



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:49 PM UTC

PDB ID : 1H81 / pdb_00001h81
Title : STRUCTURE OF POLYAMINE OXIDASE IN THE REDUCED STATE
Authors : Binda, C.; Coda, A.; Angelini, R.; Federico, R.; Ascenzi, P.; Mattevi, A.
Deposited on : 2001-01-24
Resolution : 2.10 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

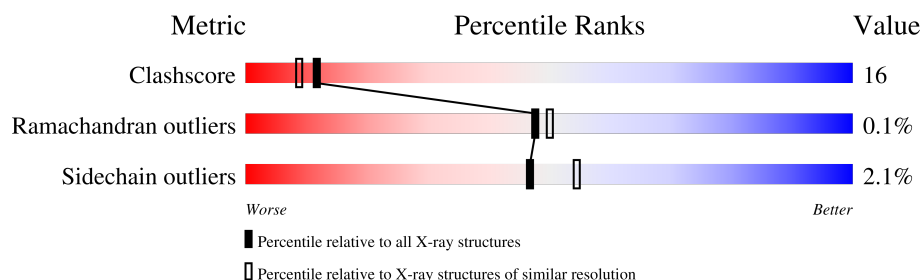
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)

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	
1	B	472	
1	C	472	
2	D	2	
2	E	2	
3	F	5	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 12113 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.

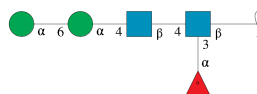
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	459	Total	C	N	O	S	55	0	0
			3684	2353	621	696	14			
1	B	462	Total	C	N	O	S	61	0	0
			3715	2374	627	700	14			
1	C	462	Total	C	N	O	S	50	0	0
			3715	2374	627	700	14			

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



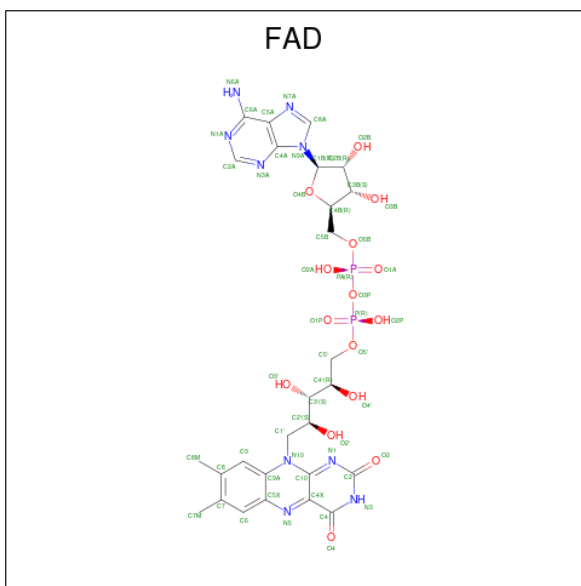
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	2	Total	C	N	O	0	0	0
			28	16	2	10			
2	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- 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 water.

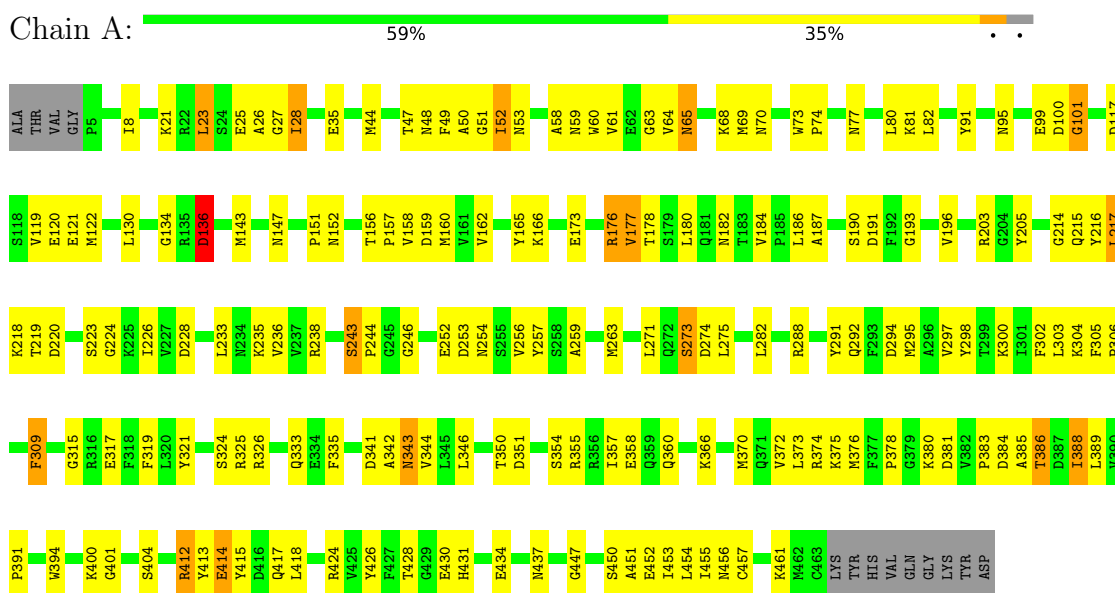
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	224	Total O 224 224	0	0
5	B	245	Total O 245 245	0	0
5	C	255	Total O 255 255	0	0

3 Residue-property plots

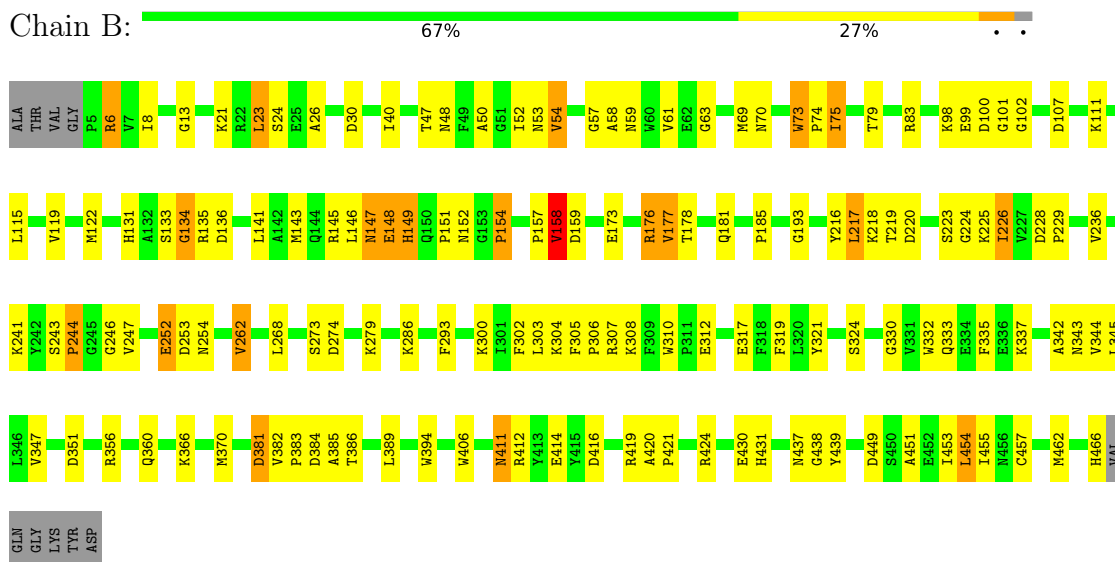
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

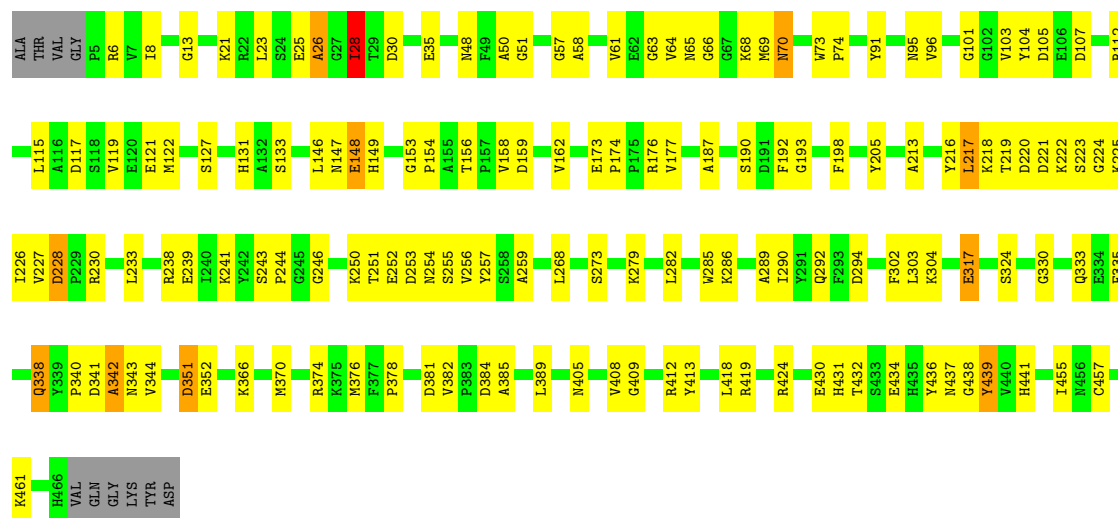


• Molecule 1: POLYAMINE OXIDASE



- Molecule 1: POLYAMINE OXIDASE

Chain C: 



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

Chain D: 



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

Chain E: 



- 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: 



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	181.77Å 181.77Å 277.53Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.10	Depositor
% Data completeness (in resolution range)	99.1 (20.00-2.10)	Depositor
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	TNT 5D	Depositor
R, R_{free}	0.191 , 0.235	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	12113	wwPDB-VP
Average B, all atoms (Å ²)	19.0	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: NAG, MAN, FAD, FCA

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	0.69	1/3775 (0.0%)	1.66	65/5116 (1.3%)
1	B	0.68	0/3808	1.62	45/5160 (0.9%)
1	C	0.70	0/3808	1.65	44/5160 (0.9%)
All	All	0.69	1/11391 (0.0%)	1.64	154/15436 (1.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	1	0

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	263	MET	SD-CE	5.12	1.92	1.79

All (154) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	61	VAL	N-CA-C	-10.50	92.66	107.99
1	C	342	ALA	N-CA-C	9.92	123.33	111.82
1	C	273	SER	CA-C-N	-9.87	107.64	122.83
1	C	273	SER	C-N-CA	-9.87	107.64	122.83
1	C	340	PRO	CA-C-N	-9.22	107.90	122.65
1	C	340	PRO	C-N-CA	-9.22	107.90	122.65
1	B	61	VAL	N-CA-C	-8.85	94.32	107.51
1	C	28	ILE	CB-CA-C	-8.83	102.61	112.68
1	A	224	GLY	N-CA-C	-8.70	103.90	115.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	409	GLY	N-CA-C	-8.39	104.60	113.58
1	C	61	VAL	N-CA-C	-8.26	95.21	107.51
1	A	447	GLY	N-CA-C	-7.95	103.20	112.73
1	A	26	ALA	N-CA-C	-7.88	103.39	113.16
1	C	26	ALA	N-CA-C	-7.84	103.44	113.16
1	B	13	GLY	N-CA-C	-7.75	100.79	112.41
1	A	273	SER	CA-C-N	-7.63	111.57	124.31
1	A	273	SER	C-N-CA	-7.63	111.57	124.31
1	B	177	VAL	N-CA-CB	-7.62	103.83	112.21
1	A	101	GLY	N-CA-C	7.51	130.99	113.18
1	B	252	GLU	N-CA-CB	-7.47	98.72	110.22
1	C	289	ALA	N-CA-C	-7.37	103.25	111.28
1	A	173	GLU	N-CA-C	-7.37	99.70	108.25
1	A	275	LEU	N-CA-C	-7.21	103.42	111.28
1	B	6	ARG	N-CA-C	-7.16	98.01	109.76
1	B	158	VAL	N-CA-C	7.08	117.19	110.53
1	C	174	PRO	O-C-N	7.00	124.44	121.15
1	B	54	VAL	N-CA-C	-6.84	99.24	108.96
1	B	386	THR	N-CA-C	-6.79	105.03	113.38
1	A	273	SER	N-CA-C	6.77	121.54	113.28
1	C	224	GLY	N-CA-C	-6.74	106.70	115.59
1	B	324	SER	N-CA-C	-6.74	105.03	113.18
1	A	309	PHE	N-CA-C	-6.73	104.20	114.16
1	A	162	VAL	N-CA-C	-6.67	104.26	110.53
1	C	177	VAL	N-CA-C	-6.59	106.24	113.43
1	C	230	ARG	NE-CZ-NH1	-6.57	114.93	121.50
1	B	351	ASP	N-CA-CB	-6.54	99.44	110.49
1	C	335	PHE	N-CA-C	6.54	121.14	112.25
1	C	324	SER	N-CA-C	-6.54	105.27	113.18
1	B	300	LYS	CA-C-N	-6.53	114.20	122.43
1	B	300	LYS	C-N-CA	-6.53	114.20	122.43
1	A	381	ASP	CA-C-N	-6.45	118.22	122.60
1	A	381	ASP	C-N-CA	-6.45	118.22	122.60
1	A	414	GLU	CA-CB-CG	-6.44	101.22	114.10
1	C	228	ASP	CA-C-O	6.37	125.13	119.59
1	A	351	ASP	N-CA-CB	-6.36	99.74	110.49
1	A	335	PHE	N-CA-CB	-6.29	102.07	111.25
1	B	224	GLY	N-CA-C	-6.25	107.05	115.36
1	C	176	ARG	CA-C-N	-6.23	114.31	122.16
1	C	176	ARG	C-N-CA	-6.23	114.31	122.16
1	B	148	GLU	N-CA-C	-6.18	105.78	113.38
1	C	205	TYR	N-CA-C	-6.13	104.66	111.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	343	ASN	CB-CA-C	-6.05	103.14	111.73
1	A	205	TYR	N-CA-C	-6.04	104.77	111.71
1	A	196	VAL	N-CA-C	-6.02	99.55	108.45
1	A	77	ASN	N-CA-C	6.01	118.79	111.82
1	C	341	ASP	CB-CA-C	6.00	120.69	110.56
1	B	356	ARG	CA-C-O	5.99	126.87	120.70
1	C	338	GLN	N-CA-C	5.95	117.56	111.14
1	A	214	GLY	N-CA-C	-5.95	106.97	114.16
1	C	104	TYR	N-CA-C	-5.94	102.87	110.53
1	A	151	PRO	N-CA-C	-5.90	107.90	114.92
1	A	386	THR	N-CA-CB	-5.85	101.28	110.30
1	A	358	GLU	N-CA-C	-5.85	104.98	111.71
1	C	13	GLY	N-CA-C	-5.83	103.04	112.31
1	A	134	GLY	N-CA-C	-5.83	107.61	115.36
1	A	357	ILE	N-CA-C	5.82	116.56	110.62
1	A	355	ARG	NE-CZ-NH2	-5.82	113.97	119.20
1	B	134	GLY	N-CA-C	-5.82	107.72	115.40
1	A	243	SER	N-CA-C	-5.81	101.46	108.14
1	B	253	ASP	N-CA-C	-5.80	106.43	112.93
1	A	381	ASP	N-CA-C	-5.79	96.97	107.75
1	B	75	ILE	CB-CA-C	-5.79	104.23	112.22
1	C	148	GLU	N-CA-C	-5.78	105.88	113.17
1	C	162	VAL	N-CA-C	-5.76	104.90	110.72
1	B	439	TYR	N-CA-C	5.76	118.45	109.52
1	B	135	ARG	NE-CZ-NH1	-5.76	115.74	121.50
1	C	408	VAL	CA-C-N	-5.75	117.21	123.30
1	C	408	VAL	C-N-CA	-5.75	117.21	123.30
1	B	268	LEU	N-CA-C	-5.70	105.06	111.28
1	A	65	ASN	CA-C-N	-5.70	117.36	122.43
1	A	65	ASN	C-N-CA	-5.70	117.36	122.43
1	C	317	GLU	N-CA-C	5.69	117.94	111.11
1	B	335	PHE	N-CA-C	5.68	119.98	112.25
1	A	136	ASP	CB-CA-C	-5.66	101.15	110.72
1	B	244	PRO	N-CA-C	-5.65	106.02	113.65
1	A	178	THR	N-CA-C	5.64	118.74	109.76
1	A	288	ARG	CA-CB-CG	-5.64	102.82	114.10
1	B	73	TRP	N-CA-C	5.64	120.42	112.75
1	A	60	TRP	CB-CA-C	-5.61	98.77	109.66
1	B	177	VAL	N-CA-C	-5.58	107.35	113.43
1	C	153	GLY	N-CA-C	-5.57	100.98	112.34
1	B	149	HIS	CA-CB-CG	-5.52	108.28	113.80
1	A	176	ARG	CB-CG-CD	-5.51	98.62	111.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	341	ASP	N-CA-C	5.51	122.10	113.72
1	A	182	ASN	N-CA-C	5.50	119.68	112.92
1	B	173	GLU	N-CA-C	-5.50	101.87	108.25
1	A	388	ILE	CA-C-N	-5.47	115.05	122.77
1	A	388	ILE	C-N-CA	-5.47	115.05	122.77
1	A	412	ARG	CA-CB-CG	-5.46	103.19	114.10
1	B	147	ASN	CA-C-N	-5.44	112.85	122.26
1	B	147	ASN	C-N-CA	-5.44	112.85	122.26
1	A	51	GLY	CA-C-N	-5.44	115.39	122.51
1	A	51	GLY	C-N-CA	-5.44	115.39	122.51
1	C	174	PRO	CB-CA-C	-5.42	106.07	111.17
1	B	345	LEU	N-CA-C	-5.42	100.94	109.50
1	A	374	ARG	CA-CB-CG	-5.42	103.27	114.10
1	A	176	ARG	CA-C-N	-5.41	113.98	121.77
1	A	176	ARG	C-N-CA	-5.41	113.98	121.77
1	B	262	VAL	N-CA-C	-5.41	100.05	108.86
1	C	268	LEU	N-CA-C	-5.39	105.41	111.28
1	B	101	GLY	N-CA-C	5.38	125.94	113.18
1	C	68	LYS	N-CA-C	-5.37	101.02	109.50
1	C	439	TYR	N-CA-C	5.34	117.99	110.14
1	C	146	LEU	N-CA-C	-5.34	105.36	111.07
1	B	100	ASP	CB-CA-C	5.33	120.30	111.23
1	B	381	ASP	N-CA-C	-5.32	97.14	107.62
1	A	48	ASN	CA-C-N	-5.32	115.27	122.77
1	A	48	ASN	C-N-CA	-5.32	115.27	122.77
1	C	432	THR	N-CA-C	-5.29	105.48	112.94
1	A	428	THR	N-CA-C	-5.29	101.44	108.74
1	B	226	ILE	N-CA-C	-5.29	102.02	109.21
1	A	456	ASN	CA-C-N	-5.25	113.30	120.44
1	A	456	ASN	C-N-CA	-5.25	113.30	120.44
1	B	48	ASN	CA-C-N	-5.23	115.40	122.77
1	B	48	ASN	C-N-CA	-5.23	115.40	122.77
1	C	95	ASN	N-CA-CB	-5.23	103.78	111.51
1	A	297	VAL	CB-CA-C	-5.22	102.45	110.50
1	B	158	VAL	N-CA-CB	5.22	117.25	110.57
1	A	413	TYR	CA-C-N	-5.22	112.38	120.31
1	A	413	TYR	C-N-CA	-5.22	112.38	120.31
1	C	381	ASP	N-CA-C	-5.21	98.82	107.99
1	A	82	LEU	N-CA-C	-5.21	101.97	110.20
1	A	68	LYS	N-CA-C	-5.21	101.16	109.23
1	B	136	ASP	CB-CA-C	-5.20	102.36	110.94
1	A	44	MET	N-CA-C	-5.20	97.38	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	380	LYS	CA-C-N	-5.19	115.64	122.85
1	A	380	LYS	C-N-CA	-5.19	115.64	122.85
1	A	28	ILE	N-CA-C	-5.18	99.66	107.73
1	C	413	TYR	N-CA-C	-5.17	105.54	111.07
1	A	27	GLY	CA-C-N	-5.16	115.93	122.43
1	A	27	GLY	C-N-CA	-5.16	115.93	122.43
1	C	351	ASP	N-CA-C	5.16	116.15	108.31
1	A	298	TYR	N-CA-CB	-5.15	102.86	110.90
1	B	176	ARG	CA-C-N	-5.14	115.68	122.16
1	B	176	ARG	C-N-CA	-5.14	115.68	122.16
1	B	330	GLY	N-CA-C	5.13	125.34	113.18
1	C	156	THR	N-CA-C	-5.11	103.51	110.36
1	B	252	GLU	CA-CB-CG	5.10	124.30	114.10
1	B	178	THR	N-CA-C	5.05	118.45	109.96
1	C	70	ASN	N-CA-C	-5.05	100.29	109.44
1	C	330	GLY	CA-C-N	-5.04	116.56	123.12
1	C	330	GLY	C-N-CA	-5.04	116.56	123.12
1	B	236	VAL	CB-CA-C	-5.03	104.86	111.25
1	A	177	VAL	N-CA-C	-5.00	107.07	113.22

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	C	386	THR	CB

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3684	0	3584	123	0
1	B	3715	0	3614	118	0
1	C	3715	0	3614	101	0
2	D	28	0	26	3	0
2	E	28	0	26	4	0
3	F	60	0	52	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	53	0	31	2	0
4	B	53	0	31	2	0
4	C	53	0	31	3	0
5	A	224	0	0	4	0
5	B	245	0	0	10	0
5	C	255	0	0	4	0
All	All	12113	0	11009	346	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 16.

All (346) 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:B:69:MET:CE	1:B:73:TRP:HB3	1.81	1.11
1:A:372:VAL:HG12	1:A:376:MET:HE2	1.12	1.09
1:B:69:MET:HE2	1:B:74:PRO:HD3	1.35	1.08
1:A:69:MET:CE	1:A:73:TRP:HB3	1.90	1.02
3:F:1:NAG:C4	3:F:2:NAG:C1	2.41	0.98
1:B:119:VAL:HA	1:B:122:MET:HE3	1.40	0.98
1:C:131:HIS:CD2	1:C:133:SER:H	1.83	0.97
1:B:411:ASN:ND2	1:B:414:GLU:H	1.66	0.93
1:C:119:VAL:HA	1:C:122:MET:HE3	1.50	0.93
1:B:69:MET:HE2	1:B:74:PRO:CD	1.99	0.93
1:C:69:MET:HE3	1:C:70:ASN:N	1.83	0.92
1:B:69:MET:HE1	1:B:73:TRP:HB3	1.52	0.92
1:A:69:MET:HE2	1:A:74:PRO:HD3	1.51	0.92
1:A:372:VAL:CG1	1:A:376:MET:HE2	1.99	0.90
1:B:69:MET:CE	1:B:74:PRO:HD3	2.01	0.90
1:C:69:MET:HE3	1:C:70:ASN:H	1.35	0.89
1:A:394:TRP:HE1	1:B:152:ASN:ND2	1.70	0.89
1:A:372:VAL:HG12	1:A:376:MET:CE	2.03	0.89
2:E:1:NAG:C4	2:E:2:NAG:C1	2.54	0.86
1:A:69:MET:HE2	1:A:74:PRO:CD	2.05	0.85
1:B:219:THR:HG22	1:B:226:ILE:HA	1.59	0.84
1:C:112:ARG:HD3	1:C:159:ASP:OD1	1.77	0.84
1:C:216:TYR:CE1	1:C:217:LEU:HD13	2.13	0.84
1:A:373:LEU:HA	1:A:376:MET:HE3	1.59	0.83
1:B:308:LYS:HE3	1:B:310:TRP:O	1.76	0.83
1:B:220:ASP:HB3	1:B:223:SER:OG	1.81	0.80
1:A:69:MET:HE1	1:A:73:TRP:HB3	1.63	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1:NAG:C4	2:D:2:NAG:C1	2.60	0.80
1:C:117:ASP:O	1:C:121:GLU:HG3	1.82	0.80
1:A:119:VAL:HA	1:A:122:MET:HE3	1.65	0.78
1:A:69:MET:HE2	1:A:74:PRO:CG	2.14	0.78
1:C:216:TYR:CD1	1:C:217:LEU:HD13	2.18	0.78
1:A:366:LYS:HD2	1:A:385:ALA:HB3	1.66	0.76
3:F:1:NAG:H3	3:F:5:FCA:O2	1.84	0.76
1:B:131:HIS:CD2	1:B:133:SER:H	2.03	0.75
1:C:220:ASP:HB3	1:C:223:SER:OG	1.86	0.75
1:A:394:TRP:HE1	1:B:152:ASN:HD22	1.35	0.75
1:A:431:HIS:CD2	1:A:431:HIS:H	2.03	0.75
1:A:50:ALA:HB1	1:A:304:LYS:HD2	1.69	0.75
1:C:131:HIS:HD2	1:C:133:SER:H	1.35	0.74
1:B:69:MET:HE3	1:B:73:TRP:HB3	1.70	0.74
1:A:69:MET:HE2	1:A:74:PRO:HG3	1.69	0.74
1:A:69:MET:CE	1:A:74:PRO:HD3	2.16	0.74
3:F:1:NAG:O4	3:F:2:NAG:C2	2.35	0.74
1:A:117:ASP:O	1:A:121:GLU:HG3	1.88	0.73
1:C:69:MET:HE3	1:C:69:MET:HA	1.70	0.73
1:B:411:ASN:HD22	1:B:414:GLU:H	1.37	0.72
1:B:69:MET:HE1	1:B:73:TRP:CD1	2.23	0.72
1:C:292:GLN:OE1	5:C:2137:HOH:O	2.07	0.72
1:A:23:LEU:HD13	1:A:451:ALA:HB1	1.71	0.71
1:C:69:MET:HE3	1:C:69:MET:CA	2.21	0.71
1:B:131:HIS:HD2	1:B:133:SER:H	1.38	0.71
1:B:419:ARG:HG2	5:B:2227:HOH:O	1.90	0.71
1:B:419:ARG:HD3	5:B:2218:HOH:O	1.90	0.71
1:A:220:ASP:HB3	1:A:223:SER:HB3	1.72	0.70
1:B:216:TYR:CD1	1:B:217:LEU:HD13	2.27	0.70
1:A:218:LYS:H	1:A:228:ASP:HB2	1.57	0.70
1:A:69:MET:HE1	1:A:73:TRP:CD1	2.28	0.69
1:A:63:GLY:HA2	1:A:193:GLY:O	1.93	0.69
1:B:107:ASP:O	1:B:111:LYS:HG3	1.93	0.69
1:C:6:ARG:HG3	1:C:6:ARG:HH11	1.57	0.69
1:C:131:HIS:HD2	1:C:133:SER:OG	1.76	0.69
1:A:117:ASP:OD1	5:A:2050:HOH:O	2.11	0.68
1:B:185:PRO:HA	5:B:2054:HOH:O	1.94	0.68
1:C:69:MET:HE2	1:C:73:TRP:HB3	1.77	0.67
1:A:373:LEU:HD23	1:A:376:MET:HE3	1.76	0.67
1:C:69:MET:CE	1:C:70:ASN:N	2.58	0.67
1:C:131:HIS:HD2	1:C:133:SER:CB	2.07	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:273:SER:O	1:A:274:ASP:HB2	1.94	0.66
1:A:370:MET:HE2	1:A:384:ASP:HA	1.78	0.66
1:A:220:ASP:CG	1:A:223:SER:HB3	2.21	0.66
1:B:449:ASP:O	1:B:453:ILE:HG13	1.97	0.65
1:A:158:VAL:HG13	1:A:159:ASP:N	2.13	0.64
3:F:1:NAG:H4	3:F:2:NAG:C1	2.28	0.64
1:B:412:ARG:HG3	5:B:2215:HOH:O	1.96	0.64
1:A:216:TYR:CD1	1:A:217:LEU:HD13	2.31	0.64
1:A:69:MET:HE3	1:A:73:TRP:HB3	1.76	0.64
1:A:412:ARG:NH1	1:A:434:GLU:OE2	2.30	0.64
1:B:69:MET:HE1	1:B:73:TRP:HD1	1.64	0.63
1:B:63:GLY:HA2	1:B:193:GLY:O	1.98	0.62
1:B:69:MET:HE2	1:B:74:PRO:CG	2.28	0.62
1:A:58:ALA:HA	4:A:579:FAD:C4X	2.30	0.62
1:A:69:MET:HE1	1:A:73:TRP:HD1	1.64	0.62
1:A:373:LEU:HD23	1:A:376:MET:CE	2.30	0.61
3:F:1:NAG:O6	3:F:2:NAG:C1	2.48	0.61
1:A:220:ASP:CB	1:A:223:SER:HB3	2.29	0.61
3:F:1:NAG:C3	3:F:5:FCA:O2	2.48	0.61
1:A:130:LEU:HD22	1:A:136:ASP:HB2	1.82	0.60
1:C:131:HIS:CD2	1:C:133:SER:OG	2.53	0.60
1:C:220:ASP:OD2	1:C:222:LYS:N	2.34	0.60
1:C:69:MET:CE	1:C:70:ASN:H	2.11	0.60
1:C:419:ARG:NH2	1:C:434:GLU:HA	2.17	0.60
1:C:131:HIS:CD2	1:C:133:SER:CB	2.85	0.60
1:C:431:HIS:H	1:C:431:HIS:CD2	2.18	0.60
1:A:49:PHE:N	1:A:52:ILE:O	2.30	0.60
1:A:177:VAL:HG11	1:B:176:ARG:HD2	1.83	0.59
1:C:412:ARG:NH1	1:C:434:GLU:OE2	2.33	0.59
1:C:69:MET:HE3	1:C:69:MET:C	2.27	0.59
2:E:1:NAG:O4	2:E:2:NAG:C2	2.47	0.59
1:A:152:ASN:ND2	1:B:394:TRP:HE1	2.01	0.59
1:B:69:MET:HE1	1:B:73:TRP:CB	2.28	0.58
1:A:218:LYS:N	1:A:228:ASP:HB2	2.18	0.58
1:C:219:THR:HG22	1:C:226:ILE:HA	1.85	0.58
1:B:119:VAL:CA	1:B:122:MET:HE3	2.24	0.58
1:B:454:LEU:C	1:B:454:LEU:HD12	2.28	0.58
1:B:431:HIS:H	1:B:431:HIS:CD2	2.20	0.58
1:B:26:ALA:HB2	1:B:455:ILE:HD13	1.85	0.58
1:B:69:MET:HE3	1:B:70:ASN:O	2.04	0.57
1:B:273:SER:O	1:B:274:ASP:HB2	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:304:LYS:HG3	1:B:305:PHE:N	2.20	0.57
1:C:6:ARG:HA	1:C:30:ASP:O	2.04	0.57
1:B:243:SER:HB2	1:B:244:PRO:CD	2.35	0.57
1:C:131:HIS:HD2	1:C:133:SER:N	2.03	0.57
1:A:243:SER:HB2	1:A:244:PRO:CD	2.34	0.56
1:A:342:ALA:O	1:A:343:ASN:HB2	2.04	0.56
1:A:50:ALA:CB	1:A:304:LYS:HD2	2.36	0.56
1:C:101:GLY:HA3	1:C:378:PRO:HG3	1.87	0.56
1:C:376:MET:C	1:C:378:PRO:HD3	2.30	0.56
1:B:6:ARG:HA	1:B:30:ASP:O	2.06	0.56
1:C:218:LYS:H	1:C:228:ASP:HB2	1.71	0.56
1:B:216:TYR:CE1	1:B:217:LEU:HD13	2.41	0.56
1:A:219:THR:HG22	1:A:226:ILE:HA	1.89	0.55
1:B:23:LEU:HD13	1:B:451:ALA:HB1	1.88	0.55
1:B:58:ALA:HA	4:B:579:FAD:C4X	2.36	0.55
1:B:457:CYS:HA	1:B:462:MET:O	2.07	0.55
1:A:47:THR:O	1:A:53:ASN:HA	2.07	0.54
1:A:64:VAL:HG12	1:A:65:ASN:N	2.21	0.54
1:C:290:ILE:HA	1:C:418:LEU:HD21	1.89	0.54
1:C:219:THR:HA	1:C:225:LYS:O	2.07	0.54
1:C:253:ASP:O	1:C:254:ASN:HB2	2.08	0.54
1:C:58:ALA:HA	4:C:579:FAD:C4X	2.38	0.54
1:B:223:SER:HB2	1:B:225:LYS:HG3	1.89	0.53
1:B:306:PRO:HG3	1:B:383:PRO:HB2	1.90	0.53
1:C:158:VAL:HG12	5:C:2073:HOH:O	2.06	0.53
1:A:216:TYR:CE1	1:A:217:LEU:HD13	2.43	0.53
1:C:105:ASP:OD1	1:C:107:ASP:HB2	2.09	0.53
1:C:131:HIS:CD2	1:C:133:SER:N	2.65	0.52
1:A:156:THR:O	1:A:160:MET:HG3	2.09	0.52
1:B:131:HIS:HD2	1:B:133:SER:OG	1.93	0.52
1:C:35:GLU:HB3	1:C:233:LEU:HD23	1.90	0.52
1:A:143:MET:SD	1:A:147:ASN:ND2	2.83	0.52
1:B:98:LYS:HG3	1:B:102:GLY:O	2.10	0.52
1:C:21:LYS:HB2	1:C:216:TYR:CE2	2.45	0.52
1:C:112:ARG:NH2	1:C:115:LEU:HD11	2.24	0.52
1:C:246:GLY:HA2	1:C:424:ARG:HD3	1.92	0.51
1:A:253:ASP:O	1:A:254:ASN:HB2	2.11	0.51
1:B:99:GLU:HA	1:B:321:TYR:CE1	2.46	0.51
1:C:57:GLY:HA2	4:C:579:FAD:C7M	2.41	0.51
1:A:317:GLU:O	1:A:333:GLN:HA	2.10	0.51
2:D:1:NAG:H4	2:D:2:NAG:C1	2.39	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:69:MET:HE2	1:B:74:PRO:HG3	1.93	0.51
1:B:219:THR:HG22	1:B:226:ILE:CA	2.37	0.51
1:B:342:ALA:O	1:B:343:ASN:HB2	2.11	0.51
1:C:119:VAL:HG13	1:C:147:ASN:HB2	1.93	0.51
1:C:73:TRP:HB3	1:C:74:PRO:HD3	1.93	0.51
1:B:419:ARG:CG	5:B:2227:HOH:O	2.55	0.50
1:A:81:LYS:O	1:A:203:ARG:NH2	2.45	0.50
1:A:376:MET:C	1:A:378:PRO:HD3	2.36	0.50
1:C:216:TYR:CE1	1:C:217:LEU:CD1	2.91	0.50
1:C:218:LYS:N	1:C:228:ASP:HB2	2.27	0.50
1:A:176:ARG:HD2	1:B:177:VAL:HG21	1.93	0.50
1:C:239:GLU:OE2	1:C:279:LYS:HD3	2.12	0.50
1:A:152:ASN:HD22	1:B:394:TRP:HE1	1.59	0.49
1:B:306:PRO:CG	1:B:383:PRO:HB2	2.42	0.49
1:B:370:MET:HE1	1:B:382:VAL:HG12	1.94	0.49
1:B:451:ALA:O	1:B:455:ILE:HG13	2.12	0.49
1:C:243:SER:HB2	1:C:244:PRO:CD	2.42	0.49
2:E:1:NAG:H4	2:E:2:NAG:C1	2.39	0.49
1:A:120:GLU:OE1	1:A:166:LYS:NZ	2.40	0.49
1:A:415:TYR:O	1:A:418:LEU:HB2	2.13	0.49
1:B:218:LYS:N	1:B:228:ASP:HB2	2.28	0.49
1:A:187:ALA:O	1:A:191:ASP:N	2.35	0.49
1:A:304:LYS:NZ	1:A:342:ALA:O	2.46	0.49
1:B:243:SER:HB2	1:B:244:PRO:HD2	1.94	0.49
1:B:247:VAL:HG11	1:B:262:VAL:HB	1.95	0.49
1:A:243:SER:CB	1:A:244:PRO:CD	2.91	0.49
1:B:143:MET:SD	1:B:147:ASN:ND2	2.86	0.49
2:E:1:NAG:O6	2:E:2:NAG:C1	2.60	0.49
1:A:430:GLU:HG2	4:A:579:FAD:O3'	2.13	0.48
1:C:63:GLY:HA2	1:C:193:GLY:O	2.14	0.48
1:A:414:GLU:HG2	1:A:414:GLU:O	2.14	0.48
1:C:69:MET:HE2	1:C:70:ASN:O	2.13	0.48
1:C:96:VAL:O	1:C:103:VAL:HA	2.13	0.48
1:C:112:ARG:NH2	1:C:115:LEU:CD1	2.76	0.48
1:A:8:ILE:HG13	1:A:259:ALA:HB2	1.95	0.48
1:C:304:LYS:NZ	1:C:342:ALA:O	2.32	0.48
1:A:21:LYS:HB2	1:A:216:TYR:CE2	2.48	0.48
1:A:157:PRO:HG3	1:A:324:SER:HA	1.96	0.48
1:C:173:GLU:OE1	1:C:294:ASP:OD2	2.32	0.48
1:A:243:SER:HB2	1:A:244:PRO:HD2	1.95	0.48
1:C:218:LYS:O	1:C:227:VAL:N	2.40	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:450:SER:HA	1:A:453:ILE:HD12	1.96	0.48
1:C:64:VAL:O	1:C:65:ASN:HB2	2.13	0.48
1:B:454:LEU:HD12	1:B:454:LEU:O	2.14	0.47
1:A:69:MET:HE1	1:A:73:TRP:CB	2.40	0.47
1:B:21:LYS:HB2	1:B:216:TYR:CE2	2.49	0.47
1:B:83:ARG:NH2	1:B:337:LYS:O	2.48	0.47
1:C:131:HIS:CD2	1:C:133:SER:HB3	2.50	0.47
1:A:431:HIS:CD2	5:A:2208:HOH:O	2.66	0.47
1:B:430:GLU:O	1:B:437:ASN:HA	2.14	0.47
1:A:95:ASN:HB3	1:A:319:PHE:HB3	1.96	0.47
1:B:241:LYS:HA	1:B:279:LYS:O	2.15	0.47
1:B:411:ASN:ND2	1:B:414:GLU:N	2.50	0.47
1:C:366:LYS:HD2	1:C:385:ALA:HB3	1.97	0.47
1:B:360:GLN:NE2	5:B:2189:HOH:O	2.48	0.47
1:B:69:MET:HE1	1:B:73:TRP:CG	2.50	0.47
1:C:370:MET:HE2	1:C:384:ASP:HA	1.95	0.47
1:A:70:ASN:O	1:A:74:PRO:HD3	2.15	0.47
1:A:238:ARG:NH1	1:A:252:GLU:OE2	2.47	0.46
1:A:305:PHE:HB3	1:A:306:PRO:HD2	1.96	0.46
1:C:26:ALA:HB2	1:C:455:ILE:HD13	1.96	0.46
1:C:69:MET:CE	1:C:73:TRP:HB3	2.44	0.46
1:C:438:GLY:O	4:C:579:FAD:H1'2	2.15	0.46
1:A:21:LYS:O	1:A:25:GLU:HG3	2.15	0.46
1:A:35:GLU:HB3	1:A:233:LEU:HD23	1.96	0.46
1:C:255:SER:HB2	1:C:257:TYR:CE1	2.50	0.46
1:A:305:PHE:HB3	1:A:306:PRO:CD	2.45	0.46
1:A:350:THR:HA	1:A:354:SER:OG	2.15	0.46
1:B:53:ASN:HB3	5:B:2099:HOH:O	2.15	0.46
1:B:145:ARG:O	1:B:149:HIS:N	2.47	0.46
1:C:187:ALA:HA	1:C:190:SER:OG	2.14	0.46
1:A:158:VAL:CG1	1:A:159:ASP:N	2.77	0.46
1:C:374:ARG:HD2	5:C:2194:HOH:O	2.15	0.46
1:B:218:LYS:H	1:B:228:ASP:HB2	1.79	0.46
2:D:1:NAG:O6	2:D:2:NAG:C1	2.63	0.46
1:A:291:TYR:CG	1:B:146:LEU:HA	2.51	0.46
1:C:285:TRP:CZ3	1:C:286:LYS:HE2	2.51	0.46
1:C:66:GLY:HA3	1:C:192:PHE:C	2.41	0.46
1:B:131:HIS:CD2	1:B:133:SER:OG	2.69	0.45
1:B:416:ASP:CG	1:B:466:HIS:HD2	2.24	0.45
1:B:131:HIS:HD2	1:B:133:SER:CB	2.29	0.45
1:B:317:GLU:O	1:B:333:GLN:HA	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:GLU:HA	1:A:321:TYR:CE1	2.51	0.45
1:B:158:VAL:HG12	5:B:2072:HOH:O	2.16	0.45
1:B:246:GLY:HA2	1:B:424:ARG:HD3	1.99	0.45
1:B:411:ASN:HD22	1:B:411:ASN:C	2.24	0.45
1:A:217:LEU:HD12	1:A:217:LEU:HA	1.65	0.45
1:A:292:GLN:OE1	5:A:2129:HOH:O	2.20	0.45
1:B:50:ALA:HB1	1:B:304:LYS:HD3	1.98	0.45
1:C:220:ASP:N	1:C:225:LYS:O	2.46	0.45
1:C:430:GLU:O	1:C:437:ASN:HA	2.16	0.45
1:C:431:HIS:CD2	5:C:2231:HOH:O	2.69	0.45
1:C:8:ILE:HG13	1:C:259:ALA:HB2	1.99	0.45
1:C:250:LYS:HG2	1:C:256:VAL:HG22	1.97	0.45
1:A:69:MET:HE3	1:A:70:ASN:O	2.16	0.45
1:A:300:LYS:HB3	1:A:346:LEU:HD11	1.98	0.45
1:B:141:LEU:HD22	1:B:176:ARG:HB3	1.97	0.45
1:B:307:ARG:HG2	1:B:383:PRO:HG3	1.99	0.45
1:B:411:ASN:HD21	1:B:414:GLU:H	1.58	0.44
1:B:411:ASN:HD21	1:B:414:GLU:HG3	1.82	0.44
1:A:303:LEU:O	1:A:344:VAL:HA	2.18	0.44
1:A:300:LYS:O	1:A:391:PRO:CD	2.65	0.44
1:A:49:PHE:O	1:A:50:ALA:HB3	2.16	0.44
1:A:256:VAL:HG12	1:A:257:TYR:N	2.32	0.44
1:C:303:LEU:O	1:C:344:VAL:HA	2.18	0.44
1:C:198:PHE:CE2	1:C:338:GLN:HG2	2.52	0.44
1:C:342:ALA:O	1:C:343:ASN:HB2	2.18	0.44
1:C:439:TYR:HB3	1:C:441:HIS:CE1	2.53	0.44
1:A:73:TRP:N	1:A:74:PRO:CD	2.80	0.44
1:A:325:ARG:O	1:A:326:ARG:C	2.61	0.44
1:C:238:ARG:HD3	1:C:252:GLU:OE2	2.18	0.44
1:C:251:THR:OG1	1:C:253:ASP:OD1	2.31	0.44
1:A:394:TRP:NE1	1:B:152:ASN:ND2	2.52	0.43
1:C:370:MET:HE1	1:C:382:VAL:HG12	2.00	0.43
1:C:457:CYS:O	1:C:461:LYS:HA	2.19	0.43
1:A:80:LEU:O	1:A:81:LYS:C	2.62	0.43
1:A:452:GLU:HA	1:A:455:ILE:HD12	1.99	0.43
1:B:52:ILE:HG13	1:B:54:VAL:HG13	2.00	0.43
1:A:426:TYR:CE1	1:A:454:LEU:HD13	2.53	0.43
1:C:302:PHE:HB2	1:C:389:LEU:HB3	2.01	0.43
1:A:253:ASP:C	1:A:253:ASP:OD1	2.61	0.43
1:A:309:PHE:CD2	1:A:383:PRO:HD2	2.54	0.43
1:B:366:LYS:HD2	1:B:385:ALA:HB3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:236:VAL:HB	1:A:252:GLU:HB2	2.01	0.43
1:A:73:TRP:HB3	1:A:74:PRO:HD3	1.99	0.43
1:B:47:THR:O	1:B:53:ASN:HA	2.19	0.43
1:B:293:PHE:CZ	1:B:406:TRP:HA	2.54	0.43
1:A:294:ASP:O	1:A:404:SER:HA	2.19	0.42
1:B:133:SER:O	1:B:411:ASN:HB2	2.19	0.42
1:C:243:SER:CB	1:C:244:PRO:CD	2.97	0.42
1:B:40:ILE:HG21	1:B:40:ILE:HD13	1.73	0.42
1:B:154:PRO:HB3	1:B:159:ASP:HB3	2.00	0.42
1:A:100:ASP:OD1	1:A:375:LYS:HE2	2.19	0.42
1:A:235:LYS:NZ	1:A:253:ASP:OD2	2.25	0.42
1:A:246:GLY:HA2	1:A:424:ARG:HD3	2.01	0.42
1:A:370:MET:HG3	1:A:384:ASP:OD2	2.19	0.42
1:A:306:PRO:HG2	1:A:383:PRO:HB2	2.01	0.42
1:C:219:THR:CA	1:C:225:LYS:O	2.67	0.42
1:A:52:ILE:HG21	1:A:52:ILE:HD13	1.77	0.42
1:A:414:GLU:HG3	1:A:417:GLN:OE1	2.20	0.42
1:C:436:TYR:O	1:C:437:ASN:C	2.61	0.42
1:A:457:CYS:O	1:A:461:LYS:HA	2.20	0.42
1:A:302:PHE:HB2	1:A:389:LEU:HB3	2.02	0.42
1:C:148:GLU:O	1:C:149:HIS:C	2.63	0.42
1:C:351:ASP:CG	1:C:352:GLU:H	2.26	0.42
1:A:64:VAL:CG1	1:A:65:ASN:N	2.82	0.42
1:A:165:TYR:CD2	1:A:165:TYR:C	2.96	0.42
1:A:180:LEU:HD12	1:A:184:VAL:HB	2.02	0.42
1:A:295:MET:HE3	1:A:401:GLY:C	2.45	0.42
1:B:134:GLY:HA2	1:B:181:GLN:OE1	2.20	0.42
1:B:243:SER:O	1:B:424:ARG:HD2	2.20	0.42
1:C:294:ASP:HB2	1:C:405:ASN:O	2.19	0.42
1:B:243:SER:CB	1:B:244:PRO:CD	2.95	0.41
1:C:91:TYR:CD1	1:C:91:TYR:N	2.87	0.41
1:B:420:ALA:HA	1:B:421:PRO:HD3	1.90	0.41
1:C:48:ASN:HD21	1:C:51:GLY:HA2	1.85	0.41
1:A:302:PHE:O	1:A:388:ILE:HA	2.19	0.41
1:C:241:LYS:HA	1:C:279:LYS:O	2.20	0.41
1:A:91:TYR:CG	1:A:315:GLY:HA3	2.55	0.41
1:A:220:ASP:OD1	1:A:223:SER:HB3	2.20	0.41
1:B:319:PHE:CZ	1:B:332:TRP:HB3	2.55	0.41
1:C:253:ASP:OD1	1:C:253:ASP:C	2.62	0.41
1:A:400:LYS:HB3	1:B:151:PRO:HG3	2.01	0.41
1:A:430:GLU:O	1:A:437:ASN:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:158:VAL:CG1	5:B:2072:HOH:O	2.68	0.41
1:B:303:LEU:O	1:B:344:VAL:HA	2.20	0.41
1:B:332:TRP:CZ3	1:B:347:VAL:HB	2.56	0.41
1:B:430:GLU:OE1	1:B:438:GLY:N	2.51	0.41
1:C:223:SER:C	1:C:225:LYS:H	2.29	0.41
1:A:271:LEU:HD23	1:A:271:LEU:HA	1.83	0.41
1:B:75:ILE:HA	1:B:79:THR:HB	2.02	0.41
1:B:302:PHE:HB2	1:B:389:LEU:HB3	2.03	0.41
1:C:6:ARG:HG3	1:C:6:ARG:NH1	2.29	0.41
1:B:252:GLU:C	1:B:254:ASN:H	2.28	0.41
1:B:312:GLU:OE2	5:B:2148:HOH:O	2.22	0.41
1:C:21:LYS:O	1:C:25:GLU:HG3	2.20	0.41
1:C:23:LEU:HB3	1:C:28:ILE:HB	2.01	0.41
1:A:235:LYS:HD3	1:A:235:LYS:HA	1.74	0.41
1:B:8:ILE:O	1:B:262:VAL:HA	2.21	0.41
1:B:216:TYR:CD1	1:B:217:LEU:CD1	3.00	0.41
1:C:213:ALA:O	1:C:217:LEU:HB2	2.21	0.41
1:A:273:SER:O	1:A:274:ASP:CB	2.57	0.40
1:A:360:GLN:NE2	5:A:2173:HOH:O	2.54	0.40
1:B:23:LEU:O	1:B:24:SER:C	2.63	0.40
1:B:220:ASP:CB	1:B:223:SER:OG	2.61	0.40
1:B:228:ASP:OD1	1:B:229:PRO:HD2	2.22	0.40
1:B:26:ALA:CB	1:B:455:ILE:HD13	2.50	0.40
1:B:57:GLY:HA2	4:B:579:FAD:C7M	2.51	0.40
1:B:286:LYS:NZ	1:B:420:ALA:O	2.44	0.40
1:C:50:ALA:HB1	1:C:304:LYS:HD3	2.03	0.40
1:C:154:PRO:HB3	1:C:159:ASP:HB3	2.03	0.40
1:C:317:GLU:O	1:C:333:GLN:HA	2.22	0.40
1:A:91:TYR:CD1	1:A:91:TYR:N	2.89	0.40
1:B:148:GLU:O	1:B:149:HIS:HB2	2.21	0.40
1:B:370:MET:HG3	1:B:384:ASP:OD2	2.21	0.40
1:B:381:ASP:O	1:B:383:PRO:HD3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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%)	437 (96%)	19 (4%)	1 (0%)	43	44
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%)	1323 (96%)	53 (4%)	1 (0%)	48	50

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	101	GLY

5.3.2 Protein sidechains ⓘ

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%)	383 (97%)	11 (3%)	38	43
1	B	397/404 (98%)	388 (98%)	9 (2%)	44	51
1	C	397/404 (98%)	392 (99%)	5 (1%)	61	69
All	All	1188/1212 (98%)	1163 (98%)	25 (2%)	47	54

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	LEU
1	A	28	ILE
1	A	52	ILE
1	A	59	ASN
1	A	136	ASP
1	A	186	LEU
1	A	190	SER
1	A	215	GLN

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Mol	Chain	Res	Type
1	A	217	LEU
1	A	282	LEU
1	A	386	THR
1	B	23	LEU
1	B	59	ASN
1	B	115	LEU
1	B	154	PRO
1	B	157	PRO
1	B	158	VAL
1	B	217	LEU
1	B	411	ASN
1	B	454	LEU
1	C	28	ILE
1	C	127	SER
1	C	217	LEU
1	C	221	ASP
1	C	282	LEU

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

Mol	Chain	Res	Type
1	A	152	ASN
1	A	215	GLN
1	A	360	GLN
1	A	431	HIS
1	B	131	HIS
1	B	152	ASN
1	B	182	ASN
1	B	360	GLN
1	B	411	ASN
1	B	431	HIS
1	B	435	HIS
1	B	466	HIS
1	C	48	ASN
1	C	131	HIS
1	C	152	ASN
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	2,1	14,14,15	0.89	0	17,19,21	1.82	6 (35%)
2	NAG	D	2	2	14,14,15	0.91	1 (7%)	17,19,21	1.43	3 (17%)
2	NAG	E	1	2,1	14,14,15	1.12	2 (14%)	17,19,21	2.01	5 (29%)
2	NAG	E	2	2	14,14,15	0.94	1 (7%)	17,19,21	1.88	4 (23%)
3	NAG	F	1	3,1	14,14,15	1.11	1 (7%)	17,19,21	2.06	4 (23%)
3	NAG	F	2	3	14,14,15	1.16	2 (14%)	17,19,21	1.87	4 (23%)
3	MAN	F	3	3	11,11,12	0.66	0	15,15,17	3.10	2 (13%)
3	MAN	F	4	3	11,11,12	0.55	0	15,15,17	1.08	2 (13%)
3	FCA	F	5	3	10,10,11	1.29	1 (10%)	14,14,16	1.77	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	2,1	-	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	2,1	-	2/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	2	2	-	2/6/23/26	0/1/1/1
3	NAG	F	1	3,1	-	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)
3	F	2	NAG	O5-C1	-3.19	1.38	1.43
3	F	5	FCA	C2-C3	-2.93	1.48	1.52
2	E	1	NAG	C1-C2	-2.56	1.48	1.52
3	F	1	NAG	C1-C2	-2.49	1.49	1.52
2	E	2	NAG	O5-C1	-2.49	1.39	1.43
3	F	2	NAG	C1-C2	-2.38	1.49	1.52
2	E	1	NAG	O5-C1	-2.31	1.39	1.43
2	D	2	NAG	O5-C1	-2.23	1.39	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	11.23	133.41	110.15
3	F	1	NAG	C1-C2-N2	-5.06	102.45	110.43
2	E	1	NAG	C2-N2-C7	-4.32	117.11	122.90
3	F	2	NAG	O5-C5-C6	-3.96	99.96	107.66
3	F	1	NAG	C1-O5-C5	3.87	117.37	112.19
2	E	2	NAG	C2-N2-C7	-3.85	117.73	122.90
2	E	2	NAG	O5-C5-C6	-3.85	100.18	107.66
3	F	5	FCA	C3-C4-C5	-3.79	104.06	109.81
2	E	1	NAG	C1-O5-C5	3.78	117.25	112.19
2	D	2	NAG	C1-C2-N2	-3.59	104.78	110.43
2	D	1	NAG	C1-C2-N2	-3.32	105.21	110.43
3	F	2	NAG	O5-C1-C2	-3.23	106.29	111.29
2	D	1	NAG	C1-O5-C5	3.15	116.41	112.19
2	E	2	NAG	C1-O5-C5	3.11	116.36	112.19
3	F	1	NAG	C8-C7-N2	-3.11	110.95	116.12
2	D	1	NAG	C8-C7-N2	-3.06	111.05	116.12
2	E	1	NAG	O5-C5-C6	-3.05	101.72	107.66
2	D	1	NAG	O5-C5-C6	-2.88	102.07	107.66
3	F	5	FCA	C1-C2-C3	2.86	113.81	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	F	4	MAN	O2-C2-C3	2.67	115.67	110.15
3	F	4	MAN	C2-C3-C4	-2.66	106.18	110.86
2	E	2	NAG	C1-C2-N2	-2.66	106.24	110.43
2	E	1	NAG	O3-C3-C2	2.59	114.79	109.40
2	E	1	NAG	C1-C2-N2	-2.57	106.38	110.43
3	F	5	FCA	C2-C3-C4	-2.37	106.69	110.86
3	F	1	NAG	C4-C3-C2	2.35	114.46	111.02
2	D	1	NAG	C6-C5-C4	2.25	118.54	113.02
2	D	2	NAG	C2-N2-C7	-2.24	119.89	122.90
3	F	3	MAN	O3-C3-C2	2.18	114.50	110.05
2	D	1	NAG	O3-C3-C4	2.15	115.45	110.38
3	F	2	NAG	C3-C4-C5	2.14	114.11	110.23
2	D	2	NAG	C8-C7-N2	-2.13	112.58	116.12
3	F	2	NAG	O3-C3-C2	-2.08	105.08	109.40
3	F	5	FCA	C1-O5-C5	2.04	117.77	112.97

There are no chirality outliers.

All (14) torsion outliers are listed below:

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

There are no ring outliers.

7 monomers are involved in 13 short contacts:

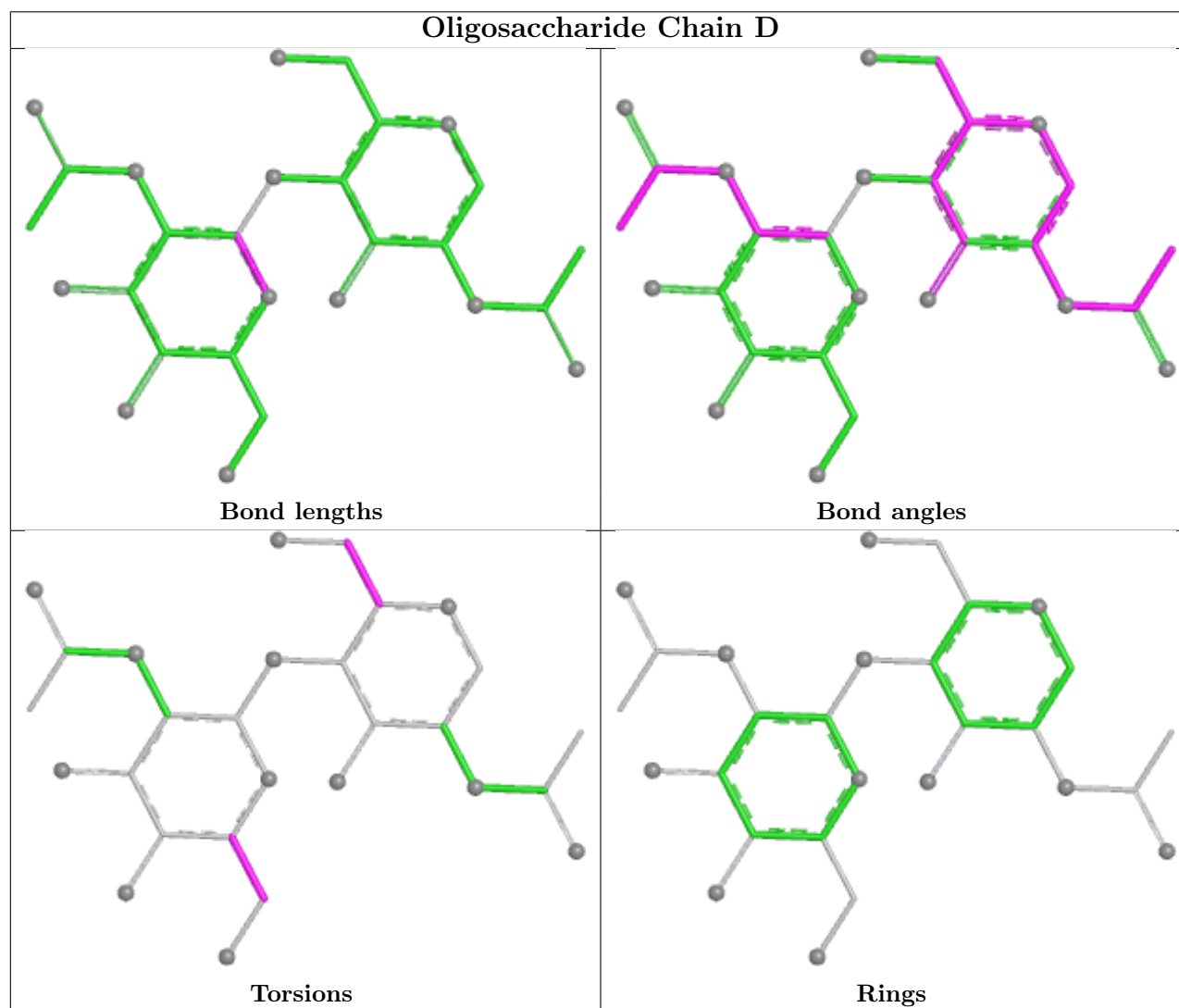
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	5	FCA	2	0
2	E	1	NAG	4	0

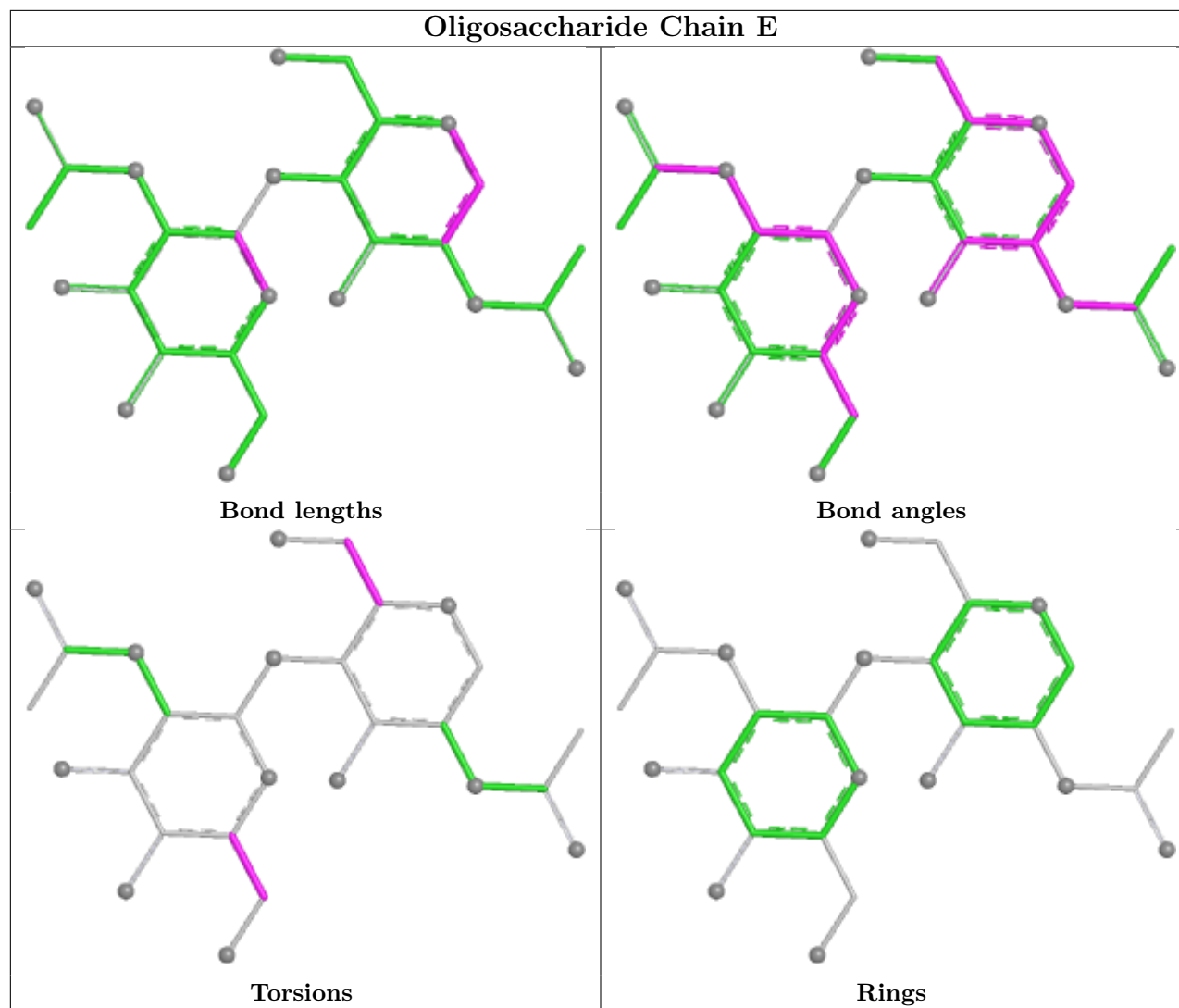
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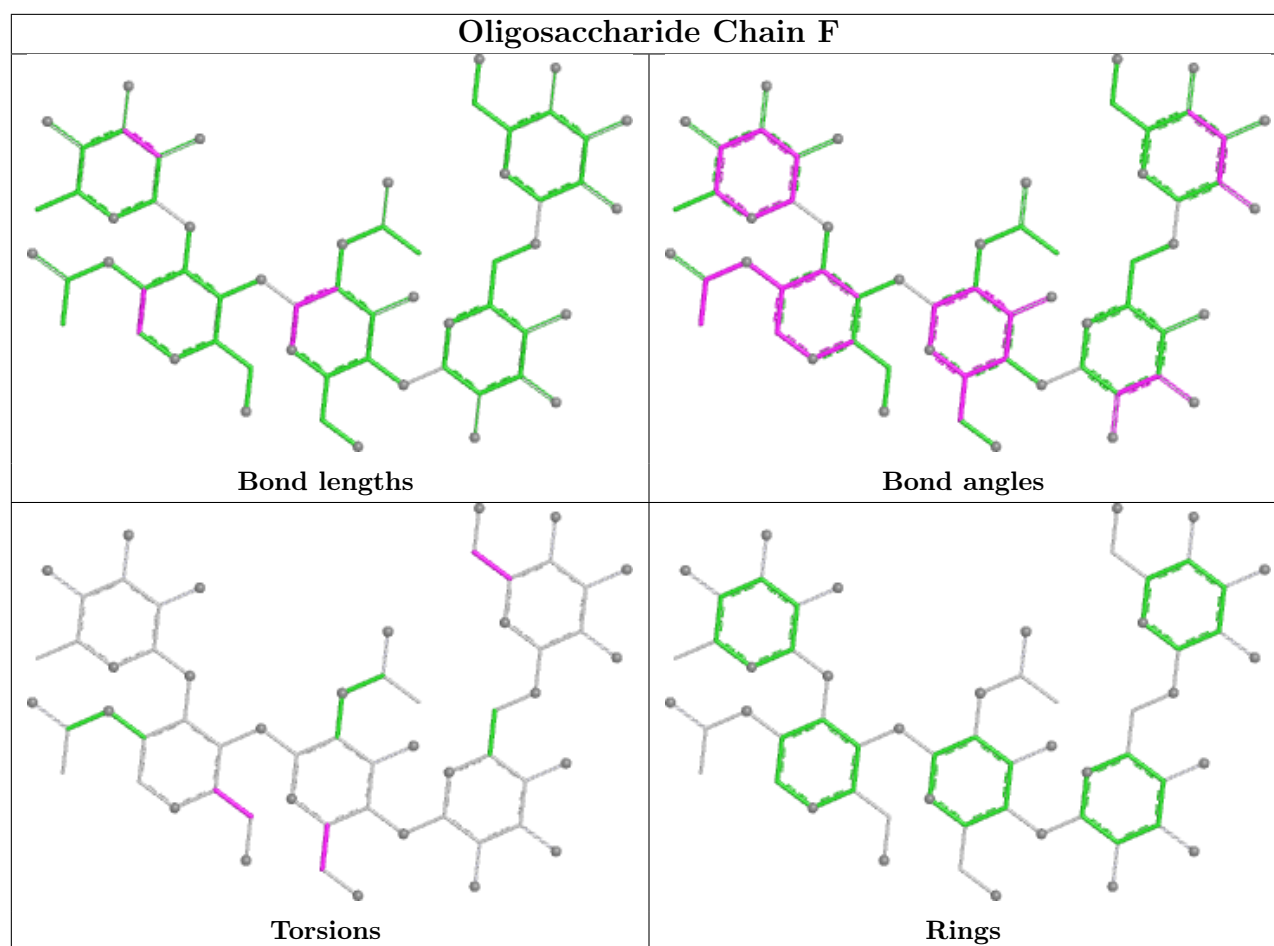
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1	NAG	3	0
2	E	2	NAG	4	0
2	D	2	NAG	3	0
3	F	2	NAG	4	0
3	F	1	NAG	6	0

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







5.6 Ligand geometry [i](#)

3 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	C	579	-	58,58,58	1.00	4 (6%)	85,89,89	1.25	10 (11%)
4	FAD	B	579	-	58,58,58	0.90	4 (6%)	85,89,89	1.28	12 (14%)
4	FAD	A	579	-	58,58,58	0.87	2 (3%)	85,89,89	1.39	12 (14%)

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	C	579	-	-	4/34/50/50	0/6/6/6
4	FAD	B	579	-	-	4/34/50/50	0/6/6/6
4	FAD	A	579	-	-	1/34/50/50	0/6/6/6

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	579	FAD	PA-O3P	3.44	1.63	1.59
4	C	579	FAD	C4X-N5	2.97	1.37	1.30
4	C	579	FAD	PA-O3P	2.91	1.62	1.59
4	B	579	FAD	P-O3P	2.77	1.62	1.59
4	A	579	FAD	C9A-N10	-2.71	1.36	1.41
4	A	579	FAD	C5X-N5	-2.45	1.34	1.39
4	B	579	FAD	C4X-N5	2.37	1.35	1.30
4	C	579	FAD	C9A-C5X	2.17	1.44	1.41
4	B	579	FAD	C9A-N10	-2.15	1.37	1.41
4	C	579	FAD	P-O3P	2.14	1.61	1.59

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	579	FAD	C9A-C5X-N5	-4.94	117.21	122.45
4	C	579	FAD	C5'-C4'-C3'	-4.13	104.43	112.22
4	A	579	FAD	C10-C4X-N5	-3.62	117.43	124.81
4	A	579	FAD	C5'-C4'-C3'	-3.34	105.91	112.22
4	C	579	FAD	C4-C4X-N5	3.12	122.51	118.21
4	C	579	FAD	O2A-PA-O1A	3.10	126.86	112.44
4	A	579	FAD	O4'-C4'-C3'	2.95	116.14	109.25
4	B	579	FAD	C10-C4X-N5	-2.94	118.80	124.81
4	B	579	FAD	C4-C4X-N5	2.91	122.23	118.21
4	B	579	FAD	C10-N1-C2	2.84	122.99	116.85
4	A	579	FAD	O3P-P-O1P	-2.80	102.28	110.70
4	A	579	FAD	C8M-C8-C9	-2.76	114.71	119.57
4	A	579	FAD	C6-C5X-C9A	2.69	122.75	119.05
4	C	579	FAD	O3P-PA-O1A	-2.67	102.68	110.70
4	B	579	FAD	C5'-C4'-C3'	-2.59	107.33	112.22
4	B	579	FAD	O3'-C3'-C4'	-2.59	103.05	108.93
4	A	579	FAD	O2A-PA-O1A	2.58	124.46	112.44
4	C	579	FAD	C10-N1-C2	2.57	122.41	116.85
4	B	579	FAD	O3P-PA-O1A	-2.46	103.30	110.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	579	FAD	O2P-P-O1P	2.46	123.87	112.44
4	B	579	FAD	C2B-C1B-N9A	2.38	119.22	113.30
4	C	579	FAD	O2P-P-O1P	2.30	123.13	112.44
4	C	579	FAD	O2P-P-O3P	-2.26	101.16	107.27
4	B	579	FAD	O2A-PA-O1A	2.24	122.87	112.44
4	A	579	FAD	O3P-PA-O1A	-2.24	103.98	110.70
4	B	579	FAD	O2A-PA-O3P	2.18	113.15	107.27
4	A	579	FAD	C9A-N10-C10	-2.17	117.44	120.75
4	C	579	FAD	O4B-C1B-C2B	-2.17	101.97	106.62
4	B	579	FAD	C5X-N5-C4X	-2.13	114.64	118.09
4	B	579	FAD	O3'-C3'-C2'	-2.12	104.11	108.93
4	C	579	FAD	C2B-C3B-C4B	2.08	106.63	102.61
4	C	579	FAD	O3'-C3'-C2'	-2.08	104.21	108.93
4	B	579	FAD	O2P-P-O1P	2.07	122.09	112.44
4	A	579	FAD	C1'-N10-C9A	2.06	124.63	120.63

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	579	FAD	C5B-O5B-PA-O1A
4	B	579	FAD	O3'-C3'-C4'-C5'
4	A	579	FAD	PA-O3P-P-O5'
4	C	579	FAD	O3'-C3'-C4'-C5'
4	C	579	FAD	C2B-C1B-N9A-C8A
4	B	579	FAD	C2B-C1B-N9A-C8A
4	B	579	FAD	O3'-C3'-C4'-O4'
4	C	579	FAD	O3'-C3'-C4'-O4'
4	C	579	FAD	O4B-C4B-C5B-O5B

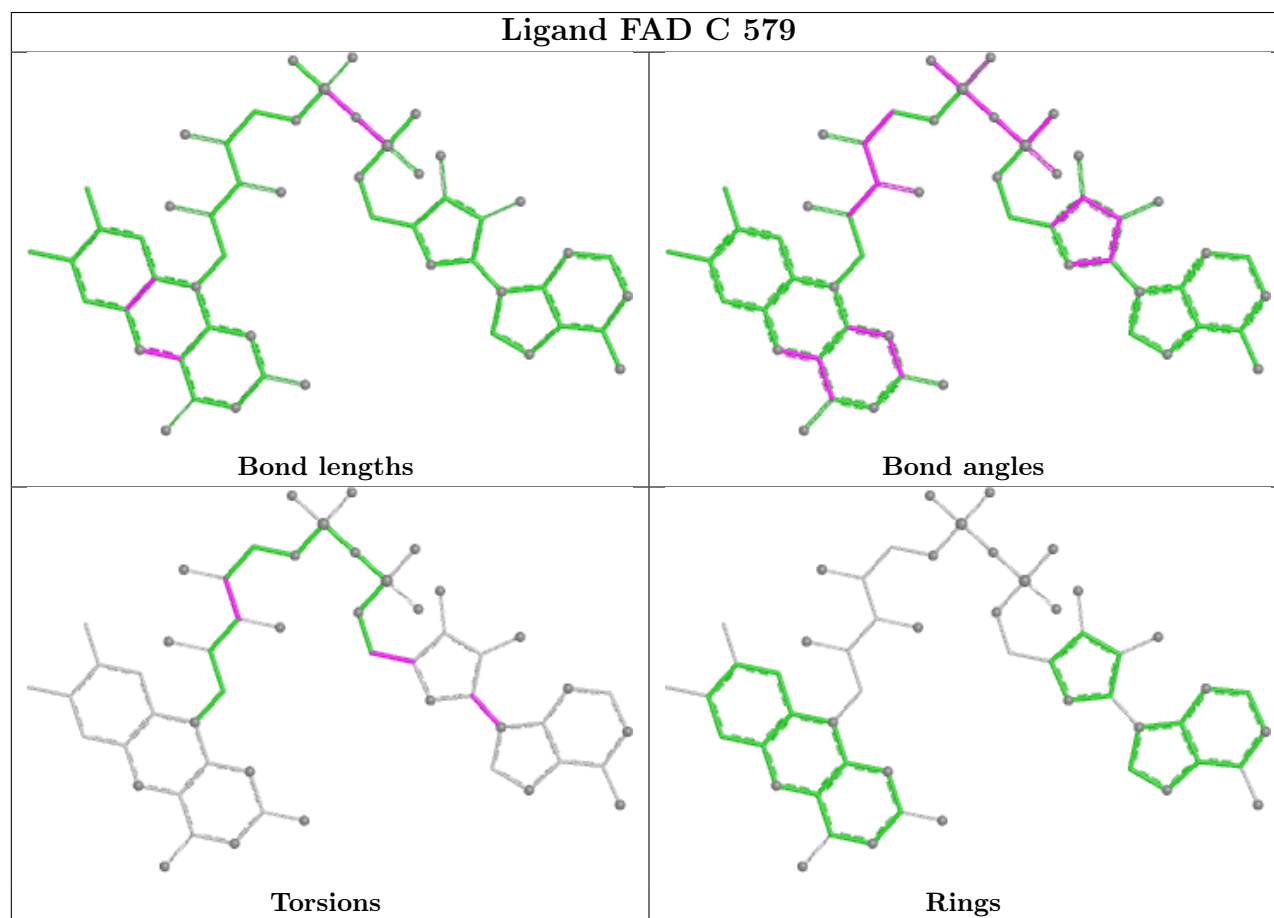
There are no ring outliers.

3 monomers are involved in 7 short contacts:

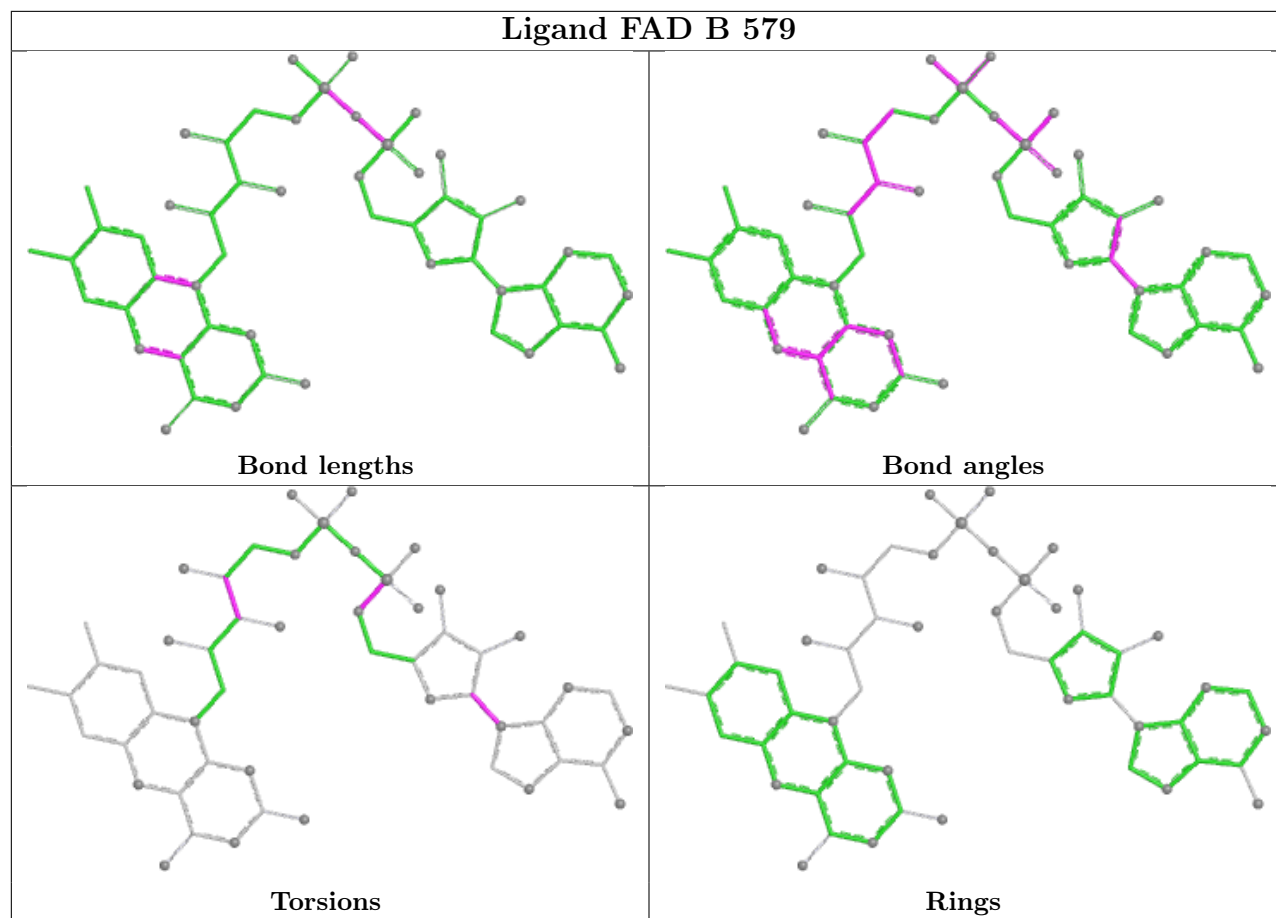
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	579	FAD	3	0
4	B	579	FAD	2	0
4	A	579	FAD	2	0

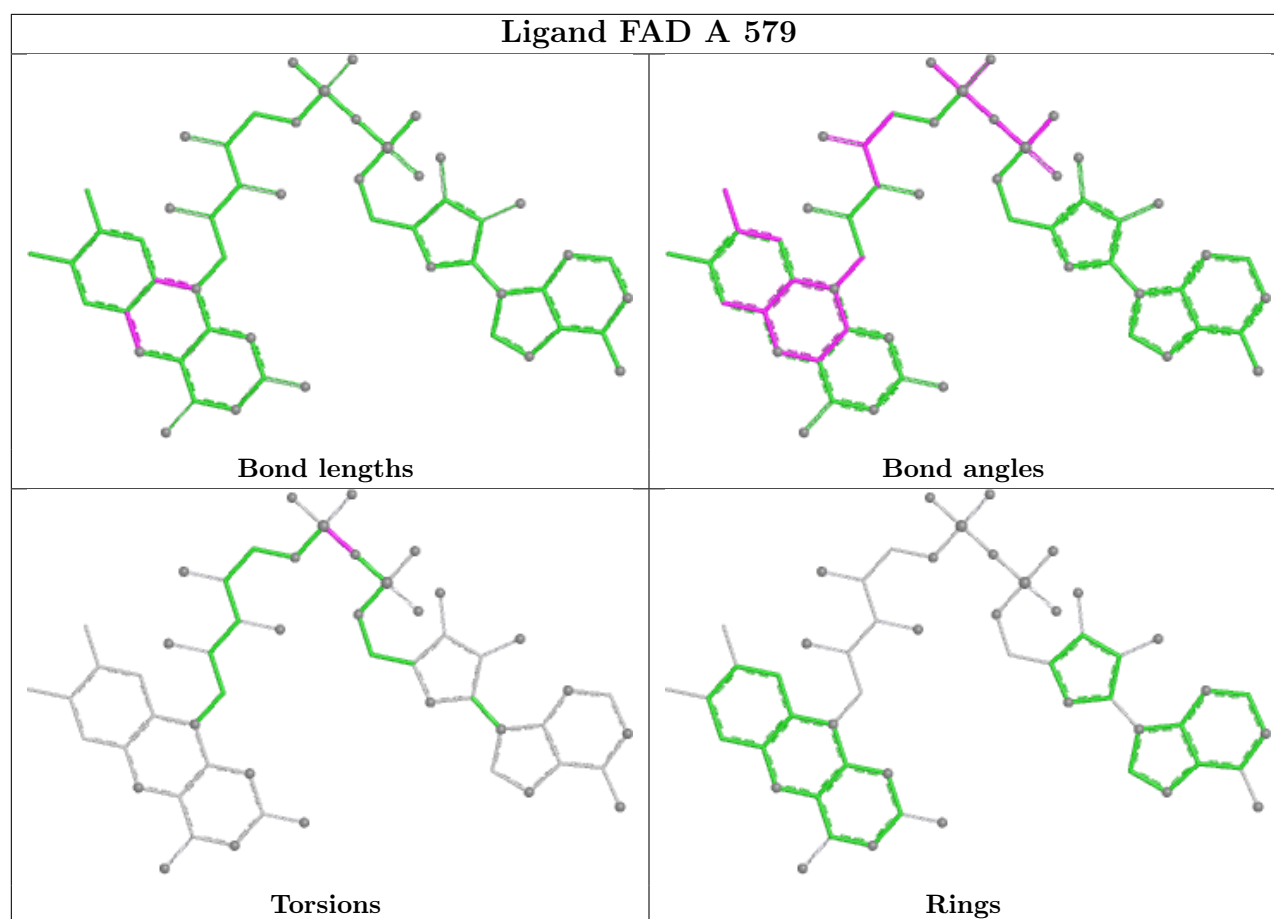
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

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.