Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 05:00 PM EDT

PDB ID	:	4PV6
Title	:	Crystal Structure Analysis of Ard1 from Thermoplasma volcanium
Authors	:	Ma, C.; Lee, S.J.; Lee, B.J.
Deposited on	:	2014-03-15
Resolution	:	3.32 Å(reported)

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

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

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

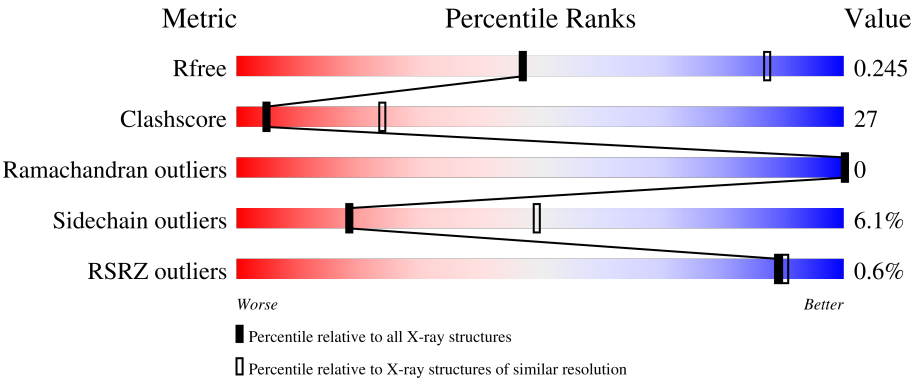
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.37.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.32 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1089 (3.36-3.28)
Clashscore	141614	1137 (3.36-3.28)
Ramachandran outliers	138981	1115 (3.36-3.28)
Sidechain outliers	138945	1114 (3.36-3.28)
RSRZ outliers	127900	1059 (3.36-3.28)

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

Mol	Chain	Length	Quality of chain
1	A	162	54% 38% · 5%
1	B	162	% 60% 26% 6% 9%
1	C	162	59% 31% · 6%
1	D	162	68% 21% · 9%
1	E	162	% 67% 22% · 7%

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Mol	Chain	Length	Quality of chain
1	F	162	70% 22% 7%
1	G	162	65% 29% 5%
1	H	162	2% 63% 30% 6%
1	I	162	67% 25% 7%
1	J	162	66% 22% 5% 7%
1	K	162	60% 30% 8%
1	L	162	60% 29% 8%
1	M	162	1% 59% 31% 9%
1	N	162	3% 53% 35% 9%
1	O	162	60% 30% 8%
1	P	162	2% 42% 40% 9% 9%

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
2	ACO	H	200	-	-	X	-
3	COA	A	201	-	-	X	-

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 20015 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 N-terminal acetyltransferase complex subunit [ARD1].

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	153	Total	C	N	O	S	0	0	0
			1248	798	214	229	7			
1	D	147	Total	C	N	O	S	0	0	0
			1196	768	201	220	7			
1	G	154	Total	C	N	O	S	0	0	0
			1256	804	215	230	7			
1	I	151	Total	C	N	O	S	0	0	0
			1226	786	206	227	7			
1	K	149	Total	C	N	O	S	0	0	0
			1215	779	205	224	7			
1	M	148	Total	C	N	O	S	0	0	0
			1205	773	202	223	7			
1	F	150	Total	C	N	O	S	0	0	0
			1220	782	206	225	7			
1	N	148	Total	C	N	O	S	0	0	0
			1205	773	202	223	7			
1	A	154	Total	C	N	O	S	0	0	0
			1256	804	215	230	7			
1	B	148	Total	C	N	O	S	0	0	0
			1205	773	202	223	7			
1	H	153	Total	C	N	O	S	0	0	0
			1248	798	214	229	7			
1	J	151	Total	C	N	O	S	0	0	0
			1228	786	208	227	7			
1	L	149	Total	C	N	O	S	0	0	0
			1210	776	203	224	7			
1	O	149	Total	C	N	O	S	0	0	0
			1215	779	205	224	7			
1	E	151	Total	C	N	O	S	0	0	0
			1230	788	209	226	7			
1	P	147	Total	C	N	O	S	0	0	0
			1196	768	201	220	7			

There are 128 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	155	LEU	-	expression tag	UNP Q97CT7
C	156	GLU	-	expression tag	UNP Q97CT7
C	157	HIS	-	expression tag	UNP Q97CT7
C	158	HIS	-	expression tag	UNP Q97CT7
C	159	HIS	-	expression tag	UNP Q97CT7
C	160	HIS	-	expression tag	UNP Q97CT7
C	161	HIS	-	expression tag	UNP Q97CT7
C	162	HIS	-	expression tag	UNP Q97CT7
D	155	LEU	-	expression tag	UNP Q97CT7
D	156	GLU	-	expression tag	UNP Q97CT7
D	157	HIS	-	expression tag	UNP Q97CT7
D	158	HIS	-	expression tag	UNP Q97CT7
D	159	HIS	-	expression tag	UNP Q97CT7
D	160	HIS	-	expression tag	UNP Q97CT7
D	161	HIS	-	expression tag	UNP Q97CT7
D	162	HIS	-	expression tag	UNP Q97CT7
G	155	LEU	-	expression tag	UNP Q97CT7
G	156	GLU	-	expression tag	UNP Q97CT7
G	157	HIS	-	expression tag	UNP Q97CT7
G	158	HIS	-	expression tag	UNP Q97CT7
G	159	HIS	-	expression tag	UNP Q97CT7
G	160	HIS	-	expression tag	UNP Q97CT7
G	161	HIS	-	expression tag	UNP Q97CT7
G	162	HIS	-	expression tag	UNP Q97CT7
I	155	LEU	-	expression tag	UNP Q97CT7
I	156	GLU	-	expression tag	UNP Q97CT7
I	157	HIS	-	expression tag	UNP Q97CT7
I	158	HIS	-	expression tag	UNP Q97CT7
I	159	HIS	-	expression tag	UNP Q97CT7
I	160	HIS	-	expression tag	UNP Q97CT7
I	161	HIS	-	expression tag	UNP Q97CT7
I	162	HIS	-	expression tag	UNP Q97CT7
K	155	LEU	-	expression tag	UNP Q97CT7
K	156	GLU	-	expression tag	UNP Q97CT7
K	157	HIS	-	expression tag	UNP Q97CT7
K	158	HIS	-	expression tag	UNP Q97CT7
K	159	HIS	-	expression tag	UNP Q97CT7
K	160	HIS	-	expression tag	UNP Q97CT7
K	161	HIS	-	expression tag	UNP Q97CT7
K	162	HIS	-	expression tag	UNP Q97CT7
M	155	LEU	-	expression tag	UNP Q97CT7
M	156	GLU	-	expression tag	UNP Q97CT7

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Chain	Residue	Modelled	Actual	Comment	Reference
M	157	HIS	-	expression tag	UNP Q97CT7
M	158	HIS	-	expression tag	UNP Q97CT7
M	159	HIS	-	expression tag	UNP Q97CT7
M	160	HIS	-	expression tag	UNP Q97CT7
M	161	HIS	-	expression tag	UNP Q97CT7
M	162	HIS	-	expression tag	UNP Q97CT7
F	155	LEU	-	expression tag	UNP Q97CT7
F	156	GLU	-	expression tag	UNP Q97CT7
F	157	HIS	-	expression tag	UNP Q97CT7
F	158	HIS	-	expression tag	UNP Q97CT7
F	159	HIS	-	expression tag	UNP Q97CT7
F	160	HIS	-	expression tag	UNP Q97CT7
F	161	HIS	-	expression tag	UNP Q97CT7
F	162	HIS	-	expression tag	UNP Q97CT7
N	155	LEU	-	expression tag	UNP Q97CT7
N	156	GLU	-	expression tag	UNP Q97CT7
N	157	HIS	-	expression tag	UNP Q97CT7
N	158	HIS	-	expression tag	UNP Q97CT7
N	159	HIS	-	expression tag	UNP Q97CT7
N	160	HIS	-	expression tag	UNP Q97CT7
N	161	HIS	-	expression tag	UNP Q97CT7
N	162	HIS	-	expression tag	UNP Q97CT7
A	155	LEU	-	expression tag	UNP Q97CT7
A	156	GLU	-	expression tag	UNP Q97CT7
A	157	HIS	-	expression tag	UNP Q97CT7
A	158	HIS	-	expression tag	UNP Q97CT7
A	159	HIS	-	expression tag	UNP Q97CT7
A	160	HIS	-	expression tag	UNP Q97CT7
A	161	HIS	-	expression tag	UNP Q97CT7
A	162	HIS	-	expression tag	UNP Q97CT7
B	155	LEU	-	expression tag	UNP Q97CT7
B	156	GLU	-	expression tag	UNP Q97CT7
B	157	HIS	-	expression tag	UNP Q97CT7
B	158	HIS	-	expression tag	UNP Q97CT7
B	159	HIS	-	expression tag	UNP Q97CT7
B	160	HIS	-	expression tag	UNP Q97CT7
B	161	HIS	-	expression tag	UNP Q97CT7
B	162	HIS	-	expression tag	UNP Q97CT7
H	155	LEU	-	expression tag	UNP Q97CT7
H	156	GLU	-	expression tag	UNP Q97CT7
H	157	HIS	-	expression tag	UNP Q97CT7
H	158	HIS	-	expression tag	UNP Q97CT7

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Chain	Residue	Modelled	Actual	Comment	Reference
H	159	HIS	-	expression tag	UNP Q97CT7
H	160	HIS	-	expression tag	UNP Q97CT7
H	161	HIS	-	expression tag	UNP Q97CT7
H	162	HIS	-	expression tag	UNP Q97CT7
J	155	LEU	-	expression tag	UNP Q97CT7
J	156	GLU	-	expression tag	UNP Q97CT7
J	157	HIS	-	expression tag	UNP Q97CT7
J	158	HIS	-	expression tag	UNP Q97CT7
J	159	HIS	-	expression tag	UNP Q97CT7
J	160	HIS	-	expression tag	UNP Q97CT7
J	161	HIS	-	expression tag	UNP Q97CT7
J	162	HIS	-	expression tag	UNP Q97CT7
L	155	LEU	-	expression tag	UNP Q97CT7
L	156	GLU	-	expression tag	UNP Q97CT7
L	157	HIS	-	expression tag	UNP Q97CT7
L	158	HIS	-	expression tag	UNP Q97CT7
L	159	HIS	-	expression tag	UNP Q97CT7
L	160	HIS	-	expression tag	UNP Q97CT7
L	161	HIS	-	expression tag	UNP Q97CT7
L	162	HIS	-	expression tag	UNP Q97CT7
O	155	LEU	-	expression tag	UNP Q97CT7
O	156	GLU	-	expression tag	UNP Q97CT7
O	157	HIS	-	expression tag	UNP Q97CT7
O	158	HIS	-	expression tag	UNP Q97CT7
O	159	HIS	-	expression tag	UNP Q97CT7
O	160	HIS	-	expression tag	UNP Q97CT7
O	161	HIS	-	expression tag	UNP Q97CT7
O	162	HIS	-	expression tag	UNP Q97CT7
E	155	LEU	-	expression tag	UNP Q97CT7
E	156	GLU	-	expression tag	UNP Q97CT7
E	157	HIS	-	expression tag	UNP Q97CT7
E	158	HIS	-	expression tag	UNP Q97CT7
E	159	HIS	-	expression tag	UNP Q97CT7
E	160	HIS	-	expression tag	UNP Q97CT7
E	161	HIS	-	expression tag	UNP Q97CT7
E	162	HIS	-	expression tag	UNP Q97CT7
P	155	LEU	-	expression tag	UNP Q97CT7
P	156	GLU	-	expression tag	UNP Q97CT7
P	157	HIS	-	expression tag	UNP Q97CT7
P	158	HIS	-	expression tag	UNP Q97CT7
P	159	HIS	-	expression tag	UNP Q97CT7
P	160	HIS	-	expression tag	UNP Q97CT7

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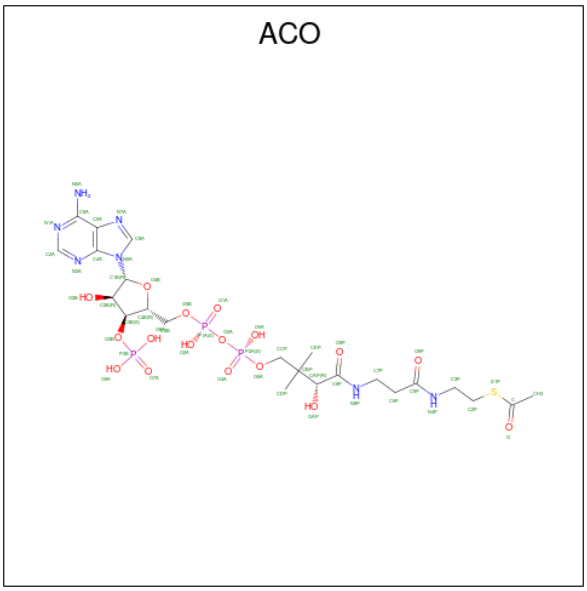
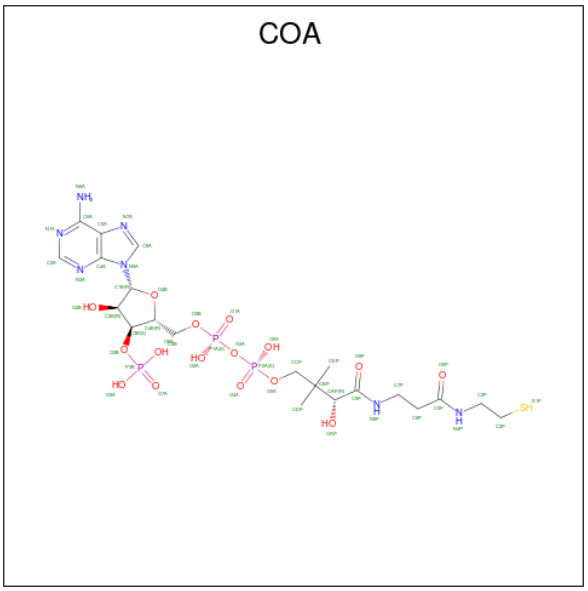
Chain	Residue	Modelled	Actual	Comment	Reference
P	161	HIS	-	expression tag	UNP Q97CT7
P	162	HIS	-	expression tag	UNP Q97CT7

- Molecule 2 is ACETYL COENZYME *A (three-letter code: ACO) (formula: $C_{23}H_{38}N_7O_{17}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	G	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	I	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	F	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	H	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	J	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	E	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 3 is COENZYME A (three-letter code: COA) (formula: $C_{21}H_{36}N_7O_{16}P_3S$).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	S	0	0
			48	21	7	16	3	1		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	4	Total	O	0	0
			4	4		
4	D	7	Total	O	0	0
			7	7		
4	G	1	Total	O	0	0
			1	1		
4	I	4	Total	O	0	0
			4	4		
4	K	1	Total	O	0	0
			1	1		
4	M	5	Total	O	0	0
			5	5		
4	F	4	Total	O	0	0
			4	4		
4	N	2	Total	O	0	0
			2	2		
4	A	5	Total	O	0	0
			5	5		
4	B	1	Total	O	0	0
			1	1		
4	H	2	Total	O	0	0
			2	2		

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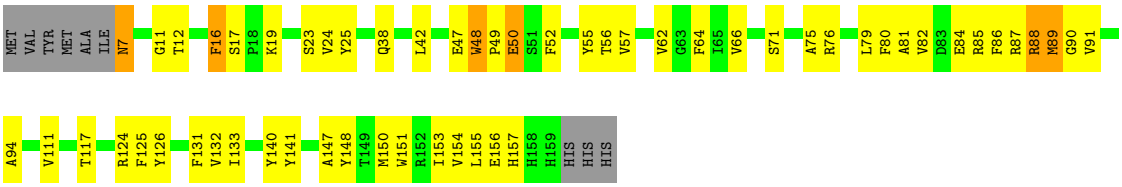
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	J	3	Total O 3 3	0	0
4	L	5	Total O 5 5	0	0
4	O	3	Total O 3 3	0	0
4	E	3	Total O 3 3	0	0
4	P	1	Total O 1 1	0	0

3 Residue-property plots (i)

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

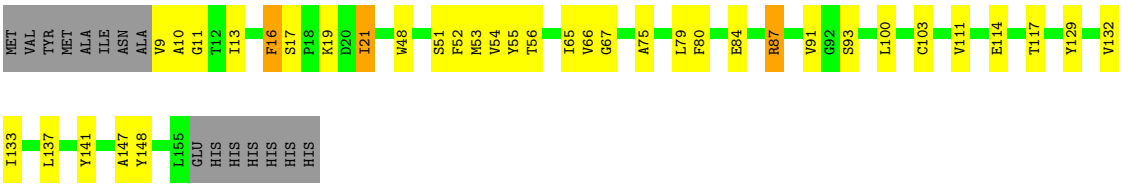
• Molecule 1: N-terminal acetyltransferase complex subunit [ARD1]

Chain C:



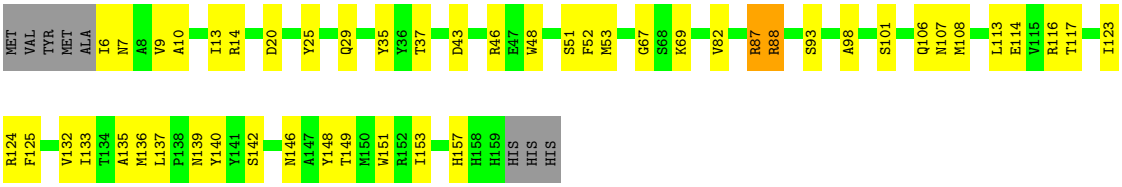
• Molecule 1: N-terminal acetyltransferase complex subunit [ARD1]

Chain D:



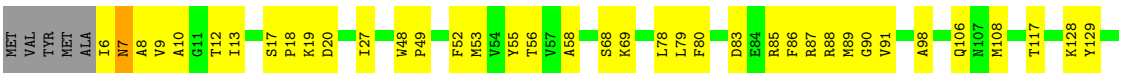
• Molecule 1: N-terminal acetyltransferase complex subunit [ARD1]

Chain G:



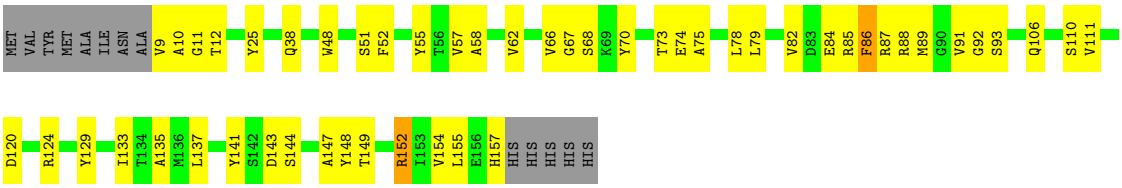
• Molecule 1: N-terminal acetyltransferase complex subunit [ARD1]

Chain I:



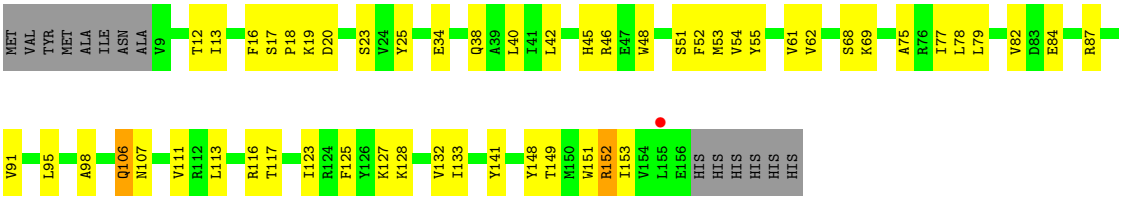
• Molecule 1: N-terminal acetyltransferase complex subunit [ARD1]

Chain K:



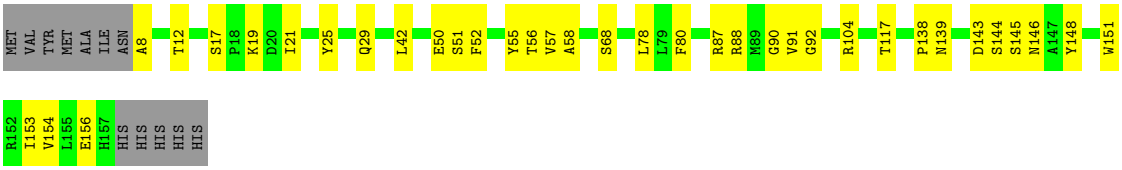
• Molecule 1: N-terminal acetyltransferase complex subunit [ARD1]

Chain M:



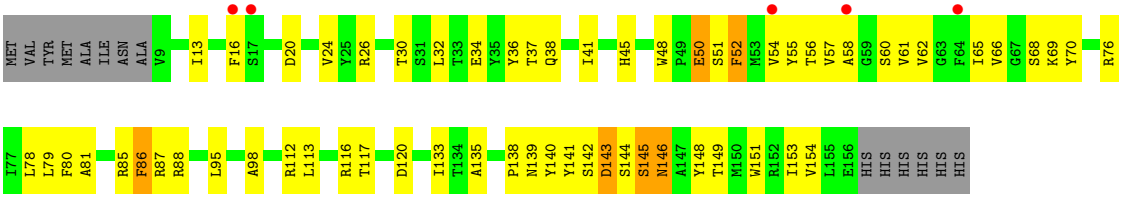
• Molecule 1: N-terminal acetyltransferase complex subunit [ARD1]

Chain F:



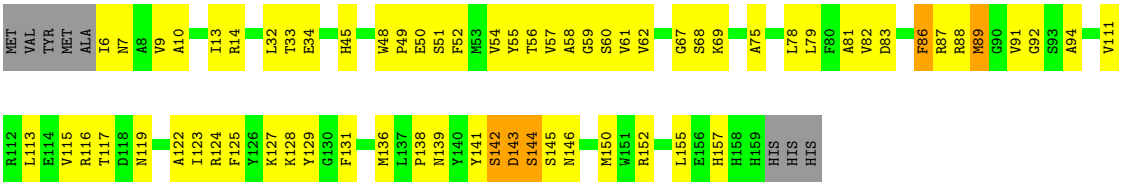
• Molecule 1: N-terminal acetyltransferase complex subunit [ARD1]

Chain N:



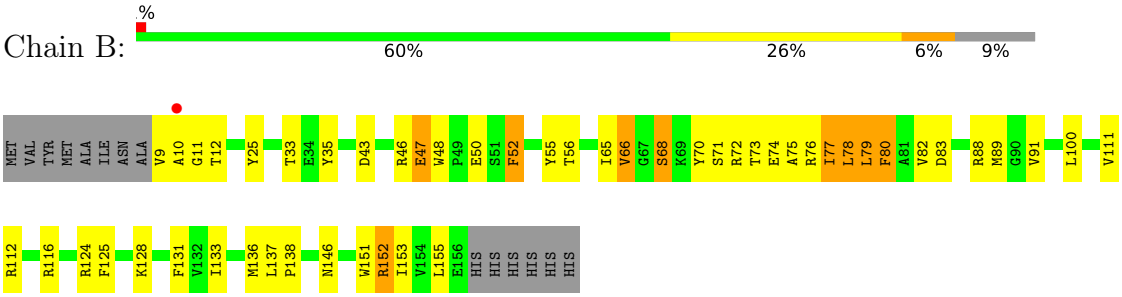
• Molecule 1: N-terminal acetyltransferase complex subunit [ARD1]

Chain A:



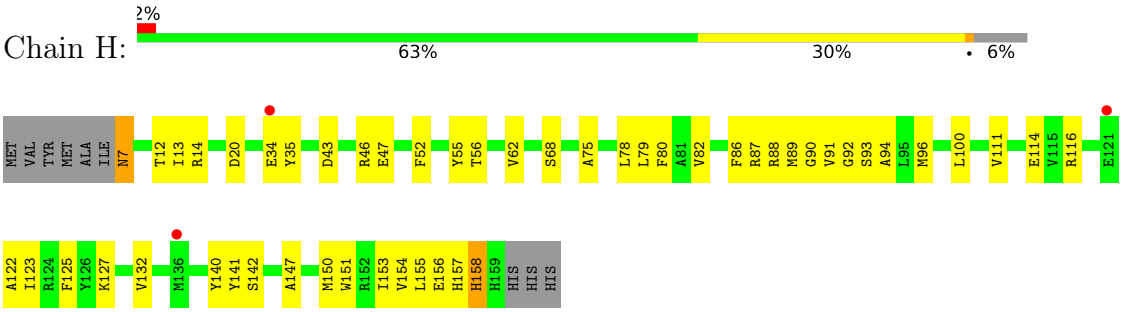
• Molecule 1: N-terminal acetyltransferase complex subunit [ARD1]

Chain B:



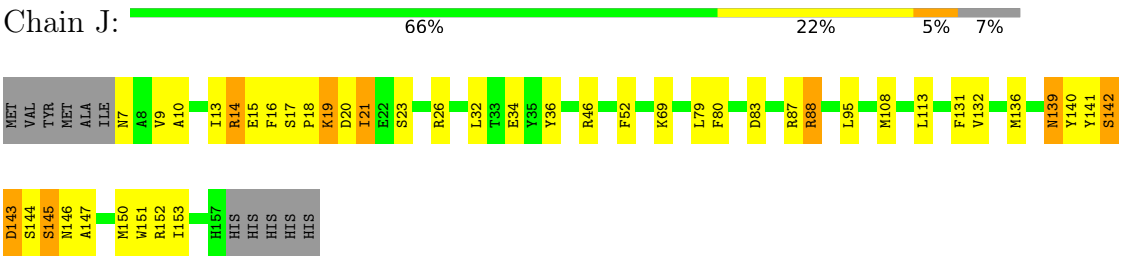
• Molecule 1: N-terminal acetyltransferase complex subunit [ARD1]

Chain H:



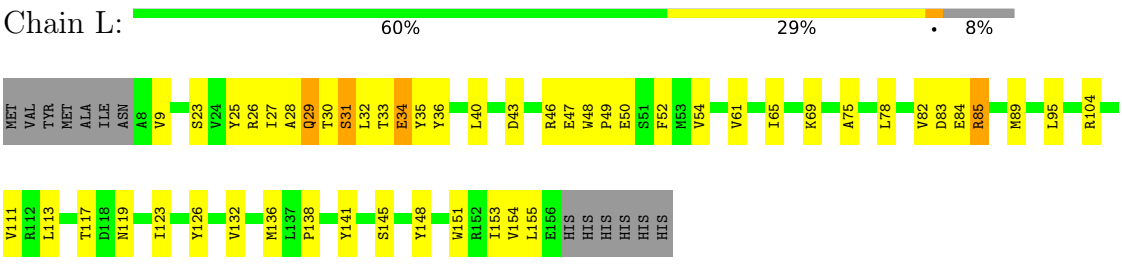
• Molecule 1: N-terminal acetyltransferase complex subunit [ARD1]

Chain J:



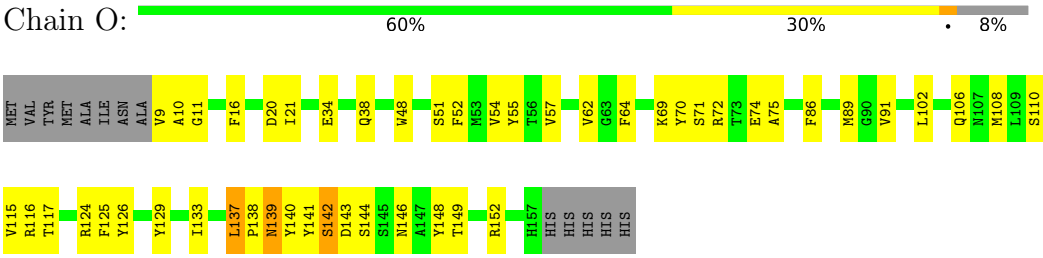
• Molecule 1: N-terminal acetyltransferase complex subunit [ARD1]

Chain L:



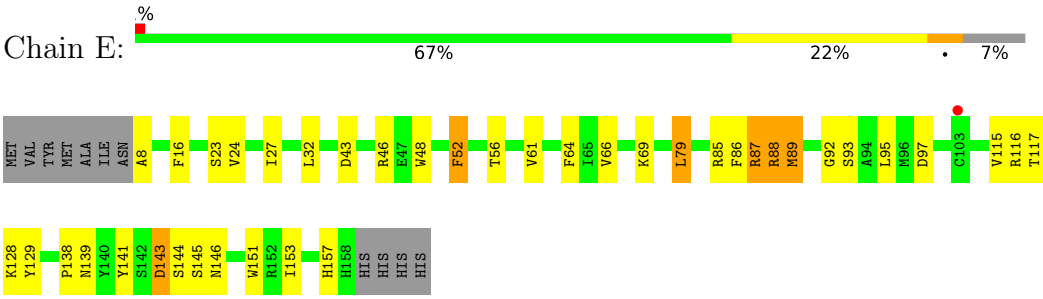
• Molecule 1: N-terminal acetyltransferase complex subunit [ARD1]

Chain O:



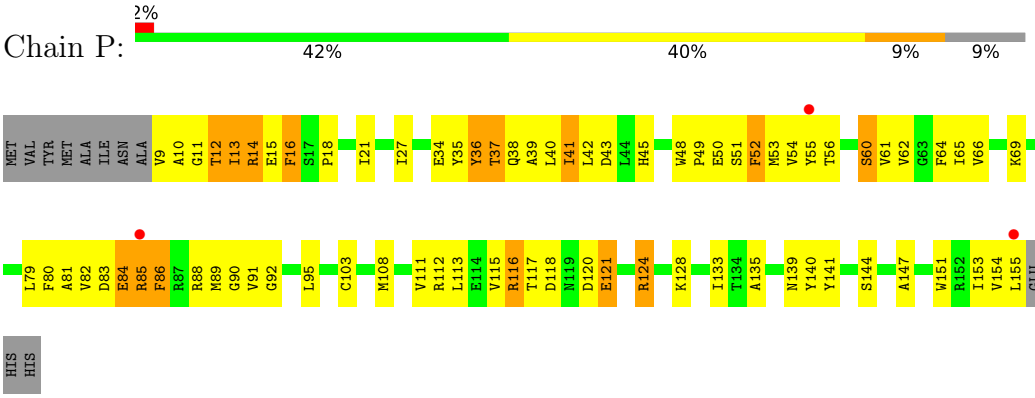
• Molecule 1: N-terminal acetyltransferase complex subunit [ARD1]

Chain E:



• Molecule 1: N-terminal acetyltransferase complex subunit [ARD1]

Chain P:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	102.24Å 129.94Å 158.58Å 90.00° 93.94° 90.00°	Depositor
Resolution (Å)	49.59 – 3.32 49.54 – 3.32	Depositor EDS
% Data completeness (in resolution range)	99.1 (49.59-3.32) 99.2 (49.54-3.32)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.70 (at 3.33Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.205 , 0.246 0.206 , 0.245	Depositor DCC
R_{free} test set	3078 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	78.0	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 62.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	20015	wwPDB-VP
Average B, all atoms (Å^2)	88.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.64	0/1284	0.81	0/1737
1	B	0.60	0/1230	0.75	0/1663
1	C	0.64	1/1276 (0.1%)	0.74	1/1726 (0.1%)
1	D	0.59	0/1221	0.77	0/1651
1	E	0.55	0/1257	0.72	0/1700
1	F	0.60	0/1246	0.78	0/1685
1	G	0.60	0/1284	0.77	1/1737 (0.1%)
1	H	0.61	0/1276	0.79	0/1726
1	I	0.64	0/1251	0.79	0/1692
1	J	0.59	0/1254	0.70	0/1696
1	K	0.58	0/1241	0.72	0/1678
1	L	0.56	0/1235	0.75	0/1670
1	M	0.72	1/1230 (0.1%)	0.83	1/1663 (0.1%)
1	N	0.59	0/1230	0.78	0/1663
1	O	0.62	0/1241	0.76	1/1678 (0.1%)
1	P	0.56	0/1221	0.78	0/1651
All	All	0.61	2/19977 (0.0%)	0.77	4/27016 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	49	PRO	N-CD	5.19	1.55	1.47
1	M	18	PRO	N-CD	5.01	1.54	1.47

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	17	SER	C-N-CD	5.82	140.63	128.40
1	C	48	TRP	C-N-CD	5.55	140.05	128.40
1	O	112	ARG	NE-CZ-NH1	5.44	123.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	116	ARG	NE-CZ-NH1	5.36	122.98	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1256	0	1237	94	0
1	B	1205	0	1194	87	0
1	C	1248	0	1226	77	0
1	D	1196	0	1188	36	0
1	E	1230	0	1213	57	0
1	F	1220	0	1206	35	0
1	G	1256	0	1237	60	0
1	H	1248	0	1226	81	0
1	I	1226	0	1216	60	0
1	J	1228	0	1212	67	0
1	K	1215	0	1201	76	0
1	L	1210	0	1199	43	0
1	M	1205	0	1194	42	0
1	N	1205	0	1194	71	0
1	O	1215	0	1201	60	0
1	P	1196	0	1188	154	0
2	C	51	0	34	18	0
2	E	51	0	34	15	0
2	F	51	0	34	6	0
2	G	51	0	34	15	0
2	H	51	0	34	37	0
2	I	51	0	34	20	0
2	J	51	0	34	19	0
3	A	48	0	32	21	0
4	A	5	0	0	0	0
4	B	1	0	0	0	0
4	C	4	0	0	1	0
4	D	7	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	3	0	0	0	0
4	F	4	0	0	0	0
4	G	1	0	0	0	0
4	H	2	0	0	0	0
4	I	4	0	0	0	0
4	J	3	0	0	0	0
4	K	1	0	0	0	0
4	L	5	0	0	0	0
4	M	5	0	0	0	0
4	N	2	0	0	0	0
4	O	3	0	0	0	0
4	P	1	0	0	0	0
All	All	20015	0	19602	1082	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 27.

All (1082) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:55:TYR:CD2	1:K:91:VAL:HG23	1.34	1.58
1:O:9:VAL:HG11	1:O:89:MET:CE	1.36	1.52
1:O:9:VAL:CG1	1:O:89:MET:HE3	1.61	1.29
1:I:136:MET:HE1	1:I:146:ASN:ND2	1.49	1.25
1:C:16:PHE:CD2	1:C:52:PHE:CE1	2.27	1.22
1:K:55:TYR:CD2	1:K:91:VAL:CG2	2.24	1.21
1:K:88:ARG:HG3	1:K:89:MET:CB	1.71	1.20
1:G:9:VAL:HG22	1:G:10:ALA:H	1.06	1.14
1:J:88:ARG:HG3	2:J:200:ACO:H52A	1.28	1.14
1:N:143:ASP:HB2	1:N:145:SER:OG	1.45	1.13
1:P:11:GLY:HA3	1:P:12:THR:HG23	1.13	1.12
1:C:16:PHE:HD2	1:C:52:PHE:CE1	1.65	1.11
1:P:9:VAL:CG2	1:P:89:MET:HB3	1.82	1.10
1:K:68:SER:HB2	1:K:78:LEU:HD11	1.15	1.09
1:P:9:VAL:HG21	1:P:89:MET:HB3	1.16	1.08
1:B:133:ILE:HG22	1:H:153:ILE:HD12	1.32	1.08
1:M:78:LEU:O	1:M:79:LEU:HD23	1.54	1.07
1:J:9:VAL:HB	1:J:10:ALA:HB2	1.09	1.07
1:P:9:VAL:HG21	1:P:89:MET:CB	1.84	1.07
1:A:138:PRO:HA	1:A:146:ASN:OD1	1.52	1.06
1:K:88:ARG:HG3	1:K:89:MET:HB2	1.08	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:VAL:HG22	1:B:89:MET:HG3	1.38	1.05
1:M:133:ILE:HG22	1:F:153:ILE:HD12	1.35	1.05
2:H:200:ACO:O5A	2:H:200:ACO:H132	1.54	1.04
1:I:136:MET:CE	1:I:146:ASN:ND2	2.21	1.03
1:N:62:VAL:HG11	1:N:86:PHE:CE2	1.93	1.03
1:B:68:SER:OG	1:B:78:LEU:HD23	1.58	1.03
1:P:56:THR:CG2	1:P:61:VAL:HG12	1.88	1.02
1:H:82:VAL:HG13	2:H:200:ACO:H142	1.41	1.01
1:E:86:PHE:O	1:E:89:MET:HG2	1.59	1.01
1:I:87:ARG:O	1:I:88:ARG:HG2	1.60	1.01
1:B:9:VAL:HA	1:B:10:ALA:HB3	1.44	1.00
1:H:34:GLU:OE2	1:P:128:LYS:HD3	1.58	1.00
1:P:13:ILE:HG22	1:P:54:VAL:O	1.62	1.00
1:A:119:ASN:HD21	3:A:201:COA:CDP	1.75	0.99
1:E:85:ARG:HD2	1:E:86:PHE:HE1	1.24	0.99
1:O:9:VAL:HG12	1:O:10:ALA:H	1.25	0.99
1:G:9:VAL:HG22	1:G:10:ALA:N	1.71	0.99
1:A:139:ASN:HA	1:A:144:SER:O	1.60	0.99
1:A:119:ASN:HD21	3:A:201:COA:H132	1.27	0.97
1:J:88:ARG:HD3	2:J:200:ACO:H2A	1.43	0.97
1:P:64:PHE:CZ	1:P:81:ALA:HB3	2.00	0.97
1:P:85:ARG:HB3	1:P:86:PHE:CE1	1.99	0.96
1:C:90:GLY:HA2	2:C:200:ACO:O1A	1.66	0.96
1:J:88:ARG:NH2	2:J:200:ACO:CEP	2.28	0.95
1:K:68:SER:CB	1:K:78:LEU:HD11	1.97	0.95
1:H:82:VAL:CG2	1:H:87:ARG:HG2	1.96	0.94
1:K:84:GLU:HG2	1:K:87:ARG:NH2	1.83	0.94
1:J:9:VAL:CB	1:J:10:ALA:HB2	1.98	0.94
1:P:13:ILE:H	1:P:13:ILE:HD12	1.30	0.94
1:G:9:VAL:CG2	1:G:10:ALA:H	1.79	0.94
1:P:9:VAL:HG12	1:P:10:ALA:H	1.31	0.93
1:B:52:PHE:CG	1:B:66:VAL:CG1	2.52	0.93
1:H:90:GLY:HA2	2:H:200:ACO:O1A	1.68	0.93
1:B:133:ILE:HG22	1:H:153:ILE:CD1	1.98	0.93
1:D:133:ILE:HG22	1:G:153:ILE:HD12	1.52	0.92
1:B:52:PHE:CD2	1:B:66:VAL:HG11	2.05	0.91
1:P:37:THR:HG21	1:P:41:ILE:HG23	1.53	0.91
1:K:55:TYR:CG	1:K:91:VAL:HG23	2.05	0.90
1:P:64:PHE:CE1	1:P:81:ALA:HB3	2.06	0.90
1:K:55:TYR:HD2	1:K:91:VAL:HG23	1.25	0.90
1:B:52:PHE:CD2	1:B:66:VAL:CG1	2.55	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:84:GLU:HG2	1:K:87:ARG:CZ	2.02	0.90
1:N:112:ARG:HG2	1:N:151:TRP:HD1	1.35	0.90
1:P:85:ARG:HG2	1:P:85:ARG:HH11	1.36	0.90
1:E:43:ASP:HA	1:E:46:ARG:NH1	1.87	0.89
1:P:11:GLY:HA3	1:P:12:THR:CG2	2.01	0.89
1:E:85:ARG:HD2	1:E:86:PHE:CE1	2.07	0.88
1:I:78:LEU:O	1:I:79:LEU:HD23	1.73	0.88
1:C:16:PHE:HD2	1:C:52:PHE:HE1	1.20	0.88
1:B:66:VAL:CG2	1:B:79:LEU:CD2	2.51	0.87
1:H:55:TYR:CD2	1:H:91:VAL:HG13	2.10	0.87
1:M:78:LEU:C	1:M:79:LEU:HD23	1.95	0.87
1:O:133:ILE:HG22	1:E:153:ILE:HD12	1.53	0.87
2:I:200:ACO:P2A	2:I:200:ACO:H142	2.14	0.87
1:K:120:ASP:HB3	1:K:124:ARG:NH1	1.90	0.87
1:L:34:GLU:OE2	1:L:35:TYR:N	2.07	0.86
1:I:136:MET:HE1	1:I:146:ASN:HD22	1.39	0.86
1:O:9:VAL:HG21	1:O:89:MET:HB3	1.59	0.85
1:L:29:GLN:HA	1:L:29:GLN:HE21	1.41	0.85
1:A:119:ASN:OD1	1:A:122:ALA:HB3	1.77	0.85
1:N:70:TYR:HB2	1:N:76:ARG:HD2	1.59	0.85
1:P:139:ASN:OD1	1:P:144:SER:HB3	1.77	0.85
1:A:55:TYR:CD2	1:A:91:VAL:HG23	2.12	0.84
2:I:200:ACO:O4A	2:I:200:ACO:H133	1.77	0.84
1:N:143:ASP:O	1:N:144:SER:OG	1.94	0.84
1:B:9:VAL:CA	1:B:10:ALA:HB3	2.07	0.84
1:B:79:LEU:HD23	1:B:79:LEU:O	1.77	0.84
1:B:9:VAL:CG2	1:B:89:MET:HG3	2.08	0.83
1:I:136:MET:HE1	1:I:146:ASN:CG	1.98	0.83
1:H:80:PHE:H	2:H:200:ACO:HH33	1.44	0.83
1:I:128:LYS:CD	2:I:200:ACO:H2A	2.07	0.83
1:E:85:ARG:HB2	1:E:86:PHE:CD1	2.12	0.83
1:J:143:ASP:O	1:J:144:SER:OG	1.96	0.83
1:H:88:ARG:NH2	2:H:200:ACO:H61A	1.77	0.83
1:P:64:PHE:CZ	1:P:81:ALA:CB	2.61	0.83
1:H:90:GLY:CA	2:H:200:ACO:O1A	2.26	0.82
1:O:9:VAL:CG1	1:O:89:MET:CE	2.32	0.82
1:P:56:THR:CG2	1:P:61:VAL:CG1	2.57	0.81
1:N:16:PHE:CE1	1:N:20:ASP:HB2	2.15	0.81
1:L:83:ASP:OD1	1:L:85:ARG:HG3	1.79	0.81
1:P:9:VAL:CG2	1:P:89:MET:SD	2.69	0.81
1:P:9:VAL:CG2	1:P:89:MET:CG	2.59	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:84:GLU:O	1:D:87:ARG:HG2	1.81	0.81
1:K:9:VAL:HG12	1:K:89:MET:O	1.79	0.81
1:A:119:ASN:OD1	1:A:122:ALA:CB	2.29	0.81
1:H:82:VAL:CG1	2:H:200:ACO:H142	2.11	0.81
1:D:75:ALA:HB3	1:D:111:VAL:HG22	1.62	0.80
1:H:140:TYR:O	1:P:124:ARG:HG2	1.81	0.80
1:P:14:ARG:HG3	1:P:14:ARG:HH11	1.47	0.80
1:P:36:TYR:HB3	1:P:37:THR:HA	1.63	0.80
1:F:8:ALA:HB3	1:N:140:TYR:OH	1.81	0.80
1:B:66:VAL:HG23	1:B:79:LEU:HD22	1.64	0.80
1:P:54:VAL:HG11	1:P:61:VAL:HG12	1.64	0.80
1:P:56:THR:HG22	1:P:61:VAL:HA	1.63	0.80
2:C:200:ACO:H133	2:C:200:ACO:P2A	2.22	0.80
1:K:88:ARG:CG	1:K:89:MET:HB2	2.03	0.79
1:A:139:ASN:CB	1:A:144:SER:O	2.30	0.79
1:A:62:VAL:HG11	1:A:86:PHE:CE2	2.17	0.79
1:H:82:VAL:HG21	2:H:200:ACO:H133	1.65	0.79
1:J:88:ARG:HD3	2:J:200:ACO:C2A	2.13	0.79
1:K:82:VAL:HG13	1:K:91:VAL:HG11	1.65	0.79
1:A:55:TYR:CG	1:A:91:VAL:HG23	2.18	0.79
1:J:21:ILE:HD12	1:J:21:ILE:O	1.83	0.78
1:P:9:VAL:CG2	1:P:89:MET:CB	2.53	0.78
1:C:55:TYR:CG	1:C:91:VAL:HG13	2.18	0.78
1:P:36:TYR:CB	1:P:37:THR:HA	2.13	0.78
1:N:62:VAL:HG11	1:N:86:PHE:HE2	1.44	0.78
1:E:43:ASP:HA	1:E:46:ARG:HH12	1.45	0.78
1:N:85:ARG:HB2	1:N:86:PHE:CD1	2.19	0.78
1:H:82:VAL:CG2	2:H:200:ACO:H133	2.14	0.78
1:I:128:LYS:HD2	2:I:200:ACO:C2A	2.14	0.78
2:I:200:ACO:H142	2:I:200:ACO:O5A	1.84	0.77
1:P:56:THR:HG22	1:P:61:VAL:CG1	2.14	0.77
1:E:85:ARG:HB2	1:E:86:PHE:CE1	2.18	0.77
1:H:87:ARG:HG2	2:H:200:ACO:H133	1.66	0.77
1:A:143:ASP:O	1:A:144:SER:HB2	1.84	0.77
2:H:200:ACO:H141	2:H:200:ACO:N8P	1.99	0.77
1:K:55:TYR:HD2	1:K:91:VAL:CG2	1.83	0.77
1:B:9:VAL:HG22	1:B:89:MET:CG	2.15	0.77
1:A:139:ASN:CA	1:A:144:SER:O	2.31	0.77
1:J:143:ASP:HB2	1:J:145:SER:OG	1.86	0.76
1:B:70:TYR:HD2	1:B:74:GLU:OE1	1.68	0.76
1:L:54:VAL:HG11	1:L:61:VAL:HG22	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:48:TRP:CD2	1:P:51:SER:HB3	2.21	0.76
1:B:65:ILE:HG13	1:B:80:PHE:HB3	1.68	0.76
1:B:66:VAL:HG23	1:B:79:LEU:CD2	2.16	0.76
1:P:85:ARG:HG2	1:P:85:ARG:NH1	1.99	0.76
1:P:11:GLY:CA	1:P:12:THR:HG23	2.06	0.75
3:A:201:COA:O5B	3:A:201:COA:O8A	2.02	0.75
1:D:55:TYR:CD2	1:D:91:VAL:HG13	2.22	0.75
1:H:155:LEU:HD23	1:H:156:GLU:N	2.01	0.75
1:O:9:VAL:CG2	1:O:89:MET:HB3	2.16	0.75
1:P:9:VAL:HG22	1:P:89:MET:SD	2.25	0.75
1:I:128:LYS:HD2	2:I:200:ACO:H2A	1.68	0.75
1:N:54:VAL:HG13	1:N:61:VAL:HG13	1.67	0.75
1:P:9:VAL:HG21	1:P:89:MET:CG	2.17	0.75
2:H:200:ACO:H141	2:H:200:ACO:C7P	2.16	0.75
1:J:9:VAL:HB	1:J:10:ALA:CB	2.03	0.75
1:C:84:GLU:HA	1:C:87:ARG:HG3	1.68	0.74
1:P:85:ARG:HB3	1:P:86:PHE:CD1	2.20	0.74
1:D:21:ILE:O	1:D:21:ILE:HD12	1.88	0.74
1:B:112:ARG:CG	1:B:151:TRP:HD1	2.01	0.74
2:H:200:ACO:H132	2:H:200:ACO:P2A	2.27	0.74
1:O:9:VAL:CG2	1:O:89:MET:O	2.36	0.74
1:G:117:THR:HG23	1:G:146:ASN:O	1.88	0.74
1:N:48:TRP:CE3	1:N:51:SER:HB3	2.22	0.74
1:B:124:ARG:HD2	1:J:140:TYR:O	1.88	0.74
1:O:139:ASN:ND2	1:O:144:SER:C	2.41	0.74
1:O:9:VAL:HG11	1:O:89:MET:HE3	0.75	0.73
1:A:6:ILE:N	1:A:6:ILE:HD12	2.03	0.73
1:C:12:THR:O	1:C:56:THR:HG22	1.88	0.73
1:P:9:VAL:HG12	1:P:10:ALA:N	2.03	0.73
1:G:69:LYS:HD3	1:G:108:MET:HE2	1.68	0.73
1:P:13:ILE:HA	1:P:54:VAL:O	1.87	0.73
1:M:78:LEU:O	1:M:79:LEU:CD2	2.36	0.73
1:I:88:ARG:HA	2:I:200:ACO:H4B	1.70	0.72
1:C:55:TYR:CG	1:C:91:VAL:CG1	2.72	0.72
1:C:86:PHE:O	1:C:89:MET:HB2	1.89	0.72
1:P:16:PHE:CE1	1:P:45:HIS:ND1	2.57	0.72
1:A:119:ASN:ND2	3:A:201:COA:CDP	2.50	0.72
1:J:19:LYS:HD2	1:J:20:ASP:OD1	1.89	0.72
1:P:54:VAL:HG11	1:P:61:VAL:CG1	2.18	0.72
1:C:16:PHE:HB2	1:C:52:PHE:HD1	1.55	0.72
1:C:16:PHE:CD2	1:C:52:PHE:CD1	2.77	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:ARG:HD2	2:E:200:ACO:H131	1.72	0.72
1:B:66:VAL:CG2	1:B:79:LEU:HD22	2.18	0.71
1:C:48:TRP:NE1	1:C:50:GLU:OE1	2.23	0.71
1:O:9:VAL:HG12	1:O:10:ALA:N	2.03	0.71
1:O:115:VAL:HG21	1:O:126:TYR:CE2	2.25	0.71
1:C:16:PHE:HB2	1:C:52:PHE:CD1	2.25	0.71
1:G:114:GLU:HG3	1:G:149:THR:HG22	1.71	0.71
1:J:139:ASN:ND2	1:J:144:SER:HB2	2.06	0.71
1:E:126:TYR:OH	2:E:200:ACO:HH32	1.91	0.71
1:K:84:GLU:CG	1:K:87:ARG:NH2	2.54	0.70
1:P:55:TYR:CD2	1:P:91:VAL:HG13	2.25	0.70
1:M:133:ILE:HG22	1:F:153:ILE:CD1	2.19	0.70
1:N:62:VAL:CG1	1:N:86:PHE:CE2	2.73	0.70
1:A:14:ARG:HA	1:B:70:TYR:CE1	2.25	0.70
1:E:151:TRP:CH2	1:E:153:ILE:HG13	2.27	0.70
1:P:56:THR:HG23	1:P:61:VAL:HG12	1.72	0.70
1:N:116:ARG:HG2	1:N:141:TYR:CE2	2.26	0.70
1:P:56:THR:HG22	1:P:61:VAL:HG12	1.69	0.70
1:I:87:ARG:O	1:I:88:ARG:CG	2.39	0.70
1:I:58:ALA:O	1:M:46:ARG:NH2	2.24	0.70
1:O:62:VAL:HG11	1:O:86:PHE:CE2	2.26	0.70
1:H:87:ARG:HG2	2:H:200:ACO:CDP	2.21	0.70
1:O:139:ASN:HD22	1:O:144:SER:CA	2.04	0.70
1:G:6:ILE:HD12	1:G:6:ILE:N	2.07	0.70
1:I:136:MET:CE	1:I:146:ASN:CG	2.58	0.69
1:M:53:MET:HE1	1:M:98:ALA:HB1	1.73	0.69
1:B:52:PHE:CD1	1:B:66:VAL:HG13	2.27	0.69
1:I:13:ILE:HG21	1:I:53:MET:HE2	1.74	0.69
1:A:6:ILE:N	1:B:78:LEU:O	2.25	0.69
1:L:50:GLU:OE2	1:L:50:GLU:N	2.23	0.69
1:G:69:LYS:HD3	1:G:108:MET:CE	2.21	0.69
1:P:54:VAL:CG1	1:P:61:VAL:HG12	2.22	0.69
1:M:48:TRP:CD2	1:M:51:SER:OG	2.44	0.69
1:I:17:SER:O	1:I:20:ASP:N	2.23	0.69
1:J:88:ARG:NH2	2:J:200:ACO:H143	2.06	0.69
1:K:82:VAL:CG1	1:K:91:VAL:HG11	2.23	0.69
1:I:69:LYS:HG2	1:I:108:MET:CE	2.22	0.69
1:C:88:ARG:HG2	1:C:88:ARG:HH11	1.58	0.68
1:P:56:THR:HG22	1:P:61:VAL:CA	2.22	0.68
1:H:88:ARG:NH2	2:H:200:ACO:N6A	2.42	0.68
1:K:88:ARG:HD2	1:K:89:MET:HG3	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:52:PHE:CE2	1:B:66:VAL:HG11	2.29	0.68
1:E:92:GLY:N	2:E:200:ACO:O5A	2.23	0.68
1:P:13:ILE:HD12	1:P:13:ILE:N	2.04	0.68
1:M:62:VAL:O	1:M:82:VAL:HG23	1.94	0.68
1:B:75:ALA:HB3	1:B:111:VAL:HG22	1.75	0.68
1:H:82:VAL:HG22	2:H:200:ACO:H142	1.75	0.68
1:E:116:ARG:HG2	1:E:141:TYR:CE2	2.28	0.68
1:G:151:TRP:CH2	1:G:153:ILE:HG13	2.29	0.68
1:N:143:ASP:CB	1:N:145:SER:OG	2.33	0.68
1:P:75:ALA:HB3	1:P:111:VAL:HG22	1.73	0.68
1:M:53:MET:CE	1:M:98:ALA:HB1	2.23	0.68
1:B:52:PHE:CG	1:B:66:VAL:HG13	2.29	0.68
1:B:77:ILE:C	1:B:77:ILE:HD12	2.14	0.68
1:N:16:PHE:CE1	1:N:24:VAL:HG21	2.29	0.68
1:G:113:LEU:C	1:G:113:LEU:HD12	2.15	0.67
1:K:88:ARG:HG3	1:K:89:MET:CG	2.24	0.67
1:P:62:VAL:CB	1:P:86:PHE:HE2	2.07	0.67
1:P:37:THR:CG2	1:P:41:ILE:HG23	2.23	0.67
1:P:116:ARG:HA	1:P:141:TYR:HE2	1.58	0.67
1:A:125:PHE:CE1	3:A:201:COA:O4B	2.47	0.67
1:O:9:VAL:HG11	1:O:89:MET:HE2	1.68	0.67
3:A:201:COA:O5B	3:A:201:COA:P3B	2.53	0.67
1:B:79:LEU:HD23	1:B:79:LEU:C	2.14	0.67
1:O:112:ARG:HD2	1:O:149:THR:CG2	2.24	0.67
1:P:83:ASP:O	1:P:84:GLU:HB3	1.93	0.67
1:F:57:VAL:HG13	1:F:58:ALA:N	2.08	0.67
1:B:52:PHE:CG	1:B:66:VAL:HG12	2.30	0.67
1:K:9:VAL:CG1	1:K:89:MET:O	2.43	0.67
1:A:54:VAL:HG11	1:A:61:VAL:HG22	1.77	0.67
1:N:85:ARG:CB	1:N:86:PHE:CD1	2.78	0.66
1:L:29:GLN:HA	1:L:29:GLN:NE2	2.10	0.66
1:P:9:VAL:HG21	1:P:89:MET:SD	2.34	0.66
1:G:53:MET:CE	1:G:98:ALA:HB1	2.24	0.66
1:I:88:ARG:HB2	2:I:200:ACO:O3B	1.96	0.66
1:P:62:VAL:HB	1:P:86:PHE:CE2	2.31	0.66
1:D:56:THR:HG23	1:D:56:THR:O	1.96	0.66
1:H:153:ILE:HG22	1:H:155:LEU:H	1.61	0.66
1:J:88:ARG:HA	2:J:200:ACO:O5B	1.95	0.66
1:O:139:ASN:HD22	1:O:144:SER:HA	1.59	0.66
1:P:37:THR:HB	1:P:40:LEU:N	2.11	0.66
1:M:54:VAL:HG13	1:M:61:VAL:HG13	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:VAL:HA	1:B:10:ALA:CB	2.14	0.66
1:M:75:ALA:HB3	1:M:111:VAL:HG22	1.78	0.66
1:H:7:ASN:N	1:L:141:TYR:HH	1.94	0.66
1:F:143:ASP:CG	1:F:145:SER:HG	1.99	0.65
1:A:125:PHE:CD1	3:A:201:COA:C5B	2.79	0.65
1:H:55:TYR:CD2	1:H:91:VAL:CG1	2.79	0.65
1:H:82:VAL:CG2	1:H:87:ARG:CG	2.74	0.65
1:P:37:THR:HG21	1:P:41:ILE:CG2	2.25	0.65
1:I:86:PHE:CD2	1:I:89:MET:HE1	2.31	0.65
1:B:112:ARG:HG2	1:B:151:TRP:HD1	1.62	0.65
1:H:7:ASN:N	1:H:7:ASN:OD1	2.29	0.65
2:H:200:ACO:O5A	2:H:200:ACO:CDP	2.39	0.65
1:L:54:VAL:HG13	1:L:61:VAL:HG13	1.77	0.65
1:G:53:MET:HE2	1:G:98:ALA:HB1	1.78	0.65
1:N:85:ARG:HB2	1:N:86:PHE:HD1	1.62	0.65
1:O:116:ARG:NH2	1:O:143:ASP:OD2	2.26	0.65
1:K:141:TYR:HE1	1:K:147:ALA:HB2	1.62	0.64
1:H:34:GLU:OE2	1:P:128:LYS:CD	2.41	0.64
1:E:86:PHE:O	1:E:89:MET:CG	2.41	0.64
1:M:55:TYR:CD1	1:M:91:VAL:HG13	2.33	0.64
1:B:65:ILE:HA	1:B:80:PHE:HB2	1.78	0.64
2:I:200:ACO:N3A	2:I:200:ACO:H51A	2.13	0.64
1:N:146:ASN:N	1:N:146:ASN:OD1	2.29	0.64
1:A:117:THR:HG23	1:A:146:ASN:O	1.97	0.64
1:C:16:PHE:CB	1:C:52:PHE:CD1	2.80	0.64
1:H:82:VAL:HG13	2:H:200:ACO:CEP	2.24	0.64
2:C:200:ACO:H142	2:C:200:ACO:O5A	1.98	0.64
1:N:85:ARG:CB	1:N:86:PHE:HD1	2.10	0.64
1:O:112:ARG:HD2	1:O:149:THR:HG21	1.80	0.64
1:P:37:THR:N	1:P:38:GLN:HA	2.13	0.64
1:P:116:ARG:HG3	1:P:116:ARG:HH11	1.62	0.64
1:K:84:GLU:OE2	1:K:87:ARG:NH2	2.30	0.64
1:P:84:GLU:HG3	1:P:84:GLU:O	1.98	0.64
2:I:200:ACO:P2A	2:I:200:ACO:CEP	2.86	0.64
1:P:48:TRP:CG	1:P:51:SER:HB3	2.32	0.64
1:K:129:TYR:O	1:K:152:ARG:NH1	2.30	0.63
1:H:155:LEU:HD21	1:H:157:HIS:CE1	2.33	0.63
1:I:6:ILE:CD1	1:M:78:LEU:HA	2.29	0.63
1:L:29:GLN:OE1	1:L:36:TYR:N	2.29	0.63
1:B:155:LEU:HD23	1:J:46:ARG:HG2	1.80	0.63
1:J:14:ARG:NH1	1:J:20:ASP:OD2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:TYR:CD2	1:C:91:VAL:HG13	2.33	0.63
1:A:55:TYR:CG	1:A:91:VAL:CG2	2.81	0.63
1:G:69:LYS:CD	1:G:108:MET:CE	2.76	0.63
1:K:55:TYR:CE2	1:K:91:VAL:HG23	2.22	0.63
1:J:153:ILE:HG21	1:P:135:ALA:HA	1.81	0.62
1:O:9:VAL:HG21	1:O:89:MET:CB	2.28	0.62
1:P:9:VAL:HG22	1:P:89:MET:CG	2.29	0.62
1:P:13:ILE:HG22	1:P:54:VAL:C	2.19	0.62
1:K:48:TRP:CZ2	1:K:106:GLN:OE1	2.53	0.62
1:K:75:ALA:HB3	1:K:111:VAL:HG22	1.80	0.62
1:M:106:GLN:O	1:M:107:ASN:HB2	1.98	0.62
1:A:9:VAL:HB	1:A:10:ALA:HA	1.82	0.62
1:O:139:ASN:ND2	1:O:144:SER:O	2.32	0.62
1:P:82:VAL:HG22	1:P:84:GLU:H	1.63	0.62
1:O:48:TRP:CD2	1:O:51:SER:HB3	2.33	0.62
1:E:24:VAL:HG23	1:E:64:PHE:CD1	2.34	0.62
1:L:31:SER:O	1:L:32:LEU:HB2	2.00	0.62
1:F:87:ARG:HD3	2:F:200:ACO:OAP	2.00	0.61
1:N:70:TYR:HB2	1:N:76:ARG:CD	2.29	0.61
1:O:75:ALA:HB2	1:O:108:MET:HE2	1.82	0.61
1:O:139:ASN:ND2	1:O:144:SER:CA	2.63	0.61
1:G:51:SER:OG	1:G:67:GLY:N	2.34	0.61
1:A:139:ASN:H	1:A:146:ASN:CG	2.04	0.61
1:I:17:SER:O	1:I:19:LYS:N	2.34	0.61
1:I:88:ARG:CB	2:I:200:ACO:O3B	2.48	0.61
1:N:112:ARG:CG	1:N:151:TRP:HD1	2.10	0.61
1:A:143:ASP:OD1	1:A:143:ASP:N	2.31	0.61
1:H:151:TRP:CH2	1:H:153:ILE:HG13	2.35	0.61
1:L:33:THR:HG22	1:L:33:THR:O	2.01	0.61
1:H:75:ALA:HB3	1:H:111:VAL:HG22	1.82	0.61
1:E:117:THR:HG23	1:E:146:ASN:O	2.00	0.61
1:P:14:ARG:HH11	1:P:14:ARG:CG	2.11	0.61
1:P:151:TRP:CH2	1:P:153:ILE:HD11	2.35	0.61
1:C:88:ARG:HH11	1:C:88:ARG:CG	2.13	0.61
1:C:52:PHE:CD2	1:C:66:VAL:HG21	2.36	0.61
1:P:13:ILE:CG2	1:P:54:VAL:O	2.45	0.61
1:G:69:LYS:CD	1:G:108:MET:HE2	2.31	0.61
1:O:55:TYR:CD2	1:O:91:VAL:HG13	2.35	0.61
1:E:143:ASP:O	1:E:144:SER:HB3	2.00	0.61
1:E:143:ASP:N	1:E:143:ASP:OD1	2.32	0.61
1:G:13:ILE:HG21	1:G:53:MET:HE2	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:48:TRP:HZ2	1:K:106:GLN:OE1	1.83	0.61
1:O:34:GLU:OE2	1:O:141:TYR:HD1	1.83	0.61
1:P:37:THR:HG21	1:P:41:ILE:HG13	1.81	0.61
1:J:139:ASN:CG	1:J:144:SER:HB2	2.21	0.60
2:H:200:ACO:P2A	2:H:200:ACO:CDP	2.89	0.60
1:C:155:LEU:HD12	1:C:156:GLU:N	2.15	0.60
1:H:82:VAL:HG23	1:H:87:ARG:CG	2.31	0.60
1:D:65:ILE:HD12	1:D:80:PHE:CD1	2.37	0.60
1:N:116:ARG:HG2	1:N:141:TYR:CD2	2.37	0.60
1:A:123:ILE:HA	1:A:150:MET:HE1	1.84	0.60
1:P:62:VAL:CB	1:P:86:PHE:CE2	2.85	0.60
1:G:69:LYS:HE2	1:G:108:MET:CE	2.32	0.60
1:B:65:ILE:CB	1:B:80:PHE:HB2	2.32	0.60
1:H:79:LEU:HA	2:H:200:ACO:CH3	2.32	0.60
1:A:55:TYR:CD2	1:A:91:VAL:CG2	2.83	0.60
1:H:79:LEU:HA	2:H:200:ACO:HH31	1.84	0.59
1:J:16:PHE:HE1	1:J:18:PRO:HA	1.67	0.59
1:C:76:ARG:NH1	4:C:304:HOH:O	2.35	0.59
1:H:55:TYR:CE2	1:H:91:VAL:HG13	2.36	0.59
1:D:87:ARG:CG	1:D:87:ARG:HH11	2.16	0.59
1:I:7:ASN:O	1:I:8:ALA:HB3	2.02	0.59
1:D:48:TRP:O	1:D:51:SER:HB3	2.02	0.59
1:K:62:VAL:HG11	1:K:86:PHE:CE2	2.38	0.59
1:B:65:ILE:CA	1:B:80:PHE:HB2	2.33	0.59
1:H:82:VAL:HG22	2:H:200:ACO:CEP	2.32	0.59
1:J:88:ARG:N	2:J:200:ACO:O5A	2.35	0.59
1:P:27:ILE:HG12	1:P:83:ASP:OD1	2.02	0.59
2:G:200:ACO:H132	2:G:200:ACO:P2A	2.43	0.59
1:A:125:PHE:HE1	3:A:201:COA:O4B	1.85	0.59
1:N:135:ALA:HB3	1:N:149:THR:HB	1.83	0.59
1:A:56:THR:HA	1:A:60:SER:O	2.03	0.59
1:B:11:GLY:HA3	1:B:55:TYR:OH	2.03	0.59
2:J:200:ACO:H133	2:J:200:ACO:O3A	2.01	0.59
1:P:139:ASN:OD1	1:P:144:SER:O	2.21	0.59
1:I:90:GLY:HA2	2:I:200:ACO:O1A	2.03	0.59
1:A:62:VAL:HG11	1:A:86:PHE:CD2	2.37	0.59
1:E:115:VAL:C	1:E:141:TYR:OH	2.41	0.58
1:N:86:PHE:HD1	1:N:86:PHE:N	2.01	0.58
1:L:75:ALA:HB3	1:L:111:VAL:HG22	1.85	0.58
1:A:91:VAL:O	1:A:94:ALA:HB3	2.04	0.58
1:H:35:TYR:CE2	1:P:90:GLY:HA3	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:27:ILE:HA	1:L:30:THR:OG1	2.04	0.58
1:I:117:THR:HG21	1:I:146:ASN:OD1	2.03	0.58
1:C:11:GLY:HA2	1:C:56:THR:O	2.03	0.58
1:A:14:ARG:HA	1:B:70:TYR:CD1	2.39	0.58
1:J:140:TYR:HD2	1:J:147:ALA:CB	2.16	0.58
1:P:116:ARG:HH11	1:P:116:ARG:CG	2.16	0.58
1:C:75:ALA:HB3	1:C:111:VAL:HG22	1.86	0.58
1:K:88:ARG:CG	1:K:89:MET:CB	2.65	0.58
1:A:139:ASN:HB2	1:A:144:SER:O	2.04	0.58
1:H:93:SER:OG	2:H:200:ACO:O2A	2.21	0.58
1:D:48:TRP:CD2	1:D:51:SER:HB2	2.39	0.58
1:E:87:ARG:HB3	2:E:200:ACO:H133	1.86	0.58
1:K:84:GLU:HG2	1:K:87:ARG:NE	2.19	0.57
1:A:113:LEU:C	1:A:113:LEU:HD12	2.23	0.57
1:A:115:VAL:HG11	1:A:150:MET:HE2	1.85	0.57
1:A:155:LEU:HD21	1:A:157:HIS:CE1	2.38	0.57
1:H:90:GLY:N	2:H:200:ACO:O1A	2.37	0.57
1:F:56:THR:HG23	1:F:56:THR:O	2.04	0.57
1:F:139:ASN:N	1:F:146:ASN:OD1	2.36	0.57
1:N:86:PHE:CD1	1:N:86:PHE:N	2.72	0.57
1:O:113:LEU:HD13	1:O:115:VAL:HG23	1.84	0.57
1:G:14:ARG:NH2	1:G:20:ASP:OD1	2.37	0.57
1:G:48:TRP:O	1:G:51:SER:HB3	2.05	0.57
1:A:34:GLU:OE2	1:A:142:SER:OG	2.22	0.57
1:C:90:GLY:HA2	2:C:200:ACO:P1A	2.44	0.57
1:K:82:VAL:CG1	1:K:91:VAL:CG1	2.82	0.57
1:M:48:TRP:CE2	1:M:69:LYS:HE2	2.39	0.57
1:B:9:VAL:HG23	1:B:9:VAL:O	2.04	0.57
1:L:29:GLN:HE21	1:L:29:GLN:CA	2.12	0.57
1:L:119:ASN:O	1:L:123:ILE:HG13	2.05	0.57
1:E:86:PHE:CD1	1:E:86:PHE:N	2.73	0.57
1:J:16:PHE:CD1	1:J:17:SER:N	2.73	0.57
1:E:88:ARG:NH2	2:E:200:ACO:C6A	2.67	0.57
1:G:88:ARG:CB	2:G:200:ACO:O3A	2.52	0.57
2:F:200:ACO:O9P	2:F:200:ACO:H141	2.05	0.57
1:E:92:GLY:O	1:E:95:LEU:N	2.38	0.57
1:P:85:ARG:CB	1:P:86:PHE:CE1	2.83	0.57
1:C:16:PHE:CD1	1:C:17:SER:N	2.72	0.57
1:O:116:ARG:HG2	1:O:141:TYR:CE2	2.40	0.57
2:C:200:ACO:H8A	2:C:200:ACO:H52A	1.87	0.56
1:I:128:LYS:HD2	2:I:200:ACO:N1A	2.20	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:141:TYR:HD2	1:E:145:SER:HB2	1.70	0.56
1:C:141:TYR:CE2	1:C:147:ALA:HB2	2.40	0.56
1:D:51:SER:OG	1:D:67:GLY:N	2.37	0.56
1:I:129:TYR:O	1:I:152:ARG:NH1	2.38	0.56
1:A:57:VAL:O	1:A:58:ALA:HB3	2.05	0.56
1:A:75:ALA:HB3	1:A:111:VAL:HG22	1.87	0.56
1:A:82:VAL:CG1	1:A:91:VAL:HG11	2.36	0.56
1:H:43:ASP:OD1	1:H:46:ARG:NH1	2.37	0.56
1:J:13:ILE:HD11	1:J:95:LEU:HD23	1.87	0.56
1:G:69:LYS:HE2	1:G:108:MET:HE2	1.86	0.56
1:F:151:TRP:CH2	1:F:153:ILE:HG13	2.40	0.56
1:B:82:VAL:HG12	1:B:83:ASP:N	2.21	0.56
2:I:200:ACO:C8A	2:I:200:ACO:H3B	2.34	0.56
1:F:90:GLY:HA2	2:F:200:ACO:H51A	1.87	0.56
1:I:68:SER:HB3	1:I:78:LEU:HD11	1.88	0.56
1:K:9:VAL:HG22	1:K:10:ALA:N	2.20	0.56
1:C:117:THR:HG23	1:C:148:TYR:CE2	2.41	0.56
1:F:80:PHE:O	2:F:200:ACO:H31	2.04	0.56
1:J:139:ASN:ND2	1:J:144:SER:CB	2.69	0.56
1:G:137:LEU:HD11	1:G:149:THR:CG2	2.35	0.56
1:N:57:VAL:O	1:N:58:ALA:HB3	2.05	0.56
1:A:119:ASN:ND2	3:A:201:COA:H131	2.21	0.56
1:P:65:ILE:HD12	1:P:80:PHE:CE1	2.41	0.56
1:O:21:ILE:HG13	1:O:38:GLN:HG2	1.88	0.56
1:B:112:ARG:HG3	1:B:151:TRP:HD1	1.70	0.56
1:H:82:VAL:CG2	2:H:200:ACO:H142	2.35	0.56
1:C:155:LEU:HD11	1:C:157:HIS:CE1	2.41	0.55
1:G:13:ILE:HD13	1:G:98:ALA:HB2	1.89	0.55
1:G:142:SER:OG	1:N:88:ARG:NH1	2.38	0.55
1:N:140:TYR:HD2	1:N:141:TYR:CE1	2.25	0.55
1:L:49:PRO:HG2	1:L:50:GLU:OE2	2.05	0.55
1:O:138:PRO:O	1:O:146:ASN:ND2	2.39	0.55
1:M:54:VAL:HG11	1:M:61:VAL:HG22	1.88	0.55
1:A:138:PRO:O	1:A:139:ASN:OD1	2.23	0.55
1:J:132:VAL:O	1:J:150:MET:HA	2.06	0.55
1:L:151:TRP:CH2	1:L:153:ILE:HG13	2.41	0.55
1:G:6:ILE:N	1:K:78:LEU:O	2.40	0.55
1:A:48:TRP:CD2	1:A:51:SER:HB2	2.41	0.55
1:B:71:SER:OG	1:B:74:GLU:HB2	2.07	0.55
1:H:82:VAL:HG23	1:H:87:ARG:HG2	1.84	0.55
1:H:92:GLY:HA3	2:H:200:ACO:CCP	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:157:HIS:CE1	1:P:72:ARG:HH12	2.24	0.55
1:M:133:ILE:CG2	1:F:153:ILE:HD12	2.24	0.55
1:N:48:TRP:CD2	1:N:51:SER:HB3	2.42	0.55
1:N:85:ARG:HB2	1:N:86:PHE:CE1	2.41	0.55
1:A:119:ASN:OD1	1:A:122:ALA:N	2.36	0.55
1:A:125:PHE:CE1	3:A:201:COA:H51A	2.42	0.55
1:P:16:PHE:HE1	1:P:45:HIS:ND1	2.04	0.55
2:H:200:ACO:H141	2:H:200:ACO:H72	1.89	0.55
1:P:9:VAL:HG23	1:P:89:MET:HB3	1.84	0.55
1:P:41:ILE:CD1	1:P:42:LEU:HD12	2.37	0.55
1:P:62:VAL:HG11	1:P:86:PHE:CE2	2.42	0.55
1:P:62:VAL:HG21	1:P:86:PHE:HE2	1.71	0.55
1:P:64:PHE:CE1	1:P:81:ALA:CB	2.85	0.55
1:K:11:GLY:O	1:K:12:THR:HG23	2.07	0.55
1:J:26:ARG:NH1	1:J:83:ASP:OD2	2.36	0.55
1:P:37:THR:OG1	1:P:41:ILE:HG13	2.06	0.55
1:C:52:PHE:CD2	1:C:66:VAL:CG2	2.90	0.54
1:P:27:ILE:HD11	1:P:83:ASP:CG	2.26	0.54
1:A:125:PHE:CD1	3:A:201:COA:H51A	2.42	0.54
1:P:16:PHE:CD1	1:P:45:HIS:CE1	2.95	0.54
1:P:37:THR:OG1	1:P:38:GLN:O	2.21	0.54
1:K:86:PHE:CD1	1:K:86:PHE:N	2.73	0.54
1:J:88:ARG:NH2	2:J:200:ACO:H141	2.16	0.54
1:B:124:ARG:CZ	1:J:139:ASN:O	2.55	0.54
1:G:43:ASP:OD1	1:G:46:ARG:NH2	2.38	0.54
1:K:84:GLU:HG2	1:K:87:ARG:HH21	1.71	0.54
1:N:138:PRO:O	1:N:139:ASN:OD1	2.26	0.54
1:E:16:PHE:HB2	1:E:52:PHE:CD1	2.43	0.54
1:P:115:VAL:HG12	1:P:116:ARG:N	2.22	0.54
1:D:13:ILE:HG21	1:D:53:MET:HE2	1.89	0.54
1:I:86:PHE:HD2	1:I:89:MET:HE1	1.73	0.54
1:K:84:GLU:HA	1:K:87:ARG:HB2	1.90	0.54
1:B:112:ARG:HG2	1:B:151:TRP:CD1	2.42	0.54
1:O:133:ILE:CG2	1:E:153:ILE:HD12	2.31	0.54
1:D:87:ARG:HG2	1:D:87:ARG:HH11	1.73	0.54
1:N:54:VAL:HG13	1:N:61:VAL:CG1	2.37	0.54
1:E:43:ASP:OD1	1:E:46:ARG:NH1	2.41	0.54
1:K:88:ARG:HG3	1:K:89:MET:CA	2.36	0.53
1:G:9:VAL:CG2	1:G:10:ALA:N	2.43	0.53
1:K:82:VAL:HG11	1:K:91:VAL:CG1	2.39	0.53
1:B:65:ILE:HB	1:B:80:PHE:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:117:THR:HG22	1:L:148:TYR:CE2	2.43	0.53
1:C:88:ARG:NH2	2:C:200:ACO:C5A	2.71	0.53
1:J:13:ILE:HG23	1:J:13:ILE:O	2.08	0.53
1:L:28:ALA:O	1:L:31:SER:O	2.26	0.53
1:I:13:ILE:CG2	1:I:53:MET:HE2	2.39	0.53
1:A:87:ARG:HB3	1:A:88:ARG:HA	1.90	0.53
1:B:70:TYR:CD2	1:B:112:ARG:NH2	2.77	0.53
1:K:141:TYR:CE1	1:K:147:ALA:HB2	2.43	0.53
2:E:200:ACO:O6A	2:E:200:ACO:O2A	2.26	0.53
1:P:139:ASN:OD1	1:P:144:SER:CB	2.51	0.53
1:I:69:LYS:HG2	1:I:108:MET:HE1	1.88	0.53
1:K:62:VAL:HG11	1:K:86:PHE:CD2	2.43	0.53
1:B:77:ILE:HD12	1:B:77:ILE:O	2.08	0.53
1:J:88:ARG:HH22	2:J:200:ACO:CEP	2.18	0.53
1:D:56:THR:O	1:D:56:THR:CG2	2.57	0.53
1:M:13:ILE:HG13	1:M:55:TYR:HD2	1.74	0.53
1:J:143:ASP:OD1	1:J:143:ASP:N	2.37	0.53
1:K:11:GLY:O	1:K:12:THR:CG2	2.57	0.53
1:A:48:TRP:O	1:A:51:SER:HB3	2.09	0.53
1:B:66:VAL:HG22	1:B:79:LEU:CD2	2.37	0.53
1:J:140:TYR:HD2	1:J:147:ALA:HB2	1.74	0.53
1:P:16:PHE:CE1	1:P:45:HIS:CE1	2.97	0.53
1:P:39:ALA:HB1	1:P:42:LEU:HD13	1.91	0.53
1:I:6:ILE:HD12	1:M:78:LEU:HA	1.90	0.52
1:K:67:GLY:C	1:K:78:LEU:HD12	2.30	0.52
1:K:86:PHE:N	1:K:86:PHE:HD1	2.07	0.52
1:H:89:MET:O	1:H:89:MET:HG2	2.08	0.52
1:D:9:VAL:HG22	1:D:10:ALA:N	2.24	0.52
1:L:117:THR:HG22	1:L:148:TYR:CD2	2.45	0.52
1:I:87:ARG:C	1:I:88:ARG:HG2	2.27	0.52
1:A:115:VAL:HG11	1:A:150:MET:CE	2.39	0.52
2:I:200:ACO:O9P	2:I:200:ACO:H61	2.08	0.52
1:F:57:VAL:CG1	1:F:58:ALA:N	2.73	0.52
1:A:125:PHE:CD1	3:A:201:COA:H52A	2.43	0.52
1:L:43:ASP:OD1	1:L:46:ARG:NH2	2.42	0.52
1:K:66:VAL:HG12	1:K:79:LEU:HB2	1.91	0.52
1:N:153:ILE:HG22	1:N:154:VAL:N	2.25	0.52
1:A:48:TRP:CE2	1:A:69:LYS:HE2	2.44	0.52
1:H:132:VAL:O	1:H:150:MET:HA	2.10	0.52
1:M:116:ARG:HG2	1:M:141:TYR:CE2	2.45	0.52
1:O:117:THR:HG22	1:O:148:TYR:CE2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:ILE:HG22	1:G:153:ILE:CD1	2.34	0.52
1:G:82:VAL:HB	2:G:200:ACO:H131	1.91	0.52
1:F:55:TYR:CD2	1:F:91:VAL:HG13	2.45	0.52
1:A:139:ASN:OD1	1:A:139:ASN:O	2.28	0.52
1:E:16:PHE:HE1	1:E:24:VAL:HG11	1.73	0.52
1:P:62:VAL:CG2	1:P:86:PHE:HE2	2.23	0.52
1:D:13:ILE:CG2	1:D:53:MET:CE	2.88	0.51
1:K:48:TRP:CD2	1:K:51:SER:HB3	2.45	0.51
1:N:116:ARG:CG	1:N:141:TYR:CE2	2.92	0.51
1:E:115:VAL:HG22	1:E:116:ARG:N	2.24	0.51
1:K:157:HIS:CE1	1:P:72:ARG:HH22	2.28	0.51
1:N:143:ASP:C	1:N:144:SER:HG	1.99	0.51
1:A:116:ARG:HG2	1:A:141:TYR:CE2	2.45	0.51
1:B:88:ARG:HD2	1:B:89:MET:HA	1.91	0.51
1:H:56:THR:O	1:H:56:THR:HG23	2.10	0.51
1:C:85:ARG:C	1:C:86:PHE:CD1	2.84	0.51
1:D:13:ILE:CG2	1:D:53:MET:HE2	2.41	0.51
1:K:74:GLU:HG3	1:K:110:SER:OG	2.10	0.51
1:K:84:GLU:CD	1:K:87:ARG:NH2	2.63	0.51
1:F:143:ASP:O	1:F:144:SER:HB3	2.10	0.51
1:P:65:ILE:HD12	1:P:80:PHE:CD1	2.46	0.51
1:C:7:ASN:C	1:C:7:ASN:HD22	2.05	0.51
1:I:6:ILE:HD11	1:M:78:LEU:HA	1.91	0.51
1:L:26:ARG:O	1:L:30:THR:N	2.43	0.51
1:P:85:ARG:C	1:P:86:PHE:CD1	2.83	0.51
1:D:13:ILE:HG21	1:D:53:MET:CE	2.41	0.51
1:C:86:PHE:CD1	1:C:86:PHE:N	2.78	0.51
1:N:133:ILE:HG21	1:N:148:TYR:CD1	2.46	0.51
1:E:89:MET:O	2:E:200:ACO:O3A	2.28	0.51
1:N:117:THR:HG23	1:N:148:TYR:CE2	2.46	0.51
1:C:88:ARG:H	2:C:200:ACO:P2A	2.33	0.51
1:H:62:VAL:HG11	1:H:86:PHE:CE2	2.45	0.51
1:J:139:ASN:HA	1:J:144:SER:O	2.11	0.51
1:C:125:PHE:CD1	1:C:125:PHE:C	2.84	0.51
1:G:135:ALA:HB3	1:G:149:THR:OG1	2.10	0.51
1:I:17:SER:O	1:I:18:PRO:C	2.49	0.51
1:N:66:VAL:CG1	1:N:79:LEU:HB2	2.41	0.51
1:J:88:ARG:H	2:J:200:ACO:P2A	2.34	0.51
1:A:51:SER:OG	1:A:67:GLY:N	2.44	0.50
1:H:82:VAL:HG22	2:H:200:ACO:H133	1.91	0.50
1:J:88:ARG:HH21	2:J:200:ACO:H143	1.72	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:143:ASP:OD1	1:F:145:SER:OG	2.28	0.50
1:K:55:TYR:CG	1:K:91:VAL:CG2	2.80	0.50
1:N:26:ARG:O	1:N:30:THR:OG1	2.27	0.50
1:H:82:VAL:HG22	1:H:87:ARG:HG2	1.87	0.50
1:J:88:ARG:HH22	2:J:200:ACO:H141	1.76	0.50
1:P:16:PHE:CD1	1:P:45:HIS:ND1	2.79	0.50
1:P:37:THR:HG21	1:P:41:ILE:H	1.76	0.50
1:G:25:TYR:CZ	1:G:29:GLN:NE2	2.79	0.50
1:M:84:GLU:HA	1:M:87:ARG:HE	1.77	0.50
1:A:119:ASN:O	1:A:123:ILE:CG1	2.59	0.50
1:B:70:TYR:CD2	1:B:74:GLU:OE1	2.57	0.50
1:B:124:ARG:NH1	1:J:139:ASN:O	2.45	0.50
1:C:84:GLU:HA	1:C:87:ARG:CG	2.37	0.50
2:C:200:ACO:O5A	2:C:200:ACO:O2A	2.29	0.50
1:D:133:ILE:CG2	1:G:153:ILE:HD12	2.34	0.50
1:N:32:LEU:HD21	1:N:81:ALA:HB2	1.93	0.50
1:H:7:ASN:CB	1:L:78:LEU:O	2.59	0.50
1:L:48:TRP:CE2	1:L:69:LYS:HE2	2.47	0.50
1:D:87:ARG:CG	1:D:87:ARG:NH1	2.73	0.50
2:G:200:ACO:O6A	2:G:200:ACO:OAP	2.28	0.50
1:H:91:VAL:O	1:H:94:ALA:HB3	2.11	0.50
1:L:65:ILE:HG22	1:L:95:LEU:HD22	1.92	0.50
1:P:37:THR:HG21	1:P:41:ILE:CB	2.42	0.50
1:K:66:VAL:CG1	1:K:79:LEU:HB2	2.42	0.50
1:J:16:PHE:CD1	1:J:16:PHE:C	2.85	0.50
1:L:48:TRP:CZ2	1:L:69:LYS:HE2	2.47	0.50
1:P:37:THR:CG2	1:P:41:ILE:H	2.25	0.50
1:C:157:HIS:HB2	1:K:137:LEU:CD2	2.42	0.49
1:A:91:VAL:HG13	1:A:92:GLY:N	2.27	0.49
1:A:87:ARG:CB	1:A:88:ARG:HA	2.42	0.49
1:J:88:ARG:NH2	2:J:200:ACO:H142	2.25	0.49
1:O:112:ARG:HH11	1:O:149:THR:HG23	1.77	0.49
1:P:115:VAL:O	1:P:147:ALA:HA	2.11	0.49
1:G:6:ILE:N	1:G:6:ILE:CD1	2.73	0.49
1:G:69:LYS:CE	1:G:108:MET:HE2	2.42	0.49
1:G:106:GLN:O	1:G:107:ASN:HB2	2.10	0.49
1:I:128:LYS:HD3	2:I:200:ACO:H2A	1.92	0.49
1:B:65:ILE:HD12	1:B:80:PHE:CD2	2.47	0.49
1:P:37:THR:CG2	1:P:41:ILE:HG13	2.43	0.49
1:C:16:PHE:CD1	1:C:16:PHE:C	2.85	0.49
1:C:24:VAL:HG13	1:C:64:PHE:CD1	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:TYR:HE2	1:C:147:ALA:HB2	1.77	0.49
1:J:16:PHE:CE1	1:J:17:SER:C	2.86	0.49
1:D:66:VAL:HG12	1:D:79:LEU:HB2	1.94	0.49
1:G:14:ARG:HH22	1:G:20:ASP:CG	2.15	0.49
1:P:62:VAL:HG21	1:P:86:PHE:CE2	2.48	0.49
1:P:74:GLU:OE1	1:P:112:ARG:HD3	2.12	0.49
1:P:116:ARG:CG	1:P:116:ARG:NH1	2.73	0.49
1:D:16:PHE:CD1	1:D:16:PHE:C	2.85	0.49
1:N:66:VAL:HG12	1:N:79:LEU:HB2	1.93	0.49
1:A:86:PHE:CD1	1:A:86:PHE:N	2.78	0.49
1:A:123:ILE:HG22	1:A:127:LYS:HD2	1.94	0.49
1:H:153:ILE:HG22	1:H:155:LEU:N	2.26	0.49
1:P:82:VAL:HG22	1:P:83:ASP:N	2.27	0.49
1:D:9:VAL:N	4:D:204:HOH:O	2.45	0.49
1:G:136:MET:HG2	1:G:148:TYR:CD1	2.47	0.49
1:M:117:THR:HG22	1:M:148:TYR:CE2	2.48	0.49
1:N:68:SER:OG	1:N:78:LEU:HD11	2.12	0.49
1:A:125:PHE:CE1	3:A:201:COA:C5B	2.96	0.49
1:B:133:ILE:C	1:H:153:ILE:HD11	2.33	0.49
1:D:48:TRP:CE3	1:D:51:SER:HB2	2.47	0.49
1:H:88:ARG:N	2:H:200:ACO:O4A	2.45	0.49
1:O:9:VAL:HG11	1:O:89:MET:HE1	1.70	0.49
1:P:16:PHE:CD1	1:P:16:PHE:C	2.86	0.49
1:P:40:LEU:O	1:P:43:ASP:N	2.46	0.49
1:P:62:VAL:HG11	1:P:86:PHE:HE2	1.76	0.49
1:D:117:THR:HG22	1:D:148:TYR:CE2	2.47	0.49
1:I:7:ASN:HD22	1:I:8:ALA:N	2.11	0.49
1:N:85:ARG:CB	1:N:86:PHE:CE1	2.96	0.49
1:B:80:PHE:CD1	1:B:80:PHE:C	2.85	0.49
1:B:136:MET:HE2	1:B:146:ASN:HD21	1.78	0.49
1:P:14:ARG:CG	1:P:14:ARG:NH1	2.72	0.49
1:O:74:GLU:HG2	1:O:110:SER:OG	2.13	0.49
1:K:67:GLY:O	1:K:78:LEU:HD12	2.13	0.48
1:E:56:THR:HG22	1:E:61:VAL:HG22	1.94	0.48
1:C:66:VAL:CG1	1:C:79:LEU:HB2	2.43	0.48
1:C:84:GLU:CA	1:C:87:ARG:HG3	2.41	0.48
1:C:88:ARG:CG	1:C:88:ARG:NH1	2.73	0.48
1:G:43:ASP:HA	1:G:46:ARG:NH2	2.28	0.48
1:F:57:VAL:HG13	1:F:58:ALA:H	1.78	0.48
1:J:16:PHE:CE1	1:J:18:PRO:HA	2.46	0.48
1:L:26:ARG:O	1:L:30:THR:HG23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:87:ARG:HD2	2:E:200:ACO:CDP	2.41	0.48
1:A:82:VAL:HG13	1:A:91:VAL:HG11	1.95	0.48
1:P:140:TYR:HD2	1:P:141:TYR:CE1	2.31	0.48
1:C:82:VAL:HB	2:C:200:ACO:H131	1.95	0.48
1:N:34:GLU:HB3	1:N:36:TYR:CE1	2.48	0.48
1:P:86:PHE:CD1	1:P:86:PHE:N	2.80	0.48
1:M:12:THR:HG22	1:M:13:ILE:N	2.29	0.48
1:F:8:ALA:HA	1:F:12:THR:HB	1.95	0.48
1:B:138:PRO:HG2	1:H:158:HIS:ND1	2.29	0.48
2:J:200:ACO:H133	2:J:200:ACO:P2A	2.54	0.48
1:N:68:SER:O	1:N:76:ARG:N	2.46	0.48
1:N:85:ARG:C	1:N:86:PHE:HD1	2.17	0.48
1:N:16:PHE:HE1	1:N:20:ASP:HB2	1.75	0.48
1:N:65:ILE:HG23	1:N:65:ILE:O	2.14	0.48
3:A:201:COA:O5B	3:A:201:COA:O7A	2.31	0.48
3:A:201:COA:O4A	3:A:201:COA:H10	2.13	0.48
1:J:34:GLU:OE1	1:J:142:SER:OG	2.31	0.48
1:M:25:TYR:CD2	1:M:38:GLN:HG2	2.49	0.48
1:N:48:TRP:NE1	1:N:50:GLU:OE1	2.47	0.48
1:A:48:TRP:CE3	1:A:51:SER:HB2	2.49	0.48
1:A:125:PHE:CE1	3:A:201:COA:C4B	2.97	0.48
1:K:55:TYR:HD2	1:K:91:VAL:HG21	1.76	0.48
1:L:54:VAL:CG1	1:L:61:VAL:HG13	2.43	0.48
1:G:88:ARG:HB2	2:G:200:ACO:O3A	2.13	0.48
1:A:32:LEU:HD21	1:A:81:ALA:HB2	1.96	0.48
1:P:39:ALA:HB1	1:P:42:LEU:CD1	2.44	0.48
1:P:62:VAL:CG1	1:P:86:PHE:HE2	2.26	0.48
1:G:87:ARG:HA	1:G:88:ARG:HA	1.71	0.47
1:B:65:ILE:HA	1:B:80:PHE:CB	2.44	0.47
1:B:112:ARG:CG	1:B:151:TRP:CD1	2.91	0.47
2:E:200:ACO:H52A	2:E:200:ACO:O7A	2.14	0.47
1:A:124:ARG:O	1:A:128:LYS:HG2	2.14	0.47
1:O:112:ARG:NH1	1:O:114:GLU:OE2	2.47	0.47
1:G:136:MET:HG2	1:G:148:TYR:CE1	2.48	0.47
1:H:153:ILE:HG22	1:H:154:VAL:N	2.29	0.47
1:E:125:PHE:CE1	2:E:200:ACO:O1A	2.67	0.47
1:P:154:VAL:HG12	1:P:155:LEU:N	2.29	0.47
1:I:78:LEU:C	1:I:79:LEU:HD23	2.33	0.47
1:I:80:PHE:O	2:I:200:ACO:H21	2.14	0.47
1:K:120:ASP:HB3	1:K:124:ARG:HH12	1.78	0.47
1:A:123:ILE:HD13	1:A:150:MET:HE2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:201:COA:O4A	3:A:201:COA:CAP	2.62	0.47
2:C:200:ACO:H141	2:C:200:ACO:O9P	2.14	0.47
1:M:20:ASP:O	1:M:23:SER:OG	2.23	0.47
1:N:34:GLU:HB3	1:N:36:TYR:CZ	2.50	0.47
1:B:125:PHE:O	1:B:128:LYS:HB3	2.15	0.47
1:C:153:ILE:HG22	1:C:154:VAL:N	2.30	0.47
1:H:123:ILE:O	1:H:127:LYS:HB2	2.14	0.47
1:C:84:GLU:HA	1:C:87:ARG:NE	2.30	0.47
2:G:200:ACO:O9P	2:G:200:ACO:H61	2.15	0.47
1:M:42:LEU:O	1:M:45:HIS:HB3	2.15	0.47
1:N:117:THR:HG23	1:N:148:TYR:CZ	2.50	0.47
3:A:201:COA:C5P	3:A:201:COA:S1P	3.03	0.47
1:J:17:SER:HB3	1:J:19:LYS:HG3	1.97	0.47
1:L:9:VAL:HB	1:L:89:MET:HB3	1.96	0.47
1:O:138:PRO:HD2	1:E:157:HIS:O	2.15	0.47
1:I:55:TYR:CD2	1:I:91:VAL:HG13	2.50	0.47
1:B:9:VAL:HA	1:B:10:ALA:C	2.35	0.47
1:B:68:SER:HG	1:B:78:LEU:HD23	1.76	0.47
1:H:122:ALA:O	1:H:125:PHE:N	2.48	0.47
1:E:138:PRO:HA	1:E:146:ASN:OD1	2.15	0.47
1:C:84:GLU:HA	1:C:87:ARG:CD	2.45	0.47
1:D:114:GLU:HA	1:D:148:TYR:O	2.15	0.47
1:F:138:PRO:HA	1:F:146:ASN:OD1	2.14	0.47
1:P:49:PRO:HG2	1:P:50:GLU:OE2	2.15	0.47
2:G:200:ACO:P2A	2:G:200:ACO:CDP	3.03	0.47
1:B:155:LEU:CD2	1:J:46:ARG:HG2	2.45	0.47
1:P:54:VAL:HG12	1:P:56:THR:HG23	1.96	0.47
1:D:66:VAL:CG1	1:D:79:LEU:HB2	2.45	0.46
1:P:16:PHE:HB2	1:P:54:VAL:HG23	1.96	0.46
1:B:65:ILE:HG13	1:B:80:PHE:CB	2.41	0.46
1:J:15:GLU:N	1:O:70:TYR:CE1	2.82	0.46
1:E:141:TYR:CD2	1:E:145:SER:HB2	2.49	0.46
1:B:100:LEU:HD22	1:B:152:ARG:NH1	2.29	0.46
1:J:88:ARG:HA	2:J:200:ACO:C5B	2.45	0.46
1:P:37:THR:H	1:P:38:GLN:HA	1.80	0.46
1:C:91:VAL:O	1:C:94:ALA:N	2.48	0.46
2:C:200:ACO:P2A	2:C:200:ACO:CDP	3.01	0.46
1:A:139:ASN:HA	1:A:144:SER:C	2.32	0.46
1:H:96:MET:HG3	1:H:100:LEU:HD12	1.97	0.46
1:P:37:THR:HG21	1:P:41:ILE:N	2.30	0.46
1:G:114:GLU:O	2:G:200:ACO:HH33	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:VAL:CG2	1:B:9:VAL:O	2.63	0.46
1:B:136:MET:O	1:B:137:LEU:HD23	2.14	0.46
1:J:141:TYR:O	1:J:144:SER:N	2.45	0.46
1:P:36:TYR:CD1	1:P:36:TYR:N	2.84	0.46
1:M:151:TRP:CH2	1:M:153:ILE:HG12	2.51	0.46
1:N:37:THR:O	1:N:41:ILE:HG13	2.16	0.46
1:A:119:ASN:O	1:A:123:ILE:HG13	2.15	0.46
1:B:11:GLY:CA	1:B:55:TYR:OH	2.64	0.46
1:B:65:ILE:O	1:B:65:ILE:HG23	2.15	0.46
1:G:88:ARG:HB3	2:G:200:ACO:O3A	2.16	0.46
1:F:88:ARG:O	1:F:88:ARG:HG2	2.16	0.46
1:B:55:TYR:CD2	1:B:91:VAL:HG13	2.50	0.46
1:P:54:VAL:CG1	1:P:61:VAL:CG1	2.87	0.46
2:G:200:ACO:O2A	2:G:200:ACO:O5A	2.31	0.46
1:I:83:ASP:OD1	1:I:85:ARG:NH2	2.49	0.46
1:K:9:VAL:CG2	1:K:10:ALA:N	2.78	0.46
1:N:140:TYR:CD2	1:N:141:TYR:CE1	3.03	0.46
1:L:151:TRP:CH2	1:L:153:ILE:CG1	2.98	0.46
1:P:52:PHE:HD1	1:P:53:MET:H	1.64	0.46
1:H:62:VAL:HG11	1:H:86:PHE:CZ	2.51	0.46
1:E:43:ASP:CA	1:E:46:ARG:HH12	2.22	0.46
1:E:88:ARG:NH2	2:E:200:ACO:C5A	2.78	0.46
1:P:37:THR:HG21	1:P:41:ILE:CG1	2.46	0.46
1:A:143:ASP:HB2	1:A:145:SER:OG	2.14	0.46
1:C:132:VAL:HG12	1:C:133:ILE:N	2.31	0.45
1:A:6:ILE:N	1:A:6:ILE:CD1	2.73	0.45
1:H:141:TYR:CE2	1:H:147:ALA:HB2	2.51	0.45
1:N:140:TYR:HD2	1:N:141:TYR:CD1	2.34	0.45
1:H:12:THR:OG1	1:H:13:ILE:N	2.50	0.45
1:G:35:TYR:CZ	1:G:37:THR:HG22	2.51	0.45
1:I:6:ILE:CD1	1:M:78:LEU:HD22	2.47	0.45
1:A:131:PHE:CE1	1:A:152:ARG:HG2	2.51	0.45
1:E:92:GLY:O	1:E:93:SER:C	2.54	0.45
1:B:137:LEU:CD2	1:H:157:HIS:HB2	2.46	0.45
1:E:24:VAL:HG23	1:E:64:PHE:CG	2.51	0.45
1:P:37:THR:N	1:P:38:GLN:CA	2.79	0.45
1:P:113:LEU:C	1:P:113:LEU:HD12	2.36	0.45
1:I:79:LEU:HA	2:I:200:ACO:HH33	1.98	0.45
1:K:88:ARG:HD2	1:K:89:MET:CG	2.45	0.45
1:K:88:ARG:HA	1:K:88:ARG:HD3	1.60	0.45
1:N:65:ILE:HG13	1:N:80:PHE:HB2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:131:PHE:CZ	1:A:152:ARG:HG2	2.51	0.45
1:B:43:ASP:OD1	1:B:46:ARG:CZ	2.64	0.45
1:H:92:GLY:HA3	2:H:200:ACO:H121	1.98	0.45
1:J:69:LYS:HE2	1:J:108:MET:HE1	1.97	0.45
1:C:85:ARG:HB2	1:C:86:PHE:CE1	2.52	0.45
1:G:125:PHE:HE2	2:G:200:ACO:O2A	1.99	0.45
1:G:132:VAL:HG12	1:G:133:ILE:N	2.31	0.45
1:M:125:PHE:O	1:M:128:LYS:HB3	2.17	0.45
1:B:131:PHE:CE1	1:B:152:ARG:HB3	2.52	0.45
1:J:88:ARG:HH11	2:J:200:ACO:C2A	2.30	0.45
1:E:8:ALA:HB2	1:P:34:GLU:OE2	2.16	0.45
1:E:48:TRP:CE2	1:E:69:LYS:HE2	2.51	0.45
1:P:117:THR:HG23	1:P:118:ASP:N	2.31	0.45
1:C:16:PHE:CE1	1:C:17:SER:C	2.90	0.45
2:E:200:ACO:P2A	2:E:200:ACO:H142	2.57	0.45
1:C:55:TYR:CD2	1:C:91:VAL:CG1	2.98	0.45
1:D:9:VAL:CG2	1:D:10:ALA:N	2.80	0.45
1:A:34:GLU:OE1	1:A:142:SER:OG	2.34	0.45
1:H:80:PHE:H	2:H:200:ACO:CH3	2.24	0.45
1:C:55:TYR:CD1	1:C:91:VAL:HG13	2.50	0.45
2:G:200:ACO:CDP	2:G:200:ACO:O5A	2.65	0.45
1:K:88:ARG:HA	1:K:89:MET:HA	1.69	0.45
1:N:85:ARG:HE	1:N:86:PHE:HE1	1.65	0.45
1:A:49:PRO:HG2	1:A:50:GLU:OE2	2.17	0.45
1:H:116:ARG:HG2	1:H:141:TYR:CE2	2.52	0.45
1:P:16:PHE:HD1	1:P:45:HIS:CE1	2.35	0.45
1:I:13:ILE:HD13	1:I:98:ALA:CB	2.47	0.44
1:L:113:LEU:HD22	1:L:126:TYR:CE1	2.53	0.44
1:P:66:VAL:HG12	1:P:79:LEU:HB2	1.99	0.44
1:C:62:VAL:HG11	1:C:86:PHE:CE2	2.53	0.44
1:N:153:ILE:CG2	1:N:154:VAL:N	2.80	0.44
1:A:143:ASP:O	1:A:144:SER:CB	2.58	0.44
1:J:153:ILE:HG13	1:P:133:ILE:HG22	1.99	0.44
1:G:48:TRP:CE2	1:G:69:LYS:HE3	2.53	0.44
1:G:69:LYS:CE	1:G:108:MET:CE	2.95	0.44
1:G:137:LEU:HD12	1:G:140:TYR:CD2	2.53	0.44
1:I:17:SER:C	1:I:19:LYS:N	2.71	0.44
1:K:91:VAL:HG13	1:K:92:GLY:N	2.32	0.44
1:F:17:SER:HB3	1:F:19:LYS:HE3	1.99	0.44
1:F:68:SER:HB3	1:F:78:LEU:HD11	1.99	0.44
1:B:136:MET:CE	1:B:146:ASN:HD21	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:23:SER:O	1:L:27:ILE:HD12	2.17	0.44
1:O:70:TYR:O	1:O:70:TYR:CD1	2.70	0.44
1:O:115:VAL:HG21	1:O:126:TYR:CD2	2.52	0.44
1:G:14:ARG:HA	1:K:70:TYR:CD1	2.52	0.44
1:F:87:ARG:CD	2:F:200:ACO:OAP	2.64	0.44
1:F:153:ILE:HG22	1:F:154:VAL:N	2.31	0.44
1:H:7:ASN:HB3	1:L:78:LEU:O	2.18	0.44
1:H:82:VAL:HG23	1:H:87:ARG:HG3	1.96	0.44
1:C:48:TRP:CD1	1:C:50:GLU:OE1	2.70	0.44
1:C:140:TYR:O	1:O:124:ARG:HD3	2.17	0.44
1:M:13:ILE:HG13	1:M:55:TYR:CD2	2.53	0.44
1:B:12:THR:HB	1:B:56:THR:O	2.18	0.44
1:O:125:PHE:CD1	1:O:125:PHE:C	2.90	0.44
1:P:139:ASN:OD1	1:P:144:SER:C	2.56	0.44
1:I:13:ILE:HD13	1:I:98:ALA:HB2	1.98	0.44
1:I:153:ILE:HD12	1:N:135:ALA:CA	2.48	0.44
1:B:79:LEU:CD2	1:B:79:LEU:C	2.86	0.44
1:H:82:VAL:HG21	1:H:87:ARG:HG2	1.92	0.44
1:J:69:LYS:HE3	1:J:108:MET:HE2	1.99	0.44
1:P:115:VAL:HG12	1:P:116:ARG:O	2.18	0.44
1:C:85:ARG:HB2	1:C:86:PHE:CD1	2.53	0.44
1:D:117:THR:HG22	1:D:148:TYR:CZ	2.53	0.44
1:N:65:ILE:O	1:N:65:ILE:CG2	2.66	0.44
1:A:54:VAL:HG11	1:A:61:VAL:CG2	2.47	0.44
1:A:119:ASN:HD21	3:A:201:COA:H131	1.69	0.44
1:J:151:TRP:HH2	1:J:153:ILE:HD11	1.82	0.44
1:O:115:VAL:CG2	1:O:126:TYR:CE2	2.99	0.44
1:C:16:PHE:CG	1:C:52:PHE:CD1	3.05	0.44
1:C:80:PHE:HB3	2:C:200:ACO:H21	2.00	0.44
1:K:57:VAL:HG22	1:K:62:VAL:HG21	1.99	0.44
1:N:48:TRP:CE3	1:N:51:SER:CB	2.98	0.44
1:N:113:LEU:C	1:N:113:LEU:HD12	2.38	0.44
1:P:56:THR:HA	1:P:60:SER:O	2.18	0.44
1:N:45:HIS:HD1	1:N:52:PHE:HD2	1.64	0.44
1:L:25:TYR:O	1:L:28:ALA:HB3	2.17	0.44
1:I:12:THR:O	1:I:56:THR:HG22	2.18	0.43
1:K:82:VAL:HG13	1:K:91:VAL:CG1	2.40	0.43
1:L:113:LEU:HD21	1:L:126:TYR:CD1	2.53	0.43
1:O:137:LEU:N	1:O:137:LEU:HD13	2.33	0.43
1:P:37:THR:CB	1:P:41:ILE:HG13	2.48	0.43
1:C:11:GLY:HA3	1:C:57:VAL:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:38:GLN:O	1:C:42:LEU:HG	2.18	0.43
1:C:64:PHE:CE1	1:C:81:ALA:HB3	2.53	0.43
1:G:139:ASN:N	1:G:146:ASN:OD1	2.38	0.43
1:E:23:SER:O	1:E:27:ILE:HG13	2.18	0.43
1:P:52:PHE:HD1	1:P:53:MET:N	2.16	0.43
1:F:92:GLY:N	2:F:200:ACO:O5A	2.50	0.43
1:B:152:ARG:CG	1:B:153:ILE:N	2.80	0.43
1:F:25:TYR:O	1:F:29:GLN:HG3	2.19	0.43
1:J:80:PHE:O	2:J:200:ACO:C2P	2.67	0.43
1:O:11:GLY:HA3	1:O:57:VAL:HG22	1.99	0.43
1:E:144:SER:O	1:E:144:SER:OG	2.36	0.43
1:G:51:SER:OG	1:G:67:GLY:CA	2.66	0.43
1:M:133:ILE:O	1:F:153:ILE:HD11	2.18	0.43
1:N:80:PHE:CD1	1:N:80:PHE:C	2.91	0.43
1:L:136:MET:O	1:L:138:PRO:HD3	2.19	0.43
1:E:66:VAL:HG12	1:E:79:LEU:HB2	2.00	0.43
1:P:55:TYR:CE2	1:P:91:VAL:HG13	2.52	0.43
1:P:85:ARG:CB	1:P:86:PHE:CD1	2.96	0.43
1:P:121:GLU:H	1:P:121:GLU:HG3	1.56	0.43
1:M:152:ARG:CG	1:M:153:ILE:N	2.81	0.43
1:F:21:ILE:HD13	1:F:42:LEU:CD2	2.48	0.43
1:H:114:GLU:N	1:H:114:GLU:OE1	2.51	0.43
1:P:41:ILE:HD12	1:P:42:LEU:H	1.83	0.43
1:P:62:VAL:CG1	1:P:86:PHE:CE2	3.01	0.43
1:A:86:PHE:N	1:A:86:PHE:HD1	2.16	0.43
1:J:16:PHE:CD1	1:J:17:SER:C	2.92	0.43
1:C:79:LEU:HA	1:C:79:LEU:HD23	1.80	0.43
1:C:88:ARG:N	2:C:200:ACO:O4A	2.51	0.43
1:K:133:ILE:HD13	1:K:148:TYR:CG	2.54	0.43
1:M:19:LYS:H	1:M:19:LYS:HG2	1.61	0.43
1:M:77:ILE:HD12	1:M:113:LEU:HD23	2.00	0.43
1:A:6:ILE:HD12	1:B:78:LEU:O	2.19	0.43
1:B:33:THR:HB	1:B:116:ARG:HH21	1.84	0.43
1:L:104:ARG:HH11	1:L:154:VAL:HG13	1.84	0.43
1:O:86:PHE:N	1:O:86:PHE:CD1	2.87	0.43
1:K:91:VAL:CG1	1:K:92:GLY:N	2.81	0.43
1:D:100:LEU:O	1:D:103:CYS:HB2	2.18	0.42
1:G:82:VAL:HB	2:G:200:ACO:CDP	2.49	0.42
1:G:114:GLU:HG2	1:G:140:TYR:CE2	2.54	0.42
2:G:200:ACO:O9P	2:G:200:ACO:H143	2.18	0.42
1:I:13:ILE:CG2	1:I:53:MET:CE	2.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:25:TYR:CD1	1:K:38:GLN:HG2	2.54	0.42
1:M:16:PHE:CE1	1:M:20:ASP:HB2	2.54	0.42
1:J:32:LEU:HD21	2:J:200:ACO:H21	2.00	0.42
1:E:87:ARG:O	1:E:88:ARG:HB2	2.19	0.42
1:E:89:MET:O	2:E:200:ACO:P2A	2.77	0.42
1:C:25:TYR:CG	1:C:38:GLN:HG2	2.54	0.42
1:I:6:ILE:CD1	1:M:78:LEU:CD2	2.97	0.42
1:K:57:VAL:O	1:K:58:ALA:HB3	2.19	0.42
1:K:154:VAL:O	1:K:155:LEU:HD23	2.18	0.42
1:B:52:PHE:CB	1:B:66:VAL:HG12	2.48	0.42
1:O:137:LEU:N	1:O:137:LEU:CD1	2.82	0.42
1:E:89:MET:O	2:E:200:ACO:O4A	2.37	0.42
1:K:135:ALA:HB3	1:K:149:THR:HB	2.01	0.42
1:K:143:ASP:O	1:K:144:SER:OG	2.35	0.42
1:A:68:SER:HB3	1:A:78:LEU:HD11	2.00	0.42
1:B:80:PHE:CD1	1:B:80:PHE:O	2.72	0.42
1:E:97:ASP:OD1	1:E:129:TYR:HE2	2.02	0.42
1:P:13:ILE:HG23	1:P:55:TYR:HD1	1.84	0.42
1:P:41:ILE:HD12	1:P:42:LEU:HD12	2.00	0.42
1:I:48:TRP:O	1:I:49:PRO:C	2.58	0.42
1:L:29:GLN:NE2	1:L:29:GLN:CA	2.73	0.42
1:M:12:THR:CG2	1:M:13:ILE:N	2.83	0.42
1:F:21:ILE:HD13	1:F:42:LEU:HD21	2.01	0.42
1:F:153:ILE:CG2	1:F:154:VAL:N	2.83	0.42
1:H:7:ASN:N	1:L:141:TYR:HE1	2.17	0.42
1:H:153:ILE:CG2	1:H:154:VAL:N	2.82	0.42
1:J:139:ASN:OD1	1:J:144:SER:HB2	2.20	0.42
1:P:37:THR:HG1	1:P:38:GLN:C	2.21	0.42
1:P:48:TRP:CZ2	1:P:69:LYS:HE2	2.55	0.42
1:C:82:VAL:HG23	2:C:200:ACO:O9P	2.20	0.42
1:A:54:VAL:CG1	1:A:61:VAL:HG22	2.48	0.42
1:A:82:VAL:HG12	1:A:83:ASP:N	2.34	0.42
1:A:131:PHE:CE1	1:A:152:ARG:CD	3.03	0.42
1:H:87:ARG:CG	2:H:200:ACO:CDP	2.96	0.42
1:J:36:TYR:CE1	1:J:79:LEU:HD21	2.55	0.42
1:L:104:ARG:HD2	1:L:155:LEU:O	2.20	0.42
1:O:102:LEU:O	1:O:106:GLN:HG3	2.20	0.42
1:P:27:ILE:CD1	1:P:83:ASP:CG	2.88	0.42
1:C:125:PHE:HE2	2:C:200:ACO:O2A	2.02	0.42
1:D:16:PHE:HB2	1:D:54:VAL:HG13	2.02	0.42
1:G:14:ARG:HA	1:K:70:TYR:HD1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:9:VAL:CG1	1:I:10:ALA:N	2.83	0.42
1:I:106:GLN:O	1:I:108:MET:N	2.48	0.42
1:K:48:TRP:HB3	1:K:51:SER:OG	2.18	0.42
1:A:59:GLY:HA2	1:B:47:GLU:OE2	2.19	0.42
1:H:114:GLU:HG2	1:H:140:TYR:CZ	2.55	0.42
2:H:200:ACO:N3A	2:H:200:ACO:H2B	2.34	0.42
1:J:7:ASN:HB2	1:O:140:TYR:HE2	1.84	0.42
1:P:9:VAL:HG22	1:P:89:MET:HG2	2.00	0.42
1:I:128:LYS:CD	2:I:200:ACO:C2A	2.81	0.42
1:F:143:ASP:CG	1:F:145:SER:OG	2.56	0.42
1:N:56:THR:HA	1:N:60:SER:O	2.20	0.42
1:B:133:ILE:O	1:H:153:ILE:HD11	2.20	0.42
1:J:140:TYR:O	1:J:140:TYR:CD1	2.73	0.42
1:C:17:SER:C	1:C:19:LYS:N	2.73	0.42
1:C:66:VAL:HG12	1:C:79:LEU:HB2	2.01	0.42
1:K:124:ARG:CZ	1:E:139:ASN:O	2.68	0.42
1:A:14:ARG:HA	1:B:70:TYR:HE1	1.82	0.42
1:J:14:ARG:HA	1:O:70:TYR:CE1	2.55	0.42
1:J:16:PHE:CE1	1:J:17:SER:O	2.73	0.42
1:O:62:VAL:HG11	1:O:86:PHE:CD2	2.55	0.42
1:E:85:ARG:H	1:E:85:ARG:HG3	1.73	0.42
1:P:37:THR:HB	1:P:40:LEU:H	1.80	0.42
1:P:124:ARG:HD3	1:P:124:ARG:HA	1.89	0.42
1:P:154:VAL:HG12	1:P:155:LEU:H	1.83	0.42
2:G:200:ACO:HO2A	2:G:200:ACO:P3B	2.43	0.41
1:I:27:ILE:CD1	1:I:83:ASP:HB2	2.50	0.41
1:A:89:MET:HE3	1:A:89:MET:HB3	1.90	0.41
1:B:66:VAL:CG2	1:B:79:LEU:HD23	2.45	0.41
1:H:68:SER:HB3	1:H:78:LEU:HD11	2.02	0.41
1:C:7:ASN:O	1:C:7:ASN:ND2	2.32	0.41
1:I:136:MET:HE2	1:I:146:ASN:CG	2.40	0.41
1:F:104:ARG:NH2	1:F:156:GLU:OE1	2.52	0.41
1:N:13:ILE:HG13	1:N:55:TYR:CD2	2.55	0.41
1:N:95:LEU:O	1:N:98:ALA:HB3	2.20	0.41
1:J:87:ARG:HH11	1:J:87:ARG:HD2	1.74	0.41
1:C:124:ARG:HD3	2:C:200:ACO:H2A	2.03	0.41
1:M:48:TRP:O	1:M:51:SER:HB2	2.19	0.41
1:H:87:ARG:HG2	2:H:200:ACO:H131	2.02	0.41
1:E:88:ARG:HH22	2:E:200:ACO:C2A	2.33	0.41
1:C:151:TRP:CZ2	1:C:153:ILE:HD13	2.55	0.41
1:D:84:GLU:O	1:D:87:ARG:NH1	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:136:MET:HE1	1:I:146:ASN:CB	2.50	0.41
1:I:153:ILE:CD1	1:N:135:ALA:N	2.83	0.41
1:M:123:ILE:HG22	1:M:127:LYS:HD2	2.02	0.41
1:F:57:VAL:CG1	1:F:58:ALA:H	2.34	0.41
1:A:136:MET:SD	1:A:146:ASN:HB3	2.60	0.41
1:H:123:ILE:HG22	1:H:127:LYS:HE2	2.02	0.41
1:J:131:PHE:CZ	1:J:152:ARG:HG2	2.55	0.41
1:I:88:ARG:H	2:I:200:ACO:P2A	2.43	0.41
1:K:120:ASP:CB	1:K:124:ARG:NH1	2.73	0.41
1:M:91:VAL:HG12	1:M:95:LEU:HD12	2.03	0.41
1:A:32:LEU:CD1	1:A:79:LEU:HD23	2.50	0.41
1:A:79:LEU:HA	3:A:201:COA:C3P	2.50	0.41
1:H:88:ARG:H	2:H:200:ACO:P2A	2.43	0.41
1:J:36:TYR:CZ	1:J:79:LEU:HD21	2.55	0.41
1:O:117:THR:HG22	1:O:148:TYR:CD2	2.56	0.41
1:E:97:ASP:OD1	1:E:129:TYR:CE2	2.73	0.41
1:C:52:PHE:HD2	1:C:66:VAL:HG21	1.86	0.41
1:C:126:TYR:HB3	1:C:131:PHE:HB2	2.01	0.41
1:D:137:LEU:HD22	1:G:157:HIS:HB2	2.02	0.41
1:G:123:ILE:O	1:G:124:ARG:C	2.59	0.41
1:N:139:ASN:HB2	1:N:144:SER:HA	2.02	0.41
1:B:48:TRP:NE1	1:B:50:GLU:OE1	2.54	0.41
1:L:82:VAL:O	1:L:83:ASP:C	2.58	0.41
1:O:16:PHE:CE1	1:O:20:ASP:HB2	2.55	0.41
1:O:34:GLU:OE2	1:O:141:TYR:CD1	2.69	0.41
1:P:18:PRO:O	1:P:21:ILE:CD1	2.68	0.41
1:E:46:ARG:NH1	1:E:46:ARG:HG3	2.35	0.41
1:D:141:TYR:CE2	1:D:147:ALA:HB2	2.56	0.41
1:I:13:ILE:HG21	1:I:53:MET:CE	2.47	0.41
1:K:55:TYR:CB	1:K:91:VAL:CG2	2.98	0.41
1:N:36:TYR:CE2	1:N:79:LEU:HD21	2.56	0.41
1:A:33:THR:HB	1:A:116:ARG:NH1	2.36	0.41
1:A:119:ASN:O	1:A:123:ILE:HG12	2.19	0.41
1:B:78:LEU:HD13	1:B:78:LEU:HA	1.65	0.41
1:H:14:ARG:NH2	1:H:20:ASP:OD2	2.53	0.41
1:H:82:VAL:HG22	2:H:200:ACO:CDP	2.50	0.41
1:H:87:ARG:HD3	2:H:200:ACO:H131	2.02	0.41
1:O:129:TYR:O	1:O:152:ARG:NH1	2.54	0.41
1:E:32:LEU:CD1	1:E:79:LEU:HD13	2.51	0.41
1:E:125:PHE:O	1:E:128:LYS:HB3	2.21	0.41
1:P:9:VAL:CG1	1:P:10:ALA:H	2.08	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:132:VAL:O	1:C:150:MET:HA	2.21	0.41
2:C:200:ACO:H8A	2:C:200:ACO:C5B	2.49	0.41
1:A:91:VAL:CG1	1:A:92:GLY:N	2.83	0.41
1:O:54:VAL:HG12	1:O:64:PHE:HB3	2.03	0.41
1:O:139:ASN:ND2	1:O:144:SER:CB	2.84	0.41
1:P:41:ILE:N	1:P:41:ILE:HD12	2.35	0.41
1:P:64:PHE:CZ	1:P:81:ALA:HB2	2.54	0.41
1:P:151:TRP:HH2	1:P:153:ILE:HD11	1.82	0.41
1:G:69:LYS:HE2	1:G:108:MET:HE3	2.01	0.40
1:I:83:ASP:OD2	1:I:85:ARG:NH2	2.54	0.40
1:A:79:LEU:HA	3:A:201:COA:H32	2.02	0.40
1:J:143:ASP:O	1:J:144:SER:CB	2.69	0.40
1:O:142:SER:C	1:O:144:SER:H	2.23	0.40
1:P:103:CYS:HB3	1:P:108:MET:HB2	2.02	0.40
1:C:55:TYR:CB	1:C:91:VAL:CG1	2.99	0.40
1:G:48:TRP:CD2	1:G:51:SER:HB2	2.56	0.40
1:F:12:THR:O	1:F:56:THR:HG22	2.22	0.40
1:J:113:LEU:HD12	1:J:113:LEU:C	2.41	0.40
1:O:139:ASN:ND2	1:O:144:SER:HB3	2.37	0.40
1:P:35:TYR:CD1	1:P:35:TYR:C	2.94	0.40
1:P:92:GLY:O	1:P:95:LEU:HB2	2.21	0.40
1:D:10:ALA:HA	1:D:11:GLY:HA3	1.67	0.40
1:L:40:LEU:O	1:L:43:ASP:N	2.51	0.40
1:C:80:PHE:O	2:C:200:ACO:H32	2.21	0.40
1:N:16:PHE:CE1	1:N:24:VAL:CG2	3.03	0.40
1:N:48:TRP:CE2	1:N:69:LYS:NZ	2.89	0.40
1:B:72:ARG:CG	1:B:73:THR:HG23	2.52	0.40
1:L:113:LEU:C	1:L:113:LEU:HD12	2.41	0.40
1:E:115:VAL:CG2	1:E:116:ARG:N	2.84	0.40
1:C:16:PHE:CE2	1:C:52:PHE:CE1	3.00	0.40
1:F:117:THR:HG22	1:F:148:TYR:CD2	2.56	0.40
1:A:55:TYR:CE2	1:A:91:VAL:HG23	2.56	0.40
1:A:119:ASN:CG	1:A:122:ALA:HB3	2.39	0.40
1:B:25:TYR:HH	1:B:35:TYR:HH	1.63	0.40
1:H:155:LEU:HD23	1:H:155:LEU:C	2.42	0.40
1:O:48:TRP:CE2	1:O:69:LYS:HE2	2.57	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	152/162 (94%)	147 (97%)	5 (3%)	0	100	100
1	B	146/162 (90%)	141 (97%)	5 (3%)	0	100	100
1	C	151/162 (93%)	146 (97%)	5 (3%)	0	100	100
1	D	145/162 (90%)	136 (94%)	9 (6%)	0	100	100
1	E	149/162 (92%)	145 (97%)	4 (3%)	0	100	100
1	F	148/162 (91%)	140 (95%)	8 (5%)	0	100	100
1	G	152/162 (94%)	144 (95%)	8 (5%)	0	100	100
1	H	151/162 (93%)	145 (96%)	6 (4%)	0	100	100
1	I	149/162 (92%)	142 (95%)	7 (5%)	0	100	100
1	J	149/162 (92%)	140 (94%)	9 (6%)	0	100	100
1	K	147/162 (91%)	144 (98%)	3 (2%)	0	100	100
1	L	147/162 (91%)	139 (95%)	8 (5%)	0	100	100
1	M	146/162 (90%)	139 (95%)	7 (5%)	0	100	100
1	N	146/162 (90%)	139 (95%)	7 (5%)	0	100	100
1	O	147/162 (91%)	144 (98%)	3 (2%)	0	100	100
1	P	145/162 (90%)	137 (94%)	8 (6%)	0	100	100
All	All	2370/2592 (91%)	2268 (96%)	102 (4%)	0	100	100

There are no Ramachandran outliers to report.

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	135/142 (95%)	125 (93%)	10 (7%)	13 41
1	B	130/142 (92%)	120 (92%)	10 (8%)	13 40
1	C	134/142 (94%)	126 (94%)	8 (6%)	19 50
1	D	129/142 (91%)	120 (93%)	9 (7%)	15 44
1	E	132/142 (93%)	126 (96%)	6 (4%)	27 60
1	F	131/142 (92%)	128 (98%)	3 (2%)	50 75
1	G	135/142 (95%)	129 (96%)	6 (4%)	28 60
1	H	134/142 (94%)	129 (96%)	5 (4%)	34 64
1	I	132/142 (93%)	129 (98%)	3 (2%)	50 75
1	J	132/142 (93%)	120 (91%)	12 (9%)	9 32
1	K	131/142 (92%)	125 (95%)	6 (5%)	27 60
1	L	130/142 (92%)	121 (93%)	9 (7%)	15 45
1	M	130/142 (92%)	122 (94%)	8 (6%)	18 49
1	N	130/142 (92%)	120 (92%)	10 (8%)	13 40
1	O	131/142 (92%)	125 (95%)	6 (5%)	27 60
1	P	129/142 (91%)	111 (86%)	18 (14%)	3 16
All	All	2105/2272 (93%)	1976 (94%)	129 (6%)	18 49

All (129) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	7	ASN
1	C	16	PHE
1	C	23	SER
1	C	47	GLU
1	C	50	GLU
1	C	71	SER
1	C	88	ARG
1	C	89	MET
1	D	16	PHE
1	D	17	SER
1	D	19	LYS
1	D	21	ILE
1	D	52	PHE
1	D	87	ARG
1	D	93	SER
1	D	129	TYR

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Mol	Chain	Res	Type
1	D	132	VAL
1	G	7	ASN
1	G	52	PHE
1	G	87	ARG
1	G	88	ARG
1	G	93	SER
1	G	101	SER
1	I	7	ASN
1	I	52	PHE
1	I	136	MET
1	K	52	PHE
1	K	73	THR
1	K	85	ARG
1	K	86	PHE
1	K	93	SER
1	K	152	ARG
1	M	34	GLU
1	M	40	LEU
1	M	52	PHE
1	M	68	SER
1	M	106	GLN
1	M	132	VAL
1	M	149	THR
1	M	152	ARG
1	F	50	GLU
1	F	51	SER
1	F	52	PHE
1	N	38	GLN
1	N	50	GLU
1	N	52	PHE
1	N	86	PHE
1	N	87	ARG
1	N	120	ASP
1	N	142	SER
1	N	143	ASP
1	N	145	SER
1	N	146	ASN
1	A	7	ASN
1	A	13	ILE
1	A	45	HIS
1	A	52	PHE
1	A	86	PHE

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Mol	Chain	Res	Type
1	A	89	MET
1	A	129	TYR
1	A	142	SER
1	A	143	ASP
1	A	144	SER
1	B	47	GLU
1	B	52	PHE
1	B	66	VAL
1	B	68	SER
1	B	76	ARG
1	B	77	ILE
1	B	78	LEU
1	B	79	LEU
1	B	80	PHE
1	B	152	ARG
1	H	7	ASN
1	H	47	GLU
1	H	52	PHE
1	H	142	SER
1	H	158	HIS
1	J	14	ARG
1	J	19	LYS
1	J	21	ILE
1	J	23	SER
1	J	52	PHE
1	J	88	ARG
1	J	136	MET
1	J	139	ASN
1	J	142	SER
1	J	143	ASP
1	J	145	SER
1	J	146	ASN
1	L	29	GLN
1	L	31	SER
1	L	34	GLU
1	L	47	GLU
1	L	52	PHE
1	L	84	GLU
1	L	85	ARG
1	L	132	VAL
1	L	145	SER
1	O	52	PHE

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Mol	Chain	Res	Type
1	O	71	SER
1	O	72	ARG
1	O	137	LEU
1	O	139	ASN
1	O	142	SER
1	E	52	PHE
1	E	79	LEU
1	E	87	ARG
1	E	88	ARG
1	E	89	MET
1	E	143	ASP
1	P	12	THR
1	P	13	ILE
1	P	14	ARG
1	P	15	GLU
1	P	16	PHE
1	P	36	TYR
1	P	37	THR
1	P	41	ILE
1	P	52	PHE
1	P	60	SER
1	P	84	GLU
1	P	85	ARG
1	P	86	PHE
1	P	88	ARG
1	P	116	ARG
1	P	120	ASP
1	P	121	GLU
1	P	124	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	29	GLN
1	G	38	GLN
1	G	107	ASN
1	I	7	ASN
1	K	107	ASN
1	K	157	HIS
1	M	29	GLN
1	M	139	ASN
1	F	157	HIS

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Mol	Chain	Res	Type
1	A	29	GLN
1	A	157	HIS
1	B	146	ASN
1	H	7	ASN
1	H	159	HIS
1	J	7	ASN
1	J	139	ASN
1	O	139	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
3	COA	A	201	-	41,50,50	1.10	3 (7%)	52,75,75	3.22	16 (30%)
2	ACO	G	200	-	45,53,53	0.90	1 (2%)	56,79,79	1.86	17 (30%)
2	ACO	C	200	-	45,53,53	0.85	1 (2%)	56,79,79	1.46	7 (12%)
2	ACO	E	200	-	45,53,53	0.90	4 (8%)	56,79,79	1.44	6 (10%)
2	ACO	H	200	-	45,53,53	0.97	2 (4%)	56,79,79	2.26	20 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	ACO	I	200	-	45,53,53	0.97	2 (4%)	56,79,79	1.90	13 (23%)
2	ACO	J	200	-	45,53,53	0.87	2 (4%)	56,79,79	1.78	12 (21%)
2	ACO	F	200	-	45,53,53	0.97	2 (4%)	56,79,79	1.86	12 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	COA	A	201	-	-	21/44/64/64	0/3/3/3
2	ACO	G	200	-	-	25/47/67/67	0/3/3/3
2	ACO	C	200	-	-	24/47/67/67	0/3/3/3
2	ACO	E	200	-	-	17/47/67/67	0/3/3/3
2	ACO	H	200	-	-	29/47/67/67	0/3/3/3
2	ACO	I	200	-	-	26/47/67/67	0/3/3/3
2	ACO	J	200	-	-	26/47/67/67	0/3/3/3
2	ACO	F	200	-	-	29/47/67/67	0/3/3/3

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	201	COA	C2B-C1B	-3.11	1.49	1.53
2	G	200	ACO	C5A-C4A	2.60	1.47	1.40
2	C	200	ACO	C5A-C4A	2.52	1.47	1.40
2	J	200	ACO	C5A-C4A	2.48	1.47	1.40
3	A	201	COA	C2B-C3B	-2.40	1.47	1.52
2	I	200	ACO	O4B-C1B	2.39	1.44	1.41
2	H	200	ACO	C4A-N3A	2.38	1.38	1.35
2	H	200	ACO	C5A-C4A	2.37	1.47	1.40
2	E	200	ACO	C5A-C4A	2.36	1.47	1.40
2	F	200	ACO	C2A-N3A	2.36	1.35	1.32
2	F	200	ACO	C5A-C4A	2.25	1.46	1.40
3	A	201	COA	C5A-C4A	2.19	1.46	1.40
2	E	200	ACO	C2A-N3A	2.15	1.35	1.32
2	E	200	ACO	O4B-C1B	2.09	1.44	1.41
2	E	200	ACO	P3B-O3B	2.04	1.63	1.59
2	J	200	ACO	C2A-N3A	2.00	1.35	1.32
2	I	200	ACO	C5A-C4A	2.00	1.46	1.40

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	201	COA	CEP-CBP-CAP	-12.54	87.08	108.82
3	A	201	COA	CEP-CBP-CCP	10.86	125.94	108.23
2	F	200	ACO	C3P-N4P-C5P	-6.71	110.37	122.84
2	H	200	ACO	C6P-C5P-N4P	6.57	127.49	116.42
3	A	201	COA	CEP-CBP-CDP	6.39	122.19	109.17
2	E	200	ACO	P2A-O3A-P1A	-5.84	112.79	132.83
3	A	201	COA	CDP-CBP-CAP	-5.80	98.77	108.82
2	G	200	ACO	P2A-O3A-P1A	-5.62	113.55	132.83
3	A	201	COA	O4B-C1B-C2B	-5.60	98.74	106.93
2	J	200	ACO	P2A-O3A-P1A	-5.55	113.78	132.83
2	H	200	ACO	O5P-C5P-C6P	-5.26	112.39	122.02
2	H	200	ACO	N3A-C2A-N1A	-5.23	120.51	128.68
2	C	200	ACO	P2A-O3A-P1A	-5.22	114.93	132.83
2	I	200	ACO	P2A-O3A-P1A	-5.12	115.25	132.83
2	H	200	ACO	P2A-O3A-P1A	-5.06	115.48	132.83
3	A	201	COA	N3A-C2A-N1A	-4.81	121.16	128.68
2	H	200	ACO	C3P-N4P-C5P	4.59	131.36	122.84
2	J	200	ACO	CDP-CBP-CAP	-4.59	100.87	108.82
2	F	200	ACO	N3A-C2A-N1A	-4.44	121.74	128.68
2	I	200	ACO	O4B-C1B-C2B	-4.41	100.48	106.93
2	I	200	ACO	CEP-CBP-CCP	4.33	115.30	108.23
2	J	200	ACO	C6P-C5P-N4P	4.31	123.67	116.42
2	F	200	ACO	P2A-O3A-P1A	-4.25	118.23	132.83
3	A	201	COA	P2A-O3A-P1A	-4.15	118.59	132.83
3	A	201	COA	C7P-C6P-C5P	-4.06	105.60	112.36
2	C	200	ACO	N3A-C2A-N1A	-3.97	122.48	128.68
2	G	200	ACO	N3A-C2A-N1A	-3.90	122.59	128.68
2	I	200	ACO	C2P-C3P-N4P	3.78	120.35	112.42
2	G	200	ACO	C6P-C7P-N8P	3.77	119.51	111.90
2	E	200	ACO	N3A-C2A-N1A	-3.75	122.82	128.68
2	G	200	ACO	CEP-CBP-CAP	3.70	115.24	108.82
2	J	200	ACO	N3A-C2A-N1A	-3.59	123.07	128.68
2	I	200	ACO	C6P-C5P-N4P	3.38	122.12	116.42
2	I	200	ACO	O5B-C5B-C4B	3.36	120.57	108.99
2	F	200	ACO	O9P-C9P-N8P	3.35	130.18	122.99
2	H	200	ACO	C5A-C6A-N6A	-3.33	115.30	120.35
2	G	200	ACO	O5P-C5P-C6P	-3.31	115.97	122.02
2	I	200	ACO	C7P-N8P-C9P	-3.30	116.69	122.59
3	A	201	COA	O2B-C2B-C3B	-3.29	101.82	111.17
2	J	200	ACO	C4A-C5A-N7A	-3.29	105.97	109.40
2	F	200	ACO	C7P-N8P-C9P	3.26	128.41	122.59
2	H	200	ACO	C6P-C7P-N8P	3.24	118.43	111.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	200	ACO	O3B-C3B-C4B	3.23	121.76	110.08
2	I	200	ACO	O5P-C5P-C6P	-3.23	116.11	122.02
2	H	200	ACO	CEP-CBP-CCP	-3.16	103.07	108.23
2	H	200	ACO	O5A-P2A-O4A	3.14	127.76	112.24
3	A	201	COA	O3B-C3B-C4B	-3.10	98.88	110.08
2	H	200	ACO	O6A-P2A-O4A	-3.06	97.12	109.07
2	H	200	ACO	N6A-C6A-N1A	2.98	124.77	118.57
3	A	201	COA	O5B-C5B-C4B	2.96	119.18	108.99
2	J	200	ACO	CEP-CBP-CDP	2.93	115.13	109.17
2	E	200	ACO	C3B-C2B-C1B	2.86	106.23	99.89
2	G	200	ACO	C4A-C5A-N7A	-2.85	106.42	109.40
2	F	200	ACO	CDP-CBP-CCP	2.80	112.80	108.23
3	A	201	COA	C3B-C2B-C1B	2.80	106.09	99.89
2	H	200	ACO	C7P-N8P-C9P	2.79	127.57	122.59
3	A	201	COA	O9A-P3B-O8A	2.79	118.30	107.64
2	G	200	ACO	C1B-N9A-C4A	-2.77	121.77	126.64
2	E	200	ACO	C4A-C5A-N7A	-2.77	106.51	109.40
2	E	200	ACO	C5B-C4B-C3B	-2.77	105.23	114.40
2	J	200	ACO	C3B-C2B-C1B	2.75	105.99	99.89
2	H	200	ACO	C7P-C6P-C5P	-2.73	107.81	112.36
3	A	201	COA	O5P-C5P-C6P	-2.73	117.03	122.02
2	F	200	ACO	C4A-C5A-N7A	-2.71	106.58	109.40
2	G	200	ACO	C7P-N8P-C9P	2.70	127.40	122.59
2	I	200	ACO	CAP-C9P-N8P	2.69	121.94	116.58
2	J	200	ACO	C6P-C7P-N8P	-2.67	106.51	111.90
2	C	200	ACO	CEP-CBP-CDP	2.65	114.58	109.17
2	F	200	ACO	C1B-N9A-C4A	-2.61	122.05	126.64
2	F	200	ACO	CAP-C9P-N8P	-2.59	111.42	116.58
2	G	200	ACO	C7P-C6P-C5P	-2.56	108.09	112.36
2	I	200	ACO	C4A-C5A-N7A	-2.56	106.73	109.40
2	G	200	ACO	C2P-C3P-N4P	2.56	117.79	112.42
2	H	200	ACO	CEP-CBP-CAP	2.55	113.25	108.82
2	I	200	ACO	C3B-C2B-C1B	-2.54	94.27	99.89
2	J	200	ACO	O5P-C5P-C6P	-2.54	117.38	122.02
2	H	200	ACO	CDP-CBP-CAP	-2.53	104.44	108.82
2	J	200	ACO	CEP-CBP-CAP	2.52	113.18	108.82
2	J	200	ACO	O5P-C5P-N4P	-2.52	118.27	123.01
2	G	200	ACO	C2A-N1A-C6A	2.47	122.98	118.75
3	A	201	COA	C2A-N1A-C6A	2.47	122.98	118.75
2	G	200	ACO	O9P-C9P-N8P	2.46	128.27	122.99
2	F	200	ACO	O6A-CCP-CBP	2.45	114.49	110.55
2	G	200	ACO	C3B-C2B-C1B	2.44	105.30	99.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	I	200	ACO	CDP-CBP-CCP	-2.44	104.25	108.23
2	F	200	ACO	C3B-C2B-C1B	2.42	105.25	99.89
2	G	200	ACO	O9A-P3B-O8A	2.41	116.84	107.64
2	G	200	ACO	CDP-CBP-CAP	-2.23	104.95	108.82
3	A	201	COA	O4B-C4B-C5B	2.22	116.68	109.37
2	E	200	ACO	OAP-CAP-CBP	2.21	115.45	110.25
2	G	200	ACO	C2B-C3B-C4B	2.19	107.11	103.22
2	J	200	ACO	C2P-C3P-N4P	2.18	117.00	112.42
2	C	200	ACO	O9A-P3B-O8A	2.17	115.91	107.64
2	F	200	ACO	CDP-CBP-CAP	-2.15	105.09	108.82
2	H	200	ACO	O9P-C9P-N8P	2.12	127.55	122.99
2	C	200	ACO	C2A-N1A-C6A	2.12	122.38	118.75
2	H	200	ACO	O6A-CCP-CBP	-2.11	107.16	110.55
2	C	200	ACO	C1B-N9A-C4A	-2.09	122.96	126.64
2	H	200	ACO	C2A-N1A-C6A	2.08	122.31	118.75
2	H	200	ACO	OAP-CAP-CBP	-2.04	105.46	110.25
2	H	200	ACO	O9A-P3B-O8A	2.02	115.36	107.64
2	G	200	ACO	O6A-CCP-CBP	-2.02	107.30	110.55
2	C	200	ACO	C2B-C3B-C4B	2.02	106.80	103.22

There are no chirality outliers.

All (197) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	200	ACO	C5B-O5B-P1A-O1A
2	C	200	ACO	C5B-O5B-P1A-O3A
2	C	200	ACO	CCP-O6A-P2A-O4A
2	C	200	ACO	CCP-O6A-P2A-O5A
2	C	200	ACO	CBP-CCP-O6A-P2A
2	C	200	ACO	CEP-CBP-CCP-O6A
2	C	200	ACO	CAP-CBP-CCP-O6A
2	C	200	ACO	O5P-C5P-N4P-C3P
2	C	200	ACO	S1P-C2P-C3P-N4P
2	C	200	ACO	C3P-C2P-S1P-C
2	C	200	ACO	O-C-S1P-C2P
2	C	200	ACO	CH3-C-S1P-C2P
2	G	200	ACO	O4B-C4B-C5B-O5B
2	G	200	ACO	C5B-O5B-P1A-O1A
2	G	200	ACO	C5B-O5B-P1A-O2A
2	G	200	ACO	CCP-O6A-P2A-O4A
2	G	200	ACO	CCP-O6A-P2A-O5A
2	G	200	ACO	CBP-CCP-O6A-P2A

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Mol	Chain	Res	Type	Atoms
2	G	200	ACO	OAP-CAP-CBP-CCP
2	G	200	ACO	C9P-CAP-CBP-CCP
2	G	200	ACO	OAP-CAP-CBP-CDP
2	G	200	ACO	C9P-CAP-CBP-CDP
2	G	200	ACO	OAP-CAP-CBP-CEP
2	G	200	ACO	C9P-CAP-CBP-CEP
2	G	200	ACO	C5P-C6P-C7P-N8P
2	G	200	ACO	O-C-S1P-C2P
2	G	200	ACO	CH3-C-S1P-C2P
2	I	200	ACO	C3B-O3B-P3B-O9A
2	I	200	ACO	C3B-C4B-C5B-O5B
2	I	200	ACO	C4B-C5B-O5B-P1A
2	I	200	ACO	C5B-O5B-P1A-O1A
2	I	200	ACO	CCP-O6A-P2A-O3A
2	I	200	ACO	CCP-O6A-P2A-O5A
2	I	200	ACO	CBP-CCP-O6A-P2A
2	I	200	ACO	CAP-CBP-CCP-O6A
2	I	200	ACO	OAP-CAP-CBP-CCP
2	I	200	ACO	C9P-CAP-CBP-CCP
2	I	200	ACO	OAP-CAP-CBP-CDP
2	I	200	ACO	C9P-CAP-CBP-CDP
2	I	200	ACO	OAP-CAP-CBP-CEP
2	I	200	ACO	C9P-CAP-CBP-CEP
2	I	200	ACO	C3P-C2P-S1P-C
2	I	200	ACO	O-C-S1P-C2P
2	I	200	ACO	CH3-C-S1P-C2P
2	F	200	ACO	C5B-O5B-P1A-O1A
2	F	200	ACO	C5B-O5B-P1A-O2A
2	F	200	ACO	CCP-O6A-P2A-O3A
2	F	200	ACO	CCP-O6A-P2A-O5A
2	F	200	ACO	CBP-CCP-O6A-P2A
2	F	200	ACO	CAP-CBP-CCP-O6A
2	F	200	ACO	OAP-CAP-CBP-CCP
2	F	200	ACO	C9P-CAP-CBP-CCP
2	F	200	ACO	OAP-CAP-CBP-CDP
2	F	200	ACO	C9P-CAP-CBP-CDP
2	F	200	ACO	OAP-CAP-CBP-CEP
2	F	200	ACO	C9P-CAP-CBP-CEP
2	F	200	ACO	C6P-C5P-N4P-C3P
2	F	200	ACO	S1P-C2P-C3P-N4P
2	F	200	ACO	C3P-C2P-S1P-C
2	H	200	ACO	CBP-CCP-O6A-P2A

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Mol	Chain	Res	Type	Atoms
2	H	200	ACO	CDP-CBP-CCP-O6A
2	H	200	ACO	CEP-CBP-CCP-O6A
2	H	200	ACO	CAP-CBP-CCP-O6A
2	H	200	ACO	OAP-CAP-CBP-CCP
2	H	200	ACO	C9P-CAP-CBP-CCP
2	H	200	ACO	OAP-CAP-CBP-CDP
2	H	200	ACO	C9P-CAP-CBP-CDP
2	H	200	ACO	OAP-CAP-CBP-CEP
2	H	200	ACO	C9P-CAP-CBP-CEP
2	H	200	ACO	N8P-C9P-CAP-CBP
2	H	200	ACO	N8P-C9P-CAP-OAP
2	H	200	ACO	CAP-C9P-N8P-C7P
2	H	200	ACO	S1P-C2P-C3P-N4P
2	H	200	ACO	C3P-C2P-S1P-C
2	H	200	ACO	O-C-S1P-C2P
2	H	200	ACO	CH3-C-S1P-C2P
2	J	200	ACO	C3B-C4B-C5B-O5B
2	J	200	ACO	O4B-C4B-C5B-O5B
2	J	200	ACO	C5B-O5B-P1A-O1A
2	J	200	ACO	C5B-O5B-P1A-O2A
2	J	200	ACO	CCP-O6A-P2A-O4A
2	J	200	ACO	CBP-CCP-O6A-P2A
2	J	200	ACO	C6P-C5P-N4P-C3P
2	J	200	ACO	O5P-C5P-N4P-C3P
2	J	200	ACO	C3P-C2P-S1P-C
2	J	200	ACO	O-C-S1P-C2P
2	J	200	ACO	CH3-C-S1P-C2P
2	E	200	ACO	C5B-O5B-P1A-O1A
2	E	200	ACO	C5B-O5B-P1A-O2A
2	E	200	ACO	CCP-O6A-P2A-O4A
2	E	200	ACO	CCP-O6A-P2A-O5A
2	E	200	ACO	CBP-CCP-O6A-P2A
2	E	200	ACO	C3P-C2P-S1P-C
2	E	200	ACO	O-C-S1P-C2P
2	E	200	ACO	CH3-C-S1P-C2P
3	A	201	COA	CEP-CBP-CCP-O6A
3	A	201	COA	C9P-CAP-CBP-CCP
3	A	201	COA	C9P-CAP-CBP-CDP
3	A	201	COA	C9P-CAP-CBP-CEP
3	A	201	COA	O9P-C9P-CAP-OAP
3	A	201	COA	N8P-C9P-CAP-OAP
3	A	201	COA	S1P-C2P-C3P-N4P

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Mol	Chain	Res	Type	Atoms
2	G	200	ACO	C6P-C7P-N8P-C9P
2	H	200	ACO	C6P-C7P-N8P-C9P
2	F	200	ACO	O5P-C5P-N4P-C3P
2	C	200	ACO	C6P-C5P-N4P-C3P
2	H	200	ACO	C6P-C5P-N4P-C3P
2	C	200	ACO	O4B-C4B-C5B-O5B
2	F	200	ACO	C2B-C3B-O3B-P3B
2	E	200	ACO	C4B-C3B-O3B-P3B
2	H	200	ACO	O5P-C5P-N4P-C3P
2	F	200	ACO	C6P-C7P-N8P-C9P
2	I	200	ACO	C6P-C7P-N8P-C9P
2	I	200	ACO	O4B-C4B-C5B-O5B
2	F	200	ACO	C3B-C4B-C5B-O5B
2	C	200	ACO	C2B-C3B-O3B-P3B
2	C	200	ACO	C4B-C3B-O3B-P3B
2	G	200	ACO	C2B-C3B-O3B-P3B
2	F	200	ACO	C4B-C3B-O3B-P3B
2	J	200	ACO	C2B-C3B-O3B-P3B
2	F	200	ACO	O4B-C4B-C5B-O5B
2	C	200	ACO	CDP-CBP-CCP-O6A
2	I	200	ACO	CDP-CBP-CCP-O6A
2	I	200	ACO	CEP-CBP-CCP-O6A
2	G	200	ACO	C4B-C3B-O3B-P3B
2	H	200	ACO	C2B-C3B-O3B-P3B
2	E	200	ACO	C2B-C3B-O3B-P3B
2	E	200	ACO	S1P-C2P-C3P-N4P
2	C	200	ACO	C3B-C4B-C5B-O5B
2	F	200	ACO	C5P-C6P-C7P-N8P
2	J	200	ACO	C5P-C6P-C7P-N8P
2	C	200	ACO	O9P-C9P-CAP-OAP
2	G	200	ACO	O9P-C9P-CAP-OAP
2	J	200	ACO	CDP-CBP-CCP-O6A
2	J	200	ACO	C4B-C3B-O3B-P3B
3	A	201	COA	C2B-C3B-O3B-P3B
2	J	200	ACO	OAP-CAP-CBP-CEP
3	A	201	COA	OAP-CAP-CBP-CDP
3	A	201	COA	OAP-CAP-CBP-CEP
2	G	200	ACO	P1A-O3A-P2A-O4A
2	C	200	ACO	O9P-C9P-CAP-CBP
3	A	201	COA	O9P-C9P-CAP-CBP
2	H	200	ACO	C4B-C5B-O5B-P1A
2	C	200	ACO	N8P-C9P-CAP-CBP

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Mol	Chain	Res	Type	Atoms
2	F	200	ACO	N8P-C9P-CAP-CBP
2	I	200	ACO	P1A-O3A-P2A-O6A
2	H	200	ACO	P2A-O3A-P1A-O5B
2	E	200	ACO	P1A-O3A-P2A-O6A
2	G	200	ACO	N8P-C9P-CAP-OAP
2	H	200	ACO	C3B-O3B-P3B-O7A
2	J	200	ACO	C3B-O3B-P3B-O7A
2	H	200	ACO	C5P-C6P-C7P-N8P
2	G	200	ACO	C5B-O5B-P1A-O3A
2	E	200	ACO	C5B-O5B-P1A-O3A
2	E	200	ACO	CCP-O6A-P2A-O3A
2	C	200	ACO	P2A-O3A-P1A-O2A
3	A	201	COA	P1A-O3A-P2A-O4A
3	A	201	COA	CBP-CCP-O6A-P2A
2	J	200	ACO	OAP-CAP-CBP-CCP
3	A	201	COA	OAP-CAP-CBP-CCP
2	E	200	ACO	O9P-C9P-CAP-OAP
2	H	200	ACO	O4B-C4B-C5B-O5B
2	F	200	ACO	CDP-CBP-CCP-O6A
2	F	200	ACO	CEP-CBP-CCP-O6A
2	J	200	ACO	CEP-CBP-CCP-O6A
3	A	201	COA	O4B-C4B-C5B-O5B
2	H	200	ACO	O9P-C9P-N8P-C7P
2	J	200	ACO	C4B-C5B-O5B-P1A
2	J	200	ACO	CAP-C9P-N8P-C7P
2	F	200	ACO	O9P-C9P-CAP-CBP
3	A	201	COA	C4B-C3B-O3B-P3B
2	G	200	ACO	S1P-C2P-C3P-N4P
2	E	200	ACO	C2P-C3P-N4P-C5P
3	A	201	COA	N8P-C9P-CAP-CBP
2	H	200	ACO	C4B-C3B-O3B-P3B
2	I	200	ACO	P1A-O3A-P2A-O4A
2	I	200	ACO	O9P-C9P-CAP-OAP
2	F	200	ACO	C3B-O3B-P3B-O7A
3	A	201	COA	C3B-O3B-P3B-O7A
2	J	200	ACO	C9P-CAP-CBP-CEP
2	C	200	ACO	CCP-O6A-P2A-O3A
2	G	200	ACO	CCP-O6A-P2A-O3A
2	I	200	ACO	C5B-O5B-P1A-O3A
2	F	200	ACO	C3B-O3B-P3B-O8A
2	F	200	ACO	C5B-O5B-P1A-O3A
2	J	200	ACO	C5B-O5B-P1A-O3A

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Mol	Chain	Res	Type	Atoms
2	J	200	ACO	CCP-O6A-P2A-O3A
3	A	201	COA	C3B-O3B-P3B-O8A
3	A	201	COA	C3B-O3B-P3B-O9A
2	C	200	ACO	P2A-O3A-P1A-O1A
2	G	200	ACO	P1A-O3A-P2A-O5A
2	E	200	ACO	P1A-O3A-P2A-O4A
2	I	200	ACO	C5B-O5B-P1A-O2A
2	J	200	ACO	CCP-O6A-P2A-O5A
3	A	201	COA	C5B-O5B-P1A-O1A
2	H	200	ACO	O9P-C9P-CAP-CBP
2	J	200	ACO	C9P-CAP-CBP-CCP

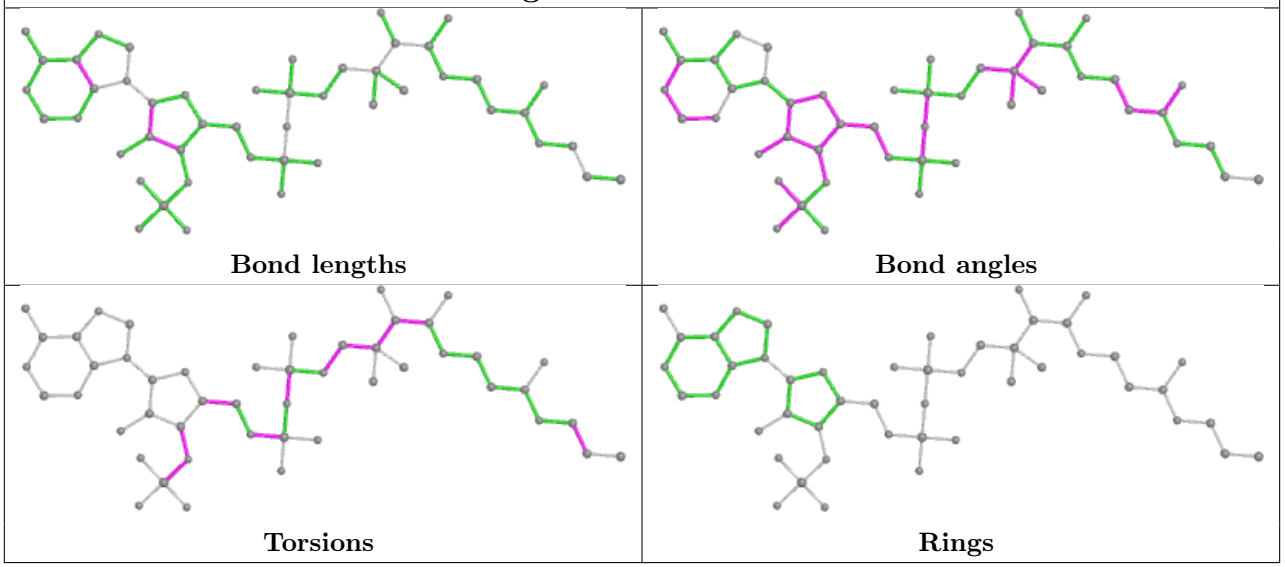
There are no ring outliers.

8 monomers are involved in 151 short contacts:

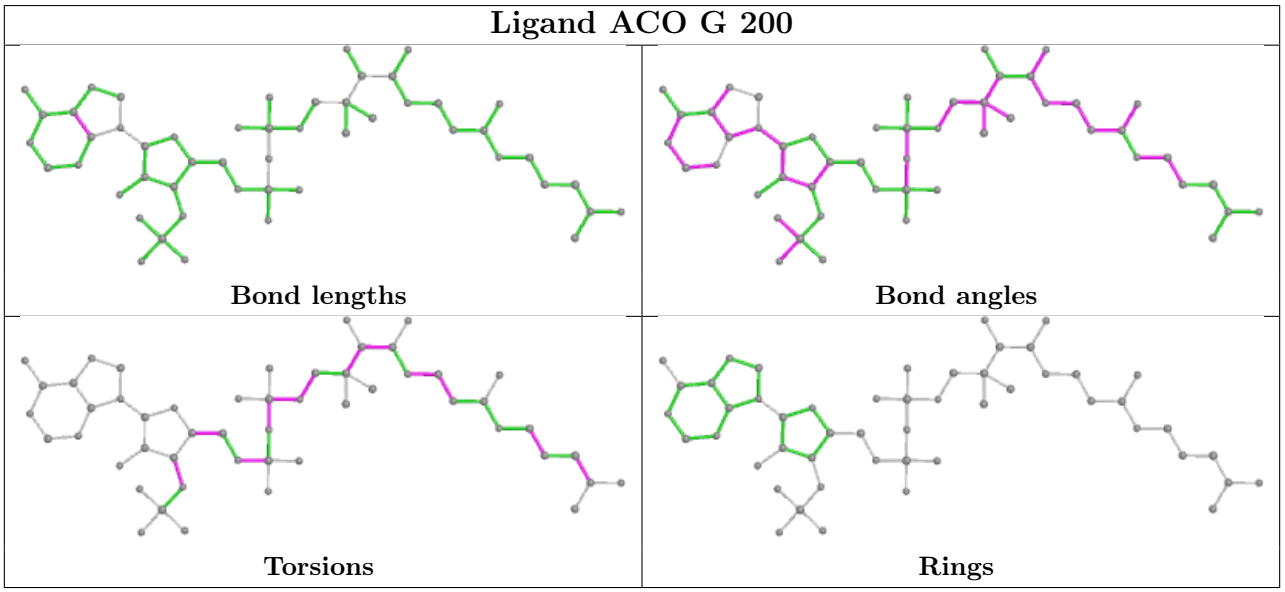
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	201	COA	21	0
2	G	200	ACO	15	0
2	C	200	ACO	18	0
2	E	200	ACO	15	0
2	H	200	ACO	37	0
2	I	200	ACO	20	0
2	J	200	ACO	19	0
2	F	200	ACO	6	0

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.

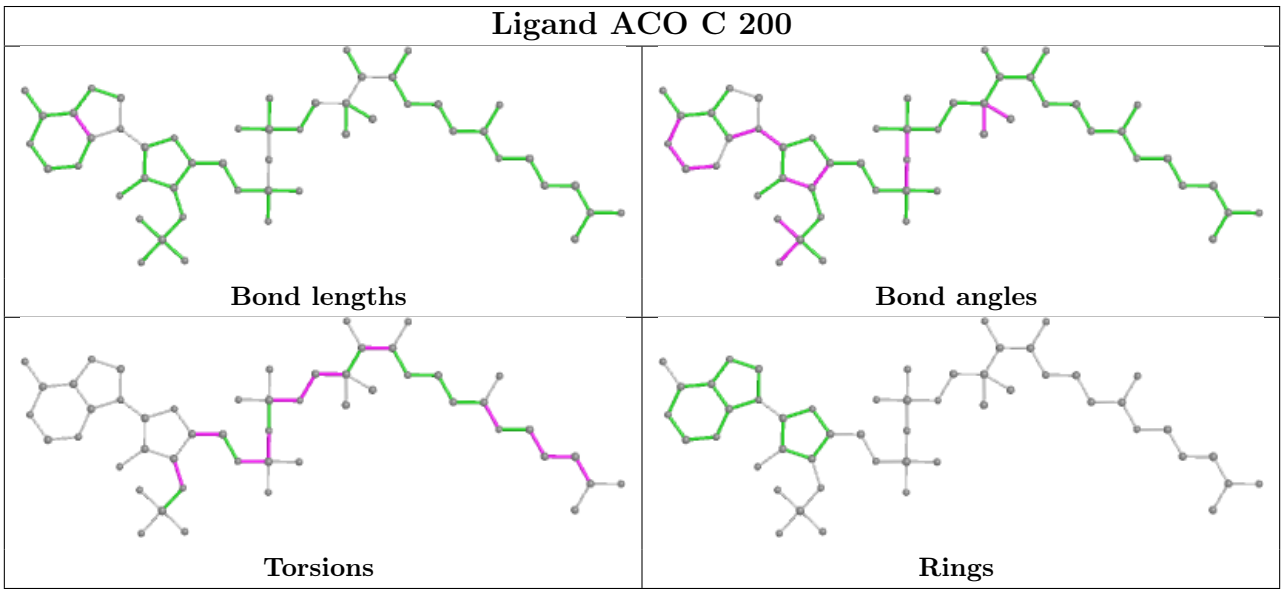
Ligand COA A 201



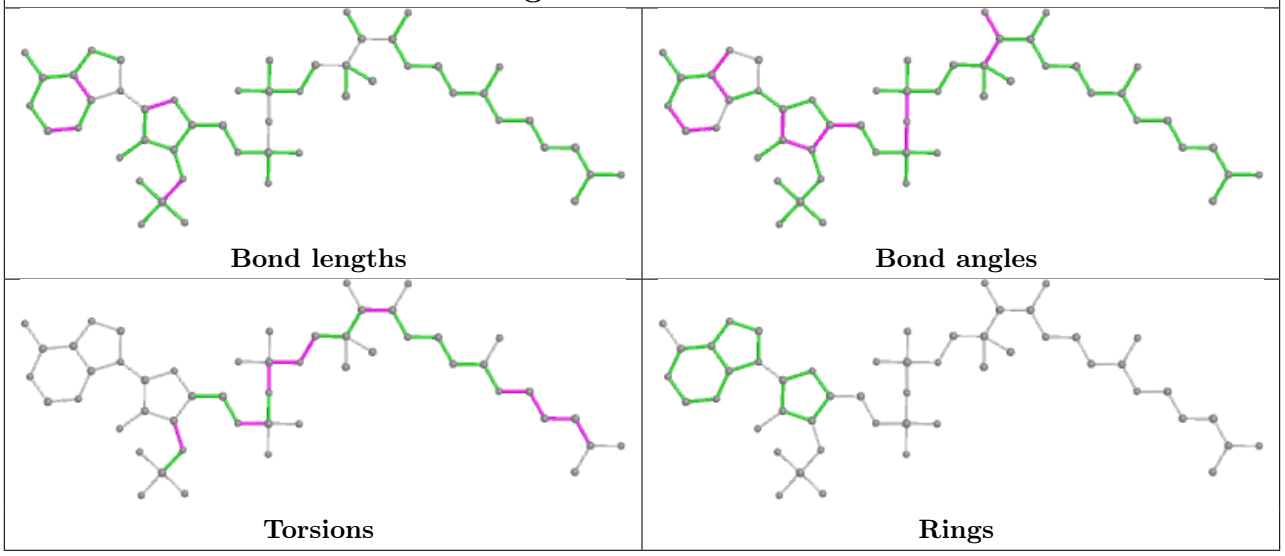
Ligand ACO G 200



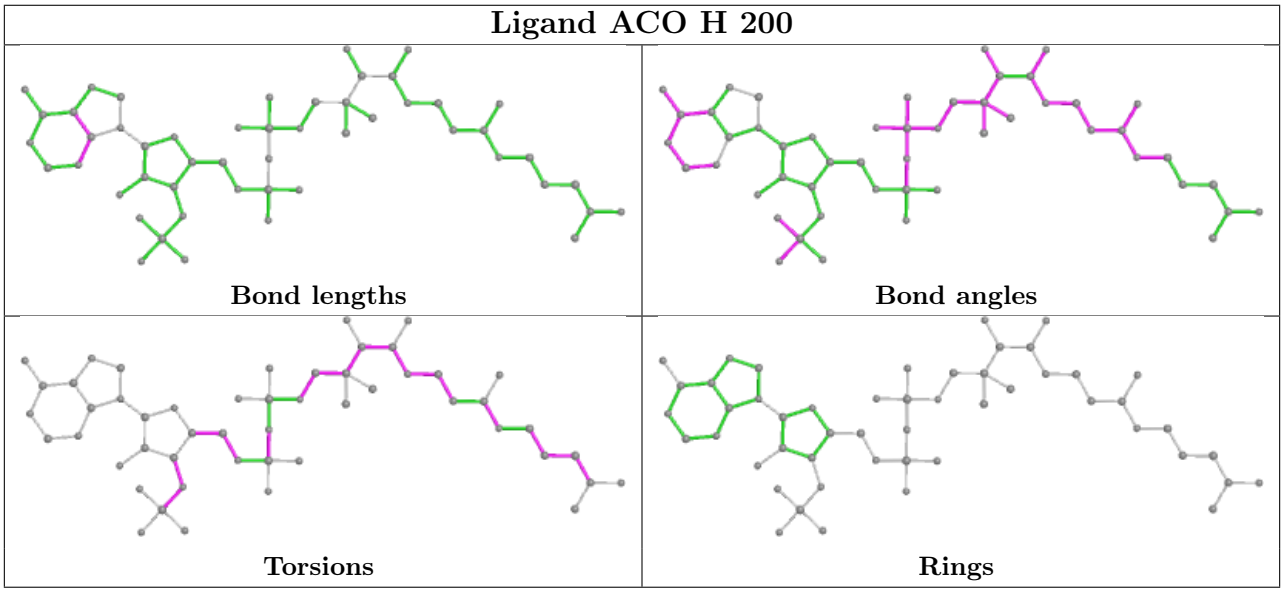
Ligand ACO C 200



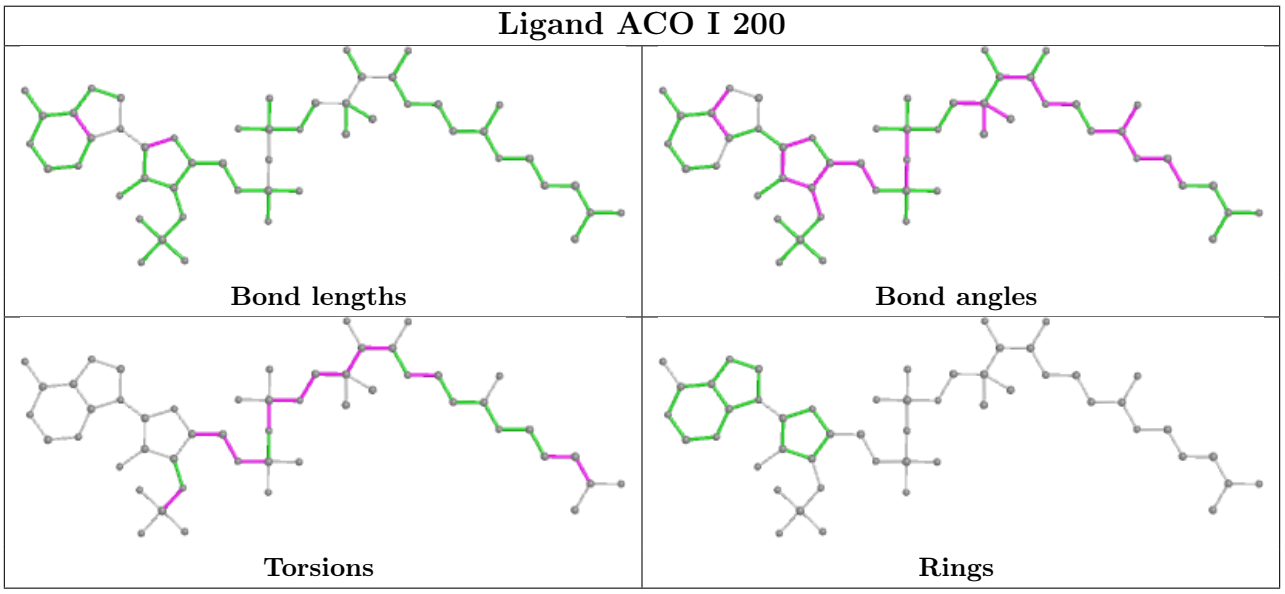
Ligand ACO E 200



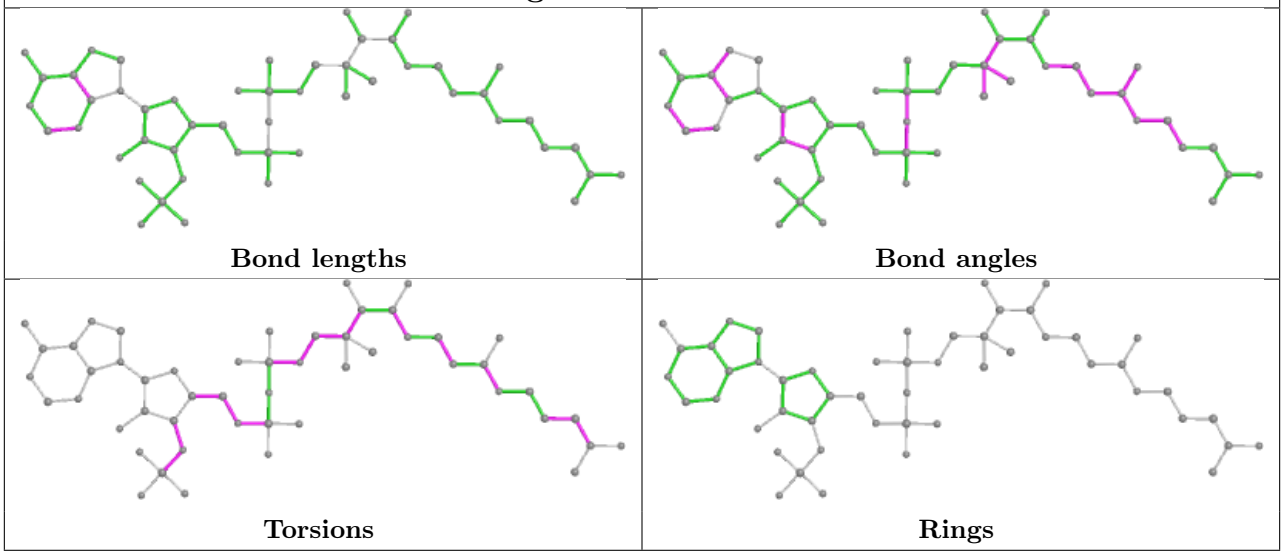
Ligand ACO H 200



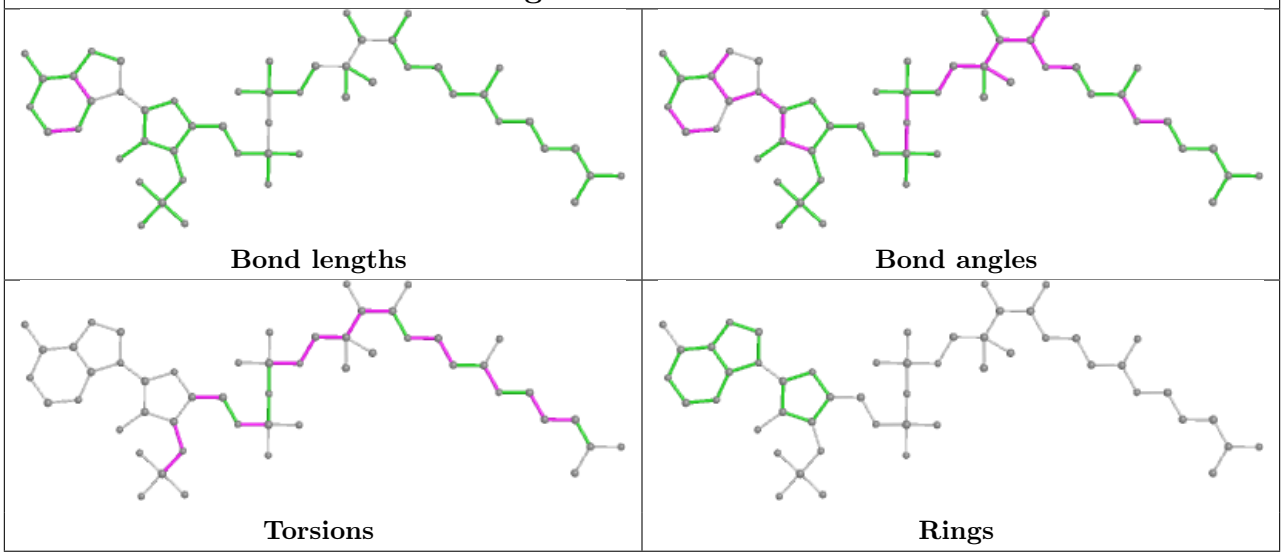
Ligand ACO I 200



Ligand ACO J 200



Ligand ACO F 200



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å^2)	Q<0.9
1	A	154/162 (95%)	-0.20	0 100 100	50, 77, 119, 138	0
1	B	148/162 (91%)	-0.14	1 (0%) 87 89	66, 91, 130, 142	0
1	C	153/162 (94%)	-0.12	0 100 100	56, 82, 113, 142	0
1	D	147/162 (90%)	-0.36	0 100 100	55, 79, 105, 132	0
1	E	151/162 (93%)	0.07	1 (0%) 87 89	61, 92, 130, 161	0
1	F	150/162 (92%)	-0.12	0 100 100	50, 80, 116, 141	0
1	G	154/162 (95%)	-0.22	0 100 100	60, 78, 110, 135	0
1	H	153/162 (94%)	-0.05	3 (1%) 65 64	56, 81, 111, 127	0
1	I	151/162 (93%)	-0.13	0 100 100	53, 80, 110, 137	0
1	J	151/162 (93%)	0.04	0 100 100	60, 88, 112, 139	0
1	K	149/162 (91%)	-0.12	0 100 100	61, 87, 122, 162	0
1	L	149/162 (91%)	-0.35	0 100 100	53, 81, 119, 135	0
1	M	148/162 (91%)	-0.03	1 (0%) 87 89	47, 73, 115, 148	0
1	N	148/162 (91%)	0.45	5 (3%) 45 43	58, 102, 139, 175	0
1	O	149/162 (91%)	-0.07	0 100 100	59, 83, 118, 153	0
1	P	147/162 (90%)	0.18	3 (2%) 65 64	66, 112, 150, 166	0
All	All	2402/2592 (92%)	-0.07	14 (0%) 89 90	47, 84, 128, 175	0

All (14) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	N	16	PHE	3.2
1	H	34	GLU	2.9
1	M	155	LEU	2.6
1	H	136	MET	2.6
1	N	54	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	N	17	SER	2.4
1	P	55	TYR	2.3
1	H	121	GLU	2.3
1	P	85	ARG	2.3
1	P	155	LEU	2.2
1	E	103	CYS	2.2
1	N	58	ALA	2.2
1	N	64	PHE	2.2
1	B	10	ALA	2.1

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

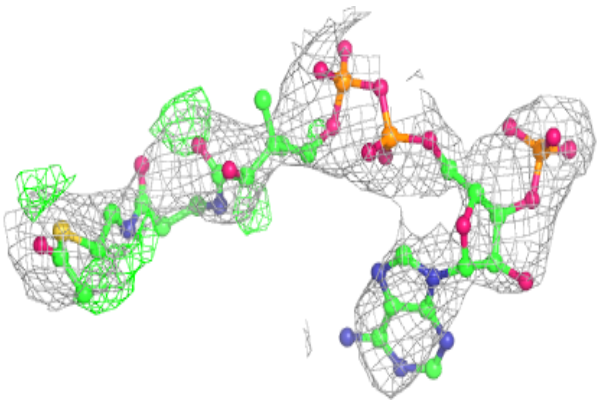
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

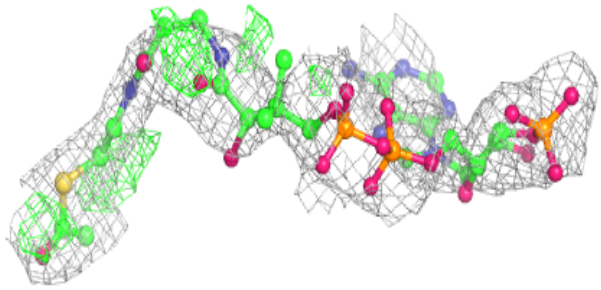
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	ACO	E	200	51/51	0.85	0.30	70,95,127,137	51
2	ACO	F	200	51/51	0.88	0.32	66,90,142,145	51
3	COA	A	201	48/48	0.88	0.31	55,94,114,124	48
2	ACO	C	200	51/51	0.90	0.27	61,77,98,107	51
2	ACO	G	200	51/51	0.91	0.26	59,71,112,113	51
2	ACO	J	200	51/51	0.91	0.26	53,73,111,123	51
2	ACO	H	200	51/51	0.92	0.24	50,70,100,104	51
2	ACO	I	200	51/51	0.93	0.28	51,70,118,122	51

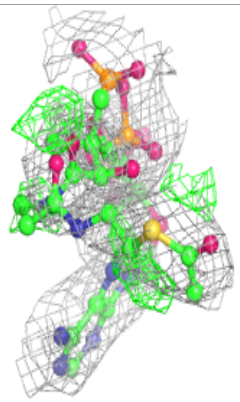
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACO E 200:

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

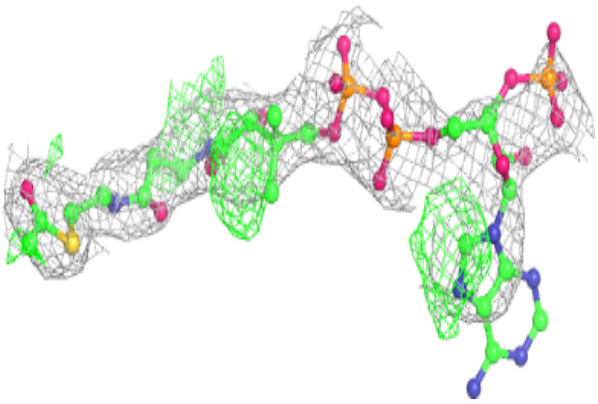


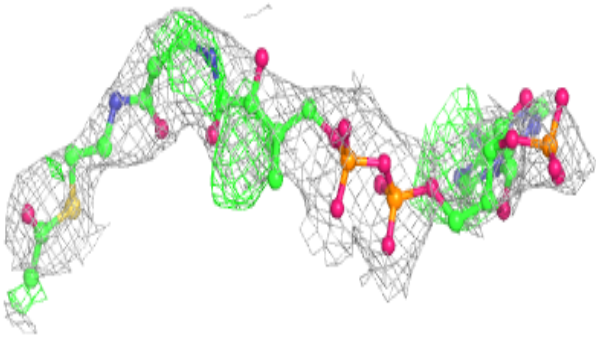


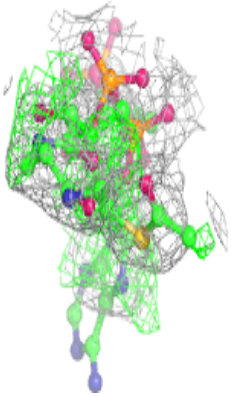


Electron density around ACO F 200:

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

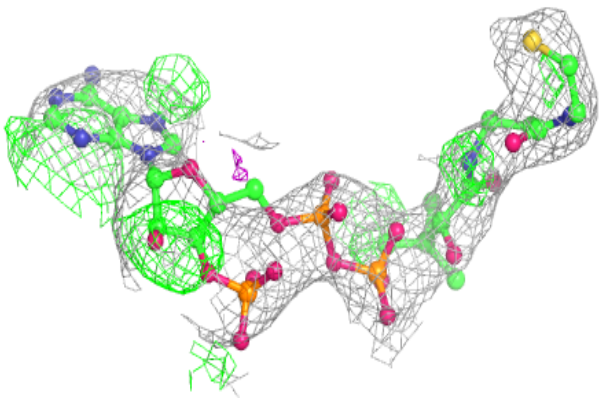


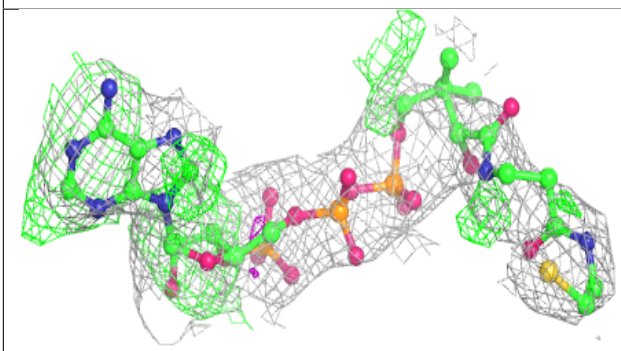


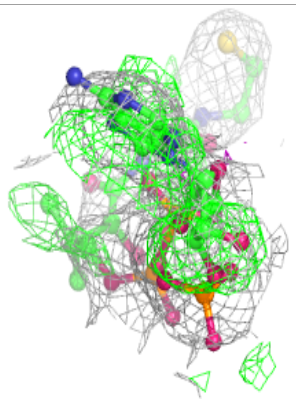


Electron density around COA A 201:

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

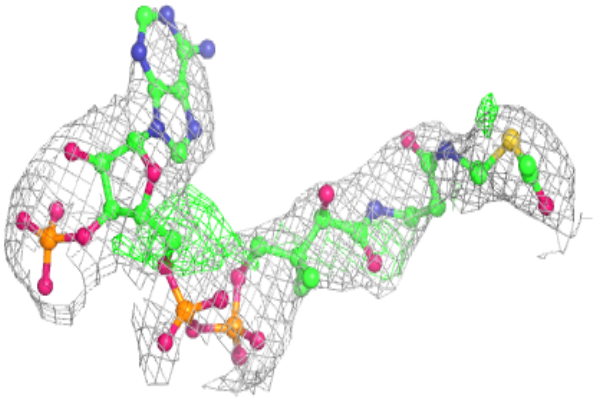


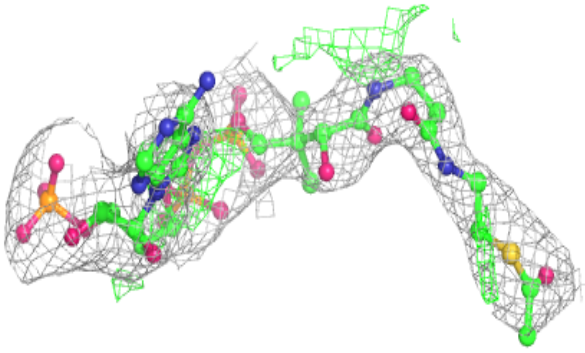


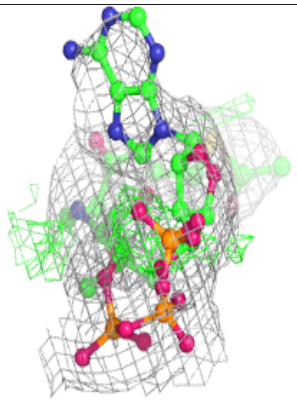


Electron density around ACO C 200:

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

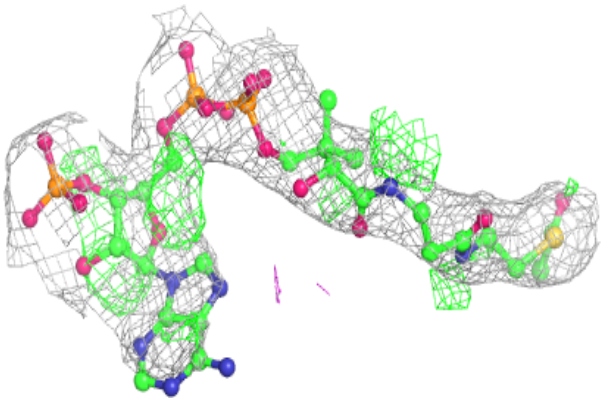


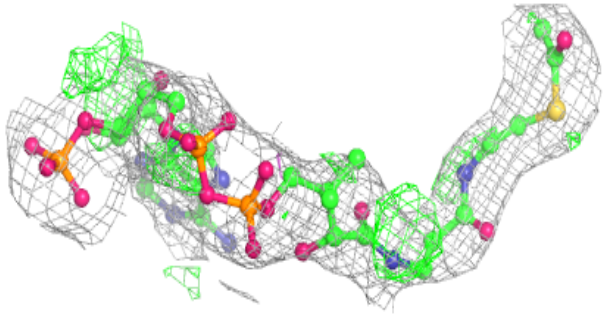


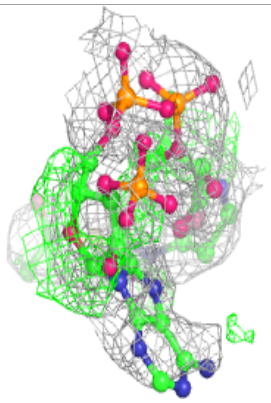


Electron density around ACO G 200:

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

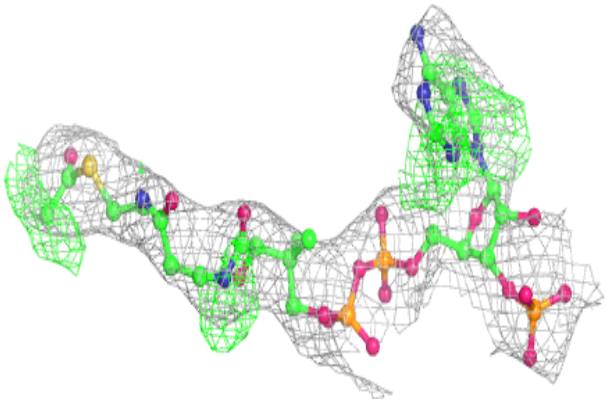


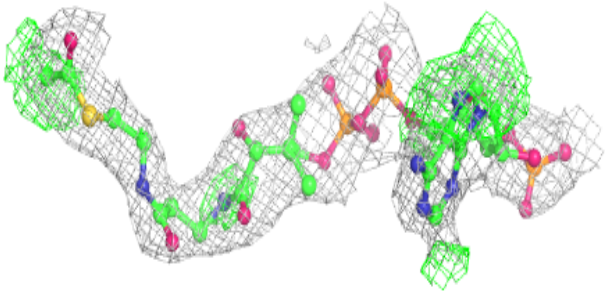


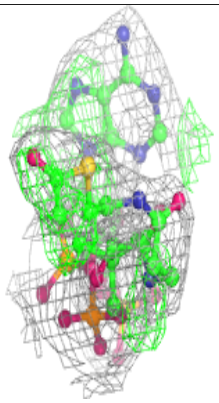


Electron density around ACO J 200:

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

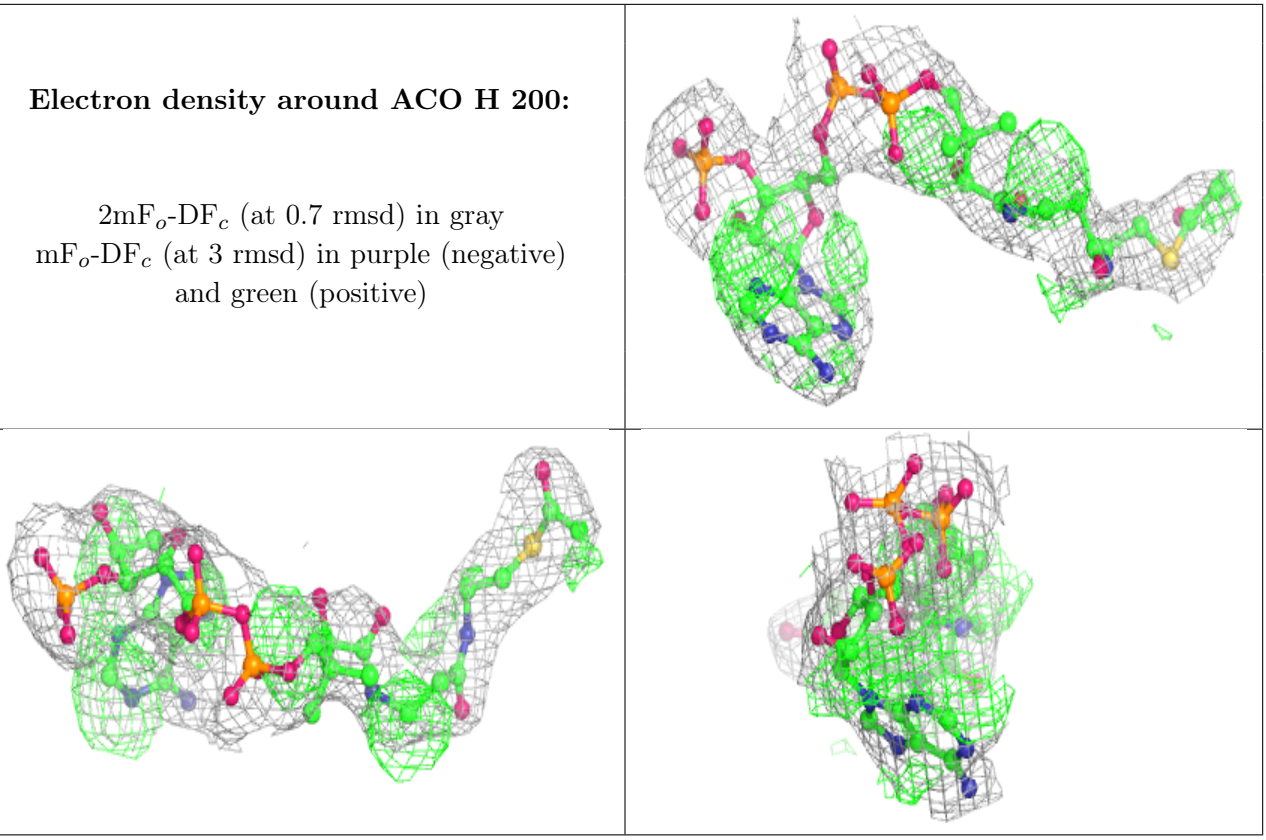






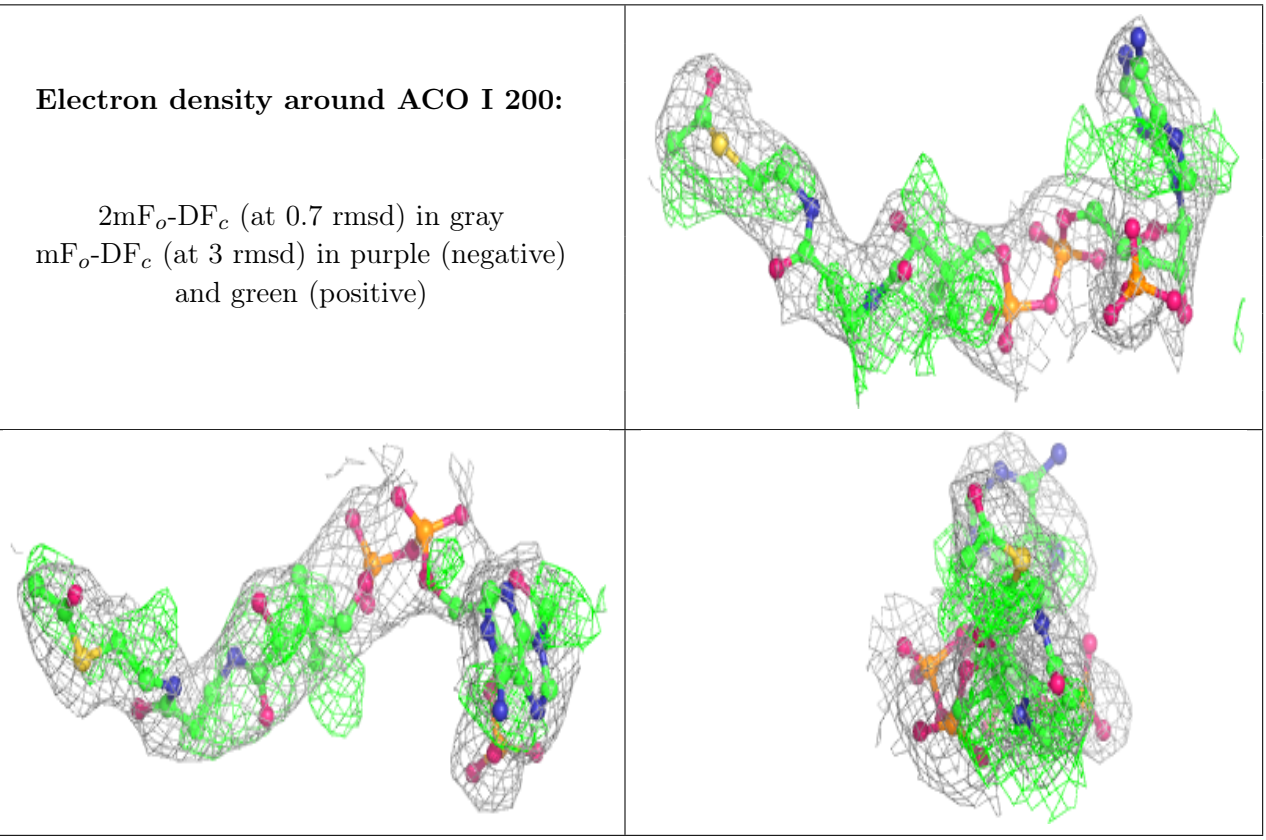
Electron density around ACO H 200:

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



Electron density around ACO I 200:

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



6.5 Other polymers (i)

There are no such residues in this entry.