



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 11:24 AM UTC

PDB ID : 1PGF / pdb_00001pgf
Title : PROSTAGLANDIN H2 SYNTHASE-1 COMPLEXED WITH 1-(4-IODOBE NZOYL)-5-METHOXY-2-METHYLINDOLE-3-ACETIC ACID (IODOIN- DOMETHACIN), CIS MODEL
Authors : Loll, P.J.; Picot, D.; Garavito, R.M.
Deposited on : 1995-12-02
Resolution : 4.50 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)
Xtrriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

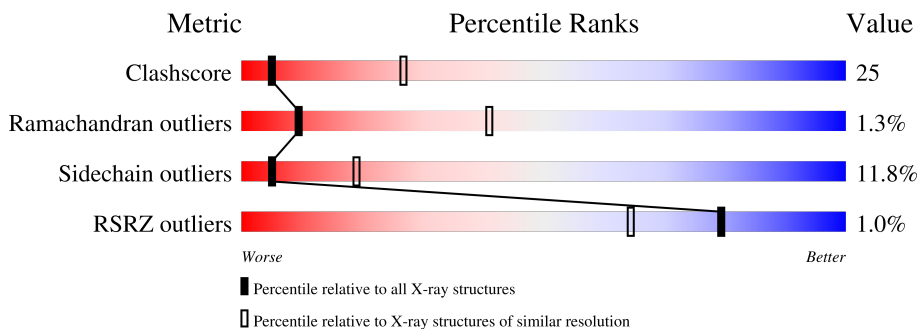
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.50 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	1002 (5.06-3.94)
Ramachandran outliers	187476	1060 (5.10-3.90)
Sidechain outliers	187428	1043 (5.10-3.90)
RSRZ outliers	180081	1122 (5.10-3.90)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	576	 2% 50% 35% 9% . .
1	B	576	 50% 36% 9% . .
2	C	2	 50% 50%
2	D	2	 50% 50%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	IMM	A	800	-	-	X	-
5	IMM	B	800	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 9202 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 PROSTAGLANDIN H2 SYNTHASE-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	551	4477	2903	758	788	28	0	0	0
1	B	551	4477	2903	758	788	28	0	0	0

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



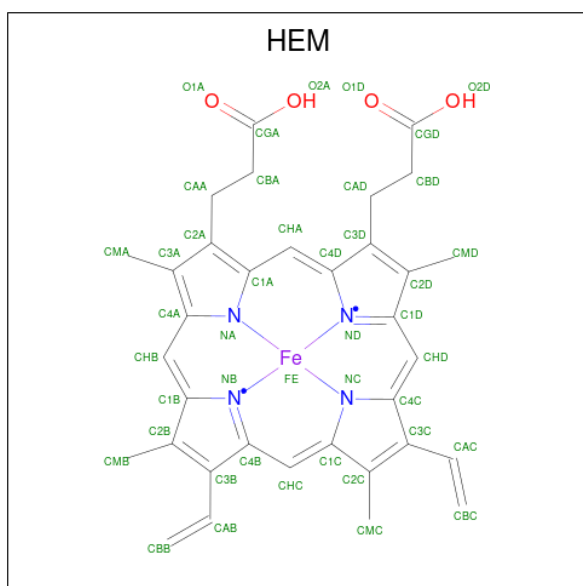
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	C	2	28	16	2	10	0	0	0
2	D	2	28	16	2	10	0	0	0

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).



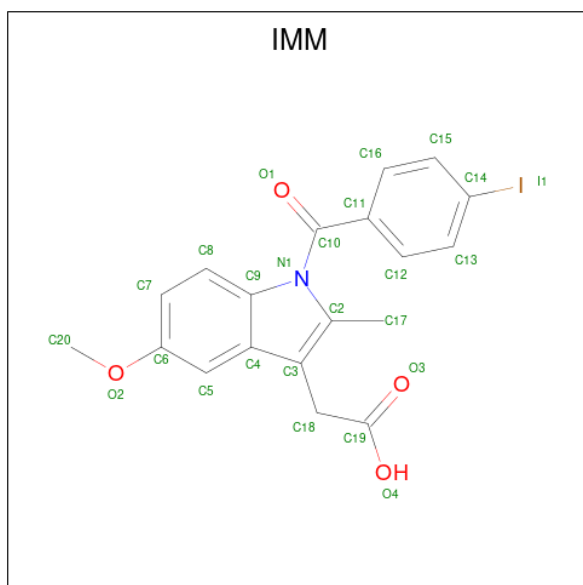
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

- Molecule 5 is 1-(4-iodobenzoyl)-5-methoxy-2-methyl indole-3-acetic acid (CCD ID: IMM) (formula: C₁₉H₁₆INO₄).

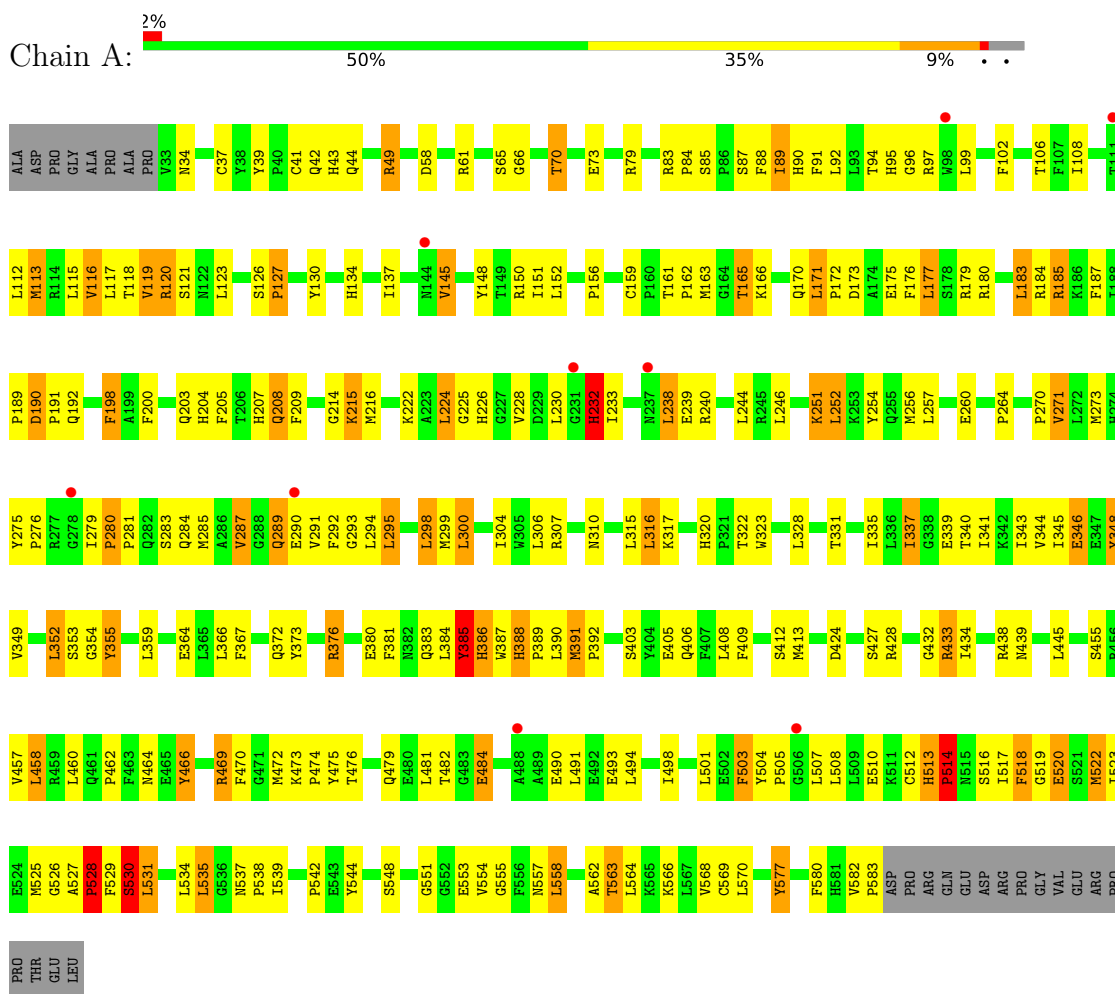


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
5	A	1	Total	C	I	N	O	0	0
			25	19	1	1	4		
5	B	1	Total	C	I	N	O	0	0
			25	19	1	1	4		

3 Residue-property plots

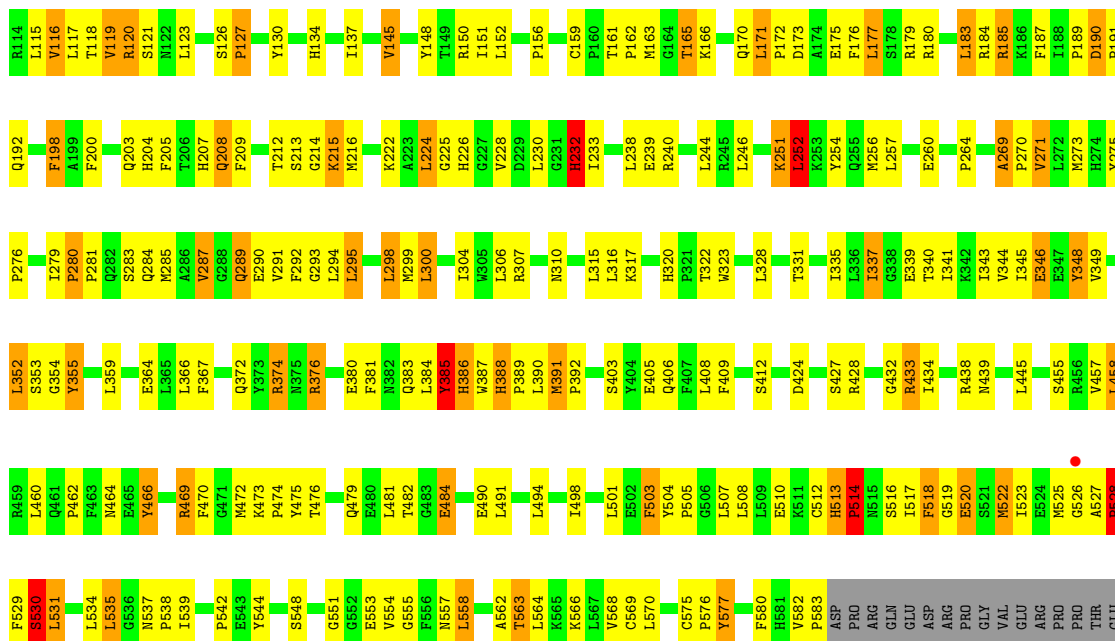
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

• Molecule 1: PROSTAGLANDIN H2 SYNTHASE-1



• Molecule 1: PROSTAGLANDIN H2 SYNTHASE-1





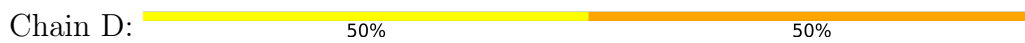
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- Molecule 2: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



MAG1
MAG2

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



MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	99.22Å 208.99Å 232.43Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 4.50 8.00 – 4.50	Depositor EDS
% Data completeness (in resolution range)	79.2 (8.00-4.50) 62.4 (8.00-4.50)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.54 (at 4.46Å)	Xtrriage
Refinement program	X-PLOR 3.1	Depositor
R, R_{free}	0.254 , 0.267 0.224 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	80.6	Xtrriage
Anisotropy	0.740	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.18 , 26.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	9202	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.16% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality i

5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: IMM, HEM, NAG

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	0.85	4/4615 (0.1%)	1.23	46/6264 (0.7%)
1	B	0.85	4/4615 (0.1%)	1.23	49/6264 (0.8%)
All	All	0.85	8/9230 (0.1%)	1.23	95/12528 (0.8%)

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	A	0	2
1	B	0	2
All	All	0	4

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	89	ILE	CA-CB	-6.50	1.46	1.54
1	B	89	ILE	CA-CB	-6.46	1.46	1.54
1	A	119	VAL	CA-CB	-5.64	1.47	1.54
1	B	119	VAL	CA-CB	-5.63	1.47	1.54
1	B	522	MET	SD-CE	-5.22	1.66	1.79
1	A	522	MET	SD-CE	-5.21	1.66	1.79
1	A	457	VAL	CA-CB	-5.05	1.48	1.54
1	B	457	VAL	CA-CB	-5.04	1.48	1.54

All (95) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	148	TYR	N-CA-C	-9.47	95.27	110.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	148	TYR	N-CA-C	-9.45	95.29	110.32
1	B	224	LEU	N-CA-C	-9.31	96.22	110.10
1	A	224	LEU	N-CA-C	-9.31	96.23	110.10
1	B	525	MET	N-CA-C	-8.15	103.16	113.43
1	A	525	MET	N-CA-C	-8.14	103.17	113.43
1	B	408	LEU	N-CA-C	8.08	128.01	110.80
1	A	408	LEU	N-CA-C	8.05	127.95	110.80
1	B	519	GLY	N-CA-C	7.81	122.50	111.10
1	A	484	GLU	N-CA-C	7.78	118.81	108.07
1	B	484	GLU	N-CA-C	7.78	118.81	108.07
1	A	519	GLY	N-CA-C	7.78	122.46	111.10
1	A	513	HIS	CA-C-N	7.37	129.06	119.84
1	A	513	HIS	C-N-CA	7.37	129.06	119.84
1	B	513	HIS	CA-C-N	7.35	129.03	119.84
1	B	513	HIS	C-N-CA	7.35	129.03	119.84
1	B	569	CYS	N-CA-C	7.32	120.13	111.71
1	A	569	CYS	N-CA-C	7.31	120.12	111.71
1	B	121	SER	N-CA-C	7.30	120.28	111.82
1	A	121	SER	N-CA-C	7.28	120.26	111.82
1	B	558	LEU	N-CA-C	-7.06	102.64	111.11
1	A	558	LEU	N-CA-C	-7.03	102.68	111.11
1	B	491	LEU	N-CA-C	-6.91	103.75	111.28
1	A	491	LEU	N-CA-C	-6.88	103.78	111.28
1	A	482	THR	N-CA-C	-6.59	101.21	110.50
1	B	482	THR	N-CA-C	-6.58	101.22	110.50
1	A	577	TYR	N-CA-C	-6.39	100.19	109.59
1	B	577	TYR	N-CA-C	-6.39	100.20	109.59
1	B	530	SER	N-CA-C	5.95	120.15	113.01
1	B	190	ASP	CA-C-N	5.94	126.36	119.47
1	B	190	ASP	C-N-CA	5.94	126.36	119.47
1	B	412	SER	N-CA-C	5.94	120.81	113.50
1	A	530	SER	N-CA-C	5.94	120.14	113.01
1	A	190	ASP	CA-C-N	5.93	126.35	119.47
1	A	190	ASP	C-N-CA	5.93	126.35	119.47
1	B	355	TYR	N-CA-C	5.91	118.39	110.35
1	A	355	TYR	N-CA-C	5.89	118.37	110.35
1	A	412	SER	N-CA-C	5.88	120.74	113.50
1	A	41	CYS	N-CA-C	5.86	118.21	109.59
1	A	225	GLY	N-CA-C	-5.84	99.33	113.18
1	B	41	CYS	N-CA-C	5.84	118.18	109.59
1	B	225	GLY	N-CA-C	-5.84	99.35	113.18
1	B	287	VAL	N-CA-C	5.75	121.30	109.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	287	VAL	N-CA-C	5.74	121.29	109.34
1	A	127	PRO	CA-C-N	5.73	127.00	119.84
1	A	127	PRO	C-N-CA	5.73	127.00	119.84
1	B	127	PRO	CA-C-N	5.71	126.98	119.84
1	B	127	PRO	C-N-CA	5.71	126.98	119.84
1	A	161	THR	CA-C-N	5.59	125.96	119.47
1	A	161	THR	C-N-CA	5.59	125.96	119.47
1	A	208	GLN	N-CA-C	-5.58	106.63	113.50
1	B	208	GLN	N-CA-C	-5.58	106.64	113.50
1	B	161	THR	CA-C-N	5.55	125.91	119.47
1	B	161	THR	C-N-CA	5.55	125.91	119.47
1	B	328	LEU	N-CA-C	-5.51	105.17	111.07
1	A	328	LEU	N-CA-C	-5.50	105.18	111.07
1	A	66	GLY	CA-C-N	5.46	125.81	119.47
1	A	66	GLY	C-N-CA	5.46	125.81	119.47
1	B	66	GLY	CA-C-N	5.46	125.81	119.47
1	B	66	GLY	C-N-CA	5.46	125.81	119.47
1	A	498	ILE	N-CA-C	-5.44	104.29	111.09
1	B	498	ILE	N-CA-C	-5.43	104.30	111.09
1	A	300	LEU	N-CA-C	-5.41	104.80	111.40
1	B	300	LEU	N-CA-C	-5.40	104.81	111.40
1	B	513	HIS	N-CA-C	-5.40	102.36	110.24
1	A	513	HIS	N-CA-C	-5.40	102.36	110.24
1	B	177	LEU	N-CA-C	-5.36	105.44	111.28
1	A	337	ILE	N-CA-C	-5.35	105.16	110.62
1	B	337	ILE	N-CA-C	-5.34	105.17	110.62
1	A	177	LEU	N-CA-C	-5.33	105.47	111.28
1	A	252	LEU	N-CA-C	-5.29	101.08	109.76
1	B	252	LEU	N-CA-C	-5.28	101.10	109.76
1	B	280	PRO	CA-C-N	5.27	125.33	119.32
1	B	280	PRO	C-N-CA	5.27	125.33	119.32
1	A	280	PRO	CA-C-N	5.26	125.32	119.32
1	A	280	PRO	C-N-CA	5.26	125.32	119.32
1	B	346	GLU	N-CA-C	5.25	119.31	113.01
1	B	385	TYR	N-CA-C	5.25	118.94	112.54
1	A	385	TYR	N-CA-C	5.25	118.94	112.54
1	A	346	GLU	N-CA-C	5.24	119.30	113.01
1	B	388	HIS	CE1-NE2-CD2	-5.24	103.76	109.00
1	A	388	HIS	CE1-NE2-CD2	-5.22	103.78	109.00
1	B	391	MET	CA-C-N	5.13	126.25	119.84
1	B	391	MET	C-N-CA	5.13	126.25	119.84
1	A	580	PHE	N-CA-C	-5.12	107.04	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	391	MET	CA-C-N	5.11	126.22	119.84
1	A	391	MET	C-N-CA	5.11	126.22	119.84
1	B	580	PHE	N-CA-C	-5.10	107.06	113.28
1	A	232	HIS	N-CA-C	-5.05	107.07	113.18
1	A	73	GLU	N-CA-C	-5.05	102.04	110.17
1	B	73	GLU	N-CA-C	-5.04	102.05	110.17
1	B	232	HIS	N-CA-C	-5.03	107.09	113.18
1	B	212	THR	N-CA-C	5.01	117.57	110.10
1	B	269	ALA	CA-C-N	5.00	126.09	119.84
1	B	269	ALA	C-N-CA	5.00	126.09	119.84

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	39	TYR	Sidechain
1	A	466	TYR	Sidechain
1	B	39	TYR	Sidechain
1	B	466	TYR	Sidechain

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	4477	0	4383	229	0
1	B	4477	0	4383	229	0
2	C	28	0	25	1	0
2	D	28	0	25	1	0
3	A	28	0	26	0	0
3	B	28	0	26	0	0
4	A	43	0	30	6	0
4	B	43	0	30	6	0
5	A	25	0	15	15	0
5	B	25	0	15	17	0
All	All	9202	0	8958	452	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 25.

All (452) 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:391:MET:HG3	4:A:601:HEM:HAB	1.41	1.00
1:B:391:MET:HG3	4:B:601:HEM:HAB	1.41	0.99
1:B:387:TRP:HE1	1:B:522:MET:HE3	1.26	0.98
1:A:387:TRP:HE1	1:A:522:MET:HE3	1.26	0.98
1:A:384:LEU:HD21	1:A:526:GLY:HA2	1.46	0.97
1:B:91:PHE:HD1	1:B:92:LEU:HD12	1.34	0.93
1:A:152:LEU:HD21	1:A:469:ARG:HG2	1.49	0.92
1:B:384:LEU:HD21	1:B:526:GLY:HA2	1.46	0.92
1:B:530:SER:HB3	5:B:800:IMM:H173	1.52	0.92
1:A:530:SER:HB3	5:A:800:IMM:H173	1.52	0.91
1:B:152:LEU:HD21	1:B:469:ARG:HG2	1.49	0.91
1:A:91:PHE:HD1	1:A:92:LEU:HD12	1.34	0.90
1:A:518:PHE:CD2	1:A:522:MET:HG2	2.07	0.90
1:A:531:LEU:HG	5:A:800:IMM:H181	1.55	0.89
1:B:531:LEU:HG	5:B:800:IMM:H181	1.55	0.88
1:B:518:PHE:CD2	1:B:522:MET:HG2	2.07	0.88
5:A:800:IMM:O3	5:A:800:IMM:H5	1.75	0.87
5:B:800:IMM:O3	5:B:800:IMM:H5	1.75	0.85
1:B:172:PRO:HB2	1:B:177:LEU:HD22	1.60	0.84
1:A:120:ARG:HH12	5:A:800:IMM:H203	1.42	0.83
1:A:380:GLU:HG2	1:A:466:TYR:CE2	2.14	0.83
1:A:172:PRO:HB2	1:A:177:LEU:HD22	1.60	0.83
1:B:120:ARG:HH12	5:B:800:IMM:H203	1.41	0.83
1:B:380:GLU:HG2	1:B:466:TYR:CE2	2.14	0.81
1:B:386:HIS:HD2	1:B:388:HIS:HE1	1.30	0.79
1:A:344:VAL:O	1:A:348:TYR:HB3	1.84	0.78
1:A:563:THR:HG22	1:A:566:LYS:H	1.50	0.77
1:B:88:PHE:O	1:B:92:LEU:HD13	1.85	0.77
1:A:386:HIS:HD2	1:A:388:HIS:HE1	1.30	0.77
1:B:563:THR:HG22	1:B:566:LYS:H	1.50	0.77
1:B:344:VAL:O	1:B:348:TYR:HB3	1.84	0.76
1:A:88:PHE:O	1:A:92:LEU:HD13	1.85	0.75
1:B:387:TRP:NE1	1:B:522:MET:HE3	1.99	0.75
1:B:294:LEU:HD22	1:B:409:PHE:CD1	2.22	0.75
1:A:387:TRP:NE1	1:A:522:MET:HE3	1.99	0.75
1:A:294:LEU:HD22	1:A:409:PHE:CD1	2.22	0.75
1:A:384:LEU:HD21	1:A:526:GLY:CA	2.16	0.75
1:B:384:LEU:HD21	1:B:526:GLY:CA	2.16	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:352:LEU:HD11	1:B:387:TRP:CH2	2.22	0.74
1:A:91:PHE:CD1	1:A:92:LEU:HD12	2.22	0.74
1:B:91:PHE:CD1	1:B:92:LEU:HD12	2.22	0.73
1:A:352:LEU:HD11	1:A:387:TRP:CH2	2.22	0.73
1:A:355:TYR:CE2	5:A:800:IMM:H201	2.24	0.73
1:B:151:ILE:HD11	1:B:529:PHE:HE1	1.53	0.73
1:B:355:TYR:CE2	5:B:800:IMM:H201	2.24	0.72
1:A:294:LEU:HD22	1:A:409:PHE:HD1	1.54	0.72
1:A:346:GLU:HG2	1:A:359:LEU:O	1.90	0.71
1:B:294:LEU:HD22	1:B:409:PHE:HD1	1.54	0.71
1:A:151:ILE:HD11	1:A:529:PHE:HE1	1.53	0.71
1:B:346:GLU:HG2	1:B:359:LEU:O	1.90	0.71
1:A:151:ILE:HG13	1:A:529:PHE:CZ	2.26	0.71
1:B:151:ILE:HG13	1:B:529:PHE:CZ	2.26	0.70
1:B:294:LEU:O	1:B:295:LEU:HG	1.91	0.70
1:A:364:GLU:HG2	1:A:367:PHE:CE2	2.26	0.70
1:B:364:GLU:HG2	1:B:367:PHE:CE2	2.26	0.70
1:A:294:LEU:O	1:A:295:LEU:HG	1.91	0.69
1:B:355:TYR:CZ	5:B:800:IMM:H201	2.28	0.69
1:A:355:TYR:CZ	5:A:800:IMM:H201	2.28	0.69
1:B:108:ILE:O	1:B:112:LEU:HG	1.93	0.69
1:A:108:ILE:O	1:A:112:LEU:HG	1.93	0.68
1:B:503:PHE:CE2	1:B:507:LEU:HD11	2.28	0.68
1:B:126:SER:HA	1:B:127:PRO:C	2.17	0.68
1:B:273:MET:HE2	1:B:285:MET:O	1.94	0.68
1:A:151:ILE:HG13	1:A:529:PHE:HZ	1.59	0.68
1:A:503:PHE:CE2	1:A:507:LEU:HD11	2.28	0.68
1:B:151:ILE:HG13	1:B:529:PHE:HZ	1.59	0.68
1:A:126:SER:HA	1:A:127:PRO:C	2.17	0.68
1:A:273:MET:HE2	1:A:285:MET:O	1.94	0.67
1:B:337:ILE:O	1:B:341:ILE:HG13	1.94	0.67
1:A:79:ARG:O	1:A:83:ARG:HG3	1.94	0.67
1:A:337:ILE:O	1:A:341:ILE:HG13	1.94	0.67
1:B:123:LEU:O	1:B:469:ARG:NH2	2.28	0.67
1:B:79:ARG:O	1:B:83:ARG:HG3	1.94	0.66
1:A:123:LEU:O	1:A:469:ARG:NH2	2.28	0.66
1:B:187:PHE:HE1	1:B:189:PRO:HB3	1.60	0.66
1:B:380:GLU:HG2	1:B:466:TYR:HE2	1.58	0.66
1:A:187:PHE:HE1	1:A:189:PRO:HB3	1.60	0.66
1:A:120:ARG:NH1	5:A:800:IMM:H203	2.10	0.65
1:A:341:ILE:HD12	1:A:539:ILE:HD11	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:GLU:HG2	1:A:466:TYR:HE2	1.57	0.65
1:B:120:ARG:NH1	5:B:800:IMM:H203	2.10	0.65
1:A:290:GLU:CD	1:A:290:GLU:H	2.06	0.64
1:A:386:HIS:HD2	1:A:388:HIS:CE1	2.15	0.64
1:B:341:ILE:HD12	1:B:539:ILE:HD11	1.79	0.63
1:B:386:HIS:HD2	1:B:388:HIS:CE1	2.15	0.63
1:A:198:PHE:HZ	1:A:352:LEU:HD21	1.65	0.62
1:B:290:GLU:H	1:B:290:GLU:CD	2.06	0.62
1:A:34:ASN:HB3	1:A:37:CYS:SG	2.39	0.62
1:A:84:PRO:CG	1:A:89:ILE:HD11	2.30	0.62
1:A:88:PHE:CE2	1:A:92:LEU:HD21	2.35	0.62
1:B:34:ASN:HB3	1:B:37:CYS:SG	2.39	0.62
1:B:553:GLU:HG3	1:B:557:ASN:HD21	1.65	0.62
1:B:518:PHE:CE2	1:B:522:MET:HG2	2.34	0.62
1:B:84:PRO:CG	1:B:89:ILE:HD11	2.30	0.62
1:B:208:GLN:NE2	1:B:230:LEU:H	1.98	0.62
1:A:528:PRO:O	1:A:529:PHE:C	2.43	0.62
1:B:306:LEU:C	1:B:306:LEU:HD23	2.25	0.61
1:B:88:PHE:CE2	1:B:92:LEU:HD21	2.35	0.61
1:A:306:LEU:HD23	1:A:306:LEU:C	2.25	0.61
1:A:518:PHE:CE2	1:A:522:MET:HG2	2.34	0.61
1:B:150:ARG:HD3	1:B:152:LEU:O	2.00	0.61
1:B:528:PRO:O	1:B:529:PHE:C	2.43	0.61
1:A:553:GLU:HG3	1:A:557:ASN:HD21	1.65	0.61
1:A:150:ARG:HD3	1:A:152:LEU:O	2.00	0.60
1:A:513:HIS:CE1	1:A:520:GLU:H	2.19	0.60
1:B:198:PHE:HZ	1:B:352:LEU:HD21	1.64	0.60
1:A:208:GLN:NE2	1:A:230:LEU:H	1.98	0.60
5:A:800:IMM:H5	5:A:800:IMM:C19	2.31	0.60
1:B:384:LEU:CD2	1:B:526:GLY:HA2	2.25	0.60
5:B:800:IMM:H5	5:B:800:IMM:C19	2.31	0.60
1:A:49:ARG:O	1:B:320:HIS:HD2	1.85	0.60
1:B:513:HIS:CE1	1:B:520:GLU:H	2.19	0.60
1:A:384:LEU:HD12	1:A:507:LEU:HD13	1.84	0.59
1:A:384:LEU:CD2	1:A:526:GLY:HA2	2.25	0.59
1:B:384:LEU:HD12	1:B:507:LEU:HD13	1.84	0.59
1:B:504:TYR:CZ	1:B:508:LEU:HD11	2.38	0.59
1:B:145:VAL:HG12	1:B:224:LEU:HD22	1.85	0.58
1:A:84:PRO:HG2	1:A:89:ILE:HD11	1.86	0.58
1:A:504:TYR:CZ	1:A:508:LEU:HD11	2.38	0.58
1:A:320:HIS:HD2	1:B:49:ARG:O	1.87	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:226:HIS:CE1	1:A:376:ARG:HD2	2.39	0.58
1:A:145:VAL:HG12	1:A:224:LEU:HD22	1.85	0.57
1:A:185:ARG:HH21	1:A:438:ARG:HG2	1.69	0.57
1:B:203:GLN:HA	4:B:601:HEM:HBC2	1.86	0.57
1:B:226:HIS:CE1	1:B:376:ARG:HD2	2.39	0.57
1:B:84:PRO:HG2	1:B:89:ILE:HD11	1.86	0.57
1:A:203:GLN:HA	4:A:601:HEM:HBC2	1.87	0.57
1:B:424:ASP:O	1:B:428:ARG:HG3	2.05	0.57
1:B:522:MET:O	1:B:526:GLY:HA3	2.05	0.57
1:A:424:ASP:O	1:A:428:ARG:HG3	2.05	0.56
1:B:504:TYR:HB3	1:B:505:PRO:HD3	1.87	0.56
1:B:185:ARG:HH21	1:B:438:ARG:HG2	1.69	0.56
1:A:348:TYR:C	1:A:348:TYR:CD1	2.83	0.56
1:A:88:PHE:O	1:A:91:PHE:HB3	2.05	0.56
1:B:102:PHE:O	1:B:106:THR:HG23	2.06	0.56
1:A:522:MET:O	1:A:526:GLY:HA3	2.05	0.56
1:B:203:GLN:HG2	1:B:298:LEU:HD11	1.88	0.56
1:A:102:PHE:O	1:A:106:THR:HG23	2.06	0.56
1:A:293:GLY:HA2	1:A:299:MET:HE3	1.88	0.56
1:B:173:ASP:OD2	1:B:175:GLU:HB3	2.06	0.56
1:B:198:PHE:CD1	1:B:198:PHE:C	2.84	0.56
1:A:504:TYR:HB3	1:A:505:PRO:HD3	1.87	0.55
1:A:289:GLN:HG3	1:A:292:PHE:CZ	2.42	0.55
1:B:88:PHE:O	1:B:91:PHE:HB3	2.05	0.55
1:B:293:GLY:HA2	1:B:299:MET:HE3	1.88	0.55
1:A:156:PRO:HB2	1:A:159:CYS:SG	2.47	0.55
1:A:173:ASP:OD2	1:A:175:GLU:HB3	2.06	0.55
1:A:352:LEU:HD13	1:A:518:PHE:HZ	1.72	0.55
1:A:79:ARG:HH11	1:A:83:ARG:HH21	1.55	0.55
1:A:345:ILE:HG12	1:A:534:LEU:HD23	1.88	0.55
1:A:349:VAL:HG12	1:A:349:VAL:O	2.06	0.55
1:A:531:LEU:HG	5:A:800:IMM:C18	2.34	0.55
1:B:176:PHE:HE2	1:B:494:LEU:HD11	1.72	0.55
1:A:198:PHE:CD1	1:A:198:PHE:C	2.84	0.55
1:A:391:MET:CG	4:A:601:HEM:HAB	2.28	0.55
1:B:289:GLN:HG3	1:B:292:PHE:CZ	2.42	0.55
1:A:120:ARG:HD3	5:A:800:IMM:H182	1.88	0.54
1:B:348:TYR:CD1	1:B:348:TYR:C	2.83	0.54
1:B:349:VAL:HG12	1:B:349:VAL:O	2.06	0.54
1:B:353:SER:OG	1:B:354:GLY:N	2.40	0.54
1:A:176:PHE:HE2	1:A:494:LEU:HD11	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:348:TYR:C	1:B:348:TYR:HD1	2.16	0.54
1:B:352:LEU:HD11	1:B:387:TRP:HH2	1.72	0.54
1:A:180:ARG:NH1	1:A:490:GLU:OE1	2.40	0.54
1:B:79:ARG:HH11	1:B:83:ARG:HH21	1.54	0.54
1:B:156:PRO:HB2	1:B:159:CYS:SG	2.47	0.54
1:B:345:ILE:HG12	1:B:534:LEU:HD23	1.88	0.54
1:A:203:GLN:HG2	1:A:298:LEU:HD11	1.88	0.54
1:A:348:TYR:C	1:A:348:TYR:HD1	2.16	0.54
1:B:120:ARG:HD3	5:B:800:IMM:H182	1.88	0.54
1:B:180:ARG:NH1	1:B:490:GLU:OE1	2.40	0.54
1:A:353:SER:OG	1:A:354:GLY:N	2.40	0.54
1:B:352:LEU:HD13	1:B:518:PHE:HZ	1.72	0.54
1:A:215:LYS:H	1:A:215:LYS:CD	2.21	0.53
1:B:531:LEU:HG	5:B:800:IMM:C18	2.34	0.53
1:B:554:VAL:HG23	1:B:555:GLY:N	2.23	0.53
5:A:800:IMM:C19	5:A:800:IMM:C5	2.87	0.53
1:A:340:THR:O	1:A:344:VAL:HG23	2.09	0.53
1:B:367:PHE:CD1	1:B:542:PRO:HG3	2.44	0.53
1:B:215:LYS:CD	1:B:215:LYS:H	2.21	0.53
1:A:388:HIS:N	1:A:389:PRO:CD	2.72	0.53
1:B:200:PHE:CE1	1:B:391:MET:HE1	2.44	0.53
1:A:200:PHE:CE1	1:A:391:MET:HE1	2.44	0.52
1:A:554:VAL:HG23	1:A:555:GLY:N	2.23	0.52
1:B:403:SER:OG	1:B:406:GLN:HG3	2.09	0.52
1:A:150:ARG:NH2	1:A:458:LEU:O	2.41	0.52
1:B:517:ILE:HG23	1:B:518:PHE:CD1	2.44	0.52
1:A:527:ALA:HB3	1:A:528:PRO:HD3	1.91	0.52
1:B:527:ALA:HB3	1:B:528:PRO:HD3	1.91	0.52
1:A:367:PHE:CD1	1:A:542:PRO:HG3	2.44	0.52
1:A:403:SER:OG	1:A:406:GLN:HG3	2.09	0.52
1:B:388:HIS:N	1:B:389:PRO:CD	2.72	0.52
1:A:294:LEU:CD2	1:A:409:PHE:HD1	2.23	0.52
1:B:150:ARG:NH2	1:B:458:LEU:O	2.42	0.52
1:A:517:ILE:HG23	1:A:518:PHE:CD1	2.44	0.52
1:B:340:THR:O	1:B:344:VAL:HG23	2.09	0.52
5:B:800:IMM:C19	5:B:800:IMM:C5	2.87	0.52
1:A:163:MET:HE3	1:A:171:LEU:HD21	1.93	0.51
1:A:470:PHE:CZ	1:A:529:PHE:CE2	2.99	0.51
1:B:187:PHE:CE1	1:B:189:PRO:HB3	2.43	0.51
1:B:464:ASN:ND2	1:B:474:PRO:HB2	2.25	0.51
1:A:205:PHE:O	1:A:208:GLN:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLN:HG3	1:A:70:THR:CG2	2.41	0.51
1:B:163:MET:HE3	1:B:171:LEU:HD21	1.93	0.51
1:B:391:MET:CG	4:B:601:HEM:HAB	2.28	0.51
1:B:470:PHE:CZ	1:B:529:PHE:CE2	2.99	0.51
1:A:352:LEU:HD13	1:A:518:PHE:CZ	2.46	0.51
1:B:205:PHE:O	1:B:208:GLN:HG2	2.10	0.51
1:A:355:TYR:OH	5:A:800:IMM:H201	2.11	0.51
1:B:42:GLN:HG3	1:B:70:THR:CG2	2.41	0.51
1:A:464:ASN:ND2	1:A:474:PRO:HB2	2.25	0.50
1:B:294:LEU:CD2	1:B:409:PHE:HD1	2.23	0.50
1:B:352:LEU:HD13	1:B:518:PHE:CZ	2.46	0.50
1:B:427:SER:HB3	1:B:577:TYR:CD2	2.46	0.50
1:A:90:HIS:CD2	1:A:90:HIS:O	2.65	0.50
1:A:116:VAL:HG12	1:A:117:LEU:N	2.27	0.50
1:B:353:SER:HB2	1:B:355:TYR:CD1	2.47	0.50
1:A:187:PHE:CE1	1:A:189:PRO:HB3	2.43	0.50
1:B:90:HIS:O	1:B:90:HIS:CD2	2.65	0.50
1:A:384:LEU:HG	5:A:800:IMM:I1	2.82	0.50
1:A:427:SER:HB3	1:A:577:TYR:CD2	2.46	0.50
1:B:175:GLU:O	1:B:179:ARG:HG3	2.11	0.50
1:A:175:GLU:O	1:A:179:ARG:HG3	2.11	0.50
1:A:352:LEU:HD11	1:A:387:TRP:HH2	1.72	0.50
1:A:353:SER:HB2	1:A:355:TYR:CD1	2.47	0.50
1:B:384:LEU:HG	5:B:800:IMM:I1	2.82	0.50
1:B:470:PHE:HZ	1:B:529:PHE:CZ	2.30	0.50
1:B:345:ILE:HG22	1:B:346:GLU:N	2.27	0.50
1:B:184:ARG:HA	1:B:438:ARG:O	2.12	0.49
1:B:355:TYR:CD1	1:B:355:TYR:N	2.79	0.49
1:B:320:HIS:HB3	1:B:323:TRP:CD1	2.48	0.49
1:A:58:ASP:HB2	1:B:548:SER:HB3	1.94	0.49
1:A:184:ARG:HA	1:A:438:ARG:O	2.12	0.49
1:A:345:ILE:HG22	1:A:346:GLU:N	2.27	0.49
1:A:355:TYR:HD1	1:A:355:TYR:N	2.10	0.49
1:A:208:GLN:HB3	1:A:232:HIS:CD2	2.47	0.49
1:B:116:VAL:O	1:B:120:ARG:HB2	2.13	0.49
1:B:355:TYR:CE2	5:B:800:IMM:C20	2.96	0.49
1:B:208:GLN:HB3	1:B:232:HIS:CD2	2.47	0.49
1:B:355:TYR:OH	5:B:800:IMM:H201	2.11	0.49
1:A:116:VAL:O	1:A:120:ARG:HB2	2.13	0.49
1:B:116:VAL:HG12	1:B:117:LEU:N	2.27	0.49
1:A:256:MET:O	1:A:257:LEU:HD23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:PHE:HZ	1:A:529:PHE:CZ	2.30	0.48
1:B:445:LEU:O	1:B:445:LEU:HG	2.12	0.48
1:A:49:ARG:O	1:B:320:HIS:CD2	2.66	0.48
1:A:445:LEU:HG	1:A:445:LEU:O	2.12	0.48
1:B:251:LYS:HG3	1:B:310:ASN:CG	2.38	0.48
1:A:280:PRO:HG2	1:A:283:SER:OG	2.13	0.48
1:B:273:MET:HE1	1:B:287:VAL:HG22	1.96	0.48
1:A:355:TYR:CE2	5:A:800:IMM:C20	2.96	0.48
1:A:355:TYR:CD1	1:A:355:TYR:N	2.79	0.48
1:B:280:PRO:HG2	1:B:283:SER:OG	2.12	0.48
1:A:251:LYS:HG3	1:A:310:ASN:CG	2.38	0.48
1:B:355:TYR:N	1:B:355:TYR:HD1	2.10	0.48
1:A:320:HIS:CD2	1:B:49:ARG:O	2.67	0.48
1:A:320:HIS:HB3	1:A:323:TRP:CD1	2.48	0.48
1:B:304:ILE:HD13	1:B:568:VAL:HG22	1.96	0.47
1:A:503:PHE:CZ	1:A:507:LEU:HD11	2.49	0.47
1:A:239:GLU:CD	1:A:239:GLU:H	2.22	0.47
1:A:273:MET:HE1	1:A:287:VAL:HG22	1.96	0.47
1:B:582:VAL:HG22	1:B:583:PRO:HD2	1.97	0.47
1:A:276:PRO:HG2	1:A:279:ILE:HD12	1.97	0.47
1:B:320:HIS:HE1	1:B:551:GLY:O	1.98	0.47
1:A:94:THR:O	1:A:95:HIS:ND1	2.47	0.47
1:B:94:THR:O	1:B:95:HIS:ND1	2.47	0.47
1:B:256:MET:O	1:B:257:LEU:HD23	2.13	0.47
1:B:320:HIS:CE1	1:B:551:GLY:O	2.67	0.47
1:A:254:TYR:HA	1:A:264:PRO:HD3	1.96	0.47
1:A:320:HIS:CE1	1:A:551:GLY:O	2.67	0.47
1:A:513:HIS:HB2	1:A:516:SER:OG	2.15	0.47
1:B:503:PHE:CZ	1:B:507:LEU:HD11	2.49	0.47
1:A:513:HIS:CE1	1:A:520:GLU:N	2.83	0.47
1:A:475:TYR:CE2	1:A:481:LEU:HD12	2.50	0.47
1:B:179:ARG:HB3	1:B:179:ARG:HH11	1.80	0.47
1:B:239:GLU:CD	1:B:239:GLU:H	2.22	0.47
1:A:130:TYR:HB3	1:A:134:HIS:O	2.15	0.46
1:B:185:ARG:HE	1:B:438:ARG:HD3	1.79	0.46
1:B:388:HIS:N	1:B:389:PRO:HD3	2.31	0.46
1:A:185:ARG:HE	1:A:438:ARG:HD3	1.79	0.46
1:A:275:TYR:CE2	1:A:284:GLN:HB3	2.51	0.46
1:B:254:TYR:HA	1:B:264:PRO:HD3	1.96	0.46
1:B:512:CYS:SG	1:B:518:PHE:HA	2.56	0.46
1:B:130:TYR:HB3	1:B:134:HIS:O	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:ARG:HH11	1:A:179:ARG:HB3	1.80	0.46
1:A:582:VAL:HG22	1:A:583:PRO:HD2	1.97	0.46
1:B:276:PRO:HG2	1:B:279:ILE:CD1	2.46	0.46
1:B:475:TYR:CE2	1:B:481:LEU:HD12	2.50	0.46
1:A:276:PRO:HG2	1:A:279:ILE:CD1	2.46	0.46
1:A:304:ILE:HD13	1:A:568:VAL:HG22	1.96	0.46
1:A:388:HIS:N	1:A:389:PRO:HD3	2.30	0.46
1:A:537:ASN:OD1	1:A:538:PRO:HD2	2.16	0.46
1:B:352:LEU:O	1:B:353:SER:C	2.59	0.46
1:B:537:ASN:OD1	1:B:538:PRO:HD2	2.16	0.46
1:A:548:SER:HB3	1:B:58:ASP:HB2	1.97	0.46
1:B:275:TYR:CE2	1:B:284:GLN:HB3	2.51	0.46
1:B:513:HIS:HB2	1:B:516:SER:OG	2.15	0.46
1:A:256:MET:HE3	1:A:256:MET:HB3	1.81	0.46
1:B:433:ARG:HH11	1:B:433:ARG:CG	2.29	0.46
1:A:214:GLY:N	1:A:215:LYS:HE2	2.31	0.45
1:A:433:ARG:HH11	1:A:433:ARG:CG	2.29	0.45
1:A:513:HIS:HB3	1:A:514:PRO:HD2	1.98	0.45
1:B:276:PRO:HG2	1:B:279:ILE:HD12	1.97	0.45
1:B:513:HIS:HB3	1:B:514:PRO:HD2	1.98	0.45
1:A:512:CYS:SG	1:A:518:PHE:HA	2.56	0.45
1:A:553:GLU:HG3	1:A:557:ASN:ND2	2.31	0.45
1:A:320:HIS:HE1	1:A:551:GLY:O	1.98	0.45
1:B:513:HIS:CE1	1:B:520:GLU:N	2.83	0.45
1:A:184:ARG:HB2	1:A:439:ASN:C	2.42	0.45
1:A:185:ARG:NE	1:A:438:ARG:HH11	2.14	0.45
1:B:120:ARG:HH12	5:B:800:IMM:C20	2.22	0.45
1:B:184:ARG:HB2	1:B:439:ASN:C	2.42	0.45
1:B:185:ARG:NE	1:B:438:ARG:HH11	2.14	0.45
1:B:208:GLN:HE22	1:B:230:LEU:H	1.64	0.45
1:B:214:GLY:N	1:B:215:LYS:HE2	2.31	0.45
1:B:280:PRO:HA	1:B:281:PRO:HD3	1.88	0.45
1:B:256:MET:HA	1:B:260:GLU:O	2.17	0.45
1:A:433:ARG:HH11	1:A:433:ARG:HG2	1.82	0.45
1:A:577:TYR:CE2	1:A:583:PRO:HD3	2.52	0.44
1:B:289:GLN:HG3	1:B:292:PHE:CE1	2.52	0.44
1:B:469:ARG:HA	1:B:469:ARG:HD2	1.52	0.44
1:A:352:LEU:O	1:A:353:SER:C	2.59	0.44
1:A:366:LEU:HD23	1:A:366:LEU:HA	1.76	0.44
1:A:208:GLN:NE2	1:A:228:VAL:HA	2.32	0.44
1:A:390:LEU:HG	1:A:434:ILE:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:MET:HA	1:A:260:GLU:O	2.17	0.44
1:A:289:GLN:HG3	1:A:292:PHE:CE1	2.52	0.44
1:B:298:LEU:HD12	1:B:298:LEU:HA	1.72	0.44
1:B:315:LEU:HD12	1:B:558:LEU:HD11	1.99	0.44
1:A:216:MET:HG2	2:C:2:NAG:H83	1.99	0.44
1:A:115:LEU:HD23	1:A:119:VAL:HG21	2.00	0.44
1:A:315:LEU:HD12	1:A:558:LEU:HD11	1.99	0.44
1:A:163:MET:HB3	1:A:462:PRO:HG3	1.99	0.44
1:B:208:GLN:NE2	1:B:228:VAL:HA	2.32	0.44
1:B:331:THR:O	1:B:335:ILE:HG13	2.18	0.44
1:A:413:MET:HB2	1:A:413:MET:HE3	1.83	0.44
1:B:216:MET:HG2	2:D:2:NAG:H83	1.99	0.44
1:A:152:LEU:HD21	1:A:469:ARG:CG	2.35	0.44
1:A:331:THR:O	1:A:335:ILE:HG13	2.18	0.44
1:B:163:MET:HB3	1:B:462:PRO:HG3	1.99	0.43
1:B:390:LEU:HG	1:B:434:ILE:HD11	1.98	0.43
1:A:96:GLY:O	1:A:97:ARG:C	2.61	0.43
1:A:387:TRP:CG	1:A:434:ILE:HD13	2.53	0.43
1:B:553:GLU:HG3	1:B:557:ASN:ND2	2.31	0.43
1:B:96:GLY:O	1:B:97:ARG:C	2.61	0.43
1:B:472:MET:HE3	1:B:472:MET:HB2	1.90	0.43
1:B:577:TYR:CE2	1:B:583:PRO:HD3	2.52	0.43
1:A:531:LEU:HD23	1:A:531:LEU:HA	1.86	0.43
1:B:115:LEU:HD23	1:B:119:VAL:HG21	2.00	0.43
1:A:189:PRO:HA	1:A:432:GLY:HA2	2.00	0.43
1:B:433:ARG:HH11	1:B:433:ARG:HG2	1.82	0.43
1:A:280:PRO:HA	1:A:281:PRO:HD3	1.88	0.43
1:B:89:ILE:C	1:B:91:PHE:H	2.27	0.43
1:B:189:PRO:HA	1:B:432:GLY:HA2	2.00	0.43
1:B:215:LYS:HE3	1:B:222:LYS:NZ	2.34	0.43
1:B:112:LEU:O	1:B:115:LEU:N	2.52	0.43
1:B:150:ARG:HA	1:B:380:GLU:OE1	2.18	0.43
1:B:190:ASP:HA	1:B:191:PRO:HD2	1.70	0.43
1:B:381:PHE:CZ	1:B:385:TYR:CD2	3.07	0.43
1:A:165:THR:HG22	1:A:166:LYS:HG2	2.01	0.43
1:A:192:GLN:OE1	1:A:516:SER:HA	2.19	0.43
1:A:494:LEU:HD23	1:A:494:LEU:HA	1.88	0.43
1:B:387:TRP:CG	1:B:434:ILE:HD13	2.53	0.43
1:A:112:LEU:O	1:A:115:LEU:N	2.52	0.43
1:A:381:PHE:CZ	1:A:385:TYR:CD2	3.07	0.43
1:A:383:GLN:O	1:A:384:LEU:C	2.61	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:HIS:O	1:B:44:GLN:HB2	2.19	0.43
1:B:165:THR:HG22	1:B:166:LYS:HG2	2.01	0.43
1:B:386:HIS:NE2	4:B:601:HEM:HAD1	2.34	0.43
1:B:575:CYS:HA	1:B:576:PRO:HD2	1.93	0.43
1:A:89:ILE:C	1:A:91:PHE:H	2.27	0.42
1:A:298:LEU:HD12	1:A:298:LEU:HA	1.72	0.42
1:A:215:LYS:HE3	1:A:222:LYS:NZ	2.34	0.42
1:A:343:ILE:O	1:A:344:VAL:C	2.61	0.42
1:A:366:LEU:HD12	1:A:535:LEU:HD12	2.01	0.42
1:A:555:GLY:O	1:A:558:LEU:HB2	2.19	0.42
1:A:61:ARG:NH1	1:B:542:PRO:O	2.52	0.42
1:B:366:LEU:HA	1:B:366:LEU:HD23	1.76	0.42
1:A:150:ARG:HA	1:A:380:GLU:OE1	2.18	0.42
1:A:240:ARG:HG3	1:A:271:VAL:CG2	2.50	0.42
1:A:387:TRP:CZ2	5:A:800:IMM:I1	3.43	0.42
1:B:391:MET:HG3	4:B:601:HEM:CAB	2.30	0.42
1:A:316:LEU:HD12	1:A:316:LEU:HA	1.94	0.42
1:A:373:TYR:O	1:B:374:ARG:NH1	2.51	0.42
1:A:504:TYR:CZ	1:A:508:LEU:CD1	3.03	0.42
1:A:127:PRO:HG2	1:B:544:TYR:CE1	2.54	0.42
1:B:256:MET:HE3	1:B:256:MET:HB3	1.81	0.42
1:B:433:ARG:HH11	1:B:433:ARG:HB3	1.84	0.42
1:A:372:GLN:HE22	1:B:372:GLN:HA	1.83	0.42
1:B:387:TRP:CZ2	5:B:800:IMM:I1	3.43	0.42
1:A:43:HIS:O	1:A:44:GLN:HB2	2.19	0.42
1:B:252:LEU:HD12	1:B:252:LEU:HA	1.92	0.42
1:A:481:LEU:HD22	1:A:501:LEU:CD2	2.50	0.42
1:B:240:ARG:HG3	1:B:271:VAL:CG2	2.50	0.42
1:A:42:GLN:HG3	1:A:70:THR:HG23	2.02	0.42
1:A:118:THR:OG1	1:A:119:VAL:N	2.53	0.42
1:A:208:GLN:HE22	1:A:230:LEU:H	1.64	0.42
1:A:339:GLU:HG2	1:A:562:ALA:HB2	2.02	0.41
1:A:433:ARG:HH11	1:A:433:ARG:HB3	1.84	0.41
1:A:566:LYS:O	1:A:570:LEU:HB2	2.20	0.41
1:B:339:GLU:HG2	1:B:562:ALA:HB2	2.02	0.41
1:A:115:LEU:O	1:A:119:VAL:HG23	2.20	0.41
1:B:294:LEU:HD22	1:B:409:PHE:CE1	2.55	0.41
1:A:183:LEU:HD23	1:A:184:ARG:N	2.35	0.41
1:B:349:VAL:O	1:B:349:VAL:CG1	2.69	0.41
1:B:383:GLN:O	1:B:384:LEU:C	2.61	0.41
1:B:566:LYS:O	1:B:570:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:238:LEU:HD23	1:A:238:LEU:HA	1.76	0.41
1:B:115:LEU:O	1:B:119:VAL:HG23	2.20	0.41
1:B:366:LEU:HD12	1:B:535:LEU:HD12	2.01	0.41
1:B:555:GLY:O	1:B:558:LEU:HB2	2.19	0.41
1:A:230:LEU:HG	1:A:233:ILE:HD12	2.03	0.41
1:A:391:MET:HG3	4:A:601:HEM:CAB	2.30	0.41
1:A:240:ARG:HG3	1:A:271:VAL:HG22	2.02	0.41
1:A:386:HIS:NE2	4:A:601:HEM:HAD1	2.34	0.41
1:B:481:LEU:HD22	1:B:501:LEU:CD2	2.50	0.41
1:A:108:ILE:H	1:A:108:ILE:HG13	1.70	0.41
1:A:544:TYR:CE1	1:B:127:PRO:HG2	2.56	0.41
1:A:557:ASN:O	1:A:558:LEU:C	2.64	0.41
1:B:42:GLN:HG3	1:B:70:THR:HG23	2.02	0.41
1:B:96:GLY:O	1:B:99:LEU:N	2.54	0.41
1:B:192:GLN:OE1	1:B:516:SER:HA	2.19	0.41
1:B:207:HIS:HE1	4:B:601:HEM:C1D	2.39	0.41
1:A:96:GLY:O	1:A:99:LEU:N	2.54	0.41
1:A:207:HIS:HE1	4:A:601:HEM:C1D	2.39	0.41
1:A:469:ARG:HA	1:A:469:ARG:HD2	1.52	0.41
1:B:152:LEU:HD21	1:B:469:ARG:CG	2.35	0.41
1:B:504:TYR:CZ	1:B:508:LEU:CD1	3.03	0.41
1:A:294:LEU:HD22	1:A:409:PHE:CE1	2.55	0.41
1:B:343:ILE:O	1:B:344:VAL:C	2.61	0.41
1:B:494:LEU:HD23	1:B:494:LEU:HA	1.88	0.41
1:A:481:LEU:HD11	1:A:510:GLU:HB2	2.03	0.40
1:A:490:GLU:HA	1:A:493:GLU:HG2	2.03	0.40
1:B:85:SER:O	1:B:89:ILE:HG12	2.22	0.40
1:B:204:HIS:CE1	1:B:292:PHE:CE2	3.09	0.40
1:B:355:TYR:CZ	5:B:800:IMM:C20	3.02	0.40
1:A:372:GLN:HA	1:B:372:GLN:HE22	1.85	0.40
1:B:88:PHE:CZ	1:B:92:LEU:HD11	2.56	0.40
1:B:269:ALA:O	1:B:271:VAL:N	2.54	0.40
1:B:531:LEU:HD23	1:B:531:LEU:HA	1.86	0.40
1:A:204:HIS:CE1	1:A:292:PHE:CE2	3.09	0.40
1:B:118:THR:OG1	1:B:119:VAL:N	2.53	0.40
1:B:183:LEU:HD23	1:B:184:ARG:N	2.35	0.40
1:A:85:SER:O	1:A:89:ILE:HG12	2.22	0.40
1:A:88:PHE:CZ	1:A:92:LEU:HD11	2.56	0.40
1:A:190:ASP:HA	1:A:191:PRO:HD2	1.70	0.40
1:B:481:LEU:HD11	1:B:510:GLU:HB2	2.03	0.40
1:B:557:ASN:O	1:B:558:LEU:C	2.64	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:113:MET:HE1	1:A:359:LEU:HD22	2.04	0.40
1:A:472:MET:HE3	1:A:472:MET:HB2	1.90	0.40
1:B:213:SER:OG	1:B:215:LYS:HG2	2.21	0.40
1:B:230:LEU:HG	1:B:233:ILE:HD12	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	549/576 (95%)	490 (89%)	52 (10%)	7 (1%)	9	41
1	B	549/576 (95%)	490 (89%)	52 (10%)	7 (1%)	9	41
All	All	1098/1152 (95%)	980 (89%)	104 (10%)	14 (1%)	9	41

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	386	HIS
1	A	514	PRO
1	A	520	GLU
1	B	386	HIS
1	B	514	PRO
1	B	520	GLU
1	A	503	PHE
1	B	503	PHE
1	A	270	PRO
1	A	295	LEU
1	A	528	PRO
1	B	270	PRO
1	B	295	LEU
1	B	528	PRO

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	486/506 (96%)	429 (88%)	57 (12%)	5	19
1	B	486/506 (96%)	428 (88%)	58 (12%)	5	19
All	All	972/1012 (96%)	857 (88%)	115 (12%)	5	19

All (115) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	65	SER
1	A	70	THR
1	A	87	SER
1	A	113	MET
1	A	116	VAL
1	A	120	ARG
1	A	137	ILE
1	A	145	VAL
1	A	162	PRO
1	A	165	THR
1	A	170	GLN
1	A	171	LEU
1	A	183	LEU
1	A	185	ARG
1	A	198	PHE
1	A	209	PHE
1	A	215	LYS
1	A	232	HIS
1	A	238	LEU
1	A	244	LEU
1	A	246	LEU
1	A	251	LYS
1	A	252	LEU
1	A	271	VAL
1	A	289	GLN
1	A	291	VAL

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Mol	Chain	Res	Type
1	A	298	LEU
1	A	300	LEU
1	A	307	ARG
1	A	316	LEU
1	A	317	LYS
1	A	322	THR
1	A	348	TYR
1	A	352	LEU
1	A	376	ARG
1	A	385	TYR
1	A	392	PRO
1	A	405	GLU
1	A	433	ARG
1	A	455	SER
1	A	458	LEU
1	A	460	LEU
1	A	469	ARG
1	A	473	LYS
1	A	476	THR
1	A	479	GLN
1	A	484	GLU
1	A	514	PRO
1	A	518	PHE
1	A	523	ILE
1	A	528	PRO
1	A	530	SER
1	A	531	LEU
1	A	535	LEU
1	A	563	THR
1	A	564	LEU
1	B	49	ARG
1	B	65	SER
1	B	70	THR
1	B	87	SER
1	B	113	MET
1	B	116	VAL
1	B	120	ARG
1	B	137	ILE
1	B	145	VAL
1	B	162	PRO
1	B	165	THR
1	B	170	GLN

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Mol	Chain	Res	Type
1	B	171	LEU
1	B	183	LEU
1	B	185	ARG
1	B	198	PHE
1	B	209	PHE
1	B	215	LYS
1	B	232	HIS
1	B	238	LEU
1	B	244	LEU
1	B	246	LEU
1	B	251	LYS
1	B	252	LEU
1	B	271	VAL
1	B	289	GLN
1	B	291	VAL
1	B	298	LEU
1	B	300	LEU
1	B	307	ARG
1	B	316	LEU
1	B	317	LYS
1	B	322	THR
1	B	348	TYR
1	B	352	LEU
1	B	374	ARG
1	B	376	ARG
1	B	385	TYR
1	B	392	PRO
1	B	405	GLU
1	B	433	ARG
1	B	455	SER
1	B	458	LEU
1	B	460	LEU
1	B	469	ARG
1	B	473	LYS
1	B	476	THR
1	B	479	GLN
1	B	484	GLU
1	B	514	PRO
1	B	518	PHE
1	B	523	ILE
1	B	528	PRO
1	B	530	SER

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Mol	Chain	Res	Type
1	B	531	LEU
1	B	535	LEU
1	B	563	THR
1	B	564	LEU

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

Mol	Chain	Res	Type
1	A	56	GLN
1	A	134	HIS
1	A	170	GLN
1	A	207	HIS
1	A	208	GLN
1	A	320	HIS
1	A	372	GLN
1	A	375	ASN
1	A	442	HIS
1	A	443	HIS
1	A	513	HIS
1	A	557	ASN
1	B	56	GLN
1	B	90	HIS
1	B	134	HIS
1	B	170	GLN
1	B	207	HIS
1	B	208	GLN
1	B	320	HIS
1	B	375	ASN
1	B	442	HIS
1	B	443	HIS
1	B	513	HIS
1	B	557	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

4 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	C	1	1,2	14,14,15	0.53	0	17,19,21	1.07	1 (5%)
2	NAG	C	2	2	14,14,15	1.14	2 (14%)	17,19,21	1.30	2 (11%)
2	NAG	D	1	1,2	14,14,15	0.53	0	17,19,21	1.07	1 (5%)
2	NAG	D	2	2	14,14,15	1.13	2 (14%)	17,19,21	1.31	2 (11%)

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	C	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	NAG	D	1	1,2	-	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	2	NAG	C4-C5	2.34	1.58	1.53
2	D	2	NAG	C4-C5	2.33	1.58	1.53
2	C	2	NAG	O5-C5	2.12	1.47	1.43
2	D	2	NAG	O5-C5	2.11	1.47	1.43

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	2	NAG	C4-C3-C2	-3.14	106.41	111.02
2	C	2	NAG	C4-C3-C2	-3.14	106.41	111.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1	NAG	C6-C5-C4	-2.33	107.29	113.02
2	C	1	NAG	C6-C5-C4	-2.33	107.29	113.02
2	C	2	NAG	O5-C1-C2	-2.26	107.80	111.29
2	D	2	NAG	O5-C1-C2	-2.26	107.80	111.29

There are no chirality outliers.

All (4) torsion outliers are listed below:

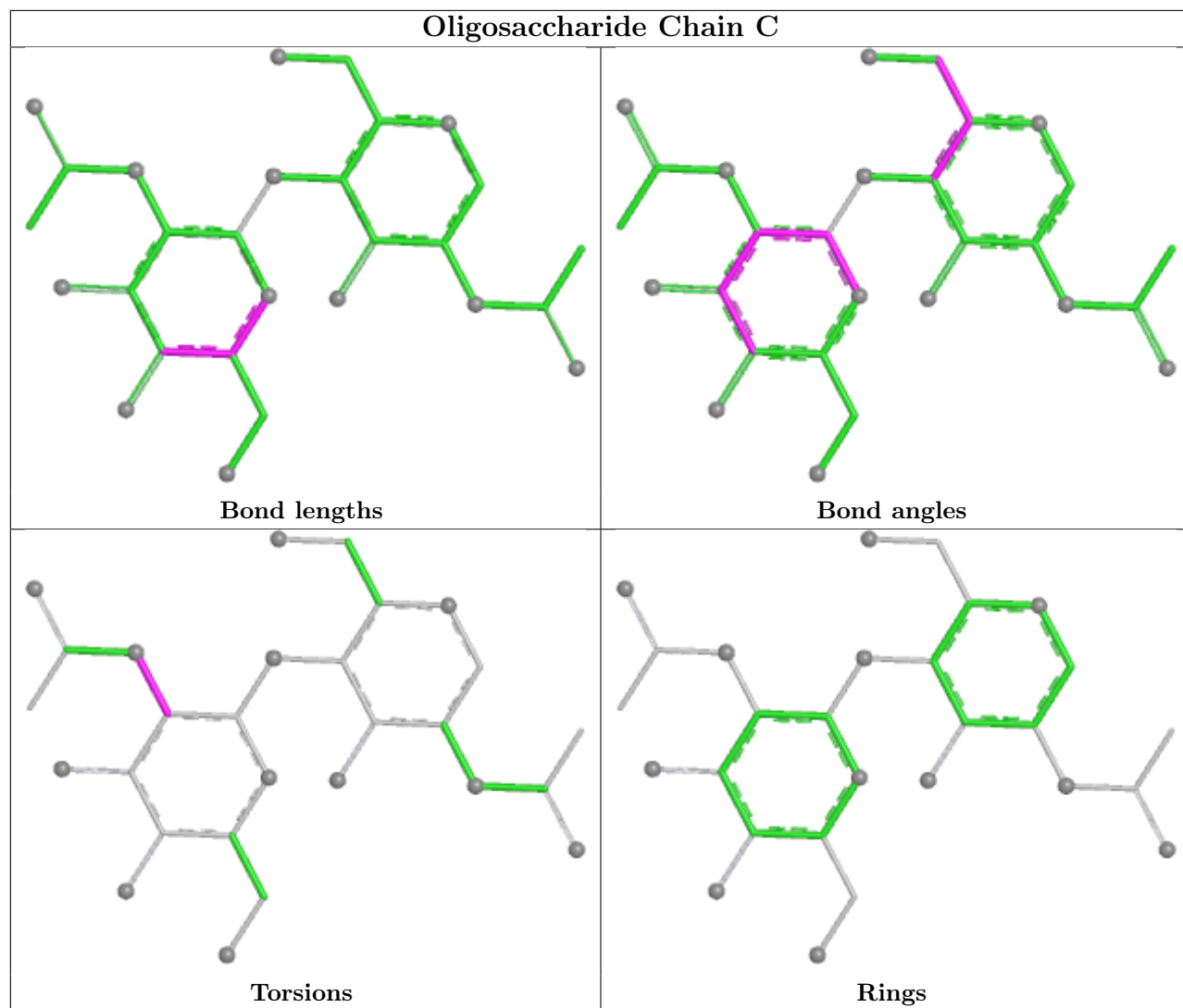
Mol	Chain	Res	Type	Atoms
2	C	2	NAG	C1-C2-N2-C7
2	D	2	NAG	C1-C2-N2-C7
2	C	2	NAG	C3-C2-N2-C7
2	D	2	NAG	C3-C2-N2-C7

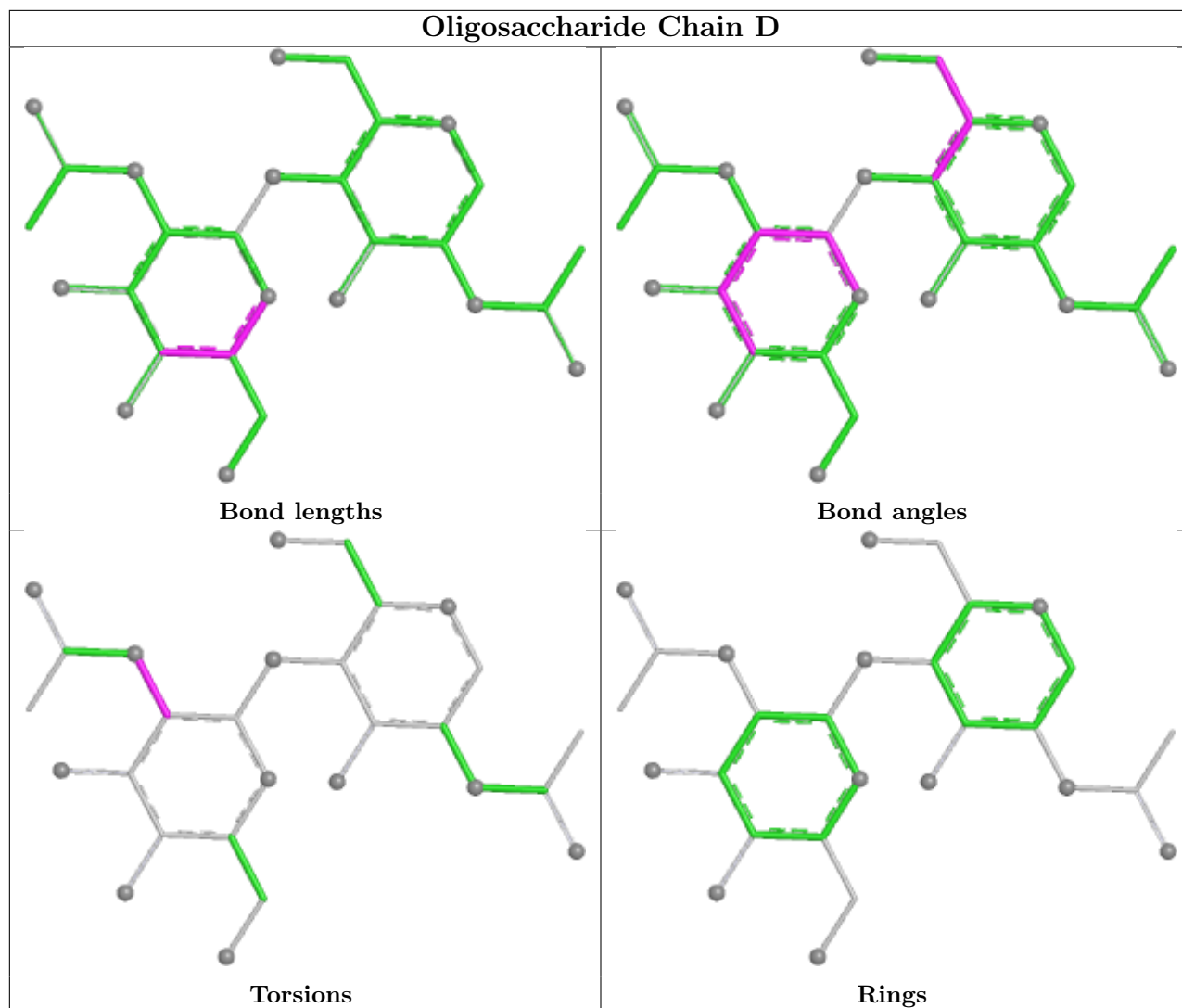
There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	2	NAG	1	0
2	C	2	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](#)

8 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	$\# Z > 2$
3	NAG	A	661	1	14,14,15	0.78	0	17,19,21	1.26	1 (5%)
3	NAG	A	681	1	14,14,15	0.77	0	17,19,21	0.85	1 (5%)
4	HEM	B	601	1	50,50,50	2.05	14 (28%)	67,82,82	2.27	24 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	IMM	B	800	-	27,27,27	1.66	4 (14%)	39,39,39	0.94	0
3	NAG	B	681	1	14,14,15	0.77	0	17,19,21	0.85	1 (5%)
5	IMM	A	800	-	27,27,27	1.66	4 (14%)	39,39,39	0.94	0
4	HEM	A	601	1	50,50,50	2.05	14 (28%)	67,82,82	2.27	24 (35%)
3	NAG	B	661	1	14,14,15	0.79	0	17,19,21	1.25	1 (5%)

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
3	NAG	A	661	1	-	0/6/23/26	0/1/1/1
3	NAG	A	681	1	-	1/6/23/26	0/1/1/1
4	HEM	B	601	1	-	6/14/54/54	-
5	IMM	B	800	-	-	7/14/14/14	0/3/3/3
3	NAG	B	681	1	-	1/6/23/26	0/1/1/1
5	IMM	A	800	-	-	7/14/14/14	0/3/3/3
4	HEM	A	601	1	-	6/14/54/54	-
3	NAG	B	661	1	-	0/6/23/26	0/1/1/1

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	800	IMM	C5-C6	-5.20	1.30	1.39
5	B	800	IMM	C5-C6	-5.18	1.30	1.39
4	A	601	HEM	C3B-C4B	5.16	1.54	1.44
4	B	601	HEM	C3B-C4B	5.13	1.54	1.44
4	A	601	HEM	CAC-C3C	-5.11	1.33	1.47
4	B	601	HEM	CAC-C3C	-5.10	1.33	1.47
4	B	601	HEM	C3C-C4C	-3.89	1.39	1.46
4	A	601	HEM	C3C-C4C	-3.85	1.39	1.46
4	B	601	HEM	CBB-CAB	3.54	1.47	1.30
4	A	601	HEM	CBB-CAB	3.54	1.47	1.30
4	B	601	HEM	C1B-C2B	3.49	1.51	1.44
4	A	601	HEM	C1B-C2B	3.46	1.51	1.44
4	B	601	HEM	C3B-C2B	-3.40	1.30	1.37
4	A	601	HEM	C3B-C2B	-3.37	1.30	1.37
4	A	601	HEM	C4A-NA	-3.37	1.33	1.39
5	B	800	IMM	C5-C4	-3.36	1.34	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	601	HEM	C4A-NA	-3.36	1.33	1.39
5	A	800	IMM	C5-C4	-3.32	1.34	1.39
4	B	601	HEM	C1B-NB	-3.28	1.34	1.40
4	A	601	HEM	C1B-NB	-3.24	1.34	1.40
4	A	601	HEM	CAB-C3B	-2.60	1.40	1.47
4	B	601	HEM	CAB-C3B	-2.59	1.40	1.47
4	B	601	HEM	C1C-NC	-2.50	1.34	1.39
4	A	601	HEM	C1C-NC	-2.49	1.34	1.39
5	A	800	IMM	C4-C3	-2.41	1.39	1.44
4	B	601	HEM	CHA-C1A	-2.41	1.34	1.39
5	B	800	IMM	C4-C3	-2.41	1.39	1.44
4	A	601	HEM	CHA-C1A	-2.41	1.34	1.39
4	B	601	HEM	CBC-CAC	2.35	1.41	1.30
4	A	601	HEM	CBC-CAC	2.33	1.41	1.30
5	B	800	IMM	C8-C9	-2.31	1.36	1.39
5	A	800	IMM	C8-C9	-2.29	1.36	1.39
4	B	601	HEM	C3C-C2C	-2.27	1.32	1.37
4	A	601	HEM	C3C-C2C	-2.26	1.32	1.37
4	B	601	HEM	CAA-C2A	2.09	1.56	1.51
4	A	601	HEM	CAA-C2A	2.08	1.56	1.51

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	HEM	C3B-C4B-NB	6.10	113.85	109.47
4	B	601	HEM	C3B-C4B-NB	6.05	113.81	109.47
4	B	601	HEM	CHC-C4B-NB	-6.05	117.92	124.42
4	A	601	HEM	CHC-C4B-NB	-6.04	117.92	124.42
4	A	601	HEM	C2A-C1A-NA	5.45	116.20	110.15
4	B	601	HEM	C2A-C1A-NA	5.42	116.17	110.15
4	A	601	HEM	C4B-C3B-C2B	-5.25	102.45	107.28
4	B	601	HEM	C4B-C3B-C2B	-5.19	102.51	107.28
3	A	661	NAG	C2-N2-C7	-4.51	116.86	122.90
3	B	661	NAG	C2-N2-C7	-4.49	116.89	122.90
4	A	601	HEM	C1A-C2A-C3A	-4.30	100.22	106.87
4	B	601	HEM	C1A-C2A-C3A	-4.29	100.22	106.87
4	A	601	HEM	CBA-CAA-C2A	3.96	123.48	112.53
4	B	601	HEM	CBA-CAA-C2A	3.95	123.46	112.53
4	B	601	HEM	C3C-C2C-C1C	-3.47	103.77	107.05
4	A	601	HEM	C3C-C2C-C1C	-3.46	103.77	107.05
4	B	601	HEM	C4D-ND-C1D	-3.41	101.17	105.21
4	A	601	HEM	C4D-ND-C1D	-3.41	101.17	105.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	601	HEM	CHA-C1A-C2A	-3.37	117.93	125.30
4	B	601	HEM	CHA-C1A-C2A	-3.33	118.00	125.30
4	B	601	HEM	C4C-C3C-C2C	3.29	109.67	106.81
4	A	601	HEM	C4C-C3C-C2C	3.29	109.67	106.81
4	A	601	HEM	CHA-C4D-C3D	-3.04	119.62	125.23
4	B	601	HEM	CHA-C4D-C3D	-3.04	119.63	125.23
4	B	601	HEM	CMD-C2D-C1D	2.97	129.67	125.03
4	A	601	HEM	CMD-C2D-C1D	2.95	129.64	125.03
4	B	601	HEM	C3D-C4D-ND	2.93	113.39	110.17
4	B	601	HEM	C4A-C3A-C2A	2.92	110.16	106.82
4	A	601	HEM	C3D-C4D-ND	2.91	113.36	110.17
4	A	601	HEM	C4A-C3A-C2A	2.90	110.14	106.82
4	A	601	HEM	CAB-C3B-C4B	2.58	135.81	124.39
4	B	601	HEM	CAB-C3B-C4B	2.57	135.75	124.39
4	B	601	HEM	C2B-C1B-NB	2.48	112.70	109.84
4	A	601	HEM	C2B-C1B-NB	2.48	112.69	109.84
4	A	601	HEM	CHB-C1B-NB	-2.43	121.36	124.37
4	B	601	HEM	CHB-C1B-NB	-2.41	121.39	124.37
4	B	601	HEM	C4A-NA-C1A	-2.39	101.92	105.82
4	A	601	HEM	C4A-NA-C1A	-2.39	101.92	105.82
4	A	601	HEM	C1B-NB-C4B	-2.38	102.39	105.21
4	B	601	HEM	C1B-NB-C4B	-2.38	102.39	105.21
4	A	601	HEM	C1A-CHA-C4D	-2.18	121.11	126.25
4	B	601	HEM	C1A-CHA-C4D	-2.17	121.15	126.25
4	B	601	HEM	CBC-CAC-C3C	-2.13	116.87	127.53
4	A	601	HEM	CBC-CAC-C3C	-2.13	116.87	127.53
4	A	601	HEM	C3B-C2B-C1B	2.12	108.00	106.41
3	B	681	NAG	C2-N2-C7	-2.08	120.11	122.90
3	A	681	NAG	C2-N2-C7	-2.08	120.11	122.90
4	B	601	HEM	CAA-C2A-C3A	2.08	131.73	127.07
4	B	601	HEM	CAB-C3B-C2B	-2.07	121.70	128.43
4	A	601	HEM	CAB-C3B-C2B	-2.07	121.71	128.43
4	B	601	HEM	C3B-C2B-C1B	2.06	107.96	106.41
4	A	601	HEM	CAA-C2A-C3A	2.06	131.68	127.07

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	601	HEM	C2C-C3C-CAC-CBC
4	B	601	HEM	C2C-C3C-CAC-CBC
5	A	800	IMM	C11-C10-N1-C2

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Mol	Chain	Res	Type	Atoms
5	A	800	IMM	O1-C10-N1-C2
5	A	800	IMM	C11-C10-N1-C9
5	A	800	IMM	O1-C10-N1-C9
5	A	800	IMM	C19-C18-C3-C2
5	A	800	IMM	C19-C18-C3-C4
5	B	800	IMM	C11-C10-N1-C2
5	B	800	IMM	O1-C10-N1-C2
5	B	800	IMM	C11-C10-N1-C9
5	B	800	IMM	O1-C10-N1-C9
5	B	800	IMM	C19-C18-C3-C2
5	B	800	IMM	C19-C18-C3-C4
4	A	601	HEM	C2B-C3B-CAB-CBB
4	B	601	HEM	C2B-C3B-CAB-CBB
5	A	800	IMM	C3-C18-C19-O3
5	B	800	IMM	C3-C18-C19-O3
4	A	601	HEM	C4C-C3C-CAC-CBC
4	B	601	HEM	C4C-C3C-CAC-CBC
3	A	681	NAG	C4-C5-C6-O6
3	B	681	NAG	C4-C5-C6-O6
4	A	601	HEM	CAA-CBA-CGA-O2A
4	B	601	HEM	CAA-CBA-CGA-O2A
4	A	601	HEM	CAA-CBA-CGA-O1A
4	B	601	HEM	CAA-CBA-CGA-O1A
4	A	601	HEM	C4B-C3B-CAB-CBB
4	B	601	HEM	C4B-C3B-CAB-CBB

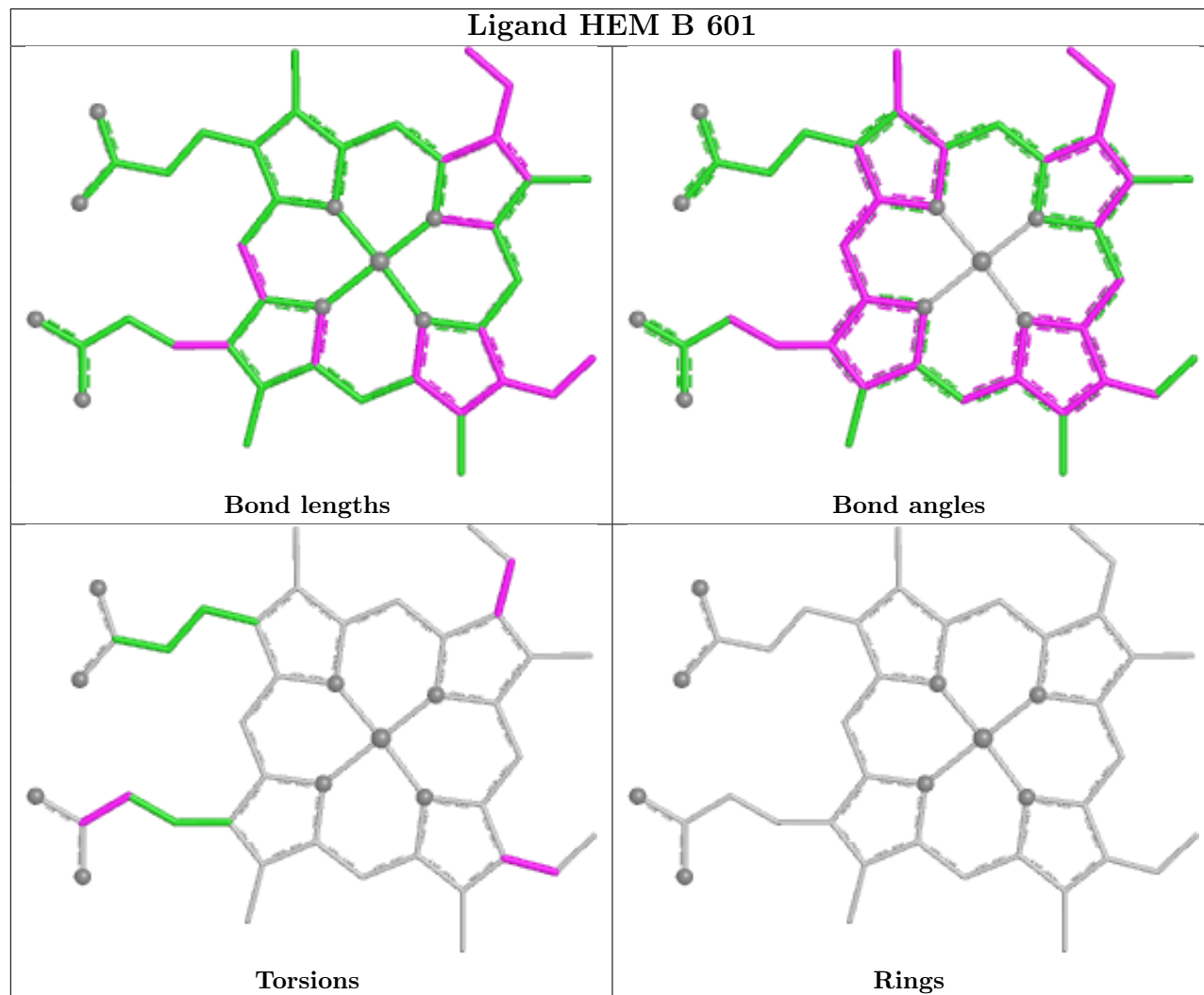
There are no ring outliers.

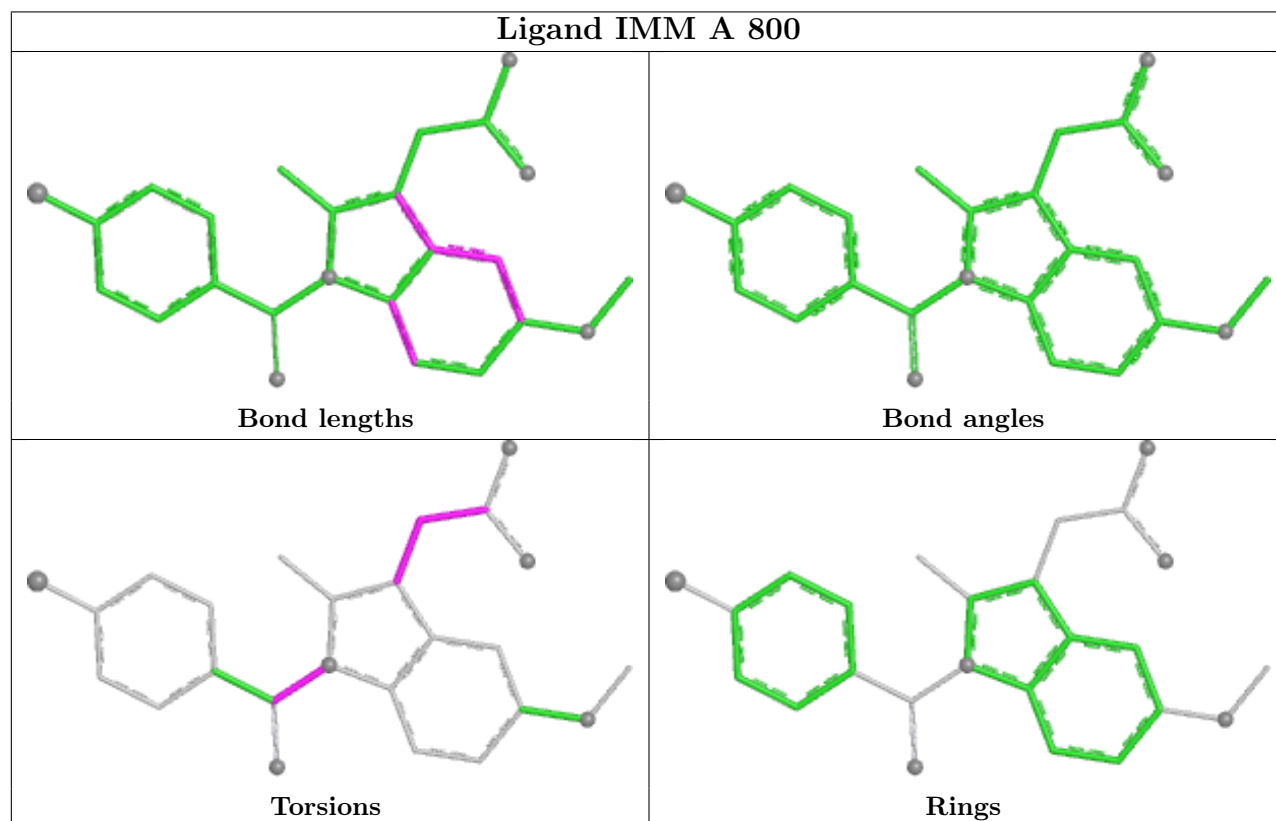
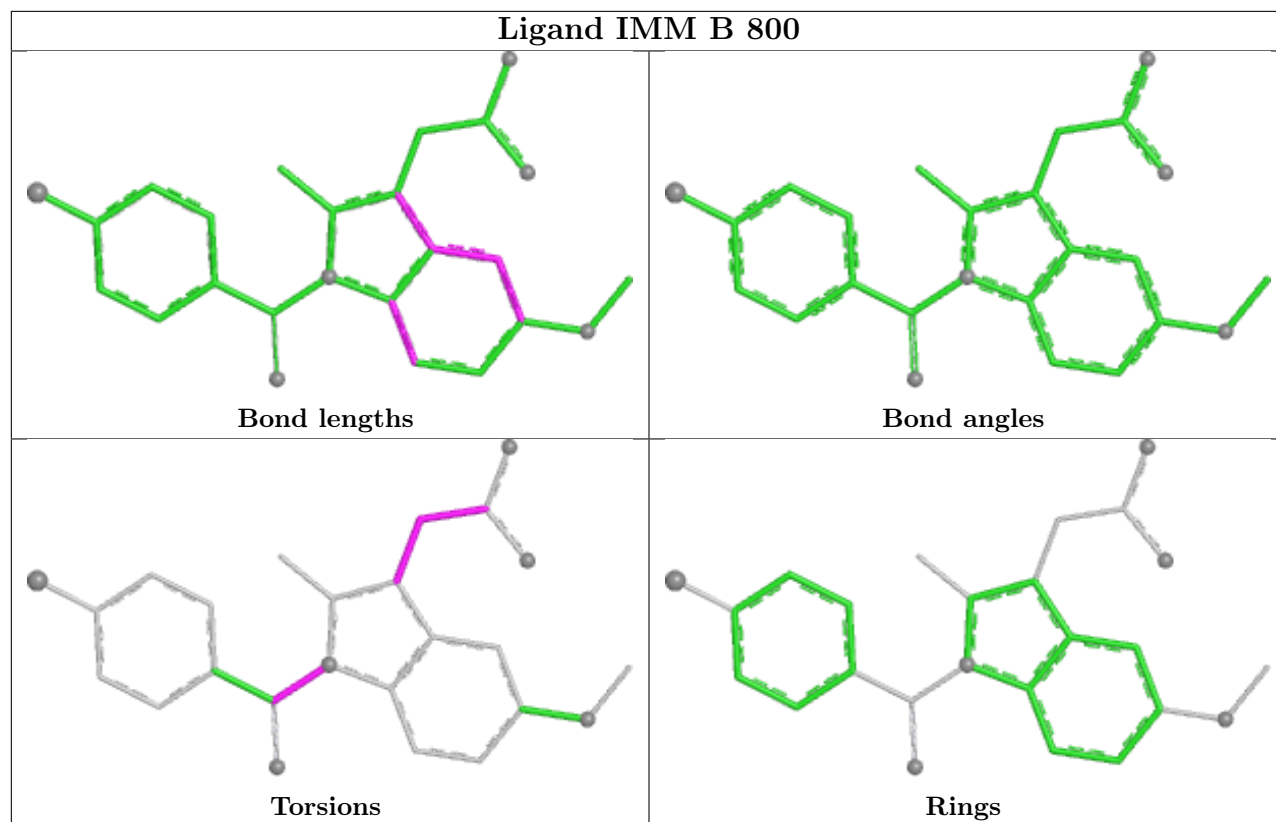
4 monomers are involved in 44 short contacts:

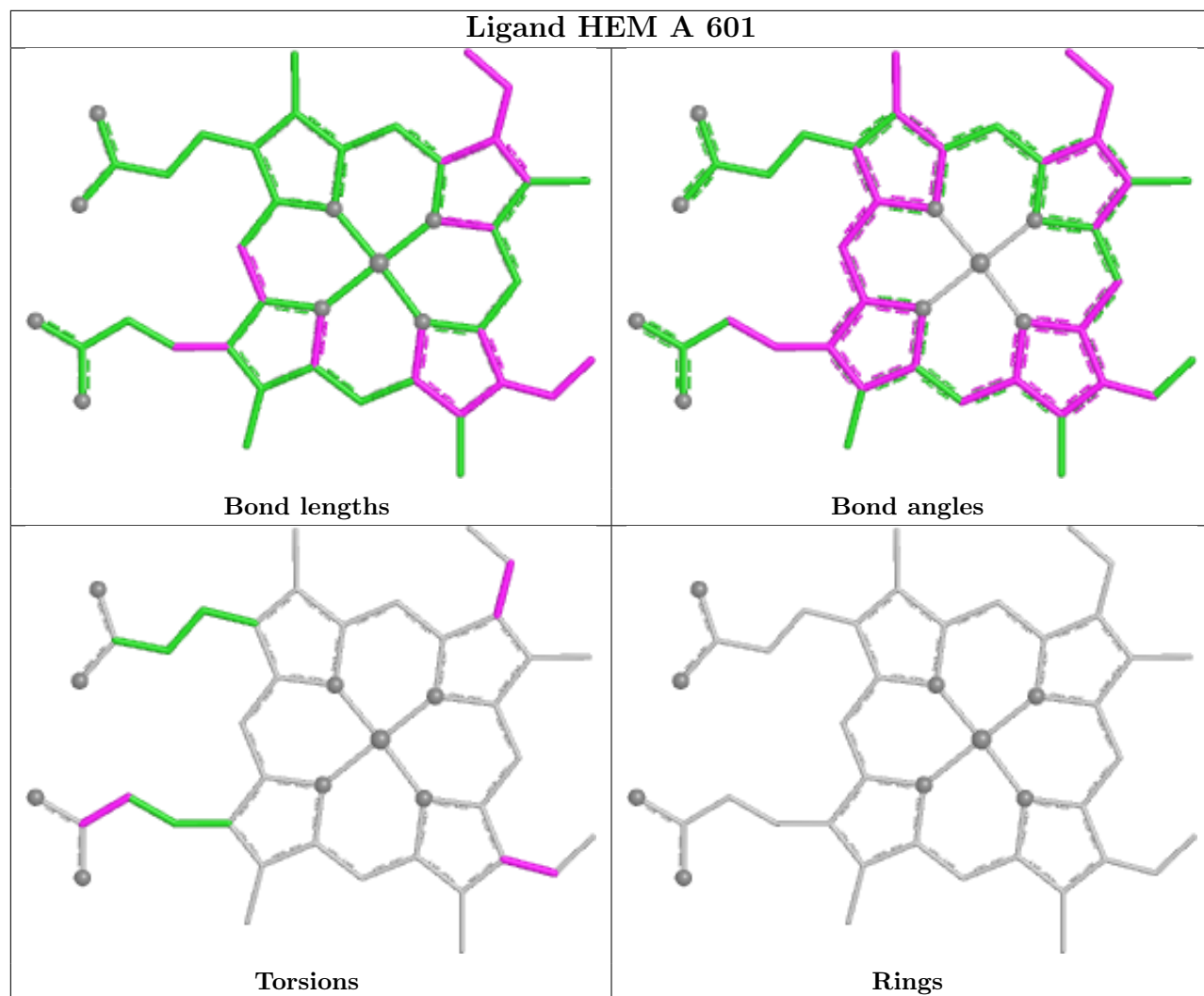
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	601	HEM	6	0
5	B	800	IMM	17	0
5	A	800	IMM	15	0
4	A	601	HEM	6	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	551/576 (95%)	-0.09	9 (1%) 70 55	4, 18, 53, 91	0
1	B	551/576 (95%)	-0.14	2 (0%) 88 77	4, 18, 53, 91	0
All	All	1102/1152 (95%)	-0.11	11 (0%) 79 64	4, 18, 53, 91	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	278	GLY	3.3
1	B	526	GLY	3.3
1	A	506	GLY	3.0
1	A	231	GLY	2.9
1	A	237	ASN	2.5
1	A	98	TRP	2.5
1	A	488	ALA	2.3
1	A	144	ASN	2.2
1	B	111	THR	2.1
1	A	111	THR	2.0
1	A	290	GLU	2.0

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

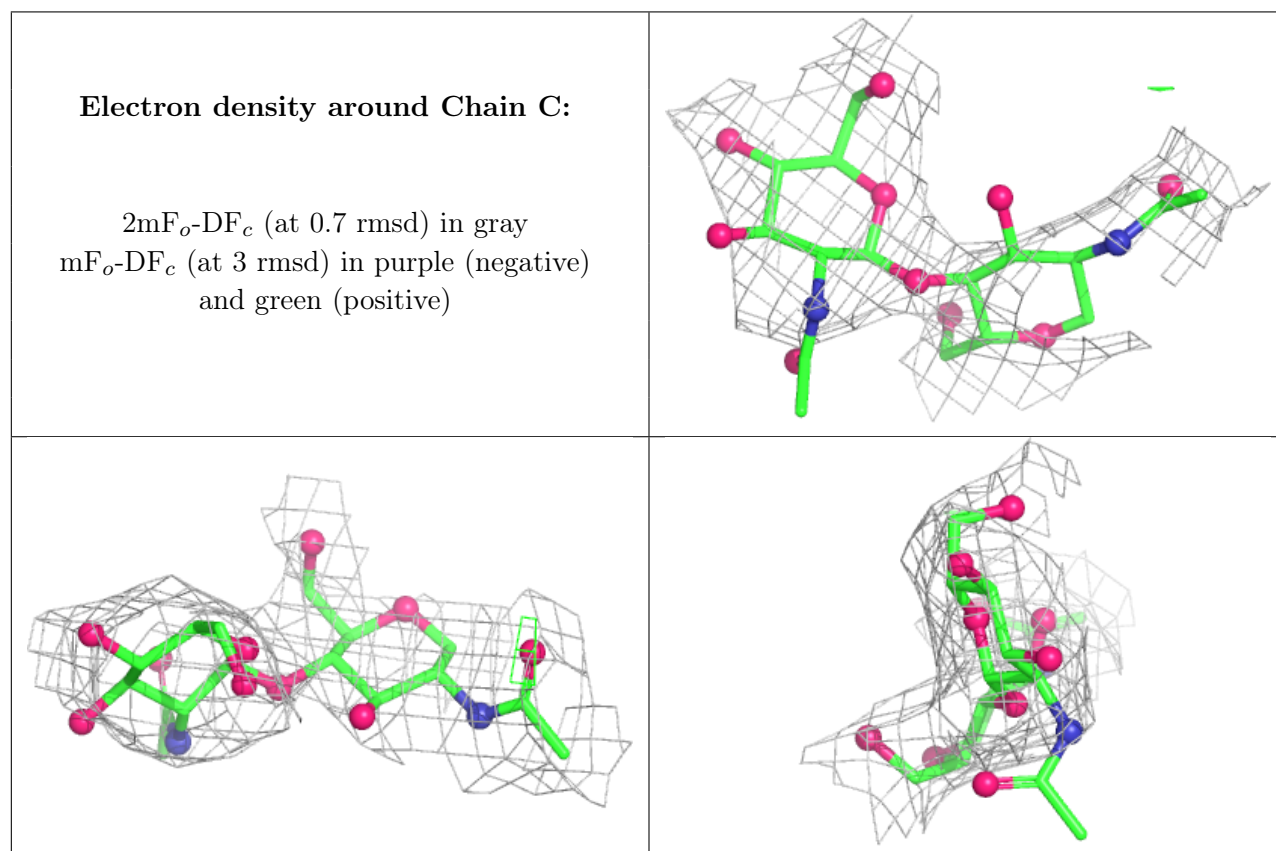
There are no non-standard protein/DNA/RNA residues in this entry.

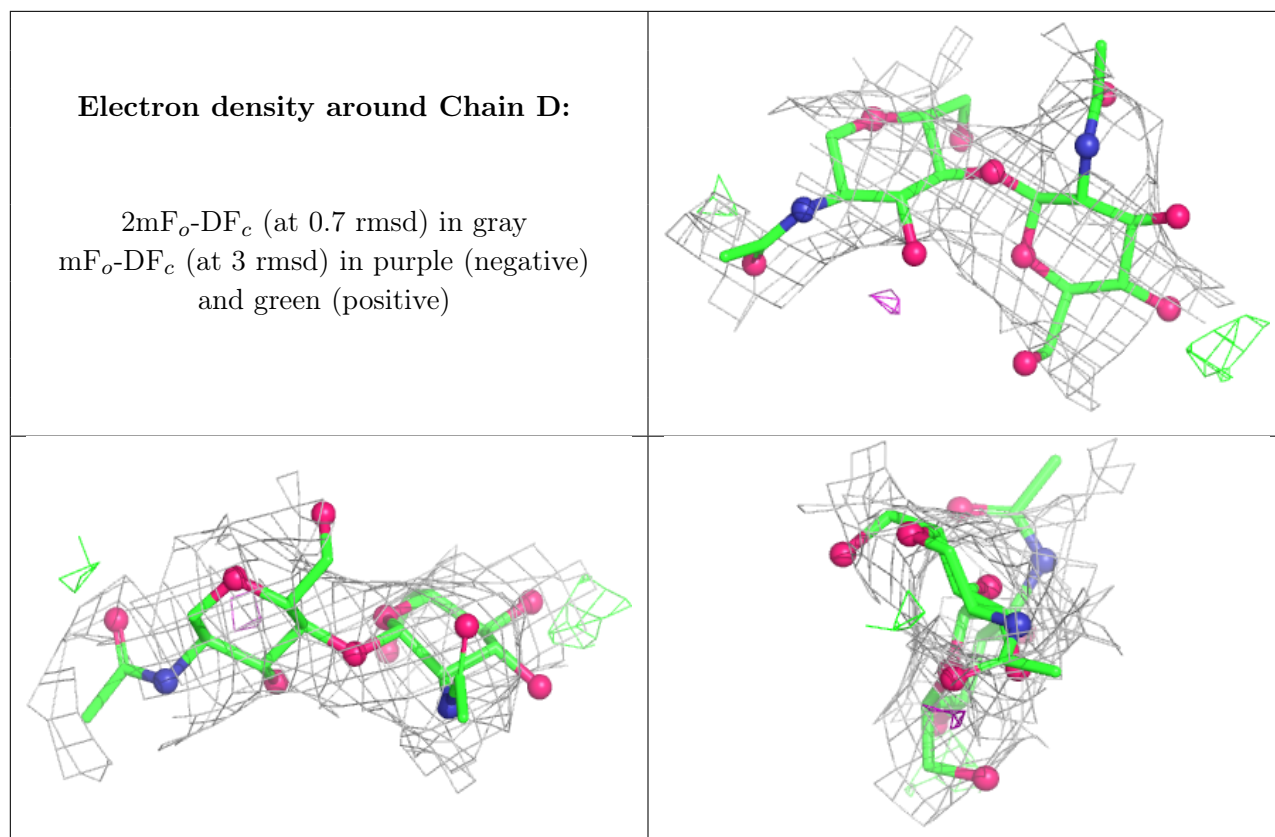
6.3 Carbohydrates [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	D	2	14/15	0.87	0.10	19,37,47,59	0
2	NAG	C	2	14/15	0.88	0.13	19,37,47,59	0
2	NAG	C	1	14/15	0.88	0.11	4,22,31,34	0
2	NAG	D	1	14/15	0.93	0.08	4,22,31,34	0

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





6.4 Ligands [i](#)

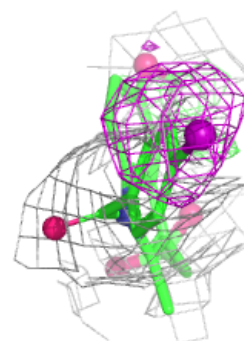
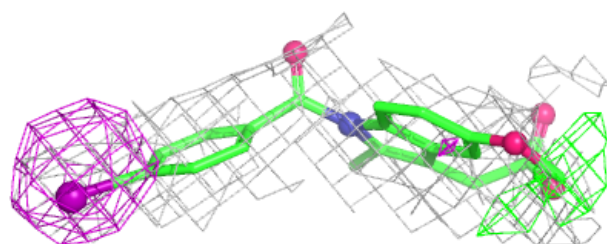
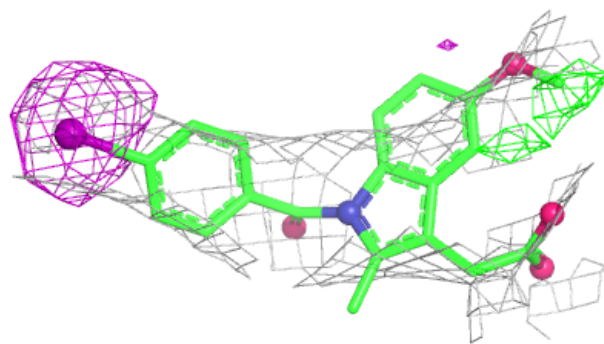
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	B	661	14/15	0.81	0.12	33,43,61,66	0
5	IMM	B	800	25/25	0.86	0.14	15,15,15,15	0
3	NAG	B	681	14/15	0.90	0.13	15,22,38,44	0
3	NAG	A	661	14/15	0.90	0.11	33,43,61,66	0
5	IMM	A	800	25/25	0.91	0.14	15,15,15,15	0
4	HEM	B	601	43/43	0.93	0.13	7,17,43,67	0
3	NAG	A	681	14/15	0.93	0.11	15,22,38,44	0
4	HEM	A	601	43/43	0.93	0.11	7,17,43,67	0

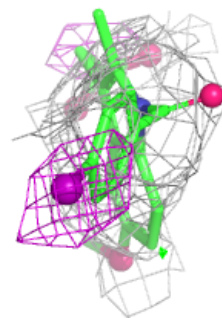
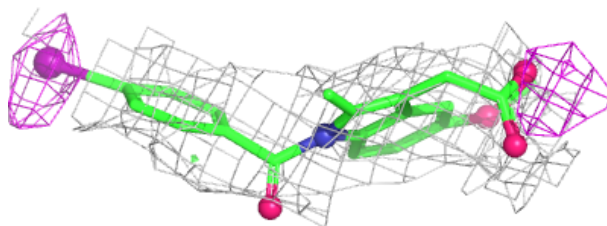
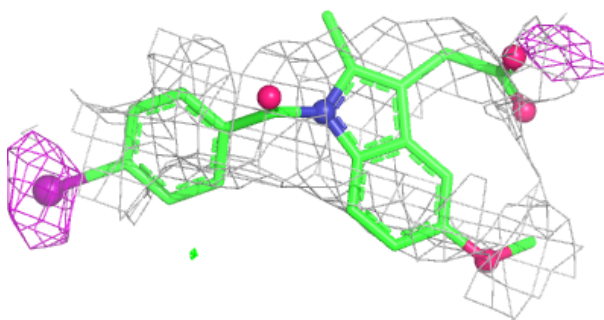
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around IMM B 800:

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

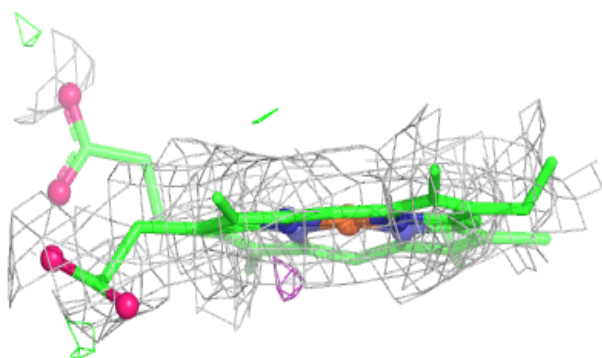
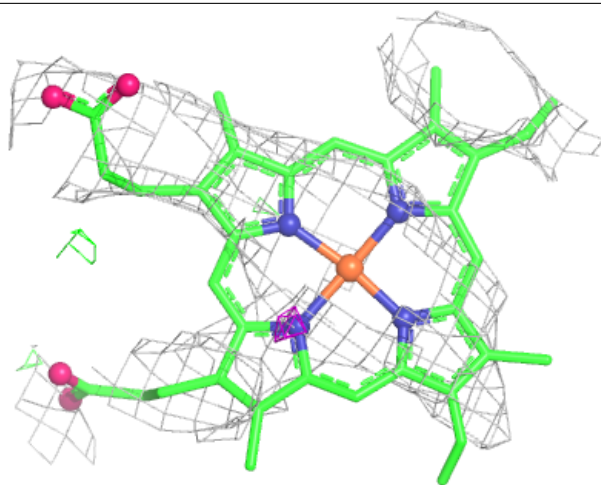
**Electron density around IMM A 800:**

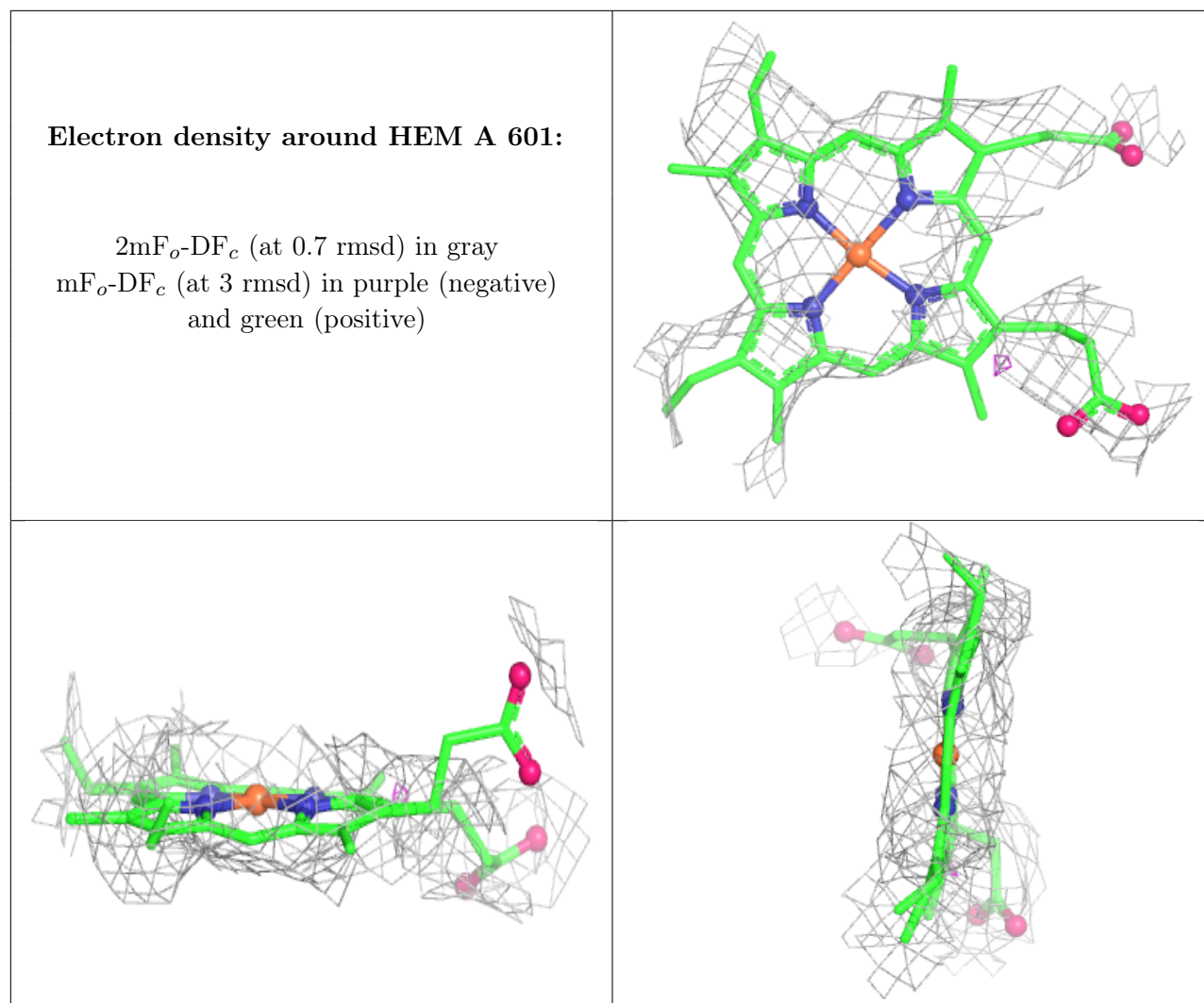
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around HEM B 601:

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





6.5 Other polymers [i](#)

There are no such residues in this entry.