



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:03 PM UTC

PDB ID : 2IPS / pdb_00002ips
Title : Crystal structure of a ternary complex of bovine lactoperoxidase with thiocyanate and iodide at 3.1 Å resolution
Authors : Singh, A.K.; Singh, N.; Sharma, S.; Singh, T.P.
Deposited on : 2006-10-12
Resolution : 3.10 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

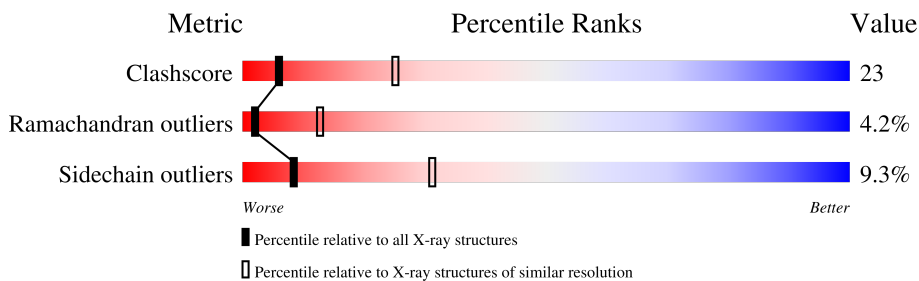
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)

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	595	 56% 34% 8% .
2	B	3	 100%
2	D	3	 33% 67%
3	C	2	 50% 50%
4	E	2	 100%

2 Entry composition [i](#)

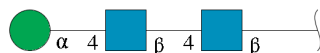
There are 10 unique types of molecules in this entry. The entry contains 5138 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Lactoperoxidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	S	0	0	0
			4770	3037	847	860	26			

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 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
3	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

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

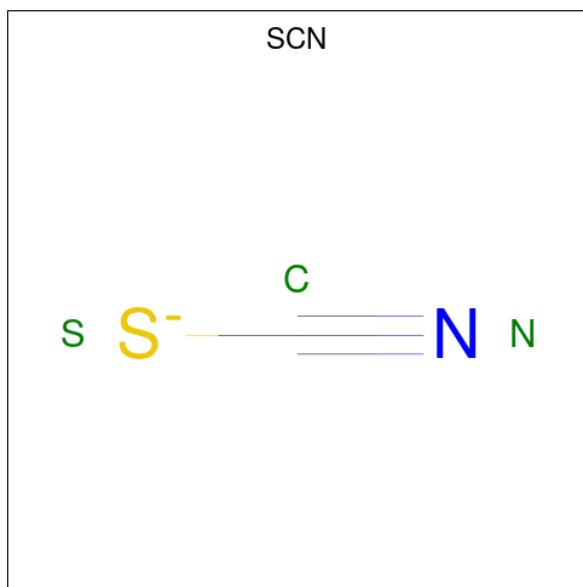


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	E	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

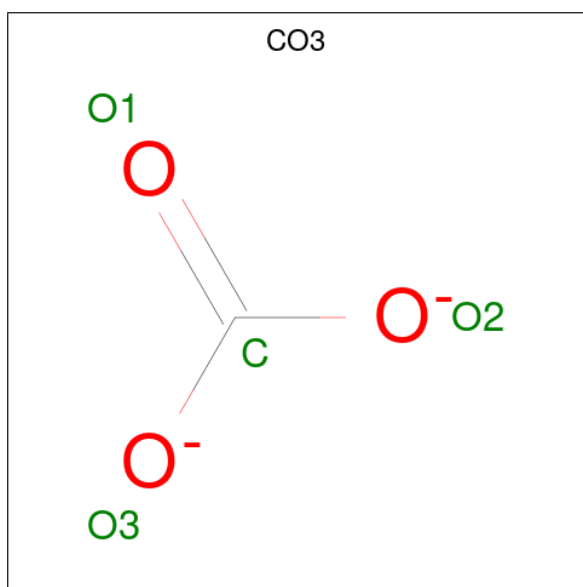
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Ca	0	0
			1	1		

- Molecule 6 is THIOCYANATE ION (CCD ID: SCN) (formula: CNS).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	S	0	0
			3	1	1	1		

- Molecule 7 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).

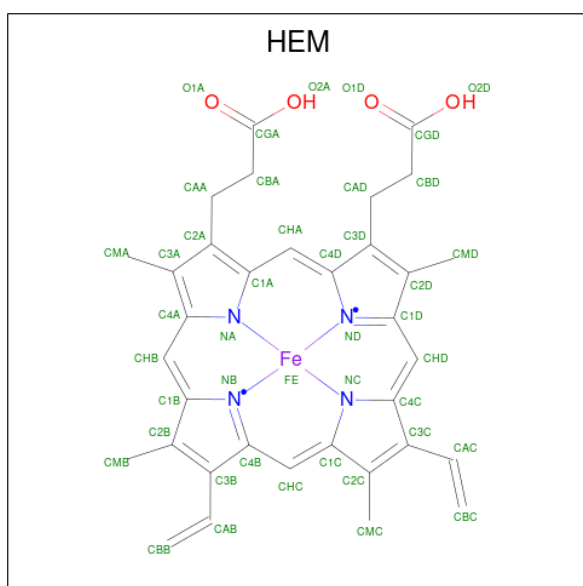


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			4	1	3		

- Molecule 8 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	6	Total	I	0	0
			6	6		

- Molecule 9 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	A	1	Total 43	C 34	Fe 1	N 4	O 4	0	0

- Molecule 10 is water.

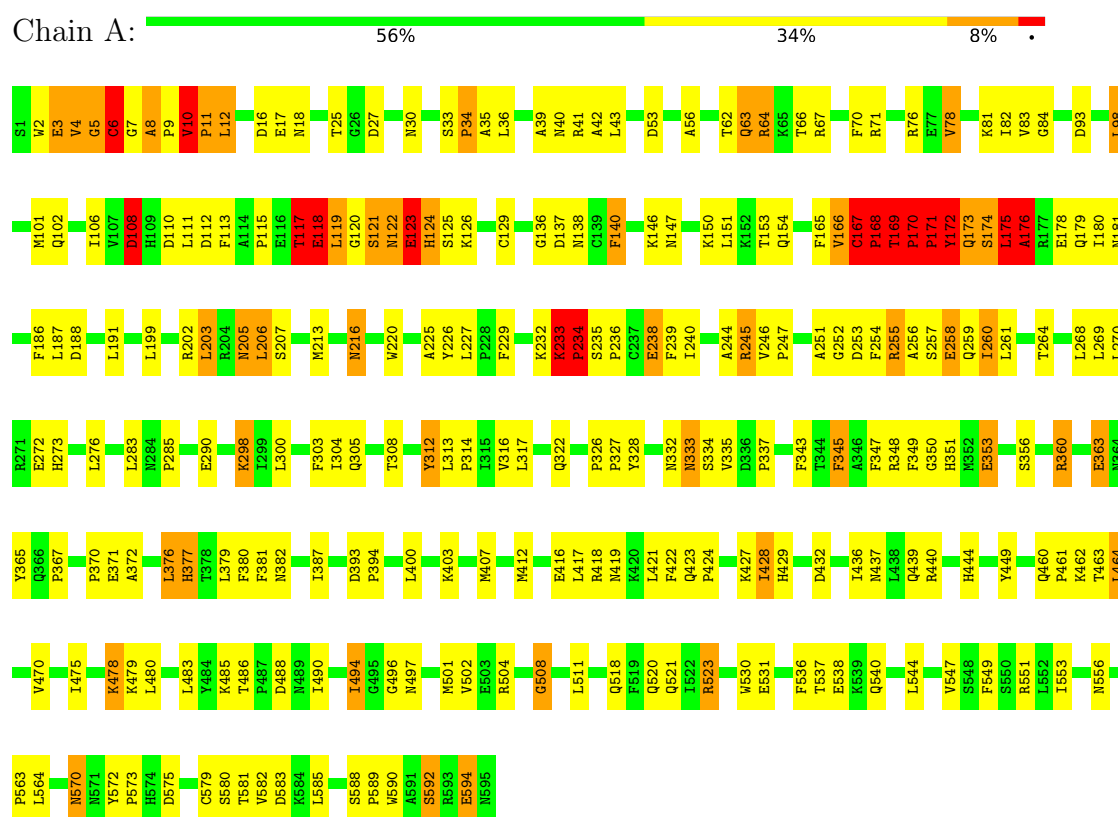
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	177	Total 177	O 177	0	0

3 Residue-property plots

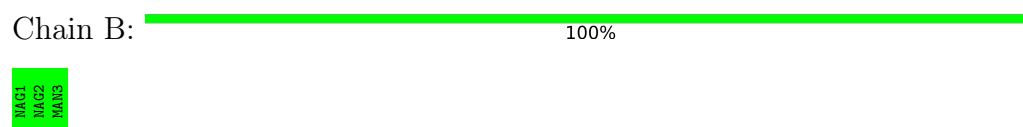
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



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



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





- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



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



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	55.54Å 80.59Å 77.92Å 90.00° 102.69° 90.00°	Depositor
Resolution (Å)	17.07 – 3.10	Depositor
% Data completeness (in resolution range)	97.4 (17.07-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.193 , 0.235	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5138	wwPDB-VP
Average B, all atoms (Å ²)	27.0	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: SCN, NAG, CO3, NDG, HEM, MAN, CA, IOD

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	0.72	7/4898 (0.1%)	1.27	71/6645 (1.1%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	PRO	N-CA	9.99	1.60	1.47
1	A	167	CYS	N-CA	-9.39	1.32	1.46
1	A	175	LEU	N-CA	8.95	1.57	1.46
1	A	234	PRO	N-CA	6.43	1.55	1.47
1	A	169	THR	CA-C	6.06	1.60	1.52
1	A	166	VAL	C-N	-5.77	1.21	1.33
1	A	332	ASN	N-CA	-5.10	1.40	1.46

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	172	TYR	CA-CB-CG	14.03	139.16	113.90
1	A	166	VAL	N-CA-C	12.99	136.37	109.34
1	A	63	GLN	OE1-CD-NE2	-10.44	112.16	122.60
1	A	170	PRO	CB-CA-C	10.36	123.56	110.92
1	A	173	GLN	OE1-CD-NE2	-9.68	112.92	122.60
1	A	81	LYS	CA-C-N	-9.27	113.67	122.66
1	A	81	LYS	C-N-CA	-9.27	113.67	122.66
1	A	172	TYR	CB-CG-CD2	8.76	133.94	120.80
1	A	4	VAL	N-CA-C	8.27	126.54	109.34
1	A	166	VAL	CB-CA-C	-8.25	97.76	111.29
1	A	172	TYR	CB-CG-CD1	-8.24	108.44	120.80
1	A	108	ASP	CA-CB-CG	7.88	120.48	112.60
1	A	205	ASN	N-CA-C	-7.79	97.89	110.20
1	A	172	TYR	N-CA-C	7.64	118.65	107.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	233	LYS	CA-C-N	-7.24	110.79	119.84
1	A	233	LYS	C-N-CA	-7.24	110.79	119.84
1	A	312	TYR	N-CA-C	7.18	122.17	113.41
1	A	172	TYR	N-CA-CB	-7.07	99.04	111.49
1	A	423	GLN	CA-C-N	6.92	128.49	119.84
1	A	423	GLN	C-N-CA	6.92	128.49	119.84
1	A	206	LEU	N-CA-C	-6.86	103.05	112.03
1	A	117	THR	N-CA-C	6.83	119.31	111.11
1	A	63	GLN	CG-CD-NE2	6.81	126.61	116.40
1	A	12	LEU	N-CA-C	6.72	119.97	110.23
1	A	508	GLY	CA-C-N	6.50	127.96	119.84
1	A	508	GLY	C-N-CA	6.50	127.96	119.84
1	A	176	ALA	N-CA-C	-6.49	96.97	110.80
1	A	111	LEU	N-CA-C	6.47	119.65	111.69
1	A	167	CYS	N-CA-C	-6.42	95.62	109.81
1	A	254	PHE	N-CA-C	6.39	119.23	111.82
1	A	11	PRO	CA-N-CD	-6.37	103.08	112.00
1	A	168	PRO	CA-N-CD	-6.36	103.10	112.00
1	A	173	GLN	CG-CD-NE2	6.22	125.74	116.40
1	A	387	ILE	N-CA-C	6.16	116.83	110.36
1	A	171	PRO	CA-C-N	-6.08	111.64	122.45
1	A	171	PRO	C-N-CA	-6.08	111.64	122.45
1	A	102	GLN	N-CA-C	5.93	117.75	111.28
1	A	175	LEU	N-CA-C	5.92	123.40	110.80
1	A	239	PHE	N-CA-C	5.88	118.16	111.11
1	A	363	GLU	N-CA-C	5.86	117.34	111.07
1	A	140	PHE	CA-C-N	5.86	125.81	119.78
1	A	140	PHE	C-N-CA	5.86	125.81	119.78
1	A	234	PRO	CA-N-CD	-5.74	103.97	112.00
1	A	78	VAL	N-CA-C	-5.72	104.78	110.62
1	A	460	GLN	CA-C-N	5.66	125.84	119.90
1	A	460	GLN	C-N-CA	5.66	125.84	119.90
1	A	112	ASP	N-CA-C	5.60	117.70	109.24
1	A	353	GLU	N-CA-C	-5.60	107.09	114.31
1	A	521	GLN	N-CA-C	5.59	117.05	111.07
1	A	260	ILE	N-CA-C	5.56	116.96	110.62
1	A	592	SER	N-CA-C	5.49	117.79	108.02
1	A	345	PHE	N-CA-C	-5.49	107.13	113.88
1	A	173	GLN	CA-C-N	-5.46	113.81	121.72
1	A	173	GLN	C-N-CA	-5.46	113.81	121.72
1	A	153	THR	N-CA-C	5.45	120.30	113.43
1	A	207	SER	N-CA-C	-5.42	106.35	113.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	34	PRO	CA-N-CD	-5.39	104.45	112.00
1	A	429	HIS	N-CA-C	-5.36	102.16	109.71
1	A	172	TYR	CB-CA-C	5.35	122.38	111.78
1	A	258	GLU	CB-CA-C	-5.30	101.68	110.68
1	A	138	ASN	N-CA-C	5.28	119.28	113.21
1	A	308	THR	N-CA-C	5.22	116.66	110.97
1	A	119	LEU	N-CA-C	-5.21	106.22	112.58
1	A	356	SER	N-CA-C	5.21	117.86	111.82
1	A	582	VAL	N-CA-C	5.20	115.39	108.11
1	A	238	GLU	N-CA-C	-5.13	105.38	111.69
1	A	556	ASN	N-CA-C	5.11	120.14	112.94
1	A	412	MET	N-CA-C	5.06	121.57	110.80
1	A	225	ALA	N-CA-C	5.05	117.20	110.53
1	A	123	GLU	N-CA-C	5.03	116.78	110.24
1	A	53	ASP	N-CA-C	-5.03	106.98	112.72

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4770	0	4689	220	0
2	B	39	0	34	0	0
2	D	39	0	34	1	0
3	C	28	0	25	3	0
4	E	28	0	24	1	0
5	A	1	0	0	0	0
6	A	3	0	0	0	0
7	A	4	0	0	0	0
8	A	6	0	0	1	0
9	A	43	0	30	4	0
10	A	177	0	0	16	0
All	All	5138	0	4836	222	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 23.

All (222) 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:A:169:THR:HB	1:A:170:PRO:CD	1.72	1.17
1:A:169:THR:HB	1:A:170:PRO:HD2	1.10	1.09
1:A:120:GLY:HA3	1:A:126:LYS:HE3	1.11	1.07
1:A:216:ASN:ND2	8:A:706:IOD:I	2.59	1.05
1:A:82:ILE:HD11	1:A:483:LEU:CD1	1.90	1.00
1:A:504:ARG:HD3	10:A:834:HOH:O	1.60	0.99
1:A:169:THR:CB	1:A:170:PRO:CD	2.40	0.98
1:A:227:LEU:HD23	1:A:270:LEU:HD22	1.49	0.93
1:A:174:SER:O	1:A:175:LEU:HB2	1.68	0.92
1:A:10:VAL:HG21	1:A:41:ARG:NH2	1.85	0.90
1:A:2:TRP:NE1	1:A:35:ALA:HB3	1.86	0.89
1:A:175:LEU:HG	10:A:731:HOH:O	1.72	0.88
1:A:381:PHE:CZ	1:A:424:PRO:HG3	2.08	0.87
1:A:238:GLU:HG2	1:A:245:ARG:O	1.74	0.87
1:A:205:ASN:CG	3:C:1:NAG:C1	2.46	0.87
1:A:169:THR:HG22	1:A:170:PRO:HD3	1.57	0.85
1:A:123:GLU:HG2	1:A:125:SER:HB3	1.61	0.83
1:A:169:THR:CG2	1:A:170:PRO:HD3	2.09	0.82
1:A:82:ILE:HD11	1:A:483:LEU:HD12	1.63	0.80
1:A:2:TRP:HB2	1:A:33:SER:HA	1.64	0.79
1:A:167:CYS:HB2	1:A:168:PRO:HD2	1.65	0.77
1:A:167:CYS:CB	1:A:168:PRO:HD2	2.17	0.75
1:A:167:CYS:CB	1:A:168:PRO:CD	2.66	0.74
1:A:333:ASN:C	1:A:333:ASN:HD22	1.96	0.73
1:A:9:PRO:HG2	10:A:766:HOH:O	1.88	0.72
1:A:205:ASN:O	1:A:206:LEU:HD23	1.88	0.72
1:A:169:THR:CB	1:A:170:PRO:HD3	2.18	0.72
1:A:2:TRP:CZ3	1:A:36:LEU:HD13	2.26	0.71
1:A:146:LYS:O	1:A:147:ASN:HB2	1.90	0.71
1:A:377:HIS:HB3	1:A:416:GLU:OE2	1.90	0.71
1:A:494:ILE:O	1:A:494:ILE:HD13	1.94	0.68
1:A:166:VAL:CG1	1:A:180:ILE:HG12	2.24	0.68
1:A:260:ILE:HG21	1:A:379:LEU:HD13	1.76	0.67
1:A:343:PHE:CD1	1:A:518:GLN:HG2	2.29	0.67
1:A:581:THR:O	1:A:581:THR:HG22	1.95	0.67
1:A:205:ASN:ND2	3:C:1:NAG:C2	2.56	0.67
1:A:82:ILE:HD11	1:A:483:LEU:HD13	1.76	0.67
1:A:4:VAL:HG13	1:A:5:GLY:H	1.60	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:VAL:HG12	1:A:180:ILE:HG12	1.77	0.67
1:A:119:LEU:HD21	1:A:170:PRO:HD3	1.76	0.67
1:A:124:HIS:HB3	10:A:824:HOH:O	1.97	0.65
1:A:120:GLY:HA3	1:A:126:LYS:CE	2.07	0.64
1:A:174:SER:O	1:A:175:LEU:CB	2.42	0.64
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.32	0.64
1:A:370:PRO:HG2	1:A:371:GLU:HG3	1.80	0.64
1:A:175:LEU:O	1:A:176:ALA:HB2	1.98	0.63
1:A:463:THR:HB	10:A:880:HOH:O	1.98	0.63
1:A:119:LEU:HD21	1:A:169:THR:CG2	2.29	0.63
1:A:272:GLU:O	1:A:276:LEU:HB2	1.99	0.63
1:A:335:VAL:HG22	4:E:1:NAG:H62	1.81	0.63
1:A:244:ALA:O	1:A:246:VAL:HG23	1.99	0.62
1:A:170:PRO:HB2	1:A:171:PRO:HD2	1.82	0.62
1:A:363:GLU:C	1:A:365:TYR:H	2.08	0.61
1:A:496:GLY:C	1:A:511:LEU:HD21	2.25	0.61
1:A:170:PRO:CB	1:A:171:PRO:HD2	2.30	0.61
1:A:570:ASN:HB3	1:A:575:ASP:CB	2.30	0.61
1:A:30:ASN:HB3	1:A:33:SER:O	2.00	0.61
1:A:167:CYS:HB3	1:A:168:PRO:CD	2.31	0.60
1:A:121:SER:O	1:A:122:ASN:HB2	2.01	0.60
1:A:171:PRO:O	1:A:172:TYR:CB	2.48	0.60
1:A:537:THR:OG1	1:A:540:GLN:HG3	2.02	0.60
1:A:98:LEU:HD22	1:A:101:MET:HE3	1.82	0.59
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.66	0.59
1:A:119:LEU:HD22	1:A:170:PRO:HG3	1.85	0.59
1:A:588:SER:OG	1:A:589:PRO:HD3	2.03	0.59
1:A:303:PHE:HD2	1:A:304:ILE:HD12	1.67	0.58
1:A:480:LEU:HG	1:A:490:ILE:HD12	1.84	0.58
1:A:475:ILE:HG22	1:A:479:LYS:HE3	1.85	0.58
1:A:113:PHE:O	1:A:115:PRO:HD3	2.04	0.58
1:A:166:VAL:HG22	1:A:178:GLU:O	2.02	0.58
1:A:258:GLU:OE1	1:A:259:GLN:HG2	2.03	0.58
1:A:260:ILE:CG2	1:A:379:LEU:HD13	2.34	0.58
1:A:36:LEU:HG	1:A:337:PRO:HD2	1.85	0.58
1:A:551:ARG:HD3	1:A:583:ASP:O	2.04	0.57
1:A:376:LEU:HD22	1:A:376:LEU:O	2.03	0.57
1:A:119:LEU:HD21	1:A:169:THR:HG22	1.85	0.57
1:A:16:ASP:C	1:A:18:ASN:H	2.12	0.57
1:A:170:PRO:CB	1:A:171:PRO:CD	2.82	0.57
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.02	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:LEU:HB3	1:A:317:LEU:HD23	1.86	0.57
1:A:407:MET:HB3	1:A:501:MET:HE2	1.87	0.56
1:A:313:LEU:N	1:A:314:PRO:CD	2.69	0.56
1:A:199:LEU:HG	1:A:203:LEU:CD2	2.36	0.56
1:A:449:TYR:CB	1:A:490:ILE:HB	2.36	0.55
9:A:708:HEM:NA	10:A:872:HOH:O	2.33	0.55
1:A:179:GLN:HG2	1:A:444:HIS:CE1	2.41	0.55
1:A:333:ASN:HD22	1:A:334:SER:N	2.04	0.55
1:A:530:TRP:CE2	1:A:531:GLU:HG3	2.41	0.55
1:A:187:LEU:HD22	1:A:304:ILE:CG2	2.36	0.55
1:A:10:VAL:HG23	1:A:10:VAL:O	2.07	0.55
1:A:259:GLN:HG2	9:A:708:HEM:HBB2	1.87	0.54
1:A:220:TRP:HD1	10:A:746:HOH:O	1.90	0.54
1:A:2:TRP:HE1	1:A:35:ALA:HB3	1.72	0.54
1:A:407:MET:HB3	1:A:501:MET:CE	2.37	0.54
1:A:461:PRO:HG3	1:A:470:VAL:HG21	1.88	0.54
1:A:63:GLN:CD	1:A:63:GLN:H	2.16	0.53
1:A:328:TYR:CD1	1:A:523:ARG:HD3	2.43	0.53
1:A:393:ASP:HB2	1:A:394:PRO:HD3	1.90	0.53
1:A:175:LEU:O	1:A:176:ALA:CB	2.55	0.53
1:A:335:VAL:O	1:A:337:PRO:HD3	2.08	0.53
1:A:10:VAL:O	1:A:10:VAL:CG2	2.56	0.53
1:A:4:VAL:HG13	1:A:5:GLY:N	2.22	0.52
1:A:106:ILE:HG23	1:A:191:LEU:HD11	1.91	0.52
1:A:187:LEU:HD22	1:A:304:ILE:HG22	1.90	0.52
1:A:199:LEU:O	1:A:203:LEU:HD22	2.09	0.52
1:A:544:LEU:O	1:A:547:VAL:HG22	2.09	0.52
1:A:475:ILE:CG2	1:A:479:LYS:HE3	2.39	0.52
1:A:328:TYR:HD1	1:A:523:ARG:HD3	1.75	0.52
1:A:35:ALA:O	1:A:36:LEU:C	2.52	0.51
1:A:16:ASP:O	1:A:18:ASN:N	2.44	0.51
1:A:272:GLU:O	1:A:272:GLU:HG3	2.10	0.51
1:A:400:LEU:HD13	1:A:563:PRO:HD2	1.94	0.51
1:A:549:PHE:CE2	1:A:553:ILE:HD11	2.46	0.50
1:A:502:VAL:HG13	1:A:508:GLY:HA2	1.93	0.50
1:A:253:ASP:OD2	1:A:255:ARG:HD3	2.12	0.50
1:A:120:GLY:CA	1:A:126:LYS:HE3	2.07	0.50
1:A:572:TYR:CD1	1:A:573:PRO:HA	2.46	0.50
1:A:165:PHE:HZ	1:A:170:PRO:O	1.94	0.49
1:A:232:LYS:HG3	10:A:854:HOH:O	2.13	0.49
1:A:118:GLU:O	1:A:119:LEU:HB2	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:570:ASN:HB3	1:A:575:ASP:HB2	1.95	0.49
1:A:117:THR:O	1:A:118:GLU:HB2	2.13	0.49
1:A:4:VAL:O	1:A:6:CYS:N	2.46	0.48
1:A:67:ARG:NH1	10:A:719:HOH:O	2.45	0.48
1:A:166:VAL:HG13	1:A:180:ILE:HG12	1.95	0.48
1:A:418:ARG:O	1:A:432:ASP:HB2	2.13	0.48
2:D:1:NAG:H62	2:D:2:NAG:C1	2.43	0.48
1:A:485:LYS:O	1:A:486:THR:HB	2.14	0.48
1:A:462:LYS:NZ	1:A:488:ASP:OD1	2.41	0.48
1:A:108:ASP:HB2	1:A:347:PHE:CD2	2.48	0.47
1:A:449:TYR:HB2	1:A:490:ILE:HB	1.95	0.47
1:A:258:GLU:O	1:A:380:PHE:HA	2.14	0.47
1:A:175:LEU:CG	10:A:731:HOH:O	2.45	0.47
1:A:360:ARG:NH1	1:A:372:ALA:HA	2.29	0.47
1:A:78:VAL:HG13	1:A:82:ILE:HD13	1.97	0.47
1:A:588:SER:N	1:A:589:PRO:HD2	2.29	0.47
1:A:42:ALA:HB2	1:A:166:VAL:HG11	1.97	0.47
1:A:418:ARG:HA	1:A:432:ASP:OD1	2.15	0.47
1:A:432:ASP:O	1:A:436:ILE:HG13	2.15	0.47
1:A:496:GLY:CA	1:A:511:LEU:HD21	2.45	0.47
1:A:588:SER:OG	1:A:589:PRO:CD	2.63	0.46
1:A:264:THR:O	1:A:268:LEU:HD13	2.14	0.46
1:A:326:PRO:HB2	1:A:327:PRO:HD2	1.97	0.46
1:A:129:CYS:HB2	10:A:721:HOH:O	2.14	0.46
1:A:76:ARG:NH2	1:A:150:LYS:HD2	2.30	0.46
1:A:220:TRP:CD1	10:A:746:HOH:O	2.66	0.46
1:A:333:ASN:C	1:A:333:ASN:ND2	2.66	0.46
1:A:579:CYS:C	1:A:581:THR:H	2.23	0.46
1:A:93:ASP:O	1:A:403:LYS:HD2	2.16	0.46
1:A:4:VAL:O	1:A:5:GLY:C	2.59	0.45
1:A:298:LYS:HD3	1:A:536:PHE:CZ	2.51	0.45
1:A:2:TRP:CD1	1:A:35:ALA:HB3	2.49	0.45
1:A:583:ASP:HB2	10:A:823:HOH:O	2.17	0.45
1:A:101:MET:SD	1:A:101:MET:C	3.00	0.45
1:A:421:LEU:HD21	9:A:708:HEM:HMA1	1.98	0.45
1:A:537:THR:O	1:A:540:GLN:N	2.50	0.45
1:A:464:LEU:C	1:A:464:LEU:HD22	2.41	0.45
1:A:140:PHE:CE2	1:A:439:GLN:NE2	2.84	0.45
1:A:187:LEU:HB3	1:A:305:GLN:HG2	1.99	0.45
1:A:462:LYS:HD2	10:A:863:HOH:O	2.16	0.45
1:A:2:TRP:HB2	1:A:33:SER:CA	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:10:VAL:HG21	1:A:41:ARG:CZ	2.45	0.45
1:A:62:THR:CG2	1:A:64:ARG:HD2	2.47	0.45
1:A:175:LEU:CD1	10:A:731:HOH:O	2.65	0.45
1:A:594:GLU:CD	1:A:594:GLU:H	2.23	0.45
1:A:251:ALA:O	1:A:253:ASP:N	2.49	0.45
1:A:350:GLY:O	1:A:353:GLU:N	2.47	0.44
1:A:16:ASP:C	1:A:18:ASN:N	2.75	0.44
1:A:113:PHE:CE2	1:A:115:PRO:HG3	2.52	0.44
1:A:167:CYS:HB3	1:A:168:PRO:HD3	2.00	0.44
1:A:229:PHE:CD1	1:A:247:PRO:HG2	2.52	0.44
1:A:233:LYS:HA	1:A:233:LYS:HD3	1.39	0.44
1:A:244:ALA:O	1:A:246:VAL:N	2.50	0.44
1:A:240:ILE:HD11	1:A:382:ASN:HA	2.00	0.44
1:A:165:PHE:CD1	1:A:165:PHE:N	2.84	0.44
1:A:579:CYS:O	1:A:581:THR:N	2.51	0.44
1:A:39:ALA:O	1:A:40:ASN:HB2	2.18	0.43
1:A:180:ILE:HG22	1:A:181:ASN:N	2.32	0.43
1:A:136:GLY:O	1:A:137:ASP:C	2.62	0.43
1:A:150:LYS:HE2	1:A:419:ASN:OD1	2.19	0.43
1:A:6:CYS:O	1:A:7:GLY:C	2.60	0.43
1:A:422:PHE:HE1	1:A:427:LYS:O	2.02	0.43
1:A:283:LEU:O	1:A:285:PRO:HD3	2.19	0.43
1:A:478:LYS:HD2	1:A:478:LYS:C	2.43	0.43
1:A:343:PHE:CE1	1:A:518:GLN:HG2	2.53	0.42
1:A:6:CYS:C	1:A:8:ALA:N	2.77	0.42
1:A:186:PHE:O	1:A:188:ASP:N	2.51	0.42
1:A:246:VAL:HA	1:A:247:PRO:HD2	1.81	0.42
1:A:283:LEU:C	1:A:285:PRO:HD3	2.44	0.42
1:A:538:GLU:HG2	10:A:723:HOH:O	2.18	0.42
1:A:169:THR:O	1:A:170:PRO:O	2.37	0.42
1:A:233:LYS:O	1:A:235:SER:N	2.53	0.42
1:A:345:PHE:CZ	1:A:440:ARG:HG3	2.55	0.42
1:A:579:CYS:C	1:A:581:THR:N	2.78	0.42
1:A:110:ASP:OD2	1:A:191:LEU:HD22	2.20	0.42
1:A:154:GLN:NE2	1:A:428:ILE:HD13	2.34	0.42
1:A:235:SER:HA	1:A:236:PRO:HD3	1.93	0.42
1:A:449:TYR:HB2	1:A:490:ILE:O	2.19	0.42
1:A:140:PHE:CZ	1:A:439:GLN:NE2	2.88	0.42
1:A:25:THR:OG1	1:A:27:ASP:OD2	2.23	0.41
1:A:64:ARG:H	1:A:64:ARG:HG3	1.49	0.41
1:A:66:THR:HB	1:A:70:PHE:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:SER:O	1:A:381:PHE:HA	2.19	0.41
1:A:300:LEU:O	1:A:303:PHE:HB3	2.20	0.41
1:A:117:THR:O	1:A:118:GLU:CB	2.69	0.41
1:A:119:LEU:HD21	1:A:169:THR:HG21	2.00	0.41
1:A:121:SER:O	1:A:122:ASN:CB	2.67	0.41
1:A:205:ASN:OD1	3:C:1:NAG:C1	2.67	0.41
1:A:165:PHE:O	1:A:180:ILE:HD11	2.21	0.41
1:A:345:PHE:HZ	1:A:440:ARG:HG3	1.86	0.41
1:A:199:LEU:HG	1:A:203:LEU:HD21	2.02	0.41
1:A:540:GLN:NE2	1:A:590:TRP:NE1	2.68	0.41
1:A:191:LEU:H	1:A:191:LEU:HD23	1.86	0.41
1:A:43:LEU:HD12	1:A:179:GLN:HB2	2.04	0.40
1:A:269:LEU:HD23	1:A:269:LEU:HA	1.91	0.40
1:A:417:LEU:HD21	9:A:708:HEM:CMB	2.50	0.40
1:A:123:GLU:HG2	1:A:125:SER:CB	2.40	0.40
1:A:377:HIS:HA	1:A:380:PHE:CE2	2.56	0.40
1:A:312:TYR:O	1:A:316:VAL:HG23	2.21	0.40
1:A:549:PHE:O	1:A:553:ILE:HG12	2.21	0.40
1:A:461:PRO:CG	1:A:470:VAL:HG21	2.51	0.40
1:A:496:GLY:HA3	1:A:511:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	593/595 (100%)	513 (86%)	55 (9%)	25 (4%)	2 13

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	5	GLY

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Mol	Chain	Res	Type
1	A	121	SER
1	A	167	CYS
1	A	168	PRO
1	A	169	THR
1	A	170	PRO
1	A	175	LEU
1	A	176	ALA
1	A	245	ARG
1	A	6	CYS
1	A	8	ALA
1	A	17	GLU
1	A	118	GLU
1	A	122	ASN
1	A	252	GLY
1	A	3	GLU
1	A	171	PRO
1	A	256	ALA
1	A	580	SER
1	A	56	ALA
1	A	83	VAL
1	A	351	HIS
1	A	234	PRO
1	A	10	VAL
1	A	84	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	518/518 (100%)	470 (91%)	48 (9%)	8 31

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	GLU
1	A	6	CYS

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Mol	Chain	Res	Type
1	A	10	VAL
1	A	11	PRO
1	A	12	LEU
1	A	34	PRO
1	A	64	ARG
1	A	71	ARG
1	A	98	LEU
1	A	108	ASP
1	A	117	THR
1	A	118	GLU
1	A	123	GLU
1	A	124	HIS
1	A	151	LEU
1	A	168	PRO
1	A	171	PRO
1	A	172	TYR
1	A	173	GLN
1	A	174	SER
1	A	175	LEU
1	A	202	ARG
1	A	203	LEU
1	A	216	ASN
1	A	226	TYR
1	A	233	LYS
1	A	234	PRO
1	A	255	ARG
1	A	261	LEU
1	A	290	GLU
1	A	298	LYS
1	A	322	GLN
1	A	333	ASN
1	A	360	ARG
1	A	367	PRO
1	A	376	LEU
1	A	377	HIS
1	A	428	ILE
1	A	464	LEU
1	A	478	LYS
1	A	494	ILE
1	A	520	GLN
1	A	523	ARG
1	A	564	LEU

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Mol	Chain	Res	Type
1	A	570	ASN
1	A	585	LEU
1	A	592	SER
1	A	594	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	109	HIS
1	A	128	GLN
1	A	147	ASN
1	A	216	ASN
1	A	333	ASN
1	A	341	ASN
1	A	377	HIS
1	A	426	HIS
1	A	468	GLN
1	A	497	ASN
1	A	520	GLN
1	A	521	GLN
1	A	545	GLN
1	A	556	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

10 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	B	1	1,2	14,14,15	0.60	0	17,19,21	0.72	0
2	NAG	B	2	2	14,14,15	0.78	0	17,19,21	0.69	0
2	MAN	B	3	2	11,11,12	0.70	0	15,15,17	0.66	0
3	NAG	C	1	3,1	14,14,15	0.59	0	17,19,21	0.79	1 (5%)
3	NAG	C	2	3	14,14,15	0.71	0	17,19,21	0.87	1 (5%)
2	NAG	D	1	1,2	14,14,15	0.54	0	17,19,21	0.87	1 (5%)
2	NAG	D	2	2	14,14,15	0.73	0	17,19,21	0.85	1 (5%)
2	MAN	D	3	2	11,11,12	0.90	1 (9%)	15,15,17	0.37	0
4	NAG	E	1	1,4	14,14,15	0.62	0	17,19,21	0.77	0
4	NDG	E	2	4	14,14,15	0.67	0	17,19,21	1.63	3 (17%)

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	B	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	MAN	B	3	2	-	1/2/19/22	1/1/1/1
3	NAG	C	1	3,1	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
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	MAN	D	3	2	-	0/2/19/22	0/1/1/1
4	NAG	E	1	1,4	-	2/6/23/26	0/1/1/1
4	NDG	E	2	4	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	3	MAN	C2-C3	2.00	1.55	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	E	2	NDG	C4-C3-C2	4.59	117.75	111.02
4	E	2	NDG	C3-C4-C5	3.76	117.05	110.23
2	D	2	NAG	C1-O5-C5	2.27	115.23	112.19
3	C	1	NAG	C2-N2-C7	-2.22	119.93	122.90
4	E	2	NDG	C2-N2-C7	-2.16	120.00	122.90
2	D	1	NAG	C2-N2-C7	-2.11	120.08	122.90
3	C	2	NAG	C2-N2-C7	-2.03	120.18	122.90

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

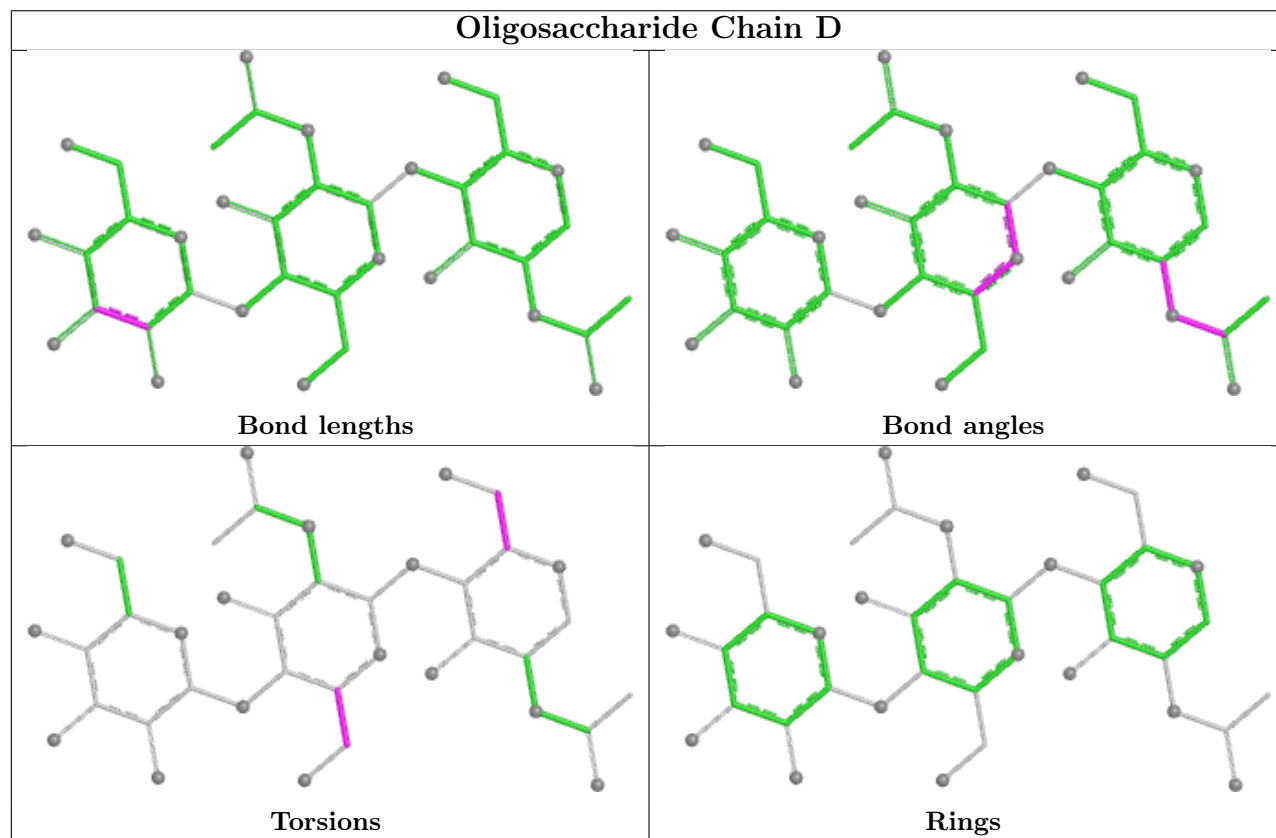
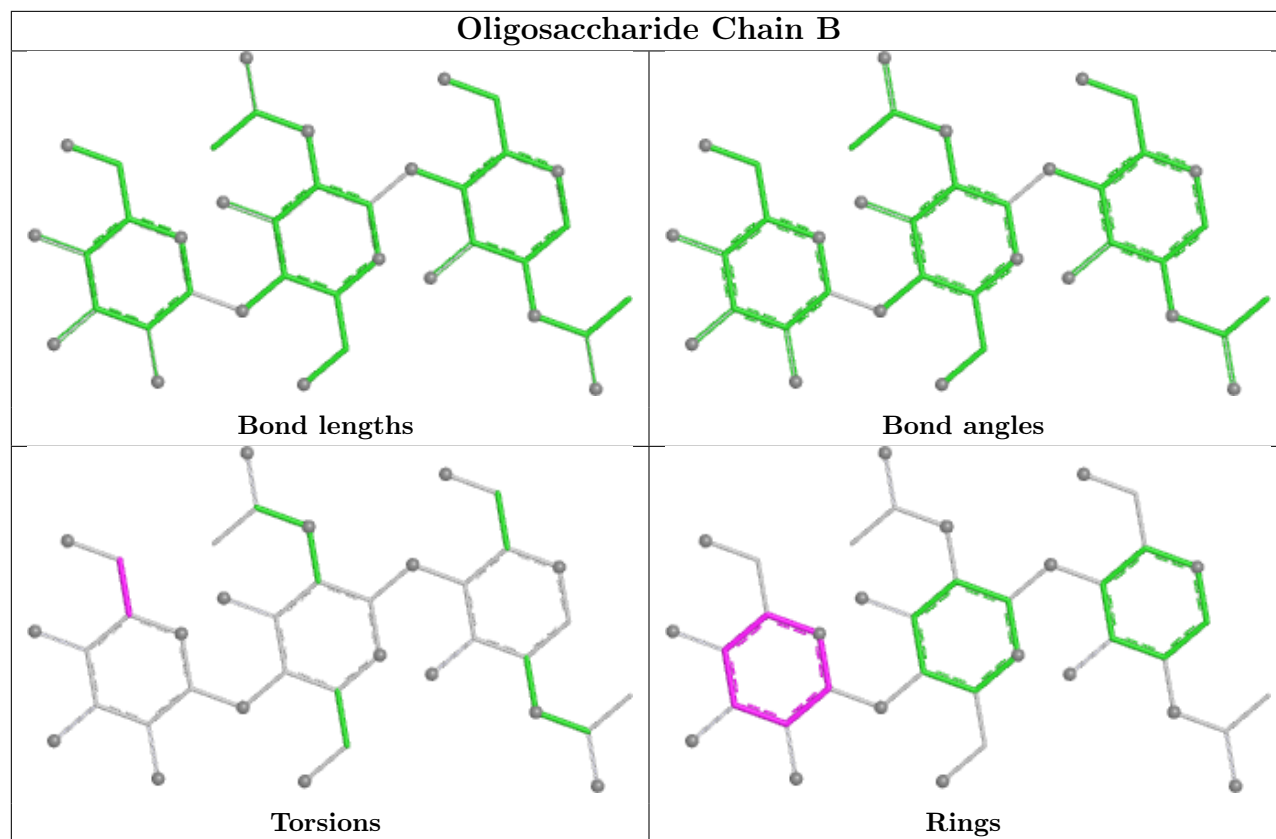
All (1) ring outliers are listed below:

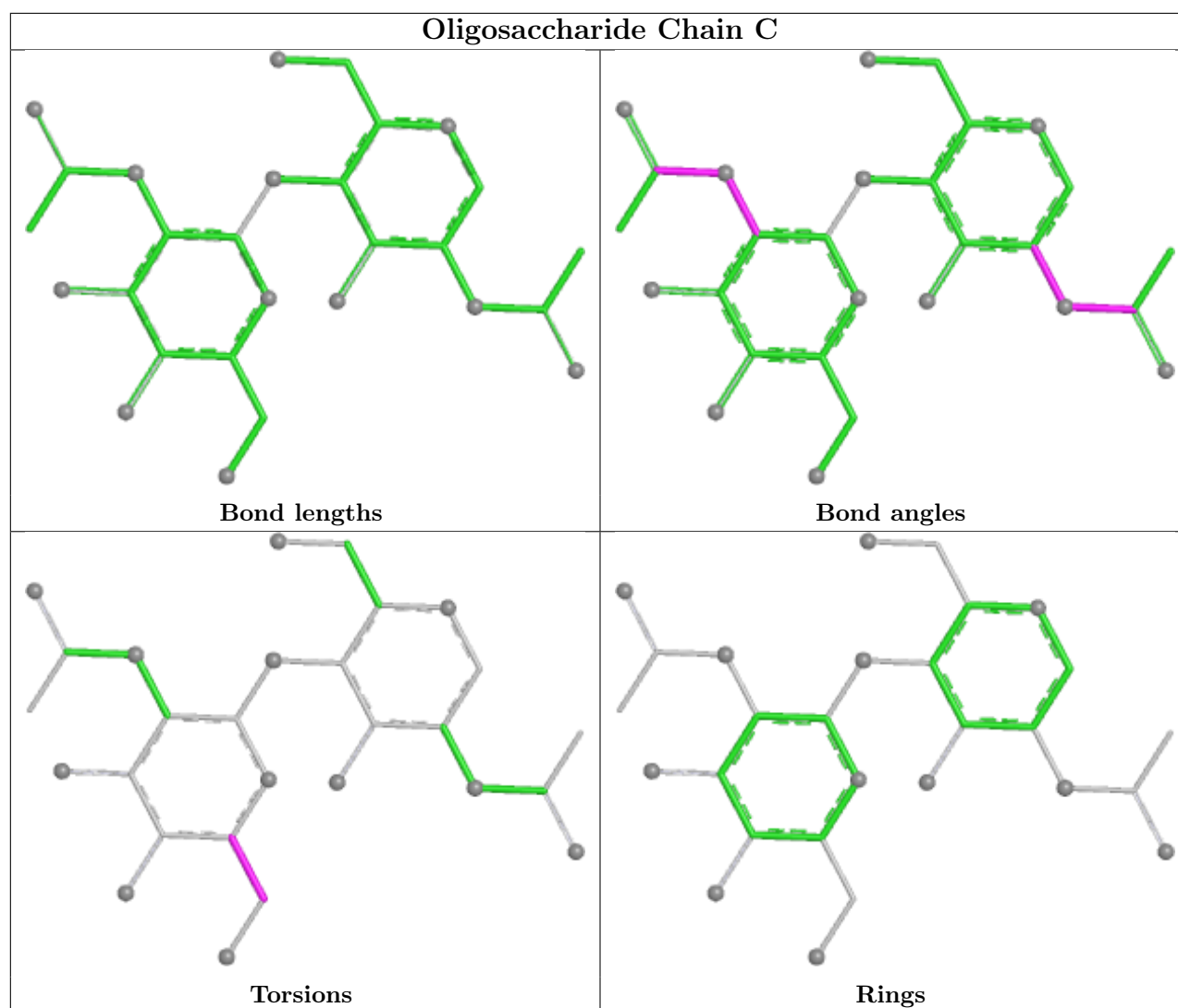
Mol	Chain	Res	Type	Atoms
2	B	3	MAN	C1-C2-C3-C4-C5-O5

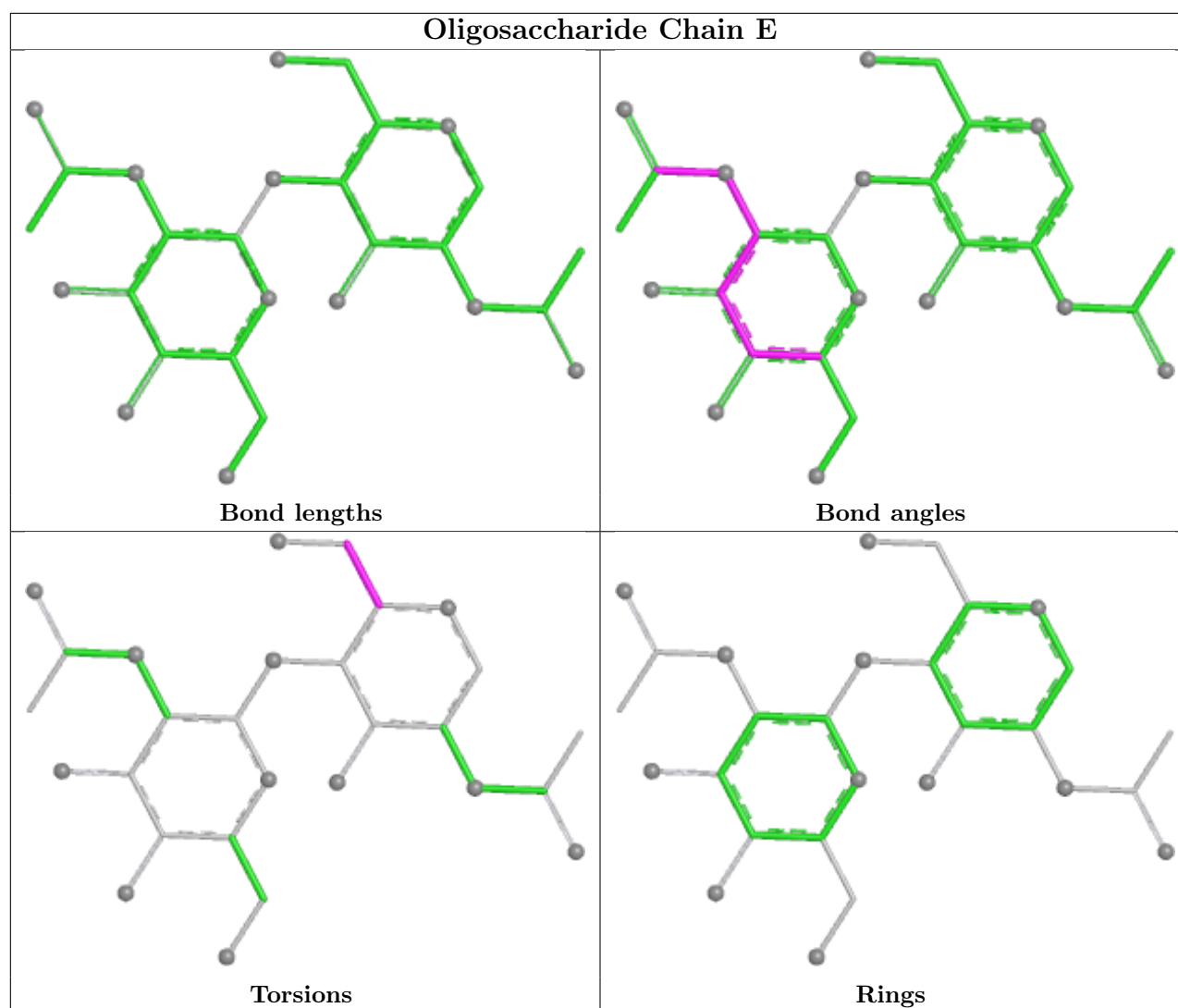
4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	1	0
3	C	1	NAG	3	0
2	D	1	NAG	1	0
4	E	1	NAG	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 oligosaccharide.







5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 7 are monoatomic - leaving 3 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
7	CO3	A	688	-	3,3,3	0.72	0	2,3,3	0.14	0
9	HEM	A	708	1,10	50,50,50	2.54	18 (36%)	67,82,82	1.67	9 (13%)
6	SCN	A	702	-	1,2,2	4.33	1 (100%)	0,1,1	-	-

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
9	HEM	A	708	1,10	-	5/14/54/54	-

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	708	HEM	FE-NA	7.61	2.20	1.95
9	A	708	HEM	C3D-C2D	6.12	1.50	1.36
9	A	708	HEM	CHA-C1A	-5.53	1.27	1.39
9	A	708	HEM	CMC-C2C	4.77	1.60	1.50
6	A	702	SCN	C-N	4.33	1.30	1.15
9	A	708	HEM	CAC-C3C	4.31	1.58	1.47
9	A	708	HEM	CAD-C3D	3.72	1.60	1.51
9	A	708	HEM	C4D-ND	-3.64	1.33	1.40
9	A	708	HEM	FE-ND	3.43	2.05	1.94
9	A	708	HEM	C4D-C3D	3.39	1.50	1.45
9	A	708	HEM	FE-NB	3.09	2.04	1.94
9	A	708	HEM	O1A-CGA	2.89	1.31	1.22
9	A	708	HEM	CAB-C3B	2.88	1.55	1.47
9	A	708	HEM	C1A-NA	-2.80	1.34	1.39
9	A	708	HEM	CHC-C4B	-2.75	1.32	1.39
9	A	708	HEM	C4B-NB	-2.59	1.33	1.38
9	A	708	HEM	CHA-C4D	-2.37	1.33	1.38
9	A	708	HEM	C2A-C3A	-2.28	1.33	1.38
9	A	708	HEM	C1B-NB	-2.16	1.36	1.40

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	A	708	HEM	CAD-C3D-C4D	6.45	135.94	124.70
9	A	708	HEM	CMD-C2D-C1D	5.16	133.10	125.03
9	A	708	HEM	C2A-C1A-NA	3.76	114.33	110.15
9	A	708	HEM	CAD-C3D-C2D	-3.57	121.17	127.87
9	A	708	HEM	C4D-C3D-C2D	-2.75	102.89	106.89
9	A	708	HEM	CHD-C1D-C2D	-2.70	120.76	125.03
9	A	708	HEM	C2D-C1D-ND	2.48	112.77	109.90
9	A	708	HEM	C3D-C4D-ND	2.05	112.42	110.17
9	A	708	HEM	CMC-C2C-C1C	2.05	128.34	124.73

There are no chirality outliers.

All (5) torsion outliers are listed below:

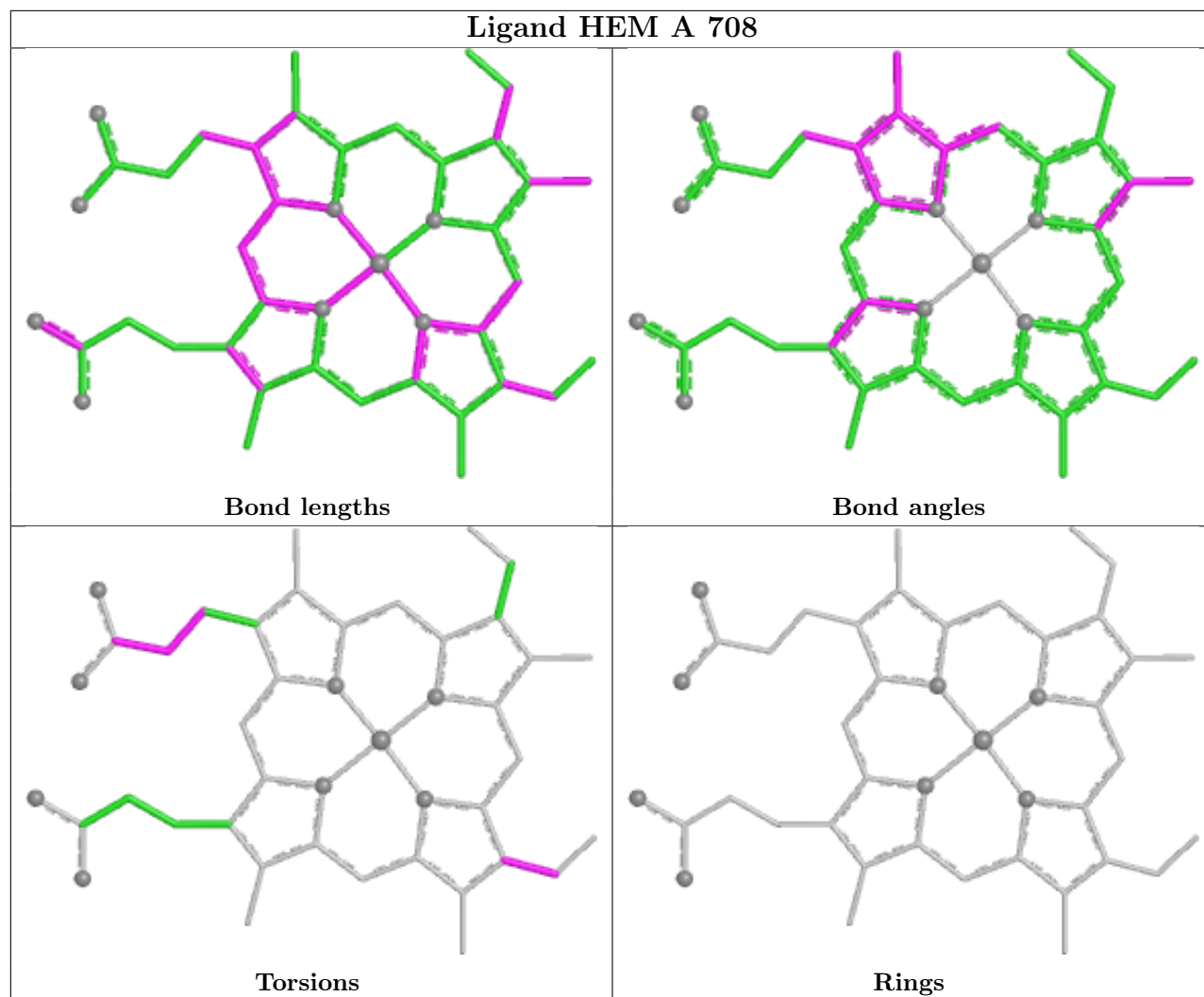
Mol	Chain	Res	Type	Atoms
9	A	708	HEM	C3D-CAD-CBD-CGD
9	A	708	HEM	CAD-CBD-CGD-O1D
9	A	708	HEM	CAD-CBD-CGD-O2D
9	A	708	HEM	C4B-C3B-CAB-CBB
9	A	708	HEM	C2B-C3B-CAB-CBB

There are no ring outliers.

1 monomer is involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
9	A	708	HEM	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 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.



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.