



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:02 AM UTC

PDB ID : 1H83 / pdb_00001h83
Title : STRUCTURE OF POLYAMINE OXIDASE IN COMPLEX WITH 1,8-DIAMINOOCCTANE
Authors : Binda, C.; Coda, A.; Angelini, R.; Federico, R.; Ascenzi, P.; Mattevi, A.
Deposited on : 2001-01-24
Resolution : 1.90 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

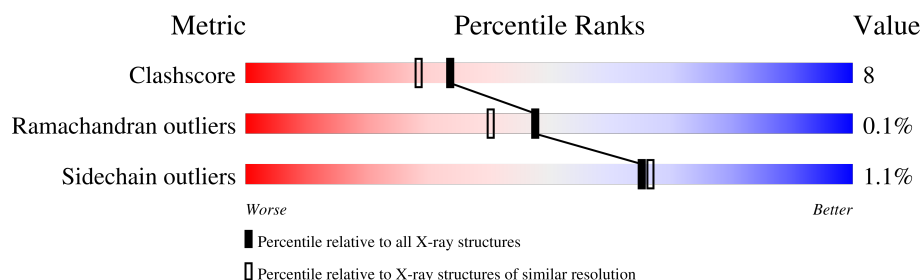
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 Å.

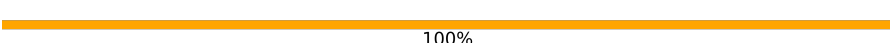
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	8410 (1.90-1.90)
Ramachandran outliers	187476	8333 (1.90-1.90)
Sidechain outliers	187428	8333 (1.90-1.90)

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	472	 75% 19% ..
1	B	472	 81% 15% ..
1	C	472	 82% 14% ..
2	D	2	 100%
2	E	2	 100%
3	F	5	 40% 60%

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 12183 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 POLYAMINE OXIDASE.

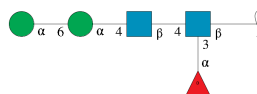
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	65	0	0
			3684	2353	621	696	14			
1	B	462	Total	C	N	O	S	66	0	0
			3715	2374	627	700	14			
1	C	462	Total	C	N	O	S	58	0	0
			3715	2374	627	700	14			

- Molecule 2 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



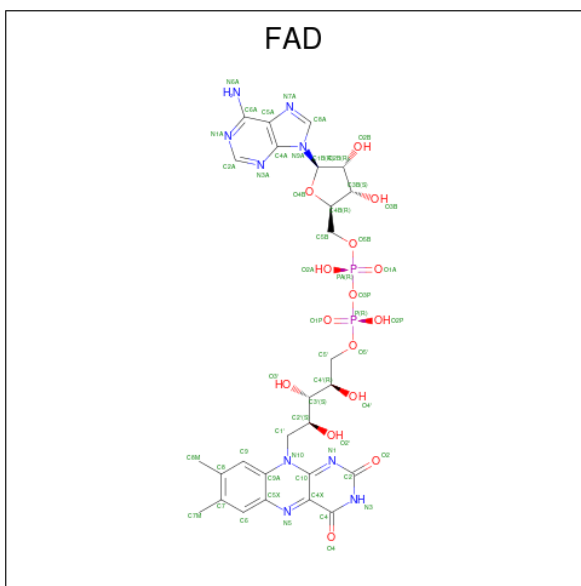
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-D-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose.



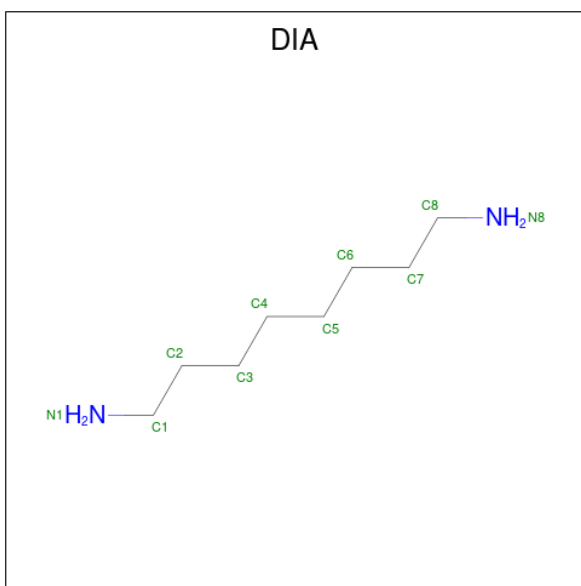
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	F	5	Total	C	N	O	0	0	0
			60	34	2	24			

- Molecule 4 is FLAVIN-ADENINE DINUCLEOTIDE (CCD ID: FAD) (formula: $\text{C}_{27}\text{H}_{33}\text{N}_9\text{O}_{15}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	B	1	Total 53	C 27	N 9	O 15	P 2	0	0
4	C	1	Total 53	C 27	N 9	O 15	P 2	0	0

- Molecule 5 is OCTANE 1,8-DIAMINE (CCD ID: DIA) (formula: $\text{C}_8\text{H}_{20}\text{N}_2$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	1
			20	16	4		
5	B	1	Total	C	N	0	1
			20	16	4		
5	C	1	Total	C	N	0	1
			20	16	4		

- Molecule 6 is water.

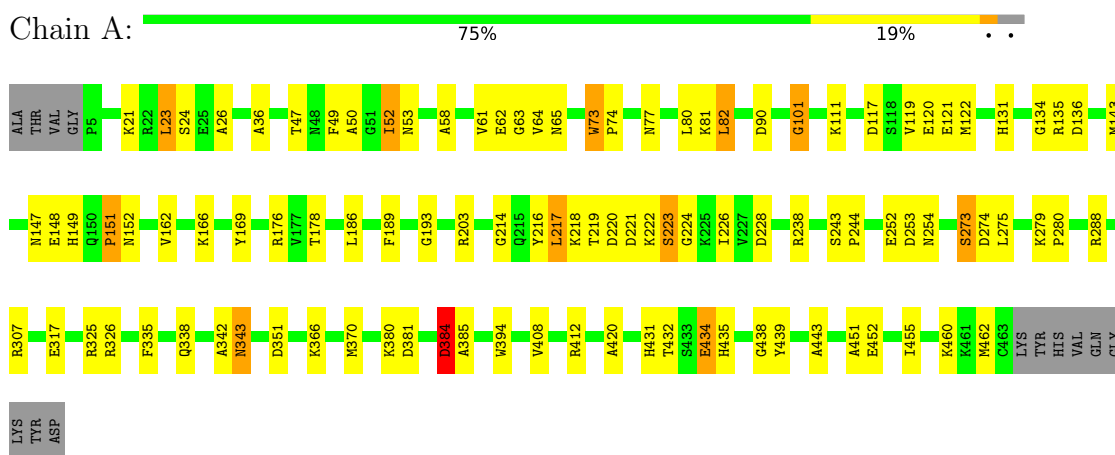
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	223	Total	O	0	0
			223	223		
6	B	242	Total	O	0	0
			242	242		
6	C	269	Total	O	0	0
			269	269		

3 Residue-property plots

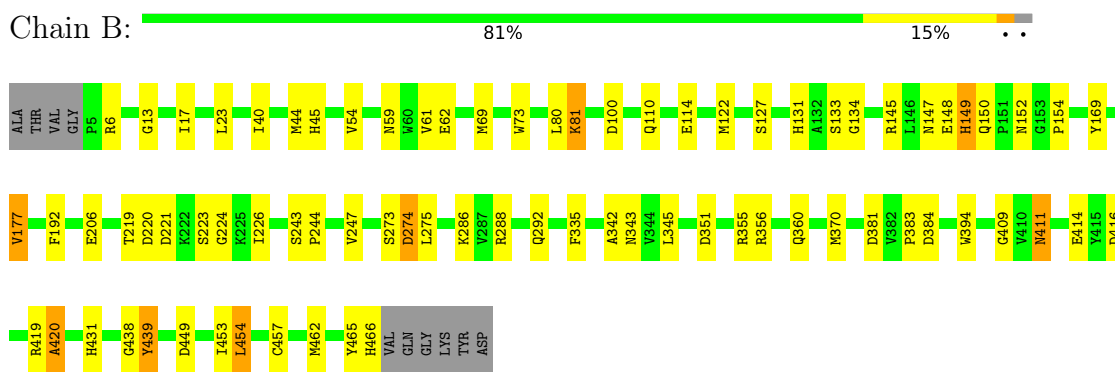
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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.

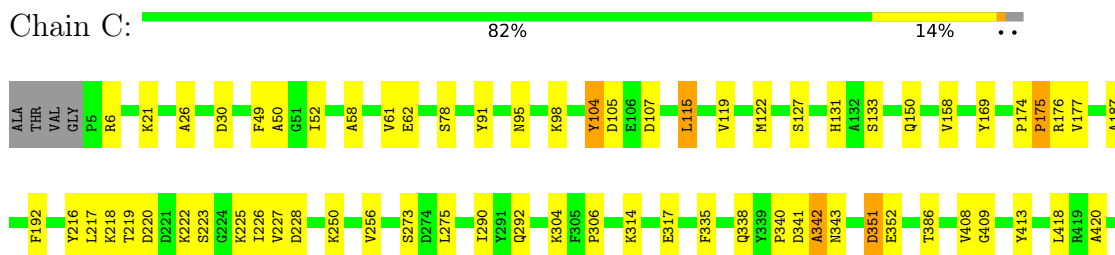
• Molecule 1: POLYAMINE OXIDASE

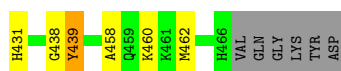


• Molecule 1: POLYAMINE OXIDASE



• Molecule 1: POLYAMINE OXIDASE





- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain D:  100%



- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain E:  100%



- Molecule 3: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-[alpha-D-fucopyranose-(1-3)]2-acetamido-2-deoxy-beta-D-glucopyranose

Chain F:  40% 60%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 65 2 2	Depositor
Cell constants a, b, c, α , β , γ	184.69Å 184.69Å 282.22Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 1.90	Depositor
% Data completeness (in resolution range)	97.9 (20.00-1.90)	Depositor
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5D	Depositor
R, R_{free}	0.196 , 0.237	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12183	wwPDB-VP
Average B, all atoms (Å ²)	15.0	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: MAN, NAG, FCA, FAD, DIA

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	0.67	1/3775 (0.0%)	1.55	40/5116 (0.8%)
1	B	0.66	1/3808 (0.0%)	1.54	33/5160 (0.6%)
1	C	0.67	0/3808	1.54	33/5160 (0.6%)
All	All	0.67	2/11391 (0.0%)	1.54	106/15436 (0.7%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	134	GLY	C-N	-6.20	1.25	1.33
1	B	149	HIS	CA-C	-5.02	1.47	1.53

All (106) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	340	PRO	CA-C-N	-12.21	103.11	122.65
1	C	340	PRO	C-N-CA	-12.21	103.11	122.65
1	C	342	ALA	N-CA-C	10.25	123.71	111.82
1	A	61	VAL	N-CA-C	-9.48	94.15	107.99
1	C	273	SER	CA-C-N	-9.31	107.74	122.73
1	C	273	SER	C-N-CA	-9.31	107.74	122.73
1	B	149	HIS	CB-CA-C	-8.75	99.33	112.11
1	B	177	VAL	N-CA-CB	-8.61	102.74	112.21
1	A	273	SER	CA-C-N	-8.52	109.65	124.82
1	A	273	SER	C-N-CA	-8.52	109.65	124.82
1	A	101	GLY	N-CA-C	8.01	132.15	113.18
1	C	420	ALA	N-CA-C	7.42	119.06	109.64
1	B	100	ASP	N-CA-C	7.22	122.06	112.25
1	C	61	VAL	N-CA-C	-7.18	96.81	107.51
1	C	338	GLN	N-CA-C	7.16	118.87	111.14
1	A	381	ASP	CA-C-N	-7.11	117.47	122.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	381	ASP	C-N-CA	-7.11	117.47	122.59
1	B	221	ASP	N-CA-C	7.10	119.02	111.28
1	B	465	TYR	N-CA-C	7.05	121.97	111.04
1	B	13	GLY	N-CA-C	-6.88	102.09	112.41
1	B	61	VAL	N-CA-C	-6.78	97.41	107.51
1	A	26	ALA	N-CA-C	-6.66	105.03	113.02
1	B	150	GLN	N-CA-C	-6.64	100.54	108.25
1	B	335	PHE	N-CA-C	6.59	121.21	112.25
1	C	176	ARG	CA-C-N	-6.53	112.97	122.69
1	C	176	ARG	C-N-CA	-6.53	112.97	122.69
1	A	221	ASP	N-CA-C	6.48	119.16	111.71
1	B	420	ALA	N-CA-C	6.43	117.80	109.64
1	A	223	SER	N-CA-C	6.43	117.94	111.07
1	B	439	TYR	N-CA-C	6.32	120.21	110.42
1	C	26	ALA	N-CA-C	-6.31	105.34	113.16
1	B	409	GLY	CA-C-N	-6.27	115.03	122.93
1	B	409	GLY	C-N-CA	-6.27	115.03	122.93
1	C	115	LEU	N-CA-CB	-6.21	100.99	110.12
1	A	384	ASP	CB-CA-C	-6.19	98.55	109.62
1	C	335	PHE	N-CA-C	6.16	120.63	112.25
1	B	351	ASP	N-CA-CB	-6.15	100.10	110.49
1	A	162	VAL	N-CA-C	-6.14	104.52	110.72
1	C	275	LEU	N-CA-C	6.07	118.39	111.11
1	C	150	GLN	CB-CA-C	-6.02	100.64	109.97
1	B	100	ASP	CB-CA-C	5.99	119.47	111.14
1	A	151	PRO	N-CA-C	-5.97	108.47	114.68
1	A	351	ASP	N-CA-CB	-5.91	100.50	110.49
1	B	149	HIS	CA-CB-CG	-5.86	107.94	113.80
1	C	439	TYR	N-CA-C	5.85	119.49	110.42
1	C	351	ASP	N-CA-C	5.84	117.19	108.31
1	A	434	GLU	N-CA-C	5.84	117.64	111.28
1	C	409	GLY	CA-C-N	-5.84	115.58	122.93
1	C	409	GLY	C-N-CA	-5.84	115.58	122.93
1	B	356	ARG	CA-C-O	5.83	126.71	120.70
1	B	122	MET	N-CA-C	-5.83	104.93	111.28
1	A	381	ASP	N-CA-C	-5.81	96.95	107.75
1	A	224	GLY	N-CA-C	-5.77	107.14	115.27
1	A	288	ARG	CA-CB-CG	-5.75	102.61	114.10
1	C	177	VAL	N-CA-C	-5.74	107.39	112.90
1	A	275	LEU	N-CA-C	-5.66	105.11	111.28
1	A	73	TRP	CA-C-O	5.66	124.27	118.73
1	A	335	PHE	N-CA-C	5.64	120.49	111.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	317	GLU	N-CA-C	5.61	117.39	111.28
1	B	275	LEU	N-CA-C	-5.61	105.25	111.36
1	A	408	VAL	CA-C-N	-5.57	116.81	123.44
1	A	408	VAL	C-N-CA	-5.57	116.81	123.44
1	C	104	TYR	N-CA-C	-5.56	103.36	110.53
1	C	458	ALA	N-CA-C	5.52	117.38	111.36
1	C	192	PHE	N-CA-C	5.51	120.01	113.28
1	C	413	TYR	N-CA-C	-5.48	105.21	111.07
1	C	317	GLU	N-CA-C	5.48	117.68	111.11
1	C	341	ASP	CB-CA-C	5.46	119.78	110.56
1	B	17	ILE	N-CA-C	-5.42	105.24	110.72
1	A	77	ASN	N-CA-C	5.42	119.06	112.23
1	A	24	SER	N-CA-C	-5.41	105.38	111.28
1	A	82	LEU	N-CA-C	-5.40	101.67	110.20
1	B	177	VAL	N-CA-C	-5.40	107.54	113.43
1	C	408	VAL	CA-C-N	-5.39	117.58	123.30
1	C	408	VAL	C-N-CA	-5.39	117.58	123.30
1	C	187	ALA	N-CA-C	5.35	117.11	111.28
1	A	443	ALA	N-CA-C	-5.33	105.47	111.28
1	B	73	TRP	N-CA-C	5.30	119.95	112.75
1	A	149	HIS	N-CA-C	5.29	118.54	111.24
1	B	6	ARG	N-CA-C	-5.26	101.11	109.59
1	A	134	GLY	N-CA-C	-5.24	108.39	115.36
1	A	338	GLN	N-CA-C	5.24	116.67	111.07
1	B	44	MET	N-CA-C	-5.24	98.72	107.99
1	B	192	PHE	N-CA-C	5.24	119.82	113.38
1	A	343	ASN	CB-CA-C	-5.22	104.32	111.73
1	B	81	LYS	CB-CA-C	-5.21	104.88	111.86
1	B	147	ASN	CA-C-N	-5.20	113.26	122.26
1	B	147	ASN	C-N-CA	-5.20	113.26	122.26
1	B	54	VAL	N-CA-C	-5.19	101.59	108.96
1	A	434	GLU	CA-C-N	-5.18	113.91	121.99
1	A	434	GLU	C-N-CA	-5.18	113.91	121.99
1	C	409	GLY	N-CA-C	-5.17	108.05	113.58
1	B	274	ASP	N-CA-C	5.16	118.84	112.24
1	A	178	THR	N-CA-C	5.15	118.62	109.96
1	A	420	ALA	N-CA-C	5.12	116.85	109.48
1	A	380	LYS	N-CA-C	5.10	118.01	110.46
1	A	214	GLY	N-CA-C	-5.10	109.06	114.67
1	C	95	ASN	N-CA-C	5.06	117.36	110.88
1	A	36	ALA	N-CA-C	5.05	116.87	111.36
1	B	345	LEU	N-CA-C	-5.05	101.69	109.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	23	LEU	N-CA-C	-5.04	105.86	111.36
1	B	134	GLY	N-CA-C	-5.04	108.65	115.21
1	C	78	SER	CA-C-N	-5.04	113.59	120.44
1	C	78	SER	C-N-CA	-5.04	113.59	120.44
1	A	90	ASP	N-CA-C	5.03	118.52	112.38
1	A	148	GLU	CB-CA-C	-5.02	101.71	110.09

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	3684	0	3585	61	0
1	B	3715	0	3614	51	0
1	C	3715	0	3614	41	0
2	D	28	0	26	5	0
2	E	28	0	26	4	0
3	F	60	0	53	6	0
4	A	53	0	31	2	0
4	B	53	0	31	1	0
4	C	53	0	31	2	0
5	A	20	0	40	5	0
5	B	20	0	40	4	0
5	C	20	0	40	5	0
6	A	223	0	0	7	1
6	B	242	0	0	4	0
6	C	269	0	0	3	2
All	All	12183	0	11131	167	2

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 8.

All (167) 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)
5:C:590[A]:DIA:HC82	6:C:2227:HOH:O	1.55	1.06
1:A:273:SER:O	1:A:274:ASP:HB2	1.72	0.88
3:F:1:NAG:C4	3:F:2:NAG:C1	2.54	0.86
2:E:1:NAG:C4	2:E:2:NAG:C1	2.55	0.84
1:C:91:TYR:OH	1:C:314:LYS:HE2	1.80	0.81
1:B:131:HIS:CD2	1:B:133:SER:H	1.98	0.81
1:C:131:HIS:CD2	1:C:133:SER:H	1.98	0.80
1:B:131:HIS:HD2	1:B:133:SER:H	1.31	0.77
3:F:1:NAG:H3	3:F:5:FCA:O2	1.85	0.76
5:B:590[A]:DIA:HC82	6:B:2212:HOH:O	1.86	0.76
2:D:1:NAG:C4	2:D:2:NAG:C1	2.64	0.76
1:B:411:ASN:ND2	1:B:414:GLU:H	1.86	0.74
1:A:216:TYR:CD1	1:A:217:LEU:HD13	2.23	0.74
1:B:62:GLU:OE2	5:B:590[A]:DIA:HC22	1.86	0.74
1:A:394:TRP:HE1	1:B:152:ASN:ND2	1.86	0.73
1:A:431:HIS:CD2	1:A:431:HIS:H	2.07	0.72
1:C:292:GLN:OE1	6:C:2144:HOH:O	2.08	0.71
1:C:460:LYS:HB3	1:C:462:MET:HE2	1.72	0.71
1:A:151:PRO:HB2	6:A:2067:HOH:O	1.91	0.70
5:A:590[A]:DIA:HC82	6:A:2196:HOH:O	1.91	0.70
1:A:216:TYR:CE1	1:A:217:LEU:HD13	2.29	0.68
1:A:370:MET:HE2	1:A:384:ASP:HA	1.76	0.68
1:C:62:GLU:OE2	5:C:590[A]:DIA:HC22	1.94	0.68
1:A:307:ARG:HG2	1:A:307:ARG:HH11	1.58	0.66
3:F:1:NAG:O4	3:F:2:NAG:C2	2.43	0.66
1:A:136:ASP:OD1	6:A:2061:HOH:O	2.13	0.66
1:C:131:HIS:HD2	1:C:133:SER:OG	1.80	0.65
1:A:307:ARG:HG2	1:A:307:ARG:NH1	2.11	0.64
2:D:1:NAG:HO4	2:D:2:NAG:C1	2.10	0.64
1:A:119:VAL:HA	1:A:122:MET:HE3	1.79	0.64
1:B:411:ASN:HD22	1:B:414:GLU:H	1.48	0.62
1:A:273:SER:O	1:A:274:ASP:CB	2.38	0.61
1:C:219:THR:HG22	1:C:226:ILE:HA	1.83	0.61
1:A:220:ASP:HB3	1:A:223:SER:OG	2.01	0.60
1:A:394:TRP:HE1	1:B:152:ASN:HD22	1.49	0.60
1:C:431:HIS:H	1:C:431:HIS:CD2	2.18	0.60
1:C:131:HIS:HD2	1:C:133:SER:H	1.47	0.59
1:B:439:TYR:CZ	5:B:590[A]:DIA:HC61	2.39	0.58
1:A:152:ASN:ND2	1:B:394:TRP:HE1	2.02	0.58
2:E:1:NAG:O4	2:E:2:NAG:C2	2.51	0.58
1:C:158:VAL:HG12	6:C:2077:HOH:O	2.04	0.58
1:B:220:ASP:HB3	1:B:223:SER:OG	2.04	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:23:LEU:HD13	1:A:451:ALA:HB1	1.87	0.57
1:A:366:LYS:HD2	1:A:385:ALA:HB3	1.87	0.57
1:A:117:ASP:O	1:A:121:GLU:HG3	2.05	0.57
1:A:73:TRP:HB3	1:A:74:PRO:HD3	1.87	0.56
1:A:218:LYS:H	1:A:228:ASP:HB2	1.71	0.56
1:A:460:LYS:HB3	1:A:462:MET:HE3	1.88	0.56
1:B:431:HIS:H	1:B:431:HIS:CD2	2.23	0.56
1:C:220:ASP:HB3	1:C:223:SER:OG	2.06	0.56
1:B:81:LYS:HZ3	1:B:81:LYS:HB3	1.71	0.55
1:C:220:ASP:OD2	1:C:222:LYS:N	2.39	0.55
1:B:81:LYS:HB3	1:B:81:LYS:NZ	2.22	0.55
1:A:111:LYS:HG2	6:A:2048:HOH:O	2.08	0.54
1:C:342:ALA:O	1:C:343:ASN:HB2	2.08	0.54
1:C:439:TYR:CZ	5:C:590[A]:DIA:HC61	2.43	0.53
1:B:169:TYR:O	5:B:590[B]:DIA:HC51	2.09	0.53
1:B:219:THR:HG22	1:B:226:ILE:HA	1.89	0.53
1:C:131:HIS:HD2	1:C:133:SER:CB	2.21	0.53
1:B:131:HIS:HD2	1:B:133:SER:OG	1.92	0.53
1:C:21:LYS:HB2	1:C:216:TYR:CE2	2.44	0.53
1:A:131:HIS:CE1	1:A:135:ARG:NH2	2.77	0.53
1:A:238:ARG:NH1	1:A:252:GLU:OE2	2.40	0.52
1:A:120:GLU:OE1	1:A:166:LYS:NZ	2.41	0.52
1:A:152:ASN:HD22	1:B:394:TRP:HE1	1.56	0.52
1:B:449:ASP:O	1:B:453:ILE:HG13	2.10	0.52
1:A:439:TYR:CZ	5:A:590[A]:DIA:HC61	2.44	0.52
1:A:63:GLY:HA2	1:A:193:GLY:O	2.10	0.51
1:C:169:TYR:O	5:C:590[B]:DIA:HC51	2.09	0.51
1:C:218:LYS:H	1:C:228:ASP:HB2	1.76	0.51
1:B:131:HIS:CD2	1:B:133:SER:OG	2.64	0.51
1:A:220:ASP:OD1	1:A:222:LYS:N	2.40	0.50
1:B:419:ARG:HD3	6:B:2217:HOH:O	2.11	0.50
1:C:131:HIS:CD2	1:C:133:SER:OG	2.61	0.50
1:A:58:ALA:HA	4:A:579:FAD:C4X	2.41	0.50
1:A:81:LYS:O	1:A:203:ARG:NH2	2.45	0.50
1:A:253:ASP:O	1:A:254:ASN:HB2	2.12	0.50
1:A:434:GLU:HG2	1:A:435:HIS:CD2	2.47	0.49
1:A:62:GLU:OE2	5:A:590[A]:DIA:HC22	2.12	0.49
1:B:148:GLU:O	1:B:149:HIS:HB2	2.12	0.49
2:E:1:NAG:H4	2:E:2:NAG:C1	2.40	0.49
1:B:131:HIS:HD2	1:B:133:SER:CB	2.26	0.48
1:B:220:ASP:O	1:B:224:GLY:N	2.45	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:GLY:O	4:B:579:FAD:H1'2	2.14	0.48
1:A:131:HIS:ND1	1:A:136:ASP:OD2	2.36	0.48
1:B:243:SER:HB2	1:B:244:PRO:CD	2.44	0.48
1:C:119:VAL:HA	1:C:122:MET:HE3	1.96	0.48
1:A:21:LYS:HB2	1:A:216:TYR:CE2	2.49	0.48
1:B:360:GLN:NE2	6:B:2188:HOH:O	2.46	0.48
1:B:110:GLN:O	1:B:114:GLU:HG2	2.13	0.47
1:C:306:PRO:HD3	1:C:386:THR:HG23	1.96	0.47
1:A:412:ARG:HH12	1:A:434:GLU:HG3	1.78	0.47
1:A:342:ALA:O	1:A:343:ASN:HB2	2.15	0.47
1:C:218:LYS:O	1:C:227:VAL:N	2.42	0.47
1:A:431:HIS:CD2	6:A:2206:HOH:O	2.67	0.47
1:B:81:LYS:NZ	1:B:81:LYS:CB	2.77	0.47
1:A:47:THR:O	1:A:53:ASN:HA	2.16	0.46
2:D:1:NAG:O6	2:D:2:NAG:C1	2.63	0.46
1:B:80:LEU:O	1:B:81:LYS:HB2	2.14	0.46
1:B:411:ASN:HD22	1:B:411:ASN:C	2.23	0.46
1:A:169:TYR:O	5:A:590[B]:DIA:HC51	2.15	0.46
1:B:131:HIS:HD2	1:B:133:SER:N	2.07	0.45
1:B:273:SER:O	1:B:274:ASP:HB2	2.16	0.45
3:F:2:NAG:H62	3:F:5:FCA:H5	1.98	0.45
1:C:131:HIS:CD2	1:C:133:SER:CB	2.99	0.45
1:C:351:ASP:CG	1:C:352:GLU:H	2.23	0.45
1:B:220:ASP:OD2	1:B:223:SER:OG	2.33	0.45
1:C:58:ALA:HA	4:C:579:FAD:C4X	2.47	0.45
1:C:105:ASP:OD1	1:C:107:ASP:HB2	2.17	0.45
1:A:49:PHE:O	1:A:50:ALA:HB3	2.17	0.45
1:B:454:LEU:HD12	1:B:454:LEU:C	2.42	0.44
1:C:6:ARG:HH11	1:C:6:ARG:HG3	1.82	0.44
1:C:6:ARG:HA	1:C:30:ASP:O	2.17	0.44
1:C:219:THR:HA	1:C:225:LYS:O	2.16	0.44
1:C:220:ASP:OD2	1:C:222:LYS:HB3	2.17	0.44
2:D:1:NAG:H4	2:D:2:NAG:C1	2.47	0.44
1:B:355:ARG:NE	6:B:2183:HOH:O	2.41	0.44
5:A:590[A]:DIA:C8	6:A:2196:HOH:O	2.59	0.44
1:B:286:LYS:NZ	1:B:420:ALA:O	2.50	0.44
1:C:62:GLU:OE2	5:C:590[B]:DIA:HC72	2.16	0.44
1:C:438:GLY:O	4:C:579:FAD:H1'2	2.17	0.44
1:A:279:LYS:HA	1:A:280:PRO:HA	1.84	0.44
1:C:49:PHE:O	1:C:52:ILE:HG12	2.18	0.44
1:A:143:MET:SD	1:A:147:ASN:ND2	2.92	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:TYR:CZ	1:C:314:LYS:HE2	2.54	0.43
1:A:186:LEU:HD23	1:A:189:PHE:CE1	2.53	0.43
1:A:452:GLU:HA	1:A:455:ILE:HD12	1.99	0.43
1:B:40:ILE:HG21	1:B:40:ILE:HD13	1.74	0.43
1:B:220:ASP:O	1:B:224:GLY:HA2	2.19	0.43
1:A:176:ARG:HD2	1:B:177:VAL:HG21	1.99	0.43
1:A:243:SER:HB2	1:A:244:PRO:CD	2.48	0.43
1:C:290:ILE:HA	1:C:418:LEU:HD21	2.01	0.43
1:A:52:ILE:HD13	1:A:52:ILE:HG21	1.73	0.42
1:A:73:TRP:N	1:A:74:PRO:CD	2.82	0.42
1:C:218:LYS:N	1:C:228:ASP:HB2	2.34	0.42
1:A:219:THR:HG22	1:A:226:ILE:HA	2.00	0.42
1:B:370:MET:HG3	1:B:384:ASP:OD2	2.19	0.42
1:A:432:THR:HA	6:A:2207:HOH:O	2.18	0.42
1:B:45:HIS:HA	1:B:206:GLU:OE2	2.19	0.42
1:A:64:VAL:HG12	1:A:65:ASN:N	2.34	0.42
1:A:217:LEU:HA	1:A:217:LEU:HD12	1.75	0.42
3:F:1:NAG:O6	3:F:2:NAG:C1	2.67	0.42
1:A:82:LEU:HA	1:A:82:LEU:HD23	1.75	0.42
1:B:381:ASP:O	1:B:383:PRO:HD3	2.19	0.42
1:C:217:LEU:HD23	1:C:217:LEU:HA	1.80	0.42
3:F:1:NAG:C3	3:F:5:FCA:O2	2.64	0.42
1:B:220:ASP:CG	1:B:223:SER:HG	2.28	0.42
1:B:69:MET:HE2	1:B:69:MET:HB2	1.82	0.42
1:B:131:HIS:CD2	1:B:133:SER:CB	3.03	0.42
1:B:243:SER:HB2	1:B:244:PRO:HD2	2.02	0.42
1:C:98:LYS:HG2	1:C:104:TYR:CE1	2.54	0.42
1:C:250:LYS:HG2	1:C:256:VAL:HG22	2.00	0.42
2:E:1:NAG:O6	2:E:2:NAG:C1	2.68	0.41
1:A:82:LEU:HD23	1:A:203:ARG:CZ	2.50	0.41
1:B:342:ALA:O	1:B:343:ASN:HB2	2.20	0.41
1:C:50:ALA:HB1	1:C:304:LYS:HD3	2.03	0.41
1:A:80:LEU:O	1:A:81:LYS:C	2.64	0.41
1:B:416:ASP:OD2	1:B:466:HIS:HD2	2.03	0.41
1:A:438:GLY:O	4:A:579:FAD:H1'2	2.20	0.41
1:B:145:ARG:O	1:B:149:HIS:N	2.52	0.41
1:A:218:LYS:N	1:A:228:ASP:HB2	2.34	0.41
1:A:325:ARG:O	1:A:326:ARG:C	2.63	0.41
2:D:1:NAG:O4	2:D:2:NAG:C2	2.60	0.41
1:B:288:ARG:O	1:B:292:GLN:HG3	2.21	0.40
1:C:174:PRO:HA	1:C:175:PRO:HD3	1.91	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:457:CYS:HA	1:B:462:MET:O	2.21	0.40
1:A:370:MET:CE	1:A:384:ASP:HA	2.49	0.40

All (2) 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)
6:C:2094:HOH:O	6:C:2094:HOH:O[10_665]	0.73	1.47
6:A:2131:HOH:O	6:C:2058:HOH:O[6_654]	1.30	0.90

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	457/472 (97%)	438 (96%)	18 (4%)	1 (0%)	43	36
1	B	460/472 (98%)	444 (96%)	16 (4%)	0	100	100
1	C	460/472 (98%)	442 (96%)	18 (4%)	0	100	100
All	All	1377/1416 (97%)	1324 (96%)	52 (4%)	1 (0%)	48	40

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	GLY

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	394/404 (98%)	390 (99%)	4 (1%)	68	70
1	B	397/404 (98%)	391 (98%)	6 (2%)	57	56
1	C	397/404 (98%)	394 (99%)	3 (1%)	73	75
All	All	1188/1212 (98%)	1175 (99%)	13 (1%)	65	67

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	52	ILE
1	A	217	LEU
1	A	384	ASP
1	B	59	ASN
1	B	127	SER
1	B	154	PRO
1	B	247	VAL
1	B	411	ASN
1	B	454	LEU
1	C	115	LEU
1	C	127	SER
1	C	175	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	149	HIS
1	A	150	GLN
1	A	152	ASN
1	A	359	GLN
1	A	360	GLN
1	A	431	HIS
1	A	437	ASN
1	B	84	ASN
1	B	131	HIS
1	B	149	HIS
1	B	150	GLN
1	B	152	ASN
1	B	182	ASN
1	B	360	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	371	GLN
1	B	411	ASN
1	B	431	HIS
1	B	437	ASN
1	C	131	HIS
1	C	215	GLN
1	C	360	GLN
1	C	431	HIS

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 ⓘ

9 monosaccharides 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	NAG	D	1	1,2	14,14,15	0.95	0	17,19,21	1.43	4 (23%)
2	NAG	D	2	2	14,14,15	0.87	1 (7%)	17,19,21	1.84	3 (17%)
2	NAG	E	1	1,2	14,14,15	1.24	2 (14%)	17,19,21	1.65	3 (17%)
2	NAG	E	2	2	14,14,15	0.95	1 (7%)	17,19,21	1.37	2 (11%)
3	NAG	F	1	1,3	14,14,15	1.08	2 (14%)	17,19,21	2.22	7 (41%)
3	NAG	F	2	3	14,14,15	0.94	1 (7%)	17,19,21	1.56	4 (23%)
3	MAN	F	3	3	11,11,12	0.72	0	15,15,17	2.89	4 (26%)
3	MAN	F	4	3	11,11,12	0.55	0	15,15,17	1.42	3 (20%)
3	FCA	F	5	3	10,10,11	1.18	1 (10%)	14,14,16	1.86	4 (28%)

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	NAG	D	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	NAG	E	1	1,2	-	2/6/23/26	0/1/1/1
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
3	NAG	F	1	1,3	-	2/6/23/26	0/1/1/1
3	NAG	F	2	3	-	2/6/23/26	0/1/1/1
3	MAN	F	3	3	-	0/2/19/22	0/1/1/1
3	MAN	F	4	3	-	2/2/19/22	0/1/1/1
3	FCA	F	5	3	-	-	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAG	C1-C2	-3.15	1.48	1.52
3	F	2	NAG	O5-C1	-2.77	1.39	1.43
3	F	5	FCA	C2-C3	-2.57	1.48	1.52
2	E	1	NAG	O5-C1	-2.43	1.39	1.43
2	E	2	NAG	O5-C1	-2.34	1.39	1.43
3	F	1	NAG	C1-C2	-2.30	1.49	1.52
2	D	2	NAG	O5-C1	-2.24	1.39	1.43
3	F	1	NAG	O5-C1	-2.15	1.40	1.43

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	3	MAN	O2-C2-C3	9.99	130.85	110.15
2	D	2	NAG	C2-N2-C7	-5.42	115.64	122.90
3	F	1	NAG	C1-C2-N2	-5.01	102.53	110.43
3	F	1	NAG	C8-C7-N2	-3.68	110.01	116.12
2	E	2	NAG	C2-N2-C7	-3.68	117.97	122.90
3	F	4	MAN	C1-C2-C3	-3.64	104.35	109.64
3	F	2	NAG	O5-C1-C2	-3.62	105.69	111.29
2	E	1	NAG	C1-C2-N2	-3.61	104.75	110.43
2	E	1	NAG	C2-N2-C7	-3.47	118.25	122.90
3	F	1	NAG	O5-C5-C6	-3.22	101.40	107.66
3	F	1	NAG	O7-C7-C8	3.18	127.72	122.05
3	F	5	FCA	C3-C4-C5	-3.03	105.20	109.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	1	NAG	O3-C3-C4	2.88	117.17	110.38
3	F	5	FCA	O5-C1-C2	-2.86	103.98	110.79
2	D	1	NAG	C1-C2-N2	-2.79	106.03	110.43
3	F	3	MAN	C1-O5-C5	2.78	115.91	112.19
2	D	2	NAG	C1-C2-N2	-2.76	106.08	110.43
3	F	2	NAG	O5-C5-C4	-2.60	104.50	110.83
3	F	4	MAN	O2-C2-C3	2.59	115.52	110.15
3	F	5	FCA	O3-C3-C4	-2.58	104.30	110.38
2	D	1	NAG	C1-O5-C5	2.53	115.58	112.19
2	D	1	NAG	O5-C5-C6	-2.48	102.84	107.66
3	F	2	NAG	C2-N2-C7	-2.48	119.58	122.90
3	F	3	MAN	O4-C4-C3	2.35	115.92	110.38
3	F	1	NAG	O5-C5-C4	-2.35	105.11	110.83
2	D	1	NAG	O3-C3-C4	2.35	115.91	110.38
3	F	3	MAN	O2-C2-C1	2.28	114.44	109.22
2	E	1	NAG	C1-O5-C5	2.27	115.23	112.19
3	F	4	MAN	C2-C3-C4	-2.17	107.05	110.86
3	F	1	NAG	O4-C4-C3	-2.15	105.30	110.38
2	D	2	NAG	C8-C7-N2	-2.08	112.67	116.12
3	F	5	FCA	C2-C3-C4	-2.06	107.24	110.86
3	F	2	NAG	C3-C4-C5	2.04	113.92	110.23
2	E	2	NAG	C1-O5-C5	2.03	114.91	112.19

There are no chirality outliers.

All (14) torsion outliers are listed below:

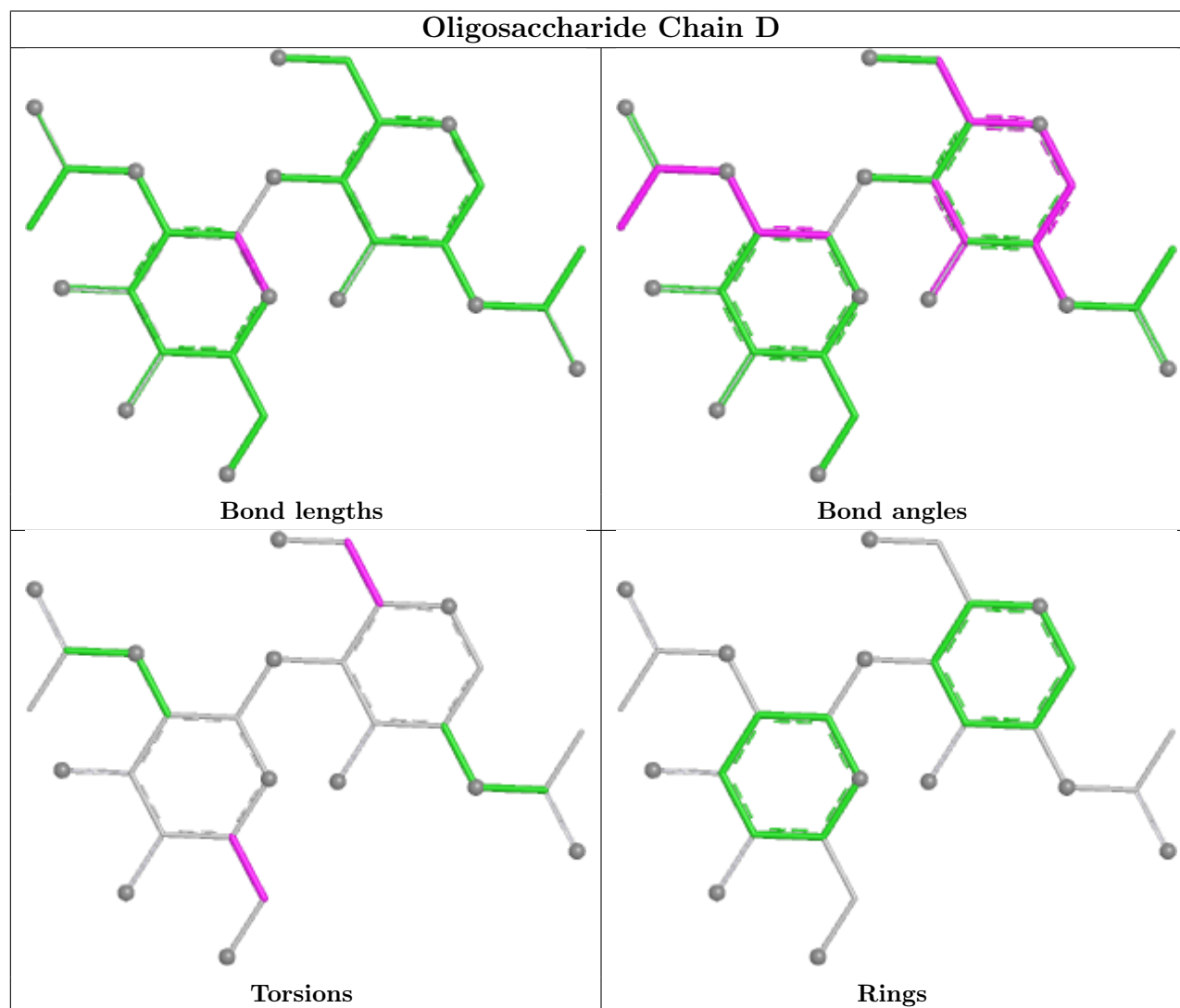
Mol	Chain	Res	Type	Atoms
2	E	2	NAG	C4-C5-C6-O6
2	D	1	NAG	C4-C5-C6-O6
2	D	2	NAG	C4-C5-C6-O6
2	E	1	NAG	C4-C5-C6-O6
3	F	2	NAG	C4-C5-C6-O6
3	F	1	NAG	C4-C5-C6-O6
3	F	4	MAN	O5-C5-C6-O6
2	D	1	NAG	O5-C5-C6-O6
2	E	1	NAG	O5-C5-C6-O6
2	E	2	NAG	O5-C5-C6-O6
3	F	2	NAG	O5-C5-C6-O6
3	F	4	MAN	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6
3	F	1	NAG	O5-C5-C6-O6

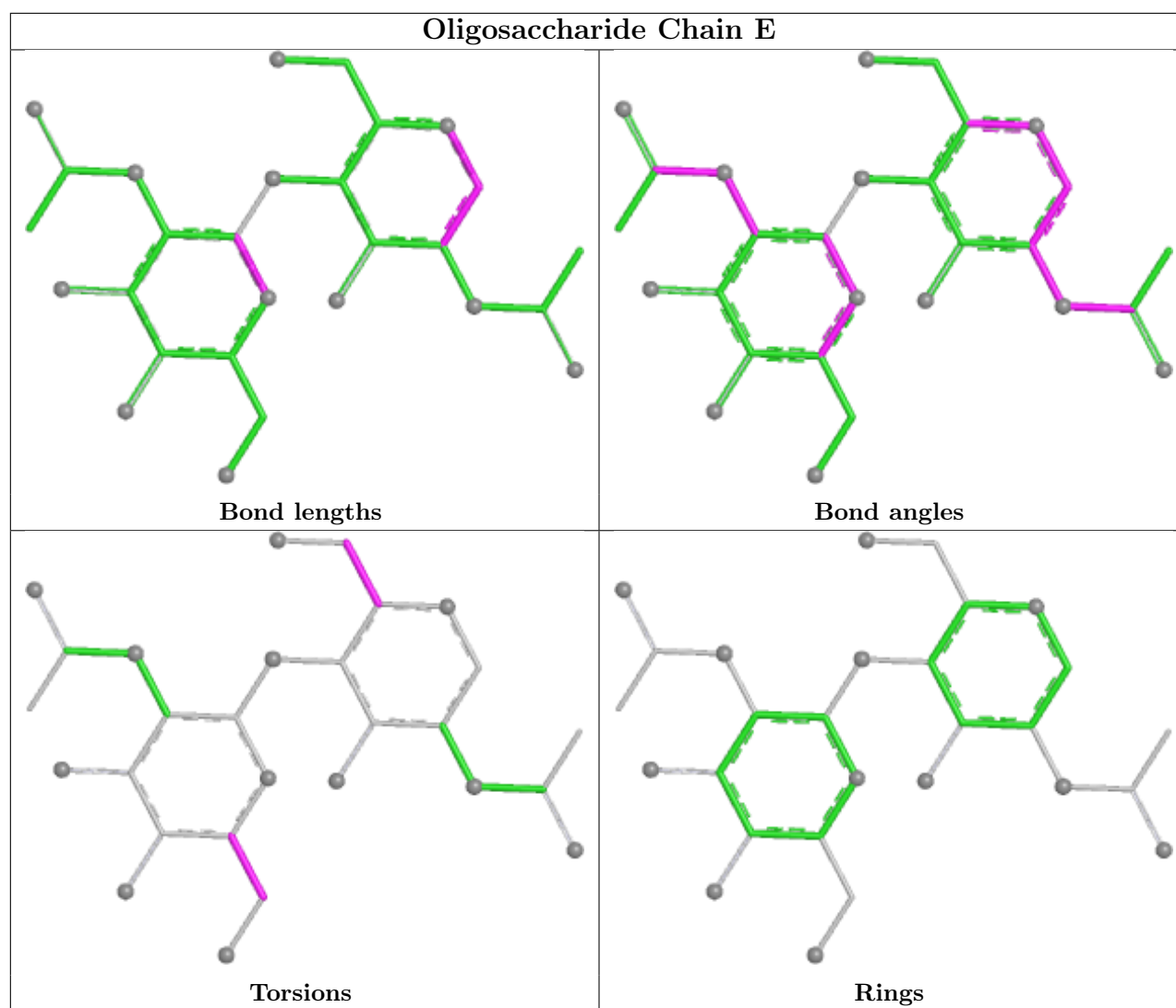
There are no ring outliers.

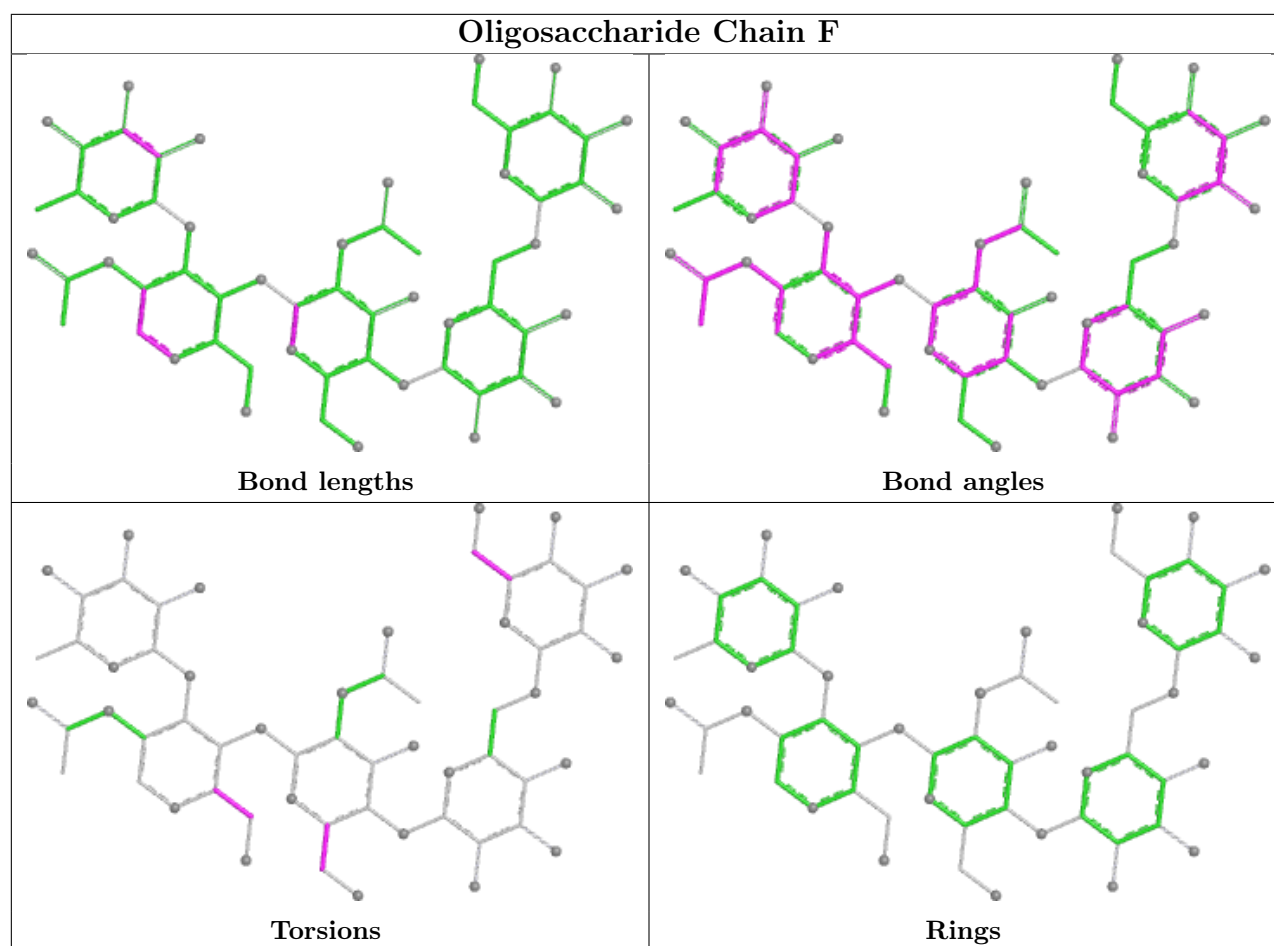
7 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	5	0
2	D	1	NAG	5	0
2	E	2	NAG	4	0
3	F	5	FCA	3	0
3	F	1	NAG	5	0
3	F	2	NAG	4	0
2	E	1	NAG	4	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.







5.6 Ligand geometry [i](#)

9 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	$\# Z > 2$
4	FAD	A	579	-	58,58,58	0.94	5 (8%)	85,89,89	1.37	12 (14%)
5	DIA	B	590[B]	-	9,9,9	0.52	0	8,8,8	0.35	0
5	DIA	A	590[A]	-	9,9,9	0.48	0	8,8,8	0.28	0
5	DIA	B	590[A]	-	9,9,9	0.49	0	8,8,8	0.45	0
5	DIA	C	590[B]	-	9,9,9	0.51	0	8,8,8	0.38	0
5	DIA	C	590[A]	-	9,9,9	0.50	0	8,8,8	0.45	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	FAD	B	579	-	58,58,58	0.89	3 (5%)	85,89,89	1.17	12 (14%)
4	FAD	C	579	-	58,58,58	1.12	4 (6%)	85,89,89	1.19	11 (12%)
5	DIA	A	590[B]	-	9,9,9	0.53	0	8,8,8	0.31	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
4	FAD	A	579	-	-	1/34/50/50	0/6/6/6
5	DIA	B	590[B]	-	-	3/7/7/7	-
5	DIA	A	590[A]	-	-	4/7/7/7	-
5	DIA	B	590[A]	-	-	5/7/7/7	-
5	DIA	C	590[B]	-	-	4/7/7/7	-
5	DIA	C	590[A]	-	-	6/7/7/7	-
4	FAD	B	579	-	-	5/34/50/50	0/6/6/6
4	FAD	C	579	-	-	1/34/50/50	0/6/6/6
5	DIA	A	590[B]	-	-	3/7/7/7	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	579	FAD	PA-O3P	3.69	1.63	1.59
4	C	579	FAD	C4X-N5	3.14	1.37	1.30
4	B	579	FAD	P-O3P	2.78	1.62	1.59
4	C	579	FAD	P-O3P	2.68	1.62	1.59
4	A	579	FAD	P-O3P	2.57	1.62	1.59
4	A	579	FAD	PA-O3P	2.48	1.62	1.59
4	B	579	FAD	PA-O3P	2.44	1.62	1.59
4	B	579	FAD	C4X-N5	2.29	1.35	1.30
4	A	579	FAD	C4X-N5	2.24	1.35	1.30
4	A	579	FAD	C5X-N5	-2.19	1.35	1.39
4	C	579	FAD	C5'-C4'	2.05	1.54	1.51
4	A	579	FAD	C5'-C4'	2.00	1.54	1.51

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	579	FAD	C9A-C5X-N5	-5.51	116.60	122.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	579	FAD	O4'-C4'-C3'	3.18	116.68	109.25
4	A	579	FAD	C6-C5X-C9A	3.08	123.28	119.05
4	A	579	FAD	O3P-PA-O1A	-2.90	101.99	110.70
4	B	579	FAD	C4-C4X-N5	2.84	122.13	118.21
4	C	579	FAD	C5'-C4'-C3'	-2.73	107.06	112.22
4	C	579	FAD	O4B-C1B-C2B	-2.73	100.77	106.62
4	A	579	FAD	C5'-C4'-C3'	-2.72	107.09	112.22
4	A	579	FAD	O4-C4-N3	2.71	125.22	120.11
4	B	579	FAD	C10-C4X-N5	-2.71	119.27	124.81
4	B	579	FAD	O3'-C3'-C4'	-2.70	102.79	108.93
4	A	579	FAD	O2A-PA-O1A	2.66	124.83	112.44
4	C	579	FAD	C9A-C5X-N5	-2.63	119.67	122.45
4	C	579	FAD	O3P-PA-O1A	-2.57	102.98	110.70
4	B	579	FAD	O4B-C1B-C2B	-2.54	101.17	106.62
4	B	579	FAD	C10-N1-C2	2.53	122.33	116.85
4	A	579	FAD	C8M-C8-C9	-2.45	115.25	119.57
4	A	579	FAD	C10-C4X-N5	-2.35	120.02	124.81
4	B	579	FAD	C7M-C7-C6	-2.34	115.45	119.57
4	C	579	FAD	O2A-PA-O1A	2.33	123.27	112.44
4	A	579	FAD	O4-C4-C4X	-2.31	120.44	126.53
4	C	579	FAD	O2P-P-O1P	2.31	123.18	112.44
4	B	579	FAD	C4'-C3'-C2'	2.30	117.40	113.57
4	B	579	FAD	O4B-C1B-N9A	-2.30	103.68	108.09
4	C	579	FAD	C10-N1-C2	2.28	121.79	116.85
4	B	579	FAD	C7M-C7-C8	2.21	125.28	120.76
4	C	579	FAD	C9-C8-C7	2.20	122.91	119.69
4	C	579	FAD	C4'-C3'-C2'	2.15	117.15	113.57
4	B	579	FAD	C5X-C9A-N10	-2.12	116.05	117.97
4	C	579	FAD	O2P-P-O3P	-2.11	101.58	107.27
4	B	579	FAD	O2P-P-O1P	2.07	122.05	112.44
4	A	579	FAD	O2P-P-O1P	2.05	121.99	112.44
4	A	579	FAD	O2'-C2'-C3'	-2.04	104.48	109.25
4	C	579	FAD	C4-C4X-N5	2.03	121.01	118.21
4	B	579	FAD	O2B-C2B-C3B	-2.02	105.36	111.82

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	579	FAD	C5B-O5B-PA-O1A
5	A	590[B]	DIA	C2-C3-C4-C5
5	B	590[B]	DIA	C2-C3-C4-C5

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
5	B	590[A]	DIA	C3-C4-C5-C6
5	B	590[A]	DIA	C2-C3-C4-C5
5	C	590[A]	DIA	C3-C4-C5-C6
5	C	590[B]	DIA	C2-C3-C4-C5
5	A	590[A]	DIA	C3-C4-C5-C6
5	A	590[A]	DIA	C2-C3-C4-C5
5	A	590[A]	DIA	C5-C6-C7-C8
5	C	590[A]	DIA	C2-C3-C4-C5
5	C	590[A]	DIA	C5-C6-C7-C8
5	B	590[A]	DIA	C5-C6-C7-C8
5	C	590[B]	DIA	C4-C5-C6-C7
5	C	590[A]	DIA	C4-C5-C6-C7
5	B	590[B]	DIA	C1-C2-C3-C4
5	C	590[B]	DIA	C1-C2-C3-C4
5	B	590[A]	DIA	C4-C5-C6-C7
5	A	590[A]	DIA	C4-C5-C6-C7
5	A	590[B]	DIA	C1-C2-C3-C4
5	A	590[B]	DIA	C4-C5-C6-C7
5	B	590[B]	DIA	C4-C5-C6-C7
5	B	590[A]	DIA	C6-C7-C8-N8
5	C	590[A]	DIA	C6-C7-C8-N8
4	B	579	FAD	C2'-C3'-C4'-O4'
4	B	579	FAD	O3'-C3'-C4'-C5'
4	B	579	FAD	O3'-C3'-C4'-O4'
5	C	590[B]	DIA	C5-C6-C7-C8
5	C	590[A]	DIA	C1-C2-C3-C4
4	B	579	FAD	C2B-C1B-N9A-C8A
4	C	579	FAD	C2B-C1B-N9A-C8A
4	B	579	FAD	O4B-C4B-C5B-O5B

There are no ring outliers.

9 monomers are involved in 19 short contacts:

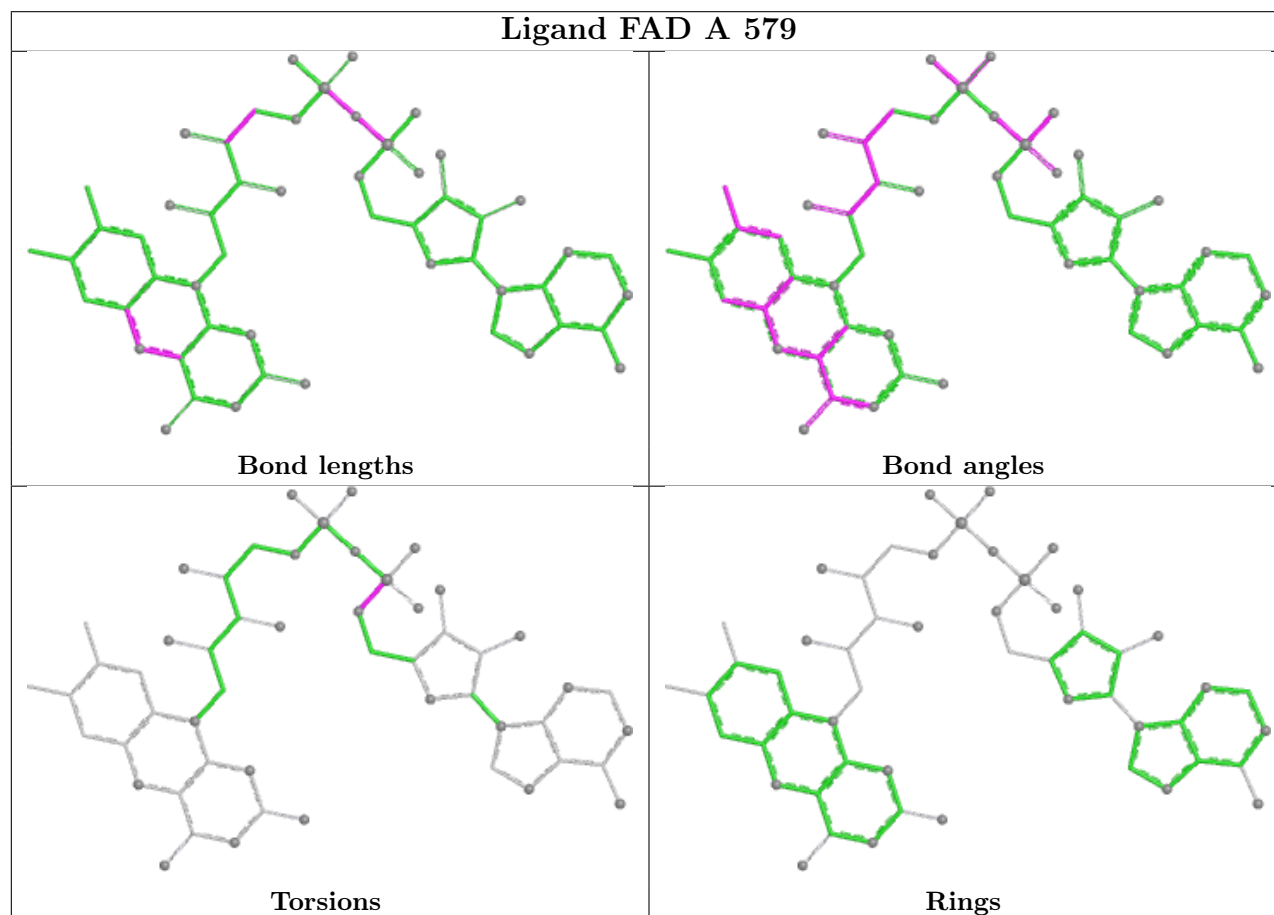
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	579	FAD	2	0
5	B	590[B]	DIA	1	0
5	A	590[A]	DIA	4	0
5	B	590[A]	DIA	3	0
5	C	590[B]	DIA	2	0
5	C	590[A]	DIA	3	0
4	B	579	FAD	1	0
4	C	579	FAD	2	0

Continued on next page...

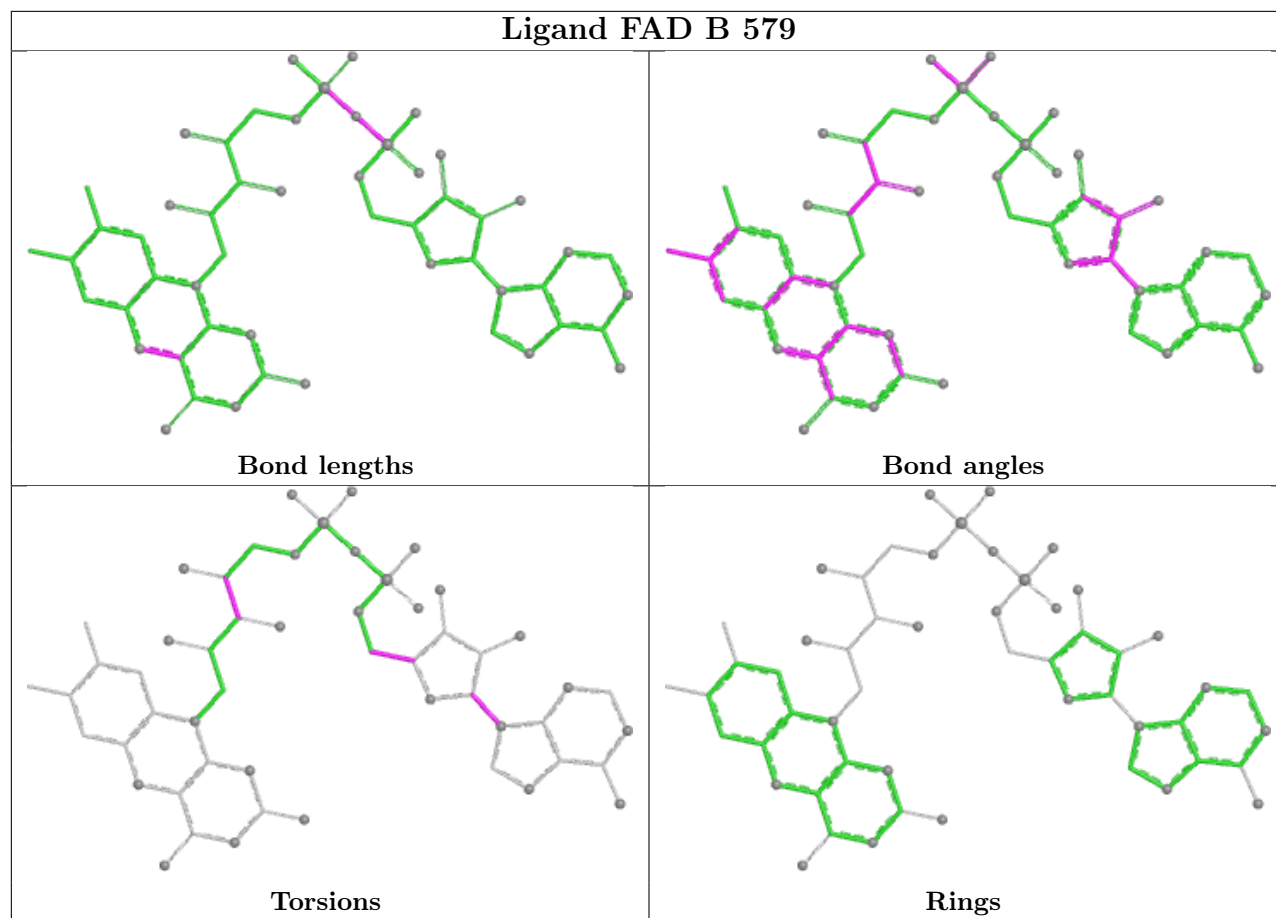
Continued from previous page...

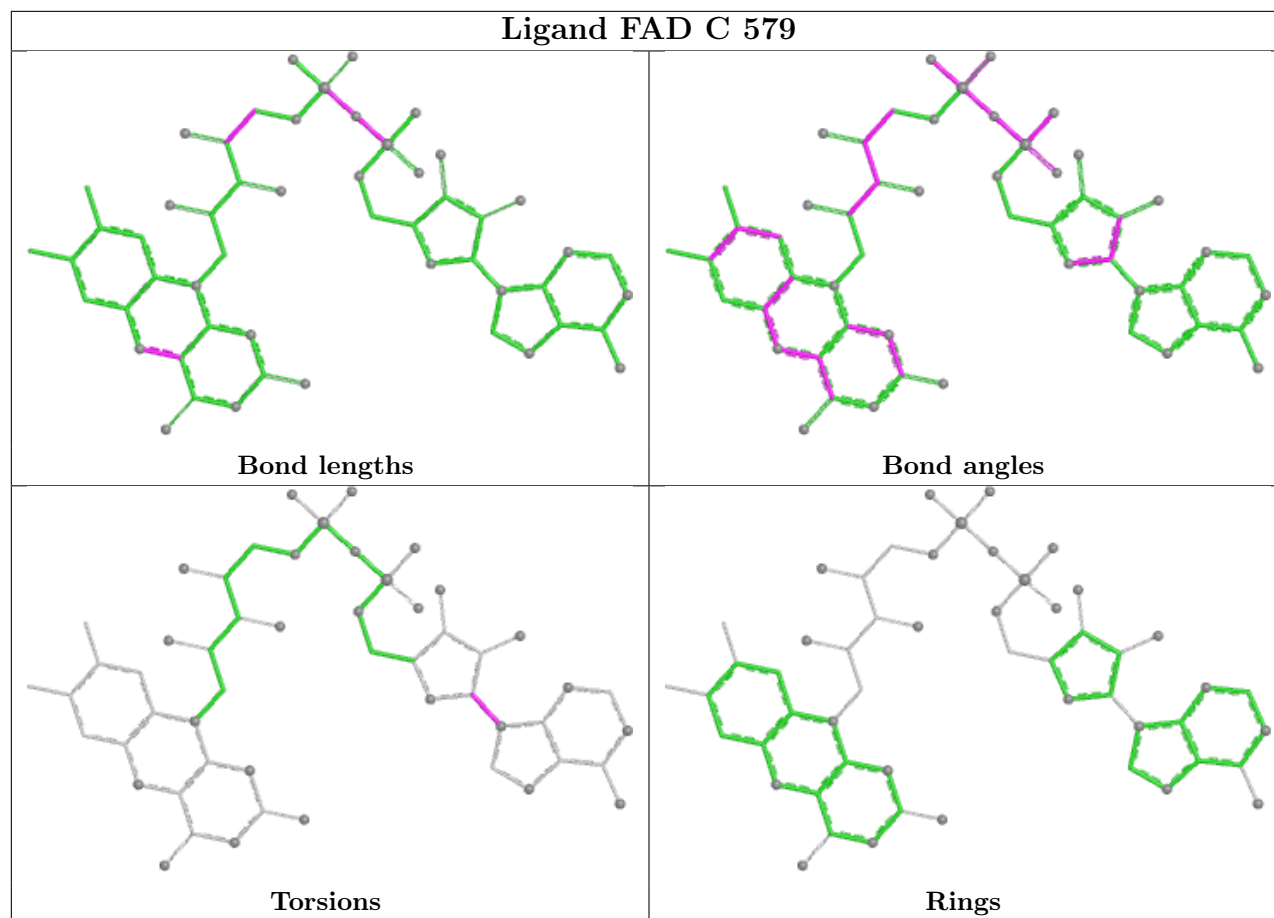
Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	590[B]	DIA	1	0

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 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 FAD B 579





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.