Full wwPDB X-ray Structure Validation Report (i)

Aug 30, 2023 – 10:24 AM EDT

PDB ID	:	3NZ2
Title	:	Crystal Structure of Hexapeptide-Repeat containing-Acetyltransferase VCA0836 Complexed with Acetyl Co Enzyme A from Vibrio cholerae O1 biovar eltor
Authors	:	Kim, Y.; Maltseva, N.; Hasseman, J.; Anderson, W.F.; Joachimiak, A.; Center for Structural Genomics of Infectious Diseases (CSGID)
Deposited on	:	2010-07-15
Resolution	:	2.35 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 (1)) were used in the production of this report:

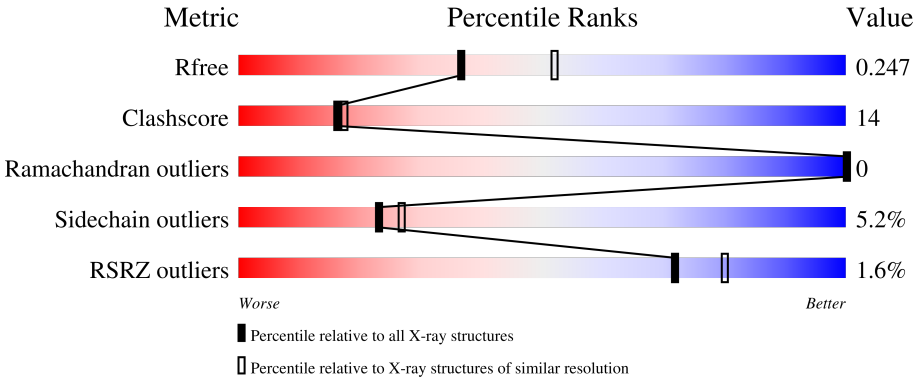
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.35 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	1164 (2.36-2.36)
Clashscore	141614	1232 (2.36-2.36)
Ramachandran outliers	138981	1211 (2.36-2.36)
Sidechain outliers	138945	1212 (2.36-2.36)
RSRZ outliers	127900	1150 (2.36-2.36)

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	195	75% 17% • 7%
1	B	195	2% 71% 23% 6%
1	C	195	% 63% 27% • 6%
1	D	195	4% 62% 28% 5% 6%
1	E	195	3% 76% 16% • 6%

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Mol	Chain	Length	Quality of chain
1	F	195	4% 70% 23% 6%
1	G	195	71% 20% 7%
1	H	195	3% 69% 24% 6%
1	I	195	67% 25% 6%
1	J	195	72% 22% 5%
1	K	195	68% 24% 6%
1	L	195	69% 23% 6%

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
3	ACY	K	198	-	-	X	-
4	GOL	E	196	-	-	X	-

2 Entry composition (i)

There are 8 unique types of molecules in this entry. The entry contains 18822 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 Hexapeptide-repeat containing-acetyltransferase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	Se	0	1	0
			1420	891	257	265	3	4			
1	B	184	Total	C	N	O	S	Se	0	1	0
			1437	902	260	267	3	5			
1	C	183	Total	C	N	O	S	Se	0	0	0
			1417	889	254	267	3	4			
1	D	183	Total	C	N	O	S	Se	0	1	0
			1431	900	256	268	3	4			
1	E	183	Total	C	N	O	S	Se	0	1	0
			1428	895	258	268	3	4			
1	F	183	Total	C	N	O	S	Se	0	0	0
			1417	889	254	267	3	4			
1	G	182	Total	C	N	O	S	Se	0	1	0
			1418	890	254	267	3	4			
1	H	183	Total	C	N	O	S	Se	0	1	0
			1428	895	258	268	3	4			
1	I	184	Total	C	N	O	S	Se	0	1	0
			1437	901	260	269	3	4			
1	J	185	Total	C	N	O	S	Se	0	0	0
			1431	899	257	267	3	5			
1	K	183	Total	C	N	O	S	Se	0	0	0
			1417	889	254	267	3	4			
1	L	183	Total	C	N	O	S	Se	0	1	0
			1428	895	258	268	3	4			

There are 48 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	SER	-	expression tag	UNP Q9KLB0
A	-1	ASN	-	expression tag	UNP Q9KLB0
A	0	ALA	-	expression tag	UNP Q9KLB0
A	1	MSE	-	expression tag	UNP Q9KLB0
B	-2	SER	-	expression tag	UNP Q9KLB0

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-1	ASN	-	expression tag	UNP Q9KLB0
B	0	ALA	-	expression tag	UNP Q9KLB0
B	1	MSE	-	expression tag	UNP Q9KLB0
C	-2	SER	-	expression tag	UNP Q9KLB0
C	-1	ASN	-	expression tag	UNP Q9KLB0
C	0	ALA	-	expression tag	UNP Q9KLB0
C	1	MSE	-	expression tag	UNP Q9KLB0
D	-2	SER	-	expression tag	UNP Q9KLB0
D	-1	ASN	-	expression tag	UNP Q9KLB0
D	0	ALA	-	expression tag	UNP Q9KLB0
D	1	MSE	-	expression tag	UNP Q9KLB0
E	-2	SER	-	expression tag	UNP Q9KLB0
E	-1	ASN	-	expression tag	UNP Q9KLB0
E	0	ALA	-	expression tag	UNP Q9KLB0
E	1	MSE	-	expression tag	UNP Q9KLB0
F	-2	SER	-	expression tag	UNP Q9KLB0
F	-1	ASN	-	expression tag	UNP Q9KLB0
F	0	ALA	-	expression tag	UNP Q9KLB0
F	1	MSE	-	expression tag	UNP Q9KLB0
G	-2	SER	-	expression tag	UNP Q9KLB0
G	-1	ASN	-	expression tag	UNP Q9KLB0
G	0	ALA	-	expression tag	UNP Q9KLB0
G	1	MSE	-	expression tag	UNP Q9KLB0
H	-2	SER	-	expression tag	UNP Q9KLB0
H	-1	ASN	-	expression tag	UNP Q9KLB0
H	0	ALA	-	expression tag	UNP Q9KLB0
H	1	MSE	-	expression tag	UNP Q9KLB0
I	-2	SER	-	expression tag	UNP Q9KLB0
I	-1	ASN	-	expression tag	UNP Q9KLB0
I	0	ALA	-	expression tag	UNP Q9KLB0
I	1	MSE	-	expression tag	UNP Q9KLB0
J	-2	SER	-	expression tag	UNP Q9KLB0
J	-1	ASN	-	expression tag	UNP Q9KLB0
J	0	ALA	-	expression tag	UNP Q9KLB0
J	1	MSE	-	expression tag	UNP Q9KLB0
K	-2	SER	-	expression tag	UNP Q9KLB0
K	-1	ASN	-	expression tag	UNP Q9KLB0
K	0	ALA	-	expression tag	UNP Q9KLB0
K	1	MSE	-	expression tag	UNP Q9KLB0
L	-2	SER	-	expression tag	UNP Q9KLB0
L	-1	ASN	-	expression tag	UNP Q9KLB0
L	0	ALA	-	expression tag	UNP Q9KLB0

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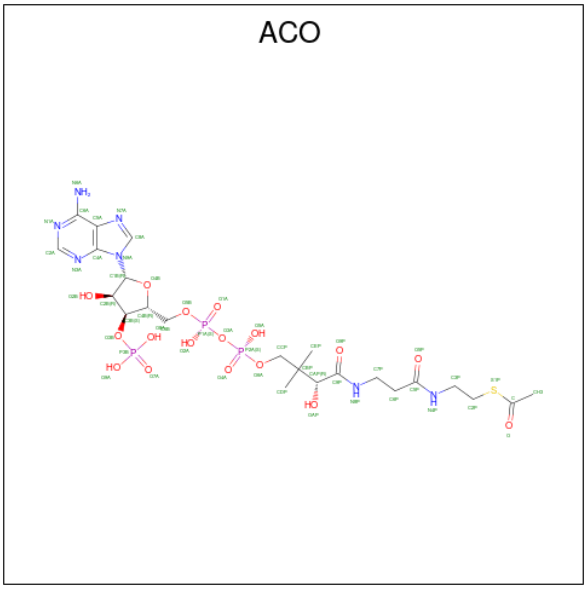
Chain	Residue	Modelled	Actual	Comment	Reference
L	1	MSE	-	expression tag	UNP Q9KLB0

- 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	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	A	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	C	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	D	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		
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	I	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	J	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		
2	L	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

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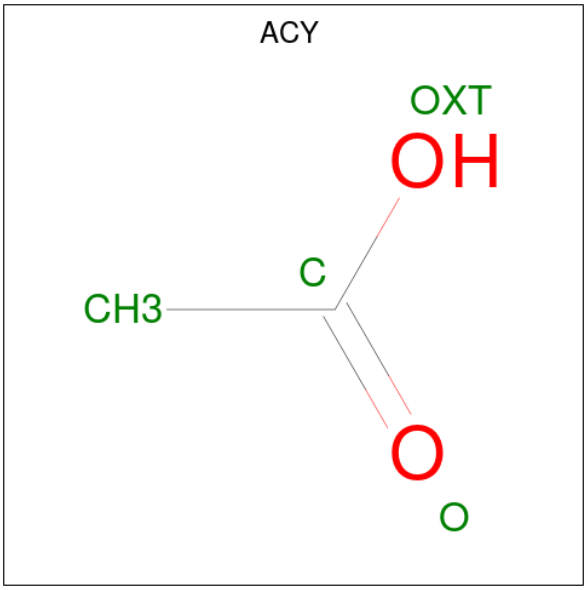
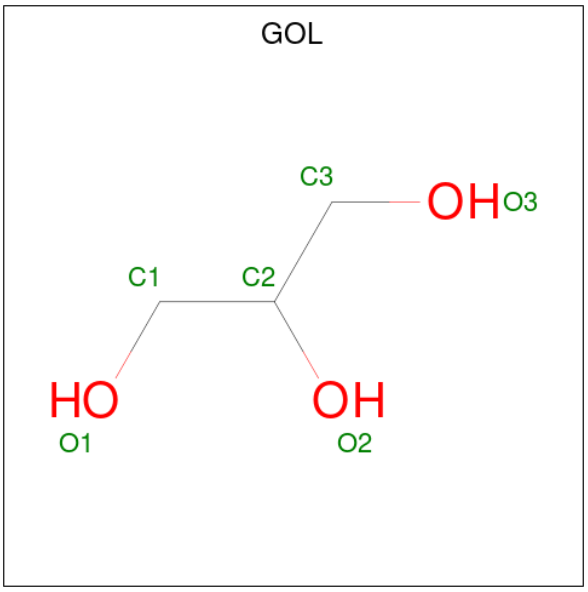
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	L	1	Total	C	N	O	P	S	0	0
			51	23	7	17	3	1		

- Molecule 3 is ACETIC ACID (three-letter code: ACY) (formula: $C_2H_4O_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O		0	0
			4	2	2			
3	A	1	Total	C	O		0	0
			4	2	2			
3	B	1	Total	C	O		0	0
			4	2	2			
3	D	1	Total	C	O		0	0
			4	2	2			
3	F	1	Total	C	O		0	0
			4	2	2			
3	G	1	Total	C	O		0	0
			4	2	2			
3	I	1	Total	C	O		0	0
			4	2	2			
3	K	1	Total	C	O		0	0
			4	2	2			
3	K	1	Total	C	O		0	0
			4	2	2			

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 6 3 3	0	0
4	E	1	Total C O 6 3 3	0	0
4	F	1	Total C O 6 3 3	0	0
4	L	1	Total C O 6 3 3	0	0

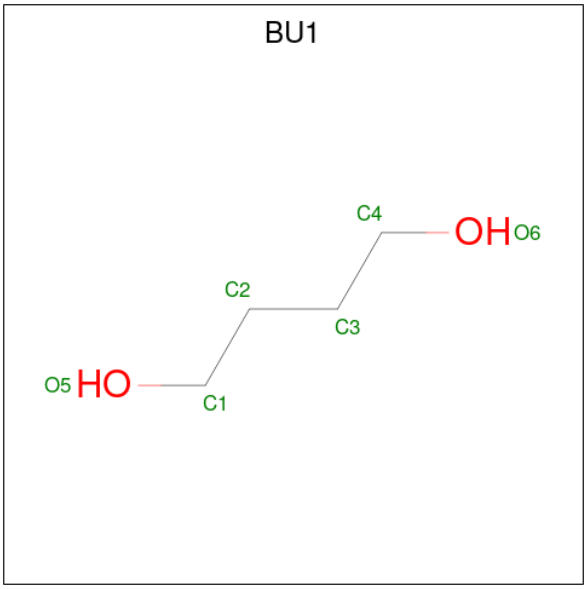
- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Cl 1 1	0	0
5	C	1	Total Cl 1 1	0	0
5	E	1	Total Cl 1 1	0	0
5	H	1	Total Cl 1 1	0	0
5	J	1	Total Cl 1 1	0	0

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total Mg 2 2	0	1

- Molecule 7 is 1,4-BUTANEDIOL (three-letter code: BU1) (formula: $C_4H_{10}O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	G	1	Total C O 6 4 2	0	0
7	K	1	Total C O 6 4 2	0	0

- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	98	Total O 98 98	0	0
8	B	88	Total O 88 88	0	0
8	C	80	Total O 80 80	0	0
8	D	66	Total O 66 66	0	0
8	E	97	Total O 97 97	0	0
8	F	93	Total O 93 93	0	0
8	G	69	Total O 69 69	0	0

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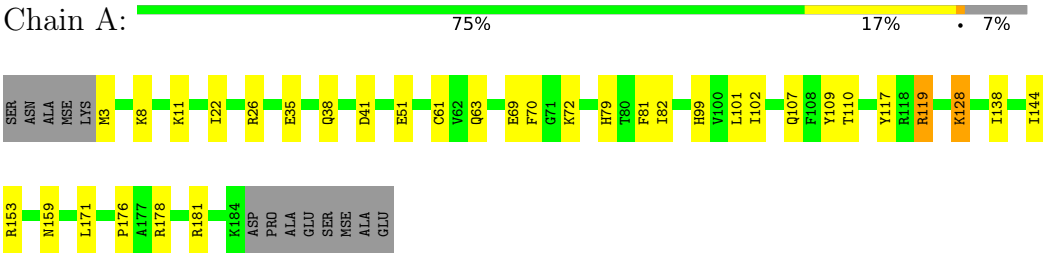
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	H	75	Total O 75 75	0	0
8	I	80	Total O 80 80	0	0
8	J	87	Total O 87 87	0	0
8	K	92	Total O 92 92	0	0
8	L	97	Total O 97 97	0	0

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.

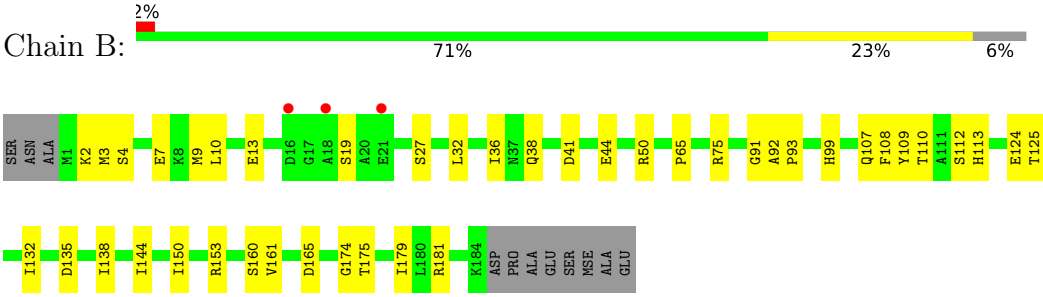
• Molecule 1: Hexapeptide-repeat containing-acetyltransferase

Chain A:



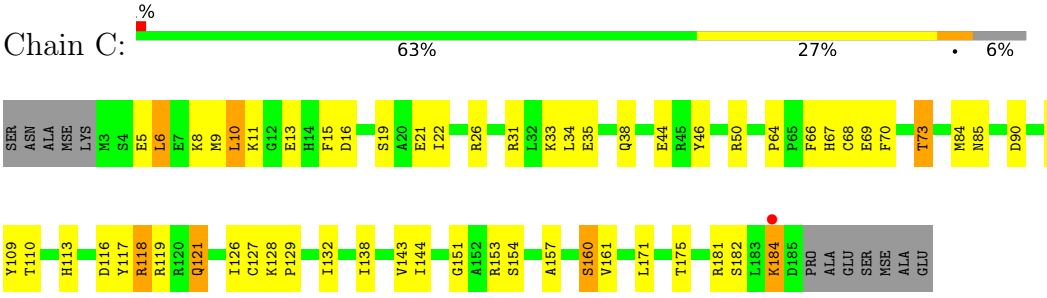
• Molecule 1: Hexapeptide-repeat containing-acetyltransferase

Chain B:



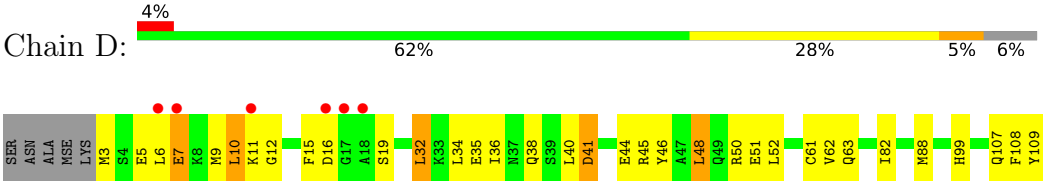
• Molecule 1: Hexapeptide-repeat containing-acetyltransferase

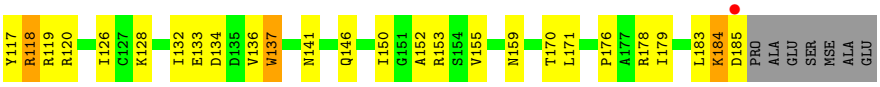
Chain C:



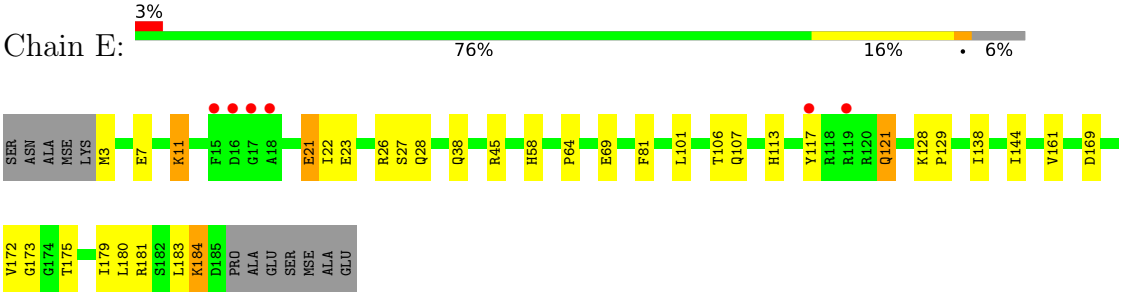
• Molecule 1: Hexapeptide-repeat containing-acetyltransferase

Chain D:

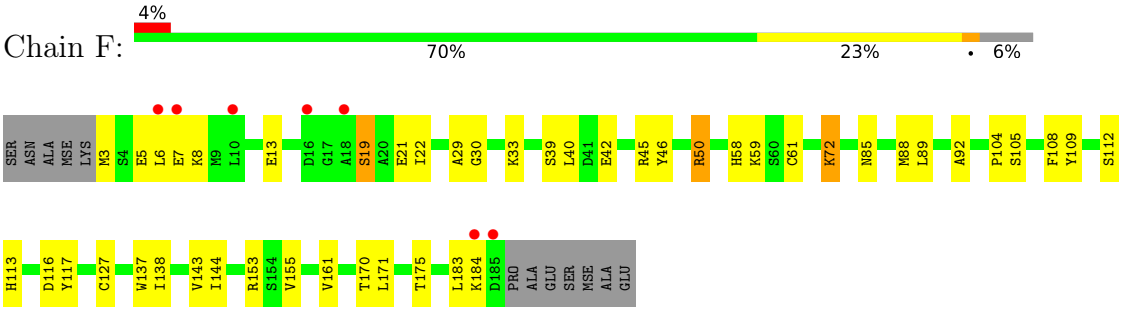




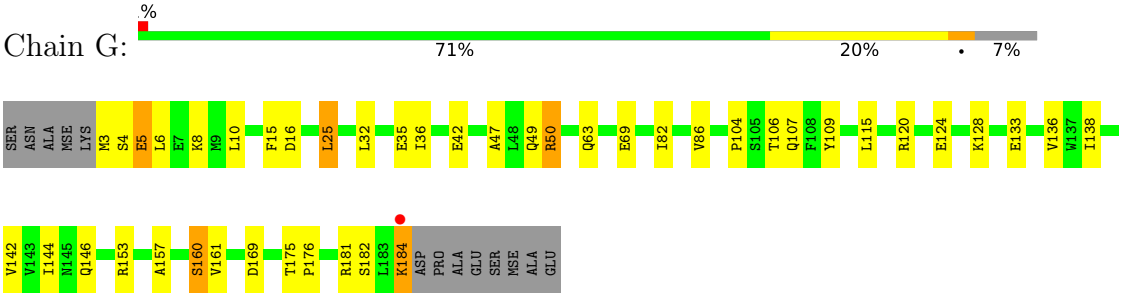
• Molecule 1: Hexapeptide-repeat containing-acetyltransferase



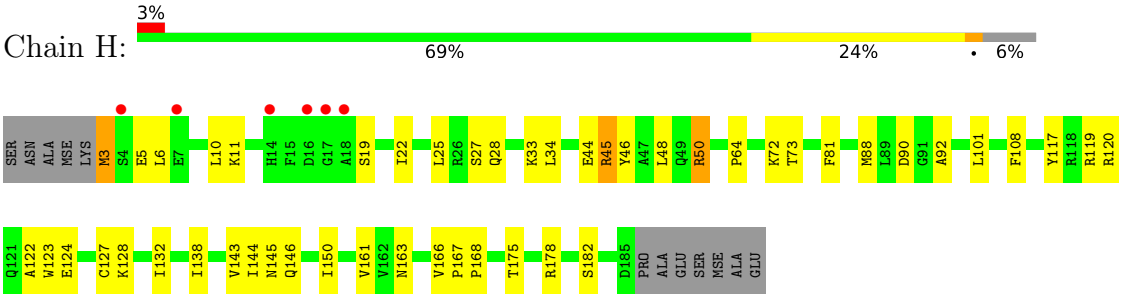
• Molecule 1: Hexapeptide-repeat containing-acetyltransferase



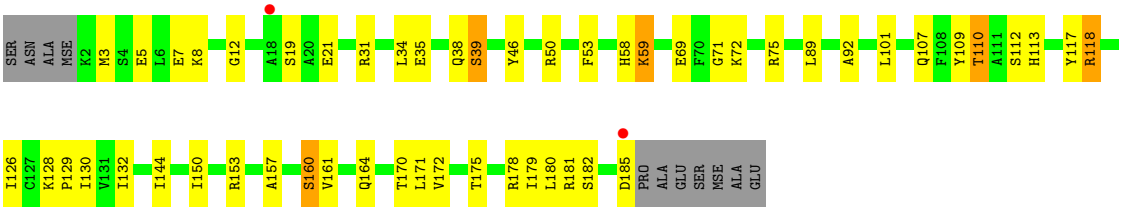
• Molecule 1: Hexapeptide-repeat containing-acetyltransferase



• Molecule 1: Hexapeptide-repeat containing-acetyltransferase

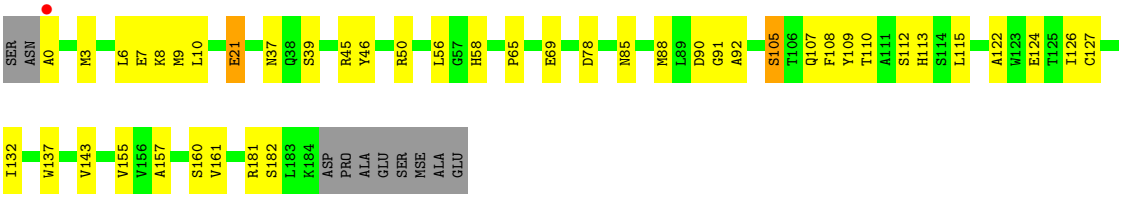


• Molecule 1: Hexapeptide-repeat containing-acetyltransferase



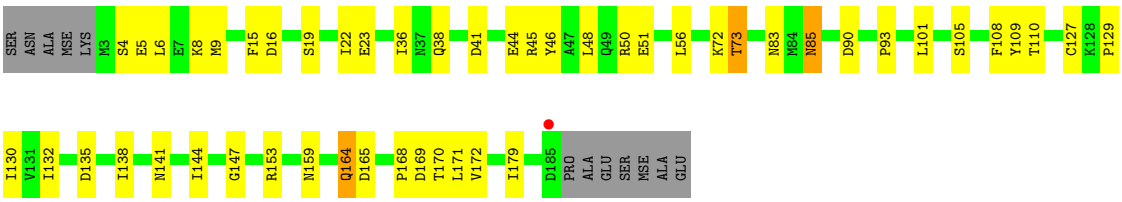
• Molecule 1: Hexapeptide-repeat containing-acetyltransferase

Chain J:



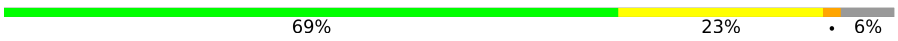
• Molecule 1: Hexapeptide-repeat containing-acetyltransferase

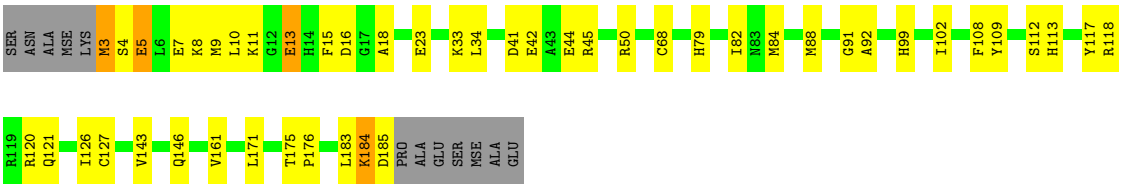
Chain K:



• Molecule 1: Hexapeptide-repeat containing-acetyltransferase

Chain L:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	77.32Å 135.80Å 120.53Å 90.00° 91.77° 90.00°	Depositor
Resolution (Å)	46.63 – 2.35 46.63 – 2.35	Depositor EDS
% Data completeness (in resolution range)	96.9 (46.63-2.35) 97.0 (46.63-2.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.18	Depositor
$< I/\sigma(I) >$ [1]	2.16 (at 2.34Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.2_432)	Depositor
R, R_{free}	0.188 , 0.253 0.182 , 0.247	Depositor DCC
R_{free} test set	5025 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å^2)	25.0	Xtriage
Anisotropy	0.767	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 57.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.056 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	18822	wwPDB-VP
Average B, all atoms (Å^2)	29.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 46.23 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.1800e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: CL, ACO, BU1, ACY, MG, GOL

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	0.61	0/1444	0.69	0/1950
1	B	0.64	0/1460	0.70	0/1968
1	C	0.60	0/1441	0.68	0/1947
1	D	0.58	0/1457	0.67	0/1970
1	E	0.66	0/1452	0.67	0/1961
1	F	0.59	0/1441	0.65	0/1947
1	G	0.61	0/1442	0.69	0/1948
1	H	0.61	0/1452	0.74	0/1961
1	I	0.64	0/1460	0.69	0/1969
1	J	0.63	0/1453	0.74	1/1958 (0.1%)
1	K	0.59	0/1441	0.67	0/1947
1	L	0.64	0/1452	0.70	0/1961
All	All	0.62	0/17395	0.69	1/23487 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	90	ASP	CB-CG-OD1	5.20	122.98	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1420	0	1416	32	0
1	B	1437	0	1441	35	0
1	C	1417	0	1407	57	0
1	D	1431	0	1417	74	0
1	E	1428	0	1420	44	0
1	F	1417	0	1408	37	0
1	G	1418	0	1409	33	0
1	H	1428	0	1420	44	0
1	I	1437	0	1433	42	0
1	J	1431	0	1434	33	0
1	K	1417	0	1408	42	0
1	L	1428	0	1420	43	0
2	A	102	0	68	17	0
2	C	51	0	34	5	0
2	D	51	0	34	2	0
2	E	51	0	34	4	0
2	F	51	0	34	11	0
2	H	51	0	34	2	0
2	I	102	0	68	8	0
2	J	51	0	34	6	0
2	L	102	0	68	6	1
3	A	8	0	6	1	0
3	B	4	0	3	0	0
3	D	4	0	3	0	0
3	F	4	0	3	0	0
3	G	4	0	3	1	0
3	I	4	0	3	0	0
3	K	8	0	6	2	0
4	B	6	0	8	1	0
4	E	6	0	8	4	0
4	F	6	0	8	1	0
4	L	6	0	8	3	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	E	1	0	0	0	0
5	H	1	0	0	0	0
5	J	1	0	0	0	0
6	C	2	0	0	0	0
7	G	6	0	10	2	0
7	K	6	0	10	0	0
8	A	98	0	0	4	0
8	B	88	0	0	9	0
8	C	80	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	66	0	0	5	0
8	E	97	0	0	8	0
8	F	93	0	0	5	0
8	G	69	0	0	3	0
8	H	75	0	0	4	0
8	I	80	0	0	3	1
8	J	87	0	0	1	0
8	K	92	0	0	2	0
8	L	97	0	0	2	0
All	All	18822	0	17520	507	1

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 14.

All (507) 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:E:3:MSE:HE2	1:E:7:GLU:OE2	1.26	1.28
2:F:195:ACO:HH33	8:F:646:HOH:O	1.39	1.20
1:E:45:ARG:HE	4:E:196:GOL:H11	0.93	1.09
1:I:92:ALA:H	1:I:110:THR:HG21	1.09	1.08
1:H:45[A]:ARG:HG2	1:H:45[A]:ARG:HH11	1.01	1.07
1:E:45:ARG:HE	4:E:196:GOL:C1	1.69	1.04
1:E:45:ARG:NE	4:E:196:GOL:H11	1.73	1.02
1:H:45[A]:ARG:HG2	1:H:45[A]:ARG:NH1	1.79	0.95
1:J:113:HIS:NE2	2:L:193:ACO:HH32	1.83	0.93
1:E:161:VAL:CG1	1:E:175:THR:HG23	1.99	0.93
1:E:11:LYS:O	1:E:11:LYS:HG3	1.69	0.90
1:D:184:LYS:O	1:D:185:ASP:HB2	1.69	0.90
1:E:3:MSE:CE	1:E:7:GLU:OE2	2.20	0.88
1:F:21:GLU:HB3	8:F:990:HOH:O	1.73	0.87
1:H:145:ASN:HD22	1:H:163:ASN:ND2	1.71	0.87
1:K:5:GLU:HG3	1:K:16:ASP:HB2	1.56	0.87
1:K:9:MSE:HE2	1:K:15:PHE:CE1	2.09	0.87
1:H:45[A]:ARG:HH11	1:H:45[A]:ARG:CG	1.89	0.85
2:A:195:ACO:O9P	2:A:195:ACO:H131	1.75	0.84
1:E:161:VAL:HG13	1:E:175:THR:HG23	1.60	0.83
1:I:113:HIS:NE2	2:I:195:ACO:HH32	1.94	0.82
1:E:161:VAL:HG13	1:E:175:THR:CG2	2.08	0.82
1:D:6:LEU:HD22	1:D:7:GLU:OE1	1.79	0.81
1:E:161:VAL:HG13	1:E:175:THR:OG1	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:5:GLU:HG3	1:L:16:ASP:H	1.44	0.80
1:I:170:THR:HG21	1:I:179:ILE:HD12	1.63	0.80
1:H:50:ARG:CG	1:H:50:ARG:HH11	1.95	0.79
1:I:92:ALA:N	1:I:110:THR:HG21	1.93	0.79
1:E:161:VAL:CG1	1:E:175:THR:CG2	2.59	0.79
1:L:3:MSE:HE1	1:L:11:LYS:HE2	1.65	0.78
1:J:9:MSE:HE2	1:J:91:GLY:HA3	1.64	0.78
2:F:195:ACO:O9A	2:F:195:ACO:H4B	1.85	0.77
1:D:6:LEU:CD2	1:D:7:GLU:OE1	2.32	0.77
1:K:108:PHE:HE1	1:K:132:ILE:HD11	1.50	0.76
1:F:88:MSE:HG2	1:F:108:PHE:HB2	1.68	0.76
1:K:108:PHE:CE1	1:K:132:ILE:HD11	2.21	0.76
1:G:107:GLN:HB3	1:G:109:TYR:CE1	2.21	0.76
8:G:777:HOH:O	2:I:195:ACO:S1P	2.45	0.75
1:A:3:MSE:HE2	1:A:8:LYS:HA	1.69	0.74
1:C:73:THR:HG21	1:C:90:ASP:O	1.87	0.74
1:H:50:ARG:HH11	1:H:50:ARG:HG3	1.50	0.74
1:A:3:MSE:HE3	1:A:11:LYS:HD3	1.69	0.74
1:D:109:TYR:CD2	2:F:195:ACO:H32	2.23	0.74
1:H:3:MSE:SE	1:H:11:LYS:HD2	2.38	0.74
1:I:89:LEU:O	1:I:110:THR:HB	1.88	0.73
1:L:113:HIS:NE2	2:L:195:ACO:HH33	2.02	0.73
1:C:26:ARG:HD3	8:C:756:HOH:O	1.87	0.73
1:H:6:LEU:HD12	1:H:22:ILE:HG13	1.69	0.73
1:A:22:ILE:HG22	1:A:26:ARG:HH12	1.53	0.72
1:C:109:TYR:CD2	2:C:195:ACO:H32	2.25	0.72
2:C:195:ACO:O9P	8:C:202:HOH:O	2.06	0.72
1:H:73:THR:HG21	1:H:90:ASP:HB2	1.70	0.72
1:G:161:VAL:HG11	8:H:975:HOH:O	1.90	0.72
1:L:5:GLU:HG2	1:L:16:ASP:HB3	1.71	0.72
1:A:107:GLN:HB3	1:A:109:TYR:CE1	2.25	0.71
1:F:3:MSE:HE1	1:F:13:GLU:HG3	1.70	0.71
1:L:42:GLU:HG2	4:L:196:GOL:H11	1.70	0.70
1:C:6:LEU:HD22	1:C:10:LEU:HD22	1.74	0.70
1:G:124:GLU:HA	7:G:197:BU1:H41	1.73	0.70
1:E:58:HIS:ND1	8:E:493:HOH:O	2.23	0.70
1:G:157:ALA:CB	2:I:195:ACO:H131	2.22	0.70
1:I:34:LEU:HD11	1:I:38:GLN:NE2	2.07	0.70
1:E:181:ARG:NH1	2:E:195:ACO:O4A	2.24	0.70
1:D:61:CYS:SG	1:D:63:GLN:NE2	2.64	0.69
1:I:172:VAL:HG12	1:I:179:ILE:HD13	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:73:THR:HG23	1:K:93:PRO:HA	1.73	0.69
1:H:145:ASN:HD22	1:H:163:ASN:HD22	1.40	0.69
2:A:195:ACO:O9P	2:A:195:ACO:CDP	2.42	0.68
1:G:4:SER:O	1:G:8:LYS:HG3	1.93	0.68
1:B:108:PHE:CE1	1:B:132:ILE:HD11	2.28	0.68
1:J:46:TYR:CE2	1:J:50:ARG:HD2	2.29	0.68
1:D:11:LYS:NZ	8:D:647:HOH:O	2.26	0.68
1:A:138:ILE:HD12	1:A:144:ILE:HD11	1.75	0.68
1:C:19:SER:HB2	1:C:22:ILE:HG12	1.75	0.68
1:D:153:ARG:HD2	1:E:117:TYR:CE2	2.29	0.68
1:E:161:VAL:HG13	1:E:175:THR:CB	2.24	0.67
1:H:143:VAL:HB	1:H:161:VAL:HG22	1.76	0.67
1:B:65:PRO:HD3	8:B:945:HOH:O	1.94	0.67
1:D:120:ARG:HG2	8:D:888:HOH:O	1.94	0.67
1:J:88:MSE:HG2	1:J:108:PHE:HB2	1.77	0.67
1:B:99:HIS:CD2	1:C:121:GLN:HG3	2.29	0.67
2:A:195:ACO:H141	1:C:157:ALA:HB2	1.77	0.66
1:C:73:THR:CG2	1:C:90:ASP:HB2	2.26	0.66
1:H:45[A]:ARG:NH1	1:H:45[A]:ARG:CG	2.54	0.66
1:H:73:THR:CG2	1:H:90:ASP:HB2	2.25	0.66
1:G:157:ALA:HB2	2:I:195:ACO:H131	1.76	0.66
1:B:113:HIS:HD2	1:B:124:GLU:O	1.78	0.66
1:I:170:THR:HG21	1:I:179:ILE:CD1	2.26	0.66
1:C:113:HIS:NE2	2:C:195:ACO:HH32	2.11	0.66
8:B:970:HOH:O	2:C:195:ACO:H52A	1.96	0.65
1:H:45[B]:ARG:HD3	1:H:64:PRO:HG3	1.79	0.65
1:H:108:PHE:CE1	1:H:132:ILE:HD11	2.31	0.65
1:B:179:ILE:HD12	1:B:179:ILE:H	1.61	0.65
1:H:88:MSE:HG2	1:H:108:PHE:HB2	1.79	0.65
2:J:195:ACO:H32	1:K:109:TYR:CD2	2.31	0.65
1:L:143:VAL:HB	1:L:161:VAL:HG22	1.79	0.65
1:B:3:MSE:HE3	1:B:13:GLU:OE1	1.96	0.65
1:D:44:GLU:HA	1:D:44:GLU:OE1	1.97	0.64
1:D:137[A]:TRP:HH2	2:D:195:ACO:H31	1.60	0.64
3:A:196:ACY:H2	1:B:27:SER:HA	1.80	0.64
1:C:9:MSE:HE3	1:C:15:PHE:CZ	2.33	0.64
1:D:7:GLU:OE1	1:D:7:GLU:N	2.30	0.64
1:K:172:VAL:HG12	1:K:179:ILE:HA	1.77	0.64
1:L:16:ASP:OD1	1:L:18:ALA:HB3	1.96	0.64
1:G:5:GLU:HG3	1:G:16:ASP:H	1.63	0.64
1:J:6:LEU:HD12	1:J:21:GLU:HB2	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:9:MSE:CE	1:K:15:PHE:CE1	2.80	0.64
1:B:125:THR:OG1	4:B:196:GOL:H11	1.98	0.64
1:K:5:GLU:CG	1:K:16:ASP:HB2	2.28	0.64
1:E:26[B]:ARG:NH2	1:E:69:GLU:OE2	2.30	0.63
1:B:108:PHE:CZ	1:B:132:ILE:HD11	2.32	0.63
2:A:195:ACO:C8A	2:A:195:ACO:H132	2.28	0.63
1:B:50[B]:ARG:NH1	8:B:791:HOH:O	2.27	0.63
1:K:73:THR:HG21	1:K:90:ASP:O	1.97	0.63
1:A:178[B]:ARG:NH2	8:A:533:HOH:O	2.31	0.63
1:B:161:VAL:HB	1:B:175:THR:HG23	1.81	0.63
1:F:138:ILE:HD13	1:F:144:ILE:HD11	1.80	0.63
2:E:195:ACO:S1P	8:E:688:HOH:O	2.56	0.63
1:H:25:LEU:HD11	1:H:72:LYS:HG2	1.81	0.63
1:C:69:GLU:HB2	1:C:90:ASP:OD1	1.99	0.63
1:D:108:PHE:HE1	1:D:132:ILE:HD13	1.63	0.63
1:A:41:ASP:HB2	1:D:35:GLU:OE2	1.99	0.62
1:I:109:TYR:CD2	2:I:195:ACO:H32	2.34	0.62
1:L:9:MSE:HE3	1:L:91:GLY:HA2	1.81	0.62
8:B:818:HOH:O	2:C:195:ACO:HH33	1.99	0.62
1:E:161:VAL:HG11	1:E:175:THR:CG2	2.30	0.62
1:K:9:MSE:HE3	1:K:22:ILE:HD13	1.82	0.61
1:F:161:VAL:HB	1:F:175:THR:HG23	1.82	0.61
1:K:141:ASN:O	1:K:159:ASN:HA	1.99	0.61
1:L:3:MSE:CE	1:L:11:LYS:HE2	2.31	0.61
1:E:58:HIS:CE1	8:E:493:HOH:O	2.53	0.61
1:D:128:LYS:HB2	1:D:146:GLN:HB2	1.81	0.61
1:B:3:MSE:HG3	1:B:7:GLU:HB2	1.81	0.61
1:D:99:HIS:CD2	1:E:121:GLN:CG	2.83	0.61
1:C:9:MSE:HE3	1:C:15:PHE:CE1	2.36	0.61
1:K:50:ARG:NH1	1:K:56:LEU:O	2.34	0.61
1:D:179:ILE:HD12	1:D:179:ILE:H	1.65	0.60
1:A:128:LYS:HD3	1:A:147:GLY:HA3	1.82	0.60
1:A:153:ARG:NH1	8:A:222:HOH:O	2.35	0.60
1:G:106:THR:HG23	1:G:142:VAL:O	2.01	0.60
1:D:170:THR:HG22	1:D:171:LEU:N	2.17	0.60
1:L:5:GLU:CG	1:L:16:ASP:H	2.13	0.60
2:A:195:ACO:H141	1:C:157:ALA:CB	2.31	0.60
1:J:69:GLU:HG3	1:L:84:MSE:HE3	1.83	0.60
2:H:195:ACO:O7A	8:H:354:HOH:O	2.17	0.60
1:K:129:PRO:O	1:K:147:GLY:HA2	2.02	0.60
1:D:99:HIS:CD2	1:E:121:GLN:HG3	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:61:CYS:SG	4:F:197:GOL:H32	2.42	0.59
1:L:118[B]:ARG:NH1	8:L:842:HOH:O	2.35	0.59
1:B:110:THR:O	1:B:127:CYS:HA	2.02	0.59
1:K:48:LEU:HD23	3:K:198:ACY:CH3	2.32	0.59
1:D:46:TYR:CE2	1:D:50:ARG:HD2	2.38	0.59
1:D:179:ILE:HD12	1:D:179:ILE:N	2.18	0.59
1:A:171:LEU:HD11	2:A:193:ACO:H143	1.85	0.59
2:A:195:ACO:H132	2:A:195:ACO:N7A	2.18	0.59
1:J:39:SER:HB3	1:J:45:ARG:HG2	1.84	0.59
1:G:138:ILE:HD13	1:G:144:ILE:HD11	1.84	0.58
1:A:26:ARG:HH11	1:A:26:ARG:HB2	1.67	0.58
1:F:29:ALA:O	1:F:33:LYS:HB2	2.04	0.58
1:L:50:ARG:NH2	8:L:590:HOH:O	2.35	0.58
1:I:34:LEU:HD11	1:I:38:GLN:HE22	1.69	0.58
1:L:9:MSE:HG3	1:L:15:PHE:CE2	2.39	0.58
1:D:7:GLU:OE1	1:D:7:GLU:CA	2.51	0.58
1:K:46:TYR:CE2	1:K:50:ARG:HD2	2.38	0.58
1:D:9:MSE:HB2	1:D:15:PHE:CG	2.38	0.58
1:D:45:ARG:HD2	8:D:985:HOH:O	2.02	0.58
1:D:36:ILE:HG23	1:D:45:ARG:HG3	1.84	0.58
1:C:73:THR:HG1	1:C:93:PRO:HA	1.67	0.57
2:D:195:ACO:S1P	1:E:113:HIS:NE2	2.77	0.57
1:G:36:ILE:HD13	1:G:49:GLN:HG3	1.85	0.57
2:A:195:ACO:H142	1:C:171:LEU:HD11	1.86	0.57
1:C:73:THR:HG23	1:C:90:ASP:HB2	1.86	0.57
1:C:9:MSE:HE1	1:C:70:PHE:CZ	2.39	0.57
1:C:157:ALA:O	1:C:160:SER:HB3	2.05	0.57
1:C:116:ASP:HB3	1:C:119:ARG:HD2	1.87	0.57
1:D:38:GLN:NE2	1:E:38:GLN:HE22	2.02	0.57
1:F:3:MSE:N	8:F:639:HOH:O	2.37	0.57
1:G:8:LYS:HD3	8:G:809:HOH:O	2.04	0.57
1:K:48:LEU:HD23	3:K:198:ACY:H2	1.85	0.57
1:G:104:PRO:HG2	1:I:109:TYR:CE1	2.40	0.57
1:D:107:GLN:HB3	1:D:109:TYR:CE1	2.40	0.56
1:J:108:PHE:HE1	1:J:132:ILE:CD1	2.18	0.56
1:L:184:LYS:O	1:L:185:ASP:HB2	2.05	0.56
1:A:26:ARG:HB2	1:A:26:ARG:NH1	2.21	0.56
2:E:195:ACO:HH32	1:F:113:HIS:NE2	2.21	0.56
1:E:138:ILE:HD13	1:E:144:ILE:HD11	1.88	0.56
1:H:108:PHE:HE1	1:H:132:ILE:HD11	1.71	0.56
1:D:178:ARG:HG2	1:D:179:ILE:N	2.20	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:108:PHE:HE1	1:D:132:ILE:CD1	2.18	0.55
1:E:161:VAL:HG11	1:E:175:THR:HG23	1.84	0.55
1:J:108:PHE:CE1	1:J:132:ILE:CD1	2.90	0.55
1:A:81:PHE:HB3	1:A:101:LEU:HD23	1.86	0.55
1:H:44:GLU:OE1	1:H:44:GLU:HA	2.05	0.55
1:F:19:SER:HB3	1:F:22:ILE:HD12	1.88	0.55
1:L:88:MSE:HG2	1:L:108:PHE:HB2	1.89	0.55
1:B:32:LEU:O	1:B:36:ILE:HD12	2.07	0.55
1:D:141:ASN:O	1:D:159:ASN:HA	2.06	0.54
1:D:6:LEU:C	1:D:6:LEU:HD23	2.27	0.54
1:B:3:MSE:CE	1:B:13:GLU:OE1	2.55	0.54
1:C:73:THR:OG1	1:C:93:PRO:HA	2.06	0.54
1:D:108:PHE:CE1	1:D:132:ILE:HD13	2.42	0.54
1:G:47:ALA:O	1:G:50:ARG:HB2	2.08	0.54
1:F:46:TYR:CE2	1:F:50:ARG:CD	2.90	0.54
1:K:164:GLN:HG2	1:K:165:ASP:O	2.08	0.54
1:F:39:SER:HB2	1:F:45:ARG:HD3	1.89	0.54
1:K:38:GLN:HA	1:L:34:LEU:HD11	1.88	0.54
1:J:107:GLN:HB3	1:J:109:TYR:CE1	2.42	0.54
1:A:119:ARG:NH2	8:A:684:HOH:O	2.41	0.54
1:H:50:ARG:CG	1:H:50:ARG:NH1	2.62	0.54
1:B:179:ILE:HD12	1:B:179:ILE:N	2.23	0.53
1:D:99:HIS:CD2	1:E:121:GLN:HG2	2.42	0.53
1:I:132:ILE:HD12	1:I:150:ILE:HD12	1.89	0.53
1:K:85:ASN:O	1:K:105:SER:HA	2.07	0.53
1:E:172:VAL:HG12	1:E:179:ILE:HA	1.89	0.53
1:J:108:PHE:HE1	1:J:132:ILE:HD12	1.74	0.53
1:C:5:GLU:HA	1:C:8:LYS:HG3	1.89	0.53
1:D:116:ASP:OD1	1:D:118:ARG:NH1	2.41	0.53
1:E:23:GLU:OE1	1:E:23:GLU:HA	2.07	0.53
1:H:45[A]:ARG:HD2	1:H:64:PRO:HG3	1.91	0.53
1:L:42:GLU:HG2	4:L:196:GOL:C1	2.36	0.53
1:D:6:LEU:HD23	1:D:7:GLU:OE1	2.07	0.53
1:G:181:ARG:HG2	1:G:182:SER:O	2.09	0.53
1:D:88:MSE:HG2	1:D:108:PHE:HB2	1.90	0.53
1:B:132:ILE:HD13	1:B:138:ILE:CD1	2.39	0.53
1:C:73:THR:HG21	1:C:90:ASP:HB2	1.91	0.53
1:C:9:MSE:HE1	1:C:70:PHE:CE2	2.44	0.52
1:J:37:ASN:OD1	1:J:65:PRO:HA	2.10	0.52
1:A:171:LEU:HD23	1:A:181:ARG:HG2	1.92	0.52
1:B:4:SER:OG	1:B:7:GLU:HG2	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:116:ASP:HB2	1:D:119:ARG:HH11	1.75	0.52
1:G:15:PHE:O	7:G:197:BU1:H42	2.10	0.52
2:A:195:ACO:CEP	1:C:157:ALA:HB2	2.40	0.52
1:K:101:LEU:HD12	1:L:120:ARG:HD2	1.91	0.52
1:E:11:LYS:O	1:E:11:LYS:CG	2.50	0.52
1:G:153:ARG:HD2	1:I:117:TYR:CE2	2.45	0.52
1:A:159:ASN:ND2	8:B:988:HOH:O	2.43	0.52
1:C:44:GLU:OE1	1:C:44:GLU:HA	2.09	0.52
1:G:157:ALA:HB1	2:I:195:ACO:H131	1.92	0.52
1:E:169:ASP:HA	8:E:697:HOH:O	2.09	0.52
1:A:3:MSE:CE	1:A:11:LYS:HD3	2.36	0.52
1:B:75:ARG:NH2	8:B:398:HOH:O	2.33	0.52
1:D:9:MSE:O	8:D:602:HOH:O	2.19	0.51
1:K:110:THR:O	1:K:127:CYS:HA	2.10	0.51
1:G:157:ALA:O	1:G:160:SER:HB2	2.10	0.51
1:J:143:VAL:HB	1:J:161:VAL:HG22	1.93	0.51
1:K:41:ASP:HB3	1:K:44:GLU:HB3	1.92	0.51
1:K:135:ASP:OD1	1:L:121:GLN:NE2	2.35	0.51
1:J:85:ASN:O	1:J:105:SER:HA	2.10	0.51
1:J:110:THR:O	1:J:127:CYS:HA	2.10	0.51
1:L:8:LYS:HB3	1:L:13:GLU:HB3	1.92	0.51
1:B:181:ARG:NH2	8:B:970:HOH:O	2.43	0.51
1:E:161:VAL:CG2	1:E:175:THR:HG23	2.40	0.51
1:I:34:LEU:CD1	1:I:38:GLN:NE2	2.73	0.51
1:J:9:MSE:HE2	1:J:91:GLY:CA	2.38	0.51
1:D:99:HIS:NE2	1:E:121:GLN:HG2	2.25	0.51
1:I:172:VAL:CG1	1:I:179:ILE:HD13	2.40	0.51
1:I:161:VAL:HB	1:I:175:THR:HG23	1.93	0.51
1:J:50:ARG:NH1	1:J:56:LEU:O	2.44	0.50
1:C:6:LEU:HB2	1:C:21:GLU:CD	2.31	0.50
1:D:9:MSE:HB2	1:D:15:PHE:CD2	2.45	0.50
1:D:108:PHE:CE1	1:D:132:ILE:CD1	2.94	0.50
1:F:46:TYR:CE2	1:F:50:ARG:HD3	2.47	0.50
1:J:108:PHE:CE1	1:J:132:ILE:HD11	2.46	0.50
1:K:168:PRO:O	1:K:169:ASP:HB2	2.11	0.50
1:D:137[A]:TRP:CD1	1:D:155:VAL:HG13	2.46	0.50
1:I:118:ARG:NH1	8:I:913:HOH:O	2.44	0.50
1:K:9:MSE:HE2	1:K:15:PHE:HE1	1.73	0.50
1:E:183:LEU:HB2	8:E:697:HOH:O	2.12	0.50
1:L:92:ALA:HB2	1:L:127:CYS:HB3	1.94	0.50
1:C:5:GLU:OE1	1:C:16:ASP:HB3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:133:GLU:O	1:G:136:VAL:HG23	2.13	0.49
1:K:138:ILE:HD13	1:K:144:ILE:HD11	1.94	0.49
2:A:193:ACO:H133	2:A:193:ACO:C8A	2.42	0.49
1:I:53:PHE:HA	1:I:71:GLY:O	2.12	0.49
1:B:108:PHE:HE1	1:B:132:ILE:HD11	1.77	0.49
1:H:45[B]:ARG:HD3	1:H:64:PRO:CG	2.43	0.49
1:A:117:TYR:CE2	1:C:153:ARG:HD2	2.47	0.49
1:H:6:LEU:O	1:H:10:LEU:HD13	2.12	0.49
2:A:195:ACO:H2B	8:A:993:HOH:O	2.13	0.49
1:H:122:ALA:HB3	1:H:124:GLU:CD	2.33	0.49
1:C:182:SER:OG	1:C:184:LYS:HD3	2.12	0.49
1:I:164:GLN:OE1	8:I:253:HOH:O	2.20	0.49
1:J:3:MSE:HB3	1:J:8:LYS:HG3	1.95	0.49
1:J:7:GLU:OE1	1:J:7:GLU:HA	2.13	0.49
1:B:99:HIS:NE2	1:C:121:GLN:HG3	2.27	0.49
2:A:195:ACO:O5B	2:A:195:ACO:O4A	2.30	0.48
1:A:110:THR:O	1:A:146:GLN:NE2	2.40	0.48
1:D:170:THR:CG2	1:D:171:LEU:N	2.76	0.48
1:F:137:TRP:NE1	2:F:195:ACO:HH32	2.29	0.48
1:D:133:GLU:CG	1:D:152:ALA:HB2	2.42	0.48
1:A:101:LEU:HB3	2:A:193:ACO:CH3	2.44	0.48
1:E:27:SER:O	1:E:28:GLN:C	2.51	0.48
1:F:3:MSE:HB3	1:F:7:GLU:HB3	1.94	0.48
1:G:5:GLU:HG2	1:G:16:ASP:HB3	1.95	0.48
2:A:195:ACO:H51A	2:A:195:ACO:H8A	1.94	0.48
1:C:64:PRO:O	1:C:84:MSE:HG2	2.14	0.48
1:C:85:ASN:O	1:C:105:SER:HA	2.14	0.48
2:F:195:ACO:HO2A	2:F:195:ACO:P3B	2.37	0.48
1:G:82:ILE:CG2	1:G:86:VAL:HG21	2.44	0.48
1:I:109:TYR:CG	2:I:195:ACO:H32	2.49	0.48
1:F:137:TRP:HB3	1:F:155:VAL:HG22	1.96	0.48
1:H:92:ALA:HB2	1:H:127:CYS:HB3	1.95	0.48
1:L:4:SER:O	1:L:8:LYS:HG3	2.14	0.48
1:D:51:GLU:OE2	8:D:206:HOH:O	2.20	0.48
1:H:3:MSE:SE	1:H:11:LYS:HE3	2.64	0.48
1:I:46:TYR:HE2	1:I:50:ARG:HE	1.62	0.48
1:J:69:GLU:HG3	1:L:84:MSE:CE	2.44	0.48
1:I:3:MSE:HE3	1:I:8:LYS:CG	2.44	0.47
1:B:3:MSE:SE	1:B:7:GLU:HB3	2.64	0.47
1:F:89:LEU:HD12	1:F:109:TYR:CD1	2.48	0.47
2:H:195:ACO:O4A	2:H:195:ACO:O5B	2.32	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:165:ASP:OD2	8:B:792:HOH:O	2.20	0.47
1:C:35:GLU:HG2	8:E:356:HOH:O	2.13	0.47
1:F:21:GLU:CB	8:F:990:HOH:O	2.47	0.47
1:K:110:THR:HG22	1:K:130:ILE:HG13	1.96	0.47
1:B:107:GLN:HB3	1:B:109:TYR:CE1	2.50	0.47
2:E:195:ACO:H32	1:F:109:TYR:CD2	2.49	0.47
1:C:6:LEU:CD2	1:C:10:LEU:HD22	2.41	0.47
1:D:126:ILE:N	1:D:126:ILE:HD12	2.30	0.47
1:I:7:GLU:OE2	8:I:624:HOH:O	2.20	0.47
1:J:181:ARG:HG2	1:J:182:SER:O	2.13	0.47
1:K:44:GLU:O	1:K:48:LEU:HG	2.15	0.47
1:A:176:PRO:HG2	1:A:178[B]:ARG:HH21	1.78	0.47
1:D:38:GLN:CG	1:E:38:GLN:HE22	2.27	0.47
1:D:184:LYS:HB2	1:D:184:LYS:HE2	1.48	0.47
1:C:46:TYR:CE2	1:C:50:ARG:HD3	2.50	0.47
1:H:119:ARG:O	8:H:266:HOH:O	2.20	0.47
1:I:126:ILE:O	1:I:126:ILE:HG23	2.15	0.47
1:L:82:ILE:HG12	1:L:102:ILE:HD12	1.96	0.47
1:B:174:GLY:HA2	8:B:987:HOH:O	2.13	0.47
1:E:21:GLU:HG2	1:E:22:ILE:N	2.29	0.47
1:E:184:LYS:HB2	1:E:184:LYS:HE2	1.61	0.47
1:H:161:VAL:HB	1:H:175:THR:HG23	1.97	0.47
1:A:51:GLU:OE1	1:D:41:ASP:OD2	2.33	0.47
1:I:5:GLU:HA	1:I:8:LYS:HD2	1.97	0.47
1:I:172:VAL:HG12	1:I:179:ILE:HA	1.97	0.47
1:G:25:LEU:HD13	1:G:25:LEU:HA	1.62	0.47
1:J:58:HIS:N	1:J:78:ASP:OD1	2.46	0.47
2:A:195:ACO:CDP	2:A:195:ACO:N7A	2.77	0.46
1:D:133:GLU:HG2	1:D:152:ALA:HB2	1.97	0.46
1:G:104:PRO:HG3	1:I:89:LEU:HD11	1.96	0.46
1:A:38:GLN:HE22	1:C:38:GLN:HG2	1.81	0.46
1:C:181:ARG:CG	1:C:182:SER:N	2.78	0.46
1:G:32:LEU:O	1:G:36:ILE:HG13	2.15	0.46
1:B:132:ILE:HD13	1:B:138:ILE:HD11	1.98	0.46
1:C:117:TYR:CE2	1:C:118:ARG:HG3	2.50	0.46
1:J:157:ALA:HB2	2:J:195:ACO:CDP	2.46	0.46
1:K:141:ASN:ND2	1:K:159:ASN:OD1	2.48	0.46
1:D:6:LEU:HD23	1:D:10:LEU:HD22	1.98	0.46
1:F:85:ASN:O	1:F:105:SER:HA	2.16	0.46
1:D:137[A]:TRP:HB3	1:D:155:VAL:HG22	1.98	0.46
1:F:116:ASP:OD1	1:F:116:ASP:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:31:ARG:HG2	1:C:31:ARG:HH11	1.80	0.46
1:I:171:LEU:HG	1:I:180:LEU:HB2	1.97	0.46
1:B:65:PRO:HG2	1:C:67:HIS:CE1	2.51	0.45
1:E:64:PRO:HD3	4:E:196:GOL:H12	1.98	0.45
1:K:51:GLU:O	1:K:72:LYS:HE2	2.16	0.45
1:C:151:GLY:O	1:C:154:SER:HB2	2.16	0.45
1:D:133:GLU:O	1:D:136:VAL:HG23	2.15	0.45
1:F:183:LEU:C	8:F:768:HOH:O	2.55	0.45
1:C:66:PHE:CE2	1:C:68:CYS:HB3	2.51	0.45
1:F:6:LEU:HD22	1:F:21:GLU:HG2	1.98	0.45
1:D:117:TYR:CE2	1:F:153:ARG:HD2	2.52	0.45
1:F:143:VAL:HB	1:F:161:VAL:HG22	1.99	0.45
1:G:128:LYS:HB2	1:G:146:GLN:HB2	1.97	0.45
1:I:31:ARG:O	1:I:35:GLU:HG3	2.17	0.45
1:D:32:LEU:HD23	1:D:52:LEU:HA	1.99	0.45
1:E:81:PHE:HB3	1:E:101:LEU:HD23	1.99	0.45
1:E:173:GLY:HA3	1:E:180:LEU:HD11	1.99	0.45
1:I:107:GLN:HB3	1:I:109:TYR:CE1	2.52	0.45
1:C:118:ARG:NH2	8:C:896:HOH:O	2.29	0.45
1:H:73:THR:HG21	1:H:90:ASP:O	2.17	0.45
1:H:167:PRO:HA	1:H:168:PRO:HD2	1.86	0.45
1:I:58:HIS:CD2	1:I:59:LYS:HG3	2.52	0.45
1:L:5:GLU:HG2	1:L:16:ASP:CB	2.42	0.45
1:L:41:ASP:HB3	1:L:44:GLU:HB3	1.99	0.44
1:D:176:PRO:HG2	2:F:195:ACO:H2B	1.98	0.44
1:G:69:GLU:CG	8:G:370:HOH:O	2.64	0.44
1:D:36:ILE:HG12	1:D:48:LEU:HB3	1.99	0.44
1:D:38:GLN:NE2	1:E:38:GLN:NE2	2.64	0.44
1:I:170:THR:CG2	1:I:179:ILE:HD12	2.43	0.44
1:K:36:ILE:HG23	1:K:45:ARG:HG3	2.00	0.44
1:C:5:GLU:HG3	1:C:19:SER:OG	2.17	0.44
2:F:195:ACO:O7A	2:F:195:ACO:O2B	2.36	0.44
1:D:12:GLY:O	1:D:126:ILE:HG23	2.18	0.44
1:I:12:GLY:O	1:I:126:ILE:HD11	2.18	0.44
1:I:72:LYS:HA	1:I:72:LYS:HD3	1.72	0.44
1:L:7:GLU:HG2	1:L:11:LYS:HD3	1.99	0.44
1:B:128:LYS:HA	1:B:129:PRO:HD3	1.83	0.44
1:C:6:LEU:HB2	1:C:21:GLU:OE2	2.18	0.44
1:E:28:GLN:NE2	8:E:208:HOH:O	2.49	0.44
1:L:45:ARG:HH21	4:L:196:GOL:C1	2.31	0.44
1:H:166:VAL:HA	1:H:167:PRO:HD2	1.68	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:157:ALA:O	1:I:160:SER:OG	2.36	0.44
1:B:41:ASP:HB3	1:B:44:GLU:HB3	1.99	0.43
1:L:9:MSE:HE3	1:L:91:GLY:CA	2.48	0.43
1:D:109:TYR:CE2	2:F:195:ACO:H32	2.52	0.43
1:K:73:THR:CG2	1:K:90:ASP:HB2	2.48	0.43
1:D:133:GLU:HG3	1:D:134:ASP:N	2.34	0.43
1:F:92:ALA:HB2	1:F:127:CYS:HB3	2.00	0.43
1:H:72:LYS:HA	1:H:72:LYS:HD2	1.76	0.43
1:H:46:TYR:HB2	8:H:704:HOH:O	2.17	0.43
1:J:108:PHE:CE1	1:J:132:ILE:HD12	2.53	0.43
1:K:9:MSE:HE3	1:K:15:PHE:CD1	2.53	0.43
1:L:113:HIS:NE2	2:L:195:ACO:CH3	2.77	0.43
1:B:144:ILE:HD12	1:B:150:ILE:HD11	2.01	0.43
1:D:32:LEU:HD12	1:D:32:LEU:HA	1.81	0.43
1:L:118[B]:ARG:HE	1:L:118[B]:ARG:HB2	1.13	0.43
1:C:110:THR:O	1:C:127:CYS:HA	2.18	0.43
1:C:132:ILE:HD12	1:C:138:ILE:HD11	2.01	0.43
1:J:137:TRP:HE1	2:J:195:ACO:HH32	1.82	0.43
1:K:129:PRO:HD3	8:K:282:HOH:O	2.19	0.43
1:L:88:MSE:HE2	1:L:108:PHE:CE2	2.53	0.43
1:L:113:HIS:CE1	2:L:195:ACO:HH33	2.54	0.43
2:A:195:ACO:C8A	2:A:195:ACO:H51A	2.48	0.43
1:C:9:MSE:HE1	1:C:70:PHE:CE1	2.54	0.43
1:D:5:GLU:HG3	1:D:16:ASP:HB3	2.00	0.43
1:D:34:LEU:O	1:D:38:GLN:HB2	2.19	0.43
1:D:44:GLU:HG3	1:D:48:LEU:HD22	2.01	0.43
1:D:184:LYS:O	1:D:185:ASP:CB	2.50	0.43
1:F:58:HIS:CE1	1:F:59:LYS:HZ2	2.36	0.43
1:A:26:ARG:NH1	1:A:70:PHE:CE1	2.87	0.43
1:D:115:LEU:HD11	2:F:195:ACO:H143	2.01	0.43
1:D:179:ILE:H	1:D:179:ILE:CD1	2.31	0.43
1:I:128:LYS:HA	1:I:129:PRO:HD3	1.77	0.43
1:F:30:GLY:HA2	1:F:33:LYS:HE2	2.01	0.43
1:G:104:PRO:HG3	1:I:89:LEU:CD1	2.49	0.43
1:K:153:ARG:HD2	1:L:117:TYR:CE2	2.54	0.43
1:H:138:ILE:HD13	1:H:144:ILE:HD11	2.00	0.43
1:J:137:TRP:HE1	2:J:195:ACO:CH3	2.31	0.43
1:K:23:GLU:HB2	8:K:963:HOH:O	2.18	0.43
1:L:171:LEU:HB2	1:L:183:LEU:HD21	2.01	0.43
1:D:5:GLU:HG3	1:D:19:SER:OG	2.19	0.42
1:H:108:PHE:CZ	1:H:132:ILE:HD11	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:33:LYS:HD2	1:L:68:CYS:H	1.84	0.42
1:A:79:HIS:O	1:A:99:HIS:HA	2.19	0.42
1:D:62:VAL:HG22	1:D:82:ILE:HD12	2.00	0.42
1:L:9:MSE:HG3	1:L:15:PHE:CZ	2.55	0.42
1:B:38:GLN:HG2	1:C:38:GLN:NE2	2.35	0.42
1:C:161:VAL:HB	1:C:175:THR:HG23	2.00	0.42
1:L:79:HIS:O	1:L:99:HIS:HA	2.18	0.42
1:C:128:LYS:HA	1:C:129:PRO:HD3	1.89	0.42
1:H:3:MSE:SE	1:H:11:LYS:CD	3.14	0.42
1:A:72:LYS:HA	1:A:72:LYS:HD2	1.93	0.42
1:D:114:SER:OG	1:D:119:ARG:HB2	2.19	0.42
1:G:169:ASP:HB3	1:G:184:LYS:HG2	1.99	0.42
1:G:175:THR:HA	1:G:176:PRO:HA	1.92	0.42
1:H:178:ARG:HD3	1:H:178:ARG:HA	1.91	0.42
1:K:170:THR:HG22	1:K:172:VAL:HG13	2.02	0.42
1:A:82:ILE:HG12	1:A:102:ILE:HD12	2.02	0.42
1:A:61:CYS:HB3	1:A:63:GLN:HE21	1.84	0.42
1:E:161:VAL:CG1	1:E:175:THR:OG1	2.61	0.42
1:F:137:TRP:HE1	2:F:195:ACO:HH32	1.83	0.42
1:H:145:ASN:ND2	1:H:163:ASN:ND2	2.53	0.42
1:J:137:TRP:HB3	1:J:155:VAL:HG22	2.01	0.42
1:K:171:LEU:HD11	2:L:195:ACO:H132	2.01	0.42
1:C:143:VAL:HB	1:C:161:VAL:HG22	2.02	0.42
1:J:122:ALA:HB3	1:J:124:GLU:CD	2.41	0.42
1:A:107:GLN:NE2	1:C:105:SER:OG	2.52	0.42
1:C:9:MSE:CE	1:C:70:PHE:CE2	3.03	0.42
1:H:128:LYS:HB2	1:H:146:GLN:HB2	2.01	0.42
1:I:130:ILE:HD13	1:I:144:ILE:HG22	2.02	0.42
1:J:0:ALA:N	8:J:516:HOH:O	2.52	0.42
1:L:126:ILE:HD11	1:L:146:GLN:HE22	1.85	0.42
1:L:175:THR:HA	1:L:176:PRO:HA	1.92	0.42
1:G:120:ARG:HD2	1:H:101:LEU:HD12	2.02	0.41
1:H:117:TYR:CE2	1:I:153:ARG:HD2	2.55	0.41
1:H:122:ALA:O	1:H:123:TRP:HB2	2.20	0.41
1:L:109:TYR:CD2	2:L:195:ACO:H32	2.55	0.41
1:C:5:GLU:OE2	1:C:8:LYS:HE3	2.19	0.41
1:G:6:LEU:HD12	1:G:6:LEU:O	2.20	0.41
1:I:3:MSE:HE3	1:I:8:LYS:HG2	2.01	0.41
1:J:115:LEU:HD23	1:J:115:LEU:HA	1.90	0.41
1:J:137:TRP:NE1	2:J:195:ACO:HH32	2.35	0.41
1:C:138:ILE:HD13	1:C:144:ILE:HD11	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:81:PHE:CD2	1:H:81:PHE:C	2.93	0.41
1:D:133:GLU:CG	1:D:134:ASP:N	2.83	0.41
1:D:133:GLU:CD	1:D:134:ASP:H	2.24	0.41
1:J:92:ALA:HB2	1:J:127:CYS:HB3	2.01	0.41
1:A:35:GLU:OE1	1:D:40:LEU:HB2	2.20	0.41
1:H:120:ARG:HD2	1:I:101:LEU:HD12	2.01	0.41
1:A:26:ARG:NH1	1:A:70:PHE:HE1	2.17	0.41
2:A:195:ACO:H8A	2:A:195:ACO:C5B	2.51	0.41
1:B:92:ALA:HB1	1:B:93:PRO:HD2	2.01	0.41
1:F:104:PRO:HD3	2:F:195:ACO:H21	2.03	0.41
1:I:39:SER:O	1:I:39:SER:OG	2.38	0.41
1:C:11:LYS:HA	1:C:11:LYS:HD3	1.83	0.41
1:E:117:TYR:CD1	1:E:117:TYR:C	2.94	0.41
8:E:205:HOH:O	1:F:117:TYR:HB3	2.20	0.41
1:F:5:GLU:HA	1:F:8:LYS:HG3	2.02	0.41
1:F:170:THR:HG22	1:F:171:LEU:N	2.35	0.41
1:G:161:VAL:HB	1:G:175:THR:HG23	2.03	0.41
1:D:116:ASP:HB3	1:D:119:ARG:HE	1.86	0.41
1:L:18:ALA:O	1:L:23:GLU:CD	2.60	0.40
1:F:72:LYS:HD2	1:F:72:LYS:HA	1.79	0.40
1:F:137:TRP:O	1:F:155:VAL:HA	2.21	0.40
1:G:63:GLN:OE1	3:G:196:ACY:H3	2.21	0.40
2:I:193:ACO:O9P	2:I:193:ACO:H131	2.20	0.40
1:B:135:ASP:O	1:B:153:ARG:HA	2.20	0.40
1:E:128:LYS:HA	1:E:129:PRO:HD3	1.87	0.40
1:F:3:MSE:CE	1:F:13:GLU:HG3	2.45	0.40
1:K:72:LYS:HD3	1:K:72:LYS:HA	1.93	0.40
2:J:195:ACO:H32	1:K:109:TYR:CE2	2.56	0.40
1:K:4:SER:O	1:K:8:LYS:HG3	2.21	0.40
1:A:178[B]:ARG:HA	1:A:178[B]:ARG:HD3	1.73	0.40
1:B:9:MSE:HG2	1:B:91:GLY:O	2.22	0.40
1:F:40:LEU:HA	1:F:40:LEU:HD23	1.74	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:L:195:ACO:O5A	8:I:624:HOH:O[1_655]	2.16	0.04

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	181/195 (93%)	178 (98%)	3 (2%)	0	100	100
1	B	183/195 (94%)	182 (100%)	1 (0%)	0	100	100
1	C	181/195 (93%)	179 (99%)	2 (1%)	0	100	100
1	D	182/195 (93%)	178 (98%)	4 (2%)	0	100	100
1	E	182/195 (93%)	181 (100%)	1 (0%)	0	100	100
1	F	181/195 (93%)	180 (99%)	1 (1%)	0	100	100
1	G	181/195 (93%)	179 (99%)	2 (1%)	0	100	100
1	H	182/195 (93%)	182 (100%)	0	0	100	100
1	I	183/195 (94%)	182 (100%)	1 (0%)	0	100	100
1	J	183/195 (94%)	179 (98%)	4 (2%)	0	100	100
1	K	181/195 (93%)	179 (99%)	2 (1%)	0	100	100
1	L	182/195 (93%)	180 (99%)	2 (1%)	0	100	100
All	All	2182/2340 (93%)	2159 (99%)	23 (1%)	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	154/157 (98%)	151 (98%)	3 (2%)	57	68
1	B	156/157 (99%)	151 (97%)	5 (3%)	39	47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	C	154/157 (98%)	143 (93%)	11 (7%)	14 15
1	D	155/157 (99%)	142 (92%)	13 (8%)	11 10
1	E	155/157 (99%)	149 (96%)	6 (4%)	32 40
1	F	154/157 (98%)	148 (96%)	6 (4%)	32 40
1	G	154/157 (98%)	144 (94%)	10 (6%)	17 18
1	H	155/157 (99%)	142 (92%)	13 (8%)	11 10
1	I	156/157 (99%)	142 (91%)	14 (9%)	9 8
1	J	155/157 (99%)	149 (96%)	6 (4%)	32 40
1	K	154/157 (98%)	148 (96%)	6 (4%)	32 40
1	L	155/157 (99%)	149 (96%)	6 (4%)	32 40
All	All	1857/1884 (99%)	1758 (95%)	99 (5%)	23 26

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

Mol	Chain	Res	Type
1	A	69	GLU
1	A	119	ARG
1	A	128	LYS
1	B	2	LYS
1	B	10	LEU
1	B	19	SER
1	B	112	SER
1	B	160	SER
1	C	6	LEU
1	C	10	LEU
1	C	13	GLU
1	C	33	LYS
1	C	34	LEU
1	C	73	THR
1	C	118	ARG
1	C	121	GLN
1	C	126	ILE
1	C	160	SER
1	C	184	LYS
1	D	3	MSE
1	D	7	GLU
1	D	10	LEU
1	D	32	LEU

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Mol	Chain	Res	Type
1	D	41	ASP
1	D	48	LEU
1	D	115	LEU
1	D	118	ARG
1	D	137[A]	TRP
1	D	137[B]	TRP
1	D	150	ILE
1	D	183	LEU
1	D	184	LYS
1	E	11	LYS
1	E	21	GLU
1	E	106	THR
1	E	107	GLN
1	E	121	GLN
1	E	184	LYS
1	F	19	SER
1	F	42	GLU
1	F	50	ARG
1	F	72	LYS
1	F	112	SER
1	F	184	LYS
1	G	3	MSE
1	G	5	GLU
1	G	10	LEU
1	G	25	LEU
1	G	35	GLU
1	G	42	GLU
1	G	50	ARG
1	G	115	LEU
1	G	160	SER
1	G	184	LYS
1	H	3	MSE
1	H	5	GLU
1	H	19	SER
1	H	27	SER
1	H	28	GLN
1	H	33	LYS
1	H	34	LEU
1	H	45[A]	ARG
1	H	45[B]	ARG
1	H	48	LEU
1	H	50	ARG

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Mol	Chain	Res	Type
1	H	150	ILE
1	H	182	SER
1	I	19	SER
1	I	21	GLU
1	I	39	SER
1	I	59	LYS
1	I	69	GLU
1	I	75	ARG
1	I	110	THR
1	I	112	SER
1	I	118	ARG
1	I	160	SER
1	I	178	ARG
1	I	181	ARG
1	I	182	SER
1	I	185	ASP
1	J	10	LEU
1	J	21	GLU
1	J	105	SER
1	J	112	SER
1	J	126	ILE
1	J	160	SER
1	K	6	LEU
1	K	19	SER
1	K	73	THR
1	K	83	ASN
1	K	85	ASN
1	K	164	GLN
1	L	3	MSE
1	L	5	GLU
1	L	10	LEU
1	L	13	GLU
1	L	112	SER
1	L	184	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	63	GLN
1	A	107	GLN
1	C	38	GLN

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Mol	Chain	Res	Type
1	C	67	HIS
1	C	145	ASN
1	D	38	GLN
1	D	55	HIS
1	D	63	GLN
1	D	107	GLN
1	D	145	ASN
1	D	159	ASN
1	E	28	GLN
1	E	38	GLN
1	E	163	ASN
1	F	28	GLN
1	F	49	GLN
1	F	58	HIS
1	F	145	ASN
1	G	38	GLN
1	G	67	HIS
1	G	107	GLN
1	G	145	ASN
1	G	146	GLN
1	H	107	GLN
1	H	163	ASN
1	I	38	GLN
1	I	58	HIS
1	I	107	GLN
1	I	164	GLN
1	J	107	GLN
1	K	14	HIS
1	K	85	ASN
1	K	107	GLN
1	K	141	ASN
1	K	159	ASN
1	K	164	GLN
1	L	28	GLN
1	L	85	ASN
1	L	145	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 34 ligands modelled in this entry, 7 are monoatomic - leaving 27 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
4	GOL	F	197	-	5,5,5	0.38	0	5,5,5	0.27	0
3	ACY	A	196	-	3,3,3	0.80	0	3,3,3	0.94	0
2	ACO	I	195	-	45,53,53	1.80	11 (24%)	56,79,79	1.47	11 (19%)
3	ACY	K	198	-	3,3,3	0.60	0	3,3,3	1.47	1 (33%)
2	ACO	E	195	-	45,53,53	1.82	11 (24%)	56,79,79	1.21	5 (8%)
2	ACO	L	195	-	45,53,53	1.87	10 (22%)	56,79,79	1.37	10 (17%)
2	ACO	J	195	-	45,53,53	1.92	12 (26%)	56,79,79	1.64	10 (17%)
3	ACY	B	198	-	3,3,3	0.83	0	3,3,3	0.50	0
2	ACO	A	195	-	45,53,53	1.88	10 (22%)	56,79,79	1.45	7 (12%)
3	ACY	I	196	-	3,3,3	0.78	0	3,3,3	0.75	0
4	GOL	E	196	-	5,5,5	0.53	0	5,5,5	1.20	1 (20%)
2	ACO	C	195	-	45,53,53	1.81	11 (24%)	56,79,79	1.44	6 (10%)
3	ACY	A	197	-	3,3,3	0.77	0	3,3,3	0.77	0
2	ACO	H	195	-	45,53,53	1.95	11 (24%)	56,79,79	1.53	9 (16%)
2	ACO	L	193	-	45,53,53	1.88	12 (26%)	56,79,79	1.43	9 (16%)
3	ACY	D	197	-	3,3,3	0.71	0	3,3,3	1.09	0
3	ACY	G	196	-	3,3,3	0.77	0	3,3,3	1.34	0
4	GOL	L	196	-	5,5,5	0.36	0	5,5,5	1.16	1 (20%)
3	ACY	K	197	-	3,3,3	0.78	0	3,3,3	0.94	0
2	ACO	F	195	-	45,53,53	1.86	11 (24%)	56,79,79	1.66	9 (16%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
7	BU1	G	197	-	5,5,5	0.33	0	4,4,4	0.60	0
7	BU1	K	196	-	5,5,5	0.35	0	4,4,4	0.36	0
2	ACO	D	195	-	45,53,53	1.77	6 (13%)	56,79,79	1.51	8 (14%)
2	ACO	A	193	-	45,53,53	1.81	10 (22%)	56,79,79	1.59	7 (12%)
2	ACO	I	193	-	45,53,53	1.79	9 (20%)	56,79,79	1.38	5 (8%)
3	ACY	F	196	-	3,3,3	0.86	0	3,3,3	0.78	0
4	GOL	B	196	-	5,5,5	0.37	0	5,5,5	0.28	0

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
2	ACO	J	195	-	-	20/47/67/67	0/3/3/3
2	ACO	L	193	-	-	18/47/67/67	0/3/3/3
4	GOL	B	196	-	-	2/4/4/4	-
2	ACO	A	195	-	-	22/47/67/67	0/3/3/3
4	GOL	F	197	-	-	0/4/4/4	-
2	ACO	F	195	-	-	16/47/67/67	0/3/3/3
7	BU1	G	197	-	-	0/3/3/3	-
7	BU1	K	196	-	-	1/3/3/3	-
4	GOL	E	196	-	-	2/4/4/4	-
2	ACO	D	195	-	-	16/47/67/67	0/3/3/3
2	ACO	C	195	-	-	20/47/67/67	0/3/3/3
4	GOL	L	196	-	-	2/4/4/4	-
2	ACO	I	195	-	-	12/47/67/67	0/3/3/3
2	ACO	A	193	-	-	18/47/67/67	0/3/3/3
2	ACO	I	193	-	-	17/47/67/67	0/3/3/3
2	ACO	H	195	-	-	18/47/67/67	0/3/3/3
2	ACO	E	195	-	-	21/47/67/67	0/3/3/3
2	ACO	L	195	-	-	13/47/67/67	0/3/3/3

All (124) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	195	ACO	C9P-N8P	7.82	1.50	1.33
2	I	193	ACO	C9P-N8P	7.37	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	195	ACO	C9P-N8P	7.36	1.49	1.33
2	A	195	ACO	C9P-N8P	7.14	1.49	1.33
2	I	195	ACO	C9P-N8P	7.12	1.49	1.33
2	A	193	ACO	C9P-N8P	6.89	1.48	1.33
2	L	195	ACO	C9P-N8P	6.85	1.48	1.33
2	F	195	ACO	C9P-N8P	6.75	1.48	1.33
2	L	193	ACO	C9P-N8P	6.51	1.47	1.33
2	C	195	ACO	C9P-N8P	6.50	1.47	1.33
2	J	195	ACO	C9P-N8P	6.47	1.47	1.33
2	E	195	ACO	C9P-N8P	6.31	1.47	1.33
2	F	195	ACO	C2B-C3B	-4.73	1.42	1.52
2	A	195	ACO	C2B-C3B	-4.58	1.42	1.52
2	L	195	ACO	C2B-C3B	-4.28	1.43	1.52
2	J	195	ACO	C2B-C3B	-4.26	1.43	1.52
2	L	193	ACO	C2B-C3B	-4.15	1.43	1.52
2	D	195	ACO	C2B-C3B	-4.13	1.43	1.52
2	J	195	ACO	C2B-C1B	-4.05	1.47	1.53
2	I	195	ACO	C2B-C3B	-4.00	1.44	1.52
2	E	195	ACO	C2B-C3B	-3.92	1.44	1.52
2	J	195	ACO	O4B-C1B	-3.89	1.35	1.41
2	H	195	ACO	C2B-C3B	-3.83	1.44	1.52
2	L	193	ACO	C2B-C1B	-3.82	1.48	1.53
2	L	195	ACO	C2B-C1B	-3.80	1.48	1.53
2	I	193	ACO	C2B-C3B	-3.77	1.44	1.52
2	H	195	ACO	C2B-C1B	-3.70	1.48	1.53
2	A	193	ACO	C2B-C3B	-3.69	1.44	1.52
2	C	195	ACO	C2B-C3B	-3.63	1.44	1.52
2	A	195	ACO	C2B-C1B	-3.60	1.48	1.53
2	I	195	ACO	C2B-C1B	-3.59	1.48	1.53
2	A	193	ACO	C2B-C1B	-3.56	1.48	1.53
2	F	195	ACO	C2B-C1B	-3.49	1.48	1.53
2	A	193	ACO	O4B-C1B	-3.46	1.36	1.41
2	E	195	ACO	O4B-C1B	-3.40	1.36	1.41
2	C	195	ACO	O4B-C1B	-3.38	1.36	1.41
2	D	195	ACO	C5P-N4P	3.23	1.40	1.33
2	H	195	ACO	O4B-C1B	-3.22	1.36	1.41
2	I	193	ACO	C2B-C1B	-3.18	1.48	1.53
2	C	195	ACO	C2B-C1B	-3.16	1.49	1.53
2	I	193	ACO	C5P-N4P	3.13	1.40	1.33
2	L	193	ACO	C3B-C4B	-2.95	1.45	1.52
2	H	195	ACO	C5P-N4P	2.91	1.40	1.33
2	L	193	ACO	O9P-C9P	-2.88	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	193	ACO	O4B-C1B	-2.82	1.37	1.41
2	L	195	ACO	O4B-C1B	-2.82	1.37	1.41
2	F	195	ACO	C3B-C4B	-2.77	1.45	1.52
2	I	195	ACO	O4B-C1B	-2.76	1.37	1.41
2	L	195	ACO	C3B-C4B	-2.75	1.45	1.52
2	E	195	ACO	O9P-C9P	-2.73	1.18	1.23
2	F	195	ACO	C5P-N4P	2.73	1.39	1.33
2	A	195	ACO	C5P-N4P	2.71	1.39	1.33
2	J	195	ACO	C6P-C5P	-2.68	1.46	1.51
2	E	195	ACO	C2B-C1B	-2.67	1.49	1.53
2	A	195	ACO	C3B-C4B	-2.66	1.45	1.52
2	F	195	ACO	O4B-C1B	-2.64	1.37	1.41
2	C	195	ACO	O9P-C9P	-2.64	1.18	1.23
2	H	195	ACO	C3B-C4B	-2.63	1.45	1.52
2	E	195	ACO	C6P-C5P	-2.56	1.46	1.51
2	J	195	ACO	O2B-C2B	-2.56	1.37	1.43
2	D	195	ACO	C6A-N6A	2.55	1.43	1.34
2	A	193	ACO	O2B-C2B	-2.52	1.37	1.43
2	C	195	ACO	C5P-N4P	2.52	1.39	1.33
2	E	195	ACO	P3B-O9A	-2.51	1.45	1.54
2	J	195	ACO	O9P-C9P	-2.51	1.18	1.23
2	E	195	ACO	O2B-C2B	-2.50	1.37	1.43
2	A	193	ACO	O9P-C9P	-2.49	1.18	1.23
2	I	193	ACO	O4B-C1B	-2.48	1.37	1.41
2	I	195	ACO	O2B-C2B	-2.48	1.37	1.43
2	I	195	ACO	C3B-C4B	-2.48	1.46	1.52
2	A	195	ACO	O4B-C1B	-2.46	1.37	1.41
2	H	195	ACO	C5B-C4B	-2.45	1.43	1.51
2	D	195	ACO	C3B-C4B	-2.45	1.46	1.52
2	H	195	ACO	P3B-O9A	-2.45	1.45	1.54
2	L	193	ACO	O2B-C2B	-2.44	1.37	1.43
2	J	195	ACO	C3B-C4B	-2.43	1.46	1.52
2	F	195	ACO	C5B-C4B	-2.42	1.44	1.51
2	L	193	ACO	P3B-O9A	-2.42	1.45	1.54
2	C	195	ACO	C3B-C4B	-2.42	1.46	1.52
2	E	195	ACO	C3B-C4B	-2.41	1.46	1.52
2	F	195	ACO	O2B-C2B	-2.41	1.37	1.43
2	D	195	ACO	C2B-C1B	-2.41	1.50	1.53
2	I	195	ACO	C5P-N4P	2.41	1.38	1.33
2	L	193	ACO	C5B-C4B	-2.37	1.44	1.51
2	A	195	ACO	C5B-C4B	-2.37	1.44	1.51
2	L	195	ACO	O9P-C9P	-2.37	1.18	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	195	ACO	P3B-O9A	-2.37	1.45	1.54
2	J	195	ACO	C5B-C4B	-2.36	1.44	1.51
2	L	195	ACO	O2B-C2B	-2.36	1.37	1.43
2	C	195	ACO	C5B-C4B	-2.35	1.44	1.51
2	A	193	ACO	C3B-C4B	-2.35	1.46	1.52
2	E	195	ACO	C5B-C4B	-2.34	1.44	1.51
2	A	195	ACO	O2B-C2B	-2.33	1.37	1.43
2	L	195	ACO	C5B-C4B	-2.32	1.44	1.51
2	E	195	ACO	P3B-O8A	-2.30	1.46	1.54
2	A	195	ACO	P3B-O9A	-2.29	1.46	1.54
2	A	193	ACO	C5P-N4P	2.29	1.38	1.33
2	F	195	ACO	O9P-C9P	-2.29	1.18	1.23
2	L	193	ACO	C6P-C5P	-2.29	1.47	1.51
2	I	193	ACO	C3B-C4B	-2.29	1.46	1.52
2	C	195	ACO	C6P-C5P	-2.28	1.47	1.51
2	L	193	ACO	P3B-O8A	-2.25	1.46	1.54
2	I	195	ACO	C5B-C4B	-2.24	1.44	1.51
2	J	195	ACO	P3B-O9A	-2.23	1.46	1.54
2	I	193	ACO	C6A-N6A	2.21	1.42	1.34
2	A	195	ACO	O9P-C9P	-2.20	1.19	1.23
2	H	195	ACO	O2B-C2B	-2.19	1.37	1.43
2	I	193	ACO	C5B-C4B	-2.17	1.44	1.51
2	A	193	ACO	C5B-C4B	-2.17	1.44	1.51
2	L	193	ACO	C5P-N4P	2.17	1.38	1.33
2	L	195	ACO	P3B-O9A	-2.14	1.46	1.54
2	I	193	ACO	O2B-C2B	-2.14	1.37	1.43
2	I	195	ACO	P3B-O9A	-2.13	1.46	1.54
2	H	195	ACO	P3B-O8A	-2.13	1.46	1.54
2	F	195	ACO	C6P-C5P	-2.11	1.47	1.51
2	L	195	ACO	C5P-N4P	2.09	1.38	1.33
2	H	195	ACO	O9P-C9P	-2.08	1.19	1.23
2	C	195	ACO	O2B-C2B	-2.05	1.38	1.43
2	I	195	ACO	C6A-N6A	2.05	1.41	1.34
2	J	195	ACO	C6A-N6A	2.04	1.41	1.34
2	A	193	ACO	C6A-N6A	2.02	1.41	1.34
2	F	195	ACO	P3B-O9A	-2.02	1.47	1.54
2	J	195	ACO	C5P-N4P	2.01	1.38	1.33
2	I	195	ACO	C6P-C5P	-2.00	1.47	1.51

All (99) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	193	ACO	O6A-CCP-CBP	6.60	121.15	110.55
2	F	195	ACO	O6A-CCP-CBP	6.06	120.29	110.55
2	J	195	ACO	O6A-CCP-CBP	5.50	119.38	110.55
2	C	195	ACO	N3A-C2A-N1A	-4.83	121.14	128.68
2	L	193	ACO	N3A-C2A-N1A	-4.65	121.41	128.68
2	A	195	ACO	N3A-C2A-N1A	-4.60	121.48	128.68
2	D	195	ACO	O6A-CCP-CBP	4.46	117.71	110.55
2	H	195	ACO	O6A-CCP-CBP	4.42	117.65	110.55
2	J	195	ACO	N3A-C2A-N1A	-4.41	121.78	128.68
2	H	195	ACO	N3A-C2A-N1A	-4.40	121.80	128.68
2	L	195	ACO	N3A-C2A-N1A	-4.37	121.84	128.68
2	D	195	ACO	N3A-C2A-N1A	-4.30	121.95	128.68
2	A	193	ACO	N3A-C2A-N1A	-4.28	121.98	128.68
2	I	193	ACO	N3A-C2A-N1A	-4.27	122.01	128.68
2	E	195	ACO	N3A-C2A-N1A	-4.13	122.22	128.68
2	D	195	ACO	O5B-C5B-C4B	4.12	123.19	108.99
2	A	195	ACO	O6A-CCP-CBP	4.12	117.17	110.55
2	I	195	ACO	N3A-C2A-N1A	-4.11	122.26	128.68
2	C	195	ACO	O6A-CCP-CBP	4.06	117.08	110.55
2	F	195	ACO	N3A-C2A-N1A	-4.03	122.39	128.68
2	L	193	ACO	O5B-C5B-C4B	3.84	122.19	108.99
2	F	195	ACO	O5B-C5B-C4B	3.81	122.09	108.99
2	I	195	ACO	O6A-CCP-CBP	3.77	116.61	110.55
2	I	193	ACO	O5B-C5B-C4B	3.66	121.57	108.99
2	I	195	ACO	O5B-C5B-C4B	3.65	121.57	108.99
2	C	195	ACO	O5B-C5B-C4B	3.58	121.33	108.99
2	L	195	ACO	O6A-CCP-CBP	3.54	116.25	110.55
2	I	193	ACO	O6A-CCP-CBP	3.50	116.17	110.55
2	I	193	ACO	C7P-C6P-C5P	3.46	118.12	112.36
2	J	195	ACO	C1B-N9A-C4A	-3.45	120.58	126.64
2	F	195	ACO	C2P-C3P-N4P	3.27	119.28	112.42
2	H	195	ACO	C7P-C6P-C5P	3.24	117.75	112.36
2	H	195	ACO	C6P-C7P-N8P	3.22	118.40	111.90
2	H	195	ACO	O5B-C5B-C4B	3.13	119.78	108.99
2	E	195	ACO	O6A-CCP-CBP	3.13	115.58	110.55
2	A	193	ACO	C7P-C6P-C5P	3.08	117.48	112.36
2	J	195	ACO	O5B-C5B-C4B	3.07	119.57	108.99
2	D	195	ACO	C3B-C2B-C1B	3.05	106.65	99.89
2	L	195	ACO	O5B-C5B-C4B	2.98	119.26	108.99
2	J	195	ACO	OAP-CAP-CBP	2.97	117.24	110.25
2	L	193	ACO	O6A-CCP-CBP	2.93	115.26	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	195	ACO	O5B-C5B-C4B	2.91	119.02	108.99
2	L	195	ACO	P2A-O3A-P1A	-2.82	123.14	132.83
2	L	193	ACO	C5B-C4B-C3B	-2.71	105.40	114.40
2	I	195	ACO	O9P-C9P-N8P	-2.69	117.22	122.99
2	A	193	ACO	P2A-O3A-P1A	-2.68	123.64	132.83
2	A	193	ACO	O9P-C9P-N8P	-2.65	117.31	122.99
2	I	193	ACO	P2A-O3A-P1A	-2.64	123.78	132.83
2	D	195	ACO	C2P-S1P-C	2.63	115.51	101.68
2	C	195	ACO	C6P-C7P-N8P	2.63	117.20	111.90
2	A	195	ACO	P2A-O3A-P1A	-2.61	123.88	132.83
2	F	195	ACO	C3P-N4P-C5P	-2.60	118.00	122.84
2	F	195	ACO	C2B-C3B-C4B	2.57	107.79	103.22
2	L	195	ACO	C6P-C7P-N8P	2.57	117.08	111.90
2	H	195	ACO	P2A-O3A-P1A	-2.55	124.09	132.83
2	D	195	ACO	O5P-C5P-C6P	-2.54	117.37	122.02
2	J	195	ACO	C7P-N8P-C9P	-2.52	118.10	122.59
2	A	195	ACO	O3B-C3B-C2B	-2.51	102.60	111.68
2	A	195	ACO	C1B-N9A-C4A	-2.47	122.31	126.64
2	C	195	ACO	C1B-N9A-C4A	-2.41	122.42	126.64
2	J	195	ACO	C6P-C5P-N4P	2.39	120.44	116.42
2	J	195	ACO	C3P-N4P-C5P	-2.38	118.41	122.84
2	F	195	ACO	O9P-C9P-N8P	-2.37	117.91	122.99
4	E	196	GOL	O2-C2-C3	2.35	119.48	109.12
2	I	195	ACO	C2P-C3P-N4P	2.35	117.36	112.42
2	D	195	ACO	C2B-C3B-C4B	2.34	107.37	103.22
2	L	195	ACO	C7P-C6P-C5P	2.34	116.25	112.36
2	H	195	ACO	O4B-C1B-C2B	-2.33	103.52	106.93
2	L	195	ACO	O5P-C5P-N4P	-2.33	118.61	123.01
2	L	193	ACO	CDP-CBP-CAP	2.32	112.84	108.82
2	E	195	ACO	O5B-C5B-C4B	2.31	116.95	108.99
2	J	195	ACO	O5P-C5P-C6P	-2.29	117.83	122.02
2	L	195	ACO	C7P-N8P-C9P	-2.29	118.51	122.59
2	D	195	ACO	C3P-N4P-C5P	2.29	127.08	122.84
2	I	195	ACO	C6P-C5P-N4P	2.27	120.25	116.42
2	L	193	ACO	C6P-C5P-N4P	2.27	120.24	116.42
2	J	195	ACO	O5P-C5P-N4P	-2.20	118.85	123.01
2	F	195	ACO	C6P-C5P-N4P	2.19	120.11	116.42
2	L	193	ACO	O9P-C9P-N8P	-2.19	118.30	122.99
2	I	195	ACO	O4B-C1B-C2B	-2.19	103.73	106.93
2	I	195	ACO	CDP-CBP-CAP	2.18	112.60	108.82
2	C	195	ACO	CEP-CBP-CAP	2.18	112.60	108.82
2	L	193	ACO	O5P-C5P-N4P	-2.17	118.92	123.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	193	ACO	C3P-N4P-C5P	-2.17	118.81	122.84
2	H	195	ACO	O9P-C9P-N8P	-2.16	118.35	122.99
2	I	195	ACO	O3B-C3B-C2B	-2.15	103.90	111.68
2	F	195	ACO	C3B-C2B-C1B	2.14	104.64	99.89
2	A	193	ACO	O5B-C5B-C4B	2.12	116.30	108.99
2	H	195	ACO	C1B-N9A-C4A	-2.11	122.94	126.64
2	A	195	ACO	C2P-S1P-C	2.10	112.72	101.68
2	L	195	ACO	O9P-C9P-N8P	-2.09	118.51	122.99
2	E	195	ACO	OAP-CAP-CBP	2.08	115.14	110.25
2	E	195	ACO	C4A-C5A-N7A	-2.06	107.25	109.40
2	A	193	ACO	C4A-C5A-N7A	-2.05	107.26	109.40
2	I	195	ACO	O-C-CH3	-2.04	114.70	123.07
4	L	196	GOL	C3-C2-C1	-2.03	103.79	111.70
2	I	195	ACO	C6P-C7P-N8P	2.03	116.00	111.90
3	K	198	ACY	O-C-CH3	-2.03	114.44	122.33
2	L	195	ACO	C1B-N9A-C4A	-2.03	123.08	126.64

There are no chirality outliers.

All (218) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	195	ACO	C3B-O3B-P3B-O7A
2	A	195	ACO	C3B-C4B-C5B-O5B
2	A	195	ACO	C5B-O5B-P1A-O1A
2	A	195	ACO	C5B-O5B-P1A-O2A
2	A	195	ACO	P2A-O3A-P1A-O5B
2	A	195	ACO	CCP-O6A-P2A-O3A
2	A	195	ACO	CCP-O6A-P2A-O5A
2	A	195	ACO	O9P-C9P-CAP-CBP
2	A	195	ACO	O9P-C9P-CAP-OAP
2	A	195	ACO	C5P-C6P-C7P-N8P
2	A	195	ACO	S1P-C2P-C3P-N4P
2	A	195	ACO	O-C-S1P-C2P
2	A	195	ACO	CH3-C-S1P-C2P
2	A	193	ACO	C3B-O3B-P3B-O7A
2	A	193	ACO	C3B-C4B-C5B-O5B
2	A	193	ACO	O4B-C4B-C5B-O5B
2	A	193	ACO	C5B-O5B-P1A-O1A
2	A	193	ACO	C5B-O5B-P1A-O2A
2	A	193	ACO	C9P-CAP-CBP-CCP
2	A	193	ACO	O9P-C9P-CAP-CBP
2	A	193	ACO	S1P-C2P-C3P-N4P

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Mol	Chain	Res	Type	Atoms
2	A	193	ACO	C3P-C2P-S1P-C
2	A	193	ACO	O-C-S1P-C2P
2	C	195	ACO	C3B-O3B-P3B-O7A
2	C	195	ACO	C3B-C4B-C5B-O5B
2	C	195	ACO	O4B-C4B-C5B-O5B
2	C	195	ACO	C5B-O5B-P1A-O2A
2	C	195	ACO	C5B-O5B-P1A-O3A
2	C	195	ACO	CCP-O6A-P2A-O4A
2	C	195	ACO	C9P-CAP-CBP-CCP
2	C	195	ACO	OAP-CAP-CBP-CDP
2	C	195	ACO	C9P-CAP-CBP-CDP
2	C	195	ACO	C9P-CAP-CBP-CEP
2	C	195	ACO	O9P-C9P-CAP-CBP
2	D	195	ACO	C4B-C3B-O3B-P3B
2	D	195	ACO	C5B-O5B-P1A-O2A
2	D	195	ACO	C5B-O5B-P1A-O3A
2	D	195	ACO	P2A-O3A-P1A-O5B
2	D	195	ACO	C5P-C6P-C7P-N8P
2	D	195	ACO	O5P-C5P-N4P-C3P
2	D	195	ACO	C3P-C2P-S1P-C
2	D	195	ACO	O-C-S1P-C2P
2	D	195	ACO	CH3-C-S1P-C2P
2	E	195	ACO	C5B-O5B-P1A-O1A
2	E	195	ACO	C5B-O5B-P1A-O2A
2	E	195	ACO	P1A-O3A-P2A-O6A
2	E	195	ACO	CCP-O6A-P2A-O4A
2	E	195	ACO	CCP-O6A-P2A-O5A
2	E	195	ACO	CDP-CBP-CCP-O6A
2	E	195	ACO	CEP-CBP-CCP-O6A
2	E	195	ACO	CAP-CBP-CCP-O6A
2	F	195	ACO	C4B-C3B-O3B-P3B
2	F	195	ACO	C3B-C4B-C5B-O5B
2	F	195	ACO	O4B-C4B-C5B-O5B
2	F	195	ACO	CCP-O6A-P2A-O5A
2	F	195	ACO	CDP-CBP-CCP-O6A
2	F	195	ACO	CEP-CBP-CCP-O6A
2	F	195	ACO	CAP-CBP-CCP-O6A
2	F	195	ACO	O-C-S1P-C2P
2	F	195	ACO	CH3-C-S1P-C2P
2	H	195	ACO	C3B-O3B-P3B-O7A
2	H	195	ACO	C3B-C4B-C5B-O5B
2	H	195	ACO	CAP-CBP-CCP-O6A

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Mol	Chain	Res	Type	Atoms
2	H	195	ACO	OAP-CAP-CBP-CCP
2	H	195	ACO	OAP-CAP-CBP-CDP
2	H	195	ACO	OAP-CAP-CBP-CEP
2	H	195	ACO	S1P-C2P-C3P-N4P
2	H	195	ACO	C3P-C2P-S1P-C
2	H	195	ACO	O-C-S1P-C2P
2	H	195	ACO	CH3-C-S1P-C2P
2	I	195	ACO	CCP-O6A-P2A-O4A
2	I	195	ACO	C3P-C2P-S1P-C
2	I	193	ACO	C3B-C4B-C5B-O5B
2	I	193	ACO	O4B-C4B-C5B-O5B
2	I	193	ACO	P2A-O3A-P1A-O5B
2	I	193	ACO	OAP-CAP-CBP-CCP
2	I	193	ACO	OAP-CAP-CBP-CDP
2	I	193	ACO	C3P-C2P-S1P-C
2	I	193	ACO	O-C-S1P-C2P
2	I	193	ACO	CH3-C-S1P-C2P
2	J	195	ACO	C3B-C4B-C5B-O5B
2	J	195	ACO	O4B-C4B-C5B-O5B
2	J	195	ACO	CDP-CBP-CCP-O6A
2	J	195	ACO	CEP-CBP-CCP-O6A
2	J	195	ACO	CAP-CBP-CCP-O6A
2	J	195	ACO	OAP-CAP-CBP-CCP
2	J	195	ACO	OAP-CAP-CBP-CDP
2	J	195	ACO	C9P-CAP-CBP-CDP
2	J	195	ACO	OAP-CAP-CBP-CEP
2	J	195	ACO	O-C-S1P-C2P
2	J	195	ACO	CH3-C-S1P-C2P
2	L	195	ACO	C5B-O5B-P1A-O3A
2	L	195	ACO	CCP-O6A-P2A-O4A
2	L	195	ACO	O-C-S1P-C2P
2	L	195	ACO	CH3-C-S1P-C2P
2	L	193	ACO	C5B-O5B-P1A-O3A
2	L	193	ACO	CCP-O6A-P2A-O3A
2	L	193	ACO	CDP-CBP-CCP-O6A
2	L	193	ACO	CAP-CBP-CCP-O6A
2	L	193	ACO	OAP-CAP-CBP-CCP
2	L	193	ACO	OAP-CAP-CBP-CDP
2	L	193	ACO	O-C-S1P-C2P
2	L	193	ACO	CH3-C-S1P-C2P
4	B	196	GOL	O1-C1-C2-C3
4	E	196	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
2	L	195	ACO	O5P-C5P-N4P-C3P
2	A	195	ACO	O4B-C4B-C5B-O5B
2	E	195	ACO	O4B-C4B-C5B-O5B
2	H	195	ACO	O4B-C4B-C5B-O5B
2	D	195	ACO	C6P-C5P-N4P-C3P
2	E	195	ACO	C3B-C4B-C5B-O5B
2	I	195	ACO	C3B-C4B-C5B-O5B
2	A	195	ACO	O5P-C5P-N4P-C3P
2	H	195	ACO	CDP-CBP-CCP-O6A
2	H	195	ACO	CEP-CBP-CCP-O6A
2	L	193	ACO	CEP-CBP-CCP-O6A
2	L	193	ACO	O5P-C5P-N4P-C3P
4	E	196	GOL	C1-C2-C3-O3
4	L	196	GOL	O1-C1-C2-C3
4	B	196	GOL	O1-C1-C2-O2
2	I	195	ACO	O4B-C4B-C5B-O5B
2	A	193	ACO	CH3-C-S1P-C2P
2	C	195	ACO	O-C-S1P-C2P
2	C	195	ACO	CH3-C-S1P-C2P
2	J	195	ACO	O9P-C9P-CAP-OAP
2	L	195	ACO	O9P-C9P-CAP-OAP
2	L	193	ACO	O9P-C9P-CAP-OAP
4	L	196	GOL	O1-C1-C2-O2
2	L	195	ACO	C6P-C5P-N4P-C3P
2	L	193	ACO	C3B-C4B-C5B-O5B
2	I	195	ACO	CDP-CBP-CCP-O6A
2	I	195	ACO	CEP-CBP-CCP-O6A
2	L	195	ACO	CDP-CBP-CCP-O6A
2	L	195	ACO	CEP-CBP-CCP-O6A
2	C	195	ACO	OAP-CAP-CBP-CEP
2	I	193	ACO	OAP-CAP-CBP-CEP
2	L	193	ACO	OAP-CAP-CBP-CEP
2	F	195	ACO	O9P-C9P-CAP-CBP
2	I	195	ACO	O9P-C9P-CAP-CBP
2	L	193	ACO	C2P-C3P-N4P-C5P
2	D	195	ACO	O4B-C4B-C5B-O5B
2	L	193	ACO	C3P-C2P-S1P-C
2	A	193	ACO	P2A-O3A-P1A-O5B
2	A	193	ACO	P1A-O3A-P2A-O6A
2	C	195	ACO	P2A-O3A-P1A-O5B
2	C	195	ACO	P1A-O3A-P2A-O6A
2	E	195	ACO	P2A-O3A-P1A-O5B

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Mol	Chain	Res	Type	Atoms
2	F	195	ACO	P2A-O3A-P1A-O5B
2	H	195	ACO	P2A-O3A-P1A-O5B
2	I	195	ACO	P2A-O3A-P1A-O5B
2	J	195	ACO	P2A-O3A-P1A-O5B
2	J	195	ACO	P1A-O3A-P2A-O6A
2	A	195	ACO	N8P-C9P-CAP-OAP
2	E	195	ACO	C3B-O3B-P3B-O7A
2	I	193	ACO	N8P-C9P-CAP-OAP
2	A	193	ACO	C9P-CAP-CBP-CEP
2	I	193	ACO	C9P-CAP-CBP-CDP
2	A	193	ACO	C5B-O5B-P1A-O3A
2	D	195	ACO	CCP-O6A-P2A-O3A
2	F	195	ACO	CCP-O6A-P2A-O3A
2	L	195	ACO	CCP-O6A-P2A-O3A
2	D	195	ACO	CCP-O6A-P2A-O5A
2	F	195	ACO	CCP-O6A-P2A-O4A
2	L	195	ACO	C5B-O5B-P1A-O1A
2	L	193	ACO	C5B-O5B-P1A-O1A
2	L	193	ACO	CCP-O6A-P2A-O4A
2	L	193	ACO	CCP-O6A-P2A-O5A
2	F	195	ACO	S1P-C2P-C3P-N4P
2	C	195	ACO	OAP-CAP-CBP-CCP
2	I	195	ACO	CAP-CBP-CCP-O6A
2	E	195	ACO	O9P-C9P-CAP-OAP
2	I	193	ACO	O9P-C9P-CAP-OAP
2	A	195	ACO	CDP-CBP-CCP-O6A
2	C	195	ACO	CDP-CBP-CCP-O6A
2	C	195	ACO	CEP-CBP-CCP-O6A
2	F	195	ACO	CAP-C9P-N8P-C7P
2	I	195	ACO	CAP-C9P-N8P-C7P
2	A	193	ACO	CDP-CBP-CCP-O6A
2	A	195	ACO	N8P-C9P-CAP-CBP
2	C	195	ACO	C3P-C2P-S1P-C
2	E	195	ACO	C3P-C2P-S1P-C
2	F	195	ACO	C3P-C2P-S1P-C
2	L	195	ACO	C3P-C2P-S1P-C
2	I	193	ACO	O9P-C9P-N8P-C7P
2	D	195	ACO	C3B-C4B-C5B-O5B
2	D	195	ACO	N8P-C9P-CAP-OAP
2	J	195	ACO	N8P-C9P-CAP-OAP
7	K	196	BU1	O5-C1-C2-C3
2	A	195	ACO	CEP-CBP-CCP-O6A

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Mol	Chain	Res	Type	Atoms
2	A	193	ACO	C9P-CAP-CBP-CDP
2	H	195	ACO	C9P-CAP-CBP-CDP
2	A	195	ACO	C3B-O3B-P3B-O9A
2	A	195	ACO	C5B-O5B-P1A-O3A
2	E	195	ACO	C3B-O3B-P3B-O8A
2	E	195	ACO	C3B-O3B-P3B-O9A
2	E	195	ACO	C5B-O5B-P1A-O3A
2	E	195	ACO	CCP-O6A-P2A-O3A
2	I	195	ACO	OAP-CAP-CBP-CEP
2	I	193	ACO	C5B-O5B-P1A-O3A
2	J	195	ACO	C5B-O5B-P1A-O3A
2	A	195	ACO	P1A-O3A-P2A-O5A
2	D	195	ACO	P2A-O3A-P1A-O1A
2	E	195	ACO	P2A-O3A-P1A-O1A
2	H	195	ACO	P2A-O3A-P1A-O1A
2	I	193	ACO	P2A-O3A-P1A-O1A
2	J	195	ACO	CBP-CCP-O6A-P2A
2	H	195	ACO	O5P-C5P-N4P-C3P
2	J	195	ACO	C4B-C5B-O5B-P1A
2	A	193	ACO	CCP-O6A-P2A-O4A
2	I	195	ACO	C5B-O5B-P1A-O1A
2	I	193	ACO	C5B-O5B-P1A-O2A
2	L	195	ACO	C5B-O5B-P1A-O2A
2	H	195	ACO	O9P-C9P-CAP-CBP
2	E	195	ACO	O9P-C9P-N8P-C7P
2	E	195	ACO	C4B-C3B-O3B-P3B
2	I	193	ACO	C4B-C5B-O5B-P1A
2	J	195	ACO	C9P-CAP-CBP-CCP
2	J	195	ACO	S1P-C2P-C3P-N4P

There are no ring outliers.

20 monomers are involved in 77 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	F	197	GOL	1	0
3	A	196	ACY	1	0
2	I	195	ACO	7	0
3	K	198	ACY	2	0
2	E	195	ACO	4	0
2	L	195	ACO	5	1
2	J	195	ACO	6	0
2	A	195	ACO	14	0

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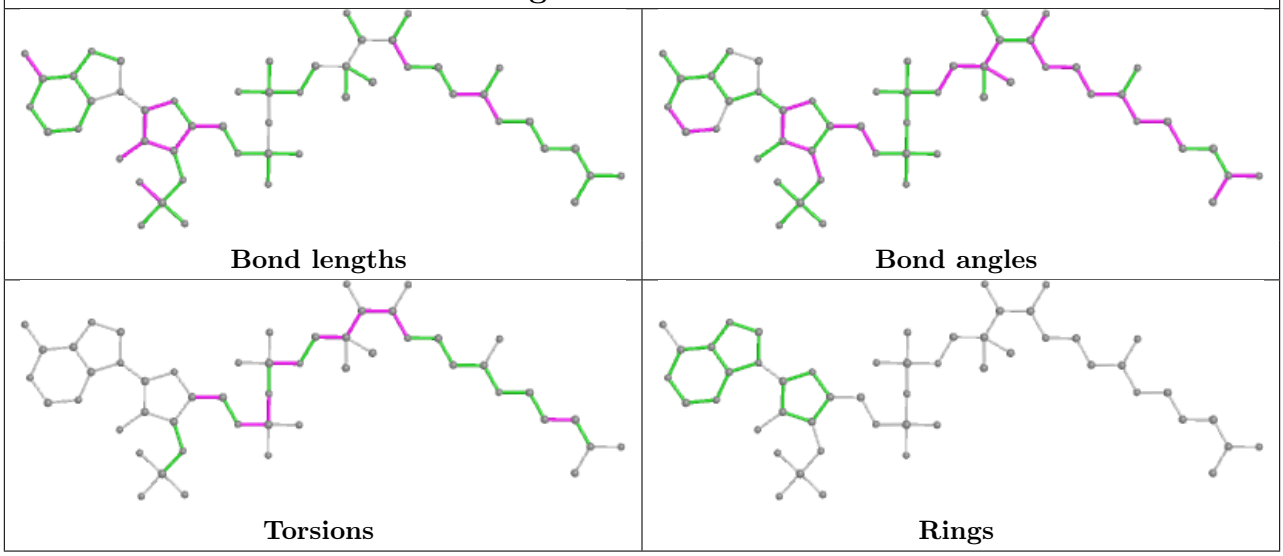
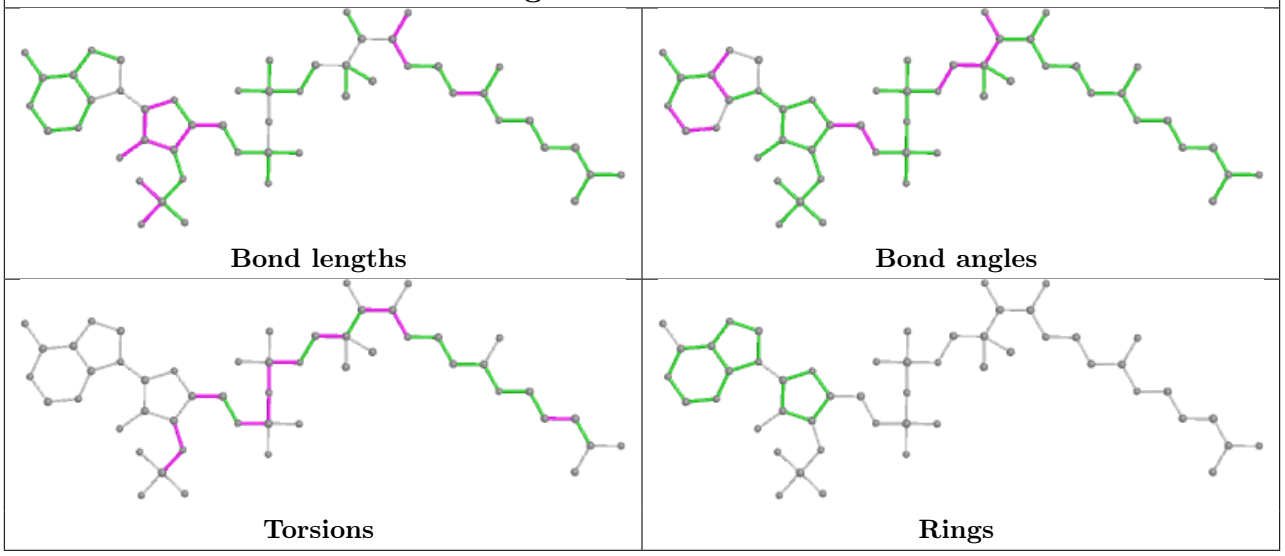
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	196	GOL	4	0
2	C	195	ACO	5	0
2	H	195	ACO	2	0
2	L	193	ACO	1	0
3	G	196	ACY	1	0
4	L	196	GOL	3	0
2	F	195	ACO	11	0
7	G	197	BU1	2	0
2	D	195	ACO	2	0
2	A	193	ACO	3	0
2	I	193	ACO	1	0
4	B	196	GOL	1	0

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.

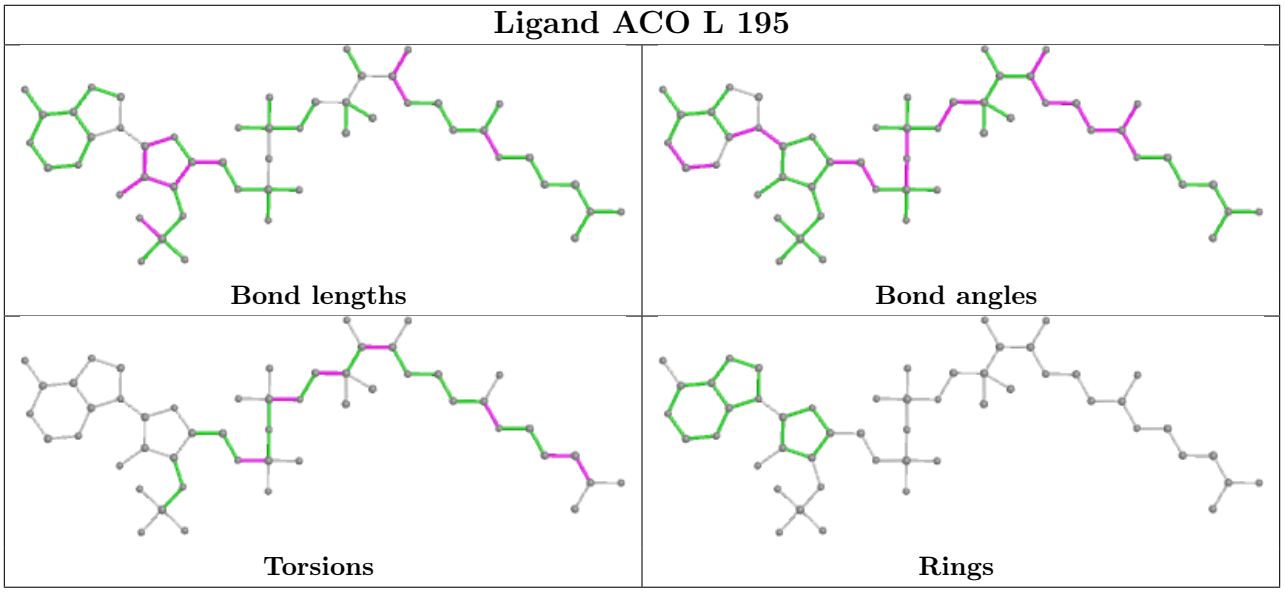
Ligand ACO I 195



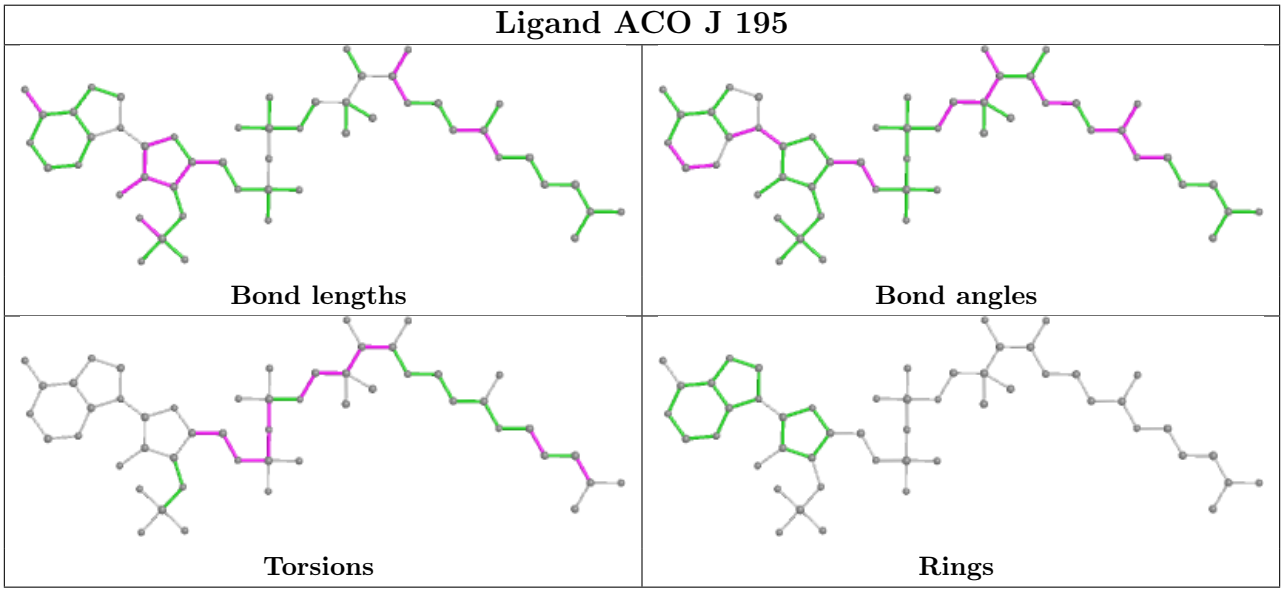
Ligand ACO E 195



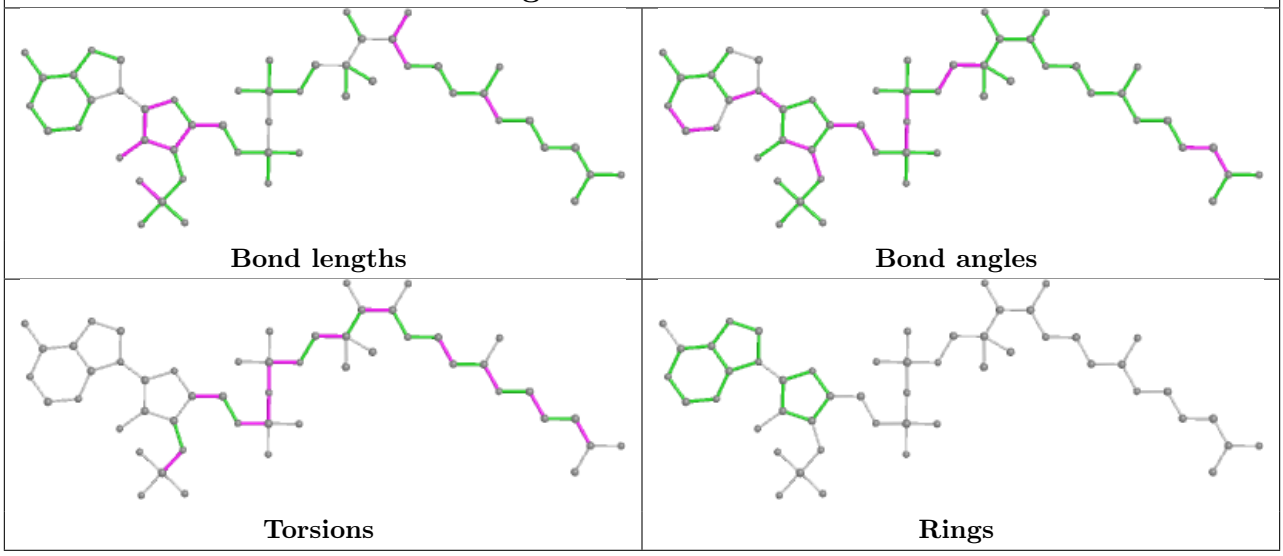
Ligand ACO L 195



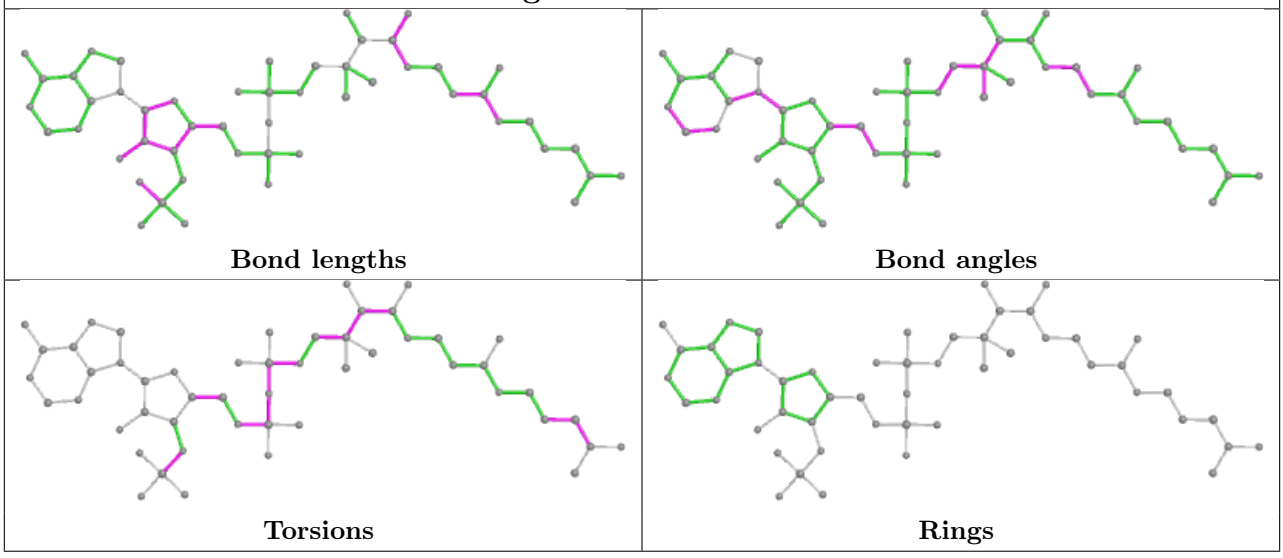
Ligand ACO J 195



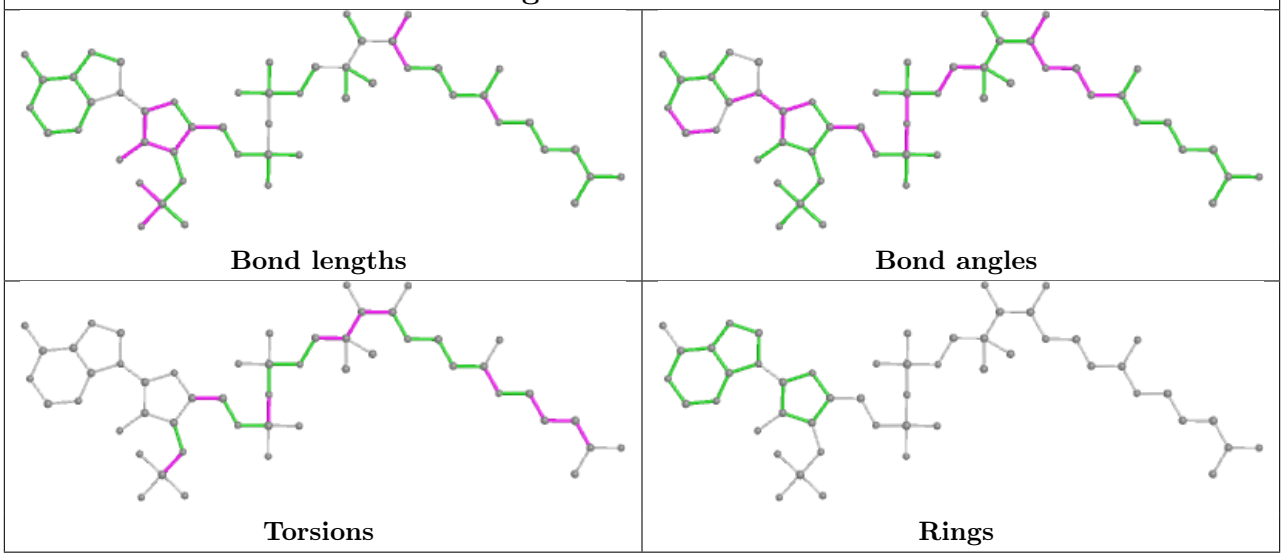
Ligand ACO A 195



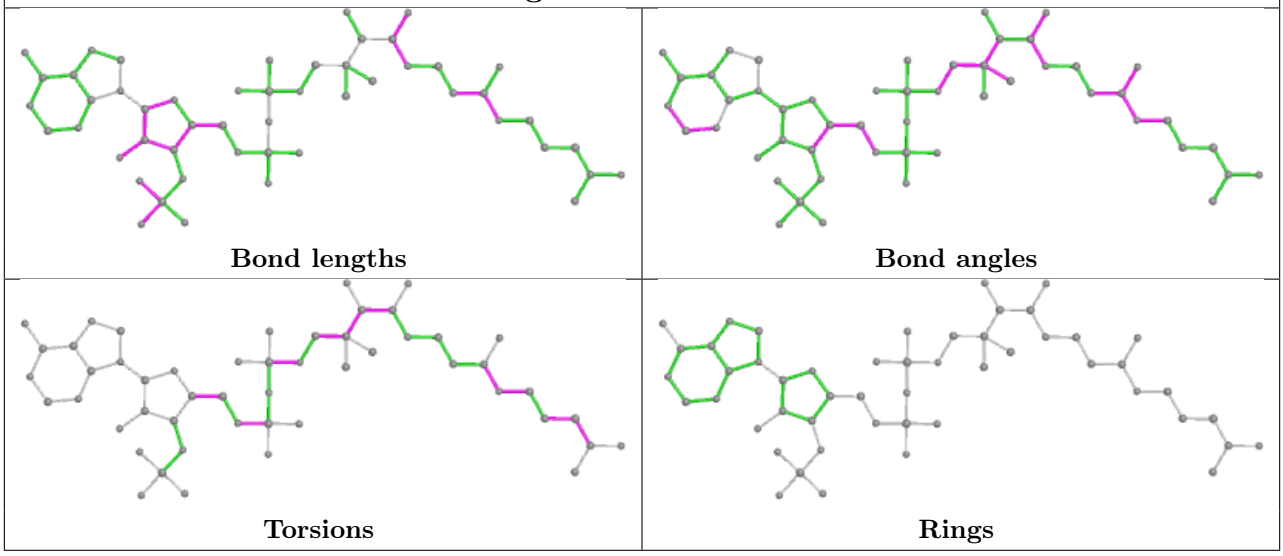
Ligand ACO C 195



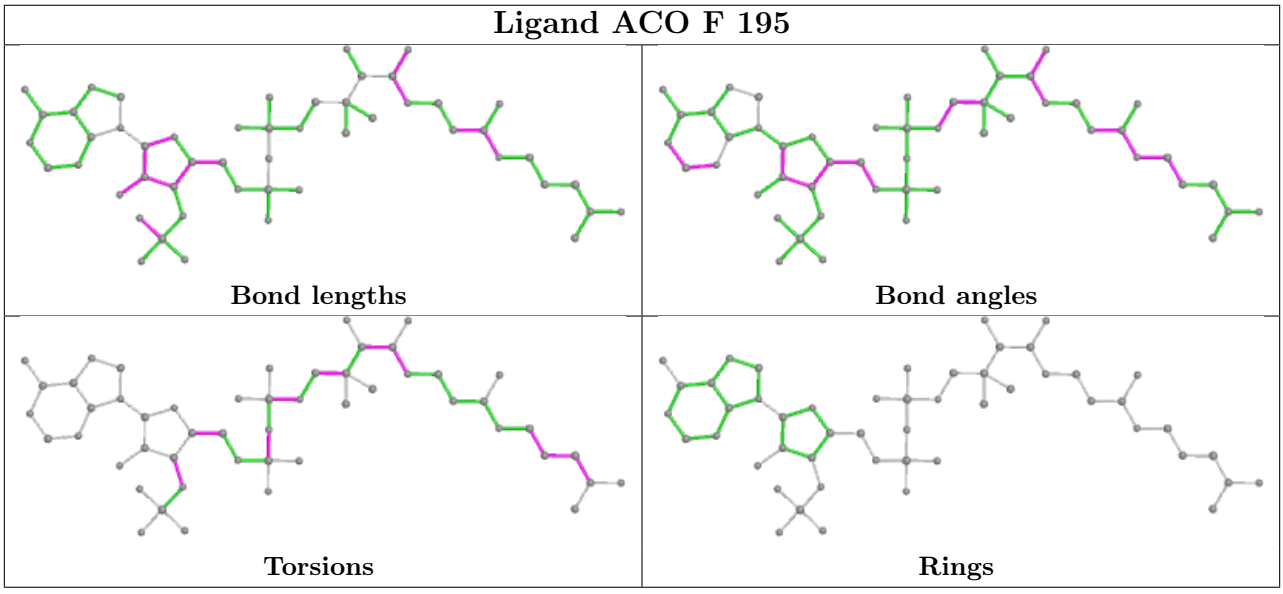
Ligand ACO H 195



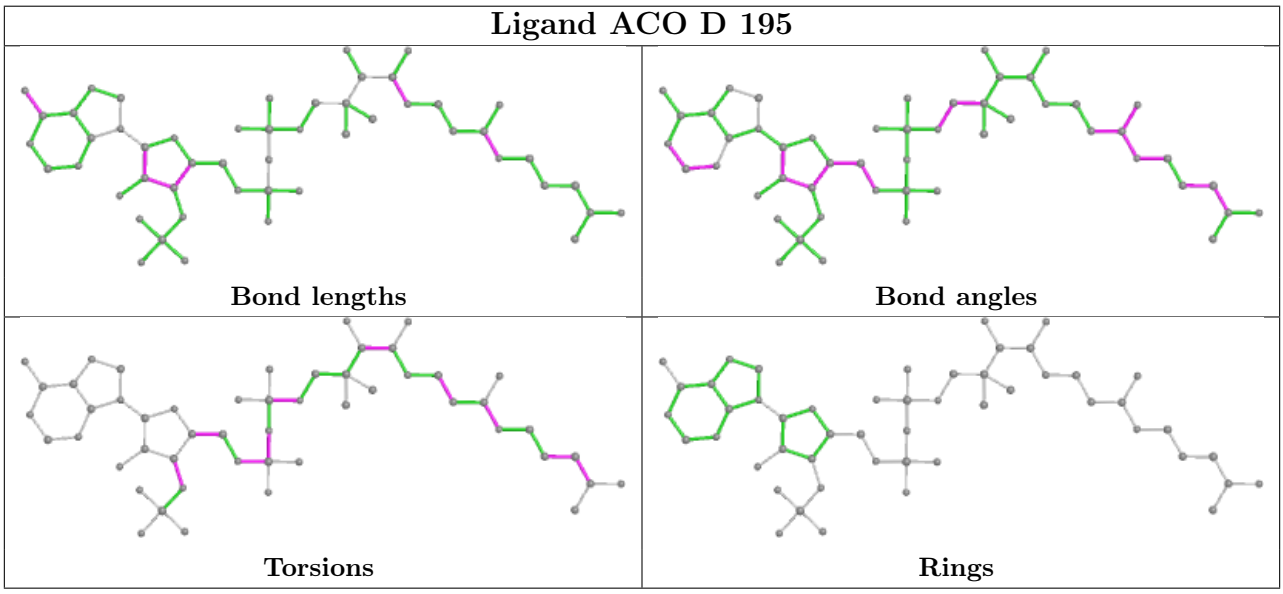
Ligand ACO L 193



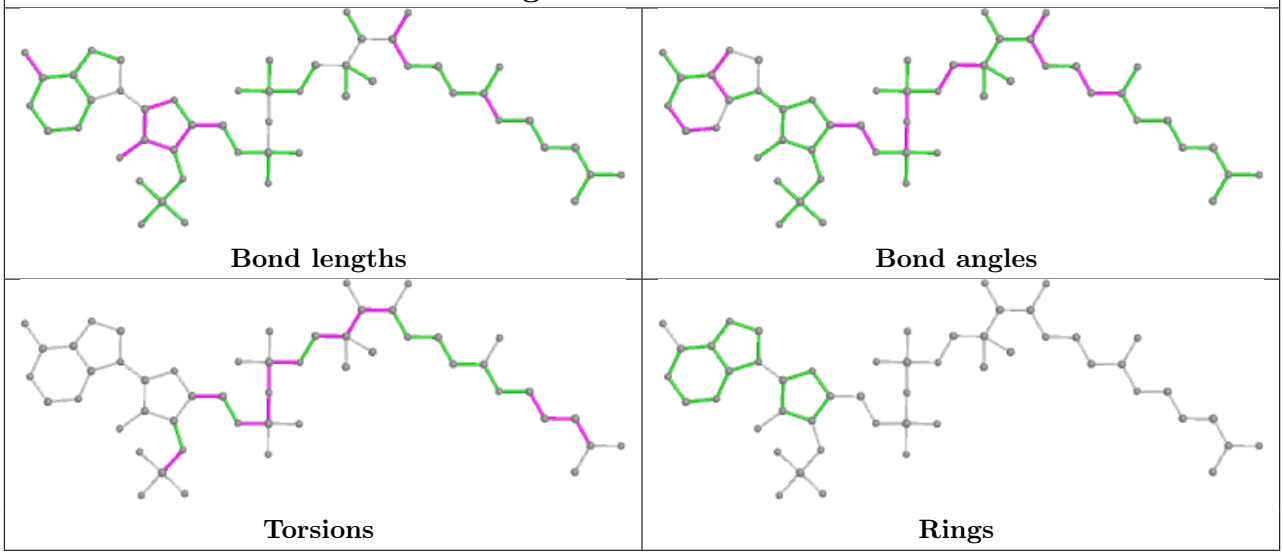
Ligand ACO F 195



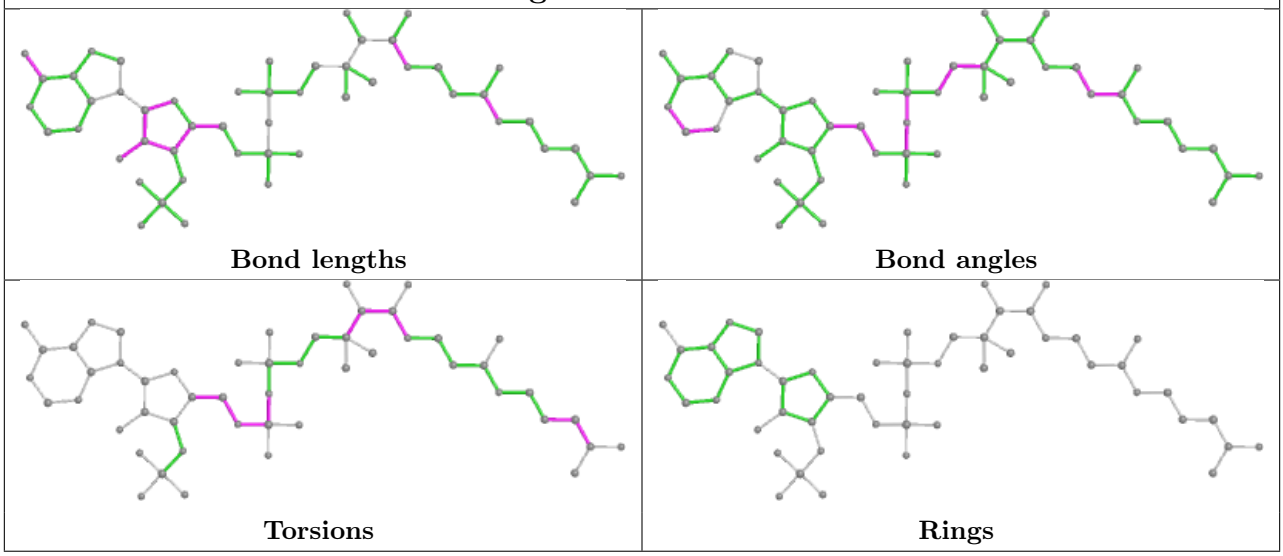
Ligand ACO D 195



Ligand ACO A 193



Ligand ACO I 193



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	178/195 (91%)	-0.32	0 100 100	10, 22, 40, 62	0
1	B	179/195 (91%)	-0.14	3 (1%) 70 78	10, 23, 47, 88	0
1	C	179/195 (91%)	-0.18	1 (0%) 89 93	11, 26, 55, 87	0
1	D	179/195 (91%)	-0.19	7 (3%) 39 52	16, 28, 59, 82	0
1	E	179/195 (91%)	-0.05	6 (3%) 45 57	11, 22, 48, 69	0
1	F	179/195 (91%)	-0.10	7 (3%) 39 52	15, 27, 53, 84	0
1	G	178/195 (91%)	-0.32	1 (0%) 89 93	13, 25, 45, 64	0
1	H	179/195 (91%)	-0.08	6 (3%) 45 57	13, 28, 61, 86	0
1	I	180/195 (92%)	-0.14	2 (1%) 80 87	15, 25, 54, 74	0
1	J	180/195 (92%)	-0.29	1 (0%) 89 93	11, 24, 48, 79	0
1	K	179/195 (91%)	-0.24	1 (0%) 89 93	10, 24, 49, 75	0
1	L	179/195 (91%)	-0.21	0 100 100	9, 20, 47, 65	0
All	All	2148/2340 (91%)	-0.19	35 (1%) 72 80	9, 24, 51, 88	0

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	K	185	ASP	4.0
1	D	6	LEU	3.7
1	H	18	ALA	3.7
1	D	185	ASP	3.4
1	I	18	ALA	3.4
1	J	0	ALA	3.3
1	C	184	LYS	3.0
1	F	184	LYS	3.0
1	E	15	PHE	2.9
1	D	18	ALA	2.8
1	F	18	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	E	18	ALA	2.7
1	B	18	ALA	2.7
1	H	4	SER	2.7
1	F	16	ASP	2.6
1	D	16	ASP	2.5
1	F	10	LEU	2.4
1	G	184	LYS	2.3
1	F	185	ASP	2.3
1	B	16	ASP	2.2
1	F	7	GLU	2.2
1	F	6	LEU	2.2
1	I	185	ASP	2.2
1	H	17	GLY	2.2
1	D	7	GLU	2.1
1	D	17	GLY	2.1
1	H	16	ASP	2.1
1	H	7	GLU	2.1
1	E	17	GLY	2.1
1	E	119	ARG	2.0
1	D	11	LYS	2.0
1	B	21	GLU	2.0
1	E	117	TYR	2.0
1	H	14	HIS	2.0
1	E	16	ASP	2.0

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

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

6.3 Carbohydrates

There are no monosaccharides in this entry.

6.4 Ligands

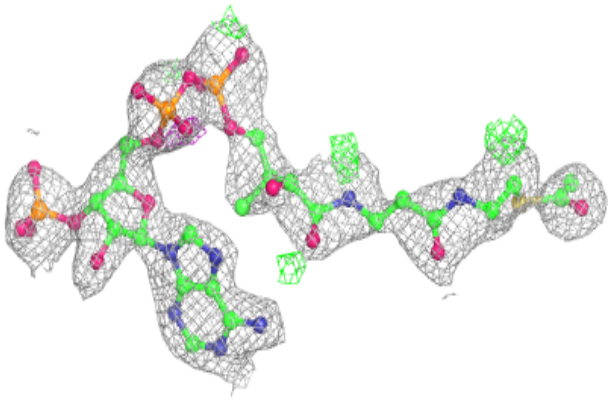
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

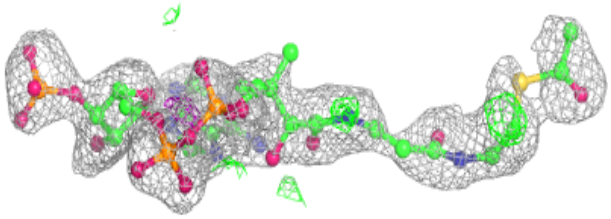
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	ACY	I	196	4/4	0.64	0.37	74,76,76,76	0
4	GOL	B	196	6/6	0.71	0.35	54,59,62,66	0
3	ACY	K	197	4/4	0.72	0.21	50,54,57,60	0
5	CL	B	197	1/1	0.79	0.16	73,73,73,73	0
3	ACY	B	198	4/4	0.81	0.30	48,64,67,68	0
3	ACY	F	196	4/4	0.81	0.21	54,59,59,59	0
6	MG	C	197[A]	1/1	0.81	0.23	38,38,38,38	1
6	MG	C	197[B]	1/1	0.81	0.23	35,35,35,35	1
2	ACO	A	193	51/51	0.83	0.19	26,59,88,114	0
3	ACY	D	197	4/4	0.83	0.22	43,45,51,54	0
4	GOL	F	197	6/6	0.83	0.25	50,57,61,64	0
7	BU1	G	197	6/6	0.83	0.20	46,50,52,52	0
2	ACO	I	195	51/51	0.85	0.18	24,67,88,93	0
2	ACO	H	195	51/51	0.85	0.17	25,51,128,131	0
3	ACY	A	196	4/4	0.87	0.21	35,36,38,42	0
2	ACO	A	195	51/51	0.87	0.18	23,60,89,152	0
2	ACO	F	195	51/51	0.88	0.16	23,52,125,132	0
2	ACO	I	193	51/51	0.88	0.18	22,64,86,104	0
3	ACY	K	198	4/4	0.88	0.19	44,49,49,50	0
2	ACO	C	195	51/51	0.89	0.18	23,40,64,70	0
5	CL	J	196	1/1	0.90	0.17	58,58,58,58	0
4	GOL	E	196	6/6	0.90	0.18	28,30,34,37	0
2	ACO	J	195	51/51	0.90	0.16	28,49,68,77	0
2	ACO	L	195	51/51	0.90	0.17	27,44,80,88	0
7	BU1	K	196	6/6	0.90	0.13	43,45,47,49	0
5	CL	C	196	1/1	0.91	0.08	61,61,61,61	0
2	ACO	D	195	51/51	0.91	0.15	5,48,85,156	0
3	ACY	G	196	4/4	0.92	0.14	24,29,33,33	0
5	CL	H	196	1/1	0.93	0.24	70,70,70,70	0
4	GOL	L	196	6/6	0.93	0.17	21,34,35,37	0
2	ACO	E	195	51/51	0.94	0.13	19,36,45,71	0
2	ACO	L	193	51/51	0.94	0.12	18,34,53,62	0
3	ACY	A	197	4/4	0.96	0.12	42,44,46,48	0
5	CL	E	193	1/1	0.96	0.12	51,51,51,51	0

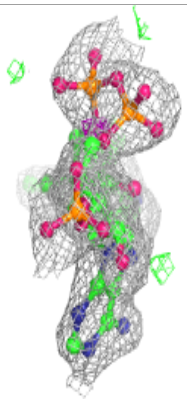
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ACO A 193:

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

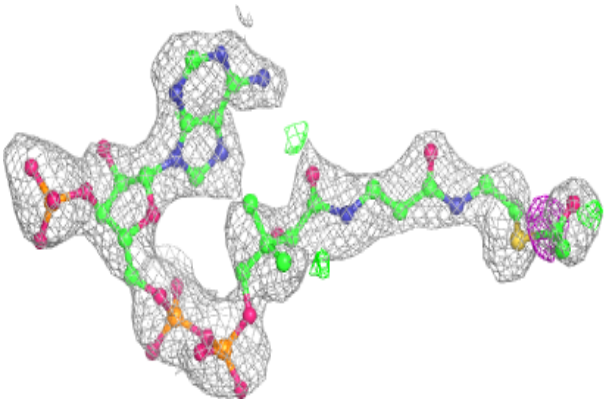


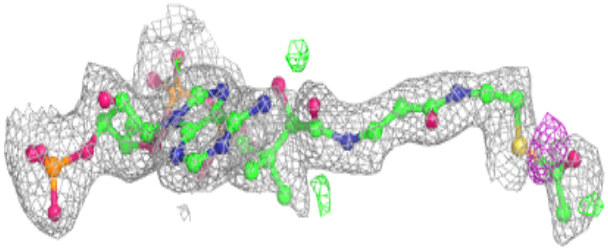


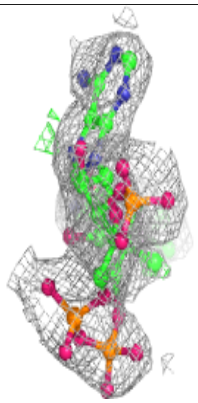


Electron density around ACO I 195:

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

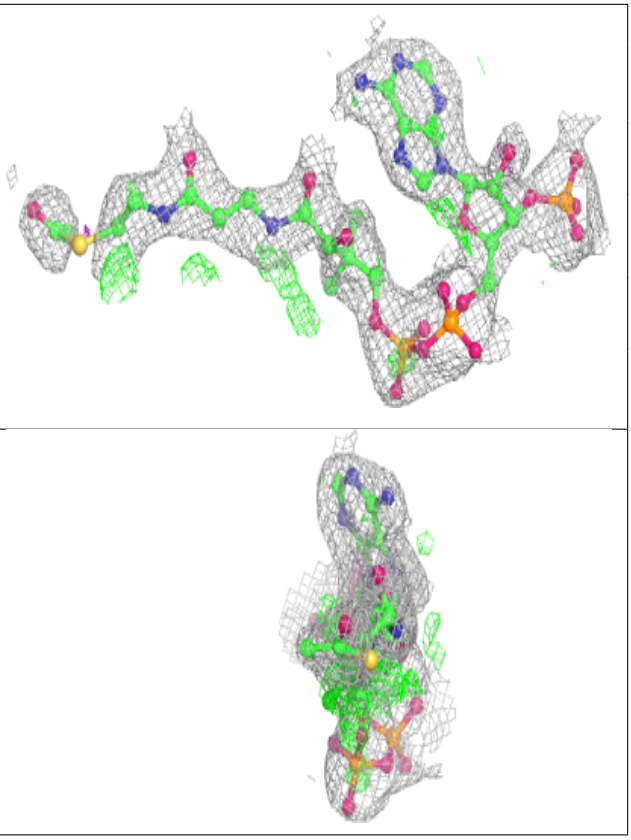






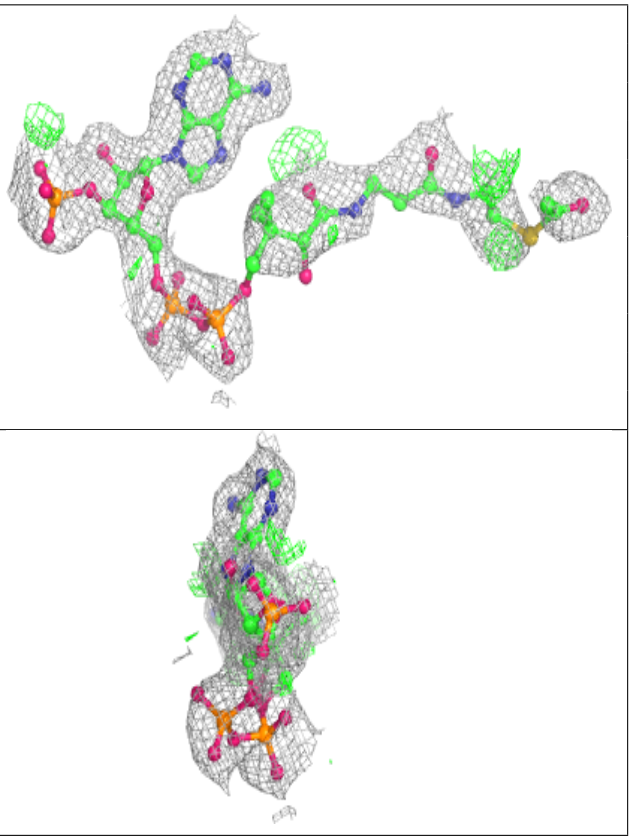
Electron density around ACO H 195:

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



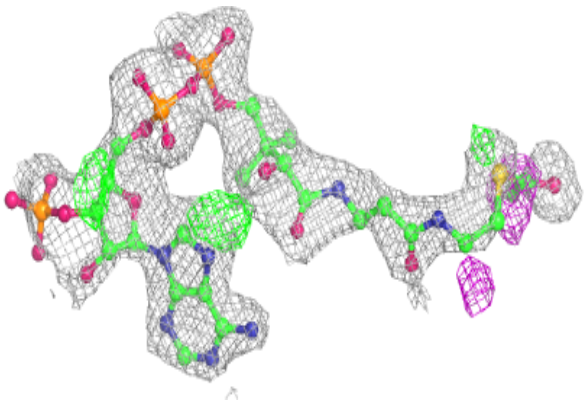
Electron density around ACO A 195:

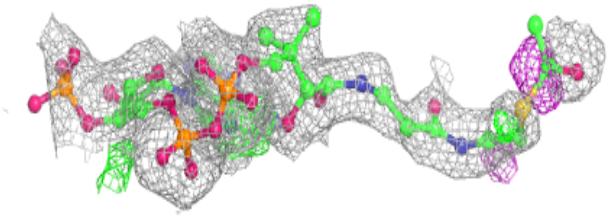
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

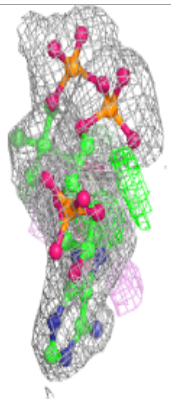


Electron density around ACO F 195:

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

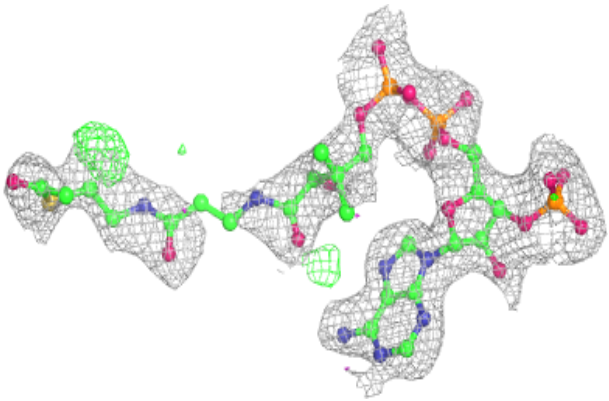


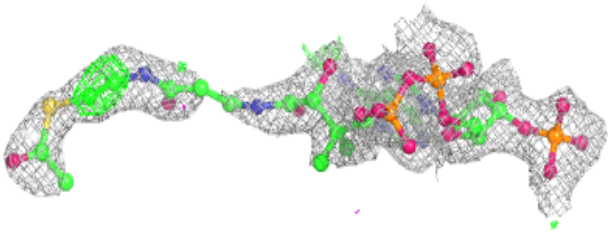


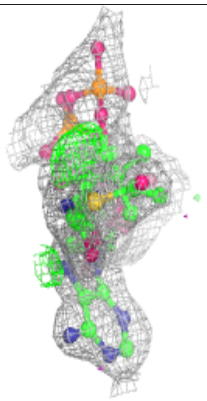


Electron density around ACO I 193:

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

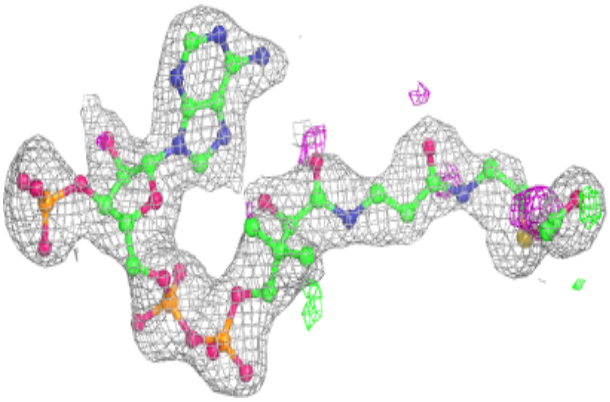


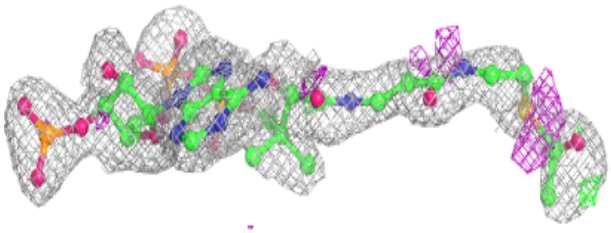


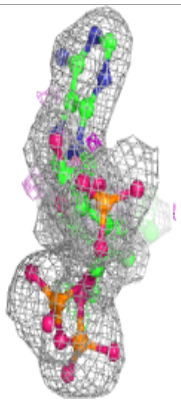


Electron density around ACO C 195:

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

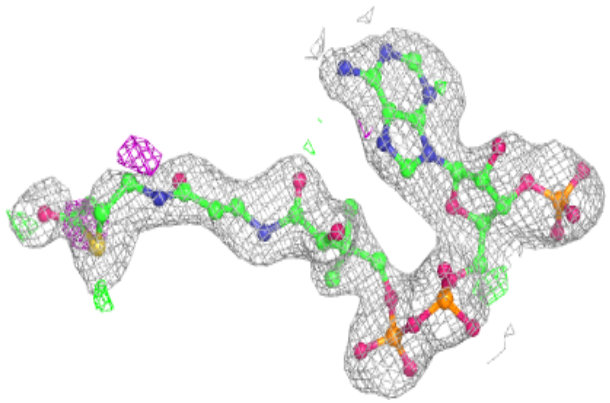


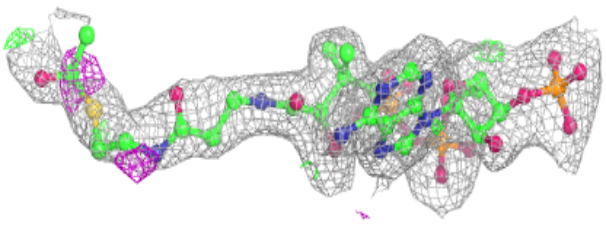


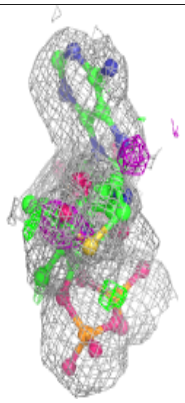


Electron density around ACO J 195:

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

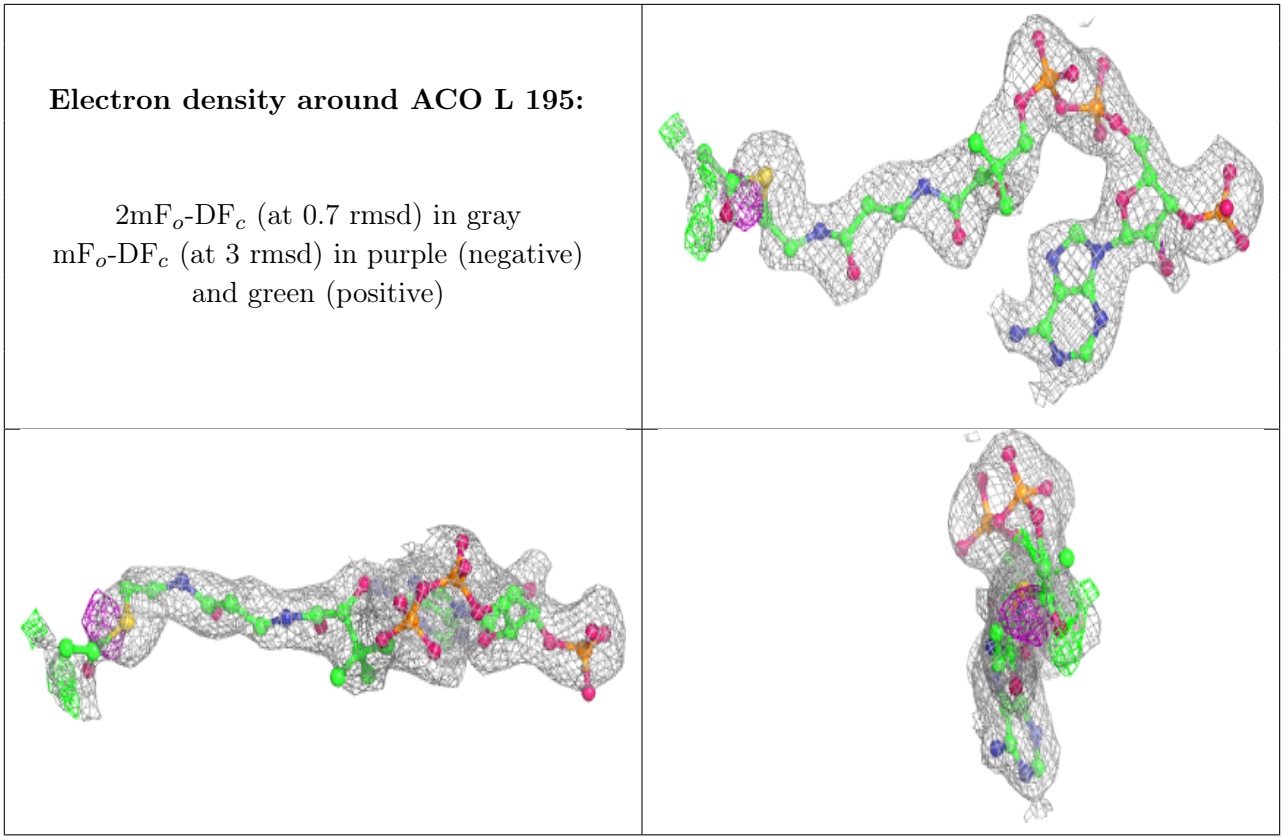






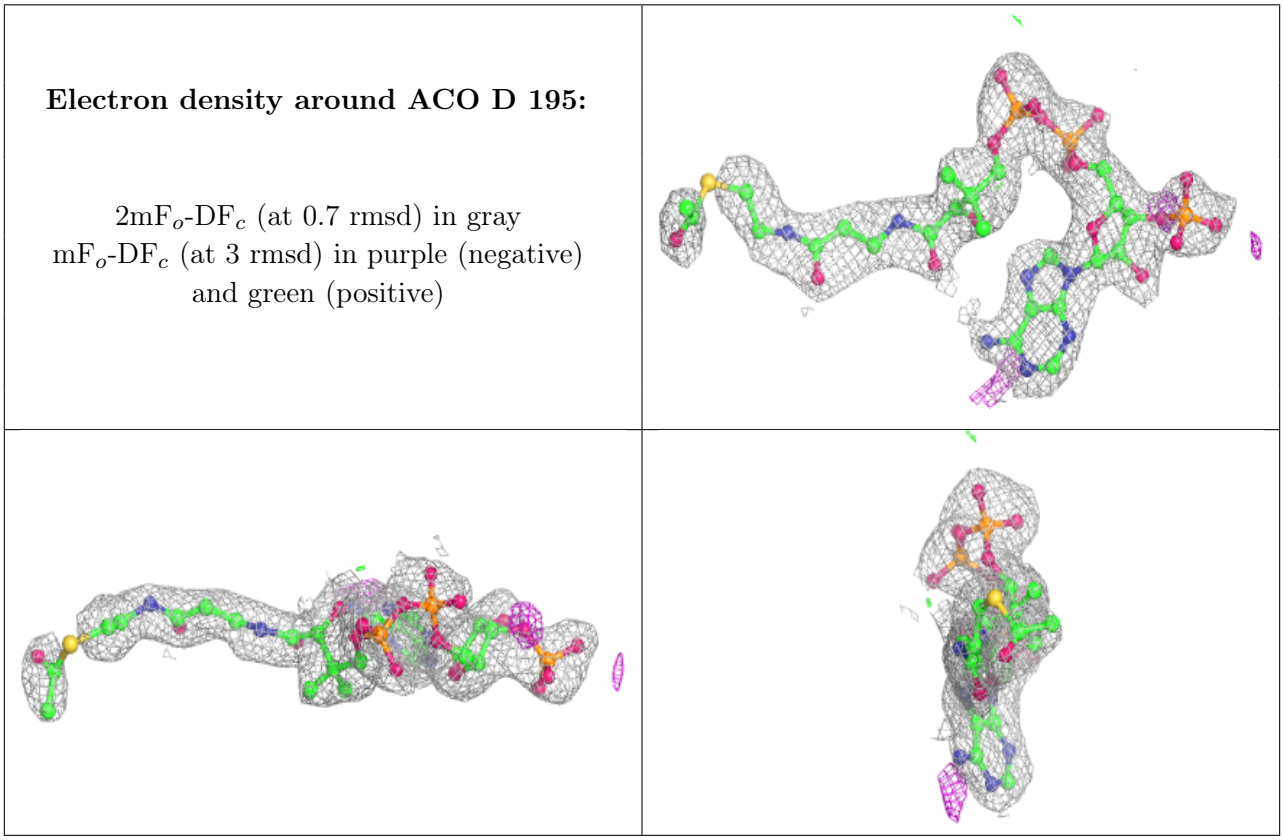
Electron density around ACO L 195:

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



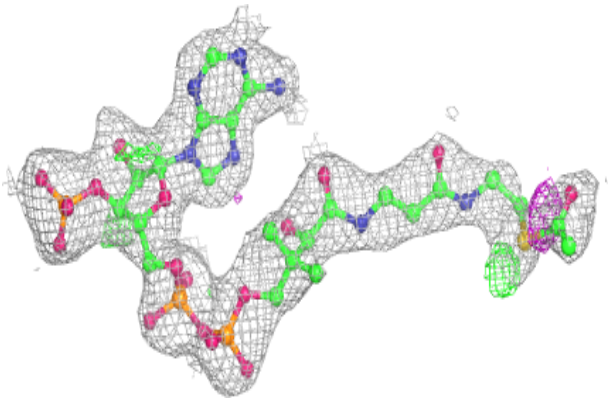
Electron density around ACO D 195:

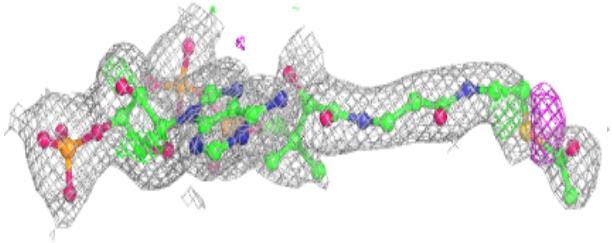
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around ACO E 195:

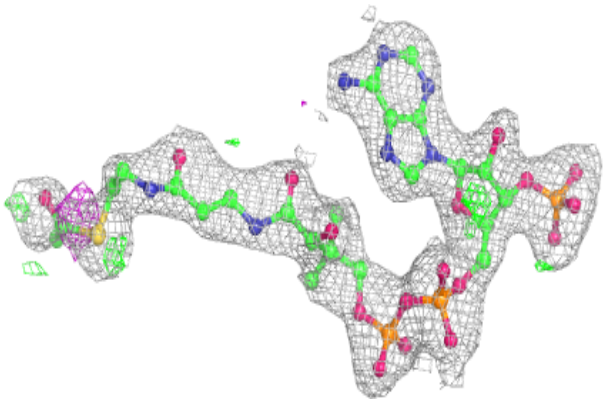
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

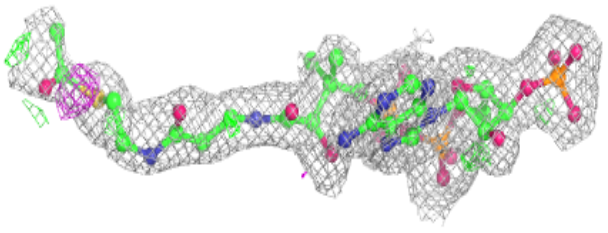


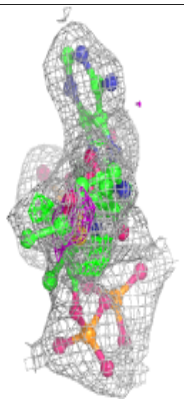


Electron density around ACO L 193:

$2mF_o$-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.