB3	8:A:1001:HEA:HBC1	1.89	0.54
1:G:311:PHE:CD1	1:G:311:PHE:C	2.80	0.54
1:A:91:ASN:OD1	1:A:91:ASN:C	2.46	0.53
1:A:541:THR:HG22	1:A:541:THR:O	2.07	0.53
1:G:282:PHE:CD1	1:G:282:PHE:C	2.79	0.53
2:H:62:LEU:HA	2:H:65:ILE:HD11	1.90	0.53
1:A:298:VAL:O	1:A:299:SER:C	2.45	0.53
1:A:426:LEU:CD2	1:A:464:ALA:HB1	2.38	0.53
9:A:2009:3PE:H2C2	9:A:2009:3PE:C3B	2.38	0.53
2:B:254:GLU:O	2:B:255:LEU:C	2.46	0.53
1:G:247:ALA:HB2	9:G:3009:3PE:C3I	2.37	0.53
1:G:273:VAL:HG13	1:G:335:MET:CE	2.38	0.53
1:G:556:LYS:N	1:G:559:ASP:OD2	2.38	0.53
2:H:220:THR:O	2:H:250:GLY:HA3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:289:LEU:HG	2:H:289:LEU:OXT	2.07	0.53
1:A:484:ILE:O	1:A:484:ILE:HG12	2.07	0.53
2:B:152:GLU:HB3	2:B:283:ARG:HH21	1.74	0.53
1:G:387:PHE:CD1	1:G:387:PHE:C	2.82	0.53
3:C:196:ASN:HB2	10:C:2027:HOH:O	2.08	0.53
4:D:18:ILE:HG22	4:D:21:GLN:HB2	1.91	0.53
1:G:17:PHE:O	1:G:21:PHE:HB2	2.08	0.53
1:G:148:ALA:O	1:G:149:GLY:C	2.47	0.53
1:G:332:ALA:HB3	1:G:348:PHE:CD2	2.42	0.53
2:B:235:LEU:HG	4:J:11:HIS:O	2.09	0.53
3:C:63:VAL:O	3:C:64:THR:C	2.45	0.53
1:G:41:GLY:O	1:G:45:VAL:HB	2.08	0.53
1:G:409:TYR:CD1	1:G:409:TYR:C	2.81	0.53
2:B:161:ILE:HG21	2:B:180:LEU:HD23	1.89	0.53
2:B:220:THR:HB	2:B:227:LYS:HG3	1.90	0.53
1:A:241:LEU:HD13	9:D:2011:3PE:H2H2	1.90	0.53
1:G:273:VAL:HG13	1:G:335:MET:HE1	1.90	0.53
1:A:112:ILE:N	1:A:113:PRO:CD	2.72	0.53
2:B:109:ILE:O	2:B:113:VAL:HG23	2.09	0.53
2:B:173:SER:H	2:B:176:VAL:HB	1.74	0.53
3:C:249:PHE:CE1	9:C:2010:3PE:H3I1	2.44	0.53
1:A:256:ASP:N	1:A:261:THR:OG1	2.41	0.53
1:A:370:MET:SD	1:A:385:LEU:HD21	2.49	0.53
1:A:398:GLY:O	1:A:402:SER:N	2.38	0.53
1:A:560:TRP:CD1	1:A:560:TRP:C	2.83	0.53
4:D:17:ASP:OD1	4:D:17:ASP:C	2.47	0.53
1:G:40:VAL:CG1	1:G:105:LEU:HD22	2.39	0.53
1:G:406:VAL:HG22	2:H:57:LEU:HD23	1.90	0.53
2:H:220:THR:OG1	2:H:221:VAL:N	2.41	0.53
1:A:64:CYS:HB2	1:A:67:HIS:CD2	2.45	0.52
2:B:43:PHE:CD2	2:B:55:HIS:CD2	2.97	0.52
2:B:248:PHE:HE2	2:B:269:VAL:CG1	2.21	0.52
9:C:2010:3PE:H2I2	4:D:36:ALA:HB1	1.91	0.52
9:G:3009:3PE:H2C2	9:G:3009:3PE:H3B2	1.92	0.52
1:A:49:VAL:O	1:A:50:TYR:C	2.47	0.52
3:I:103:LYS:HD3	3:I:103:LYS:O	2.08	0.52
3:I:245:TRP:HE1	9:I:3013:3PE:H322	1.74	0.52
4:J:17:ASP:OD2	10:J:1143:HOH:O	2.19	0.52
4:J:20:GLN:NE2	10:J:1130:HOH:O	2.40	0.52
1:A:263:PHE:HE1	3:C:201:ASN:HD22	1.58	0.52
1:A:407:ASP:O	1:A:408:ARG:C	2.47	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:PHE:O	1:A:424:MET:HB2	2.09	0.52
1:A:493:TRP:HA	1:A:493:TRP:CE3	2.43	0.52
2:B:76:ILE:O	2:B:80:VAL:HG23	2.08	0.52
3:I:245:TRP:NE1	9:I:3013:3PE:H322	2.25	0.52
3:C:249:PHE:HE1	9:C:2010:3PE:H3I1	1.74	0.52
2:B:107:VAL:HG13	2:B:108:PRO:HD3	1.90	0.52
3:C:168:LEU:O	3:C:172:ILE:HG13	2.09	0.52
1:G:294:ALA:O	1:G:298:VAL:HG23	2.10	0.52
3:I:136:ILE:HG21	3:I:181:PHE:CE2	2.45	0.52
1:A:54:GLU:HG2	1:A:63:MET:CE	2.40	0.52
1:A:432:ILE:O	1:A:436:ILE:HG13	2.09	0.52
1:A:486:TYR:HD2	1:A:490:PHE:HB2	1.73	0.52
2:B:192:LEU:HB3	2:B:249:PHE:CD2	2.45	0.52
3:I:112:GLU:HB2	3:I:116:ILE:HB	1.91	0.52
1:A:415:TYR:CD1	1:A:415:TYR:O	2.63	0.52
4:D:50:ASN:O	9:D:2011:3PE:H112	2.09	0.52
1:G:91:ASN:CG	1:G:165:GLN:HE22	2.13	0.52
1:G:213:LEU:HB3	3:I:81:TRP:CH2	2.44	0.52
2:H:182:GLU:HA	2:H:182:GLU:OE1	2.08	0.52
9:I:3010:3PE:H2B1	9:I:3010:3PE:H381	1.92	0.52
3:C:226:ARG:HB3	3:C:231:HIS:HB2	1.92	0.52
1:A:26:HIS:C	1:A:26:HIS:CD2	2.83	0.52
1:A:148:ALA:O	1:A:151:SER:HB2	2.09	0.52
9:A:2009:3PE:H221	3:C:58:TRP:NE1	2.25	0.52
3:C:152:HIS:HB2	3:C:244:ILE:HD13	1.91	0.52
9:C:2013:3PE:H261	9:C:2013:3PE:C3B	2.39	0.52
1:G:52:ARG:HD3	1:G:498:SER:HA	1.91	0.52
1:G:400:VAL:HG11	1:G:410:TYR:HE2	1.75	0.52
1:G:403:GLN:O	1:G:404:ALA:C	2.47	0.52
1:G:539:GLU:HG2	1:G:540:TRP:N	2.23	0.52
1:A:249:ALA:HB2	1:A:278:ILE:CG2	2.39	0.52
2:B:190:PHE:CD1	2:B:190:PHE:C	2.82	0.52
1:G:262:THR:HG22	10:I:3030:HOH:O	2.09	0.52
1:G:331:TRP:CH2	9:I:3010:3PE:H251	2.45	0.52
1:G:433:PHE:HE1	1:G:511:PHE:CZ	2.28	0.52
3:I:130:PRO:HD2	10:I:3038:HOH:O	2.10	0.52
1:A:100:THR:O	1:A:104:ILE:HG13	2.10	0.51
1:A:506:ALA:HA	1:A:509:LEU:HD12	1.93	0.51
1:G:442:LYS:HE2	1:G:539:GLU:O	2.10	0.51
3:I:51:VAL:O	3:I:55:MET:HG3	2.09	0.51
1:A:262:THR:HG22	10:C:2028:HOH:O	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:VAL:CB	1:A:358:PRO:HD3	2.36	0.51
2:B:156:PHE:CD2	2:B:196:THR:HG21	2.45	0.51
2:B:214:ASP:OD1	2:B:214:ASP:N	2.44	0.51
1:G:29:ILE:HD12	1:G:139:ASN:HD22	1.75	0.51
1:G:71:GLY:HA3	1:G:74:LYS:NZ	2.26	0.51
1:G:112:ILE:HB	1:G:113:PRO:HD3	1.92	0.51
1:A:141:LEU:O	1:A:141:LEU:HD12	2.11	0.51
1:A:213:LEU:HB3	3:C:81:TRP:HH2	1.75	0.51
3:C:130:PRO:O	3:C:134:PRO:HB2	2.10	0.51
3:C:212:HIS:HD2	3:C:246:TYR:OH	1.94	0.51
1:G:397:THR:HG21	1:G:419:HIS:CB	2.35	0.51
1:G:445:GLY:HA2	1:G:525:VAL:HG12	1.93	0.51
9:I:3013:3PE:H2B2	9:I:3013:3PE:H3D2	1.93	0.51
1:A:274:LEU:HD22	3:C:103:LYS:HD2	1.91	0.51
2:B:226:VAL:O	2:B:226:VAL:HG23	2.10	0.51
3:C:81:TRP:O	3:C:82:GLY:C	2.46	0.51
1:A:22:MET:HG2	3:C:16:ILE:CA	2.35	0.51
1:A:133:MET:HE3	1:A:211:THR:HG21	1.91	0.51
1:A:436:ILE:HD11	8:A:1001:HEA:H251	1.93	0.51
2:B:98:SER:O	2:B:99:PRO:C	2.48	0.51
2:H:258:ILE:O	2:H:258:ILE:HG22	2.11	0.51
3:I:66:SER:HB2	3:I:71:HIS:CE1	2.46	0.51
3:I:152:HIS:CA	3:I:240:PHE:HE1	2.23	0.51
1:A:525:VAL:HG11	1:A:544:SER:HB3	1.93	0.51
3:C:63:VAL:O	3:C:66:SER:N	2.44	0.51
1:G:91:ASN:HD21	1:G:165:GLN:NE2	2.09	0.51
1:G:318:TYR:O	1:G:319:ALA:C	2.49	0.51
1:G:325:VAL:HG22	9:G:3012:3PE:H3D1	1.93	0.51
3:I:147:ALA:HB1	3:I:170:LEU:HD23	1.92	0.51
3:I:249:PHE:HE1	9:I:3010:3PE:H3I1	1.76	0.51
1:A:105:LEU:O	1:A:110:VAL:HG23	2.11	0.51
1:A:282:PHE:CD1	1:A:282:PHE:C	2.80	0.51
1:G:122:TYR:HD1	1:G:122:TYR:O	1.94	0.51
1:G:127:HIS:CE1	1:G:300:HIS:HE1	2.29	0.51
1:G:422:TYR:CD2	1:G:426:LEU:HD12	2.46	0.51
3:I:107:TYR:OH	4:J:51:ALA:HA	2.11	0.51
3:I:236:LYS:O	3:I:237:HIS:HB3	2.09	0.51
1:G:91:ASN:HD21	1:G:165:GLN:CD	2.14	0.51
3:I:133:LEU:HD23	3:I:185:GLU:CG	2.41	0.51
1:A:65:ALA:HB3	1:A:89:THR:HB	1.93	0.51
2:B:134:VAL:HG12	2:B:135:THR:N	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:152:HIS:O	3:C:156:VAL:HG23	2.11	0.51
3:I:212:HIS:O	3:I:213:VAL:C	2.48	0.51
1:A:216:ARG:NH1	1:A:220:MET:O	2.36	0.51
2:B:160:MET:HB2	2:B:264:PRO:HD2	1.93	0.51
3:C:152:HIS:CA	3:C:240:PHE:HE1	2.20	0.51
1:G:24:THR:HG21	3:I:13:PRO:O	2.11	0.51
1:G:308:LYS:NZ	1:G:371:TRP:O	2.32	0.51
1:G:416:VAL:O	1:G:419:HIS:N	2.39	0.51
1:A:199:ALA:HA	9:A:2009:3PE:H3D1	1.92	0.50
1:A:450:GLU:O	1:A:454:LYS:HG3	2.11	0.50
2:H:145:TRP:CZ2	2:H:265:ILE:HD11	2.46	0.50
3:I:161:ARG:HH22	3:I:232:PHE:H	1.58	0.50
9:I:3013:3PE:H3H2	9:I:3013:3PE:H2E1	1.92	0.50
4:J:12:VAL:CG1	4:J:15:SER:HB2	2.41	0.50
1:A:74:LYS:H	1:A:74:LYS:HD2	1.76	0.50
1:A:125:PRO:O	1:A:126:LEU:C	2.49	0.50
1:G:148:ALA:CB	1:G:196:LEU:HD13	2.42	0.50
2:H:158:SER:OG	2:H:194:THR:OG1	2.25	0.50
1:A:74:LYS:H	1:A:74:LYS:CD	2.24	0.50
1:A:347:TYR:CE2	9:D:2011:3PE:H252	2.46	0.50
3:C:120:PHE:CD1	3:C:120:PHE:C	2.85	0.50
3:C:161:ARG:HH22	3:C:232:PHE:H	1.59	0.50
1:G:127:HIS:HE1	1:G:300:HIS:CE1	2.29	0.50
1:G:323:ILE:HG22	1:G:324:GLY:N	2.26	0.50
1:G:243:LEU:N	1:G:244:PRO:CD	2.74	0.50
1:G:377:LEU:HD21	2:H:80:VAL:HG13	1.94	0.50
2:H:221:VAL:O	2:H:222:PRO:C	2.50	0.50
3:I:101:PHE:CE2	3:I:261:ILE:HG12	2.47	0.50
1:A:213:LEU:CD1	3:C:81:TRP:CZ2	2.95	0.50
1:A:394:GLY:O	1:A:397:THR:HB	2.12	0.50
2:B:211:THR:HG22	2:B:212:GLY:N	2.26	0.50
1:G:274:LEU:O	1:G:277:HIS:N	2.45	0.50
1:G:450:GLU:OE2	1:G:454:LYS:HE3	2.12	0.50
2:B:145:TRP:CZ2	2:B:265:ILE:HD11	2.46	0.50
1:G:274:LEU:HD22	3:I:103:LYS:HD2	1.92	0.50
1:G:379:THR:CB	1:G:380:PRO:HD3	2.32	0.50
1:G:409:TYR:C	1:G:409:TYR:HD1	2.14	0.50
1:G:427:GLY:O	1:G:430:PHE:HB2	2.11	0.50
1:A:137:ARG:NH2	9:A:2009:3PE:H112	2.23	0.50
3:C:124:GLY:CA	1:G:557:ARG:HH12	2.25	0.50
1:A:481:ARG:O	1:A:482:ARG:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:62:LEU:HA	2:B:65:ILE:HD11	1.94	0.49
3:C:201:ASN:O	3:C:202:PHE:C	2.49	0.49
2:H:143:TRP:CD1	2:H:143:TRP:N	2.79	0.49
2:H:158:SER:HG	2:H:194:THR:HG1	1.60	0.49
2:H:221:VAL:HB	2:H:224:PHE:HD2	1.77	0.49
3:I:249:PHE:CE1	9:I:3010:3PE:H3I1	2.47	0.49
1:A:52:ARG:HD3	1:A:498:SER:HA	1.93	0.49
3:C:136:ILE:HG21	3:C:181:PHE:CE2	2.48	0.49
2:H:152:GLU:HB2	2:H:154:ILE:HD12	1.94	0.49
3:I:155:LEU:O	3:I:155:LEU:HG	2.12	0.49
3:I:227:VAL:HG22	3:I:232:PHE:HD2	1.77	0.49
1:A:427:GLY:O	1:A:430:PHE:HB2	2.13	0.49
1:A:556:LYS:N	1:A:559:ASP:OD2	2.45	0.49
1:G:350:MET:HA	1:G:353:MET:CE	2.42	0.49
1:G:474:LEU:HD11	1:G:494:ASN:ND2	2.27	0.49
3:C:147:ALA:CB	3:C:170:LEU:HD23	2.42	0.49
3:C:221:LEU:O	3:C:225:ILE:HG13	2.11	0.49
1:G:100:THR:O	1:G:104:ILE:HG13	2.12	0.49
2:H:160:MET:HG3	2:H:264:PRO:HG2	1.95	0.49
1:A:300:HIS:H	1:A:300:HIS:CD2	2.31	0.49
3:C:249:PHE:O	3:C:253:VAL:HG23	2.13	0.49
1:G:241:LEU:HD13	9:J:3011:3PE:C2I	2.42	0.49
1:G:336:TYR:HD2	1:G:407:ASP:OD2	1.96	0.49
1:G:477:GLN:NE2	2:H:42:GLY:O	2.46	0.49
1:G:493:TRP:HA	1:G:493:TRP:HE3	1.73	0.49
3:I:152:HIS:HB2	3:I:244:ILE:HD13	1.94	0.49
2:B:78:TYR:CD1	2:B:78:TYR:C	2.85	0.49
3:C:212:HIS:O	3:C:213:VAL:C	2.51	0.49
2:H:138:VAL:HG23	2:H:208:VAL:HG13	1.93	0.49
1:A:42:LEU:O	1:A:43:ILE:C	2.49	0.49
1:G:222:MET:HE1	9:G:3012:3PE:O32	2.13	0.49
1:G:476:ARG:HD3	2:H:41:THR:O	2.12	0.49
2:H:71:PHE:CD1	2:H:71:PHE:C	2.85	0.49
2:H:214:ASP:OD1	2:H:214:ASP:N	2.46	0.49
3:I:114:PRO:O	3:I:115:ILE:C	2.48	0.49
9:A:2012:3PE:H2D1	9:D:2011:3PE:C2I	2.42	0.49
3:C:152:HIS:CG	3:C:244:ILE:HD13	2.48	0.49
1:G:239:ILE:HG12	1:G:289:ILE:HD13	1.94	0.49
2:H:152:GLU:HB2	2:H:154:ILE:CD1	2.43	0.49
3:I:197:ILE:O	3:I:198:TYR:C	2.50	0.49
9:I:3010:3PE:C2I	9:I:3013:3PE:H3H1	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:LEU:HD22	1:A:282:PHE:CD2	2.47	0.49
1:G:539:GLU:HA	1:G:542:LEU:HD12	1.95	0.49
9:G:3009:3PE:H2C2	9:G:3009:3PE:C3A	2.40	0.49
3:I:162:ARG:HG3	3:I:163:ASP:H	1.76	0.49
1:A:300:HIS:CD2	1:A:300:HIS:N	2.79	0.49
2:B:71:PHE:CE1	2:B:75:LEU:HD11	2.48	0.49
2:B:142:GLN:HG3	2:B:214:ASP:OD2	2.12	0.49
3:C:74:VAL:HG23	3:C:75:VAL:N	2.27	0.49
3:C:199:GLY:O	3:C:203:PHE:HB2	2.12	0.49
1:G:133:MET:CE	1:G:211:THR:HG21	2.43	0.49
3:I:211:PHE:O	3:I:215:VAL:HG23	2.13	0.49
1:A:482:ARG:HD3	2:B:255:LEU:HB2	1.94	0.48
2:B:137:LYS:HZ3	4:J:11:HIS:HB2	1.78	0.48
1:G:44:SER:HB2	1:G:105:LEU:HB2	1.94	0.48
1:G:91:ASN:ND2	1:G:165:GLN:NE2	2.61	0.48
4:J:11:HIS:O	4:J:12:VAL:HG23	2.12	0.48
1:A:74:LYS:HD2	1:A:74:LYS:N	2.28	0.48
1:A:127:HIS:HB3	1:A:226:PRO:CG	2.29	0.48
1:A:396:VAL:HG13	2:B:65:ILE:HB	1.95	0.48
8:A:1001:HEA:H263	8:A:1001:HEA:C12	2.43	0.48
2:B:141:TYR:HE2	2:B:146:GLY:HA3	1.77	0.48
2:B:175:GLU:HA	2:B:178:GLN:NE2	2.28	0.48
2:B:221:VAL:CB	2:B:224:PHE:HD2	2.26	0.48
3:C:255:LEU:HB3	9:D:2011:3PE:C3I	2.37	0.48
9:C:2013:3PE:H2G2	4:D:37:VAL:HG23	1.95	0.48
1:G:65:ALA:HB3	1:G:89:THR:HB	1.94	0.48
1:G:387:PHE:O	1:G:388:LEU:C	2.52	0.48
1:A:347:TYR:CE1	1:A:351:ALA:HB2	2.48	0.48
2:B:129:ILE:HD13	2:B:237:GLN:HB3	1.95	0.48
2:H:120:LEU:N	2:H:121:PRO:HD2	2.29	0.48
2:H:152:GLU:HB3	2:H:283:ARG:HH21	1.78	0.48
4:D:18:ILE:CG2	4:D:21:GLN:HB2	2.43	0.48
9:G:3009:3PE:H3E1	9:G:3009:3PE:C2E	2.39	0.48
2:H:192:LEU:HB3	2:H:249:PHE:CD2	2.48	0.48
3:I:32:ALA:O	3:I:36:MET:HG3	2.13	0.48
1:A:314:LEU:HD12	1:A:314:LEU:HA	1.77	0.48
1:A:329:VAL:HB	1:A:347:TYR:OH	2.13	0.48
2:B:182:GLU:OE1	2:B:182:GLU:HA	2.13	0.48
2:B:263:MET:N	2:B:264:PRO:CD	2.76	0.48
1:G:191:ILE:HG21	1:G:254:LEU:HD13	1.95	0.48
2:H:252:CYS:HB2	2:H:263:MET:HG3	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:LEU:CB	1:A:315:PRO:HD3	2.43	0.48
1:A:525:VAL:CG1	1:A:544:SER:HB3	2.44	0.48
4:J:18:ILE:HG22	4:J:21:GLN:HB2	1.95	0.48
1:A:54:GLU:HG2	1:A:63:MET:HE2	1.95	0.48
1:A:81:TRP:CG	1:A:82:PRO:HD2	2.49	0.48
3:C:177:LEU:O	3:C:178:PHE:C	2.52	0.48
2:H:252:CYS:HB2	2:H:263:MET:CG	2.44	0.48
3:I:214:ILE:O	3:I:218:ILE:HG12	2.14	0.48
3:I:231:HIS:O	9:I:3008:3PE:H121	2.14	0.48
1:A:154:VAL:O	1:A:155:ALA:C	2.52	0.48
1:A:374:SER:HA	2:B:83:PHE:O	2.14	0.48
2:B:220:THR:OG1	2:B:221:VAL:N	2.47	0.48
3:C:209:HIS:NE2	3:C:254:TRP:HB2	2.29	0.48
1:G:396:VAL:HG13	2:H:65:ILE:HG21	1.95	0.48
1:A:26:HIS:NE2	1:A:27:LYS:HG3	2.29	0.48
1:A:477:GLN:HA	1:A:477:GLN:NE2	2.29	0.48
3:C:253:VAL:HG22	9:C:2010:3PE:H3H1	1.96	0.48
1:G:46:ALA:O	1:G:49:VAL:HG12	2.14	0.48
1:G:111:VAL:HG11	1:G:290:ILE:HG23	1.96	0.48
1:G:284:HIS:N	1:G:285:PRO:CD	2.77	0.48
3:I:128:PHE:O	3:I:130:PRO:HD3	2.13	0.48
1:A:106:MET:CB	8:A:1001:HEA:HAC	2.36	0.47
1:A:112:ILE:HD12	10:A:2037:HOH:O	2.13	0.47
1:A:556:LYS:HD2	1:A:556:LYS:HA	1.52	0.47
3:C:62:VAL:HG12	9:C:2008:3PE:H31	1.93	0.47
3:C:135:LEU:O	3:C:139:LEU:HG	2.14	0.47
3:C:245:TRP:NE1	9:C:2013:3PE:H322	2.29	0.47
1:G:397:THR:O	1:G:400:VAL:HB	2.13	0.47
1:G:456:HIS:O	1:G:457:PHE:C	2.53	0.47
1:G:498:SER:O	1:G:502:PHE:CD2	2.65	0.47
1:G:538:LEU:HD21	1:G:560:TRP:HE3	1.79	0.47
2:H:137:LYS:HB3	2:H:148:GLU:HB2	1.95	0.47
1:A:137:ARG:NE	9:A:2009:3PE:O14	2.42	0.47
2:B:209:GLN:OE1	4:J:11:HIS:HD2	1.96	0.47
1:G:280:TRP:O	1:G:331:TRP:HB2	2.14	0.47
1:A:473:PHE:O	1:A:474:LEU:C	2.49	0.47
3:C:74:VAL:O	3:C:77:LEU:N	2.46	0.47
3:C:131:TRP:HE3	3:C:135:LEU:HD22	1.79	0.47
1:G:62:PHE:CE2	1:G:82:PRO:HD3	2.49	0.47
1:G:153:ALA:O	1:G:156:SER:HB3	2.13	0.47
1:G:168:SER:HB3	1:G:170:ILE:CD1	2.44	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:129:ILE:HA	2:H:130:PRO:HD2	1.67	0.47
2:H:248:PHE:HE2	2:H:269:VAL:CG1	2.27	0.47
3:I:74:VAL:CG1	4:J:18:ILE:HG12	2.44	0.47
1:A:285:PRO:O	1:A:289:ILE:HG13	2.14	0.47
1:A:455:LEU:HD23	1:A:510:PHE:CE2	2.49	0.47
1:A:511:PHE:CE1	1:A:515:ILE:HD11	2.48	0.47
8:A:1002:HEA:C22	2:B:68:ILE:HD13	2.44	0.47
2:B:107:VAL:HG12	2:B:108:PRO:HD3	1.97	0.47
1:A:418:ALA:O	1:A:419:HIS:C	2.53	0.47
2:B:35:ARG:HG2	2:B:36:PRO:O	2.14	0.47
3:C:80:ARG:HH22	9:C:2013:3PE:C11	2.26	0.47
1:G:414:TYR:OH	10:G:3020:HOH:O	2.20	0.47
1:G:505:PHE:O	1:G:509:LEU:HG	2.14	0.47
1:G:511:PHE:CE1	1:G:515:ILE:HD11	2.49	0.47
1:A:109:PHE:O	1:A:146:TYR:OH	2.30	0.47
9:A:2012:3PE:H3E1	9:D:2011:3PE:H2I3	1.95	0.47
1:G:456:HIS:CE1	1:G:511:PHE:HB2	2.49	0.47
1:G:551:PHE:CD1	1:G:555:PRO:HD3	2.49	0.47
2:H:78:TYR:CD1	2:H:78:TYR:C	2.88	0.47
2:H:248:PHE:HE2	2:H:269:VAL:HG12	1.80	0.47
9:I:3013:3PE:C3H	9:I:3013:3PE:H2E1	2.44	0.47
1:A:66:GLU:OE2	1:A:89:THR:OG1	2.31	0.47
1:A:176:PRO:CB	1:A:177:PRO:HA	2.44	0.47
1:A:424:MET:O	1:A:429:VAL:HG23	2.15	0.47
1:A:447:GLN:HG3	1:A:448:TYR:N	2.30	0.47
1:A:469:PHE:N	1:A:470:PRO:CD	2.76	0.47
1:A:470:PRO:HA	1:A:473:PHE:CD2	2.49	0.47
2:B:137:LYS:HE2	10:B:1072:HOH:O	2.14	0.47
3:C:72:THR:O	3:C:73:PRO:C	2.53	0.47
1:G:506:ALA:HA	1:G:509:LEU:HD12	1.96	0.47
2:H:164:PRO:HB3	10:H:1122:HOH:O	2.15	0.47
3:I:226:ARG:HE	3:I:231:HIS:CD2	2.32	0.47
1:A:91:ASN:ND2	1:A:165:GLN:HE22	2.13	0.47
9:A:2012:3PE:H2D1	9:D:2011:3PE:H2I2	1.97	0.47
3:C:147:ALA:HB1	3:C:170:LEU:HD23	1.96	0.47
1:G:48:THR:CG2	1:G:102:HIS:CE1	2.97	0.47
1:G:329:VAL:HB	1:G:347:TYR:OH	2.14	0.47
1:G:370:MET:SD	1:G:385:LEU:HD21	2.54	0.47
2:H:136:VAL:HG11	2:H:198:MET:CE	2.37	0.47
3:I:141:LEU:O	3:I:142:LEU:C	2.53	0.47
3:I:201:ASN:O	3:I:202:PHE:C	2.53	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:126:LEU:HD23	10:A:2049:HOH:O	2.14	0.47
1:A:135:PHE:CE1	3:C:79:LEU:HD23	2.49	0.47
2:B:152:GLU:HB2	2:B:154:ILE:HD12	1.97	0.47
2:B:172:MET:HE1	2:B:187:ARG:O	2.15	0.47
1:G:86:GLU:O	2:H:171:ARG:NH1	2.48	0.47
1:G:112:ILE:H	1:G:113:PRO:HD2	1.78	0.47
1:G:312:GLY:HA2	10:H:1132:HOH:O	2.14	0.47
1:G:344:GLN:O	1:G:348:PHE:HD2	1.98	0.47
1:G:350:MET:HA	1:G:353:MET:HE3	1.97	0.47
1:G:378:LYS:O	1:G:379:THR:C	2.52	0.47
1:G:416:VAL:O	1:G:419:HIS:HB3	2.14	0.47
3:I:221:LEU:O	3:I:225:ILE:HG13	2.14	0.47
2:H:138:VAL:HG23	2:H:208:VAL:CG1	2.45	0.47
1:A:415:TYR:CD1	1:A:415:TYR:C	2.89	0.46
2:B:86:LYS:HE3	10:B:1054:HOH:O	2.15	0.46
2:B:143:TRP:HZ2	2:B:257:GLY:HA3	1.78	0.46
4:D:12:VAL:HG12	4:D:15:SER:HB2	1.97	0.46
1:G:213:LEU:CB	3:I:81:TRP:CH2	2.98	0.46
2:H:200:VAL:N	2:H:268:LYS:O	2.47	0.46
1:A:491:ALA:O	1:A:492:THR:C	2.54	0.46
9:A:2009:3PE:H221	3:C:58:TRP:CE2	2.50	0.46
1:G:307:LYS:HD2	1:G:374:SER:OG	2.16	0.46
1:G:556:LYS:HD2	1:G:556:LYS:HA	1.68	0.46
3:I:76:ARG:O	3:I:80:ARG:HG3	2.15	0.46
1:A:428:ALA:O	1:A:432:ILE:HG13	2.15	0.46
1:G:85:VAL:HG23	10:G:3116:HOH:O	2.15	0.46
1:G:241:LEU:HD13	9:J:3011:3PE:H2I1	1.96	0.46
1:G:246:LEU:HD22	1:G:282:PHE:CZ	2.50	0.46
2:H:194:THR:HG22	2:H:266:THR:CB	2.45	0.46
1:A:539:GLU:HA	1:A:542:LEU:HD12	1.98	0.46
2:B:209:GLN:CG	2:B:235:LEU:HD22	2.45	0.46
1:G:26:HIS:HD2	1:G:122:TYR:HA	1.80	0.46
1:G:470:PRO:O	1:G:473:PHE:HB2	2.16	0.46
9:G:3012:3PE:H3C1	9:J:3011:3PE:H2I1	1.96	0.46
1:A:424:MET:CE	8:A:1002:HEA:HMD3	2.46	0.46
1:G:27:LYS:HZ3	1:G:27:LYS:HB2	1.79	0.46
1:G:198:GLY:O	1:G:202:ILE:HD12	2.16	0.46
1:G:401:LEU:O	1:G:402:SER:C	2.54	0.46
2:H:234:ARG:NH1	3:I:114:PRO:HG3	2.30	0.46
4:J:12:VAL:HG12	4:J:12:VAL:O	2.15	0.46
1:G:538:LEU:HD21	1:G:560:TRP:CE3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:G:1002:HEA:O11	8:G:1002:HEA:CHC	2.64	0.46
1:A:392:THR:O	1:A:393:VAL:C	2.54	0.46
1:A:411:HIS:CD2	1:A:412:ASP:HB2	2.51	0.46
1:G:264:PHE:HB3	1:G:272:PRO:HA	1.97	0.46
1:A:88:CYS:O	1:A:90:PRO:HD3	2.14	0.46
1:G:525:VAL:CG1	1:G:544:SER:HB3	2.46	0.46
2:H:71:PHE:O	2:H:75:LEU:HD12	2.15	0.46
2:H:97:ASN:O	2:H:101:GLU:HG3	2.16	0.46
3:I:196:ASN:HD21	3:I:199:GLY:HA3	1.80	0.46
1:A:280:TRP:O	1:A:331:TRP:HB2	2.16	0.46
2:B:251:GLN:O	2:B:252:CYS:C	2.54	0.46
3:C:220:LEU:CD2	3:C:243:ALA:HB1	2.46	0.46
1:G:206:ILE:HG22	1:G:207:ASN:N	2.31	0.46
1:G:307:LYS:HA	1:G:534:HIS:CG	2.51	0.46
3:I:172:ILE:CD1	3:I:221:LEU:HA	2.46	0.46
1:A:107:MET:H	1:A:107:MET:HG2	1.45	0.46
1:A:239:ILE:HG12	1:A:289:ILE:CD1	2.38	0.46
1:A:510:PHE:O	1:A:514:VAL:HG23	2.16	0.46
3:C:46:ILE:O	3:C:47:GLY:C	2.54	0.46
3:C:66:SER:HB2	3:C:71:HIS:CE1	2.50	0.46
3:C:186:TYR:O	3:C:187:SER:C	2.54	0.46
1:G:199:ALA:HA	9:G:3009:3PE:H3D1	1.97	0.46
1:G:396:VAL:HG11	2:H:65:ILE:HD12	1.97	0.46
1:A:70:SER:C	1:A:71:GLY:O	2.54	0.45
2:B:37:GLN:O	2:B:38:PRO:C	2.51	0.45
2:B:211:THR:HG22	2:B:212:GLY:H	1.80	0.45
1:G:122:TYR:CD1	1:G:122:TYR:C	2.89	0.45
1:A:347:TYR:CD2	9:D:2011:3PE:H252	2.51	0.45
2:B:59:GLY:HA2	10:B:1016:HOH:O	2.16	0.45
1:G:148:ALA:O	1:G:151:SER:N	2.49	0.45
1:G:212:PHE:CD1	1:G:212:PHE:C	2.90	0.45
3:I:115:ILE:H	3:I:115:ILE:HG13	1.55	0.45
3:I:209:HIS:CE1	3:I:254:TRP:HB2	2.52	0.45
1:A:311:PHE:CD1	1:A:311:PHE:C	2.90	0.45
1:A:357:VAL:CB	1:A:358:PRO:CD	2.91	0.45
1:A:422:TYR:OH	1:A:469:PHE:HD1	1.98	0.45
1:A:426:LEU:HD21	1:A:464:ALA:HB1	1.98	0.45
1:A:469:PHE:N	1:A:470:PRO:HD2	2.31	0.45
9:A:2009:3PE:H3A1	9:A:2009:3PE:C2C	2.41	0.45
1:G:556:LYS:HB3	1:G:559:ASP:OD1	2.16	0.45
1:A:299:SER:O	1:A:302:ILE:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:ILE:HG22	8:A:1001:HEA:H252	1.95	0.45
1:G:328:PHE:HA	10:G:3100:HOH:O	2.15	0.45
2:H:209:GLN:CD	2:H:235:LEU:HD22	2.37	0.45
4:J:47:ALA:CA	9:J:3011:3PE:H321	2.45	0.45
9:C:2013:3PE:H261	9:C:2013:3PE:H3A2	1.99	0.45
1:G:198:GLY:HA2	1:G:243:LEU:HD12	1.98	0.45
1:G:243:LEU:N	1:G:243:LEU:HD23	2.32	0.45
1:G:384:ALA:O	1:G:388:LEU:HG	2.16	0.45
3:I:20:MET:HG2	3:I:54:THR:OG1	2.16	0.45
3:I:133:LEU:N	3:I:134:PRO:HD2	2.26	0.45
4:J:39:ILE:O	4:J:42:ALA:HB3	2.16	0.45
1:A:26:HIS:HB3	1:A:132:ASP:OD1	2.17	0.45
1:A:262:THR:HG21	3:C:196:ASN:N	2.31	0.45
1:A:326:LEU:O	1:A:328:PHE:N	2.50	0.45
8:A:1002:HEA:HMC1	8:A:1002:HEA:CBC	2.38	0.45
1:G:137:ARG:NH2	9:G:3009:3PE:H112	2.31	0.45
1:G:479:MET:HA	1:G:480:PRO:HD3	1.82	0.45
3:I:136:ILE:HG21	3:I:181:PHE:HE2	1.81	0.45
4:J:51:ALA:O	9:J:3011:3PE:H122	2.16	0.45
3:C:52:LEU:HD23	3:C:55:MET:HE2	1.99	0.45
1:G:300:HIS:CD2	1:G:300:HIS:N	2.85	0.45
2:H:136:VAL:HG12	2:H:137:LYS:N	2.32	0.45
2:H:195:ASP:OD1	2:H:196:THR:N	2.50	0.45
3:I:74:VAL:HG12	4:J:18:ILE:CG2	2.47	0.45
4:J:46:LEU:O	4:J:47:ALA:C	2.52	0.45
1:A:213:LEU:HD12	3:C:81:TRP:CZ2	2.52	0.45
1:A:225:VAL:HG13	1:A:226:PRO:HD2	1.99	0.45
2:B:231:VAL:O	2:B:232:PRO:C	2.55	0.45
3:C:52:LEU:HD22	9:C:2008:3PE:H3C2	1.99	0.45
3:C:252:VAL:HG12	9:C:2010:3PE:H3H2	1.98	0.45
1:G:155:ALA:HB1	10:G:3085:HOH:O	2.15	0.45
1:G:420:PHE:HB2	8:G:1002:HEA:HMD3	1.99	0.45
2:H:173:SER:O	2:H:174:PRO:C	2.55	0.45
3:I:135:LEU:O	3:I:139:LEU:HG	2.17	0.45
1:A:163:ASN:HA	3:I:159:ASN:HB3	1.99	0.45
2:B:120:LEU:O	2:B:123:LEU:N	2.47	0.45
3:C:12:LEU:HA	3:C:13:PRO:HD2	1.80	0.45
1:G:84:ALA:O	1:G:85:VAL:C	2.55	0.45
1:G:379:THR:O	1:G:380:PRO:C	2.53	0.45
2:H:134:VAL:CG1	2:H:135:THR:N	2.80	0.45
2:H:176:VAL:O	2:H:180:LEU:HG	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:176:ALA:O	3:I:179:THR:HB	2.17	0.45
3:C:245:TRP:HE1	9:C:2013:3PE:H322	1.81	0.45
1:G:463:GLY:CA	1:G:503:LEU:HD23	2.47	0.45
3:I:122:PRO:HB2	3:I:125:ILE:CG1	2.47	0.45
1:A:45:VAL:HG21	8:A:1001:HEA:H162	1.98	0.44
2:B:171:ARG:O	2:B:176:VAL:HG21	2.17	0.44
2:B:217:HIS:HB2	2:B:230:ALA:HB3	1.98	0.44
4:D:17:ASP:OD1	4:D:18:ILE:N	2.50	0.44
1:G:44:SER:HB2	1:G:105:LEU:CB	2.47	0.44
1:G:192:PHE:CE1	3:I:29:LEU:HD22	2.52	0.44
1:G:424:MET:O	1:G:429:VAL:HG23	2.17	0.44
4:J:18:ILE:HG23	4:J:21:GLN:OE1	2.16	0.44
1:A:170:ILE:O	2:B:255:LEU:HD23	2.17	0.44
1:A:249:ALA:HB2	1:A:278:ILE:HG22	1.98	0.44
2:B:141:TYR:O	2:B:142:GLN:C	2.53	0.44
3:C:253:VAL:HG22	9:C:2010:3PE:C3I	2.47	0.44
1:G:257:ARG:HH11	1:G:257:ARG:HD3	1.55	0.44
1:G:262:THR:OG1	1:G:268:GLY:HA3	2.17	0.44
1:G:331:TRP:HH2	9:I:3010:3PE:H251	1.81	0.44
1:A:379:THR:HA	1:A:382:LEU:HD12	1.98	0.44
2:B:129:ILE:HA	2:B:130:PRO:HD2	1.69	0.44
2:B:221:VAL:O	2:B:222:PRO:C	2.55	0.44
4:D:39:ILE:HD13	9:D:2011:3PE:H2G2	1.98	0.44
1:G:81:TRP:CE3	1:G:82:PRO:HD2	2.52	0.44
1:G:176:PRO:HB2	1:G:177:PRO:HA	1.99	0.44
2:H:122:VAL:O	2:H:126:GLN:HG2	2.18	0.44
2:H:195:ASP:OD1	2:H:196:THR:OG1	2.33	0.44
3:I:127:THR:HG21	3:I:266:GLN:HA	1.99	0.44
1:A:341:SER:HB3	1:A:344:GLN:HG3	1.98	0.44
1:G:54:GLU:HG2	1:G:63:MET:CE	2.47	0.44
1:G:129:GLY:HA2	1:G:551:PHE:CE2	2.53	0.44
1:G:396:VAL:CG1	2:H:65:ILE:HD12	2.47	0.44
3:I:103:LYS:HD3	3:I:103:LYS:C	2.38	0.44
3:I:149:THR:O	3:I:152:HIS:HB3	2.17	0.44
9:A:2012:3PE:C3E	9:D:2011:3PE:H2I3	2.48	0.44
2:B:161:ILE:CD1	2:B:180:LEU:HD23	2.48	0.44
2:B:218:SER:HA	2:B:229:ASP:HA	2.00	0.44
3:C:80:ARG:NH2	9:C:2013:3PE:O13	2.27	0.44
3:C:140:ILE:CD1	3:C:177:LEU:HD23	2.47	0.44
2:H:98:SER:HB2	2:H:99:PRO:CD	2.47	0.44
2:H:169:ASP:O	2:H:170:ASN:HB2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:228:GLN:HG3	2:H:229:ASP:N	2.29	0.44
9:I:3010:3PE:H362	9:I:3010:3PE:H391	1.63	0.44
1:A:62:PHE:CE2	1:A:82:PRO:HD3	2.53	0.44
1:A:314:LEU:HB3	1:A:315:PRO:CD	2.45	0.44
1:G:168:SER:HB3	1:G:170:ILE:HD11	2.00	0.44
1:G:422:TYR:OH	1:G:469:PHE:HD1	2.00	0.44
4:J:40:VAL:O	4:J:44:ILE:HG13	2.17	0.44
4:J:42:ALA:O	4:J:43:LEU:C	2.55	0.44
1:A:36:THR:O	1:A:40:VAL:HG23	2.18	0.44
1:A:417:VAL:HA	1:A:420:PHE:CE2	2.53	0.44
1:A:477:GLN:NE2	2:B:42:GLY:O	2.51	0.44
9:A:2012:3PE:H3C1	9:D:2011:3PE:H2I1	1.98	0.44
3:C:212:HIS:O	3:C:215:VAL:N	2.50	0.44
3:C:246:TYR:O	3:C:247:TRP:C	2.55	0.44
1:G:357:VAL:CB	1:G:358:PRO:CD	2.96	0.44
2:H:275:TYR:O	2:H:279:LEU:HG	2.17	0.44
3:I:2:ALA:HB3	3:I:5:LYS:HD3	2.00	0.44
3:I:83:PHE:CE1	9:I:3008:3PE:H262	2.43	0.44
2:B:132:ALA:HB1	2:B:134:VAL:O	2.18	0.44
4:D:47:ALA:CA	9:D:2011:3PE:H321	2.46	0.44
1:G:159:ALA:HB1	1:G:160:PRO:HD2	1.99	0.44
1:G:450:GLU:O	1:G:454:LYS:HG3	2.17	0.44
2:H:45:PRO:HB3	2:H:244:ARG:NH2	2.31	0.44
3:I:20:MET:HE3	3:I:20:MET:HB2	1.96	0.44
3:I:73:PRO:HD2	4:J:14:GLY:HA2	2.00	0.44
1:A:153:ALA:HB2	1:A:193:ALA:HB1	2.00	0.44
1:A:449:PRO:O	1:A:450:GLU:C	2.55	0.44
1:G:148:ALA:O	1:G:151:SER:HB2	2.18	0.44
1:A:346:SER:O	1:A:350:MET:HG3	2.18	0.43
1:A:380:PRO:HG3	1:A:437:TYR:HB3	1.99	0.43
1:G:81:TRP:CG	1:G:82:PRO:HD2	2.53	0.43
1:G:161:GLY:O	1:G:162:GLY:C	2.56	0.43
1:G:362:LYS:NZ	10:G:3057:HOH:O	2.37	0.43
1:G:398:GLY:O	1:G:402:SER:N	2.38	0.43
1:G:449:PRO:O	1:G:450:GLU:C	2.54	0.43
1:G:477:GLN:NE2	1:G:477:GLN:HA	2.33	0.43
3:I:212:HIS:HD2	3:I:246:TYR:OH	2.01	0.43
3:I:266:GLN:HG2	3:I:266:GLN:OXT	2.18	0.43
1:G:421:HIS:O	1:G:425:SER:N	2.45	0.43
1:G:470:PRO:HA	1:G:473:PHE:CD2	2.53	0.43
3:I:77:LEU:O	3:I:77:LEU:HG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:255:LEU:HB3	9:J:3011:3PE:C3I	2.42	0.43
1:A:307:LYS:HA	1:A:534:HIS:CG	2.52	0.43
3:C:72:THR:CG2	3:C:73:PRO:N	2.77	0.43
1:G:22:MET:CG	3:I:16:ILE:HD12	2.49	0.43
2:H:206:VAL:HB	2:H:240:PHE:CE1	2.53	0.43
1:A:213:LEU:HB3	3:C:81:TRP:CH2	2.50	0.43
1:A:218:PRO:HB3	1:A:557:ARG:HH21	1.84	0.43
1:A:456:HIS:O	1:A:457:PHE:C	2.57	0.43
1:G:176:PRO:CB	1:G:177:PRO:HA	2.48	0.43
1:G:263:PHE:HE1	3:I:201:ASN:HD22	1.64	0.43
1:A:307:LYS:NZ	10:A:2068:HOH:O	2.48	0.43
1:G:48:THR:HG22	1:G:102:HIS:CE1	2.53	0.43
1:G:314:LEU:HB3	1:G:315:PRO:HD3	2.00	0.43
1:G:401:LEU:HD13	8:G:1002:HEA:HBA2	2.00	0.43
1:G:546:PRO:HA	1:G:547:PRO:HD3	1.93	0.43
3:I:104:HIS:HB2	10:I:3022:HOH:O	2.17	0.43
1:A:361:ILE:HD11	2:B:105:THR:OG1	2.18	0.43
3:C:168:LEU:O	3:C:169:ALA:C	2.57	0.43
4:D:18:ILE:HA	4:D:21:GLN:OE1	2.19	0.43
1:G:239:ILE:HG12	1:G:289:ILE:CD1	2.49	0.43
1:G:401:LEU:CD1	1:G:416:VAL:HG22	2.49	0.43
2:H:156:PHE:HD2	2:H:196:THR:HG21	1.82	0.43
3:I:180:VAL:O	3:I:183:ALA:HB3	2.19	0.43
4:J:16:MET:HG2	4:J:17:ASP:N	2.34	0.43
1:A:238:LEU:HD22	1:A:328:PHE:CE2	2.54	0.43
2:B:289:LEU:HG	2:B:289:LEU:OXT	2.17	0.43
1:G:122:TYR:HD1	1:G:122:TYR:C	2.22	0.43
1:G:507:SER:O	1:G:510:PHE:N	2.51	0.43
2:H:98:SER:N	2:H:99:PRO:HD2	2.33	0.43
3:I:120:PHE:CD1	3:I:120:PHE:C	2.92	0.43
9:I:3013:3PE:H261	9:I:3013:3PE:C3A	2.48	0.43
1:A:29:ILE:HD12	1:A:139:ASN:HD22	1.83	0.43
1:A:148:ALA:O	1:A:149:GLY:C	2.55	0.43
4:D:18:ILE:HG23	4:D:21:GLN:OE1	2.19	0.43
1:G:74:LYS:H	1:G:74:LYS:CD	2.31	0.43
1:G:329:VAL:HG12	9:J:3011:3PE:H281	2.01	0.43
2:H:190:PHE:CD1	2:H:190:PHE:C	2.89	0.43
3:I:99:TRP:HD1	3:I:99:TRP:O	2.02	0.43
3:I:133:LEU:O	3:I:136:ILE:HB	2.19	0.43
1:A:40:VAL:O	1:A:40:VAL:HG12	2.18	0.43
9:C:2013:3PE:C3H	9:C:2013:3PE:C2D	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:77:LEU:O	2:H:78:TYR:C	2.54	0.43
3:I:74:VAL:HG23	3:I:75:VAL:N	2.33	0.43
1:A:262:THR:O	1:A:262:THR:HG23	2.19	0.43
3:C:105:ALA:HB2	10:C:2020:HOH:O	2.18	0.43
2:H:175:GLU:HA	2:H:178:GLN:NE2	2.34	0.43
2:H:185:TYR:CD2	2:H:193:ALA:HB1	2.53	0.43
9:A:2009:3PE:H3E1	9:A:2009:3PE:H3B2	1.70	0.42
9:A:2012:3PE:H2I3	3:C:91:VAL:HG11	2.01	0.42
2:B:194:THR:HG22	2:B:266:THR:CB	2.49	0.42
3:C:130:PRO:HD3	3:C:266:GLN:NE2	2.34	0.42
1:G:422:TYR:HH	1:G:469:PHE:HD1	1.67	0.42
8:G:1002:HEA:HHA	8:G:1002:HEA:HAD2	1.78	0.42
2:H:120:LEU:O	2:H:123:LEU:N	2.52	0.42
3:I:21:ALA:CB	3:I:54:THR:HG21	2.37	0.42
2:B:48:SER:HB2	2:B:49:PRO:HD2	2.01	0.42
3:C:32:ALA:O	3:C:36:MET:HG3	2.19	0.42
4:D:39:ILE:O	4:D:40:VAL:C	2.57	0.42
1:G:217:ALA:O	1:G:218:PRO:C	2.56	0.42
1:A:130:ALA:HB2	1:A:215:MET:O	2.18	0.42
1:A:131:PRO:HG2	3:C:9:TYR:CD2	2.54	0.42
1:G:132:ASP:CG	1:G:133:MET:H	2.21	0.42
1:G:191:ILE:HD13	1:G:191:ILE:HA	1.67	0.42
2:H:194:THR:CG2	2:H:266:THR:HB	2.49	0.42
1:A:43:ILE:O	1:A:44:SER:C	2.56	0.42
1:A:112:ILE:HB	1:A:113:PRO:HD3	2.00	0.42
2:B:186:SER:O	2:B:187:ARG:C	2.55	0.42
2:B:276:ALA:O	2:B:277:ALA:C	2.57	0.42
1:G:189:LEU:HD23	3:I:33:VAL:HG21	2.02	0.42
1:G:317:VAL:O	1:G:320:MET:HB2	2.20	0.42
1:G:506:ALA:O	1:G:509:LEU:HB2	2.19	0.42
8:G:1002:HEA:C22	2:H:68:ILE:HD13	2.49	0.42
3:I:219:PHE:HE1	9:I:3008:3PE:H342	1.84	0.42
1:A:188:ASP:OD1	1:A:257:ARG:NH1	2.41	0.42
1:A:284:HIS:N	1:A:285:PRO:CD	2.83	0.42
3:C:13:PRO:HD2	10:C:2018:HOH:O	2.19	0.42
1:G:43:ILE:O	1:G:44:SER:C	2.57	0.42
1:G:493:TRP:CZ3	1:G:496:VAL:HG21	2.54	0.42
1:G:525:VAL:HG11	1:G:544:SER:HB3	2.02	0.42
3:I:72:THR:O	3:I:73:PRO:C	2.58	0.42
3:I:80:ARG:HH12	9:I:3013:3PE:H111	1.83	0.42
1:A:403:GLN:O	1:A:404:ALA:C	2.57	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:17:TRP:O	3:C:20:MET:HB3	2.19	0.42
3:C:226:ARG:HH22	9:C:2008:3PE:C12	2.32	0.42
9:C:2010:3PE:H322	9:D:2011:3PE:O32	2.20	0.42
1:G:246:LEU:O	1:G:246:LEU:HG	2.19	0.42
1:G:481:ARG:O	1:G:482:ARG:HB2	2.19	0.42
1:G:511:PHE:O	1:G:515:ILE:HG13	2.19	0.42
8:G:1001:HEA:HMA	8:G:1001:HEA:HAA1	1.81	0.42
2:H:129:ILE:HD13	2:H:237:GLN:HB3	2.02	0.42
2:H:211:THR:O	2:H:230:ALA:HB1	2.19	0.42
3:I:238:VAL:HB	9:I:3008:3PE:O14	2.20	0.42
9:I:3010:3PE:H322	9:J:3011:3PE:O32	2.19	0.42
4:J:50:ASN:O	9:J:3011:3PE:H112	2.19	0.42
1:A:26:HIS:HD2	1:A:122:TYR:HA	1.84	0.42
1:A:201:SER:HB3	1:A:239:ILE:HG21	2.01	0.42
9:C:2010:3PE:H3E2	9:C:2010:3PE:C3I	2.37	0.42
9:C:2010:3PE:H2A1	9:D:2011:3PE:H2E1	2.02	0.42
1:G:284:HIS:H	1:G:285:PRO:CD	2.32	0.42
1:G:375:ILE:HD12	2:H:80:VAL:HA	2.02	0.42
10:G:3036:HOH:O	3:I:109:MET:HG2	2.18	0.42
1:A:71:GLY:CA	1:A:74:LYS:HD3	2.50	0.42
1:A:368:ALA:O	1:A:369:THR:C	2.56	0.42
1:A:466:LEU:O	1:A:470:PRO:HD2	2.20	0.42
1:A:498:SER:O	1:A:502:PHE:HD2	2.03	0.42
8:A:1002:HEA:H252	2:B:108:PRO:HB3	2.02	0.42
2:B:252:CYS:HB2	2:B:263:MET:HG3	2.02	0.42
4:D:43:LEU:HD23	4:D:43:LEU:HA	1.72	0.42
1:G:48:THR:HG21	1:G:102:HIS:CE1	2.54	0.42
1:G:188:ASP:CG	1:G:257:ARG:HH12	2.22	0.42
1:G:396:VAL:HG12	1:G:397:THR:N	2.29	0.42
9:G:3009:3PE:H392	9:G:3009:3PE:H291	2.00	0.42
2:H:220:THR:HB	2:H:227:LYS:CG	2.49	0.42
3:I:80:ARG:HH12	9:I:3013:3PE:C11	2.33	0.42
3:I:83:PHE:CE1	9:I:3008:3PE:H241	2.55	0.42
3:I:152:HIS:O	3:I:156:VAL:HG23	2.20	0.42
1:A:132:ASP:CG	1:A:133:MET:H	2.20	0.42
1:A:191:ILE:HD13	1:A:191:ILE:HA	1.68	0.42
2:B:120:LEU:N	2:B:121:PRO:HD2	2.34	0.42
2:B:137:LYS:NZ	4:J:11:HIS:CD2	2.88	0.42
1:G:337:THR:HA	10:H:1069:HOH:O	2.20	0.42
1:G:442:LYS:HD2	1:G:442:LYS:HA	1.91	0.42
8:A:1002:HEA:O11	8:A:1002:HEA:CHC	2.68	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:143:TRP:CD1	2:B:143:TRP:N	2.84	0.42
4:D:46:LEU:O	4:D:47:ALA:C	2.57	0.42
1:G:205:ALA:O	1:G:209:ILE:HG13	2.20	0.42
1:G:286:GLU:O	1:G:290:ILE:HG13	2.20	0.42
1:G:473:PHE:O	1:G:474:LEU:C	2.58	0.42
3:I:110:GLY:H	3:I:113:SER:HG	1.66	0.42
3:I:172:ILE:HD13	3:I:221:LEU:HA	2.01	0.42
1:A:22:MET:CG	3:C:16:ILE:HD12	2.49	0.41
9:A:2012:3PE:C2I	3:C:91:VAL:HG11	2.50	0.41
2:B:211:THR:OG1	2:B:235:LEU:HD23	2.20	0.41
1:G:52:ARG:CD	1:G:498:SER:HA	2.50	0.41
1:G:406:VAL:HG12	1:G:410:TYR:CE2	2.55	0.41
9:I:3013:3PE:H3B1	9:I:3013:3PE:C26	2.39	0.41
1:A:74:LYS:CD	1:A:74:LYS:N	2.82	0.41
1:A:481:ARG:O	10:A:2021:HOH:O	2.21	0.41
3:C:133:LEU:HD12	3:C:133:LEU:HA	1.98	0.41
9:C:2010:3PE:H231	9:C:2010:3PE:C33	2.50	0.41
1:G:103:GLY:O	1:G:104:ILE:C	2.58	0.41
1:G:284:HIS:CB	1:G:285:PRO:HD3	2.49	0.41
3:I:72:THR:CG2	3:I:73:PRO:N	2.77	0.41
1:A:133:MET:CE	1:A:211:THR:HG21	2.50	0.41
1:A:251:THR:O	1:A:251:THR:CG2	2.68	0.41
3:C:46:ILE:O	3:C:49:VAL:N	2.53	0.41
3:C:226:ARG:HE	3:C:231:HIS:CD2	2.38	0.41
9:C:2013:3PE:H3D2	9:C:2013:3PE:C2B	2.51	0.41
4:D:36:ALA:O	4:D:40:VAL:HG23	2.21	0.41
1:G:178:LEU:HD12	10:G:3028:HOH:O	2.20	0.41
1:G:312:GLY:O	1:G:313:TYR:C	2.58	0.41
2:H:231:VAL:HB	2:H:234:ARG:HB2	2.01	0.41
1:A:497:SER:O	1:A:498:SER:C	2.58	0.41
2:B:98:SER:CB	2:B:99:PRO:CD	2.98	0.41
2:B:137:LYS:HD2	4:J:11:HIS:NE2	2.35	0.41
3:C:91:VAL:HG22	9:C:2010:3PE:H3I2	2.02	0.41
3:C:136:ILE:HG21	3:C:181:PHE:HE2	1.84	0.41
4:D:50:ASN:O	4:D:51:ALA:C	2.59	0.41
1:G:133:MET:O	1:G:134:ALA:C	2.59	0.41
1:G:529:ASN:OD1	1:G:529:ASN:C	2.59	0.41
2:H:136:VAL:HG11	2:H:147:TYR:HD2	1.85	0.41
3:I:23:VAL:O	3:I:24:GLY:C	2.56	0.41
1:A:106:MET:HG3	8:A:1001:HEA:C3C	2.50	0.41
1:A:239:ILE:O	1:A:240:LEU:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:314:LEU:O	1:A:317:VAL:N	2.53	0.41
1:A:400:VAL:CG1	1:A:410:TYR:HE2	2.31	0.41
1:A:539:GLU:CG	1:A:540:TRP:N	2.82	0.41
10:A:2040:HOH:O	2:B:143:TRP:HH2	2.02	0.41
3:C:155:LEU:HB2	3:C:164:VAL:CG2	2.50	0.41
3:C:172:ILE:HD13	3:C:221:LEU:HA	2.02	0.41
1:G:202:ILE:HD11	1:G:243:LEU:HB2	2.01	0.41
1:G:463:GLY:HA2	1:G:503:LEU:HD23	2.01	0.41
2:H:289:LEU:OXT	2:H:289:LEU:CG	2.68	0.41
3:I:27:VAL:O	3:I:28:MET:C	2.58	0.41
3:I:110:GLY:O	3:I:112:GLU:N	2.53	0.41
3:I:253:VAL:HG22	9:I:3010:3PE:H3I1	2.02	0.41
1:A:81:TRP:CE3	1:A:82:PRO:HD2	2.56	0.41
1:A:189:LEU:HD21	3:C:30:PHE:CD1	2.55	0.41
2:B:35:ARG:HG3	2:B:36:PRO:HD2	2.02	0.41
4:D:51:ALA:O	9:D:2011:3PE:H122	2.21	0.41
1:G:115:LEU:HG	1:G:432:ILE:HG12	2.03	0.41
1:G:138:MET:HE3	9:G:3009:3PE:O21	2.20	0.41
1:G:225:VAL:C	1:G:226:PRO:O	2.57	0.41
1:G:482:ARG:HH21	8:G:1001:HEA:CGD	2.33	0.41
2:H:62:LEU:HD12	2:H:65:ILE:HD11	2.03	0.41
2:H:107:VAL:HG12	2:H:108:PRO:HD3	1.99	0.41
9:I:3010:3PE:H382	9:I:3010:3PE:H3B2	1.85	0.41
1:A:44:SER:O	1:A:45:VAL:C	2.59	0.41
1:A:131:PRO:HG2	3:C:9:TYR:HD2	1.85	0.41
1:A:282:PHE:C	1:A:285:PRO:HD2	2.40	0.41
1:A:295:PHE:HB3	1:A:362:LYS:HE2	2.02	0.41
1:A:382:LEU:HD11	1:A:454:LYS:HE2	2.03	0.41
1:G:469:PHE:N	1:G:470:PRO:CD	2.84	0.41
1:G:558:GLU:O	1:G:560:TRP:N	2.53	0.41
1:A:318:TYR:HD1	1:A:318:TYR:HA	1.71	0.41
1:A:493:TRP:CE3	1:A:496:VAL:HG21	2.55	0.41
9:A:2012:3PE:H2I3	9:C:2010:3PE:H2F1	2.02	0.41
2:B:208:VAL:HG12	2:B:210:VAL:HG23	2.03	0.41
9:C:2013:3PE:H3H2	9:C:2013:3PE:H2E1	2.01	0.41
1:G:467:THR:HG21	8:G:1001:HEA:HMB2	2.02	0.41
9:G:3009:3PE:H3E1	9:G:3009:3PE:H3B2	1.67	0.41
9:G:3012:3PE:H231	4:J:31:MET:CE	2.50	0.41
2:H:106:ILE:O	2:H:107:VAL:O	2.38	0.41
2:H:185:TYR:CE1	2:H:247:ILE:HD13	2.49	0.41
3:I:187:SER:HG	3:I:188:HIS:CE1	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:17:ASP:OD1	4:J:17:ASP:C	2.59	0.41
1:A:38:GLY:HA2	8:A:1001:HEA:H22	2.02	0.41
1:A:103:GLY:HA2	8:A:1001:HEA:HMD3	2.03	0.41
1:A:213:LEU:HD13	3:C:81:TRP:CZ2	2.55	0.41
1:A:396:VAL:O	1:A:397:THR:C	2.59	0.41
1:A:433:PHE:HA	1:A:436:ILE:HD12	2.03	0.41
2:B:161:ILE:HD12	2:B:180:LEU:HD23	2.03	0.41
3:C:114:PRO:O	3:C:115:ILE:C	2.59	0.41
3:C:120:PHE:HA	3:C:121:PRO:C	2.41	0.41
3:C:187:SER:HG	3:C:188:HIS:CE1	2.31	0.41
9:C:2010:3PE:H2I2	4:D:36:ALA:CB	2.49	0.41
1:G:26:HIS:HB3	1:G:132:ASP:OD1	2.19	0.41
1:G:243:LEU:N	1:G:244:PRO:HD2	2.35	0.41
1:G:308:LYS:HD3	1:G:369:THR:O	2.21	0.41
1:G:361:ILE:HD11	2:H:105:THR:OG1	2.21	0.41
1:G:381:MET:O	1:G:381:MET:HG3	2.21	0.41
9:G:3009:3PE:H221	3:I:58:TRP:CE2	2.56	0.41
3:I:253:VAL:HG22	9:I:3010:3PE:C3I	2.51	0.41
4:J:12:VAL:HG12	4:J:15:SER:HB2	2.03	0.41
9:C:2013:3PE:H3D2	9:C:2013:3PE:H2B2	2.02	0.41
1:G:314:LEU:CB	1:G:315:PRO:HD3	2.51	0.41
1:G:392:THR:O	1:G:393:VAL:C	2.58	0.41
2:H:83:PHE:O	2:H:84:HIS:C	2.57	0.41
3:I:81:TRP:NE1	4:J:28:PHE:CE2	2.88	0.41
9:I:3010:3PE:H2I2	4:J:36:ALA:CB	2.51	0.41
1:A:260:GLY:O	3:C:194:ALA:HB1	2.21	0.40
3:C:240:PHE:CD1	3:C:244:ILE:HD11	2.56	0.40
1:G:29:ILE:HD12	1:G:139:ASN:ND2	2.37	0.40
1:G:173:VAL:O	1:G:174:LEU:HB2	2.21	0.40
1:G:357:VAL:N	1:G:358:PRO:HD2	2.36	0.40
2:H:251:GLN:O	2:H:252:CYS:C	2.59	0.40
3:I:177:LEU:O	3:I:178:PHE:C	2.59	0.40
1:A:122:TYR:C	1:A:122:TYR:CD1	2.95	0.40
1:A:201:SER:HB3	1:A:239:ILE:CG2	2.51	0.40
2:B:148:GLU:O	2:B:150:PRO:HD3	2.21	0.40
2:B:254:GLU:H	2:B:260:HIS:HE1	1.69	0.40
3:C:84:ILE:HG23	9:C:2013:3PE:H272	2.04	0.40
1:G:493:TRP:CE3	1:G:496:VAL:HG21	2.57	0.40
2:H:68:ILE:O	2:H:69:THR:C	2.58	0.40
2:H:98:SER:CB	2:H:99:PRO:CD	2.99	0.40
9:I:3010:3PE:H231	9:I:3010:3PE:C33	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:3013:3PE:H3D2	9:I:3013:3PE:C2B	2.51	0.40
1:A:152:LEU:HD23	1:A:152:LEU:HA	1.91	0.40
1:A:388:LEU:HD23	1:A:388:LEU:HA	1.96	0.40
1:G:180:THR:HA	1:G:257:ARG:CG	2.52	0.40
2:H:71:PHE:CE1	2:H:75:LEU:HD11	2.56	0.40
1:A:136:PRO:HA	10:A:2052:HOH:O	2.21	0.40
1:A:547:PRO:HD2	1:A:550:THR:HG22	2.03	0.40
8:A:1001:HEA:HAA1	8:A:1001:HEA:HMA	1.70	0.40
8:A:1001:HEA:HHC	8:A:1001:HEA:H11	1.81	0.40
2:H:234:ARG:HH12	3:I:114:PRO:HG3	1.86	0.40
3:I:113:SER:HA	3:I:114:PRO:HA	1.82	0.40
1:A:323:ILE:HG22	1:A:324:GLY:N	2.34	0.40
1:A:476:ARG:HD3	2:B:41:THR:O	2.21	0.40
2:B:165:ALA:HB2	10:I:3042:HOH:O	2.20	0.40
3:C:111:PRO:HA	4:J:12:VAL:CB	2.44	0.40
3:C:135:LEU:HD12	3:C:135:LEU:HA	1.83	0.40
1:G:74:LYS:HD2	1:G:74:LYS:N	2.36	0.40
1:G:292:LEU:HD23	1:G:292:LEU:HA	1.98	0.40
1:G:396:VAL:O	1:G:399:ILE:N	2.54	0.40
1:G:541:THR:O	1:G:541:THR:HG22	2.20	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	545/566 (96%)	479 (88%)	54 (10%)	12 (2%)	6 5
1	G	545/566 (96%)	466 (86%)	67 (12%)	12 (2%)	6 5
2	B	258/264 (98%)	222 (86%)	32 (12%)	4 (2%)	9 9
2	H	258/264 (98%)	220 (85%)	33 (13%)	5 (2%)	8 7

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	C	263/266 (99%)	229 (87%)	30 (11%)	4 (2%)	10	10
3	I	263/266 (99%)	234 (89%)	25 (10%)	4 (2%)	10	10
4	D	40/51 (78%)	37 (92%)	2 (5%)	1 (2%)	5	4
4	J	40/51 (78%)	32 (80%)	7 (18%)	1 (2%)	5	4
All	All	2212/2294 (96%)	1919 (87%)	250 (11%)	43 (2%)	8	7

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	544	SER
3	C	111	PRO
1	G	327	GLY
1	G	544	SER
2	H	264	PRO
3	I	111	PRO
4	J	12	VAL
1	A	487	PRO
1	A	492	THR
4	D	12	VAL
1	G	162	GLY
1	G	487	PRO
1	G	492	THR
1	G	545	PRO
1	G	559	ASP
3	I	195	GLY
1	A	58	PRO
1	A	256	ASP
1	A	419	HIS
2	H	252	CYS
2	H	255	LEU
1	A	71	GLY
1	A	106	MET
1	A	327	GLY
1	A	545	PRO
2	B	85	GLU
2	B	255	LEU
1	G	90	PRO
1	G	405	SER
2	H	45	PRO
2	H	187	ARG
3	I	237	HIS

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Mol	Chain	Res	Type
2	B	99	PRO
3	C	237	HIS
1	A	131	PRO
3	C	73	PRO
1	G	393	VAL
3	I	133	LEU
1	G	43	ILE
1	G	323	ILE
2	B	34	GLY
3	C	133	LEU
1	A	90	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	446/459 (97%)	422 (95%)	24 (5%)	22	30
1	G	446/459 (97%)	410 (92%)	36 (8%)	11	15
2	B	216/220 (98%)	204 (94%)	12 (6%)	21	29
2	H	216/220 (98%)	209 (97%)	7 (3%)	39	54
3	C	215/216 (100%)	207 (96%)	8 (4%)	34	48
3	I	215/216 (100%)	206 (96%)	9 (4%)	30	42
4	D	30/37 (81%)	28 (93%)	2 (7%)	16	21
4	J	30/37 (81%)	29 (97%)	1 (3%)	38	53
All	All	1814/1864 (97%)	1715 (94%)	99 (6%)	21	30

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	SER
1	A	45	VAL
1	A	52	ARG
1	A	55	LEU

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Mol	Chain	Res	Type
1	A	70	SER
1	A	79	SER
1	A	89	THR
1	A	122	TYR
1	A	133	MET
1	A	137	ARG
1	A	151	SER
1	A	206	ILE
1	A	212	PHE
1	A	243	LEU
1	A	262	THR
1	A	282	PHE
1	A	310	ILE
1	A	409	TYR
1	A	412	ASP
1	A	446	ARG
1	A	460	MET
1	A	484	ILE
1	A	520	THR
1	A	525	VAL
2	B	69	THR
2	B	74	LEU
2	B	104	TRP
2	B	125	ASN
2	B	149	TYR
2	B	199	VAL
2	B	214	ASP
2	B	222	PRO
2	B	241	ARG
2	B	253	SER
2	B	263	MET
2	B	264	PRO
3	C	60	SER
3	C	155	LEU
3	C	157	HIS
3	C	166	TRP
3	C	188	HIS
3	C	193	PHE
3	C	196	ASN
3	C	231	HIS
4	D	15	SER
4	D	50	ASN

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Mol	Chain	Res	Type
1	G	23	SER
1	G	45	VAL
1	G	49	VAL
1	G	52	ARG
1	G	55	LEU
1	G	70	SER
1	G	79	SER
1	G	89	THR
1	G	113	PRO
1	G	122	TYR
1	G	125	PRO
1	G	131	PRO
1	G	133	MET
1	G	137	ARG
1	G	182	GLU
1	G	191	ILE
1	G	195	HIS
1	G	208	MET
1	G	212	PHE
1	G	243	LEU
1	G	252	MET
1	G	262	THR
1	G	267	SER
1	G	274	LEU
1	G	282	PHE
1	G	291	VAL
1	G	293	PRO
1	G	379	THR
1	G	409	TYR
1	G	412	ASP
1	G	446	ARG
1	G	460	MET
1	G	484	ILE
1	G	520	THR
1	G	525	VAL
1	G	532	ASN
2	H	104	TRP
2	H	149	TYR
2	H	214	ASP
2	H	238	LEU
2	H	241	ARG
2	H	253	SER

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Mol	Chain	Res	Type
2	H	263	MET
3	I	60	SER
3	I	72	THR
3	I	111	PRO
3	I	155	LEU
3	I	159	ASN
3	I	166	TRP
3	I	193	PHE
3	I	196	ASN
3	I	231	HIS
4	J	50	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	26	HIS
1	A	127	HIS
1	A	139	ASN
1	A	345	GLN
1	A	494	ASN
2	B	55	HIS
2	B	84	HIS
2	B	127	GLN
2	B	178	GLN
2	B	209	GLN
2	B	237	GLN
3	C	153	HIS
3	C	159	ASN
3	C	201	ASN
3	C	212	HIS
3	C	231	HIS
1	G	25	ASN
1	G	26	HIS
1	G	96	ASN
1	G	139	ASN
1	G	163	ASN
1	G	345	GLN
1	G	494	ASN
2	H	55	HIS
2	H	84	HIS
3	I	37	HIS

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Mol	Chain	Res	Type
3	I	153	HIS
3	I	159	ASN
3	I	201	ASN
3	I	212	HIS
3	I	231	HIS
4	J	11	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 26 ligands modelled in this entry, 10 are monoatomic - leaving 16 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	3PE	I	3008	-	50,50,50	1.54	2 (4%)	53,55,55	1.15	4 (7%)
9	3PE	C	2013	-	50,50,50	1.59	3 (6%)	53,55,55	1.11	3 (5%)
8	HEA	G	1002	1	44,67,67	1.98	7 (15%)	37,103,103	2.31	14 (37%)
8	HEA	A	1002	1	44,67,67	1.68	6 (13%)	37,103,103	2.00	12 (32%)
9	3PE	C	2010	-	50,50,50	1.61	2 (4%)	53,55,55	0.99	3 (5%)
8	HEA	A	1001	1	44,67,67	1.68	7 (15%)	37,103,103	2.48	15 (40%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
9	3PE	G	3009	-	50,50,50	1.55	2 (4%)	53,55,55	1.02	1 (1%)
9	3PE	C	2008	-	50,50,50	1.58	2 (4%)	53,55,55	1.17	5 (9%)
9	3PE	A	2012	-	50,50,50	1.59	3 (6%)	53,55,55	1.07	5 (9%)
9	3PE	A	2009	-	50,50,50	1.52	2 (4%)	53,55,55	1.01	3 (5%)
9	3PE	G	3012	-	50,50,50	1.58	3 (6%)	53,55,55	1.11	4 (7%)
8	HEA	G	1001	1	44,67,67	1.60	9 (20%)	37,103,103	2.49	18 (48%)
9	3PE	I	3013	-	50,50,50	1.55	4 (8%)	53,55,55	1.08	4 (7%)
9	3PE	J	3011	-	50,50,50	1.54	2 (4%)	53,55,55	1.30	4 (7%)
9	3PE	I	3010	-	50,50,50	1.61	2 (4%)	53,55,55	0.97	3 (5%)
9	3PE	D	2011	-	50,50,50	1.54	2 (4%)	53,55,55	1.28	4 (7%)

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
9	3PE	I	3008	-	-	35/54/54/54	-
9	3PE	C	2013	-	-	27/54/54/54	-
8	HEA	G	1002	1	3/3/7/16	2/24/76/76	-
8	HEA	A	1002	1	3/3/7/16	4/24/76/76	-
9	3PE	C	2010	-	-	29/54/54/54	-
8	HEA	A	1001	1	3/3/7/16	10/24/76/76	-
9	3PE	G	3009	-	-	27/54/54/54	-
9	3PE	C	2008	-	-	35/54/54/54	-
9	3PE	A	2012	-	-	23/54/54/54	-
9	3PE	A	2009	-	-	31/54/54/54	-
9	3PE	G	3012	-	-	24/54/54/54	-
8	HEA	G	1001	1	3/3/7/16	8/24/76/76	-
9	3PE	I	3013	-	-	28/54/54/54	-
9	3PE	J	3011	-	-	26/54/54/54	-
9	3PE	I	3010	-	-	25/54/54/54	-
9	3PE	D	2011	-	-	22/54/54/54	-

All (58) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	C	2013	3PE	O21-C21	7.70	1.56	1.34
9	C	2010	3PE	O31-C31	7.64	1.55	1.33
9	G	3009	3PE	O21-C21	7.52	1.55	1.34
9	C	2008	3PE	O21-C21	7.50	1.55	1.34
9	J	3011	3PE	O21-C21	7.48	1.55	1.34
9	C	2008	3PE	O31-C31	7.47	1.55	1.33
9	I	3010	3PE	O21-C21	7.46	1.55	1.34
9	I	3010	3PE	O31-C31	7.46	1.55	1.33
9	A	2012	3PE	O31-C31	7.43	1.55	1.33
9	I	3008	3PE	O31-C31	7.42	1.55	1.33
9	G	3012	3PE	O31-C31	7.39	1.55	1.33
9	D	2011	3PE	O21-C21	7.38	1.55	1.34
9	C	2010	3PE	O21-C21	7.26	1.54	1.34
9	A	2009	3PE	O21-C21	7.25	1.54	1.34
9	G	3012	3PE	O21-C21	7.24	1.54	1.34
9	I	3013	3PE	O21-C21	7.20	1.54	1.34
9	A	2012	3PE	O21-C21	7.11	1.54	1.34
9	I	3013	3PE	O31-C31	7.05	1.54	1.33
9	C	2013	3PE	O31-C31	7.03	1.53	1.33
9	I	3008	3PE	O21-C21	7.02	1.54	1.34
9	A	2009	3PE	O31-C31	7.01	1.53	1.33
9	D	2011	3PE	O31-C31	6.89	1.53	1.33
8	G	1002	HEA	C3B-C11	-6.83	1.47	1.52
9	J	3011	3PE	O31-C31	6.78	1.53	1.33
9	G	3009	3PE	O31-C31	6.77	1.53	1.33
8	G	1002	HEA	C3A-C2A	-6.40	1.31	1.40
8	A	1002	HEA	C3A-C2A	-5.44	1.32	1.40
8	G	1002	HEA	C3C-C2C	-4.55	1.34	1.40
8	A	1001	HEA	C3C-CAC	-4.46	1.38	1.47
8	A	1002	HEA	C3C-CAC	-4.41	1.38	1.47
8	A	1001	HEA	C3C-C2C	-4.20	1.34	1.40
8	G	1001	HEA	C3A-C2A	-3.89	1.35	1.40
8	G	1001	HEA	C3C-CAC	-3.87	1.40	1.47
8	A	1001	HEA	C3A-C2A	-3.69	1.35	1.40
8	G	1002	HEA	C3C-CAC	-3.57	1.40	1.47
8	G	1001	HEA	C3C-C2C	-3.50	1.35	1.40
8	A	1002	HEA	C3B-C11	-3.37	1.50	1.52
8	G	1001	HEA	C3B-C11	-3.28	1.50	1.52
8	A	1001	HEA	C16-C15	-3.15	1.44	1.51
8	A	1002	HEA	C3C-C2C	-3.14	1.36	1.40
8	A	1002	HEA	C3A-CMA	3.00	1.53	1.46
8	G	1002	HEA	CAA-C2A	2.72	1.57	1.52
8	G	1001	HEA	C3B-C2B	-2.71	1.32	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	1001	HEA	C1C-NC	2.67	1.41	1.36
8	A	1001	HEA	C3B-C2B	-2.66	1.32	1.41
9	A	2012	3PE	O21-C2	-2.49	1.40	1.46
8	A	1001	HEA	O11-C11	2.43	1.48	1.42
8	G	1001	HEA	C3A-CMA	2.43	1.52	1.46
9	I	3013	3PE	O32-C31	2.21	1.29	1.22
8	A	1002	HEA	C3B-C2B	-2.16	1.34	1.41
9	G	3012	3PE	O21-C2	-2.15	1.41	1.46
8	G	1002	HEA	C3B-C2B	-2.11	1.34	1.41
8	G	1001	HEA	C1D-C2D	2.10	1.47	1.42
9	C	2013	3PE	O21-C2	-2.06	1.41	1.46
8	G	1002	HEA	C1C-NC	2.06	1.40	1.36
8	G	1001	HEA	C4B-C3B	2.06	1.47	1.42
9	I	3013	3PE	O21-C2	-2.05	1.41	1.46
8	G	1001	HEA	C16-C15	-2.02	1.47	1.51

All (102) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	A	1001	HEA	C13-C14-C15	-6.96	110.89	127.66
8	G	1001	HEA	CBA-CAA-C2A	5.73	123.03	112.48
9	J	3011	3PE	C2-O21-C21	-5.46	104.36	117.79
8	G	1001	HEA	C13-C14-C15	-5.39	114.68	127.66
8	A	1002	HEA	C17-C18-C19	-5.12	115.34	127.66
8	G	1002	HEA	CBD-CAD-C3D	4.92	121.56	112.49
9	G	3009	3PE	C3-C2-C1	-4.92	100.15	111.79
8	G	1002	HEA	OMA-CMA-C3A	-4.90	114.24	124.91
8	A	1001	HEA	CAA-C2A-C3A	-4.85	114.90	126.86
8	A	1001	HEA	C26-C15-C14	-4.63	111.81	123.68
9	C	2008	3PE	C2-O21-C21	-4.57	106.53	117.79
9	D	2011	3PE	C2-O21-C21	-4.50	106.72	117.79
8	G	1002	HEA	C27-C19-C20	4.47	122.78	115.27
8	G	1001	HEA	C17-C18-C19	-4.25	117.43	127.66
8	G	1002	HEA	CAA-CBA-CGA	4.17	119.67	112.67
9	C	2013	3PE	C2-O21-C21	-4.13	107.63	117.79
9	J	3011	3PE	C3-C2-C1	-4.11	102.06	111.79
9	A	2009	3PE	C3-C2-C1	-4.00	102.34	111.79
8	A	1002	HEA	CBD-CAD-C3D	3.98	119.82	112.49
8	A	1001	HEA	C17-C18-C19	-3.95	118.15	127.66
9	D	2011	3PE	C3-C2-C1	-3.95	102.46	111.79
8	G	1002	HEA	CMC-C2C-C1C	-3.89	122.48	128.46
9	I	3008	3PE	O21-C2-C3	-3.89	94.31	108.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	G	1001	HEA	CAA-CBA-CGA	3.78	119.01	112.67
8	A	1001	HEA	C26-C15-C16	3.63	121.38	115.27
8	A	1001	HEA	C3C-C4C-NC	3.63	113.90	109.21
9	I	3008	3PE	C2-O21-C21	-3.63	108.86	117.79
9	I	3013	3PE	C2-O21-C21	-3.61	108.89	117.79
8	G	1002	HEA	C17-C18-C19	-3.52	119.18	127.66
8	G	1001	HEA	CMB-C2B-C1B	-3.48	123.12	128.46
8	A	1002	HEA	C3C-C4C-NC	3.48	113.70	109.21
8	G	1001	HEA	C16-C15-C14	3.46	128.11	121.12
9	G	3012	3PE	C3-C2-C1	-3.42	103.70	111.79
9	G	3012	3PE	O21-C21-O22	3.36	131.83	123.70
8	G	1001	HEA	CAA-C2A-C3A	-3.32	118.69	126.86
8	G	1002	HEA	CBA-CAA-C2A	3.20	118.37	112.48
8	A	1002	HEA	C13-C14-C15	-3.19	119.98	127.66
9	C	2008	3PE	C3-O31-C31	-3.17	105.37	117.12
8	A	1002	HEA	C12-C11-C3B	3.07	120.62	112.56
8	G	1001	HEA	C27-C19-C20	3.06	120.41	115.27
9	C	2010	3PE	C3-C2-C1	-3.05	104.56	111.79
9	C	2010	3PE	O31-C3-C2	3.05	117.32	108.43
8	A	1001	HEA	C25-C23-C24	-3.04	107.88	114.60
9	A	2012	3PE	O21-C21-O22	3.02	131.00	123.70
8	A	1001	HEA	C4B-C3B-C2B	-3.00	104.77	106.87
9	C	2013	3PE	C3-O31-C31	-2.98	106.08	117.12
9	C	2008	3PE	O21-C2-C3	-2.96	97.70	108.40
9	I	3008	3PE	O31-C3-C2	2.92	116.94	108.43
8	A	1001	HEA	C13-C12-C11	2.92	118.73	114.35
9	G	3012	3PE	O21-C2-C1	2.87	118.80	108.40
8	G	1001	HEA	CMB-C2B-C3B	2.86	130.28	124.69
8	A	1002	HEA	O11-C11-C3B	-2.82	103.87	112.00
8	A	1001	HEA	C16-C15-C14	2.81	126.81	121.12
8	A	1002	HEA	CMC-C2C-C1C	-2.81	124.15	128.46
8	A	1002	HEA	CMC-C2C-C3C	2.74	129.80	124.68
8	G	1002	HEA	C27-C19-C18	-2.72	116.69	123.68
8	A	1001	HEA	CMB-C2B-C1B	-2.72	124.29	128.46
8	G	1002	HEA	CMC-C2C-C3C	2.71	129.75	124.68
9	A	2012	3PE	C3-C2-C1	-2.71	105.39	111.79
9	D	2011	3PE	P-O13-C11	-2.70	108.29	121.59
8	A	1002	HEA	C16-C17-C18	-2.67	103.09	111.88
8	G	1001	HEA	C24-C23-C22	2.67	130.37	122.65
9	I	3008	3PE	C3-O31-C31	-2.64	107.35	117.12
8	G	1001	HEA	C3C-C4C-NC	2.64	112.62	109.21
8	G	1002	HEA	C3C-C4C-NC	2.63	112.61	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	3013	3PE	C23-C22-C21	-2.59	104.19	113.62
8	G	1002	HEA	C13-C14-C15	-2.58	121.45	127.66
8	A	1002	HEA	CAD-CBD-CGD	2.56	116.96	112.67
9	A	2012	3PE	C3-O31-C31	-2.55	107.69	117.12
9	A	2009	3PE	O21-C2-C3	-2.54	99.20	108.40
9	I	3010	3PE	C2-O21-C21	-2.54	111.54	117.79
8	G	1001	HEA	CBD-CAD-C3D	-2.54	107.81	112.49
8	A	1002	HEA	CBA-CAA-C2A	2.51	117.11	112.48
8	G	1002	HEA	C12-C11-C3B	2.49	119.09	112.56
8	G	1001	HEA	CMC-C2C-C1C	-2.46	124.68	128.46
8	G	1002	HEA	C26-C15-C16	-2.44	111.16	115.27
8	G	1001	HEA	C26-C15-C16	-2.41	111.22	115.27
9	J	3011	3PE	P-O11-C1	-2.40	107.59	121.68
8	A	1001	HEA	CAD-CBD-CGD	2.38	116.66	112.67
8	G	1001	HEA	CMC-C2C-C3C	2.36	129.09	124.68
9	I	3010	3PE	C3-O31-C31	-2.34	108.46	117.12
9	J	3011	3PE	P-O13-C11	-2.32	110.17	121.59
8	A	1001	HEA	CBA-CAA-C2A	2.32	116.75	112.48
9	C	2013	3PE	O31-C31-C32	2.27	119.02	111.91
9	D	2011	3PE	P-O11-C1	-2.27	108.39	121.68
9	I	3010	3PE	C3-C2-C1	-2.26	106.43	111.79
9	C	2008	3PE	O13-C11-C12	-2.22	100.78	109.10
8	G	1001	HEA	CMD-C2D-C3D	2.22	129.13	124.94
8	A	1001	HEA	CAA-CBA-CGA	2.20	116.36	112.67
8	G	1001	HEA	C21-C22-C23	-2.19	120.25	127.75
9	A	2012	3PE	C2E-C2D-C2C	-2.18	103.37	114.42
9	A	2009	3PE	C3-O31-C31	-2.17	109.08	117.12
9	I	3013	3PE	C2B-C2A-C29	-2.16	103.46	114.42
9	A	2012	3PE	O21-C2-C1	2.16	116.21	108.40
8	G	1001	HEA	C16-C17-C18	-2.15	104.81	111.88
8	A	1001	HEA	C21-C20-C19	2.10	119.90	112.98
8	A	1002	HEA	C4B-C3B-C2B	-2.06	105.43	106.87
9	C	2008	3PE	P-O13-C11	-2.05	111.51	121.59
9	G	3012	3PE	O21-C21-C22	-2.04	107.11	111.50
9	C	2010	3PE	C2-O21-C21	-2.03	112.80	117.79
9	I	3013	3PE	O32-C31-C32	-2.02	115.85	123.73
8	G	1002	HEA	CMB-C2B-C3B	-2.01	120.75	124.69

All (12) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
8	A	1001	HEA	ND

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Mol	Chain	Res	Type	Atom
8	A	1001	HEA	NB
8	A	1001	HEA	NA
8	A	1002	HEA	ND
8	A	1002	HEA	NB
8	A	1002	HEA	NA
8	G	1001	HEA	ND
8	G	1001	HEA	NB
8	G	1001	HEA	NA
8	G	1002	HEA	ND
8	G	1002	HEA	NB
8	G	1002	HEA	NA

All (356) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	1001	HEA	C1A-C2A-CAA-CBA
8	A	1001	HEA	C3A-C2A-CAA-CBA
8	A	1001	HEA	C3B-C11-C12-C13
8	A	1001	HEA	O11-C11-C12-C13
8	A	1001	HEA	C11-C12-C13-C14
8	A	1002	HEA	C3B-C11-C12-C13
8	A	1002	HEA	O11-C11-C12-C13
8	G	1001	HEA	C1A-C2A-CAA-CBA
8	G	1001	HEA	C3A-C2A-CAA-CBA
8	G	1001	HEA	C3B-C11-C12-C13
8	G	1001	HEA	O11-C11-C12-C13
8	G	1001	HEA	C11-C12-C13-C14
8	G	1002	HEA	C3B-C11-C12-C13
8	G	1002	HEA	O11-C11-C12-C13
9	A	2009	3PE	C11-O13-P-O12
9	A	2009	3PE	C11-O13-P-O14
9	A	2009	3PE	O13-C11-C12-N
9	A	2012	3PE	C1-O11-P-O14
9	A	2012	3PE	O13-C11-C12-N
9	A	2012	3PE	O11-C1-C2-O21
9	C	2008	3PE	C1-O11-P-O12
9	C	2008	3PE	C1-O11-P-O14
9	C	2008	3PE	O13-C11-C12-N
9	C	2010	3PE	C1-O11-P-O12
9	C	2010	3PE	C11-O13-P-O12
9	C	2010	3PE	O13-C11-C12-N
9	C	2013	3PE	C12-C11-O13-P

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Mol	Chain	Res	Type	Atoms
9	C	2013	3PE	C22-C21-O21-C2
9	D	2011	3PE	C11-O13-P-O11
9	D	2011	3PE	C11-O13-P-O12
9	D	2011	3PE	C11-O13-P-O14
9	G	3009	3PE	C11-O13-P-O11
9	G	3009	3PE	C11-O13-P-O12
9	G	3009	3PE	C11-O13-P-O14
9	G	3009	3PE	O13-C11-C12-N
9	G	3012	3PE	C1-O11-P-O12
9	G	3012	3PE	C1-O11-P-O14
9	G	3012	3PE	O13-C11-C12-N
9	G	3012	3PE	O11-C1-C2-O21
9	I	3008	3PE	C1-O11-P-O12
9	I	3008	3PE	C1-O11-P-O14
9	I	3008	3PE	O13-C11-C12-N
9	I	3010	3PE	C1-O11-P-O12
9	I	3010	3PE	O13-C11-C12-N
9	I	3013	3PE	C12-C11-O13-P
9	I	3013	3PE	C22-C21-O21-C2
9	J	3011	3PE	C11-O13-P-O11
9	J	3011	3PE	C11-O13-P-O12
9	J	3011	3PE	C11-O13-P-O14
9	C	2013	3PE	O22-C21-O21-C2
9	I	3013	3PE	O22-C21-O21-C2
9	C	2008	3PE	O32-C31-O31-C3
9	I	3008	3PE	O32-C31-O31-C3
9	C	2013	3PE	C32-C33-C34-C35
9	I	3008	3PE	C32-C31-O31-C3
9	I	3013	3PE	C32-C33-C34-C35
9	A	2009	3PE	C3B-C3C-C3D-C3E
9	G	3009	3PE	C3B-C3C-C3D-C3E
9	I	3010	3PE	C38-C39-C3A-C3B
9	C	2008	3PE	C32-C31-O31-C3
9	C	2010	3PE	C38-C39-C3A-C3B
8	A	1001	HEA	C27-C19-C20-C21
8	G	1001	HEA	C27-C19-C20-C21
8	A	1001	HEA	C18-C19-C20-C21
8	G	1001	HEA	C18-C19-C20-C21
9	D	2011	3PE	C31-C32-C33-C34
9	A	2012	3PE	C31-C32-C33-C34
9	G	3012	3PE	C31-C32-C33-C34
9	J	3011	3PE	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
9	J	3011	3PE	C28-C29-C2A-C2B
9	A	2009	3PE	C31-C32-C33-C34
9	I	3013	3PE	C25-C26-C27-C28
9	J	3011	3PE	C21-C22-C23-C24
9	I	3010	3PE	C36-C37-C38-C39
9	D	2011	3PE	C21-C22-C23-C24
9	G	3009	3PE	C31-C32-C33-C34
9	A	2009	3PE	C11-O13-P-O11
9	C	2008	3PE	C1-O11-P-O13
9	C	2010	3PE	C1-O11-P-O13
9	C	2013	3PE	C1-O11-P-O13
9	C	2013	3PE	C11-O13-P-O11
9	G	3009	3PE	C1-O11-P-O13
9	G	3012	3PE	C1-O11-P-O13
9	I	3008	3PE	C1-O11-P-O13
9	I	3010	3PE	C1-O11-P-O13
9	I	3013	3PE	C1-O11-P-O13
9	I	3013	3PE	C11-O13-P-O11
9	C	2010	3PE	C36-C37-C38-C39
9	C	2013	3PE	C22-C23-C24-C25
9	G	3009	3PE	C3D-C3E-C3F-C3G
9	I	3008	3PE	C26-C27-C28-C29
9	A	2012	3PE	C28-C29-C2A-C2B
9	A	2009	3PE	C24-C25-C26-C27
9	C	2008	3PE	C26-C27-C28-C29
9	C	2013	3PE	C39-C3A-C3B-C3C
9	C	2008	3PE	C24-C25-C26-C27
9	G	3012	3PE	C26-C27-C28-C29
9	I	3013	3PE	C22-C23-C24-C25
9	A	2009	3PE	C3D-C3E-C3F-C3G
9	A	2012	3PE	C36-C37-C38-C39
9	I	3013	3PE	C39-C3A-C3B-C3C
9	A	2009	3PE	C36-C37-C38-C39
9	D	2011	3PE	C26-C27-C28-C29
9	G	3012	3PE	C36-C37-C38-C39
9	G	3009	3PE	C24-C25-C26-C27
9	G	3009	3PE	C29-C2A-C2B-C2C
9	C	2013	3PE	C2C-C2D-C2E-C2F
9	I	3013	3PE	C3D-C3E-C3F-C3G
9	C	2008	3PE	C23-C24-C25-C26
9	D	2011	3PE	C2B-C2C-C2D-C2E
9	G	3012	3PE	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
9	C	2013	3PE	C3D-C3E-C3F-C3G
9	D	2011	3PE	C28-C29-C2A-C2B
9	G	3009	3PE	C38-C39-C3A-C3B
9	G	3009	3PE	C39-C3A-C3B-C3C
9	G	3009	3PE	C3E-C3F-C3G-C3H
9	I	3008	3PE	C24-C25-C26-C27
9	I	3013	3PE	C33-C34-C35-C36
9	A	2009	3PE	C39-C3A-C3B-C3C
9	A	2012	3PE	C38-C39-C3A-C3B
9	A	2012	3PE	C3C-C3D-C3E-C3F
9	A	2012	3PE	C26-C27-C28-C29
9	C	2013	3PE	C33-C34-C35-C36
9	I	3008	3PE	C23-C24-C25-C26
9	A	2009	3PE	C38-C39-C3A-C3B
9	A	2012	3PE	C27-C28-C29-C2A
9	C	2008	3PE	C32-C33-C34-C35
9	C	2008	3PE	C3A-C3B-C3C-C3D
9	G	3009	3PE	C36-C37-C38-C39
9	J	3011	3PE	C26-C27-C28-C29
9	J	3011	3PE	C2B-C2C-C2D-C2E
9	C	2008	3PE	C2A-C2B-C2C-C2D
9	I	3008	3PE	C3A-C3B-C3C-C3D
9	A	2009	3PE	C3E-C3F-C3G-C3H
9	C	2008	3PE	C29-C2A-C2B-C2C
9	I	3008	3PE	C32-C33-C34-C35
9	C	2013	3PE	C3C-C3D-C3E-C3F
9	I	3013	3PE	C2C-C2D-C2E-C2F
9	I	3008	3PE	C29-C2A-C2B-C2C
9	A	2009	3PE	C29-C2A-C2B-C2C
9	I	3008	3PE	C36-C37-C38-C39
9	I	3013	3PE	C3C-C3D-C3E-C3F
9	D	2011	3PE	C29-C2A-C2B-C2C
9	G	3012	3PE	C27-C28-C29-C2A
9	C	2008	3PE	C27-C28-C29-C2A
9	G	3012	3PE	C38-C39-C3A-C3B
9	C	2010	3PE	C2C-C2D-C2E-C2F
9	A	2009	3PE	C22-C21-O21-C2
9	C	2010	3PE	C22-C23-C24-C25
9	C	2013	3PE	C25-C26-C27-C28
9	I	3008	3PE	C2A-C2B-C2C-C2D
9	C	2008	3PE	C2D-C2E-C2F-C2G
9	I	3013	3PE	C36-C37-C38-C39

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Mol	Chain	Res	Type	Atoms
9	I	3013	3PE	C38-C39-C3A-C3B
9	A	2012	3PE	C3E-C3F-C3G-C3H
9	C	2013	3PE	C3A-C3B-C3C-C3D
9	C	2013	3PE	C36-C37-C38-C39
9	C	2010	3PE	C23-C24-C25-C26
9	J	3011	3PE	C27-C28-C29-C2A
9	A	2009	3PE	O22-C21-O21-C2
9	G	3009	3PE	C2E-C2F-C2G-C2H
9	A	2009	3PE	C1-O11-P-O13
9	A	2012	3PE	C1-O11-P-O13
9	C	2010	3PE	C11-O13-P-O11
9	C	2008	3PE	C36-C37-C38-C39
9	I	3013	3PE	O11-C1-C2-C3
9	D	2011	3PE	C27-C28-C29-C2A
9	C	2008	3PE	C38-C39-C3A-C3B
9	C	2010	3PE	C1-C2-C3-O31
9	G	3012	3PE	C1-C2-C3-O31
9	I	3010	3PE	C1-C2-C3-O31
9	C	2013	3PE	C38-C39-C3A-C3B
9	I	3008	3PE	C39-C3A-C3B-C3C
9	C	2010	3PE	C21-C22-C23-C24
9	J	3011	3PE	C29-C2A-C2B-C2C
9	A	2012	3PE	C24-C25-C26-C27
9	D	2011	3PE	C2F-C2G-C2H-C2I
9	I	3008	3PE	C38-C39-C3A-C3B
9	I	3008	3PE	C2F-C2G-C2H-C2I
9	I	3008	3PE	C34-C35-C36-C37
9	I	3013	3PE	C3E-C3F-C3G-C3H
9	J	3011	3PE	C39-C3A-C3B-C3C
9	C	2013	3PE	C3E-C3F-C3G-C3H
9	G	3012	3PE	C24-C25-C26-C27
9	G	3012	3PE	C29-C2A-C2B-C2C
9	C	2013	3PE	O11-C1-C2-O21
9	I	3008	3PE	C37-C38-C39-C3A
9	C	2008	3PE	C37-C38-C39-C3A
9	C	2008	3PE	C21-C22-C23-C24
9	C	2008	3PE	C2F-C2G-C2H-C2I
9	J	3011	3PE	C2F-C2G-C2H-C2I
9	A	2009	3PE	C2E-C2F-C2G-C2H
9	I	3008	3PE	C2D-C2E-C2F-C2G
9	C	2010	3PE	C26-C27-C28-C29
9	A	2012	3PE	O11-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
9	C	2013	3PE	O11-C1-C2-C3
9	D	2011	3PE	C33-C34-C35-C36
9	D	2011	3PE	C36-C37-C38-C39
9	A	2009	3PE	C3C-C3D-C3E-C3F
9	A	2012	3PE	C22-C23-C24-C25
9	G	3009	3PE	C3C-C3D-C3E-C3F
9	G	3012	3PE	C3C-C3D-C3E-C3F
9	A	2009	3PE	C1-C2-C3-O31
9	A	2012	3PE	C1-C2-C3-O31
9	I	3013	3PE	C1-C2-C3-O31
9	I	3013	3PE	C3A-C3B-C3C-C3D
9	I	3008	3PE	C21-C22-C23-C24
9	G	3012	3PE	C22-C23-C24-C25
9	I	3010	3PE	C28-C29-C2A-C2B
9	I	3010	3PE	C3D-C3E-C3F-C3G
9	C	2008	3PE	O11-C1-C2-O21
9	I	3013	3PE	O11-C1-C2-O21
9	D	2011	3PE	C32-C31-O31-C3
9	I	3010	3PE	C21-C22-C23-C24
9	I	3010	3PE	C2C-C2D-C2E-C2F
9	I	3013	3PE	C26-C27-C28-C29
9	C	2008	3PE	O21-C2-C3-O31
9	C	2013	3PE	O21-C2-C3-O31
9	I	3008	3PE	O21-C2-C3-O31
9	I	3010	3PE	O21-C2-C3-O31
9	I	3013	3PE	O21-C2-C3-O31
9	C	2010	3PE	C2F-C2G-C2H-C2I
9	G	3009	3PE	C2B-C2C-C2D-C2E
9	A	2009	3PE	C2B-C2C-C2D-C2E
9	G	3009	3PE	C2F-C2G-C2H-C2I
9	I	3008	3PE	C27-C28-C29-C2A
9	A	2012	3PE	C29-C2A-C2B-C2C
9	C	2013	3PE	C37-C38-C39-C3A
9	C	2008	3PE	O11-C1-C2-C3
9	G	3012	3PE	O11-C1-C2-C3
9	I	3008	3PE	O11-C1-C2-C3
9	C	2008	3PE	C39-C3A-C3B-C3C
9	C	2010	3PE	C25-C26-C27-C28
9	C	2013	3PE	C1-C2-C3-O31
9	G	3012	3PE	C3E-C3F-C3G-C3H
9	A	2012	3PE	C23-C24-C25-C26
9	G	3009	3PE	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
9	C	2010	3PE	O21-C2-C3-O31
9	J	3011	3PE	C37-C38-C39-C3A
8	A	1001	HEA	C26-C15-C16-C17
9	C	2008	3PE	C3D-C3E-C3F-C3G
9	D	2011	3PE	O32-C31-O31-C3
9	C	2010	3PE	C3D-C3E-C3F-C3G
9	I	3010	3PE	C26-C27-C28-C29
9	I	3008	3PE	C2E-C2F-C2G-C2H
9	A	2009	3PE	C1-O11-P-O12
9	A	2012	3PE	C1-O11-P-O12
9	C	2010	3PE	C1-O11-P-O14
9	C	2010	3PE	C11-O13-P-O14
9	C	2013	3PE	C1-O11-P-O14
9	C	2013	3PE	C11-O13-P-O12
9	G	3009	3PE	C1-O11-P-O12
9	I	3013	3PE	C1-O11-P-O14
9	I	3013	3PE	C11-O13-P-O12
9	G	3012	3PE	C21-C22-C23-C24
9	C	2008	3PE	C34-C35-C36-C37
9	D	2011	3PE	C39-C3A-C3B-C3C
9	A	2012	3PE	C12-C11-O13-P
9	G	3012	3PE	C12-C11-O13-P
9	I	3008	3PE	C3D-C3E-C3F-C3G
9	I	3008	3PE	O11-C1-C2-O21
9	A	2009	3PE	C2F-C2G-C2H-C2I
9	I	3010	3PE	C2F-C2G-C2H-C2I
9	C	2008	3PE	C22-C21-O21-C2
9	D	2011	3PE	C24-C25-C26-C27
9	J	3011	3PE	C36-C37-C38-C39
9	C	2008	3PE	C1-C2-C3-O31
9	I	3008	3PE	C1-C2-C3-O31
9	J	3011	3PE	C1-C2-C3-O31
9	A	2009	3PE	C25-C26-C27-C28
9	I	3013	3PE	C3F-C3G-C3H-C3I
9	C	2010	3PE	C22-C21-O21-C2
9	C	2013	3PE	C26-C27-C28-C29
9	C	2008	3PE	O22-C21-O21-C2
9	C	2010	3PE	O22-C21-O21-C2
9	C	2013	3PE	C24-C25-C26-C27
9	I	3010	3PE	C22-C23-C24-C25
9	C	2013	3PE	C3F-C3G-C3H-C3I
9	I	3013	3PE	C28-C29-C2A-C2B

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Mol	Chain	Res	Type	Atoms
9	C	2008	3PE	C11-O13-P-O11
9	I	3008	3PE	C11-O13-P-O11
9	I	3010	3PE	C11-O13-P-O11
9	C	2010	3PE	C28-C29-C2A-C2B
9	I	3010	3PE	C3E-C3F-C3G-C3H
9	I	3013	3PE	C24-C25-C26-C27
9	J	3011	3PE	C3B-C3C-C3D-C3E
8	A	1001	HEA	C14-C15-C16-C17
9	A	2009	3PE	C27-C28-C29-C2A
9	I	3008	3PE	C22-C23-C24-C25
9	J	3011	3PE	C33-C34-C35-C36
9	G	3009	3PE	C23-C24-C25-C26
9	G	3012	3PE	C23-C24-C25-C26
9	A	2012	3PE	C21-C22-C23-C24
9	I	3008	3PE	O22-C21-O21-C2
9	C	2010	3PE	C2D-C2E-C2F-C2G
9	I	3008	3PE	C35-C36-C37-C38
9	C	2008	3PE	C33-C34-C35-C36
9	I	3010	3PE	C23-C24-C25-C26
9	G	3009	3PE	O22-C21-O21-C2
9	C	2008	3PE	C2E-C2F-C2G-C2H
9	G	3012	3PE	C2E-C2F-C2G-C2H
9	C	2010	3PE	C3F-C3G-C3H-C3I
8	A	1002	HEA	C20-C21-C22-C23
9	C	2008	3PE	C35-C36-C37-C38
9	G	3009	3PE	C3F-C3G-C3H-C3I
9	C	2010	3PE	C3A-C3B-C3C-C3D
9	G	3009	3PE	C22-C21-O21-C2
9	I	3010	3PE	C33-C34-C35-C36
9	A	2009	3PE	C21-C22-C23-C24
9	D	2011	3PE	C3A-C3B-C3C-C3D
9	I	3008	3PE	C22-C21-O21-C2
9	I	3010	3PE	C2D-C2E-C2F-C2G
9	C	2010	3PE	O31-C31-C32-C33
9	I	3010	3PE	O31-C31-C32-C33
9	J	3011	3PE	C32-C31-O31-C3
8	A	1002	HEA	C26-C15-C16-C17
9	J	3011	3PE	O32-C31-O31-C3
9	A	2012	3PE	O21-C21-C22-C23
9	I	3008	3PE	C2B-C2C-C2D-C2E
9	C	2008	3PE	C3-C2-O21-C21
9	G	3009	3PE	O31-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
9	A	2009	3PE	O31-C31-C32-C33
9	A	2009	3PE	C23-C24-C25-C26
9	D	2011	3PE	C1-C2-C3-O31
9	D	2011	3PE	C3D-C3E-C3F-C3G
9	I	3010	3PE	C35-C36-C37-C38
9	J	3011	3PE	C3F-C3G-C3H-C3I
9	A	2009	3PE	O21-C2-C3-O31
9	J	3011	3PE	O21-C2-C3-O31
9	C	2010	3PE	O21-C21-C22-C23
9	G	3012	3PE	O21-C21-C22-C23
9	C	2010	3PE	O32-C31-C32-C33
9	I	3010	3PE	C3F-C3G-C3H-C3I
8	G	1001	HEA	C14-C15-C16-C17
9	C	2008	3PE	C28-C29-C2A-C2B
9	I	3010	3PE	O32-C31-C32-C33
9	A	2009	3PE	C3A-C3B-C3C-C3D
9	D	2011	3PE	C37-C38-C39-C3A
9	A	2009	3PE	O32-C31-C32-C33
9	G	3009	3PE	O32-C31-C32-C33
9	J	3011	3PE	O21-C21-C22-C23
9	J	3011	3PE	C2A-C2B-C2C-C2D
9	C	2010	3PE	O22-C21-C22-C23
9	G	3009	3PE	C1-O11-P-O14
9	I	3010	3PE	C11-O13-P-O14
9	I	3013	3PE	C1-O11-P-O12
9	A	2012	3PE	O22-C21-C22-C23
9	G	3012	3PE	O22-C21-C22-C23
9	J	3011	3PE	C2C-C2D-C2E-C2F
9	I	3008	3PE	C3-C2-O21-C21
9	D	2011	3PE	O21-C21-C22-C23
9	A	2009	3PE	C22-C23-C24-C25
9	I	3010	3PE	O21-C21-C22-C23
9	J	3011	3PE	O22-C21-C22-C23
9	J	3011	3PE	C3A-C3B-C3C-C3D
8	A	1001	HEA	C19-C20-C21-C22

There are no ring outliers.

16 monomers are involved in 226 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	I	3008	3PE	9	0
9	C	2013	3PE	21	0

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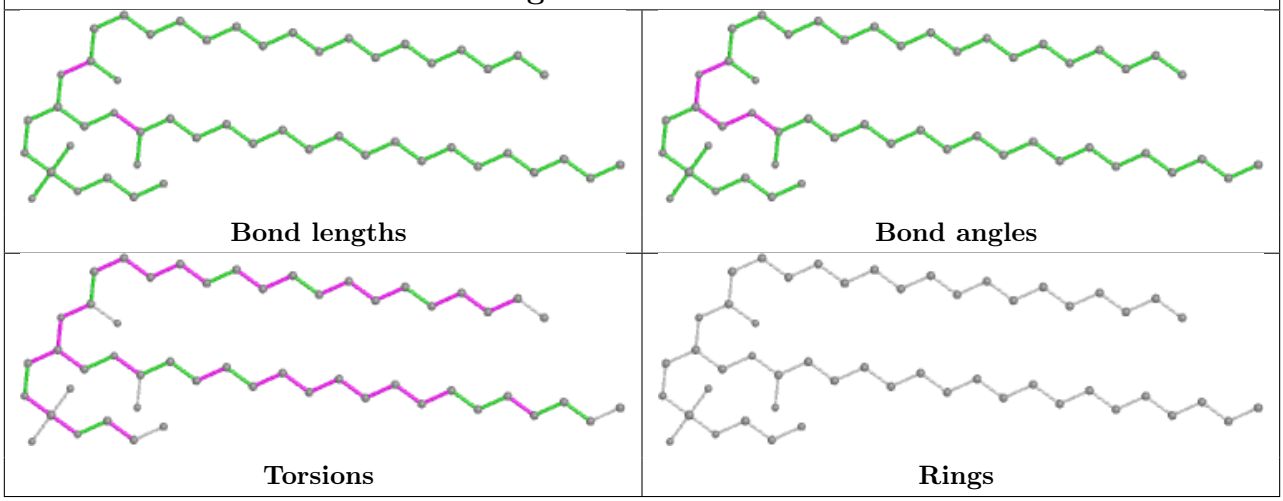
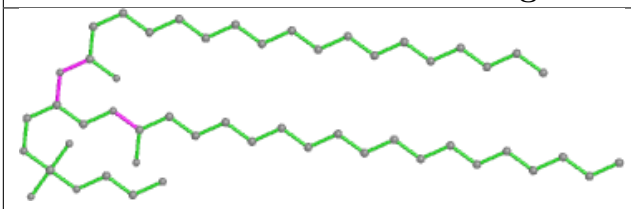
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	G	1002	HEA	7	0
8	A	1002	HEA	9	0
9	C	2010	3PE	20	0
8	A	1001	HEA	17	0
9	G	3009	3PE	17	0
9	C	2008	3PE	7	0
9	A	2012	3PE	14	0
9	A	2009	3PE	20	0
9	G	3012	3PE	12	0
8	G	1001	HEA	11	0
9	I	3013	3PE	22	0
9	J	3011	3PE	16	0
9	I	3010	3PE	21	0
9	D	2011	3PE	21	0

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

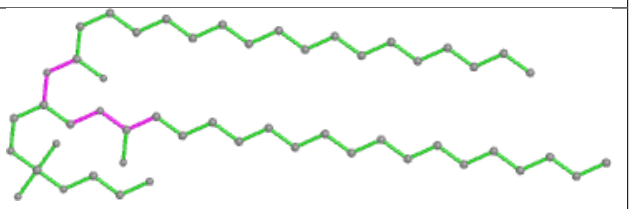
Ligand 3PE I 3008



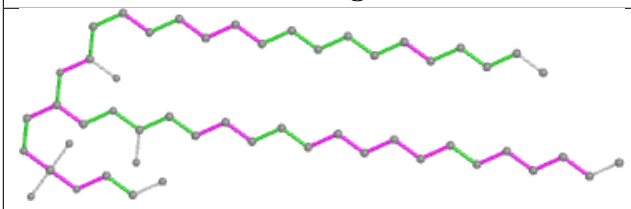
Ligand 3PE C 2013



Bond lengths



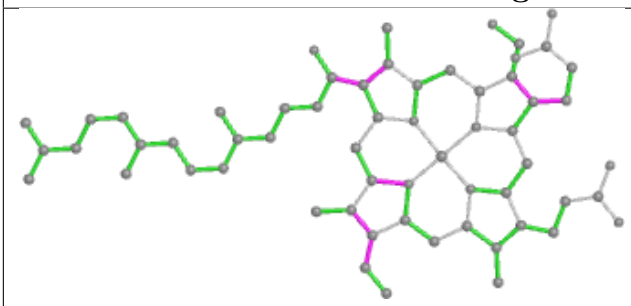
Bond angles



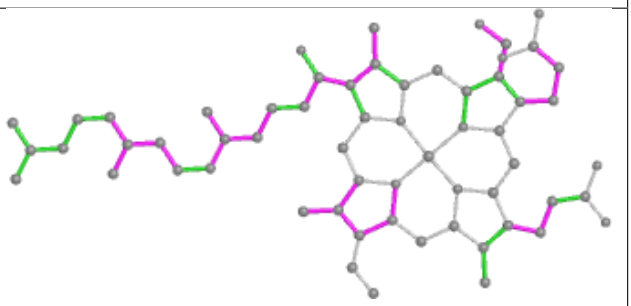
Torsions

Rings

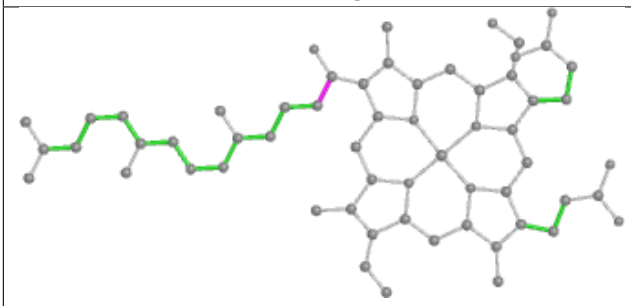
Ligand HEA G 1002



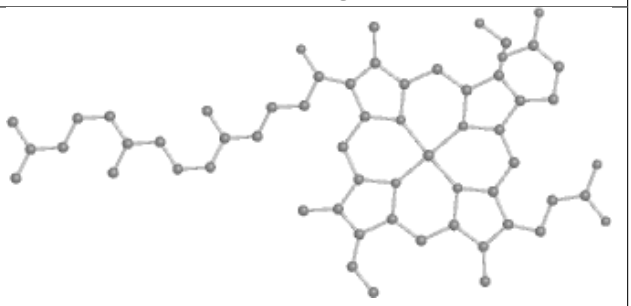
Bond lengths



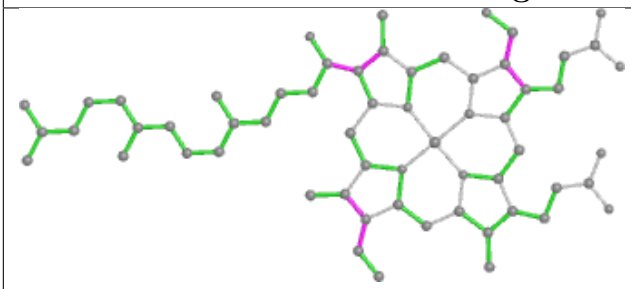
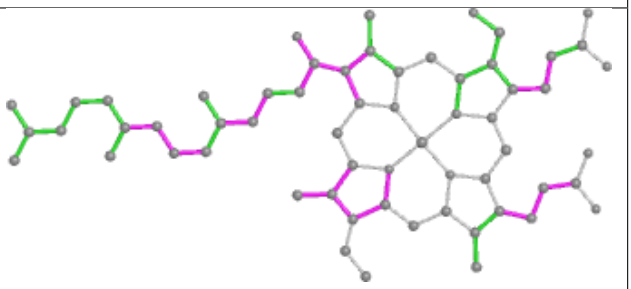
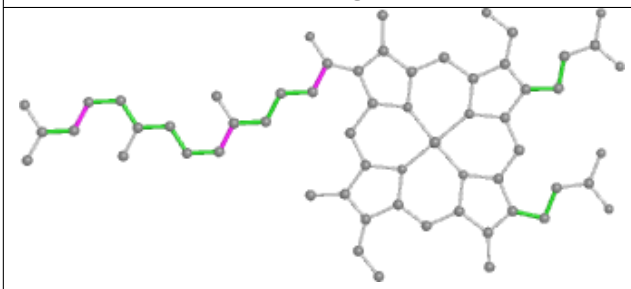
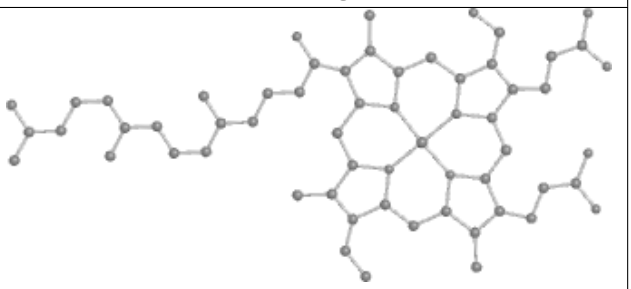
Bond angles

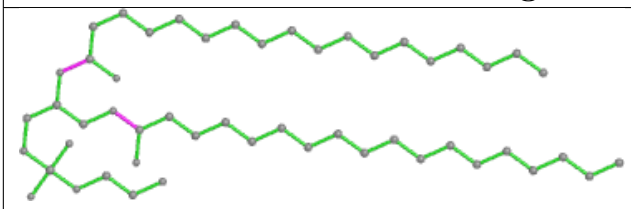
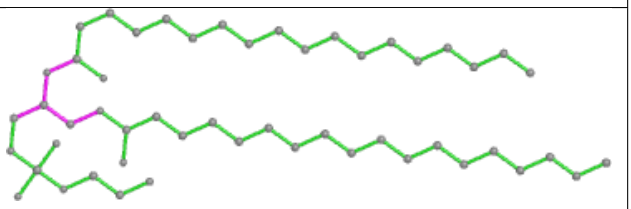
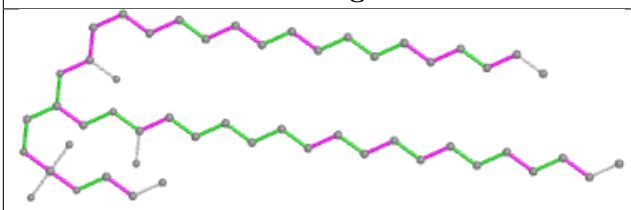
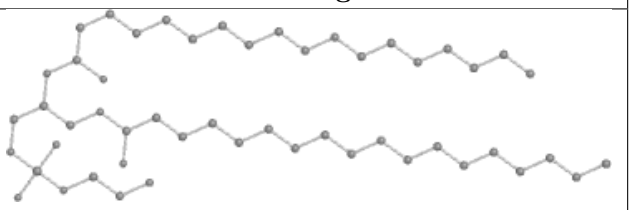


Torsions

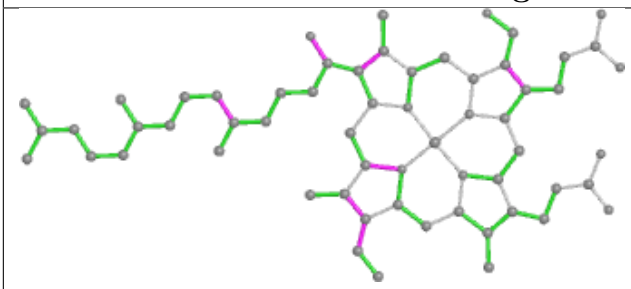


Rings

Ligand HEA A 1002	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand 3PE C 2010	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand HEA A 1001



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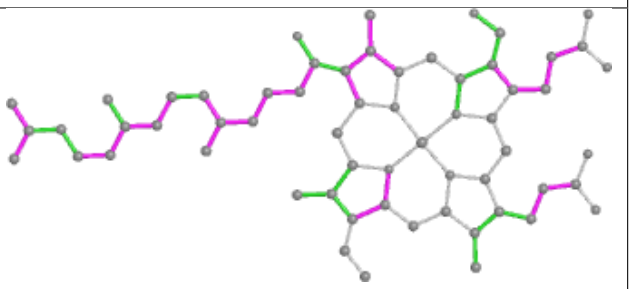

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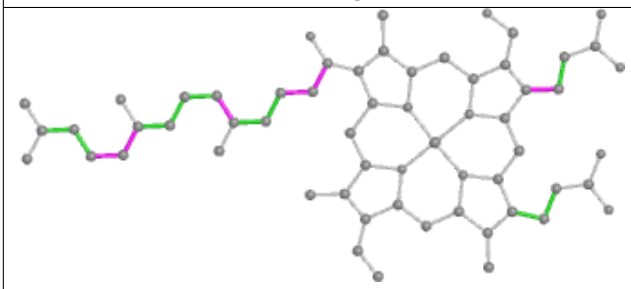

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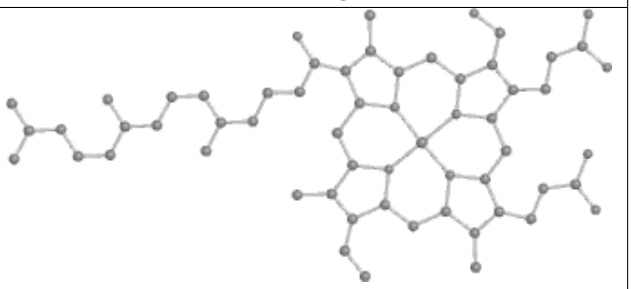
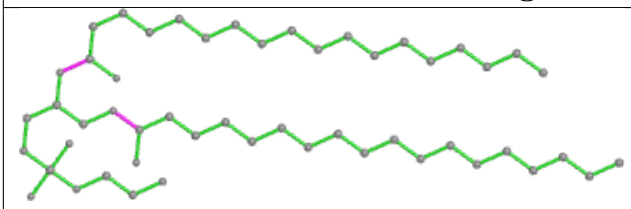


Rings

Ligand 3PE G 3009



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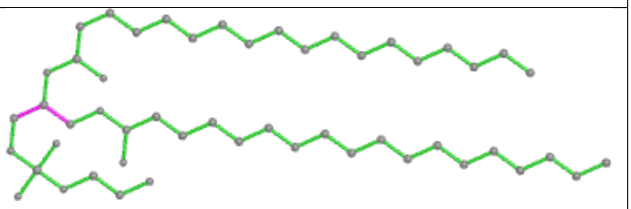

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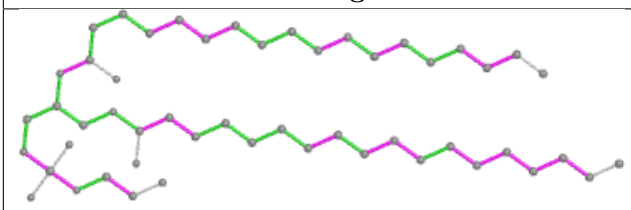

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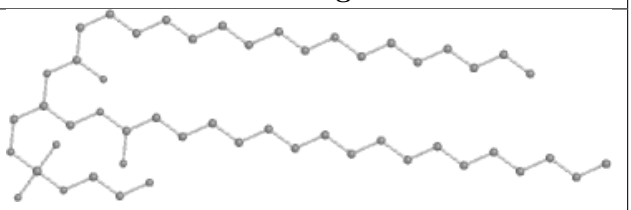
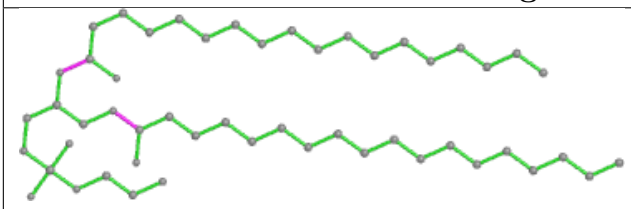


Rings

Ligand 3PE C 2008



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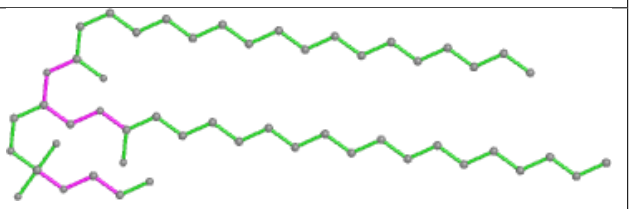

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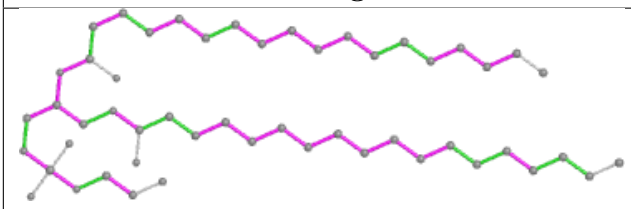

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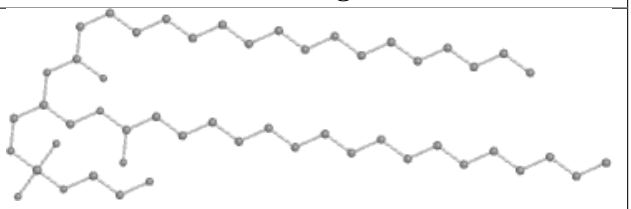
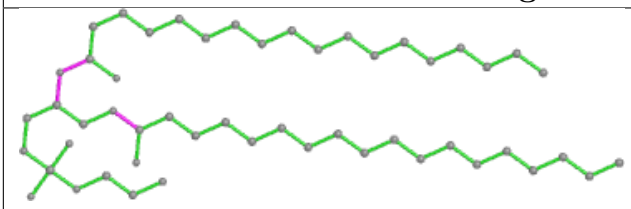


Rings

Ligand 3PE A 2012



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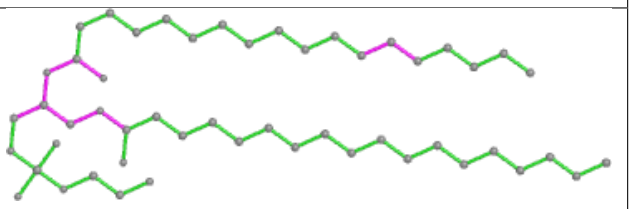
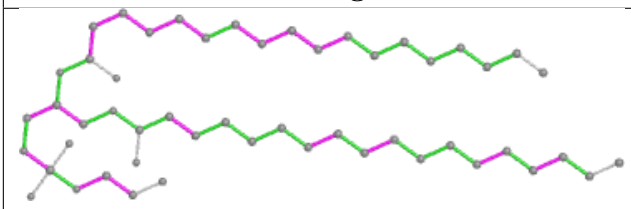


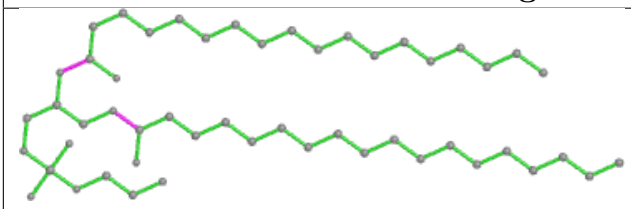
Bond angles



Torsions

Rings

Ligand 3PE A 2009



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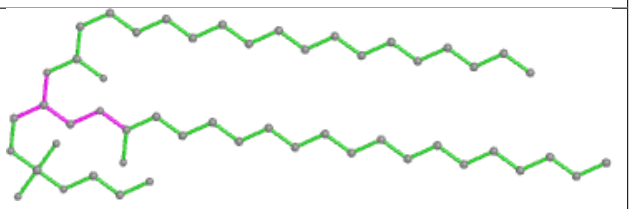

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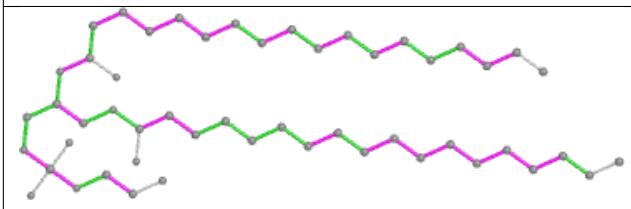

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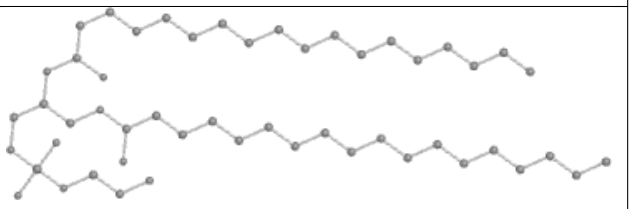
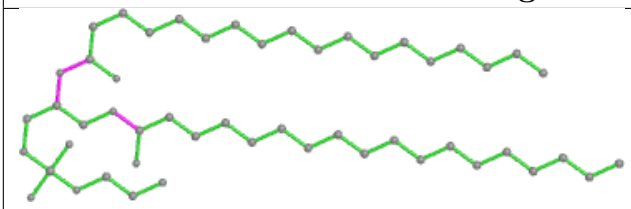


Rings

Ligand 3PE G 3012



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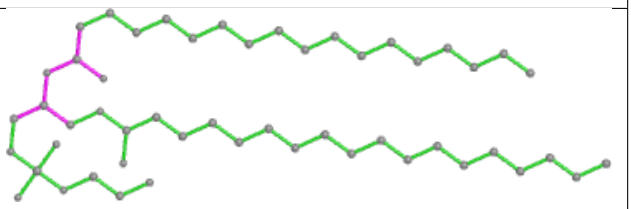

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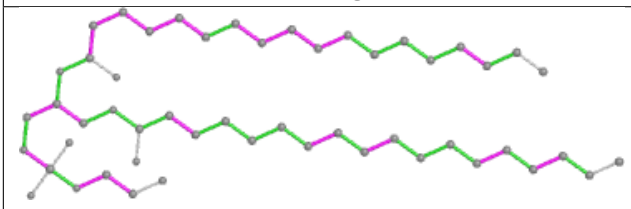

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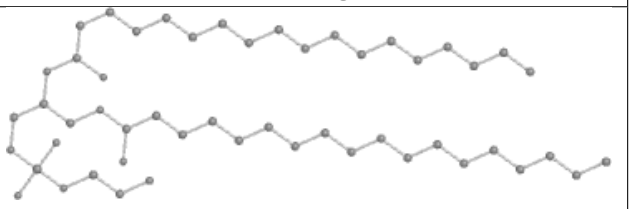
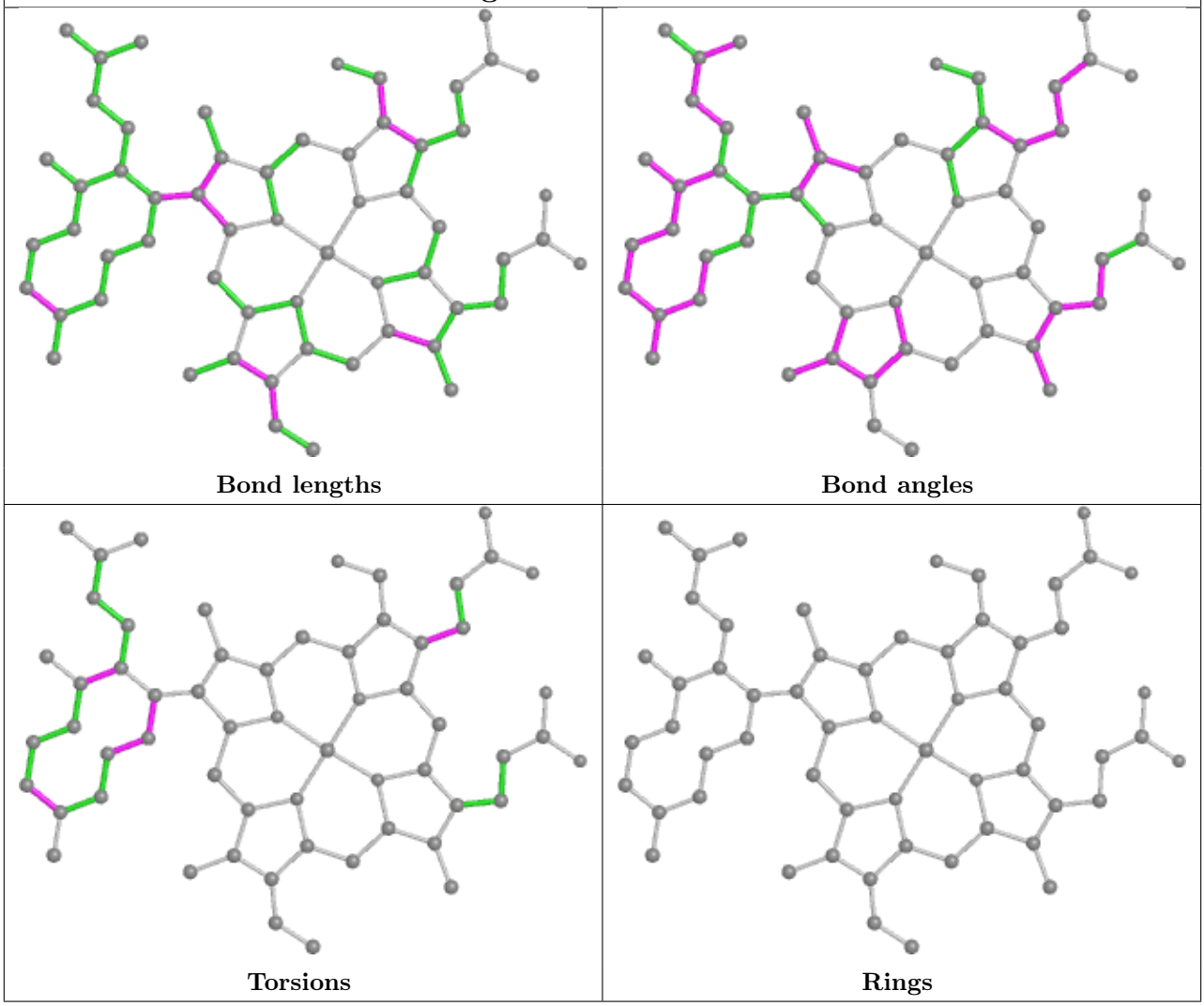


Rings

Ligand HEA G 1001



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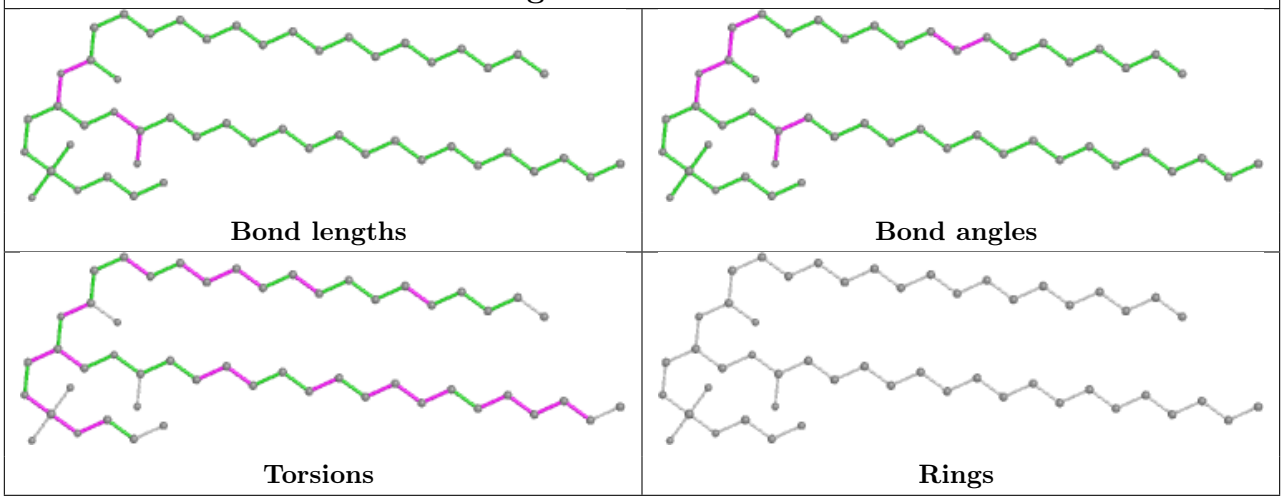

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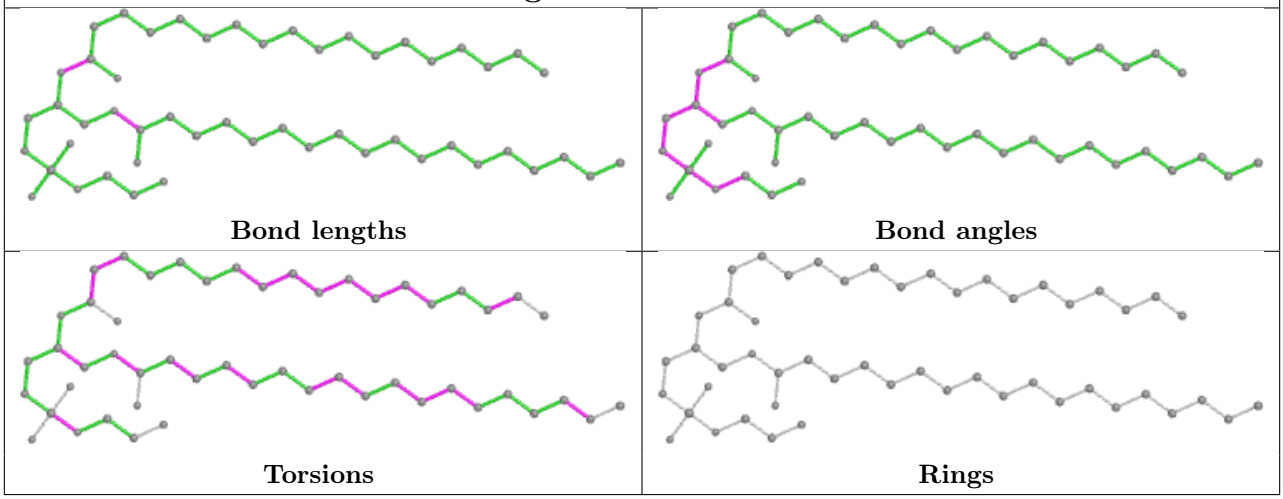

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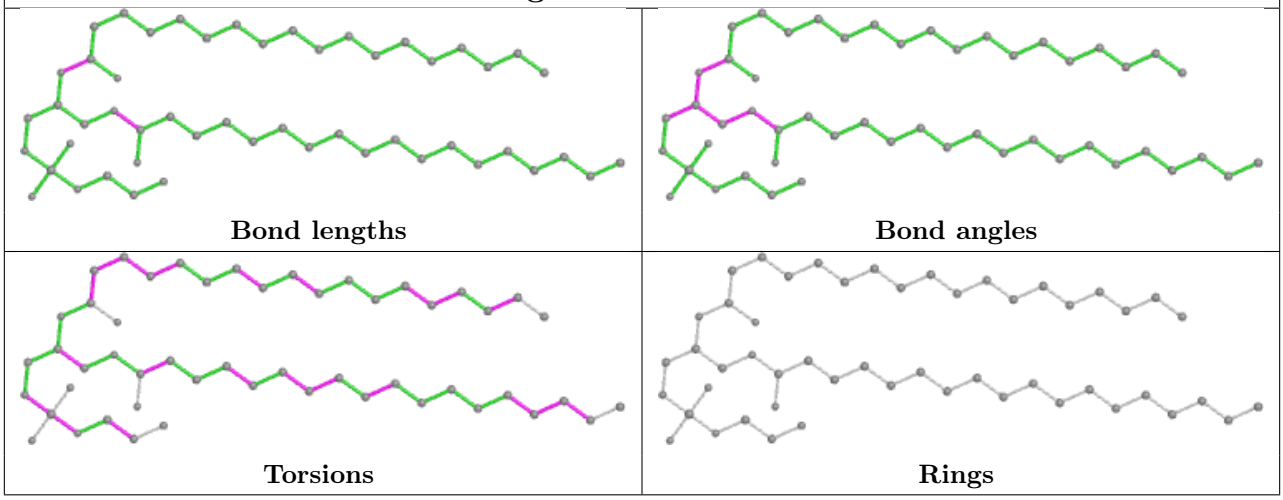
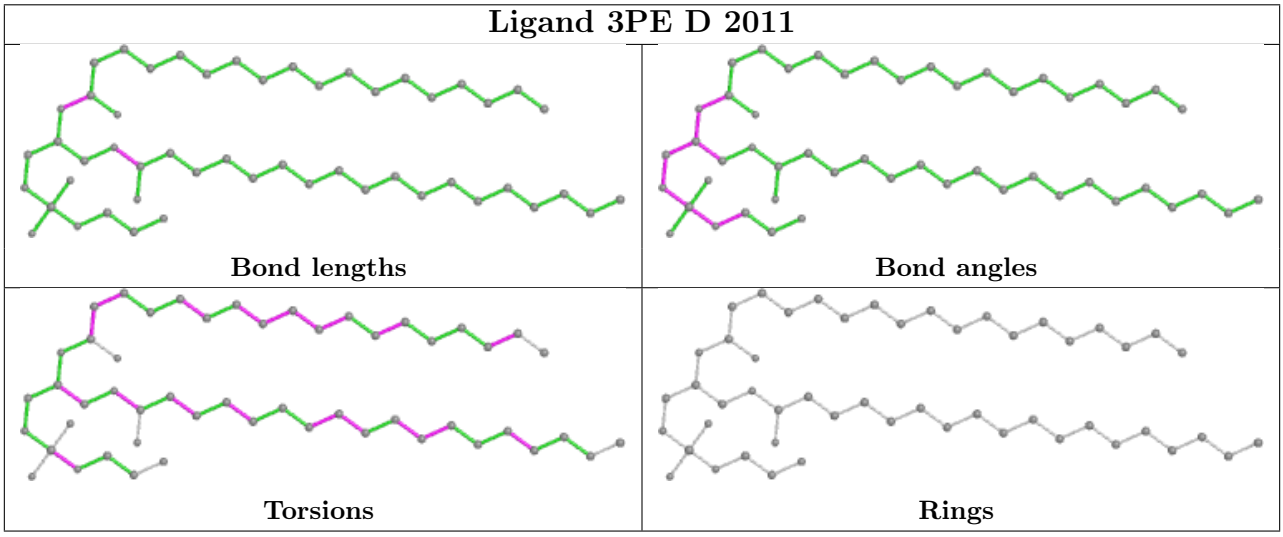


Ligand 3PE D 2011



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates (i)

EDS was not executed - this section is therefore empty.

6.4 Ligands (i)

EDS was not executed - this section is therefore empty.

6.5 Other polymers (i)

EDS was not executed - this section is therefore empty.