



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 09:27 AM UTC

PDB ID : 1KK4 / pdb_00001kk4
Title : Crystal Structure of Vat(D) in Complex with Acetyl-CoA
Authors : Sugantino, M.; Roderick, S.L.
Deposited on : 2001-12-06
Resolution : 2.70 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

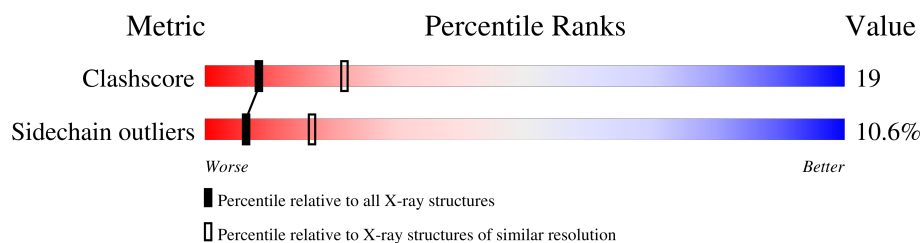
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.70 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	3843 (2.70-2.70)
Sidechain outliers	187428	3778 (2.70-2.70)

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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	209	55% 34% 10% .
1	B	209	61% 30% 7% .
1	C	209	55% 38% . .
1	D	209	59% 32% 7% ..
1	E	209	64% 28% 7% .
1	F	209	60% 33% 5% .

2 Entry composition [i](#)

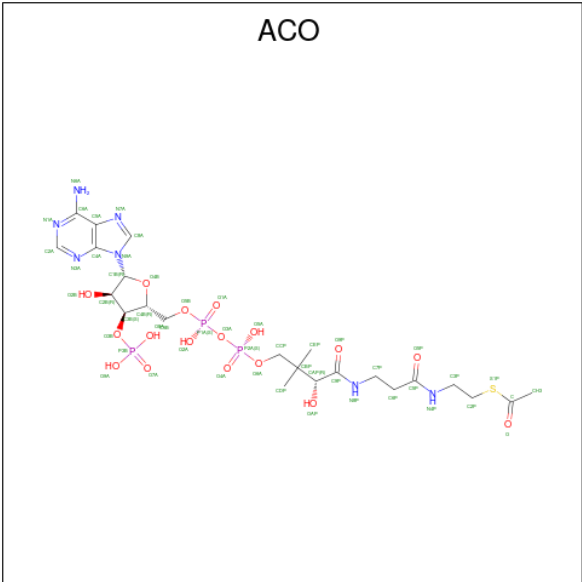
There are 3 unique types of molecules in this entry. The entry contains 10155 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 STREPTOGRAMIN A ACETYLTRANSFERASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	205	Total	C	N	O	S	0	0	0
			1621	1044	267	301	9			
1	B	205	Total	C	N	O	S	0	0	0
			1614	1040	266	299	9			
1	C	205	Total	C	N	O	S	0	0	0
			1617	1041	266	301	9			
1	D	206	Total	C	N	O	S	0	0	0
			1625	1047	267	302	9			
1	E	206	Total	C	N	O	S	0	0	0
			1613	1037	265	302	9			
1	F	206	Total	C	N	O	S	0	0	0
			1624	1045	268	302	9			

- Molecule 2 is ACETYL COENZYME *A (CCD ID: ACO) (formula: C₂₃H₃₈N₇O₁₇P₃S).



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

- Molecule 3 is water.

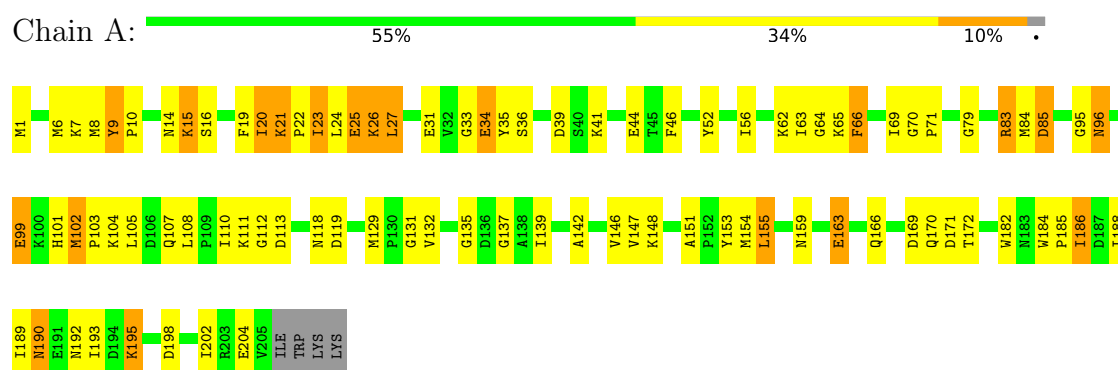
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	25	Total	O	0	0
			25	25		
3	C	21	Total	O	0	0
			21	21		
3	D	24	Total	O	0	0
			24	24		
3	E	21	Total	O	0	0
			21	21		
3	F	24	Total	O	0	0
			24	24		

3 Residue-property plots [i](#)

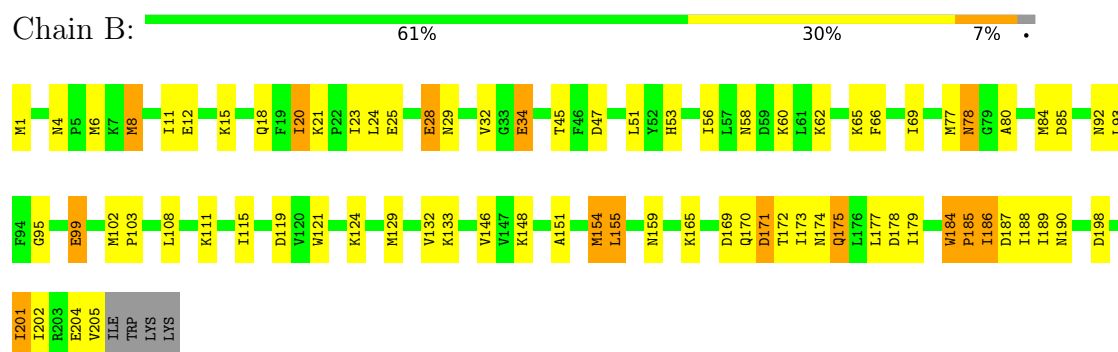
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

Note EDS was not executed.

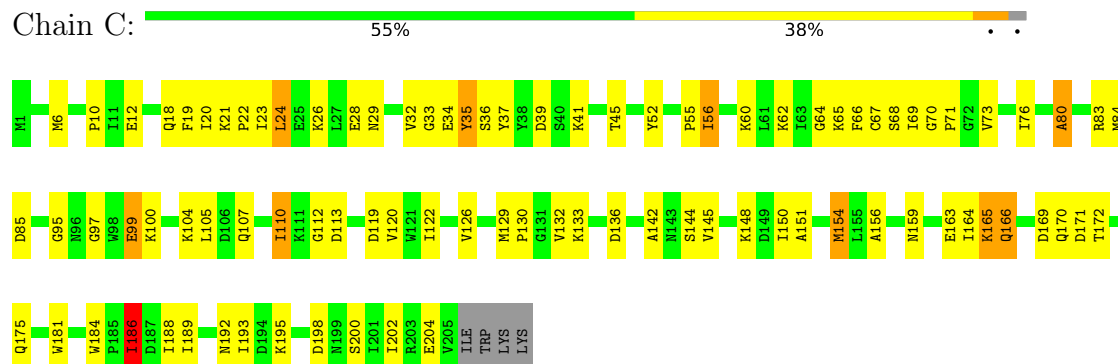
• Molecule 1: STREPTOGRAMIN A ACETYLTRANSFERASE



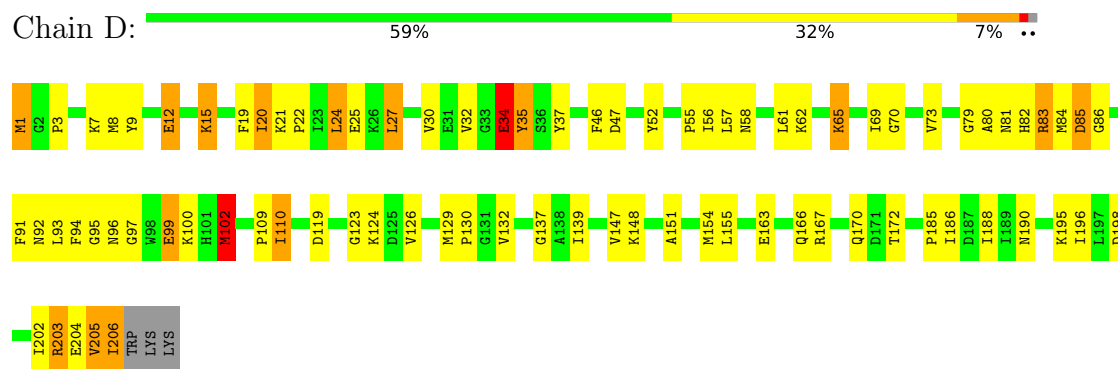
• Molecule 1: STREPTOGRAMIN A ACETYLTRANSFERASE



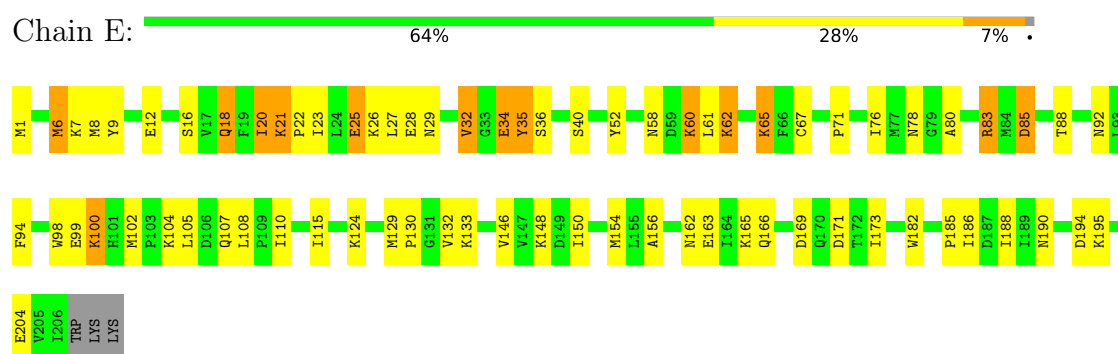
• Molecule 1: STREPTOGRAMIN A ACETYLTRANSFERASE



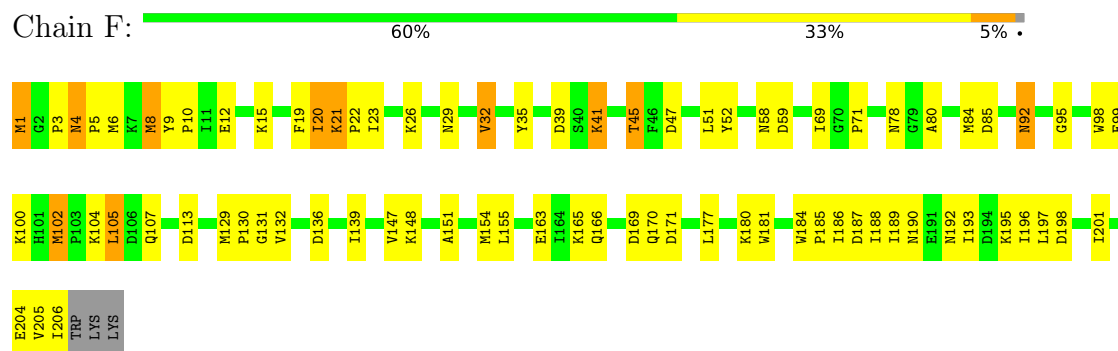
• Molecule 1: STREPTOGRAMIN A ACETYLTRANSFERASE



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4 Data and refinement statistics

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

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	186.30Å 186.30Å 186.50Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 2.70	Depositor
% Data completeness (in resolution range)	94.0 (99.00-2.70)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.188 , 0.246	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	10155	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section:
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	0.60	2/1660 (0.1%)	1.10	14/2251 (0.6%)
1	B	0.56	0/1653	1.13	17/2243 (0.8%)
1	C	0.50	0/1656	1.01	8/2247 (0.4%)
1	D	0.53	0/1664	1.07	14/2258 (0.6%)
1	E	0.52	0/1652	1.04	9/2245 (0.4%)
1	F	0.54	0/1663	1.04	12/2255 (0.5%)
All	All	0.54	2/9948 (0.0%)	1.07	74/13499 (0.5%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	14	ASN	CA-C	6.55	1.61	1.52
1	A	15	LYS	N-CA	5.84	1.53	1.46

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	205	VAL	N-CA-C	10.02	139.05	111.00
1	D	34	GLU	N-CA-C	9.06	120.84	110.97
1	D	205	VAL	N-CA-C	-8.37	105.33	113.53
1	A	34	GLU	N-CA-C	7.87	121.00	111.40
1	E	20	ILE	N-CA-C	7.83	118.61	110.62
1	B	34	GLU	N-CA-C	7.77	120.50	111.02
1	E	34	GLU	N-CA-C	7.75	119.42	110.97
1	F	20	ILE	N-CA-C	7.72	117.83	110.42
1	A	26	LYS	N-CA-C	-7.42	104.33	113.15
1	B	184	TRP	CA-C-N	7.35	128.51	119.98
1	B	184	TRP	C-N-CA	7.35	128.51	119.98
1	D	20	ILE	N-CA-C	7.23	117.36	110.42
1	B	78	ASN	N-CA-C	7.17	121.87	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	20	ILE	N-CA-C	7.03	117.82	110.72
1	E	83	ARG	N-CA-C	-6.86	101.02	110.35
1	F	78	ASN	N-CA-C	6.81	121.29	113.19
1	A	135	GLY	N-CA-C	6.80	121.25	112.54
1	B	185	PRO	N-CA-C	-6.78	99.97	110.95
1	D	206	ILE	N-CA-C	6.71	129.80	111.00
1	A	27	LEU	N-CA-C	6.71	120.46	109.72
1	E	85	ASP	N-CA-C	-6.69	104.59	112.89
1	B	205	VAL	CA-C-O	6.59	132.00	120.80
1	D	102	MET	N-CA-C	-6.53	101.54	109.83
1	B	20	ILE	N-CA-C	6.52	117.30	110.72
1	C	80	ALA	N-CA-C	6.49	120.81	113.02
1	D	46	PHE	N-CA-C	6.44	120.71	112.34
1	E	78	ASN	N-CA-C	6.42	120.71	113.01
1	C	20	ILE	N-CA-C	6.39	116.56	110.42
1	C	26	LYS	N-CA-C	-6.37	105.51	113.28
1	D	24	LEU	N-CA-C	6.36	118.30	111.36
1	D	85	ASP	N-CA-C	-6.35	105.60	113.15
1	F	165	LYS	N-CA-C	6.30	116.76	107.88
1	B	205	VAL	CB-CA-C	-6.26	99.50	111.40
1	E	35	TYR	N-CA-C	6.23	120.89	113.16
1	F	35	TYR	N-CA-C	6.05	120.28	113.02
1	A	9	TYR	CA-C-N	6.04	127.39	119.84
1	A	9	TYR	C-N-CA	6.04	127.39	119.84
1	D	83	ARG	N-CA-C	-5.94	102.13	110.50
1	B	129	MET	CA-C-N	5.91	125.67	119.76
1	B	129	MET	C-N-CA	5.91	125.67	119.76
1	F	32	VAL	N-CA-C	5.84	116.29	108.11
1	E	32	VAL	N-CA-C	5.82	117.13	108.46
1	A	66	PHE	N-CA-C	-5.80	103.26	111.56
1	F	51	LEU	N-CA-C	5.80	119.52	110.17
1	F	4	ASN	CA-C-N	5.80	125.50	119.82
1	F	4	ASN	C-N-CA	5.80	125.50	119.82
1	F	84	MET	N-CA-C	5.79	119.55	111.56
1	E	173	ILE	N-CA-C	5.78	115.91	110.30
1	F	85	ASP	N-CA-C	-5.64	106.37	113.20
1	A	129	MET	CA-C-N	5.63	125.57	119.78
1	A	129	MET	C-N-CA	5.63	125.57	119.78
1	B	32	VAL	N-CA-C	5.53	116.70	108.46
1	C	35	TYR	N-CA-C	5.50	118.78	112.57
1	A	23	ILE	N-CA-C	5.49	115.62	110.30
1	D	35	TYR	N-CA-C	5.47	119.59	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	206	ILE	CA-C-O	5.47	130.09	120.80
1	F	26	LYS	N-CA-C	-5.46	105.41	111.36
1	D	196	ILE	N-CA-C	-5.43	105.55	110.82
1	A	56	ILE	N-CA-C	5.31	116.04	110.62
1	C	24	LEU	N-CA-C	5.29	119.83	113.17
1	B	204	GLU	CA-C-N	5.28	131.20	121.70
1	B	204	GLU	C-N-CA	5.28	131.20	121.70
1	A	83	ARG	N-CA-C	-5.19	102.60	110.28
1	B	4	ASN	CA-C-N	5.17	124.88	119.82
1	B	4	ASN	C-N-CA	5.17	124.88	119.82
1	C	202	ILE	CB-CA-C	-5.15	105.37	111.81
1	E	40	SER	N-CA-C	5.13	117.47	110.24
1	C	164	ILE	CB-CA-C	-5.07	105.28	111.92
1	B	51	LEU	N-CA-C	5.05	117.98	109.95
1	F	58	ASN	N-CA-C	5.04	119.00	112.86
1	D	58	ASN	N-CA-C	5.03	118.68	112.24
1	D	82	HIS	N-CA-C	-5.02	103.09	110.52
1	A	46	PHE	N-CA-C	5.02	118.17	111.75
1	C	186	ILE	N-CA-C	5.01	116.33	110.62

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	1621	0	1611	85	0
1	B	1614	0	1601	54	0
1	C	1617	0	1600	51	0
1	D	1625	0	1614	74	0
1	E	1613	0	1575	59	0
1	F	1624	0	1609	67	0
2	A	51	0	27	5	0
2	B	51	0	27	3	0
2	C	51	0	27	6	0
2	D	51	0	27	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	51	0	27	0	0
2	F	51	0	27	1	0
3	A	20	0	0	2	0
3	B	25	0	0	4	0
3	C	21	0	0	0	0
3	D	24	0	0	9	0
3	E	21	0	0	9	0
3	F	24	0	0	4	0
All	All	10155	0	9772	377	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 19.

All (377) 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:26:LYS:O	1:E:27:LEU:HD23	1.53	1.05
1:B:60:LYS:HE3	3:B:3512:HOH:O	1.58	1.01
1:F:195:LYS:NZ	1:F:204:GLU:HG3	1.77	0.99
1:A:195:LYS:HZ1	1:A:204:GLU:CD	1.70	0.97
1:A:154:MET:HE3	1:A:163:GLU:HG2	1.47	0.94
1:B:186:ILE:HG23	1:B:187:ASP:H	1.30	0.93
1:D:95:GLY:HA2	1:D:99:GLU:HG3	1.52	0.92
1:A:195:LYS:NZ	1:A:204:GLU:CD	2.30	0.89
1:F:195:LYS:HZ2	1:F:204:GLU:HG3	1.33	0.89
1:F:154:MET:HE3	1:F:163:GLU:HB3	1.56	0.85
1:B:184:TRP:CH2	1:B:201:ILE:HD11	2.12	0.84
1:D:24:LEU:O	1:D:27:LEU:HB2	1.78	0.83
1:F:95:GLY:HA2	1:F:99:GLU:HG3	1.62	0.81
1:C:151:ALA:HB3	1:C:154:MET:HG3	1.62	0.81
1:E:62:LYS:HD2	1:E:115:ILE:HG12	1.62	0.80
1:F:196:ILE:HG12	1:F:201:ILE:HD12	1.64	0.79
1:E:26:LYS:O	1:E:27:LEU:CD2	2.30	0.79
1:B:187:ASP:HA	1:B:190:ASN:HD22	1.48	0.79
1:D:204:GLU:OE1	1:D:204:GLU:HA	1.84	0.78
1:F:184:TRP:CZ3	1:F:201:ILE:HD11	2.19	0.77
1:B:155:LEU:HD11	2:B:302:ACO:H131	1.67	0.77
1:D:205:VAL:O	1:D:206:ILE:CB	2.33	0.77
1:A:21:LYS:HB3	1:A:22:PRO:HD3	1.68	0.76
1:C:95:GLY:HA2	1:C:99:GLU:HG3	1.68	0.75
1:F:92:ASN:HB2	1:F:102:MET:HE3	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:169:ASP:OD1	1:B:171:ASP:HB2	1.87	0.74
1:B:173:ILE:HG22	1:B:177:LEU:HD12	1.69	0.73
1:B:23:ILE:HG22	1:B:24:LEU:HD23	1.70	0.73
1:F:1:MET:N	3:F:3634:HOH:O	2.22	0.73
1:D:203:ARG:HD2	3:D:3582:HOH:O	1.87	0.73
1:B:186:ILE:HG23	1:B:187:ASP:N	2.03	0.72
1:A:169:ASP:OD1	1:A:171:ASP:HB3	1.89	0.72
1:D:20:ILE:HG22	1:D:32:VAL:HG11	1.72	0.71
1:D:34:GLU:HG2	1:D:65:LYS:HD2	1.72	0.71
1:D:130:PRO:HG3	3:D:3543:HOH:O	1.91	0.71
1:B:186:ILE:O	1:B:189:ILE:N	2.24	0.71
1:A:10:PRO:HG3	1:A:19:PHE:CD1	2.26	0.71
1:D:172:THR:HG23	1:D:202:ILE:HD11	1.73	0.71
1:A:35:TYR:OH	1:A:186:ILE:HD13	1.91	0.70
1:D:25:GLU:C	1:D:27:LEU:H	1.98	0.70
1:F:147:VAL:HB	3:F:3557:HOH:O	1.91	0.70
1:D:130:PRO:CG	3:D:3543:HOH:O	2.39	0.69
1:D:151:ALA:HB3	1:D:154:MET:HG3	1.72	0.69
1:E:25:GLU:HG3	3:E:3517:HOH:O	1.92	0.69
1:A:186:ILE:O	1:A:190:ASN:HB2	1.91	0.69
1:D:52:TYR:CD1	1:D:80:ALA:HB2	2.28	0.69
1:D:195:LYS:NZ	1:D:204:GLU:HG3	2.08	0.68
1:E:148:LYS:HE3	3:E:3644:HOH:O	1.92	0.68
1:D:102:MET:HE1	3:D:3566:HOH:O	1.93	0.68
1:A:31:GLU:OE2	1:A:62:LYS:HE2	1.94	0.67
1:F:204:GLU:OE1	1:F:204:GLU:HA	1.94	0.67
1:F:41:LYS:HB2	1:F:71:PRO:HB2	1.77	0.67
1:A:70:GLY:HA2	2:A:301:ACO:CH3	2.25	0.67
1:A:113:ASP:O	1:A:131:GLY:HA2	1.94	0.67
1:B:184:TRP:CZ3	1:B:201:ILE:HD11	2.29	0.67
1:D:57:LEU:HD22	1:D:110:ILE:HD11	1.76	0.66
1:C:23:ILE:HG22	1:C:24:LEU:HD23	1.76	0.66
1:E:102:MET:HE3	3:E:3553:HOH:O	1.96	0.66
1:D:94:PHE:HB3	1:F:3:PRO:HG3	1.76	0.66
1:F:139:ILE:HB	1:F:155:LEU:HD12	1.78	0.66
1:B:186:ILE:O	1:B:188:ILE:N	2.28	0.66
1:D:185:PRO:HD2	1:D:188:ILE:HD12	1.79	0.65
1:C:69:ILE:HG12	1:C:122:ILE:HD12	1.79	0.65
1:F:184:TRP:CH2	1:F:201:ILE:HD11	2.31	0.65
1:D:21:LYS:HE3	1:D:25:GLU:OE2	1.97	0.64
1:A:41:LYS:HG3	1:A:41:LYS:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1:MET:HE3	1:D:190:ASN:CG	2.22	0.64
1:F:195:LYS:HZ3	1:F:204:GLU:HG3	1.61	0.64
1:A:70:GLY:HA2	2:A:301:ACO:HH32	1.79	0.63
1:A:41:LYS:HB2	1:A:71:PRO:HB2	1.80	0.63
1:C:37:TYR:CE2	1:C:68:SER:HA	2.33	0.63
1:A:35:TYR:CZ	1:A:186:ILE:HD13	2.34	0.63
1:A:26:LYS:O	1:A:26:LYS:HG3	1.98	0.62
1:F:151:ALA:HB3	1:F:154:MET:HG3	1.80	0.62
1:D:154:MET:HE2	1:D:163:GLU:HB3	1.81	0.62
1:B:95:GLY:HA2	1:B:99:GLU:HG3	1.82	0.62
1:A:9:TYR:CD2	1:A:15:LYS:HA	2.35	0.61
1:E:71:PRO:HG2	1:E:124:LYS:HB2	1.83	0.61
1:F:205:VAL:O	1:F:206:ILE:C	2.44	0.61
1:C:165:LYS:HG2	1:C:166:GLN:N	2.15	0.60
1:D:19:PHE:O	1:D:22:PRO:HD2	2.01	0.60
1:B:169:ASP:OD1	1:B:171:ASP:CB	2.49	0.60
1:A:83:ARG:HG2	3:A:3613:HOH:O	2.02	0.60
1:F:151:ALA:O	1:F:154:MET:HB2	2.02	0.60
1:A:8:MET:O	1:A:10:PRO:HD3	2.02	0.60
1:F:186:ILE:HG23	1:F:187:ASP:H	1.65	0.60
1:B:20:ILE:CD1	1:B:69:ILE:HD12	2.31	0.59
1:A:154:MET:HE3	1:A:163:GLU:CG	2.28	0.59
1:C:195:LYS:HG2	1:C:200:SER:OG	2.03	0.59
1:A:65:LYS:O	1:A:66:PHE:HB2	2.02	0.59
1:B:6:MET:HE1	1:B:21:LYS:HE2	1.85	0.59
1:D:91:PHE:HD1	1:F:197:LEU:HD21	1.67	0.59
1:A:172:THR:HG23	1:A:202:ILE:CD1	2.33	0.59
1:F:139:ILE:HB	1:F:155:LEU:CD1	2.33	0.58
1:B:186:ILE:CG2	1:B:187:ASP:H	2.10	0.58
1:A:36:SER:OG	1:A:65:LYS:HA	2.04	0.58
1:D:25:GLU:HG3	3:D:3628:HOH:O	2.02	0.58
1:E:21:LYS:HB2	3:E:3529:HOH:O	2.03	0.58
1:B:173:ILE:HG22	1:B:177:LEU:CD1	2.33	0.58
1:F:169:ASP:OD1	1:F:171:ASP:HB3	2.02	0.58
1:D:20:ILE:CG2	1:D:32:VAL:HG11	2.35	0.57
1:E:83:ARG:HG2	3:E:3519:HOH:O	2.04	0.57
1:A:26:LYS:O	1:A:27:LEU:HD23	2.05	0.56
1:A:69:ILE:C	2:A:301:ACO:HH31	2.31	0.56
1:B:172:THR:HG23	1:B:202:ILE:HD11	1.86	0.56
3:B:3505:HOH:O	1:C:83:ARG:HG2	2.05	0.56
1:D:172:THR:HG23	1:D:202:ILE:CD1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:70:GLY:O	1:C:73:VAL:HG23	2.05	0.56
1:E:20:ILE:HG22	1:E:32:VAL:HG11	1.87	0.56
1:F:21:LYS:HB3	1:F:22:PRO:HD3	1.88	0.56
1:C:28:GLU:O	1:C:29:ASN:HB2	2.06	0.56
1:E:20:ILE:CG2	1:E:32:VAL:HG11	2.36	0.55
1:A:154:MET:CE	1:A:163:GLU:HG2	2.28	0.55
1:F:20:ILE:HG22	1:F:32:VAL:HG11	1.88	0.55
1:A:188:ILE:O	1:A:189:ILE:C	2.50	0.55
1:E:100:LYS:C	1:E:102:MET:H	2.14	0.55
1:C:69:ILE:C	2:C:303:ACO:HH31	2.31	0.55
1:B:184:TRP:CH2	1:B:201:ILE:CD1	2.89	0.54
1:C:66:PHE:O	1:C:119:ASP:HA	2.06	0.54
1:D:91:PHE:CD1	1:F:197:LEU:HD21	2.41	0.54
1:A:1:MET:CE	1:A:190:ASN:OD1	2.55	0.54
1:B:174:ASN:O	1:B:178:ASP:HB2	2.08	0.54
1:B:186:ILE:HG12	1:B:190:ASN:HD21	1.70	0.54
1:C:24:LEU:HD12	1:C:32:VAL:HG21	1.88	0.54
1:B:66:PHE:O	1:B:119:ASP:HA	2.08	0.54
1:C:19:PHE:O	1:C:22:PRO:HD2	2.08	0.54
1:E:76:ILE:O	1:E:130:PRO:HG3	2.07	0.54
1:F:10:PRO:HB3	1:F:19:PHE:CE1	2.42	0.54
1:D:35:TYR:OH	1:D:186:ILE:HD13	2.08	0.53
1:F:29:ASN:ND2	3:F:3545:HOH:O	2.42	0.53
1:F:69:ILE:C	2:F:306:ACO:HH31	2.33	0.53
1:D:97:GLY:N	1:D:99:GLU:OE2	2.39	0.53
1:E:52:TYR:CD1	1:E:80:ALA:HB2	2.43	0.53
1:A:66:PHE:O	1:A:119:ASP:HA	2.08	0.53
1:A:21:LYS:HB3	1:A:22:PRO:CD	2.38	0.53
1:E:6:MET:HE1	1:E:21:LYS:CD	2.38	0.53
1:D:195:LYS:HZ3	1:D:204:GLU:HG3	1.73	0.53
1:E:34:GLU:HG2	1:E:65:LYS:HD2	1.91	0.53
1:E:92:ASN:HB2	3:E:3553:HOH:O	2.08	0.53
1:F:185:PRO:HD2	1:F:188:ILE:HD12	1.90	0.53
1:B:20:ILE:HD11	1:B:69:ILE:HD12	1.90	0.53
1:E:1:MET:HE2	1:E:190:ASN:HB3	1.91	0.52
1:E:65:LYS:HE3	1:E:182:TRP:O	2.09	0.52
1:B:102:MET:HG3	1:B:103:PRO:HD2	1.91	0.52
1:D:123:GLY:O	1:D:126:VAL:HG23	2.10	0.52
1:E:21:LYS:HB3	1:E:22:PRO:HD3	1.92	0.52
1:C:21:LYS:HB3	1:C:22:PRO:HD3	1.92	0.52
1:C:126:VAL:HG22	1:C:144:SER:H	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:20:ILE:CD1	1:D:69:ILE:HD12	2.40	0.52
1:D:195:LYS:HZ2	1:D:204:GLU:HG3	1.74	0.52
1:E:154:MET:HE3	1:E:163:GLU:HB3	1.92	0.52
1:A:96:ASN:N	1:A:96:ASN:HD22	2.08	0.52
1:F:9:TYR:CD2	1:F:15:LYS:HA	2.45	0.52
1:A:195:LYS:HE3	1:A:204:GLU:OE2	2.10	0.51
1:B:159:ASN:HB2	1:C:159:ASN:HD22	1.76	0.51
1:F:39:ASP:O	1:F:71:PRO:HB3	2.10	0.51
1:B:28:GLU:O	1:B:29:ASN:HB2	2.10	0.51
1:D:9:TYR:CE2	1:D:15:LYS:HA	2.46	0.51
1:C:104:LYS:HB2	1:C:107:GLN:OE1	2.10	0.51
1:A:142:ALA:HB2	2:A:301:ACO:O5P	2.10	0.51
1:B:18:GLN:OE1	1:B:45:THR:HA	2.11	0.51
1:D:56:ILE:O	1:D:56:ILE:CG1	2.59	0.51
1:A:111:LYS:HE2	2:C:303:ACO:O4A	2.10	0.51
1:B:187:ASP:HA	1:B:190:ASN:ND2	2.23	0.51
1:A:195:LYS:NZ	1:A:204:GLU:CG	2.72	0.51
1:F:99:GLU:H	1:F:99:GLU:CD	2.19	0.51
1:E:132:VAL:HG11	1:E:146:VAL:HG12	1.93	0.50
1:D:93:LEU:HG	1:D:93:LEU:O	2.11	0.50
1:A:111:LYS:NZ	2:C:303:ACO:CBP	2.74	0.50
1:B:132:VAL:HG11	1:B:146:VAL:HG12	1.93	0.50
1:B:198:ASP:HA	1:C:85:ASP:OD1	2.11	0.50
1:C:60:LYS:O	1:C:113:ASP:HB3	2.11	0.50
1:A:44:GLU:N	1:A:44:GLU:OE1	2.43	0.50
1:A:195:LYS:HZ2	1:A:204:GLU:CG	2.25	0.50
3:B:3567:HOH:O	1:C:129:MET:HE2	2.11	0.50
1:D:186:ILE:HD11	1:E:98:TRP:HZ2	1.77	0.50
1:E:186:ILE:HD11	1:F:98:TRP:HZ2	1.76	0.50
1:F:185:PRO:O	1:F:186:ILE:C	2.55	0.50
1:A:101:HIS:CD2	1:C:193:ILE:HG21	2.47	0.49
1:D:81:ASN:HB3	1:D:109:PRO:HG2	1.94	0.49
1:F:177:LEU:O	1:F:180:LYS:HG3	2.12	0.49
1:A:1:MET:HB2	1:A:190:ASN:OD1	2.13	0.49
1:A:25:GLU:C	1:A:27:LEU:H	2.18	0.49
1:B:175:GLN:OE1	1:B:202:ILE:CG2	2.61	0.49
1:E:169:ASP:O	1:E:171:ASP:N	2.46	0.49
1:F:129:MET:HB3	1:F:130:PRO:HD2	1.95	0.49
1:E:115:ILE:O	1:E:133:LYS:HA	2.13	0.49
1:F:169:ASP:HA	3:F:3560:HOH:O	2.13	0.49
1:B:151:ALA:HB3	1:B:154:MET:HG3	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:184:TRP:HZ3	1:F:201:ILE:HD11	1.76	0.49
1:A:172:THR:HG23	1:A:202:ILE:HD11	1.95	0.49
1:A:188:ILE:C	1:A:190:ASN:N	2.70	0.48
1:C:10:PRO:HB3	1:C:19:PHE:CE1	2.48	0.48
1:D:1:MET:HE3	1:D:190:ASN:OD1	2.12	0.48
1:D:8:MET:HE2	1:D:8:MET:HB3	1.78	0.48
1:E:102:MET:HB2	3:E:3553:HOH:O	2.13	0.48
1:F:104:LYS:N	1:F:107:GLN:OE1	2.43	0.48
1:C:39:ASP:O	1:C:71:PRO:HB3	2.13	0.48
1:D:37:TYR:OH	2:D:304:ACO:HH33	2.13	0.48
1:D:95:GLY:O	1:D:96:ASN:HB2	2.13	0.48
1:D:20:ILE:HG23	1:D:24:LEU:HG	1.94	0.48
1:D:186:ILE:HD11	1:E:98:TRP:CZ2	2.49	0.48
1:E:8:MET:HE2	1:E:9:TYR:CE1	2.48	0.48
1:C:172:THR:O	1:C:175:GLN:HB2	2.13	0.48
1:F:1:MET:HE3	1:F:1:MET:HB3	1.82	0.48
1:F:20:ILE:CG2	1:F:32:VAL:HG11	2.43	0.48
1:A:6:MET:HE1	1:A:21:LYS:HD2	1.96	0.48
1:E:104:LYS:O	1:E:105:LEU:C	2.56	0.48
1:A:101:HIS:O	1:A:102:MET:C	2.55	0.48
1:B:58:ASN:ND2	3:B:3512:HOH:O	2.47	0.48
1:A:6:MET:HE1	1:A:21:LYS:CD	2.44	0.48
1:F:47:ASP:OD1	1:F:47:ASP:N	2.45	0.48
1:A:8:MET:HE3	1:A:23:ILE:HG12	1.95	0.48
1:F:1:MET:HE3	1:F:190:ASN:CG	2.39	0.48
1:F:184:TRP:O	1:F:185:PRO:C	2.57	0.48
1:A:95:GLY:HA2	1:A:99:GLU:HG2	1.95	0.48
1:E:29:ASN:O	1:E:60:LYS:HA	2.13	0.48
1:A:198:ASP:OD1	1:A:198:ASP:C	2.57	0.47
1:D:12:GLU:CG	3:D:3532:HOH:O	2.62	0.47
1:F:8:MET:HG2	1:F:23:ILE:HG12	1.96	0.47
1:A:1:MET:HE2	1:A:190:ASN:OD1	2.14	0.47
1:D:119:ASP:O	1:D:137:GLY:HA2	2.15	0.47
1:E:36:SER:HB3	1:E:67:CYS:HB2	1.97	0.47
1:C:18:GLN:OE1	1:C:45:THR:HA	2.14	0.47
1:F:92:ASN:H	1:F:92:ASN:HD22	1.63	0.47
1:F:154:MET:CE	1:F:163:GLU:HB3	2.36	0.47
1:C:198:ASP:OD1	1:C:198:ASP:C	2.57	0.47
1:D:129:MET:HB3	1:D:130:PRO:CD	2.45	0.47
1:D:154:MET:HE2	1:D:163:GLU:HG2	1.95	0.47
1:E:21:LYS:HB3	1:E:22:PRO:CD	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:169:ASP:C	1:E:171:ASP:N	2.72	0.47
1:F:186:ILE:O	1:F:187:ASP:C	2.57	0.47
1:D:52:TYR:HB3	1:D:79:GLY:HA3	1.96	0.47
1:D:56:ILE:O	1:D:56:ILE:HG12	2.15	0.47
1:E:71:PRO:HG2	1:E:124:LYS:CB	2.44	0.47
1:E:104:LYS:O	1:E:107:GLN:N	2.38	0.47
1:E:6:MET:HE1	1:E:21:LYS:HE2	1.96	0.47
1:F:113:ASP:O	1:F:131:GLY:HA2	2.15	0.46
1:A:8:MET:HE2	1:A:9:TYR:CE1	2.49	0.46
1:D:3:PRO:HG3	1:E:94:PHE:HB3	1.97	0.46
1:A:104:LYS:O	1:A:105:LEU:C	2.57	0.46
1:A:111:LYS:HZ3	2:C:303:ACO:CBP	2.27	0.46
1:D:25:GLU:C	1:D:27:LEU:N	2.65	0.46
1:E:169:ASP:C	1:E:171:ASP:H	2.22	0.46
1:A:39:ASP:O	1:A:71:PRO:HB3	2.16	0.46
1:B:185:PRO:O	1:B:186:ILE:C	2.59	0.46
1:E:154:MET:CE	1:E:163:GLU:HB3	2.45	0.46
1:F:186:ILE:O	1:F:189:ILE:N	2.48	0.46
1:B:175:GLN:OE1	1:B:202:ILE:HG23	2.15	0.46
1:C:154:MET:HE3	1:C:165:LYS:O	2.15	0.46
1:E:35:TYR:CZ	1:E:186:ILE:HD12	2.51	0.46
1:F:59:ASP:OD1	1:F:59:ASP:N	2.47	0.46
1:F:196:ILE:CG1	1:F:201:ILE:HD12	2.41	0.46
1:D:130:PRO:HG2	3:D:3543:HOH:O	2.11	0.46
1:D:129:MET:HB3	1:D:130:PRO:HD2	1.98	0.46
1:E:1:MET:HE2	1:E:190:ASN:CG	2.41	0.46
1:A:6:MET:HA	1:A:6:MET:HE2	1.98	0.46
1:A:34:GLU:HG2	1:A:65:LYS:HD2	1.98	0.46
1:C:97:GLY:N	1:C:99:GLU:OE2	2.41	0.46
1:A:151:ALA:O	1:A:154:MET:HB2	2.16	0.45
1:D:92:ASN:OD1	1:D:102:MET:HE2	2.16	0.45
1:F:192:ASN:O	1:F:193:ILE:C	2.59	0.45
1:A:33:GLY:HA3	1:A:65:LYS:HB3	1.98	0.45
1:D:55:PRO:C	1:D:57:LEU:H	2.24	0.45
1:D:94:PHE:CB	1:F:3:PRO:HG3	2.44	0.45
1:E:62:LYS:CD	1:E:115:ILE:HG12	2.38	0.45
1:E:129:MET:O	1:E:132:VAL:HG23	2.17	0.45
1:E:156:ALA:HB1	1:E:162:ASN:O	2.15	0.45
1:F:21:LYS:HG3	1:F:32:VAL:O	2.17	0.45
1:A:52:TYR:HB3	1:A:79:GLY:HA3	1.99	0.45
1:B:115:ILE:HD12	1:B:133:LYS:HE2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ILE:O	1:B:187:ASP:C	2.58	0.45
1:C:142:ALA:HB2	2:C:303:ACO:O5P	2.17	0.45
1:E:108:LEU:HD23	1:E:108:LEU:HA	1.86	0.45
1:B:170:GLN:O	1:B:171:ASP:C	2.59	0.45
1:D:97:GLY:O	1:D:100:LYS:HG2	2.17	0.45
1:C:33:GLY:HA3	1:C:64:GLY:C	2.42	0.45
1:C:36:SER:HB3	1:C:67:CYS:HB2	1.98	0.45
1:E:190:ASN:ND2	3:E:3631:HOH:O	2.49	0.45
1:D:12:GLU:HG2	3:D:3532:HOH:O	2.16	0.45
1:B:175:GLN:O	1:B:179:ILE:HG13	2.16	0.45
1:D:30:VAL:HG22	1:D:61:LEU:HB3	1.99	0.45
1:D:139:ILE:HD12	1:D:167:ARG:HD2	1.99	0.45
1:B:62:LYS:HD2	1:B:115:ILE:HG12	1.99	0.44
1:F:52:TYR:CD1	1:F:80:ALA:HB2	2.52	0.44
1:C:188:ILE:O	1:C:189:ILE:C	2.60	0.44
1:E:25:GLU:HG2	3:E:3565:HOH:O	2.18	0.44
1:A:63:ILE:O	1:A:64:GLY:O	2.36	0.44
1:E:1:MET:HE2	1:E:190:ASN:CB	2.47	0.44
1:B:8:MET:HG2	1:B:23:ILE:HG13	2.00	0.44
1:C:181:TRP:HA	1:C:184:TRP:CE2	2.52	0.44
1:A:65:LYS:HE3	1:A:182:TRP:O	2.18	0.43
1:A:192:ASN:O	1:A:193:ILE:C	2.61	0.43
1:D:186:ILE:O	1:D:190:ASN:HB2	2.18	0.43
1:F:12:GLU:CD	1:F:12:GLU:H	2.27	0.43
1:A:99:GLU:H	1:A:99:GLU:HG3	1.29	0.43
1:C:145:VAL:HB	1:C:159:ASN:OD1	2.17	0.43
1:A:1:MET:HE3	1:A:190:ASN:OD1	2.18	0.43
1:A:137:GLY:O	1:A:153:TYR:HA	2.19	0.43
1:A:147:VAL:HG11	2:C:303:ACO:N7A	2.33	0.43
1:B:132:VAL:HG11	1:B:146:VAL:CG1	2.48	0.43
1:D:84:MET:C	1:D:86:GLY:H	2.26	0.43
1:B:108:LEU:HD23	1:B:108:LEU:HA	1.81	0.43
1:B:121:TRP:NE1	2:B:302:ACO:O	2.45	0.43
1:B:132:VAL:HG12	1:B:133:LYS:N	2.33	0.43
1:F:105:LEU:HD23	1:F:105:LEU:HA	1.78	0.43
1:A:20:ILE:O	1:A:21:LYS:C	2.61	0.43
1:A:132:VAL:HG11	1:A:146:VAL:HG12	1.99	0.43
1:C:154:MET:HE2	1:C:163:GLU:HG2	2.01	0.43
1:F:129:MET:HB3	1:F:130:PRO:CD	2.49	0.42
1:C:55:PRO:O	1:C:56:ILE:C	2.60	0.42
1:D:9:TYR:CD2	1:D:15:LYS:HA	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:6:MET:HE1	1:E:21:LYS:CE	2.49	0.42
1:A:9:TYR:CE2	1:A:15:LYS:HA	2.54	0.42
1:A:1:MET:HB2	1:A:190:ASN:HD21	1.84	0.42
1:A:8:MET:HE3	1:A:23:ILE:CD1	2.49	0.42
1:A:151:ALA:HB3	1:A:154:MET:HG3	2.00	0.42
1:B:121:TRP:CZ2	2:B:302:ACO:H61	2.54	0.42
1:D:21:LYS:HB3	1:D:22:PRO:HD3	2.01	0.42
1:D:55:PRO:O	1:D:57:LEU:N	2.53	0.42
1:B:92:ASN:ND2	1:B:103:PRO:HD3	2.35	0.42
1:C:6:MET:HE1	1:C:21:LYS:CE	2.50	0.42
1:C:192:ASN:O	1:C:193:ILE:C	2.62	0.42
1:D:198:ASP:OD1	1:D:198:ASP:C	2.63	0.42
1:A:103:PRO:CG	1:A:108:LEU:HD21	2.49	0.42
1:B:45:THR:OG1	1:B:47:ASP:OD1	2.35	0.42
1:D:70:GLY:O	1:D:73:VAL:HG23	2.20	0.42
1:E:195:LYS:HD2	1:E:204:GLU:HG3	2.02	0.42
1:A:195:LYS:CE	1:A:204:GLU:CD	2.93	0.42
1:D:83:ARG:HE	1:D:85:ASP:CG	2.27	0.42
1:A:70:GLY:N	2:A:301:ACO:HH31	2.35	0.42
1:F:195:LYS:NZ	1:F:204:GLU:CG	2.66	0.42
1:D:27:LEU:HD23	1:D:27:LEU:HA	1.86	0.42
1:E:8:MET:HE2	1:E:8:MET:HB3	1.70	0.42
1:F:192:ASN:O	1:F:195:LYS:N	2.52	0.42
1:F:198:ASP:OD1	1:F:198:ASP:C	2.63	0.42
1:C:34:GLU:HG2	1:C:65:LYS:HE2	2.02	0.41
1:A:8:MET:HE2	1:A:8:MET:HB3	1.91	0.41
1:A:95:GLY:HA2	1:A:99:GLU:CG	2.50	0.41
1:D:25:GLU:CG	3:D:3628:HOH:O	2.66	0.41
1:A:83:ARG:HG3	1:A:85:ASP:OD1	2.20	0.41
1:E:185:PRO:HD2	1:E:188:ILE:HD12	2.02	0.41
1:F:181:TRP:CE3	1:F:196:ILE:HD13	2.55	0.41
1:A:20:ILE:CG2	1:A:24:LEU:HG	2.49	0.41
1:A:184:TRP:O	1:A:185:PRO:C	2.63	0.41
1:C:165:LYS:HG2	1:C:166:GLN:O	2.21	0.41
1:F:4:ASN:HA	1:F:5:PRO:HD2	1.89	0.41
1:C:35:TYR:OH	1:C:186:ILE:HD13	2.20	0.41
1:E:58:ASN:ND2	1:E:60:LYS:HE3	2.36	0.41
1:F:154:MET:HE3	1:F:163:GLU:CB	2.41	0.41
1:A:34:GLU:H	1:A:65:LYS:HB3	1.86	0.41
1:B:78:ASN:C	1:B:80:ALA:H	2.29	0.41
1:E:18:GLN:HE21	1:E:18:GLN:HB3	1.70	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ASN:HD22	1:C:159:ASN:HB2	1.86	0.41
1:D:95:GLY:HA2	1:D:99:GLU:CG	2.36	0.41
1:C:150:ILE:HD12	1:C:156:ALA:CB	2.51	0.41
1:B:53:HIS:CG	1:B:77:MET:HG3	2.55	0.41
1:B:159:ASN:CB	1:C:159:ASN:HD22	2.34	0.41
1:C:110:ILE:HG22	1:C:112:GLY:H	1.86	0.41
1:C:171:ASP:O	1:C:172:THR:C	2.63	0.41
1:C:52:TYR:CD2	1:C:80:ALA:HB2	2.56	0.41
1:D:139:ILE:HB	1:D:155:LEU:HD13	2.03	0.41
1:B:11:ILE:O	1:B:12:GLU:C	2.65	0.40
1:C:33:GLY:HA3	1:C:64:GLY:O	2.21	0.40
1:C:169:ASP:O	1:C:170:GLN:C	2.64	0.40
1:C:76:ILE:O	1:C:130:PRO:HG3	2.21	0.40
1:D:129:MET:HG3	1:D:147:VAL:HG12	2.03	0.40
1:F:45:THR:HB	1:F:47:ASP:OD1	2.20	0.40
1:A:110:ILE:HG22	1:A:112:GLY:H	1.87	0.40
1:E:8:MET:HE3	1:E:23:ILE:HG12	2.04	0.40
1:E:25:GLU:O	1:E:27:LEU:N	2.47	0.40
1:E:28:GLU:O	1:E:29:ASN:HB2	2.22	0.40
1:E:154:MET:SD	1:E:166:GLN:HG3	2.61	0.40
1:A:107:GLN:OE1	3:A:3615:HOH:O	2.22	0.40
1:A:139:ILE:HB	1:A:155:LEU:HD13	2.02	0.40
1:B:198:ASP:OD1	1:B:198:ASP:C	2.63	0.40
1:F:195:LYS:HZ3	1:F:204:GLU:CG	2.31	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

There are no protein backbone outliers to report in this entry.

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	176/183 (96%)	158 (90%)	18 (10%)	7	18
1	B	175/183 (96%)	153 (87%)	22 (13%)	4	11
1	C	175/183 (96%)	156 (89%)	19 (11%)	6	16
1	D	177/183 (97%)	159 (90%)	18 (10%)	7	18
1	E	172/183 (94%)	153 (89%)	19 (11%)	6	15
1	F	176/183 (96%)	161 (92%)	15 (8%)	10	25
All	All	1051/1098 (96%)	940 (89%)	111 (11%)	6	17

All (111) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	LYS
1	A	16	SER
1	A	21	LYS
1	A	25	GLU
1	A	84	MET
1	A	85	ASP
1	A	96	ASN
1	A	99	GLU
1	A	102	MET
1	A	118	ASN
1	A	148	LYS
1	A	155	LEU
1	A	163	GLU
1	A	166	GLN
1	A	170	GLN
1	A	186	ILE
1	A	190	ASN
1	A	195	LYS
1	B	1	MET
1	B	8	MET
1	B	15	LYS
1	B	25	GLU
1	B	28	GLU
1	B	34	GLU
1	B	56	ILE
1	B	65	LYS
1	B	84	MET
1	B	85	ASP
1	B	93	LEU
1	B	99	GLU

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Mol	Chain	Res	Type
1	B	111	LYS
1	B	124	LYS
1	B	148	LYS
1	B	154	MET
1	B	155	LEU
1	B	165	LYS
1	B	171	ASP
1	B	175	GLN
1	B	186	ILE
1	B	201	ILE
1	C	12	GLU
1	C	41	LYS
1	C	56	ILE
1	C	62	LYS
1	C	84	MET
1	C	99	GLU
1	C	100	LYS
1	C	105	LEU
1	C	110	ILE
1	C	120	VAL
1	C	132	VAL
1	C	133	LYS
1	C	136	ASP
1	C	148	LYS
1	C	154	MET
1	C	165	LYS
1	C	166	GLN
1	C	186	ILE
1	C	204	GLU
1	D	1	MET
1	D	7	LYS
1	D	12	GLU
1	D	15	LYS
1	D	27	LEU
1	D	34	GLU
1	D	47	ASP
1	D	62	LYS
1	D	65	LYS
1	D	99	GLU
1	D	102	MET
1	D	110	ILE
1	D	124	LYS

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Mol	Chain	Res	Type
1	D	132	VAL
1	D	148	LYS
1	D	166	GLN
1	D	170	GLN
1	D	203	ARG
1	E	6	MET
1	E	7	LYS
1	E	12	GLU
1	E	16	SER
1	E	18	GLN
1	E	21	LYS
1	E	25	GLU
1	E	60	LYS
1	E	61	LEU
1	E	62	LYS
1	E	65	LYS
1	E	85	ASP
1	E	88	THR
1	E	99	GLU
1	E	100	LYS
1	E	110	ILE
1	E	150	ILE
1	E	165	LYS
1	E	194	ASP
1	F	1	MET
1	F	6	MET
1	F	8	MET
1	F	21	LYS
1	F	41	LYS
1	F	45	THR
1	F	92	ASN
1	F	100	LYS
1	F	102	MET
1	F	105	LEU
1	F	132	VAL
1	F	136	ASP
1	F	148	LYS
1	F	166	GLN
1	F	170	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	96	ASN
1	A	118	ASN
1	A	166	GLN
1	A	174	ASN
1	A	192	ASN
1	B	49	GLN
1	B	58	ASN
1	B	143	ASN
1	B	166	GLN
1	B	174	ASN
1	B	190	ASN
1	C	92	ASN
1	C	166	GLN
1	C	174	ASN
1	D	49	GLN
1	D	101	HIS
1	D	143	ASN
1	D	175	GLN
1	E	58	ASN
1	E	92	ASN
1	E	166	GLN
1	E	170	GLN
1	E	174	ASN
1	F	29	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 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
2	ACO	A	301	-	51,53,53	11.09	18 (35%)	73,79,79	11.23	25 (34%)
2	ACO	D	304	-	51,53,53	11.04	19 (37%)	73,79,79	11.21	24 (32%)
2	ACO	F	306	-	51,53,53	11.09	18 (35%)	73,79,79	11.21	25 (34%)
2	ACO	B	302	-	51,53,53	11.07	18 (35%)	73,79,79	11.23	25 (34%)
2	ACO	E	305	-	51,53,53	11.07	18 (35%)	73,79,79	11.23	25 (34%)
2	ACO	C	303	-	51,53,53	11.02	18 (35%)	73,79,79	11.21	25 (34%)

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	A	301	-	-	18/51/67/67	0/3/3/3
2	ACO	D	304	-	-	17/51/67/67	0/3/3/3
2	ACO	F	306	-	-	18/51/67/67	0/3/3/3
2	ACO	B	302	-	-	19/51/67/67	0/3/3/3
2	ACO	E	305	-	-	18/51/67/67	0/3/3/3
2	ACO	C	303	-	-	17/51/67/67	0/3/3/3

All (109) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	ACO	CEP-CBP	49.82	2.56	1.53
2	F	306	ACO	CEP-CBP	49.79	2.56	1.53
2	E	305	ACO	CEP-CBP	49.75	2.56	1.53
2	A	301	ACO	CEP-CBP	49.69	2.56	1.53
2	C	303	ACO	CEP-CBP	49.61	2.56	1.53
2	D	304	ACO	CEP-CBP	49.50	2.55	1.53
2	A	301	ACO	CDP-CBP	48.93	2.54	1.53
2	F	306	ACO	CDP-CBP	48.82	2.54	1.53
2	E	305	ACO	CDP-CBP	48.75	2.54	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	304	ACO	CDP-CBP	48.67	2.54	1.53
2	B	302	ACO	CDP-CBP	48.64	2.54	1.53
2	C	303	ACO	CDP-CBP	48.41	2.53	1.53
2	F	306	ACO	O6A-CCP	34.92	2.55	1.43
2	C	303	ACO	O6A-CCP	34.83	2.55	1.43
2	B	302	ACO	O6A-CCP	34.82	2.55	1.43
2	E	305	ACO	O6A-CCP	34.81	2.55	1.43
2	A	301	ACO	O6A-CCP	34.78	2.55	1.43
2	D	304	ACO	O6A-CCP	34.65	2.55	1.43
2	A	301	ACO	C7P-N8P	4.64	1.56	1.46
2	E	305	ACO	C6P-C5P	4.63	1.60	1.51
2	D	304	ACO	C7P-N8P	4.60	1.56	1.46
2	E	305	ACO	C7P-N8P	4.58	1.56	1.46
2	C	303	ACO	C7P-N8P	4.55	1.56	1.46
2	D	304	ACO	C6P-C5P	4.52	1.60	1.51
2	F	306	ACO	C7P-N8P	4.44	1.56	1.46
2	F	306	ACO	C6P-C5P	4.43	1.60	1.51
2	B	302	ACO	C7P-N8P	4.42	1.56	1.46
2	B	302	ACO	C6P-C5P	4.42	1.60	1.51
2	A	301	ACO	C6P-C5P	4.30	1.59	1.51
2	C	303	ACO	C6P-C5P	4.28	1.59	1.51
2	E	305	ACO	P2A-O3A	4.27	1.64	1.59
2	D	304	ACO	P2A-O3A	4.24	1.64	1.59
2	A	301	ACO	P2A-O3A	4.10	1.63	1.59
2	A	301	ACO	C3P-N4P	3.99	1.55	1.46
2	C	303	ACO	C3P-N4P	3.97	1.55	1.46
2	F	306	ACO	C3P-N4P	3.92	1.55	1.46
2	B	302	ACO	C3P-N4P	3.88	1.54	1.46
2	E	305	ACO	C3P-N4P	3.85	1.54	1.46
2	D	304	ACO	C3P-N4P	3.80	1.54	1.46
2	F	306	ACO	P2A-O3A	3.75	1.63	1.59
2	B	302	ACO	P2A-O3A	3.73	1.63	1.59
2	C	303	ACO	P2A-O3A	3.51	1.63	1.59
2	B	302	ACO	OAP-CAP	3.41	1.48	1.42
2	B	302	ACO	C2P-S1P	3.34	1.96	1.81
2	A	301	ACO	CCP-CBP	3.32	1.58	1.52
2	A	301	ACO	C2P-S1P	3.28	1.95	1.81
2	D	304	ACO	OAP-CAP	3.27	1.48	1.42
2	D	304	ACO	C2P-S1P	3.27	1.95	1.81
2	F	306	ACO	OAP-CAP	3.26	1.48	1.42
2	A	301	ACO	C2A-N1A	3.24	1.39	1.33
2	E	305	ACO	CCP-CBP	3.21	1.57	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	ACO	C8A-N7A	3.20	1.37	1.31
2	E	305	ACO	C2P-S1P	3.17	1.95	1.81
2	F	306	ACO	C2P-S1P	3.15	1.95	1.81
2	F	306	ACO	CCP-CBP	3.11	1.57	1.52
2	B	302	ACO	C2A-N1A	3.11	1.39	1.33
2	C	303	ACO	C2P-S1P	3.11	1.95	1.81
2	C	303	ACO	O5P-C5P	3.02	1.29	1.23
2	D	304	ACO	CCP-CBP	3.00	1.57	1.52
2	F	306	ACO	C2A-N1A	2.99	1.39	1.33
2	E	305	ACO	P2A-O6A	2.99	1.71	1.59
2	B	302	ACO	CCP-CBP	2.98	1.57	1.52
2	C	303	ACO	C8A-N7A	2.95	1.37	1.31
2	B	302	ACO	C8A-N7A	2.94	1.37	1.31
2	A	301	ACO	P2A-O6A	2.94	1.70	1.59
2	E	305	ACO	O5P-C5P	2.93	1.29	1.23
2	D	304	ACO	P2A-O6A	2.93	1.70	1.59
2	B	302	ACO	O5P-C5P	2.93	1.29	1.23
2	C	303	ACO	P2A-O6A	2.91	1.70	1.59
2	F	306	ACO	P2A-O6A	2.88	1.70	1.59
2	F	306	ACO	C8A-N7A	2.86	1.37	1.31
2	E	305	ACO	C8A-N7A	2.86	1.37	1.31
2	C	303	ACO	CCP-CBP	2.86	1.57	1.52
2	C	303	ACO	C2A-N1A	2.85	1.39	1.33
2	E	305	ACO	C2A-N1A	2.84	1.39	1.33
2	D	304	ACO	P3B-O9A	-2.84	1.44	1.54
2	D	304	ACO	C8A-N7A	2.82	1.37	1.31
2	D	304	ACO	C2A-N1A	2.81	1.38	1.33
2	B	302	ACO	P2A-O6A	2.79	1.70	1.59
2	A	301	ACO	O5P-C5P	2.77	1.28	1.23
2	D	304	ACO	O5P-C5P	2.76	1.28	1.23
2	F	306	ACO	P3B-O9A	-2.63	1.45	1.54
2	F	306	ACO	O5P-C5P	2.57	1.28	1.23
2	C	303	ACO	OAP-CAP	2.49	1.46	1.42
2	B	302	ACO	P3B-O9A	-2.48	1.45	1.54
2	A	301	ACO	OAP-CAP	2.42	1.46	1.42
2	E	305	ACO	P3B-O9A	-2.40	1.45	1.54
2	A	301	ACO	P3B-O9A	-2.38	1.45	1.54
2	F	306	ACO	P2A-O5A	-2.34	1.44	1.55
2	D	304	ACO	P2A-O5A	-2.32	1.44	1.55
2	C	303	ACO	P3B-O9A	-2.28	1.46	1.54
2	C	303	ACO	P2A-O5A	-2.28	1.44	1.55
2	A	301	ACO	P2A-O5A	-2.25	1.44	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	302	ACO	P2A-O5A	-2.18	1.45	1.55
2	D	304	ACO	C5P-N4P	2.18	1.38	1.33
2	E	305	ACO	P2A-O5A	-2.15	1.45	1.55
2	A	301	ACO	P2A-O4A	-2.14	1.43	1.50
2	D	304	ACO	O-C	2.14	1.31	1.21
2	B	302	ACO	O-C	2.14	1.31	1.21
2	B	302	ACO	C5P-N4P	2.11	1.38	1.33
2	E	305	ACO	O-C	2.09	1.31	1.21
2	E	305	ACO	P1A-O2A	-2.09	1.45	1.55
2	C	303	ACO	O-C	2.09	1.31	1.21
2	F	306	ACO	O-C	2.08	1.31	1.21
2	C	303	ACO	C5P-N4P	2.04	1.38	1.33
2	A	301	ACO	O-C	2.03	1.31	1.21
2	D	304	ACO	P1A-O2A	-2.03	1.45	1.55
2	E	305	ACO	C5P-N4P	2.02	1.38	1.33
2	F	306	ACO	C2P-C3P	2.01	1.59	1.51

All (149) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	303	ACO	O6A-CCP-CBP	-48.62	32.37	110.55
2	B	302	ACO	O6A-CCP-CBP	-48.59	32.42	110.55
2	D	304	ACO	O6A-CCP-CBP	-48.53	32.51	110.55
2	E	305	ACO	O6A-CCP-CBP	-48.52	32.53	110.55
2	A	301	ACO	O6A-CCP-CBP	-48.46	32.63	110.55
2	F	306	ACO	O6A-CCP-CBP	-48.44	32.67	110.55
2	A	301	ACO	CDP-CBP-CCP	-45.65	32.86	108.22
2	B	302	ACO	CDP-CBP-CCP	-45.63	32.90	108.22
2	F	306	ACO	CDP-CBP-CCP	-45.59	32.97	108.22
2	E	305	ACO	CDP-CBP-CCP	-45.57	33.00	108.22
2	D	304	ACO	CDP-CBP-CCP	-45.55	33.04	108.22
2	C	303	ACO	CDP-CBP-CCP	-45.43	33.23	108.22
2	E	305	ACO	CEP-CBP-CCP	-44.83	34.22	108.22
2	A	301	ACO	CEP-CBP-CCP	-44.83	34.22	108.22
2	F	306	ACO	CEP-CBP-CCP	-44.81	34.25	108.22
2	B	302	ACO	CEP-CBP-CCP	-44.80	34.27	108.22
2	C	303	ACO	CEP-CBP-CCP	-44.80	34.27	108.22
2	D	304	ACO	CEP-CBP-CCP	-44.78	34.30	108.22
2	B	302	ACO	CDP-CBP-CAP	-28.30	60.52	108.77
2	E	305	ACO	CDP-CBP-CAP	-28.27	60.58	108.77
2	A	301	ACO	CDP-CBP-CAP	-28.25	60.60	108.77
2	F	306	ACO	CDP-CBP-CAP	-28.18	60.72	108.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	304	ACO	CDP-CBP-CAP	-28.18	60.73	108.77
2	C	303	ACO	CDP-CBP-CAP	-28.13	60.81	108.77
2	E	305	ACO	CEP-CBP-CAP	-28.02	61.00	108.77
2	A	301	ACO	CEP-CBP-CAP	-27.92	61.18	108.77
2	C	303	ACO	CEP-CBP-CAP	-27.88	61.24	108.77
2	D	304	ACO	CEP-CBP-CAP	-27.87	61.26	108.77
2	F	306	ACO	CEP-CBP-CAP	-27.84	61.31	108.77
2	B	302	ACO	CEP-CBP-CAP	-27.83	61.33	108.77
2	A	301	ACO	CEP-CBP-CDP	-26.63	56.11	109.20
2	F	306	ACO	CEP-CBP-CDP	-26.58	56.21	109.20
2	B	302	ACO	CEP-CBP-CDP	-26.56	56.26	109.20
2	E	305	ACO	CEP-CBP-CDP	-26.55	56.27	109.20
2	D	304	ACO	CEP-CBP-CDP	-26.52	56.33	109.20
2	C	303	ACO	CEP-CBP-CDP	-26.49	56.40	109.20
2	C	303	ACO	OAP-CAP-CBP	-10.29	86.33	110.18
2	E	305	ACO	OAP-CAP-CBP	-10.28	86.36	110.18
2	F	306	ACO	OAP-CAP-CBP	-10.26	86.41	110.18
2	B	302	ACO	OAP-CAP-CBP	-10.19	86.57	110.18
2	A	301	ACO	OAP-CAP-CBP	-10.18	86.59	110.18
2	D	304	ACO	OAP-CAP-CBP	-10.17	86.61	110.18
2	D	304	ACO	C3P-N4P-C5P	8.42	138.50	122.82
2	F	306	ACO	C3P-N4P-C5P	8.37	138.41	122.82
2	A	301	ACO	C3P-N4P-C5P	8.34	138.35	122.82
2	E	305	ACO	C3P-N4P-C5P	8.34	138.34	122.82
2	C	303	ACO	C3P-N4P-C5P	8.30	138.28	122.82
2	B	302	ACO	C3P-N4P-C5P	8.23	138.15	122.82
2	B	302	ACO	C7P-N8P-C9P	-6.71	110.50	122.55
2	E	305	ACO	C7P-N8P-C9P	-6.62	110.65	122.55
2	D	304	ACO	C7P-N8P-C9P	-6.60	110.69	122.55
2	A	301	ACO	C7P-N8P-C9P	-6.53	110.81	122.55
2	F	306	ACO	C7P-N8P-C9P	-6.51	110.85	122.55
2	C	303	ACO	C7P-N8P-C9P	-6.49	110.89	122.55
2	E	305	ACO	C6P-C5P-N4P	-6.21	105.02	116.34
2	A	301	ACO	C6P-C5P-N4P	-6.20	105.05	116.34
2	C	303	ACO	C6P-C5P-N4P	-6.19	105.06	116.34
2	D	304	ACO	C6P-C5P-N4P	-6.18	105.08	116.34
2	F	306	ACO	C6P-C5P-N4P	-6.16	105.12	116.34
2	B	302	ACO	C6P-C5P-N4P	-6.16	105.12	116.34
2	C	303	ACO	C6P-C7P-N8P	6.03	124.82	112.00
2	F	306	ACO	C6P-C7P-N8P	6.00	124.76	112.00
2	D	304	ACO	C6P-C7P-N8P	6.00	124.76	112.00
2	A	301	ACO	C6P-C7P-N8P	5.95	124.67	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	302	ACO	C6P-C7P-N8P	5.92	124.61	112.00
2	E	305	ACO	C6P-C7P-N8P	5.89	124.54	112.00
2	B	302	ACO	C4A-N9A-C1B	-4.30	116.58	126.63
2	D	304	ACO	C4A-N9A-C1B	-4.28	116.62	126.63
2	C	303	ACO	C4A-N9A-C1B	-4.27	116.64	126.63
2	F	306	ACO	C4A-N9A-C1B	-4.26	116.67	126.63
2	E	305	ACO	C4A-N9A-C1B	-4.25	116.69	126.63
2	A	301	ACO	C4A-N9A-C1B	-4.25	116.70	126.63
2	E	305	ACO	O5P-C5P-N4P	3.93	130.75	123.03
2	B	302	ACO	O5P-C5P-N4P	3.89	130.67	123.03
2	C	303	ACO	O5P-C5P-N4P	3.89	130.66	123.03
2	D	304	ACO	O5P-C5P-N4P	3.87	130.62	123.03
2	F	306	ACO	O5P-C5P-N4P	3.86	130.60	123.03
2	A	301	ACO	O5P-C5P-N4P	3.81	130.51	123.03
2	B	302	ACO	C2P-C3P-N4P	-3.77	104.54	112.41
2	C	303	ACO	C2P-C3P-N4P	-3.73	104.62	112.41
2	A	301	ACO	C2P-C3P-N4P	-3.73	104.62	112.41
2	D	304	ACO	C4A-N9A-C8A	3.73	109.65	105.74
2	A	301	ACO	O5A-P2A-O4A	-3.73	95.11	112.44
2	F	306	ACO	C2P-C3P-N4P	-3.68	104.73	112.41
2	D	304	ACO	C2P-C3P-N4P	-3.67	104.75	112.41
2	B	302	ACO	O5A-P2A-O4A	-3.65	95.45	112.44
2	B	302	ACO	C4A-N9A-C8A	3.64	109.56	105.74
2	F	306	ACO	C4A-N9A-C8A	3.64	109.56	105.74
2	E	305	ACO	C2P-C3P-N4P	-3.63	104.84	112.41
2	C	303	ACO	C4A-N9A-C8A	3.62	109.54	105.74
2	A	301	ACO	C4A-N9A-C8A	3.61	109.53	105.74
2	D	304	ACO	O5A-P2A-O4A	-3.61	95.65	112.44
2	C	303	ACO	O5A-P2A-O4A	-3.56	95.88	112.44
2	E	305	ACO	O5A-P2A-O4A	-3.54	95.99	112.44
2	E	305	ACO	C4A-N9A-C8A	3.53	109.44	105.74
2	F	306	ACO	O5A-P2A-O4A	-3.46	96.34	112.44
2	F	306	ACO	CAP-C9P-N8P	3.37	122.88	116.48
2	B	302	ACO	CAP-C9P-N8P	3.34	122.82	116.48
2	E	305	ACO	CAP-C9P-N8P	3.30	122.75	116.48
2	A	301	ACO	CAP-C9P-N8P	3.30	122.74	116.48
2	D	304	ACO	CAP-C9P-N8P	3.29	122.73	116.48
2	C	303	ACO	CAP-C9P-N8P	3.24	122.64	116.48
2	E	305	ACO	C1B-N9A-C8A	3.05	133.85	127.09
2	B	302	ACO	C1B-N9A-C8A	3.04	133.85	127.09
2	C	303	ACO	C1B-N9A-C8A	3.03	133.82	127.09
2	A	301	ACO	N9A-C8A-N7A	-3.01	109.67	113.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	ACO	C1B-N9A-C8A	3.01	133.77	127.09
2	F	306	ACO	C1B-N9A-C8A	3.00	133.76	127.09
2	D	304	ACO	C1B-N9A-C8A	2.99	133.72	127.09
2	B	302	ACO	C7P-C6P-C5P	2.97	117.34	112.39
2	C	303	ACO	N9A-C8A-N7A	-2.88	109.85	113.94
2	B	302	ACO	N9A-C8A-N7A	-2.86	109.88	113.94
2	A	301	ACO	C7P-C6P-C5P	2.84	117.12	112.39
2	E	305	ACO	C7P-C6P-C5P	2.83	117.11	112.39
2	D	304	ACO	N9A-C8A-N7A	-2.83	109.92	113.94
2	F	306	ACO	N9A-C8A-N7A	-2.81	109.95	113.94
2	A	301	ACO	O5A-P2A-O6A	2.81	120.30	107.57
2	C	303	ACO	C7P-C6P-C5P	2.80	117.06	112.39
2	D	304	ACO	C7P-C6P-C5P	2.80	117.06	112.39
2	F	306	ACO	C7P-C6P-C5P	2.80	117.05	112.39
2	D	304	ACO	O5A-P2A-O6A	2.74	119.99	107.57
2	F	306	ACO	O5A-P2A-O6A	2.74	119.99	107.57
2	B	302	ACO	O5A-P2A-O6A	2.74	119.96	107.57
2	E	305	ACO	O5A-P2A-O6A	2.73	119.93	107.57
2	C	303	ACO	O5A-P2A-O6A	2.68	119.69	107.57
2	E	305	ACO	N9A-C8A-N7A	-2.66	110.16	113.94
2	A	301	ACO	P2A-O6A-CCP	2.58	135.18	121.12
2	F	306	ACO	P2A-O6A-CCP	2.57	135.13	121.12
2	D	304	ACO	P2A-O6A-CCP	2.57	135.13	121.12
2	C	303	ACO	P2A-O6A-CCP	2.54	134.94	121.12
2	E	305	ACO	P2A-O6A-CCP	2.53	134.91	121.12
2	B	302	ACO	P2A-O6A-CCP	2.53	134.90	121.12
2	B	302	ACO	O6A-P2A-O4A	2.35	118.26	108.94
2	D	304	ACO	O6A-P2A-O4A	2.33	118.19	108.94
2	E	305	ACO	O6A-P2A-O4A	2.32	118.13	108.94
2	C	303	ACO	O6A-P2A-O4A	2.29	118.02	108.94
2	F	306	ACO	O5A-P2A-O3A	2.25	113.36	107.27
2	C	303	ACO	O5A-P2A-O3A	2.25	113.35	107.27
2	B	302	ACO	O5A-P2A-O3A	2.24	113.32	107.27
2	A	301	ACO	O5A-P2A-O3A	2.22	113.27	107.27
2	E	305	ACO	O5A-P2A-O3A	2.16	113.12	107.27
2	F	306	ACO	O3A-P1A-O1A	2.15	117.17	110.70
2	D	304	ACO	O5A-P2A-O3A	2.15	113.08	107.27
2	F	306	ACO	O6A-P2A-O4A	2.13	117.37	108.94
2	A	301	ACO	O3A-P1A-O1A	2.11	117.04	110.70
2	A	301	ACO	O6A-P2A-O4A	2.08	117.19	108.94
2	E	305	ACO	O3A-P1A-O1A	2.07	116.93	110.70
2	B	302	ACO	O3A-P1A-O1A	2.07	116.92	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	303	ACO	O3A-P1A-O1A	2.04	116.85	110.70

There are no chirality outliers.

All (107) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	ACO	CCP-O6A-P2A-O3A
2	A	301	ACO	CCP-O6A-P2A-O4A
2	A	301	ACO	CCP-O6A-P2A-O5A
2	A	301	ACO	CBP-CCP-O6A-P2A
2	A	301	ACO	OAP-CAP-CBP-CCP
2	A	301	ACO	C9P-CAP-CBP-CCP
2	A	301	ACO	OAP-CAP-CBP-CDP
2	A	301	ACO	C9P-CAP-CBP-CDP
2	A	301	ACO	C5P-C6P-C7P-N8P
2	A	301	ACO	S1P-C2P-C3P-N4P
2	A	301	ACO	C3P-C2P-S1P-C
2	A	301	ACO	O-C-S1P-C2P
2	A	301	ACO	CH3-C-S1P-C2P
2	B	302	ACO	CCP-O6A-P2A-O3A
2	B	302	ACO	CCP-O6A-P2A-O4A
2	B	302	ACO	CCP-O6A-P2A-O5A
2	B	302	ACO	CBP-CCP-O6A-P2A
2	B	302	ACO	OAP-CAP-CBP-CCP
2	B	302	ACO	C9P-CAP-CBP-CCP
2	B	302	ACO	OAP-CAP-CBP-CDP
2	B	302	ACO	C9P-CAP-CBP-CDP
2	B	302	ACO	C5P-C6P-C7P-N8P
2	B	302	ACO	S1P-C2P-C3P-N4P
2	B	302	ACO	C3P-C2P-S1P-C
2	C	303	ACO	CCP-O6A-P2A-O3A
2	C	303	ACO	CCP-O6A-P2A-O4A
2	C	303	ACO	CCP-O6A-P2A-O5A
2	C	303	ACO	CBP-CCP-O6A-P2A
2	C	303	ACO	OAP-CAP-CBP-CCP
2	C	303	ACO	C9P-CAP-CBP-CCP
2	C	303	ACO	OAP-CAP-CBP-CDP
2	C	303	ACO	C9P-CAP-CBP-CDP
2	C	303	ACO	C5P-C6P-C7P-N8P
2	C	303	ACO	S1P-C2P-C3P-N4P
2	C	303	ACO	C3P-C2P-S1P-C
2	C	303	ACO	O-C-S1P-C2P

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Mol	Chain	Res	Type	Atoms
2	D	304	ACO	CCP-O6A-P2A-O3A
2	D	304	ACO	CCP-O6A-P2A-O4A
2	D	304	ACO	CCP-O6A-P2A-O5A
2	D	304	ACO	CBP-CCP-O6A-P2A
2	D	304	ACO	OAP-CAP-CBP-CCP
2	D	304	ACO	C9P-CAP-CBP-CCP
2	D	304	ACO	OAP-CAP-CBP-CDP
2	D	304	ACO	C9P-CAP-CBP-CDP
2	D	304	ACO	C5P-C6P-C7P-N8P
2	D	304	ACO	S1P-C2P-C3P-N4P
2	D	304	ACO	C3P-C2P-S1P-C
2	E	305	ACO	CCP-O6A-P2A-O3A
2	E	305	ACO	CCP-O6A-P2A-O4A
2	E	305	ACO	CCP-O6A-P2A-O5A
2	E	305	ACO	CBP-CCP-O6A-P2A
2	E	305	ACO	OAP-CAP-CBP-CCP
2	E	305	ACO	C9P-CAP-CBP-CCP
2	E	305	ACO	OAP-CAP-CBP-CDP
2	E	305	ACO	C9P-CAP-CBP-CDP
2	E	305	ACO	C5P-C6P-C7P-N8P
2	E	305	ACO	S1P-C2P-C3P-N4P
2	E	305	ACO	C3P-C2P-S1P-C
2	E	305	ACO	O-C-S1P-C2P
2	F	306	ACO	CCP-O6A-P2A-O3A
2	F	306	ACO	CCP-O6A-P2A-O4A
2	F	306	ACO	CCP-O6A-P2A-O5A
2	F	306	ACO	CBP-CCP-O6A-P2A
2	F	306	ACO	OAP-CAP-CBP-CCP
2	F	306	ACO	C9P-CAP-CBP-CCP
2	F	306	ACO	OAP-CAP-CBP-CDP
2	F	306	ACO	C9P-CAP-CBP-CDP
2	F	306	ACO	C5P-C6P-C7P-N8P
2	F	306	ACO	S1P-C2P-C3P-N4P
2	F	306	ACO	C3P-C2P-S1P-C
2	F	306	ACO	O-C-S1P-C2P
2	A	301	ACO	C2B-C3B-O3B-P3B
2	A	301	ACO	C4B-C3B-O3B-P3B
2	B	302	ACO	C2B-C3B-O3B-P3B
2	B	302	ACO	C4B-C3B-O3B-P3B
2	C	303	ACO	C2B-C3B-O3B-P3B
2	C	303	ACO	C4B-C3B-O3B-P3B
2	D	304	ACO	C2B-C3B-O3B-P3B

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Mol	Chain	Res	Type	Atoms
2	D	304	ACO	C4B-C3B-O3B-P3B
2	E	305	ACO	C2B-C3B-O3B-P3B
2	E	305	ACO	C4B-C3B-O3B-P3B
2	F	306	ACO	C2B-C3B-O3B-P3B
2	F	306	ACO	C4B-C3B-O3B-P3B
2	B	302	ACO	O-C-S1P-C2P
2	B	302	ACO	CH3-C-S1P-C2P
2	C	303	ACO	CH3-C-S1P-C2P
2	E	305	ACO	CH3-C-S1P-C2P
2	F	306	ACO	CH3-C-S1P-C2P
2	D	304	ACO	O-C-S1P-C2P
2	A	301	ACO	C3B-O3B-P3B-O8A
2	B	302	ACO	C3B-O3B-P3B-O8A
2	C	303	ACO	C3B-O3B-P3B-O8A
2	D	304	ACO	C3B-O3B-P3B-O8A
2	E	305	ACO	C3B-O3B-P3B-O8A
2	F	306	ACO	C3B-O3B-P3B-O8A
2	D	304	ACO	CH3-C-S1P-C2P
2	A	301	ACO	C2B-C1B-N9A-C8A
2	B	302	ACO	C2B-C1B-N9A-C8A
2	A	301	ACO	N8P-C9P-CAP-OAP
2	B	302	ACO	N8P-C9P-CAP-OAP
2	C	303	ACO	N8P-C9P-CAP-OAP
2	D	304	ACO	N8P-C9P-CAP-OAP
2	E	305	ACO	N8P-C9P-CAP-OAP
2	F	306	ACO	N8P-C9P-CAP-OAP
2	B	302	ACO	P2A-O3A-P1A-O2A
2	E	305	ACO	P2A-O3A-P1A-O2A
2	F	306	ACO	P2A-O3A-P1A-O2A

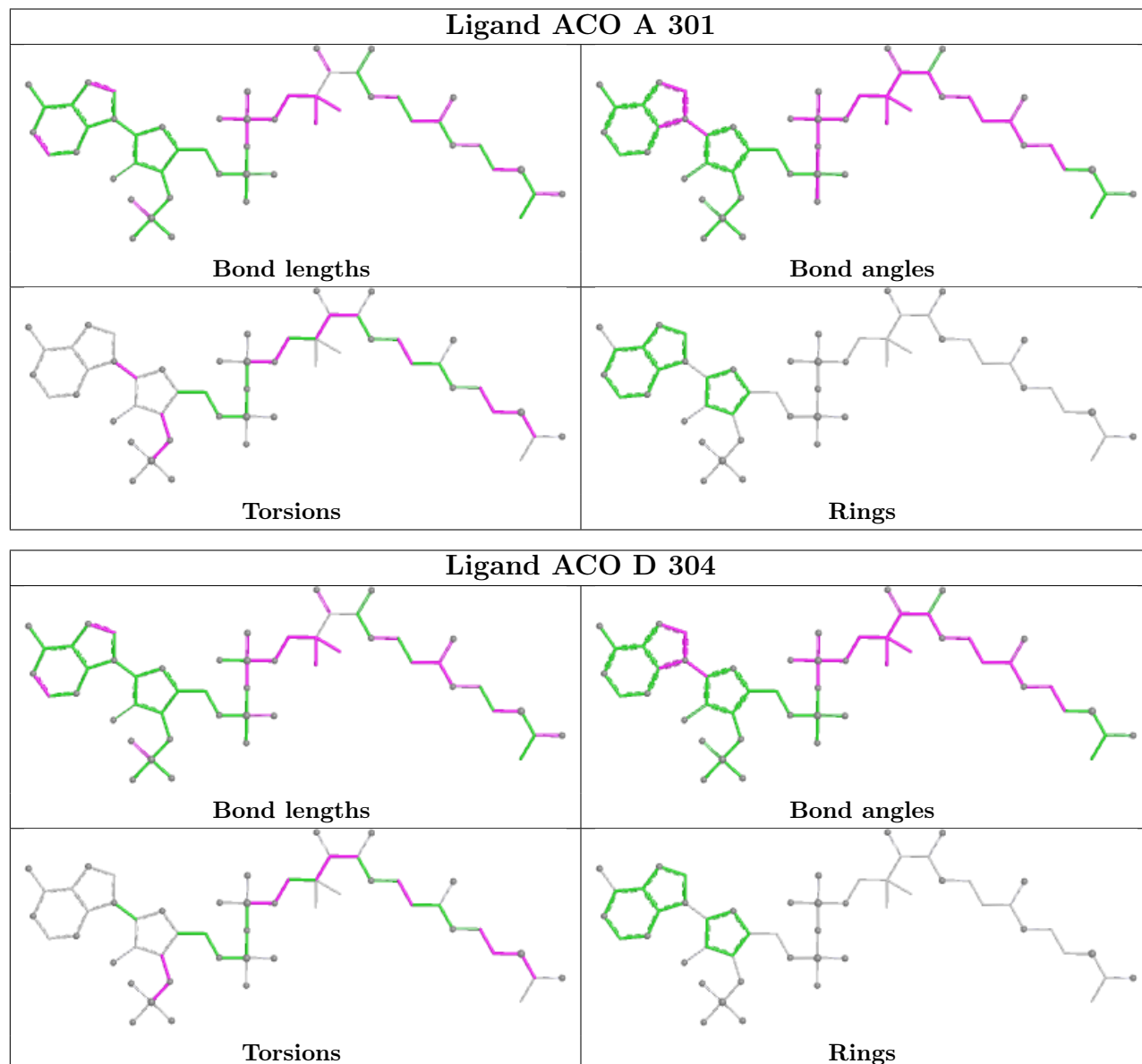
There are no ring outliers.

5 monomers are involved in 16 short contacts:

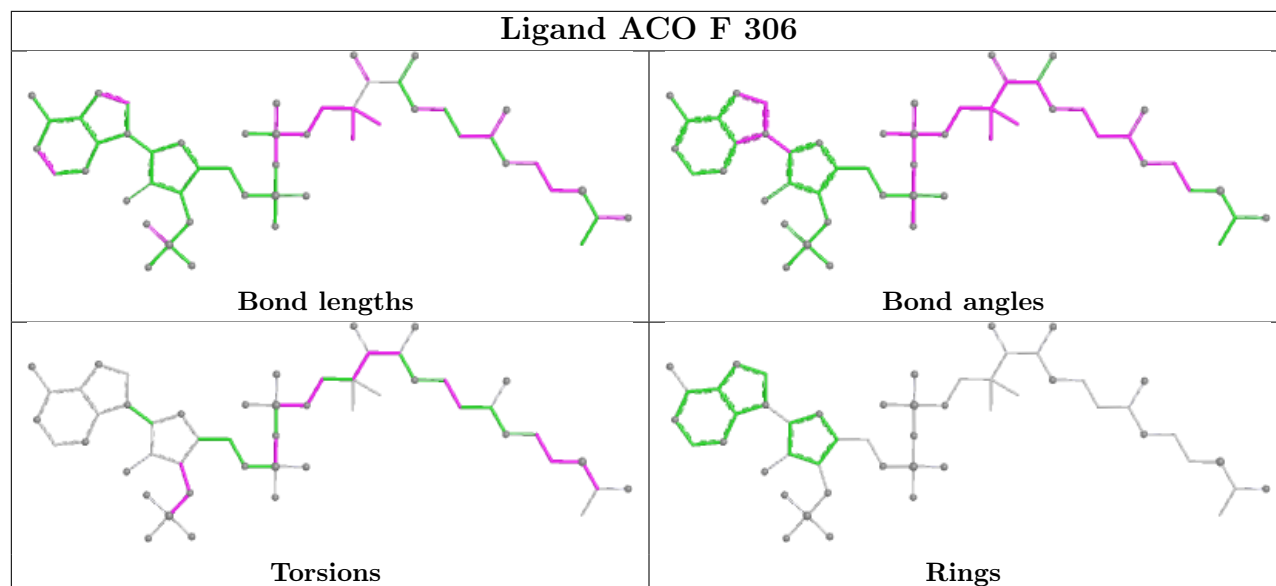
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	ACO	5	0
2	D	304	ACO	1	0
2	F	306	ACO	1	0
2	B	302	ACO	3	0
2	C	303	ACO	6	0

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

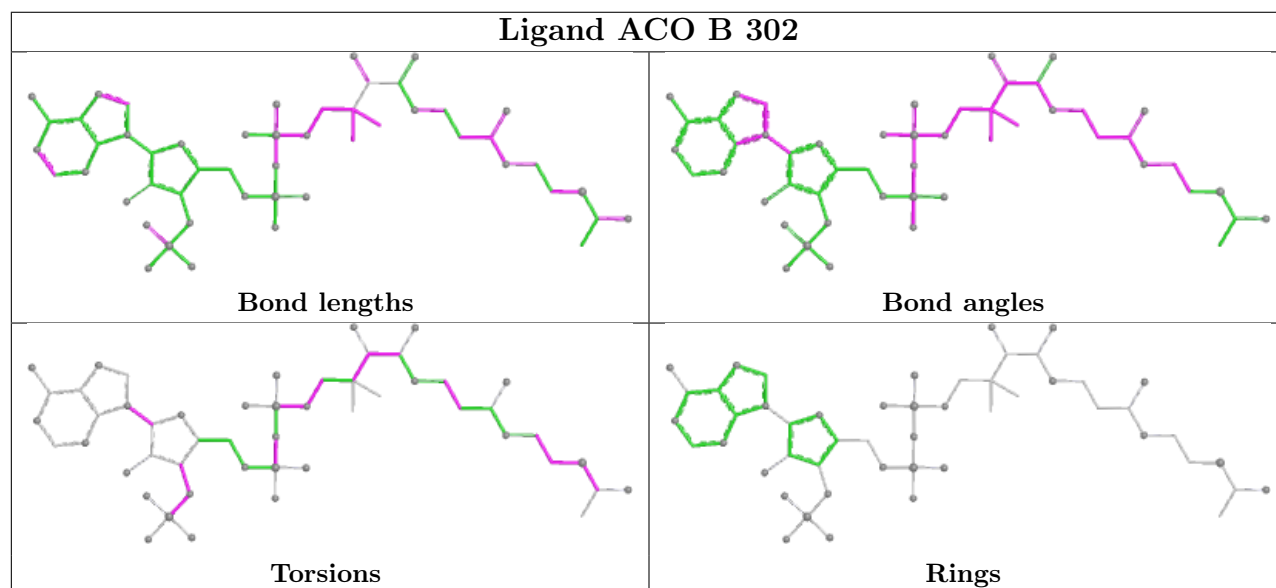
addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.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



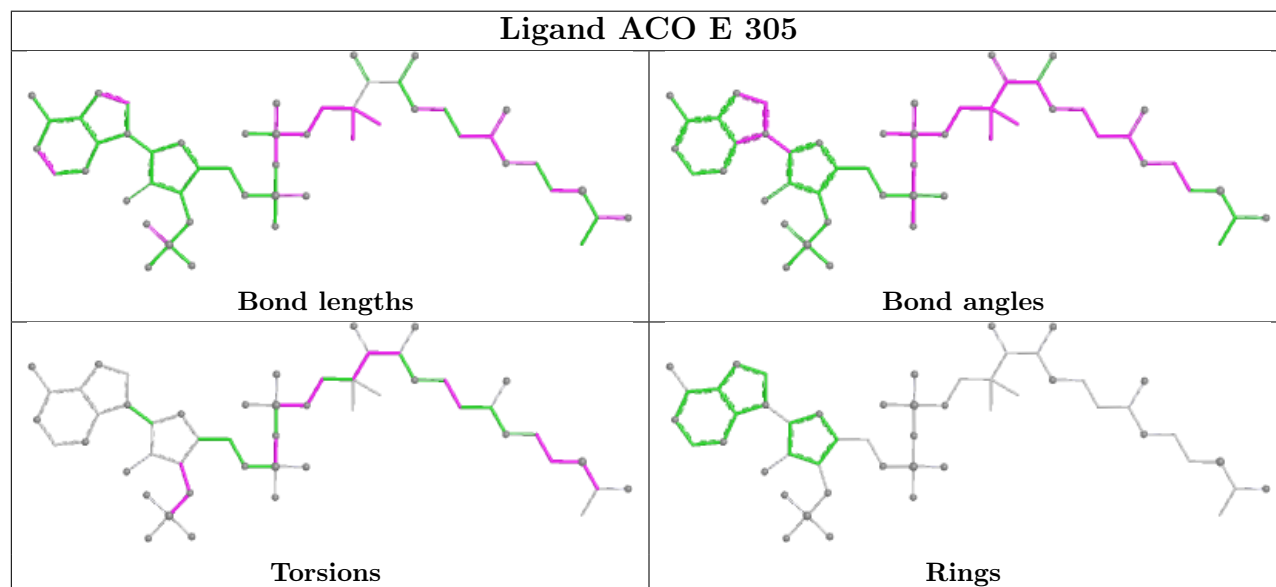
Ligand ACO F 306

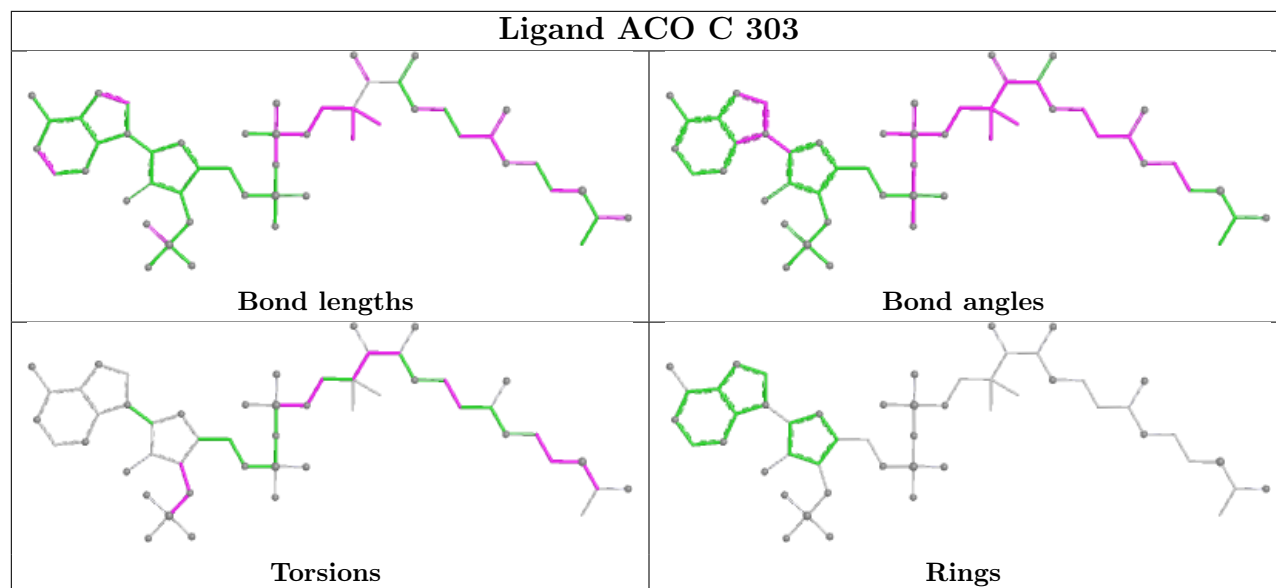


Ligand ACO B 302



Ligand ACO E 305





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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.