



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:37 PM UTC

PDB ID : 1QPA / pdb_00001qpa
Title : LIGNIN PEROXIDASE ISOZYME LIP4.65 (PI 4.65)
Authors : Choinowski, T.H.; Piontek, K.
Deposited on : 1996-10-08
Resolution : 1.80 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) : 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

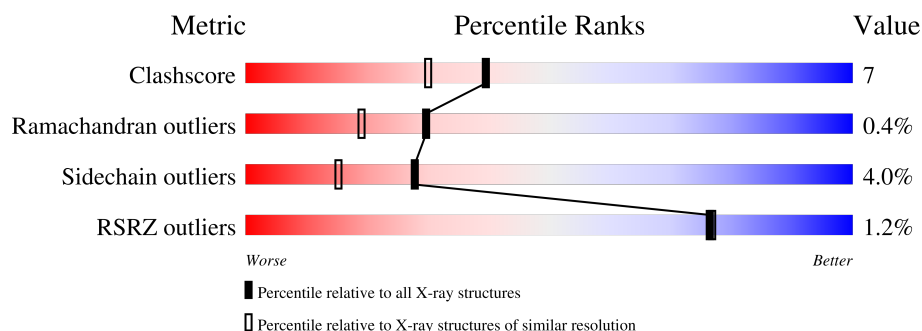
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	345	% 57% 37% 5%
1	B	345	2% 62% 34%
2	C	3	67% 33%
3	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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	FUC	C	3	X	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 5821 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.

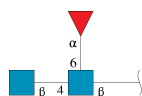
- Molecule 1 is a protein called LIGNIN PEROXIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	0	0
			2569	1630	432	492	15			
1	B	344	Total	C	N	O	S	0	0	0
			2569	1630	432	492	15			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	105	PRO	ARG	conflict	UNP P11542
A	171	HTR	TRP	modified residue	UNP P11542
A	283	ILE	THR	conflict	UNP P11542
B	105	PRO	ARG	conflict	UNP P11542
B	171	HTR	TRP	modified residue	UNP P11542
B	283	ILE	THR	conflict	UNP P11542

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



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	3	Total	C	N	O	0	0	0
			38	22	2	14			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose.



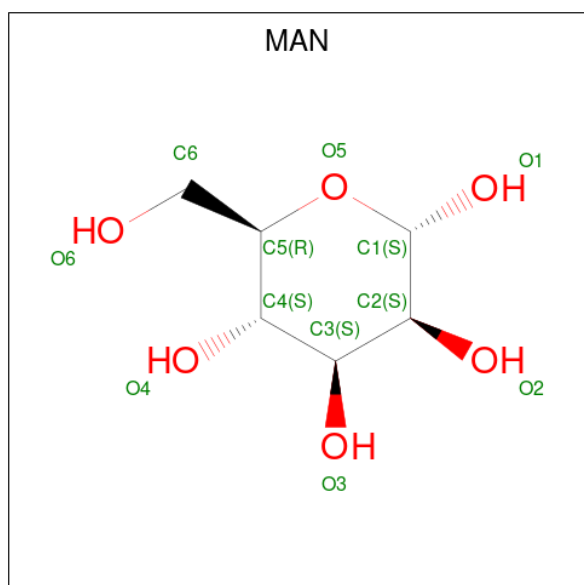
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
3	D	2	Total	C	O	0	0	0
			22	12	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

- Molecule 5 is alpha-D-mannopyranose (CCD ID: MAN) (formula: $C_6H_{12}O_6$).

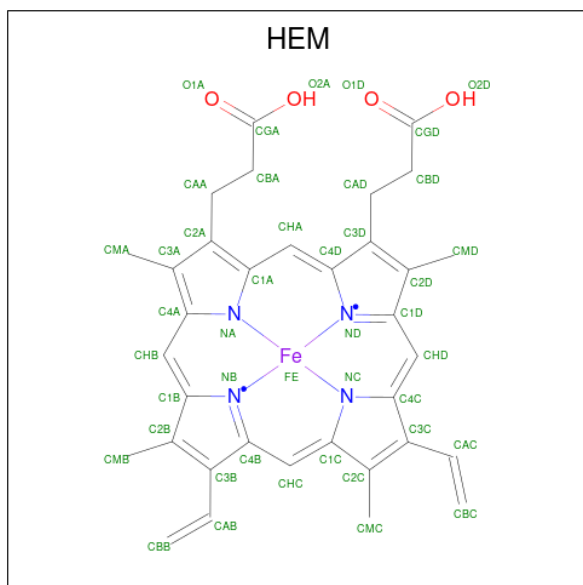


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 11	C 6	O 5	0	0
5	A	1	Total 11	C 6	O 5	0	0
5	B	1	Total 11	C 6	O 5	0	0
5	B	1	Total 11	C 6	O 5	0	0
5	B	1	Total 11	C 6	O 5	0	0

- Molecule 6 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	2	Total Ca 2 2	0	0
6	B	2	Total Ca 2 2	0	0

- Molecule 7 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

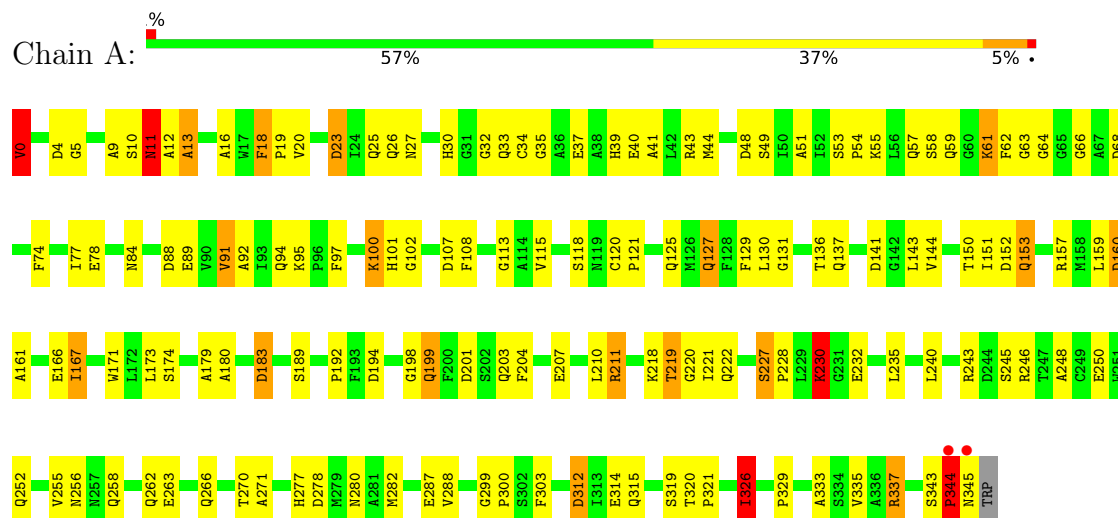
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	267	Total 267	O 267	0	0
8	B	197	Total 197	O 197	0	0

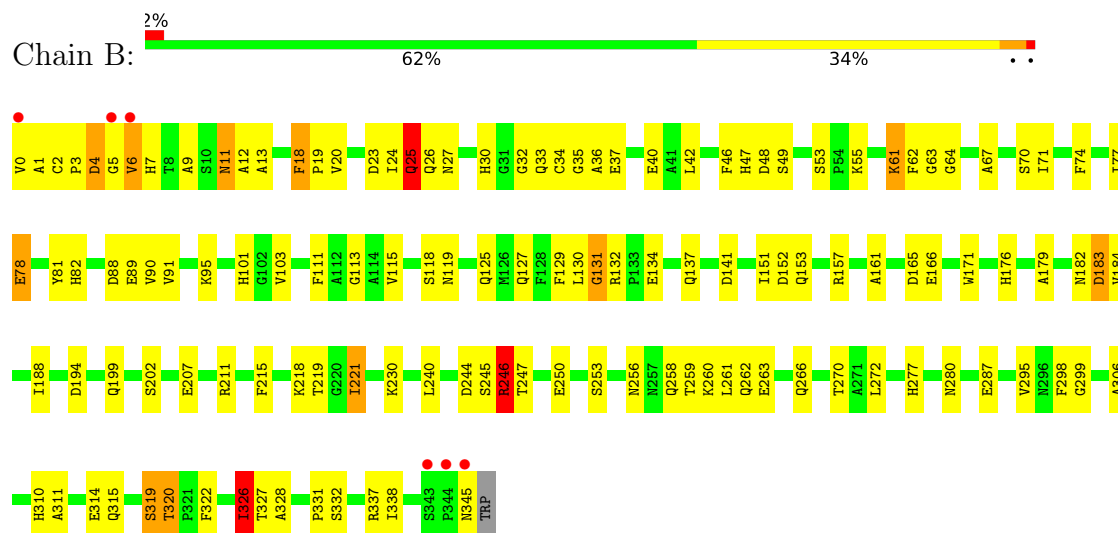
3 Residue-property plots

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 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: LIGNIN PEROXIDASE



• Molecule 1: LIGNIN PEROXIDASE



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





- Molecule 3: alpha-D-mannopyranose-(1-4)-alpha-D-mannopyranose

Chain D:  50% 50%

A horizontal progress bar for Chain D. The bar is divided into two equal halves, each labeled '50%'. The left half is yellow and the right half is orange.



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.79Å 94.02Å 81.26Å 90.00° 106.47° 90.00°	Depositor
Resolution (Å)	10.00 – 1.80 10.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (10.00-1.80) 95.5 (10.00-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.55 (at 1.80Å)	Xtriage
Refinement program	PROLSQ, X-PLOR	Depositor
R, R_{free}	(Not available) , (Not available) (Not available) , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	20.8	Xtriage
Anisotropy	0.330	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 63.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5821	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% 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: CA, HTR, NAG, HEM, MAN, FUC

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	1.31	9/2625 (0.3%)	2.43	190/3581 (5.3%)
1	B	1.14	2/2625 (0.1%)	2.39	156/3581 (4.4%)
All	All	1.23	11/5250 (0.2%)	2.41	346/7162 (4.8%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	11	ASN	CG-OD1	6.79	1.36	1.23
1	B	153	GLN	CD-OE1	6.59	1.36	1.23
1	B	26	GLN	CD-OE1	6.29	1.35	1.23
1	A	166	GLU	C-N	-5.68	1.26	1.33
1	A	49	SER	N-CA	-5.64	1.39	1.46
1	A	48	ASP	C-N	-5.54	1.26	1.33
1	A	222	GLN	CD-OE1	5.51	1.34	1.23
1	A	63	GLY	C-O	-5.38	1.19	1.24
1	A	66	GLY	CA-C	5.24	1.58	1.52
1	A	250	GLU	CA-C	5.20	1.59	1.52
1	A	27	ASN	CG-OD1	5.18	1.33	1.23

All (346) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	337	ARG	CD-NE-CZ	22.63	156.09	124.40
1	B	246	ARG	NE-CZ-NH1	19.62	141.12	121.50
1	A	53	SER	O-C-N	14.14	129.76	121.27
1	B	199	GLN	OE1-CD-NE2	13.33	135.93	122.60
1	B	115	VAL	CA-C-N	13.24	134.95	119.99
1	B	115	VAL	C-N-CA	13.24	134.95	119.99
1	A	246	ARG	NE-CZ-NH2	11.57	129.62	119.20
1	B	3	PRO	CA-C-N	11.55	142.43	122.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	3	PRO	C-N-CA	11.55	142.43	122.79
1	B	345	ASN	CA-CB-CG	11.20	123.80	112.60
1	A	329	PRO	CA-C-O	10.78	134.82	121.67
1	A	11	ASN	CB-CG-ND2	10.69	132.43	116.40
1	B	5	GLY	N-CA-C	-10.39	100.47	115.64
1	A	48	ASP	CA-C-N	10.15	134.71	120.29
1	A	48	ASP	C-N-CA	10.15	134.71	120.29
1	B	53	SER	O-C-N	10.15	127.36	121.27
1	A	280	ASN	CA-CB-CG	-10.04	102.56	112.60
1	B	153	GLN	OE1-CD-NE2	9.99	132.59	122.60
1	A	258	GLN	OE1-CD-NE2	-9.85	112.75	122.60
1	B	280	ASN	CA-CB-CG	-9.76	102.84	112.60
1	B	246	ARG	NE-CZ-NH2	-9.30	110.83	119.20
1	A	144	VAL	CA-C-O	-9.23	113.19	119.19
1	A	343	SER	CA-C-N	9.23	131.38	119.84
1	A	343	SER	C-N-CA	9.23	131.38	119.84
1	A	337	ARG	CD-NE-CZ	8.98	136.97	124.40
1	A	113	GLY	O-C-N	-8.90	113.65	122.19
1	A	344	PRO	CB-CA-C	8.69	125.89	111.56
1	B	246	ARG	NH1-CZ-NH2	-8.66	108.05	119.30
1	A	194	ASP	N-CA-CB	8.65	125.63	111.62
1	A	199	GLN	OE1-CD-NE2	8.63	131.23	122.60
1	B	315	GLN	OE1-CD-NE2	8.26	130.85	122.60
1	A	333	ALA	CA-C-O	8.22	130.23	121.19
1	A	166	GLU	CA-C-O	-8.18	110.56	119.97
1	B	37	GLU	CA-C-O	-8.18	111.88	120.55
1	A	94	GLN	OE1-CD-NE2	-8.17	114.43	122.60
1	A	35	GLY	CA-C-O	-8.12	113.32	121.93
1	A	326	ILE	CA-C-O	-8.09	112.57	121.23
1	A	211	ARG	CD-NE-CZ	-8.08	113.09	124.40
1	B	183	ASP	CA-CB-CG	8.04	120.64	112.60
1	A	34	CYS	CA-C-N	7.97	132.50	122.85
1	A	34	CYS	C-N-CA	7.97	132.50	122.85
1	A	256	ASN	OD1-CG-ND2	-7.90	114.70	122.60
1	B	125	GLN	CB-CG-CD	7.86	125.97	112.60
1	B	4	ASP	CA-C-O	7.86	130.67	120.07
1	A	30	HIS	CA-CB-CG	-7.83	105.97	113.80
1	B	263	GLU	O-C-N	7.83	130.13	122.07
1	A	23	ASP	CA-CB-CG	7.79	120.39	112.60
1	B	35	GLY	CA-C-N	7.78	131.04	120.54
1	B	35	GLY	C-N-CA	7.78	131.04	120.54
1	B	55	LYS	CA-C-O	-7.76	112.32	120.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	199	GLN	O-C-N	7.75	132.38	123.31
1	A	199	GLN	CG-CD-NE2	-7.74	104.79	116.40
1	A	160	ASP	CB-CG-OD2	7.72	136.16	118.40
1	B	48	ASP	CA-CB-CG	7.71	120.31	112.60
1	B	27	ASN	CA-CB-CG	-7.70	104.90	112.60
1	B	141	ASP	CA-C-O	-7.70	112.50	121.82
1	B	12	ALA	CA-C-O	-7.64	111.47	120.10
1	B	90	VAL	O-C-N	-7.58	114.03	121.83
1	B	63	GLY	CA-C-N	7.50	134.82	121.92
1	B	63	GLY	C-N-CA	7.50	134.82	121.92
1	A	319	SER	CA-CB-OG	7.46	126.03	111.10
1	A	143	LEU	CA-C-N	-7.34	116.28	123.04
1	A	143	LEU	C-N-CA	-7.34	116.28	123.04
1	B	337	ARG	NE-CZ-NH1	7.34	128.84	121.50
1	A	39	HIS	ND1-CE1-NE2	7.28	115.67	108.40
1	A	100	LYS	CA-CB-CG	7.26	128.62	114.10
1	A	48	ASP	CA-C-O	-7.24	113.20	120.80
1	A	40	GLU	CA-C-N	7.20	129.92	120.28
1	A	40	GLU	C-N-CA	7.20	129.92	120.28
1	B	259	THR	O-C-N	7.18	129.74	122.12
1	B	47	HIS	CA-CB-CG	-7.16	106.64	113.80
1	A	115	VAL	CA-C-O	-7.12	113.14	121.05
1	A	287	GLU	CA-C-N	7.04	132.18	120.64
1	A	287	GLU	C-N-CA	7.04	132.18	120.64
1	A	107	ASP	CA-C-O	-7.03	112.97	120.42
1	B	4	ASP	N-CA-C	-7.00	103.62	112.93
1	B	215	PHE	CA-C-O	-6.98	113.11	120.23
1	B	182	ASN	OD1-CG-ND2	6.95	129.55	122.60
1	B	27	ASN	OD1-CG-ND2	6.95	129.55	122.60
1	B	322	PHE	CA-CB-CG	-6.94	106.86	113.80
1	B	337	ARG	CB-CA-C	-6.93	95.47	109.68
1	B	30	HIS	CA-CB-CG	-6.92	106.88	113.80
1	B	179	ALA	N-CA-CB	-6.90	100.86	111.56
1	B	134	GLU	CB-CG-CD	-6.88	100.90	112.60
1	A	278	ASP	O-C-N	6.86	131.77	123.13
1	A	32	GLY	O-C-N	6.86	129.54	122.54
1	B	153	GLN	N-CA-CB	-6.83	100.06	110.16
1	A	55	LYS	CA-C-O	-6.78	113.70	120.82
1	A	189	SER	CA-C-O	-6.77	113.29	121.28
1	B	262	GLN	OE1-CD-NE2	-6.77	115.83	122.60
1	B	199	GLN	CA-C-O	-6.76	112.82	120.32
1	A	108	PHE	CA-CB-CG	-6.73	107.07	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	5	GLY	CA-C-O	6.73	126.17	119.04
1	B	89	GLU	CB-CG-CD	6.72	124.02	112.60
1	A	43	ARG	NE-CZ-NH2	6.72	125.25	119.20
1	A	243	ARG	N-CA-CB	-6.72	100.78	110.65
1	A	89	GLU	CA-CB-CG	-6.67	100.77	114.10
1	A	314	GLU	CB-CG-CD	6.67	123.93	112.60
1	A	32	GLY	CA-C-O	-6.64	112.25	119.82
1	A	299	GLY	O-C-N	6.64	128.41	121.77
1	A	337	ARG	NE-CZ-NH2	6.64	125.18	119.20
1	B	77	ILE	CA-C-O	-6.63	112.49	120.78
1	A	84	ASN	OD1-CG-ND2	-6.60	116.00	122.60
1	A	183	ASP	CA-C-O	-6.59	111.40	119.18
1	B	326	ILE	N-CA-CB	-6.59	101.23	110.26
1	B	338	ILE	N-CA-C	-6.58	101.64	108.15
1	B	295	VAL	O-C-N	6.56	129.36	122.67
1	B	272	LEU	O-C-N	-6.54	115.19	122.12
1	A	263	GLU	CA-C-O	-6.54	113.96	120.82
1	A	203	GLN	OE1-CD-NE2	-6.51	116.09	122.60
1	A	127	GLN	CG-CD-NE2	6.50	126.14	116.40
1	B	78	GLU	N-CA-C	6.50	118.36	111.28
1	A	344	PRO	N-CA-C	6.47	125.80	112.47
1	A	344	PRO	CA-N-CD	-6.47	102.95	112.00
1	B	245	SER	CA-CB-OG	-6.41	98.28	111.10
1	A	107	ASP	O-C-N	6.40	129.44	122.15
1	B	157	ARG	CD-NE-CZ	6.40	133.35	124.40
1	A	210	LEU	CA-C-O	-6.39	114.27	121.81
1	A	252	GLN	OE1-CD-NE2	6.39	128.99	122.60
1	B	161	ALA	N-CA-C	6.32	117.84	111.07
1	B	119	ASN	CA-C-N	6.32	131.69	121.83
1	B	119	ASN	C-N-CA	6.32	131.69	121.83
1	B	277	HIS	CA-CB-CG	-6.32	107.48	113.80
1	B	74	PHE	CA-CB-CG	-6.29	107.51	113.80
1	B	18	PHE	CA-C-O	6.26	124.87	118.73
1	A	92	ALA	CA-C-O	-6.25	113.93	120.55
1	A	115	VAL	CA-C-N	6.23	126.89	119.98
1	A	115	VAL	C-N-CA	6.23	126.89	119.98
1	A	68	ASP	CA-CB-CG	6.21	118.81	112.60
1	A	26	GLN	N-CA-C	6.21	117.84	111.14
1	B	91	VAL	CA-C-N	6.20	128.59	120.28
1	B	91	VAL	C-N-CA	6.20	128.59	120.28
1	A	280	ASN	OD1-CG-ND2	-6.18	116.42	122.60
1	B	113	GLY	CA-C-N	6.17	128.83	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	113	GLY	C-N-CA	6.17	128.83	120.44
1	B	298	PHE	CA-C-O	-6.16	113.91	121.06
1	B	46	PHE	CA-C-N	6.14	129.12	120.28
1	B	46	PHE	C-N-CA	6.14	129.12	120.28
1	A	320	THR	CA-CB-OG1	6.14	118.81	109.60
1	B	137	GLN	O-C-N	6.14	130.26	123.33
1	A	314	GLU	CA-C-N	6.13	129.46	120.82
1	A	314	GLU	C-N-CA	6.13	129.46	120.82
1	A	102	GLY	O-C-N	-6.11	117.01	122.57
1	B	48	ASP	CB-CG-OD2	6.09	132.42	118.40
1	A	10	SER	N-CA-C	-6.08	105.83	113.18
1	A	174	SER	CA-C-N	6.08	129.25	120.38
1	A	174	SER	C-N-CA	6.08	129.25	120.38
1	A	118	SER	CA-CB-OG	-6.07	98.96	111.10
1	B	30	HIS	CB-CA-C	-6.07	102.75	112.09
1	B	42	LEU	CA-C-N	6.06	128.40	120.28
1	B	42	LEU	C-N-CA	6.06	128.40	120.28
1	A	255	VAL	CA-C-O	6.05	128.34	120.78
1	A	44	MET	CA-C-N	6.04	128.17	120.56
1	A	44	MET	C-N-CA	6.04	128.17	120.56
1	A	130	LEU	CA-C-O	-6.02	114.33	120.71
1	A	4	ASP	CA-C-O	-6.02	111.22	119.05
1	B	134	GLU	N-CA-CB	-6.02	100.29	109.92
1	B	287	GLU	CA-C-O	-6.00	112.22	119.49
1	B	306	ALA	CA-C-O	6.00	127.50	120.96
1	B	247	THR	CA-C-N	5.98	128.61	120.54
1	B	247	THR	C-N-CA	5.98	128.61	120.54
1	A	152	ASP	CA-C-O	-5.96	114.23	120.55
1	A	161	ALA	O-C-N	-5.95	115.94	122.07
1	B	221	ILE	CA-C-N	5.94	129.81	121.02
1	B	221	ILE	C-N-CA	5.94	129.81	121.02
1	A	16	ALA	CA-C-O	-5.93	111.33	119.05
1	B	261	LEU	O-C-N	-5.92	115.93	122.09
1	A	337	ARG	CB-CA-C	5.92	120.43	109.54
1	A	312	ASP	O-C-N	5.91	130.80	122.41
1	A	89	GLU	CA-C-O	-5.88	113.21	119.97
1	B	320	THR	O-C-N	5.87	128.72	121.79
1	B	49	SER	N-CA-C	5.87	117.76	111.36
1	A	77	ILE	CA-CB-CG1	-5.87	100.43	110.40
1	A	51	ALA	CA-C-N	5.86	131.45	122.25
1	A	51	ALA	C-N-CA	5.86	131.45	122.25
1	A	252	GLN	CG-CD-NE2	-5.86	107.61	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	40	GLU	CA-C-N	5.86	128.13	120.28
1	B	40	GLU	C-N-CA	5.86	128.13	120.28
1	A	11	ASN	CB-CG-OD1	-5.85	109.10	120.80
1	A	144	VAL	O-C-N	5.84	126.92	121.61
1	B	2	CYS	CA-C-O	-5.83	114.88	119.66
1	B	337	ARG	NH1-CZ-NH2	-5.83	111.72	119.30
1	B	3	PRO	O-C-N	-5.82	114.78	122.64
1	A	41	ALA	N-CA-CB	5.82	118.68	110.12
1	A	26	GLN	O-C-N	-5.82	115.81	122.09
1	B	266	GLN	OE1-CD-NE2	-5.79	116.81	122.60
1	A	277	HIS	CA-CB-CG	-5.79	108.01	113.80
1	B	152	ASP	CA-C-O	5.79	126.68	120.55
1	A	221	ILE	CB-CG1-CD1	-5.77	101.69	113.80
1	B	115	VAL	O-C-N	-5.76	116.27	121.91
1	B	137	GLN	OE1-CD-NE2	5.75	128.35	122.60
1	A	12	ALA	CA-C-O	-5.74	113.62	120.10
1	A	161	ALA	CA-C-O	5.73	126.84	120.82
1	A	49	SER	N-CA-C	5.73	117.60	111.36
1	B	113	GLY	O-C-N	-5.73	116.63	122.19
1	B	130	LEU	CA-C-O	-5.73	114.19	120.43
1	B	131	GLY	CA-C-N	5.72	130.81	122.98
1	B	131	GLY	C-N-CA	5.72	130.81	122.98
1	A	250	GLU	O-C-N	5.71	128.66	122.15
1	B	215	PHE	N-CA-C	-5.71	102.85	109.93
1	A	37	GLU	CA-C-N	5.71	127.92	120.28
1	A	37	GLU	C-N-CA	5.71	127.92	120.28
1	A	57	GLN	CB-CG-CD	5.71	122.30	112.60
1	B	111	PHE	CA-C-O	-5.70	114.83	120.70
1	A	74	PHE	CA-CB-CG	-5.70	108.11	113.80
1	B	101	HIS	CA-CB-CG	-5.69	108.11	113.80
1	A	321	PRO	O-C-N	5.68	130.22	123.06
1	B	179	ALA	N-CA-C	5.67	117.46	108.79
1	B	24	ILE	CA-C-O	-5.66	114.35	120.47
1	A	282	MET	CA-C-O	-5.66	114.76	121.66
1	B	36	ALA	CA-C-N	5.66	127.86	120.28
1	B	36	ALA	C-N-CA	5.66	127.86	120.28
1	A	137	GLN	N-CA-CB	-5.65	101.01	111.52
1	B	199	GLN	CG-CD-NE2	-5.64	107.93	116.40
1	B	82	HIS	CA-CB-CG	-5.63	108.17	113.80
1	B	202	SER	CA-C-O	-5.63	112.61	119.43
1	B	25	GLN	OE1-CD-NE2	-5.63	116.97	122.60
1	A	125	GLN	CG-CD-NE2	5.62	124.83	116.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	ALA	CA-C-O	-5.61	115.02	121.47
1	A	20	VAL	CA-C-O	-5.60	114.91	120.85
1	B	23	ASP	N-CA-CB	-5.59	101.90	110.01
1	A	20	VAL	N-CA-C	-5.59	105.07	110.72
1	A	219	THR	CA-C-N	5.59	130.50	120.77
1	A	219	THR	C-N-CA	5.59	130.50	120.77
1	A	43	ARG	CD-NE-CZ	5.58	132.21	124.40
1	B	48	ASP	CA-C-N	5.55	128.17	120.29
1	B	48	ASP	C-N-CA	5.55	128.17	120.29
1	A	173	LEU	CA-C-N	5.55	128.27	120.28
1	A	173	LEU	C-N-CA	5.55	128.27	120.28
1	A	222	GLN	CG-CD-NE2	5.54	124.71	116.40
1	B	247	THR	N-CA-C	5.54	120.31	113.50
1	A	18	PHE	CA-CB-CG	-5.53	108.27	113.80
1	A	230	LYS	CG-CD-CE	5.51	123.97	111.30
1	B	81	TYR	O-C-N	5.51	129.18	122.96
1	B	24	ILE	O-C-N	5.50	128.02	121.80
1	B	95	LYS	N-CA-C	5.50	121.03	113.77
1	A	137	GLN	OE1-CD-NE2	5.49	128.09	122.60
1	A	248	ALA	N-CA-C	5.48	117.69	111.11
1	B	32	GLY	CA-C-O	-5.48	113.57	119.82
1	B	188	ILE	N-CA-C	5.48	116.17	108.17
1	B	2	CYS	O-C-N	5.47	129.48	121.54
1	B	327	THR	CA-C-N	5.47	129.00	120.68
1	B	327	THR	C-N-CA	5.47	129.00	120.68
1	A	57	GLN	CB-CA-C	-5.47	102.29	110.88
1	A	329	PRO	O-C-N	-5.47	116.33	123.06
1	B	259	THR	CA-C-O	-5.47	114.75	120.55
1	A	227	SER	O-C-N	5.46	126.12	121.20
1	A	88	ASP	CA-CB-CG	5.46	118.06	112.60
1	B	328	ALA	O-C-N	5.45	127.52	121.53
1	A	143	LEU	O-C-N	5.41	129.02	122.48
1	B	327	THR	O-C-N	-5.41	116.89	123.16
1	A	33	GLN	CA-CB-CG	5.41	124.91	114.10
1	B	77	ILE	O-C-N	5.39	129.31	122.57
1	B	88	ASP	CA-CB-CG	5.38	117.98	112.60
1	B	299	GLY	CA-C-N	5.38	126.56	119.84
1	B	299	GLY	C-N-CA	5.38	126.56	119.84
1	A	280	ASN	CB-CA-C	5.37	121.54	110.31
1	B	118	SER	CA-CB-OG	-5.37	100.35	111.10
1	A	344	PRO	N-CA-CB	-5.37	97.61	103.25
1	A	16	ALA	O-C-N	5.37	129.87	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	201	ASP	OD1-CG-OD2	-5.37	110.01	122.90
1	A	153	GLN	CB-CG-CD	-5.37	103.48	112.60
1	A	263	GLU	O-C-N	5.35	127.58	122.07
1	A	30	HIS	N-CA-CB	-5.34	103.80	111.70
1	A	159	LEU	CA-C-N	5.33	127.36	120.44
1	A	159	LEU	C-N-CA	5.33	127.36	120.44
1	A	250	GLU	N-CA-CB	5.32	118.03	110.16
1	B	263	GLU	CG-CD-OE2	-5.32	106.17	118.40
1	A	303	PHE	CA-C-O	5.32	127.41	121.40
1	B	34	CYS	CA-C-N	5.31	129.27	122.85
1	B	34	CYS	C-N-CA	5.31	129.27	122.85
1	A	91	VAL	CA-C-N	5.30	127.38	120.28
1	A	91	VAL	C-N-CA	5.30	127.38	120.28
1	A	120	CYS	CA-C-O	-5.30	115.40	119.32
1	A	220	GLY	N-CA-C	5.29	122.09	114.10
1	B	90	VAL	CA-C-O	5.29	126.46	120.85
1	A	335	VAL	CA-C-O	5.29	126.08	120.48
1	B	184	VAL	N-CA-C	-5.29	105.98	111.58
1	A	157	ARG	NE-CZ-NH2	5.29	123.96	119.20
1	A	37	GLU	CA-C-O	-5.28	114.96	120.55
1	A	203	GLN	CG-CD-NE2	5.27	124.31	116.40
1	B	256	ASN	CA-C-O	-5.26	114.28	120.81
1	A	113	GLY	CA-C-N	5.26	127.76	120.29
1	A	113	GLY	C-N-CA	5.26	127.76	120.29
1	A	271	ALA	O-C-N	-5.25	116.66	122.07
1	A	63	GLY	CA-C-O	-5.25	112.49	119.10
1	A	61	LYS	CA-C-O	-5.25	115.23	121.16
1	A	204	PHE	CA-C-N	5.24	127.73	120.29
1	A	204	PHE	C-N-CA	5.24	127.73	120.29
1	A	101	HIS	O-C-N	5.24	129.29	122.42
1	B	256	ASN	CB-CG-ND2	-5.24	108.55	116.40
1	A	35	GLY	CA-C-N	5.23	127.61	120.54
1	A	35	GLY	C-N-CA	5.23	127.61	120.54
1	B	165	ASP	CA-CB-CG	5.23	117.83	112.60
1	A	167	ILE	CA-CB-CG2	5.23	119.39	110.50
1	A	235	LEU	CA-C-N	-5.23	113.28	120.28
1	A	235	LEU	C-N-CA	-5.23	113.28	120.28
1	A	0	VAL	CG1-CB-CG2	-5.22	99.31	110.80
1	A	218	LYS	CA-C-O	5.22	127.01	121.16
1	A	255	VAL	O-C-N	-5.21	116.05	122.57
1	A	222	GLN	CG-CD-OE1	-5.21	110.37	120.80
1	B	48	ASP	N-CA-CB	5.21	117.73	110.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	39	HIS	CA-C-N	5.21	127.26	120.28
1	A	39	HIS	C-N-CA	5.21	127.26	120.28
1	B	23	ASP	CB-CA-C	5.20	119.05	110.88
1	A	258	GLN	CG-CD-NE2	5.20	124.20	116.40
1	B	176	HIS	CA-CB-CG	-5.20	108.60	113.80
1	A	141	ASP	CA-C-O	-5.19	115.97	121.94
1	B	129	PHE	CA-CB-CG	-5.19	108.61	113.80
1	B	207	GLU	N-CA-C	5.19	117.02	111.36
1	A	315	GLN	CG-CD-NE2	5.18	124.18	116.40
1	A	127	GLN	CA-CB-CG	-5.18	103.75	114.10
1	A	39	HIS	ND1-CG-CD2	5.17	111.27	106.10
1	B	166	GLU	CA-C-N	5.17	127.03	120.72
1	B	166	GLU	C-N-CA	5.17	127.03	120.72
1	A	219	THR	CA-C-O	5.17	126.94	121.05
1	A	220	GLY	O-C-N	5.17	127.47	122.41
1	A	78	GLU	CA-C-O	-5.16	114.04	119.97
1	A	94	GLN	CA-C-O	-5.15	113.72	119.79
1	B	250	GLU	N-CA-C	-5.14	105.75	111.36
1	A	13	ALA	CA-C-N	5.14	128.12	120.31
1	A	13	ALA	C-N-CA	5.14	128.12	120.31
1	B	33	GLN	CA-C-O	-5.13	115.66	121.72
1	B	20	VAL	N-CA-C	-5.13	105.54	110.72
1	B	314	GLU	CG-CD-OE1	5.12	130.18	118.40
1	A	33	GLN	CA-C-N	5.11	129.70	122.24
1	A	33	GLN	C-N-CA	5.11	129.70	122.24
1	B	26	GLN	CA-CB-CG	-5.11	103.88	114.10
1	A	97	PHE	CA-CB-CG	-5.11	108.69	113.80
1	A	179	ALA	N-CA-C	5.10	116.82	108.76
1	A	153	GLN	CG-CD-NE2	-5.09	108.76	116.40
1	B	103	VAL	N-CA-C	-5.09	102.06	109.29
1	B	184	VAL	CA-C-O	-5.09	114.81	120.46
1	B	338	ILE	CB-CA-C	-5.08	106.25	111.08
1	A	266	GLN	CA-CB-CG	-5.08	103.94	114.10
1	B	194	ASP	N-CA-CB	5.08	119.84	111.62
1	A	167	ILE	CB-CG1-CD1	5.07	124.44	113.80
1	B	61	LYS	CA-C-O	-5.05	115.45	121.16
1	A	59	GLN	CB-CA-C	-5.04	102.05	110.56
1	A	246	ARG	NH1-CZ-NH2	-5.04	112.75	119.30
1	A	77	ILE	CB-CG1-CD1	-5.03	103.23	113.80
1	B	258	GLN	OE1-CD-NE2	-5.01	117.59	122.60
1	A	262	GLN	O-C-N	5.01	127.50	122.09
1	B	134	GLU	CA-CB-CG	-5.01	104.09	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	259	THR	CA-CB-OG1	-5.00	102.10	109.60
1	A	129	PHE	CA-CB-CG	-5.00	108.80	113.80

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2569	0	2449	28	0
1	B	2569	0	2447	33	0
2	C	38	0	34	7	0
3	D	22	0	19	4	0
4	A	14	0	13	0	0
5	A	22	0	20	0	0
5	B	33	0	30	5	0
6	A	2	0	0	0	0
6	B	2	0	0	0	0
7	A	43	0	30	4	0
7	B	43	0	30	4	0
8	A	267	0	0	3	0
8	B	197	0	0	1	0
All	All	5821	0	5072	70	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 7.

All (70) 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:11:ASN:HD22	1:A:13:ALA:H	0.99	0.93
1:B:260:LYS:HE3	2:C:3:FUC:H2	1.54	0.90
1:B:4:ASP:HB3	1:B:6:VAL:H	1.36	0.89
1:B:211:ARG:NH1	1:B:211:ARG:HB2	1.95	0.82
1:B:4:ASP:OD2	1:B:7:HIS:ND1	2.12	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:ILE:HD11	1:B:240:LEU:HB2	1.64	0.79
1:A:11:ASN:ND2	1:A:13:ALA:H	1.78	0.79
1:B:253:SER:HB2	2:C:3:FUC:H63	1.65	0.78
5:B:380:MAN:H62	2:C:3:FUC:H62	1.67	0.77
1:B:211:ARG:HB2	1:B:211:ARG:HH11	1.50	0.77
1:B:11:ASN:HD22	1:B:13:ALA:H	1.34	0.75
1:B:319:SER:HB2	5:B:380:MAN:H2	1.69	0.75
1:A:25:GLN:HE21	1:A:25:GLN:HA	1.51	0.74
5:B:380:MAN:C6	2:C:3:FUC:H62	2.20	0.72
1:A:11:ASN:HD22	1:A:13:ALA:N	1.83	0.71
1:B:25:GLN:HE21	1:B:25:GLN:HA	1.56	0.69
1:B:260:LYS:CE	2:C:3:FUC:H2	2.22	0.69
8:B:591:HOH:O	2:C:3:FUC:H61	1.92	0.68
1:A:150:THR:OG1	1:A:153:GLN:HG3	1.93	0.68
1:A:227:SER:HB2	1:A:228:PRO:HD2	1.79	0.65
1:B:311:ALA:HA	3:D:2:MAN:O4	1.98	0.64
1:A:127:GLN:NE2	1:A:270:THR:OG1	2.30	0.63
1:A:25:GLN:HA	1:A:25:GLN:NE2	2.15	0.62
1:A:23:ASP:OD2	1:A:100:LYS:HE3	2.01	0.60
1:A:300:PRO:HG3	1:B:326:ILE:HG13	1.85	0.59
7:A:350:HEM:HHC	7:A:350:HEM:HBB2	1.85	0.59
1:B:218:LYS:HB3	1:B:221:ILE:HD11	1.85	0.58
1:B:244:ASP:OD1	1:B:246:ARG:HD3	2.03	0.58
1:A:230:LYS:HD2	8:A:472:HOH:O	2.03	0.57
1:A:326:ILE:H	1:A:326:ILE:HD13	1.70	0.56
7:B:350:HEM:HHC	7:B:350:HEM:HBB2	1.88	0.56
1:B:151:ILE:HD11	1:B:240:LEU:CB	2.35	0.53
1:B:18:PHE:HB2	1:B:19:PRO:HD3	1.90	0.53
1:B:310:HIS:HB3	3:D:2:MAN:H5	1.91	0.53
1:B:11:ASN:ND2	1:B:13:ALA:H	2.03	0.52
1:B:320:THR:HG21	5:B:380:MAN:O6	2.10	0.52
1:B:311:ALA:N	3:D:2:MAN:H62	2.26	0.50
7:A:350:HEM:HBB2	7:A:350:HEM:CHC	2.41	0.50
1:A:0:VAL:HG13	1:A:9:ALA:O	2.11	0.50
1:B:4:ASP:HB3	1:B:6:VAL:N	2.17	0.50
1:B:25:GLN:HA	1:B:25:GLN:NE2	2.22	0.48
1:B:211:ARG:HH11	1:B:211:ARG:CB	2.23	0.47
1:A:151:ILE:HD11	1:A:240:LEU:HB2	1.96	0.46
1:B:62:PHE:CE2	1:B:64:GLY:HA2	2.51	0.45
1:B:0:VAL:HB	1:B:9:ALA:O	2.16	0.45
1:A:18:PHE:HB2	1:A:19:PRO:HD3	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:SER:HA	8:A:700:HOH:O	2.17	0.45
1:A:211:ARG:HG3	1:A:312:ASP:O	2.16	0.45
1:A:121:PRO:HD2	1:A:198:GLY:O	2.16	0.45
5:B:380:MAN:H61	2:C:3:FUC:H62	1.94	0.44
1:B:70:SER:OG	1:B:78:GLU:OE2	2.35	0.44
7:B:350:HEM:HBB2	7:B:350:HEM:CHC	2.48	0.44
1:A:207:GLU:OE1	1:A:232:GLU:OE1	2.35	0.44
1:A:230:LYS:HD3	1:A:230:LYS:HA	1.37	0.43
1:B:127:GLN:NE2	1:B:270:THR:OG1	2.48	0.43
1:A:62:PHE:CE2	1:A:64:GLY:HA2	2.54	0.42
1:A:91:VAL:HG12	1:A:95:LYS:HE3	2.01	0.42
1:B:311:ALA:H	3:D:2:MAN:H62	1.85	0.42
1:A:183:ASP:OD2	7:A:350:HEM:O2A	2.37	0.42
1:A:54:PRO:HD2	1:A:160:ASP:OD1	2.20	0.41
7:B:350:HEM:HHC	7:B:350:HEM:CBB	2.49	0.41
1:B:67:ALA:O	1:B:132:ARG:HD3	2.20	0.41
1:A:344:PRO:O	1:A:345:ASN:C	2.63	0.41
1:A:230:LYS:CD	8:A:472:HOH:O	2.67	0.41
1:B:183:ASP:OD2	7:B:350:HEM:O2A	2.39	0.41
1:A:288:VAL:O	1:A:288:VAL:HG12	2.20	0.41
1:B:62:PHE:CZ	1:B:64:GLY:HA2	2.56	0.41
7:A:350:HEM:HHC	7:A:350:HEM:CBB	2.49	0.41
1:B:331:PRO:O	1:B:332:SER:C	2.65	0.40
1:A:180:ALA:HA	1:A:192:PRO:HA	2.02	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	341/345 (99%)	332 (97%)	7 (2%)	2 (1%)	21 11

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	341/345 (99%)	326 (96%)	14 (4%)	1 (0%)	36	25
All	All	682/690 (99%)	658 (96%)	21 (3%)	3 (0%)	30	19

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	344	PRO
1	A	131	GLY
1	B	131	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	274/275 (100%)	262 (96%)	12 (4%)	25	13
1	B	274/275 (100%)	264 (96%)	10 (4%)	31	18
All	All	548/550 (100%)	526 (96%)	22 (4%)	28	15

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	0	VAL
1	A	11	ASN
1	A	61	LYS
1	A	136	THR
1	A	167	ILE
1	A	199	GLN
1	A	219	THR
1	A	230	LYS
1	A	245	SER
1	A	326	ILE
1	A	337	ARG
1	A	344	PRO
1	B	6	VAL

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Mol	Chain	Res	Type
1	B	11	ASN
1	B	25	GLN
1	B	61	LYS
1	B	71	ILE
1	B	219	THR
1	B	230	LYS
1	B	246	ARG
1	B	319	SER
1	B	326	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	11	ASN
1	A	25	GLN
1	A	59	GLN
1	A	119	ASN
1	A	125	GLN
1	A	127	GLN
1	A	182	ASN
1	B	11	ASN
1	B	25	GLN
1	B	33	GLN
1	B	94	GLN
1	B	119	ASN
1	B	127	GLN
1	B	239	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

2 non-standard protein/DNA/RNA residues 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	$\# Z > 2$
1	HTR	A	171	1	13,16,17	1.04	0	17,22,24	1.73	5 (29%)
1	HTR	B	171	1	13,16,17	1.11	1 (7%)	17,22,24	1.60	4 (23%)

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
1	HTR	A	171	1	-	3/9/10/12	0/2/2/2
1	HTR	B	171	1	-	4/9/10/12	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	171	HTR	OH-CB	2.51	1.47	1.42

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	171	HTR	OH-CB-CA	3.91	116.07	107.49
1	A	171	HTR	CZ3-CH2-CZ2	3.26	124.26	120.24
1	A	171	HTR	OH-CB-CA	3.06	114.20	107.49
1	A	171	HTR	O-C-CA	-3.05	116.93	124.77
1	B	171	HTR	O-C-CA	-2.48	118.39	124.77
1	A	171	HTR	CG-CD1-NE1	-2.42	108.34	110.31
1	B	171	HTR	CD2-CG-CD1	2.42	108.10	106.25
1	B	171	HTR	CG-CD1-NE1	-2.21	108.52	110.31
1	A	171	HTR	CD2-CG-CD1	2.09	107.85	106.25

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	171	HTR	O-C-CA-CB
1	B	171	HTR	O-C-CA-CB
1	A	171	HTR	CA-CB-CG-CD1

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Mol	Chain	Res	Type	Atoms
1	B	171	HTR	CA-CB-CG-CD1
1	B	171	HTR	CA-CB-CG-CD2
1	A	171	HTR	N-CA-CB-OH
1	B	171	HTR	N-CA-CB-OH

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

5 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	1.41	2 (14%)	17,19,21	3.49	5 (29%)
2	NAG	C	2	2	14,14,15	1.22	1 (7%)	17,19,21	3.19	10 (58%)
2	FUC	C	3	2	10,10,11	1.57	2 (20%)	14,14,16	2.41	5 (35%)
3	MAN	D	1	1,3	11,11,12	0.68	0	15,15,17	2.26	6 (40%)
3	MAN	D	2	3	11,11,12	0.85	1 (9%)	15,15,17	1.89	4 (26%)

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	-	4/6/23/26	0/1/1/1
2	NAG	C	2	2	-	2/6/23/26	0/1/1/1
2	FUC	C	3	2	1/1/4/5	-	0/1/1/1
3	MAN	D	1	1,3	-	2/2/19/22	0/1/1/1
3	MAN	D	2	3	-	0/2/19/22	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	3	FUC	O5-C5	3.63	1.50	1.43
2	C	1	NAG	O7-C7	-3.16	1.16	1.23
2	C	2	NAG	O7-C7	-2.90	1.16	1.23
2	C	1	NAG	O6-C6	-2.46	1.32	1.42
3	D	2	MAN	C1-C2	2.16	1.57	1.52
2	C	3	FUC	O2-C2	2.12	1.47	1.43

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1	NAG	C1-O5-C5	9.05	124.31	112.19
2	C	1	NAG	C4-C3-C2	-6.81	101.04	111.02
2	C	1	NAG	O4-C4-C5	6.42	125.14	109.32
2	C	2	NAG	C1-O5-C5	-5.70	104.55	112.19
2	C	2	NAG	C1-C2-N2	5.45	119.01	110.43
2	C	3	FUC	C3-C4-C5	5.33	117.91	109.81
2	C	2	NAG	C3-C4-C5	4.92	119.14	110.23
2	C	2	NAG	O6-C6-C5	4.50	126.67	111.33
2	C	3	FUC	O5-C5-C4	4.25	117.20	109.55
2	C	2	NAG	O5-C1-C2	-4.10	104.95	111.29
3	D	2	MAN	O4-C4-C5	4.06	119.33	109.32
2	C	1	NAG	O5-C5-C6	-4.00	99.88	107.66
2	C	2	NAG	C4-C3-C2	-3.86	105.37	111.02
3	D	2	MAN	C6-C5-C4	3.80	122.34	113.02
3	D	1	MAN	O4-C4-C3	-3.72	101.61	110.38
3	D	1	MAN	C1-O5-C5	3.62	117.04	112.19
3	D	1	MAN	O2-C2-C3	-3.62	102.66	110.15
2	C	3	FUC	C1-O5-C5	-3.49	104.73	112.97
3	D	1	MAN	C2-C3-C4	3.44	116.92	110.86
2	C	3	FUC	C2-C3-C4	3.40	116.85	110.86
2	C	2	NAG	O3-C3-C2	3.12	115.88	109.40
3	D	2	MAN	O5-C5-C6	-2.77	102.27	107.66
2	C	2	NAG	C8-C7-N2	-2.63	111.76	116.12
3	D	1	MAN	C1-C2-C3	2.54	113.34	109.64
3	D	2	MAN	O4-C4-C3	-2.52	104.44	110.38
2	C	1	NAG	C3-C4-C5	-2.52	105.67	110.23
2	C	2	NAG	O7-C7-C8	2.40	126.33	122.05
2	C	3	FUC	O4-C4-C5	2.15	114.48	109.74
2	C	2	NAG	O5-C5-C4	2.14	116.03	110.83
3	D	1	MAN	O3-C3-C2	-2.00	105.96	110.05

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	3	FUC	C1

All (8) torsion outliers are listed below:

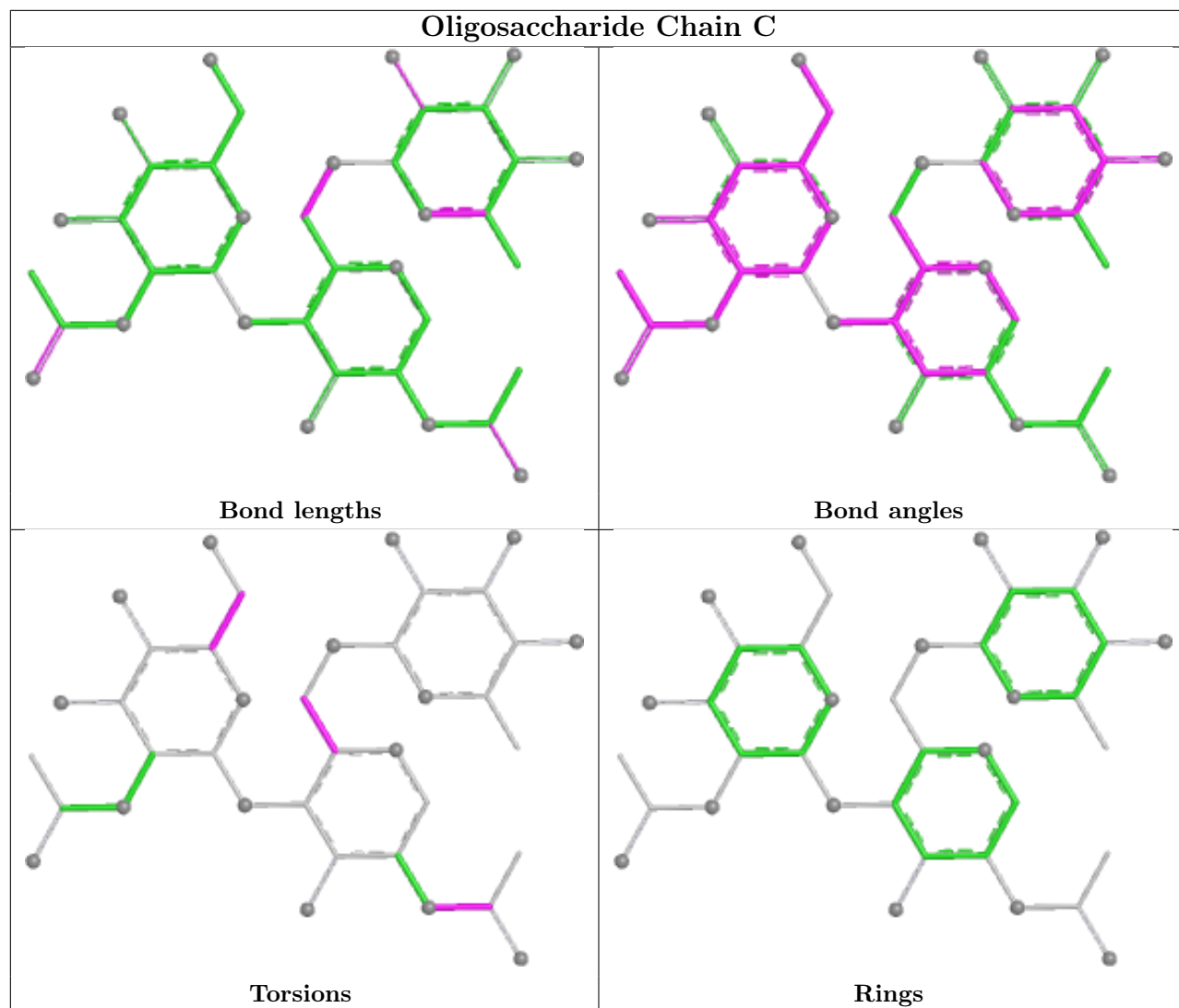
Mol	Chain	Res	Type	Atoms
2	C	1	NAG	C4-C5-C6-O6
2	C	1	NAG	O5-C5-C6-O6
3	D	1	MAN	C4-C5-C6-O6
2	C	1	NAG	C8-C7-N2-C2
2	C	1	NAG	O7-C7-N2-C2
2	C	2	NAG	O5-C5-C6-O6
3	D	1	MAN	O5-C5-C6-O6
2	C	2	NAG	C4-C5-C6-O6

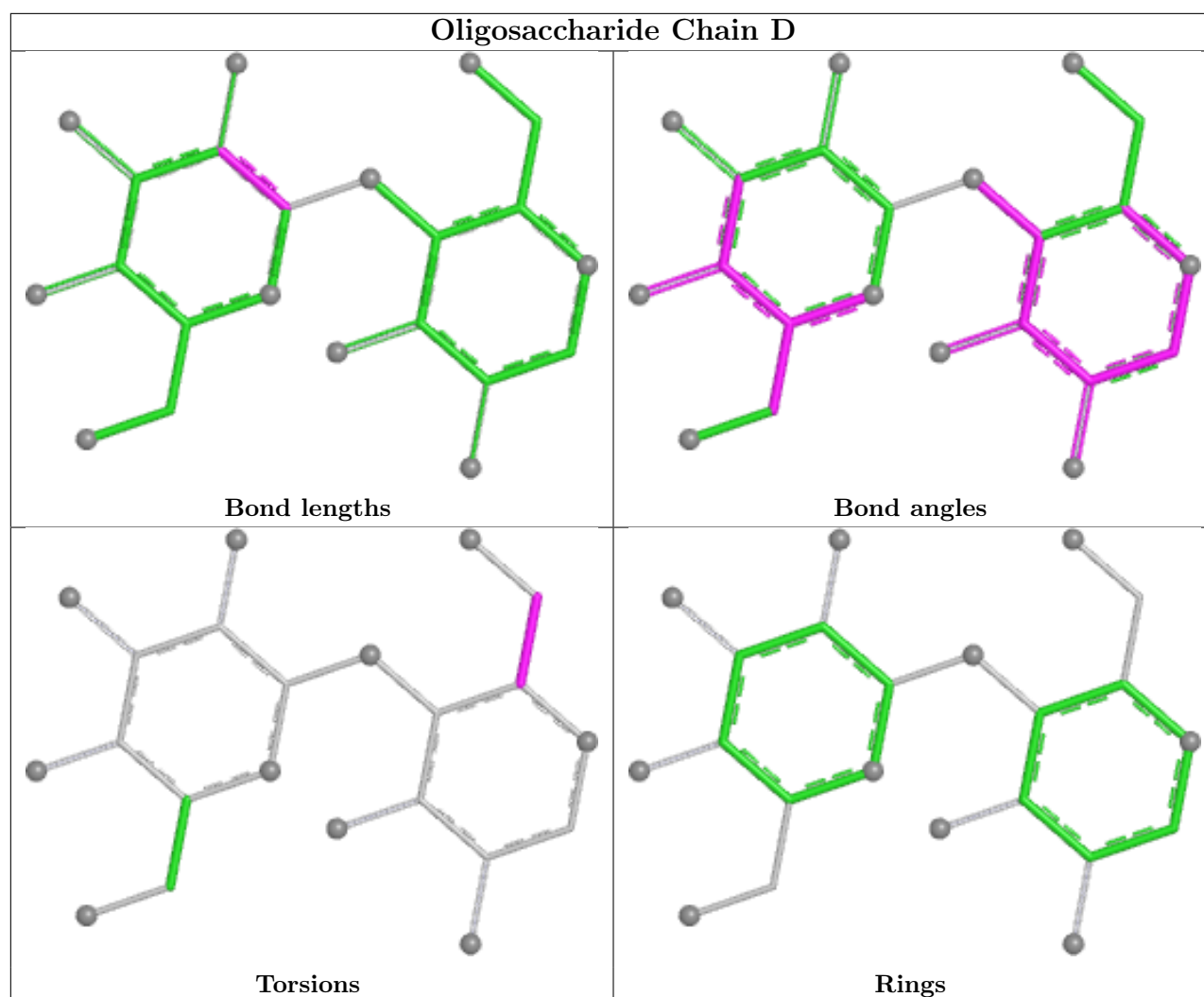
There are no ring outliers.

2 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	3	FUC	7	0
3	D	2	MAN	4	0

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





5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 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	HEM	A	350	1,8	50,50,50	2.11	13 (26%)	67,82,82	2.28	24 (35%)
5	MAN	A	370	1	11,11,12	1.18	1 (9%)	15,15,17	2.24	7 (46%)
5	MAN	B	380	1	11,11,12	0.90	0	15,15,17	1.41	1 (6%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
7	HEM	B	350	1,8	50,50,50	1.44	5 (10%)	67,82,82	1.52	14 (20%)
5	MAN	A	375	1	11,11,12	1.09	2 (18%)	15,15,17	2.12	6 (40%)
5	MAN	B	375	1	11,11,12	1.08	1 (9%)	15,15,17	2.35	5 (33%)
4	NAG	A	360	1	14,14,15	1.01	1 (7%)	17,19,21	2.02	5 (29%)
5	MAN	B	370	1	11,11,12	1.16	1 (9%)	15,15,17	1.55	1 (6%)

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
7	HEM	A	350	1,8	-	3/14/54/54	-
5	MAN	A	370	1	-	1/2/19/22	0/1/1/1
5	MAN	B	380	1	-	2/2/19/22	0/1/1/1
7	HEM	B	350	1,8	-	0/14/54/54	-
5	MAN	A	375	1	-	0/2/19/22	0/1/1/1
5	MAN	B	375	1	-	2/2/19/22	0/1/1/1
4	NAG	A	360	1	-	2/6/23/26	0/1/1/1
5	MAN	B	370	1	-	2/2/19/22	0/1/1/1

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	350	HEM	FE-NB	8.09	2.19	1.94
7	A	350	HEM	FE-ND	5.74	2.12	1.94
7	A	350	HEM	C1A-NA	5.16	1.49	1.39
7	B	350	HEM	FE-NB	4.74	2.09	1.94
7	B	350	HEM	CMC-C2C	3.81	1.58	1.50
4	A	360	NAG	O7-C7	-3.21	1.16	1.23
5	B	370	MAN	C1-C2	2.97	1.59	1.52
7	B	350	HEM	CAB-C3B	2.84	1.55	1.47
7	A	350	HEM	CAC-C3C	2.79	1.54	1.47
7	A	350	HEM	C1D-C2D	2.65	1.49	1.44
5	A	370	MAN	C1-C2	2.64	1.58	1.52
7	A	350	HEM	CMC-C2C	2.51	1.55	1.50
5	B	375	MAN	C1-C2	2.49	1.58	1.52
7	A	350	HEM	CAB-C3B	2.47	1.54	1.47
5	A	375	MAN	C4-C5	2.46	1.58	1.53
7	A	350	HEM	C1B-NB	-2.45	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	350	HEM	CHD-C4C	2.40	1.43	1.38
7	B	350	HEM	FE-NA	2.29	2.02	1.95
7	B	350	HEM	CAC-C3C	2.21	1.53	1.47
7	A	350	HEM	C1C-C2C	-2.14	1.41	1.45
7	A	350	HEM	C4A-NA	2.14	1.43	1.39
7	A	350	HEM	O2A-CGA	-2.06	1.24	1.30
5	A	375	MAN	C1-C2	2.06	1.57	1.52
7	A	350	HEM	C1C-NC	2.02	1.43	1.39

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	375	MAN	C1-O5-C5	6.34	120.69	112.19
7	A	350	HEM	C4D-ND-C1D	5.55	111.78	105.21
7	A	350	HEM	C1B-NB-C4B	5.55	111.78	105.21
4	A	360	NAG	C2-N2-C7	5.00	129.60	122.90
7	A	350	HEM	C3B-C4B-NB	-4.94	105.92	109.47
7	A	350	HEM	C3D-C4D-ND	-4.89	104.81	110.17
5	A	375	MAN	O3-C3-C2	-4.85	100.15	110.05
5	A	370	MAN	C6-C5-C4	4.66	124.47	113.02
5	B	370	MAN	C1-O5-C5	4.65	118.42	112.19
7	A	350	HEM	C2B-C1B-NB	-4.27	104.94	109.84
7	A	350	HEM	CAA-CBA-CGA	4.20	124.80	113.67
5	A	370	MAN	C2-C3-C4	4.11	118.08	110.86
7	A	350	HEM	C4A-NA-C1A	-4.10	99.13	105.82
7	A	350	HEM	C2D-C1D-ND	-3.90	105.39	109.90
5	B	380	MAN	C6-C5-C4	3.87	122.52	113.02
7	B	350	HEM	C4C-CHD-C1D	-3.85	117.83	126.02
7	A	350	HEM	O2A-CGA-CBA	3.70	125.70	114.00
7	A	350	HEM	CMB-C2B-C1B	-3.62	119.37	125.03
7	A	350	HEM	CHC-C4B-C3B	3.52	132.09	125.07
5	B	375	MAN	C2-C3-C4	3.43	116.90	110.86
7	A	350	HEM	O1A-CGA-CBA	-3.23	112.85	123.09
5	A	375	MAN	O6-C6-C5	-3.21	100.42	111.33
5	B	375	MAN	O2-C2-C1	-2.94	102.50	109.22
7	A	350	HEM	C4C-NC-C1C	-2.92	101.06	105.82
7	A	350	HEM	CMD-C2D-C1D	-2.90	120.51	125.03
7	B	350	HEM	CHD-C4C-NC	2.89	127.59	124.45
5	B	375	MAN	O5-C5-C6	-2.88	102.06	107.66
7	A	350	HEM	CAD-C3D-C4D	-2.85	119.73	124.70
4	A	360	NAG	O5-C5-C4	-2.81	104.00	110.83
4	A	360	NAG	O4-C4-C5	2.80	116.22	109.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	375	MAN	C6-C5-C4	2.73	119.73	113.02
5	A	370	MAN	C1-O5-C5	2.72	115.83	112.19
5	A	375	MAN	O2-C2-C1	-2.59	103.30	109.22
5	A	370	MAN	C1-C2-C3	2.59	113.41	109.64
7	B	350	HEM	CMD-C2D-C1D	-2.58	121.00	125.03
7	A	350	HEM	C3A-C4A-NA	2.58	114.27	110.14
7	B	350	HEM	CHD-C4C-C3C	-2.57	120.88	125.21
7	B	350	HEM	CMA-C3A-C2A	2.56	131.06	125.62
4	A	360	NAG	O5-C5-C6	-2.55	102.70	107.66
7	A	350	HEM	CHC-C4B-NB	-2.54	121.69	124.42
4	A	360	NAG	O3-C3-C4	-2.52	104.42	110.38
7	A	350	HEM	CHB-C4A-NA	-2.51	119.31	123.86
5	A	370	MAN	O3-C3-C2	-2.50	104.95	110.05
7	B	350	HEM	CMD-C2D-C3D	2.50	132.90	126.15
7	B	350	HEM	CAD-C3D-C4D	-2.49	120.35	124.70
7	B	350	HEM	CHA-C4D-ND	2.46	127.41	124.37
7	A	350	HEM	C3B-C2B-C1B	2.40	108.21	106.41
5	A	375	MAN	O3-C3-C4	2.34	115.90	110.38
7	B	350	HEM	CAC-C3C-C4C	-2.33	119.27	124.82
5	A	375	MAN	C2-C3-C4	2.24	114.79	110.86
7	B	350	HEM	C3B-C4B-NB	-2.22	107.88	109.47
5	A	370	MAN	O2-C2-C3	2.22	114.74	110.15
7	B	350	HEM	CHC-C4B-C3B	2.16	129.38	125.07
7	B	350	HEM	CMB-C2B-C1B	-2.13	121.71	125.03
7	A	350	HEM	CBB-CAB-C3B	-2.08	117.11	127.53
7	B	350	HEM	C3B-C2B-C1B	2.07	107.97	106.41
7	A	350	HEM	CAC-C3C-C4C	-2.07	119.89	124.82
5	A	370	MAN	O3-C3-C4	2.06	115.23	110.38
7	A	350	HEM	CHD-C1D-C2D	2.04	128.25	125.03
5	B	375	MAN	C6-C5-C4	2.04	118.03	113.02
7	A	350	HEM	C3C-C2C-C1C	2.03	108.97	107.05
7	A	350	HEM	CHD-C4C-C3C	-2.03	121.79	125.21
7	B	350	HEM	C4A-NA-C1A	-2.02	102.53	105.82

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	360	NAG	C8-C7-N2-C2
5	B	380	MAN	C4-C5-C6-O6
4	A	360	NAG	O7-C7-N2-C2
5	B	380	MAN	O5-C5-C6-O6

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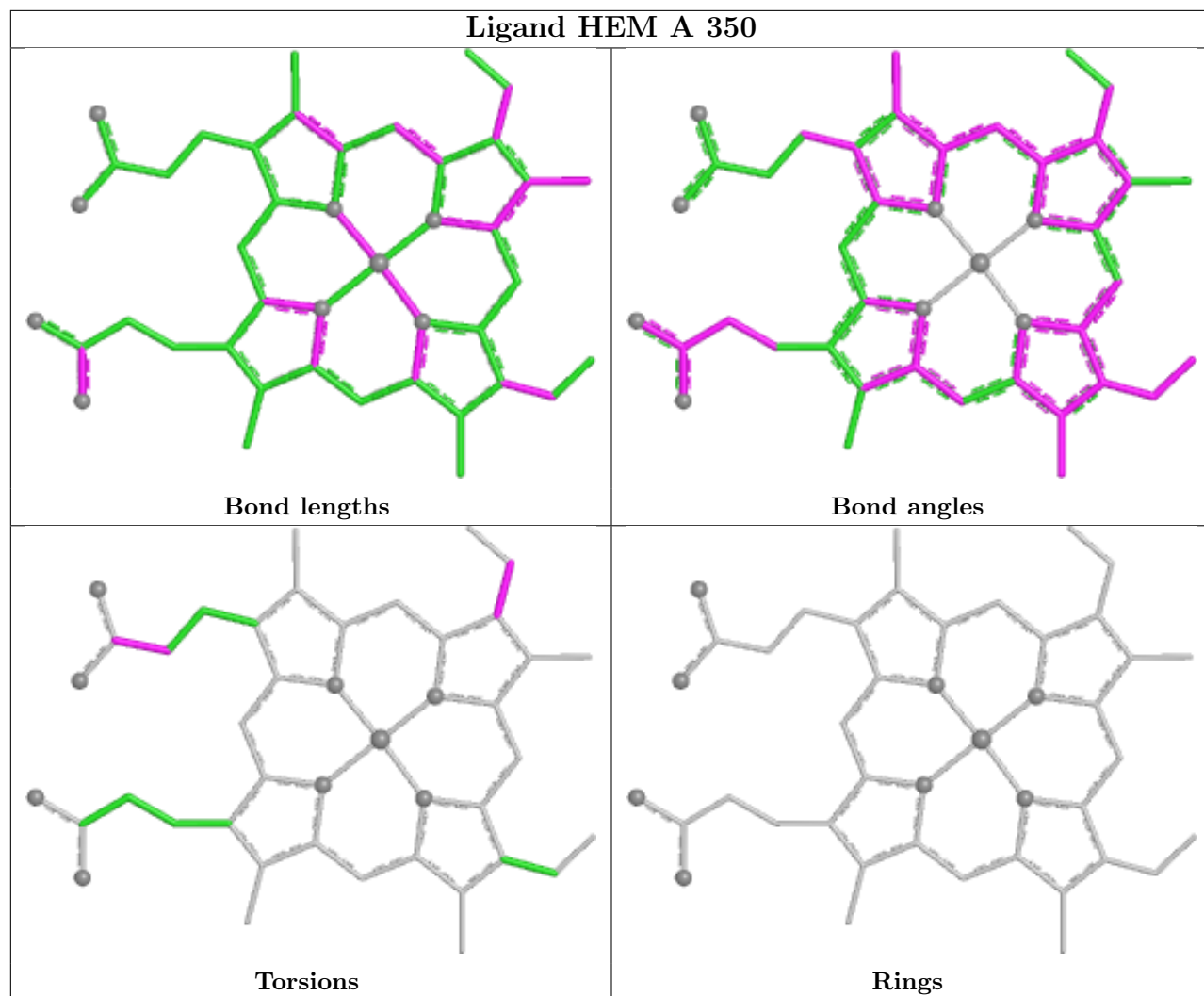
Mol	Chain	Res	Type	Atoms
5	B	370	MAN	O5-C5-C6-O6
5	B	375	MAN	C4-C5-C6-O6
5	A	370	MAN	O5-C5-C6-O6
7	A	350	HEM	C2C-C3C-CAC-CBC
5	B	375	MAN	O5-C5-C6-O6
7	A	350	HEM	CAD-CBD-CGD-O2D
5	B	370	MAN	C4-C5-C6-O6
7	A	350	HEM	CAD-CBD-CGD-O1D

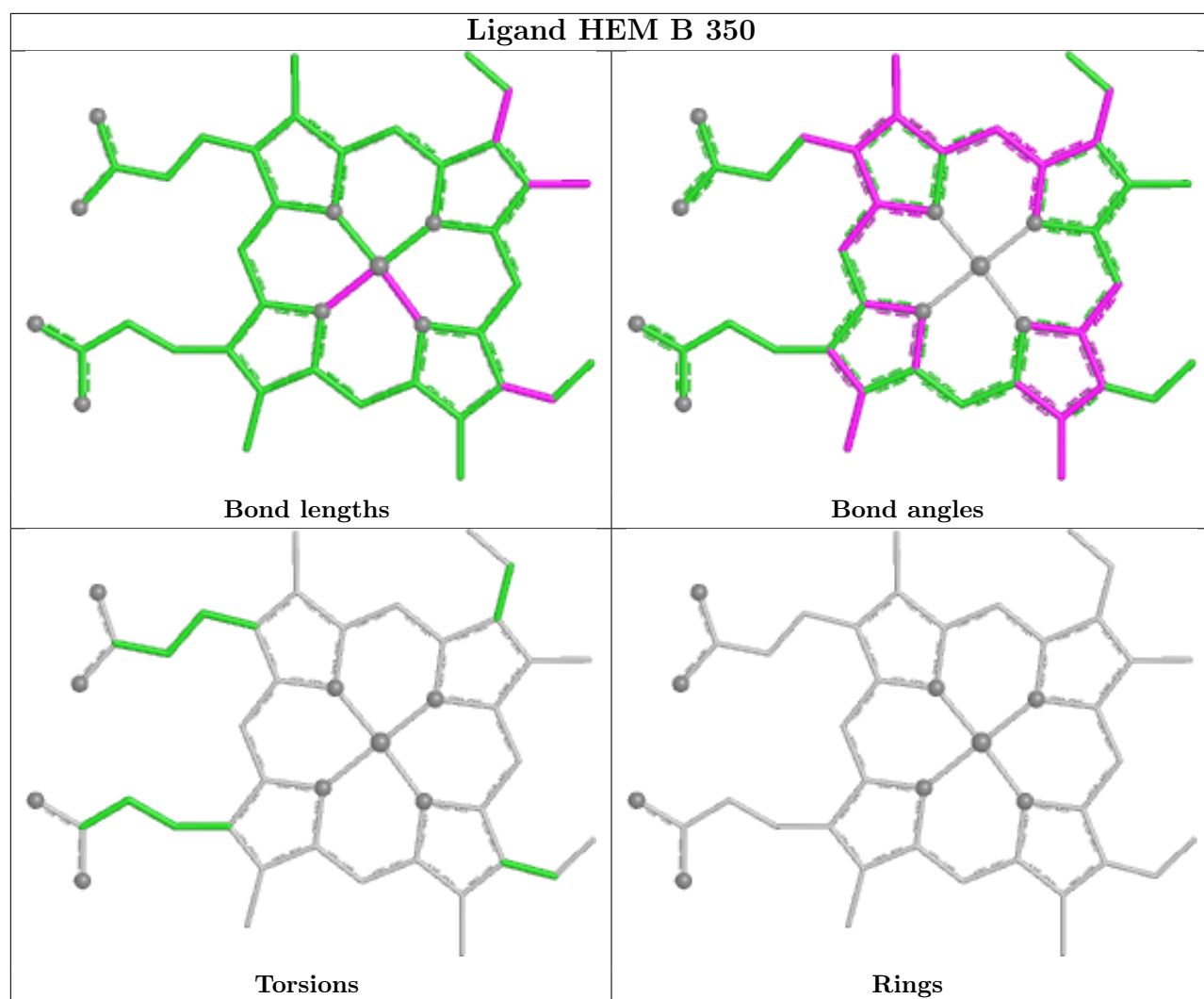
There are no ring outliers.

3 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	350	HEM	4	0
5	B	380	MAN	5	0
7	B	350	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 [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	343/345 (99%)	-0.63	2 (0%) 85 86	10, 18, 33, 91	0
1	B	343/345 (99%)	-0.37	6 (1%) 69 69	12, 22, 45, 97	0
All	All	686/690 (99%)	-0.50	8 (1%) 76 77	10, 20, 38, 97	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	GLY	3.3
1	A	344	PRO	3.1
1	B	6	VAL	3.1
1	B	343	SER	3.0
1	B	345	ASN	2.8
1	B	344	PRO	2.6
1	A	345	ASN	2.2
1	B	0	VAL	2.0

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

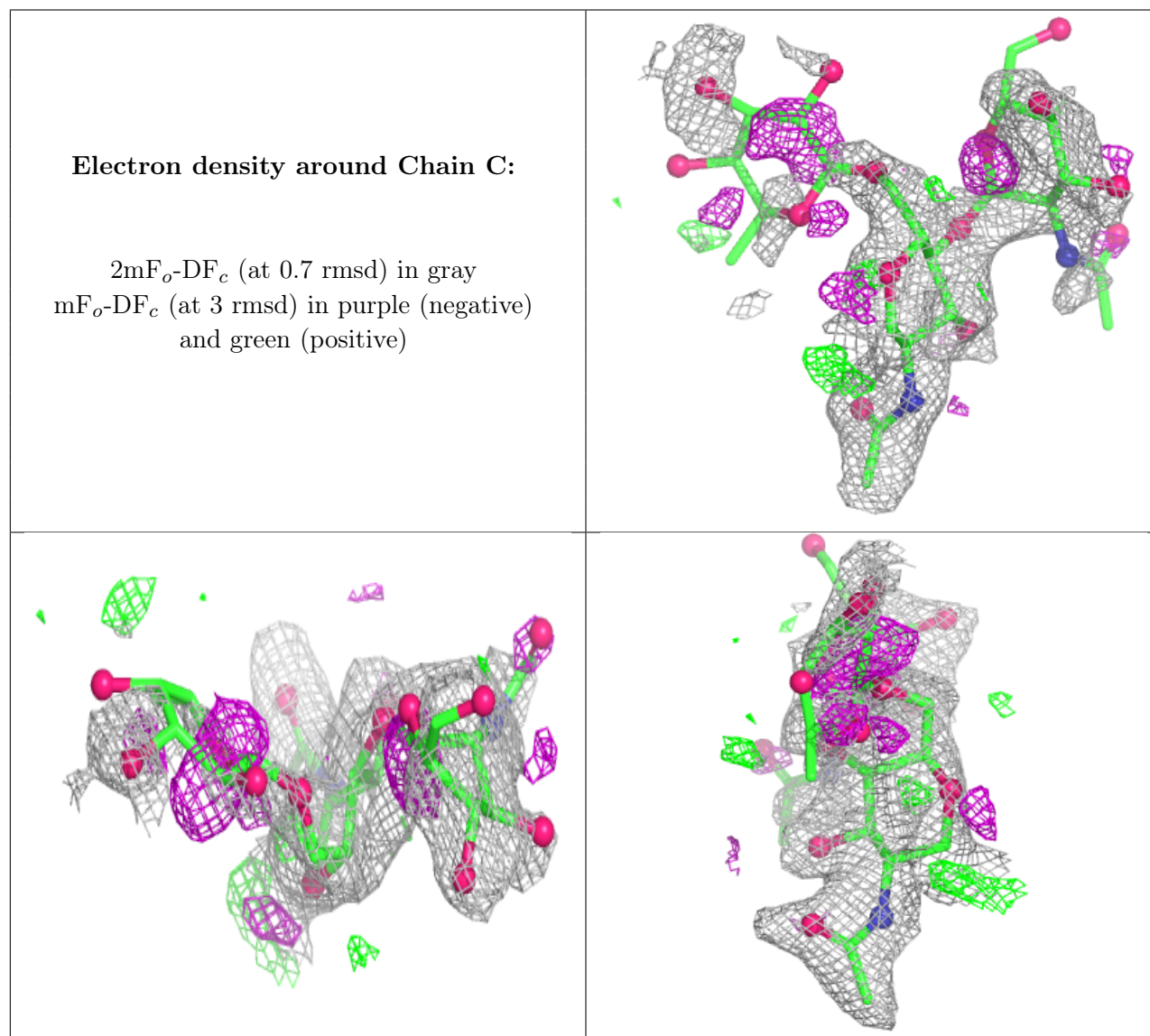
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	HTR	B	171	15/16	0.96	0.04	14,15,17,17	0
1	HTR	A	171	15/16	0.98	0.03	14,16,16,16	0

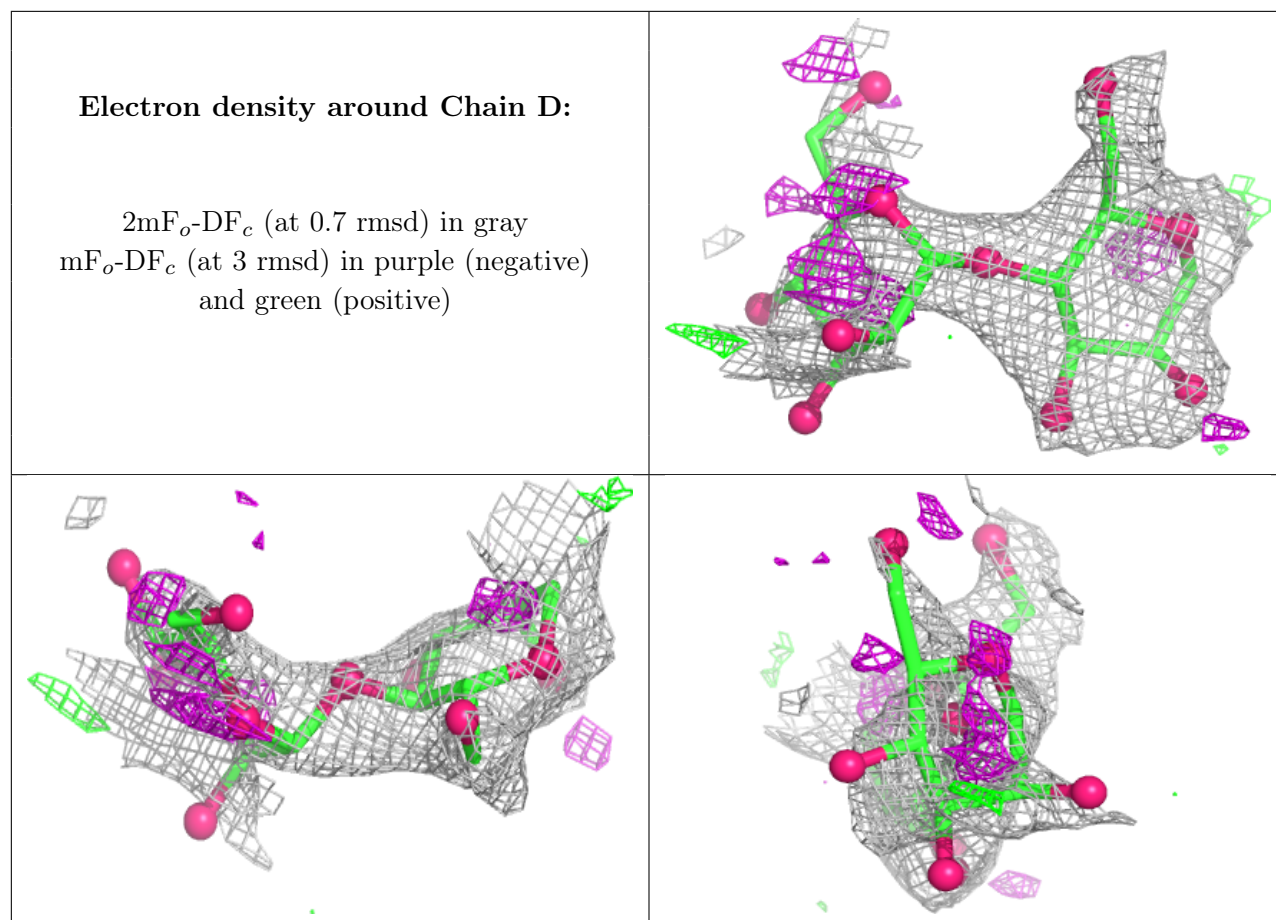
6.3 Carbohydrates ⓘ

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
2	NAG	C	2	14/15	0.50	0.14	77,81,84,85	0
2	FUC	C	3	10/11	0.52	0.22	73,75,75,76	0
2	NAG	C	1	14/15	0.68	0.13	54,60,72,74	0
3	MAN	D	1	11/12	0.76	0.10	52,58,62,65	0
3	MAN	D	2	11/12	0.76	0.15	68,71,72,72	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.



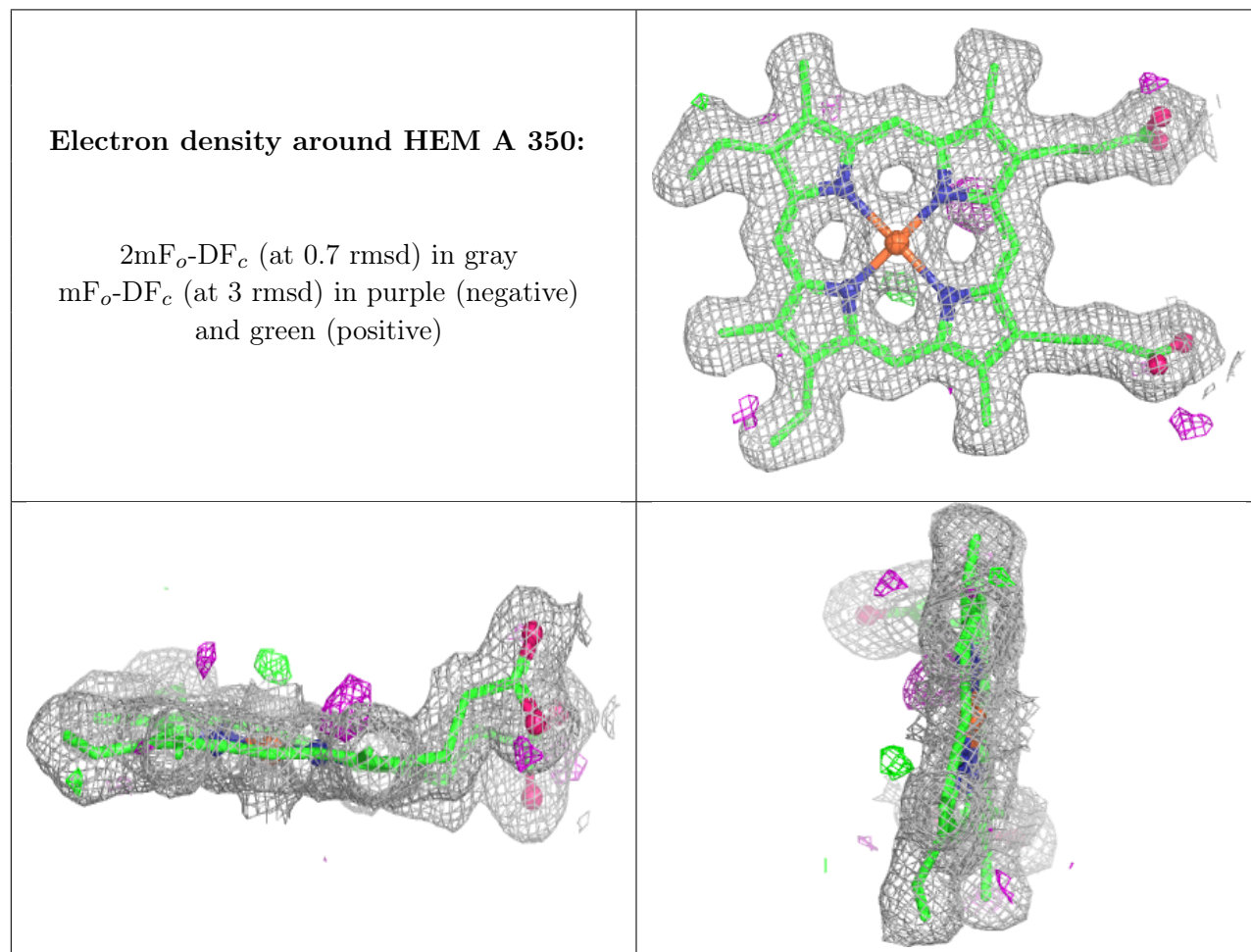


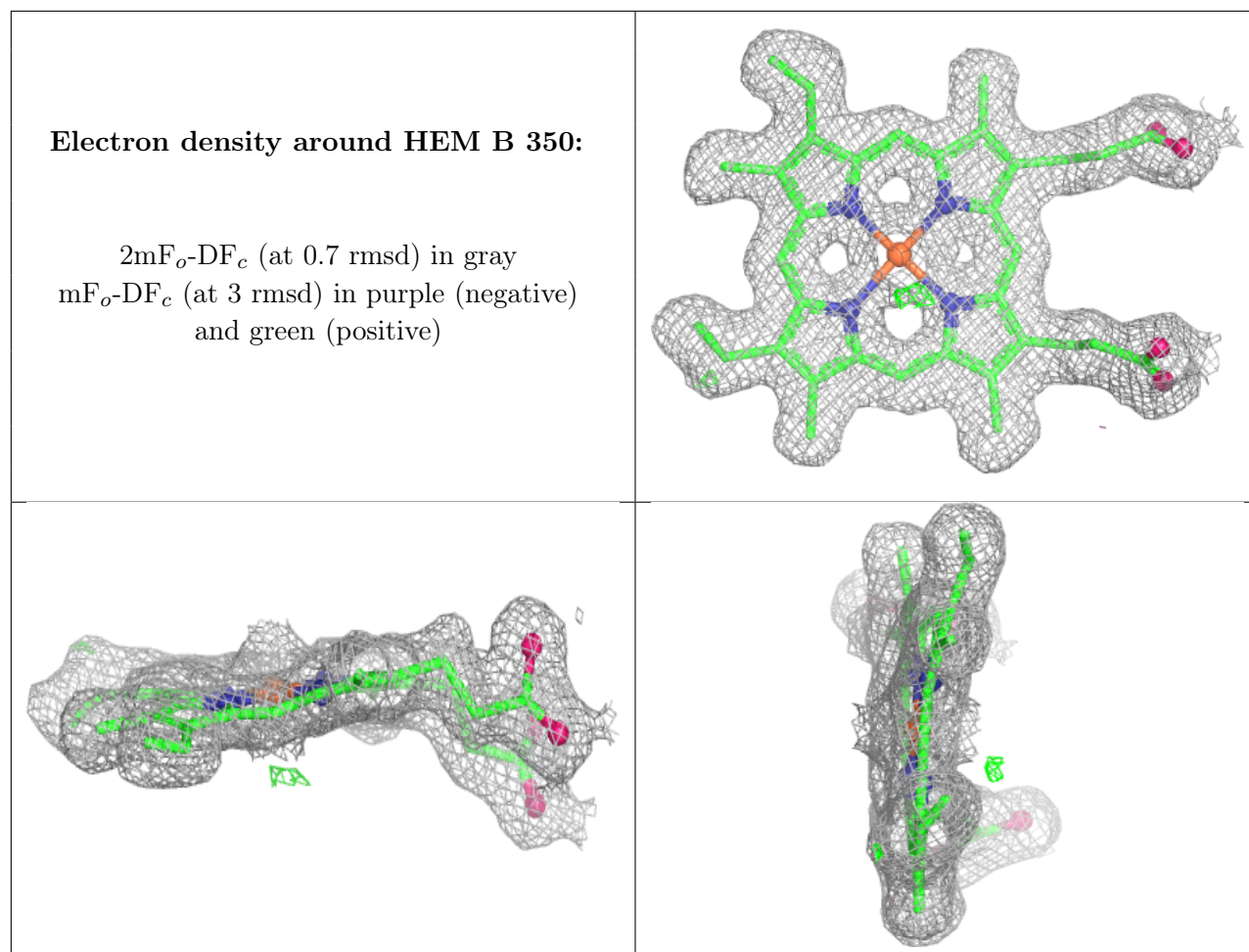
6.4 Ligands [i](#)

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
5	MAN	B	380	11/12	0.74	0.10	55,58,59,60	0
5	MAN	B	370	11/12	0.79	0.10	39,43,45,46	0
4	NAG	A	360	14/15	0.83	0.09	36,42,47,47	0
5	MAN	B	375	11/12	0.86	0.08	34,35,38,41	0
5	MAN	A	370	11/12	0.86	0.08	34,37,39,42	0
5	MAN	A	375	11/12	0.89	0.08	30,32,34,37	0
6	CA	A	352	1/1	0.99	0.02	14,14,14,14	0
6	CA	B	351	1/1	0.99	0.02	13,13,13,13	0
6	CA	B	352	1/1	0.99	0.02	18,18,18,18	0
7	HEM	A	350	43/43	0.99	0.04	9,11,14,15	0
7	HEM	B	350	43/43	0.99	0.04	12,16,18,21	0
6	CA	A	351	1/1	1.00	0.02	13,13,13,13	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.





6.5 Other polymers ⓘ

There are no such residues in this entry.