



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 5, 2026 – 01:47 PM EDT

PDB ID : 3GC1 / pdb_00003gc1
Title : Crystal structure of bovine lactoperoxidase
Authors : Singh, A.K.; Singh, N.; Sinha, M.; Kaur, P.; Srinivasan, A.; Sharma, S.; Singh, T.P.
Deposited on : 2009-02-21
Resolution : 2.50 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)
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	:	9.0.015 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.50

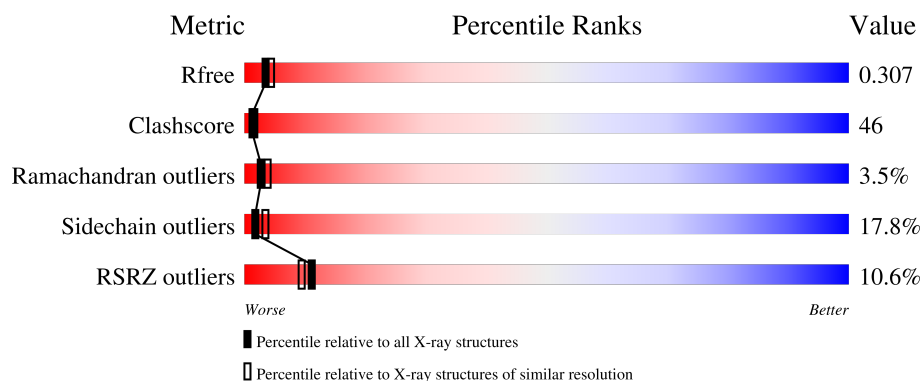
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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))
R_{free}	180053	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	595	11% 34% 44% 16% 6%
2	B	3	67% 33%
2	D	3	67% 33%
3	C	2	100%
3	E	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	NAG	B	1	X	-	-	-
2	NAG	D	1	X	-	-	-
4	HEM	A	605	-	-	X	-
7	IOD	A	610	-	-	X	-
7	IOD	A	613	-	-	X	-

2 Entry composition [i](#)

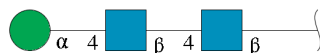
There are 8 unique types of molecules in this entry. The entry contains 5258 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Lactoperoxidase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	595	Total	C	N	O	P	S	0	0	0
			4774	3037	847	863	1	26			

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



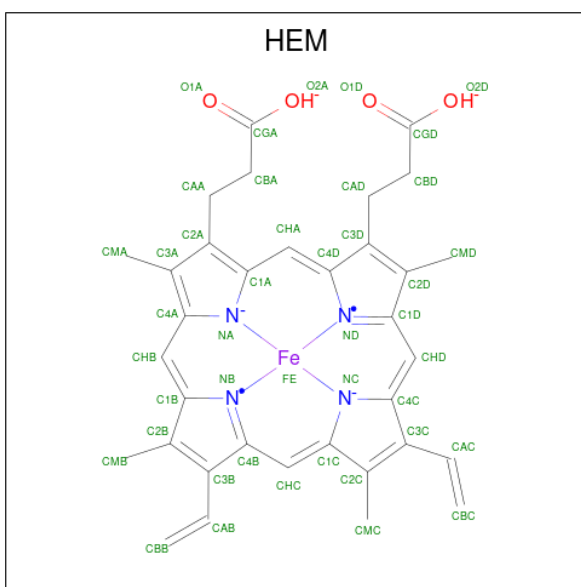
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	3	Total	C	N	O	0	0	0
			39	22	2	15			
2	D	3	Total	C	N	O	0	0	0
			39	22	2	15			

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



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

- Molecule 4 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: C₃₄H₃₂FeN₄O₄).

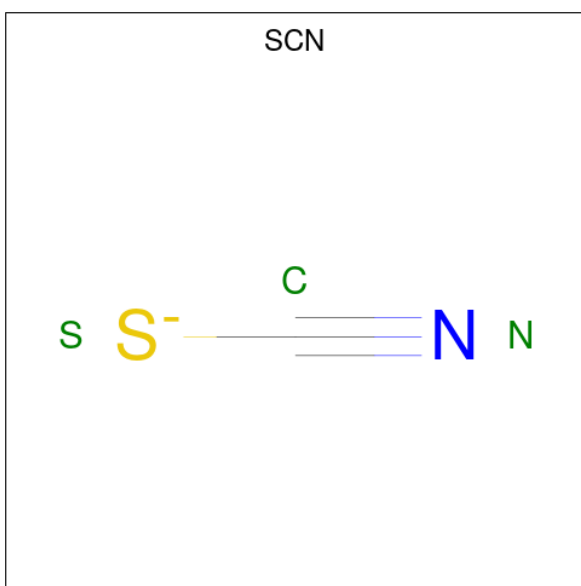


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	Fe	N	O	0	0
			43	34	1	4	4		

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

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

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



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

- Molecule 7 is IODIDE ION (CCD ID: IOD) (formula: I).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	7	Total	I	0	0
			7	7		

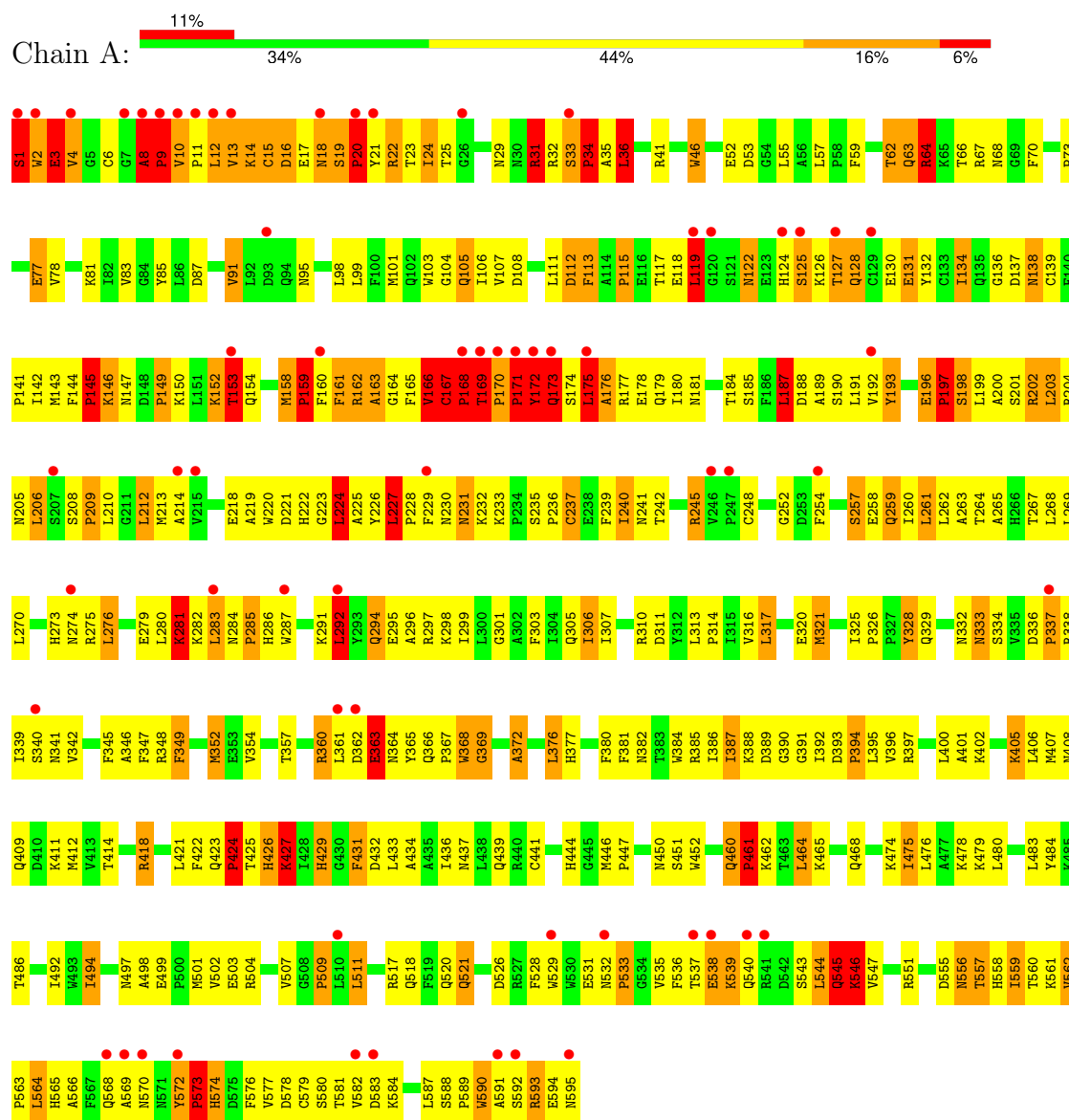
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	296	Total	O	0	0
			296	296		

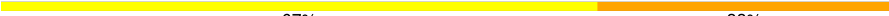
3 Residue-property plots

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: Lactoperoxidase



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

Chain B:  67% 33%

MAG1
MAG2
MAN3

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

Chain D:  67% 33%

MAG1
MAG2
MAN3

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

Chain C:  100%

MAG1
MAG2

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

Chain E:  50% 50%

MAG1
MAG2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	53.65Å 80.71Å 75.68Å 90.00° 101.75° 90.00°	Depositor
Resolution (Å)	24.97 – 2.50 24.97 – 2.50	Depositor EDS
% Data completeness (in resolution range)	95.3 (24.97-2.50) 95.2 (24.97-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.47 (at 2.50Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, R_{free}	0.247 , 0.268 0.259 , 0.307	Depositor DCC
R_{free} test set	1073 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å ²)	46.9	Xtriage
Anisotropy	0.751	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 85.7	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	0.90	EDS
Total number of atoms	5258	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.65% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SEP, MAN, SCN, HEM, CA, NAG, IOD

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.00	29/4891 (0.6%)	1.96	185/6634 (2.8%)

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	461	PRO	CA-C	-9.80	1.40	1.52
1	A	33	SER	CA-C	9.64	1.64	1.52
1	A	145	PRO	CA-C	-9.01	1.39	1.52
1	A	336	ASP	CA-C	8.13	1.62	1.52
1	A	171	PRO	N-CA	8.06	1.57	1.47
1	A	173	GLN	N-CA	-7.62	1.40	1.47
1	A	257	SER	C-N	7.35	1.42	1.33
1	A	19	SER	CA-C	-7.15	1.43	1.52
1	A	33	SER	C-N	7.02	1.44	1.33
1	A	14	LYS	N-CA	6.59	1.55	1.45
1	A	573	PRO	N-CA	6.31	1.55	1.47
1	A	34	PRO	N-CA	6.27	1.56	1.47
1	A	159	PRO	N-CA	6.26	1.54	1.47
1	A	337	PRO	N-CA	5.90	1.54	1.47
1	A	174	SER	CA-C	5.89	1.60	1.52
1	A	170	PRO	CA-C	5.75	1.57	1.52
1	A	460	GLN	CA-C	5.74	1.57	1.52
1	A	168	PRO	N-CA	5.72	1.54	1.47
1	A	13	VAL	C-N	5.62	1.40	1.33
1	A	171	PRO	CA-C	5.57	1.60	1.52
1	A	167	CYS	CA-C	5.55	1.59	1.52
1	A	8	ALA	CA-C	5.53	1.59	1.52
1	A	13	VAL	CA-C	5.39	1.58	1.52
1	A	33	SER	N-CA	5.36	1.52	1.46
1	A	196	GLU	CA-C	5.30	1.57	1.52
1	A	145	PRO	C-N	-5.27	1.26	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	537	THR	CA-C	-5.26	1.45	1.53
1	A	363	GLU	CA-C	5.13	1.59	1.52
1	A	461	PRO	CA-CB	-5.02	1.47	1.53

All (185) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	572	TYR	CA-C-N	43.97	174.80	119.84
1	A	572	TYR	C-N-CA	43.97	174.80	119.84
1	A	573	PRO	CA-N-CD	-18.43	86.20	112.00
1	A	2	TRP	N-CA-C	16.76	146.51	110.80
1	A	15	CYS	N-CA-C	16.62	130.85	110.41
1	A	573	PRO	N-CA-CB	15.03	119.03	103.25
1	A	573	PRO	N-CD-CG	12.27	121.61	103.20
1	A	581	THR	N-CA-C	-12.13	100.11	112.97
1	A	562	VAL	N-CA-C	11.58	120.70	107.84
1	A	63	GLN	OE1-CD-NE2	-10.93	111.67	122.60
1	A	461	PRO	CA-N-CD	-10.86	96.80	112.00
1	A	170	PRO	CB-CA-C	10.84	124.14	110.92
1	A	173	GLN	OE1-CD-NE2	-10.61	111.99	122.60
1	A	409	GLN	OE1-CD-NE2	-10.46	112.14	122.60
1	A	232	LYS	N-CA-C	10.32	125.48	110.10
1	A	128	GLN	OE1-CD-NE2	-10.27	112.33	122.60
1	A	105	GLN	OE1-CD-NE2	-10.25	112.35	122.60
1	A	545	GLN	OE1-CD-NE2	-10.16	112.44	122.60
1	A	231	ASN	N-CA-C	10.04	121.98	111.14
1	A	259	GLN	OE1-CD-NE2	-9.97	112.62	122.60
1	A	222	HIS	CA-CB-CG	-9.97	103.83	113.80
1	A	316	VAL	N-CA-C	-9.88	102.28	111.67
1	A	294	GLN	OE1-CD-NE2	-9.66	112.94	122.60
1	A	233	LYS	N-CA-C	-9.63	94.61	109.64
1	A	29	ASN	N-CA-C	-9.62	100.75	111.14
1	A	460	GLN	OE1-CD-NE2	-9.62	112.98	122.60
1	A	83	VAL	N-CA-C	9.56	123.04	111.09
1	A	366	GLN	OE1-CD-NE2	-9.45	113.15	122.60
1	A	254	PHE	N-CA-C	9.37	122.69	111.82
1	A	12	LEU	CA-C-N	-9.14	107.47	121.18
1	A	12	LEU	C-N-CA	-9.14	107.47	121.18
1	A	281	LYS	N-CA-C	-9.11	101.32	111.07
1	A	4	VAL	N-CA-C	8.96	120.76	111.00
1	A	349	PHE	N-CA-C	-8.93	101.46	111.82
1	A	332	ASN	N-CA-C	-8.90	95.01	109.96

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	176	ALA	N-CA-C	8.89	121.80	110.24
1	A	227	LEU	CA-C-N	8.84	128.88	119.78
1	A	227	LEU	C-N-CA	8.84	128.88	119.78
1	A	572	TYR	C-N-CD	-8.74	89.15	125.00
1	A	401	ALA	N-CA-C	8.48	123.86	113.17
1	A	408	ASN	CA-CB-CG	8.48	121.08	112.60
1	A	166	VAL	N-CA-C	8.35	126.71	109.34
1	A	159	PRO	CA-N-CD	-8.32	100.34	112.00
1	A	9	PRO	CA-N-CD	-8.32	100.36	112.00
1	A	390	GLY	N-CA-C	8.27	126.60	114.95
1	A	172	TYR	N-CA-C	8.02	121.42	110.35
1	A	202	ARG	N-CA-C	-7.96	102.19	112.23
1	A	171	PRO	N-CA-C	7.94	128.82	112.47
1	A	18	ASN	CA-CB-CG	7.92	120.52	112.60
1	A	426	HIS	N-CA-C	7.86	122.93	112.25
1	A	153	THR	N-CA-C	7.85	124.53	114.56
1	A	111	LEU	N-CA-C	7.81	123.13	112.90
1	A	544	LEU	N-CA-C	7.79	120.52	111.02
1	A	369	GLY	CA-C-N	7.76	127.30	118.85
1	A	369	GLY	C-N-CA	7.76	127.30	118.85
1	A	224	LEU	N-CA-C	7.75	121.98	110.52
1	A	427	LYS	N-CA-C	7.72	127.25	110.80
1	A	321	MET	N-CA-C	7.68	119.29	111.07
1	A	64	ARG	N-CA-C	7.63	121.06	112.97
1	A	219	ALA	N-CA-C	7.63	120.97	108.99
1	A	10	VAL	N-CA-CB	7.53	121.75	111.21
1	A	167	CYS	N-CA-C	-7.51	93.21	109.81
1	A	158	MET	N-CA-C	-7.50	99.68	110.40
1	A	77	GLU	N-CA-C	-7.42	102.56	111.69
1	A	328	TYR	N-CA-C	7.38	121.38	110.30
1	A	2	TRP	CB-CA-C	-7.38	95.74	110.42
1	A	574	HIS	N-CA-C	7.34	126.43	110.80
1	A	87	ASP	N-CA-C	7.30	119.98	108.67
1	A	105	GLN	CG-CD-NE2	7.14	127.11	116.40
1	A	13	VAL	N-CA-C	7.10	118.21	108.84
1	A	169	THR	N-CA-C	-6.96	94.42	109.81
1	A	23	THR	N-CA-C	-6.94	100.20	110.48
1	A	173	GLN	N-CA-C	6.92	122.90	113.21
1	A	294	GLN	CG-CD-NE2	6.90	126.75	116.40
1	A	372	ALA	N-CA-C	6.88	118.44	111.07
1	A	405	LYS	N-CA-C	-6.88	100.61	110.59
1	A	429	HIS	N-CA-C	-6.86	99.33	109.62

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	14	LYS	N-CA-C	6.86	119.17	110.33
1	A	173	GLN	CG-CD-NE2	6.81	126.61	116.40
1	A	424	PRO	CA-C-N	-6.77	111.94	122.37
1	A	424	PRO	C-N-CA	-6.77	111.94	122.37
1	A	63	GLN	CG-CD-NE2	6.75	126.52	116.40
1	A	128	GLN	CG-CD-NE2	6.73	126.49	116.40
1	A	13	VAL	CB-CA-C	6.70	120.30	111.33
1	A	1	SER	CA-C-N	6.67	134.28	121.54
1	A	1	SER	C-N-CA	6.67	134.28	121.54
1	A	167	CYS	CB-CA-C	6.66	123.30	110.17
1	A	326	PRO	N-CA-C	-6.61	102.63	110.70
1	A	521	GLN	N-CA-C	6.57	118.52	111.36
1	A	545	GLN	CG-CD-NE2	6.56	126.23	116.40
1	A	17	GLU	N-CA-C	6.54	122.40	113.37
1	A	197	PRO	CA-N-CD	-6.53	102.85	112.00
1	A	193	TYR	N-CA-C	6.52	121.44	112.90
1	A	409	GLN	CG-CD-NE2	6.51	126.16	116.40
1	A	572	TYR	CA-C-O	6.51	125.66	120.19
1	A	145	PRO	CA-N-CD	-6.48	102.92	112.00
1	A	336	ASP	CA-C-N	6.43	127.88	119.84
1	A	336	ASP	C-N-CA	6.43	127.88	119.84
1	A	187	LEU	N-CA-C	-6.36	97.28	108.23
1	A	122	ASN	N-CA-C	-6.35	97.28	110.80
1	A	306	ILE	N-CA-C	6.32	117.10	110.72
1	A	34	PRO	CA-N-CD	-6.26	103.23	112.00
1	A	570	ASN	N-CA-C	6.26	118.61	108.34
1	A	296	ALA	N-CA-C	-6.25	104.09	111.03
1	A	334	SER	N-CA-C	-6.25	105.48	113.23
1	A	366	GLN	CG-CD-NE2	6.24	125.76	116.40
1	A	112	ASP	CA-CB-CG	6.24	118.84	112.60
1	A	447	PRO	N-CA-C	-6.23	101.28	111.68
1	A	528	PHE	CA-CB-CG	-6.20	107.60	113.80
1	A	163	ALA	N-CA-C	6.19	119.22	110.50
1	A	34	PRO	N-CA-C	6.15	122.92	113.75
1	A	225	ALA	N-CA-C	6.15	118.85	110.55
1	A	263	ALA	N-CA-C	-6.11	104.53	111.07
1	A	460	GLN	CG-CD-NE2	6.11	125.56	116.40
1	A	418	ARG	N-CA-C	6.04	120.38	112.89
1	A	461	PRO	CB-CA-C	-6.04	102.00	110.63
1	A	484	TYR	N-CA-C	6.04	120.81	113.38
1	A	33	SER	CA-C-N	6.04	126.20	119.32
1	A	33	SER	C-N-CA	6.04	126.20	119.32

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	113	PHE	CA-CB-CG	6.02	119.82	113.80
1	A	284	ASN	CA-C-N	6.01	127.36	119.84
1	A	284	ASN	C-N-CA	6.01	127.36	119.84
1	A	546	LYS	N-CA-C	-5.99	105.93	113.72
1	A	35	ALA	N-CA-C	5.96	117.86	111.36
1	A	145	PRO	N-CA-C	-5.91	100.30	112.47
1	A	269	LEU	N-CA-C	5.90	117.71	111.28
1	A	590	TRP	N-CA-C	-5.86	106.17	113.38
1	A	259	GLN	CG-CD-NE2	5.82	125.13	116.40
1	A	170	PRO	CA-C-N	5.79	127.08	119.84
1	A	170	PRO	C-N-CA	5.79	127.08	119.84
1	A	192	VAL	CB-CA-C	-5.76	104.37	111.92
1	A	451	SER	N-CA-C	-5.75	105.10	111.36
1	A	131	GLU	N-CA-C	5.73	117.98	111.11
1	A	78	VAL	N-CA-C	-5.71	104.80	110.62
1	A	169	THR	N-CA-CB	5.70	120.52	110.37
1	A	145	PRO	CB-CA-C	-5.70	102.16	111.56
1	A	537	THR	CA-C-N	-5.68	111.68	120.31
1	A	537	THR	C-N-CA	-5.68	111.68	120.31
1	A	316	VAL	CB-CA-C	-5.67	105.11	111.80
1	A	545	GLN	N-CA-CB	5.66	120.05	110.49
1	A	13	VAL	CA-C-N	5.62	130.96	120.95
1	A	13	VAL	C-N-CA	5.62	130.96	120.95
1	A	138	ASN	N-CA-C	5.61	119.82	113.15
1	A	556	ASN	N-CA-C	5.58	119.27	111.56
1	A	460	GLN	CA-C-N	5.57	126.04	120.14
1	A	460	GLN	C-N-CA	5.57	126.04	120.14
1	A	520	GLN	N-CA-C	-5.51	104.49	111.11
1	A	46	TRP	N-CA-C	-5.50	106.41	113.23
1	A	557	THR	CA-C-N	-5.49	113.84	122.95
1	A	557	THR	C-N-CA	-5.49	113.84	122.95
1	A	573	PRO	CA-C-N	5.46	131.98	121.54
1	A	573	PRO	C-N-CA	5.46	131.98	121.54
1	A	239	PHE	N-CA-C	5.45	118.14	111.82
1	A	237	CYS	N-CA-C	-5.44	106.59	113.18
1	A	6	CYS	N-CA-C	-5.44	96.91	107.62
1	A	436	ILE	CB-CA-C	-5.43	104.73	112.22
1	A	204	ARG	N-CA-C	5.42	118.54	110.52
1	A	59	PHE	N-CA-C	-5.41	102.38	110.23
1	A	317	LEU	N-CA-C	5.38	117.14	111.28
1	A	337	PRO	CA-N-CD	-5.36	104.50	112.00
1	A	166	VAL	CB-CA-C	-5.35	102.52	111.29

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	175	LEU	N-CA-C	-5.35	101.32	108.86
1	A	159	PRO	N-CA-C	5.33	119.46	111.14
1	A	533	PRO	CB-CA-C	5.31	120.32	111.56
1	A	332	ASN	CA-C-N	-5.30	114.34	122.60
1	A	332	ASN	C-N-CA	-5.30	114.34	122.60
1	A	20	PRO	N-CA-C	5.29	123.37	112.47
1	A	31	ARG	N-CA-C	5.29	117.85	111.40
1	A	223	GLY	N-CA-C	-5.28	106.43	115.61
1	A	10	VAL	CB-CA-C	-5.27	101.77	111.36
1	A	262	LEU	N-CA-C	-5.25	105.15	112.45
1	A	538	GLU	CA-C-N	-5.21	111.82	120.68
1	A	538	GLU	C-N-CA	-5.21	111.82	120.68
1	A	336	ASP	C-N-CD	-5.21	103.66	125.00
1	A	395	LEU	N-CA-C	-5.16	106.14	112.90
1	A	125	SER	CA-C-N	5.13	129.19	120.88
1	A	125	SER	C-N-CA	5.13	129.19	120.88
1	A	368	TRP	N-CA-C	-5.10	100.76	108.67
1	A	292	LEU	N-CA-C	-5.08	106.93	113.23
1	A	313	LEU	CA-C-N	-5.07	113.70	119.28
1	A	313	LEU	C-N-CA	-5.07	113.70	119.28
1	A	178	GLU	N-CA-C	5.04	116.62	108.41
1	A	280	LEU	CA-C-N	-5.00	113.94	120.44
1	A	280	LEU	C-N-CA	-5.00	113.94	120.44
1	A	159	PRO	O-C-N	-5.00	116.98	123.03

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4774	0	4688	440	0
2	B	39	0	34	6	0
2	D	39	0	34	2	0
3	C	28	0	25	1	0
3	E	28	0	25	2	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	43	0	30	32	0
5	A	1	0	0	0	0
6	A	3	0	0	0	0
7	A	7	0	0	6	0
8	A	296	0	0	43	0
All	All	5258	0	4836	448	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 46.

All (448) 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:105:GLN:HB2	4:A:605:HEM:C2C	1.64	1.32
1:A:221:ASP:HB2	1:A:226:TYR:CZ	1.81	1.16
1:A:104:GLY:HA3	4:A:605:HEM:HBC1	1.26	1.09
1:A:22:ARG:HH11	1:A:22:ARG:CG	1.66	1.08
1:A:22:ARG:HG2	1:A:22:ARG:NH1	1.53	1.06
1:A:202:ARG:HH22	1:A:231:ASN:HB2	1.14	1.06
1:A:504:ARG:NH2	2:B:1:NAG:H4	1.73	1.03
1:A:3:GLU:HG2	1:A:175:LEU:HD22	1.41	1.03
1:A:504:ARG:HH22	2:B:1:NAG:H4	1.18	1.03
1:A:104:GLY:HA3	4:A:605:HEM:CBC	1.91	1.01
1:A:105:GLN:HB2	4:A:605:HEM:CMC	1.91	1.01
1:A:104:GLY:CA	4:A:605:HEM:HBC1	1.96	0.96
1:A:9:PRO:HG2	1:A:167:CYS:O	1.66	0.95
1:A:213:MET:HG2	1:A:273:HIS:CD2	2.01	0.95
1:A:260:ILE:HD11	1:A:386:ILE:HG13	1.46	0.95
1:A:167:CYS:HB3	1:A:168:PRO:HD2	1.48	0.94
1:A:21:TYR:CG	1:A:294:GLN:HB3	2.06	0.90
1:A:104:GLY:C	4:A:605:HEM:CBC	2.43	0.90
1:A:539:LYS:HE2	1:A:589:PRO:HB3	1.53	0.89
1:A:424:PRO:O	7:A:610:IOD:I	2.61	0.89
1:A:202:ARG:NH2	1:A:231:ASN:HB2	1.88	0.88
1:A:64:ARG:HH11	1:A:64:ARG:HG2	1.36	0.87
1:A:465:LYS:HA	1:A:468:GLN:NE2	1.89	0.87
1:A:19:SER:N	1:A:20:PRO:HD3	1.88	0.87
1:A:196:GLU:HB3	1:A:198:SEP:O2P	1.75	0.87
1:A:392:ILE:O	1:A:396:VAL:HG23	1.75	0.87
1:A:161:PHE:HD1	1:A:161:PHE:N	1.72	0.86
1:A:105:GLN:N	4:A:605:HEM:CAC	2.40	0.85

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:GLY:CA	4:A:605:HEM:CBC	2.54	0.85
1:A:494:ILE:O	1:A:494:ILE:HD13	1.77	0.85
1:A:227:LEU:HD21	1:A:267:THR:HA	1.57	0.84
1:A:105:GLN:HB2	4:A:605:HEM:HMC3	1.56	0.84
1:A:18:ASN:HB3	1:A:20:PRO:HD3	1.58	0.84
1:A:105:GLN:CB	4:A:605:HEM:C2C	2.57	0.83
1:A:260:ILE:HD13	1:A:382:ASN:O	1.79	0.83
1:A:3:GLU:CG	1:A:175:LEU:HD22	2.08	0.82
1:A:568:GLN:HE21	2:B:1:NAG:C6	1.93	0.82
1:A:141:PRO:HB2	1:A:143:MET:CE	2.11	0.81
1:A:224:LEU:HD13	8:A:778:HOH:O	1.79	0.81
1:A:161:PHE:N	1:A:161:PHE:CD1	2.45	0.81
1:A:175:LEU:HG	1:A:176:ALA:H	1.45	0.80
1:A:104:GLY:C	4:A:605:HEM:CAC	2.54	0.80
1:A:446:MET:HA	1:A:446:MET:HE2	1.62	0.79
1:A:544:LEU:O	1:A:547:VAL:HG13	1.82	0.78
1:A:199:LEU:HD12	1:A:199:LEU:O	1.83	0.78
1:A:504:ARG:HH22	2:B:1:NAG:C4	1.97	0.78
1:A:8:ALA:HB3	1:A:9:PRO:HD2	1.67	0.76
1:A:105:GLN:N	4:A:605:HEM:CBC	2.48	0.76
1:A:19:SER:N	1:A:20:PRO:CD	2.49	0.76
1:A:199:LEU:CD1	1:A:203:LEU:HD22	2.16	0.76
1:A:295:GLU:O	1:A:299:ILE:HG13	1.86	0.75
8:A:904:HOH:O	3:E:2:NAG:H4	1.87	0.74
1:A:231:ASN:HB3	8:A:847:HOH:O	1.87	0.74
1:A:166:VAL:CG1	1:A:180:ILE:HG12	2.18	0.74
1:A:521:GLN:NE2	8:A:753:HOH:O	2.20	0.74
1:A:283:LEU:C	1:A:285:PRO:HD3	2.13	0.74
1:A:161:PHE:HD1	1:A:161:PHE:H	1.36	0.73
1:A:105:GLN:CB	4:A:605:HEM:HMC3	2.19	0.73
1:A:22:ARG:HH11	1:A:22:ARG:HG2	0.72	0.72
1:A:18:ASN:CB	1:A:20:PRO:HD3	2.19	0.72
1:A:146:LYS:O	1:A:147:ASN:HB2	1.89	0.71
1:A:504:ARG:HD3	8:A:791:HOH:O	1.89	0.71
1:A:551:ARG:HD3	1:A:584:LYS:HA	1.73	0.71
1:A:545:GLN:N	1:A:545:GLN:HE21	1.88	0.71
1:A:200:ALA:O	1:A:203:LEU:HB2	1.90	0.71
1:A:565:HIS:CB	1:A:568:GLN:HG2	2.21	0.71
1:A:105:GLN:HA	4:A:605:HEM:C3C	2.27	0.70
1:A:16:ASP:OD1	1:A:16:ASP:N	2.25	0.69
1:A:64:ARG:HG2	1:A:64:ARG:NH1	2.04	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:GLN:HB3	8:A:844:HOH:O	1.91	0.69
1:A:242:THR:O	1:A:245:ARG:HG2	1.91	0.69
1:A:465:LYS:HD2	1:A:468:GLN:NE2	2.07	0.69
1:A:14:LYS:HE3	1:A:34:PRO:CG	2.23	0.68
1:A:346:ALA:HA	8:A:802:HOH:O	1.93	0.68
1:A:365:TYR:CE1	1:A:576:PHE:CE2	2.81	0.68
1:A:465:LYS:HA	1:A:468:GLN:HE21	1.59	0.68
1:A:565:HIS:HB2	1:A:568:GLN:HG2	1.76	0.68
1:A:579:CYS:O	1:A:582:VAL:HB	1.93	0.68
1:A:294:GLN:NE2	8:A:829:HOH:O	2.25	0.68
1:A:593:ARG:C	1:A:595:ASN:H	2.02	0.68
1:A:245:ARG:NH2	8:A:909:HOH:O	2.26	0.68
1:A:341:ASN:OD1	1:A:444:HIS:ND1	2.23	0.68
1:A:150:LYS:HD2	1:A:158:MET:HE3	1.76	0.67
1:A:221:ASP:HB2	1:A:226:TYR:OH	1.94	0.67
1:A:105:GLN:HB2	4:A:605:HEM:C3C	2.25	0.66
1:A:159:PRO:HB3	1:A:161:PHE:HE1	1.60	0.66
1:A:531:GLU:O	1:A:533:PRO:HD3	1.95	0.66
1:A:568:GLN:HB3	2:B:1:NAG:O6	1.95	0.66
1:A:173:GLN:HG2	1:A:173:GLN:O	1.96	0.66
1:A:2:TRP:N	1:A:2:TRP:CE3	2.64	0.66
1:A:199:LEU:HD11	1:A:203:LEU:CD2	2.26	0.66
1:A:517:ARG:HD3	8:A:753:HOH:O	1.96	0.66
1:A:433:LEU:HD13	4:A:605:HEM:HMA3	1.78	0.66
1:A:18:ASN:ND2	1:A:20:PRO:HG3	2.12	0.65
1:A:166:VAL:HG12	1:A:180:ILE:HG12	1.76	0.65
1:A:113:PHE:O	1:A:115:PRO:HD2	1.97	0.65
1:A:158:MET:SD	8:A:692:HOH:O	2.54	0.65
1:A:237:CYS:HA	1:A:381:PHE:O	1.96	0.65
1:A:310:ARG:NE	1:A:311:ASP:OD1	2.24	0.65
1:A:342:VAL:HG12	7:A:608:IOD:I	2.66	0.65
1:A:127:THR:HB	8:A:711:HOH:O	1.97	0.65
1:A:214:ALA:O	1:A:228:PRO:HG3	1.97	0.65
1:A:588:SER:N	1:A:589:PRO:HD2	2.12	0.65
1:A:224:LEU:HD11	1:A:558:HIS:CE1	2.32	0.65
1:A:461:PRO:O	1:A:462:LYS:HD3	1.97	0.65
1:A:105:GLN:CA	4:A:605:HEM:CAC	2.74	0.64
1:A:1:SER:N	1:A:2:TRP:CE3	2.64	0.64
1:A:360:ARG:HH11	1:A:372:ALA:HA	1.62	0.64
1:A:551:ARG:HD3	1:A:583:ASP:O	1.98	0.64
3:C:1:NAG:H61	3:C:2:NAG:C7	2.27	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:GLN:CA	4:A:605:HEM:C3C	2.81	0.64
1:A:139:CYS:SG	1:A:141:PRO:HG3	2.37	0.64
1:A:545:GLN:H	1:A:545:GLN:NE2	1.95	0.64
1:A:119:LEU:HD21	1:A:138:ASN:ND2	2.13	0.64
1:A:257:SER:O	1:A:381:PHE:HA	1.97	0.64
1:A:105:GLN:HA	4:A:605:HEM:CAC	2.29	0.63
1:A:1:SER:C	1:A:2:TRP:HE3	2.07	0.63
1:A:321:MET:SD	1:A:325:ILE:HD12	2.39	0.63
1:A:117:THR:CG2	1:A:164:GLY:HA2	2.29	0.63
1:A:130:GLU:HG3	1:A:159:PRO:CG	2.29	0.63
1:A:425:THR:HG22	1:A:425:THR:O	1.98	0.63
1:A:199:LEU:HD11	1:A:203:LEU:HD22	1.79	0.62
4:A:605:HEM:HMB1	4:A:605:HEM:HBB2	1.81	0.62
1:A:209:PRO:HB3	8:A:635:HOH:O	1.99	0.62
1:A:400:LEU:HD13	1:A:563:PRO:HD3	1.81	0.62
1:A:425:THR:O	1:A:425:THR:CG2	2.48	0.62
1:A:314:PRO:HG3	1:A:321:MET:HE2	1.80	0.62
1:A:166:VAL:CG1	1:A:180:ILE:CG1	2.78	0.61
1:A:2:TRP:N	1:A:2:TRP:HE3	1.99	0.61
1:A:275:ARG:CD	1:A:555:ASP:HB3	2.30	0.61
1:A:544:LEU:C	1:A:546:LYS:H	2.09	0.61
1:A:227:LEU:HD23	1:A:267:THR:HG23	1.82	0.61
1:A:545:GLN:HE21	1:A:545:GLN:H	1.48	0.61
1:A:139:CYS:O	1:A:141:PRO:HD3	2.00	0.60
1:A:276:LEU:CD1	1:A:587:LEU:HD21	2.30	0.60
1:A:303:PHE:CE1	1:A:307:ILE:HD11	2.35	0.60
1:A:117:THR:HB	1:A:119:LEU:CD2	2.30	0.60
1:A:205:ASN:HD22	1:A:212:LEU:HD12	1.65	0.60
1:A:494:ILE:HD13	1:A:494:ILE:C	2.26	0.60
1:A:14:LYS:HG3	1:A:15:CYS:H	1.66	0.60
1:A:407:MET:HB3	1:A:501:MET:HE2	1.84	0.59
1:A:499:GLU:OE1	1:A:509:PRO:HD2	2.01	0.59
1:A:283:LEU:HD23	1:A:591:ALA:HB2	1.82	0.59
1:A:153:THR:HG22	1:A:154:GLN:HG3	1.83	0.59
1:A:21:TYR:HB3	8:A:796:HOH:O	2.01	0.59
1:A:221:ASP:HB2	1:A:226:TYR:CE2	2.35	0.58
1:A:265:ALA:HA	1:A:268:LEU:HD23	1.83	0.58
1:A:328:TYR:CE2	1:A:531:GLU:HB2	2.37	0.58
1:A:578:ASP:OD1	1:A:579:CYS:N	2.37	0.58
1:A:130:GLU:HG3	1:A:159:PRO:CD	2.33	0.58
1:A:8:ALA:HB3	1:A:9:PRO:CD	2.32	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:14:LYS:CG	1:A:15:CYS:H	2.16	0.58
1:A:160:PHE:CE1	1:A:439:GLN:HB3	2.39	0.58
1:A:8:ALA:CB	1:A:9:PRO:CD	2.80	0.58
1:A:138:ASN:O	1:A:161:PHE:HA	2.04	0.58
1:A:276:LEU:HD12	1:A:587:LEU:HD21	1.86	0.58
1:A:475:ILE:HG13	1:A:479:LYS:HE3	1.86	0.57
1:A:167:CYS:HB3	1:A:168:PRO:CD	2.27	0.57
1:A:188:ASP:O	1:A:189:ALA:HB3	2.04	0.57
1:A:203:LEU:HB3	1:A:213:MET:CE	2.33	0.57
1:A:393:ASP:N	1:A:394:PRO:HD2	2.19	0.57
1:A:175:LEU:HD23	8:A:863:HOH:O	2.04	0.57
1:A:339:ILE:HA	1:A:518:GLN:NE2	2.20	0.57
1:A:556:ASN:O	1:A:557:THR:CG2	2.53	0.57
1:A:169:THR:HG22	1:A:170:PRO:HD3	1.86	0.57
1:A:465:LYS:CD	1:A:468:GLN:NE2	2.67	0.57
1:A:433:LEU:CD1	4:A:605:HEM:HMA3	2.34	0.57
1:A:464:LEU:HD22	1:A:468:GLN:HG3	1.86	0.57
1:A:544:LEU:O	1:A:546:LYS:N	2.38	0.57
1:A:227:LEU:CD2	1:A:267:THR:HA	2.31	0.57
1:A:21:TYR:OH	1:A:291:LYS:HD2	2.05	0.56
1:A:210:LEU:O	1:A:292:LEU:HD23	2.06	0.56
1:A:294:GLN:O	1:A:298:LYS:HB2	2.05	0.56
1:A:431:PHE:N	1:A:431:PHE:CD1	2.73	0.56
1:A:259:GLN:OE1	1:A:261:LEU:HB2	2.05	0.56
1:A:431:PHE:N	1:A:431:PHE:HD1	2.04	0.56
1:A:21:TYR:CD1	1:A:294:GLN:HB3	2.40	0.56
1:A:565:HIS:HB3	1:A:568:GLN:HG2	1.87	0.56
1:A:117:THR:HG23	1:A:164:GLY:HA2	1.86	0.55
1:A:180:ILE:HG22	1:A:181:ASN:N	2.21	0.55
1:A:338:ARG:CD	8:A:859:HOH:O	2.54	0.55
1:A:146:LYS:O	1:A:147:ASN:CB	2.54	0.55
1:A:287:TRP:HB2	1:A:292:LEU:HD11	1.88	0.55
1:A:365:TYR:CD2	1:A:572:TYR:CD1	2.95	0.55
1:A:465:LYS:HD3	1:A:468:GLN:HE22	1.70	0.55
1:A:574:HIS:C	1:A:574:HIS:CD2	2.84	0.55
1:A:301:GLY:O	1:A:305:GLN:HG3	2.06	0.55
1:A:529:TRP:O	1:A:535:VAL:HG11	2.07	0.55
1:A:14:LYS:HE3	1:A:34:PRO:HG3	1.87	0.55
1:A:138:ASN:HA	1:A:162:ARG:HG3	1.89	0.55
1:A:465:LYS:CD	1:A:468:GLN:HE22	2.20	0.55
1:A:113:PHE:CG	1:A:115:PRO:HD3	2.43	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:ASN:O	1:A:149:PRO:HD3	2.07	0.54
1:A:166:VAL:HG13	1:A:180:ILE:CG1	2.38	0.54
1:A:568:GLN:NE2	2:B:1:NAG:O6	2.34	0.54
1:A:25:THR:CG2	1:A:197:PRO:HD3	2.38	0.54
1:A:62:THR:O	1:A:63:GLN:C	2.49	0.54
1:A:393:ASP:HB2	1:A:394:PRO:CD	2.37	0.54
1:A:393:ASP:CB	1:A:394:PRO:CD	2.85	0.54
1:A:580:SER:C	1:A:582:VAL:H	2.16	0.54
1:A:532:ASN:O	1:A:535:VAL:HB	2.07	0.54
1:A:63:GLN:CB	8:A:844:HOH:O	2.52	0.54
1:A:185:SER:HB3	1:A:337:PRO:O	2.08	0.54
1:A:169:THR:N	1:A:170:PRO:CD	2.68	0.53
1:A:175:LEU:HG	1:A:176:ALA:N	2.19	0.53
1:A:214:ALA:O	1:A:228:PRO:CG	2.56	0.53
1:A:264:THR:HG23	1:A:392:ILE:HB	1.89	0.53
1:A:283:LEU:O	1:A:285:PRO:HD3	2.09	0.53
1:A:376:LEU:HG	8:A:824:HOH:O	2.09	0.53
1:A:259:GLN:HG2	4:A:605:HEM:CBB	2.38	0.53
1:A:101:MET:SD	4:A:605:HEM:CMC	2.97	0.53
1:A:166:VAL:HG12	1:A:180:ILE:CG1	2.38	0.53
1:A:465:LYS:HD2	1:A:468:GLN:HE21	1.71	0.53
8:A:659:HOH:O	2:D:3:MAN:H3	2.07	0.53
1:A:1:SER:CA	1:A:2:TRP:HE3	2.22	0.53
1:A:105:GLN:CB	4:A:605:HEM:C3C	2.89	0.53
1:A:275:ARG:NE	1:A:555:ASP:HB3	2.23	0.53
1:A:539:LYS:HB3	1:A:589:PRO:HB3	1.91	0.52
1:A:360:ARG:NH2	1:A:389:ASP:OD2	2.40	0.52
1:A:22:ARG:CG	1:A:22:ARG:NH1	2.38	0.52
1:A:360:ARG:C	1:A:361:LEU:HD23	2.34	0.52
1:A:393:ASP:HB2	1:A:394:PRO:HD3	1.92	0.52
1:A:169:THR:H	1:A:170:PRO:CD	2.17	0.52
1:A:240:ILE:HG12	1:A:241:ASN:N	2.24	0.52
1:A:407:MET:HB3	1:A:501:MET:CE	2.39	0.52
1:A:560:THR:O	1:A:561:LYS:HD3	2.09	0.52
1:A:188:ASP:HA	8:A:679:HOH:O	2.10	0.52
1:A:66:THR:HB	1:A:70:PHE:N	2.25	0.52
1:A:117:THR:HB	1:A:119:LEU:HD21	1.91	0.52
1:A:199:LEU:HD12	1:A:203:LEU:HD22	1.88	0.52
1:A:365:TYR:CE1	1:A:576:PHE:HE2	2.28	0.52
1:A:556:ASN:C	1:A:557:THR:HG23	2.34	0.52
1:A:593:ARG:C	1:A:595:ASN:N	2.67	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ARG:HD2	8:A:768:HOH:O	2.09	0.52
1:A:187:LEU:CD1	1:A:305:GLN:HA	2.40	0.52
1:A:345:PHE:CE2	1:A:441:CYS:HA	2.45	0.52
1:A:108:ASP:OD1	4:A:605:HEM:C2D	2.59	0.51
1:A:532:ASN:O	1:A:533:PRO:C	2.51	0.51
1:A:64:ARG:HG2	1:A:64:ARG:O	2.10	0.51
1:A:187:LEU:HD13	1:A:305:GLN:HA	1.92	0.51
1:A:77:GLU:HB2	1:A:145:PRO:HG3	1.91	0.51
1:A:113:PHE:CD1	1:A:115:PRO:HD3	2.46	0.51
1:A:193:TYR:O	1:A:200:ALA:HA	2.10	0.51
1:A:77:GLU:OE2	1:A:81:LYS:NZ	2.41	0.51
1:A:173:GLN:O	1:A:173:GLN:CG	2.59	0.51
1:A:229:PHE:HD2	7:A:613:IOD:I	2.64	0.51
1:A:167:CYS:CB	1:A:168:PRO:HD2	2.29	0.51
1:A:275:ARG:HH11	1:A:275:ARG:HG2	1.76	0.51
1:A:36:LEU:HD12	8:A:709:HOH:O	2.09	0.51
1:A:104:GLY:C	4:A:605:HEM:HBC1	2.25	0.51
1:A:561:LYS:NZ	1:A:578:ASP:HB2	2.25	0.51
1:A:22:ARG:HD3	8:A:783:HOH:O	2.11	0.50
1:A:53:ASP:C	1:A:55:LEU:H	2.18	0.50
1:A:21:TYR:CD2	1:A:294:GLN:HB3	2.46	0.50
1:A:1:SER:CA	1:A:2:TRP:CE3	2.95	0.50
1:A:202:ARG:NH2	1:A:231:ASN:CB	2.66	0.50
1:A:551:ARG:CZ	1:A:584:LYS:HG2	2.41	0.50
1:A:540:GLN:HG2	1:A:590:TRP:CD2	2.46	0.50
1:A:260:ILE:HG23	1:A:261:LEU:HD13	1.93	0.50
1:A:433:LEU:HD11	4:A:605:HEM:C3A	2.47	0.50
1:A:543:SER:OG	1:A:589:PRO:HG3	2.11	0.50
1:A:352:MET:HE3	1:A:497:ASN:CB	2.42	0.50
1:A:53:ASP:HB2	8:A:678:HOH:O	2.12	0.49
1:A:113:PHE:C	1:A:115:PRO:CD	2.85	0.49
1:A:393:ASP:CB	1:A:394:PRO:HD3	2.42	0.49
1:A:286:HIS:ND1	1:A:286:HIS:N	2.55	0.49
1:A:361:LEU:O	1:A:397:ARG:HD2	2.12	0.49
1:A:106:ILE:HG22	1:A:107:VAL:N	2.28	0.49
1:A:556:ASN:O	1:A:557:THR:HG23	2.11	0.49
1:A:14:LYS:HE3	1:A:34:PRO:HG2	1.94	0.49
1:A:41:ARG:O	1:A:180:ILE:HG23	2.13	0.49
1:A:113:PHE:CE2	1:A:115:PRO:HG3	2.48	0.49
1:A:342:VAL:HG11	1:A:452:TRP:CH2	2.47	0.49
1:A:22:ARG:CD	8:A:783:HOH:O	2.60	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:THR:HG22	1:A:128:GLN:N	2.28	0.49
1:A:136:GLY:O	1:A:137:ASP:C	2.56	0.49
1:A:166:VAL:HG13	1:A:180:ILE:HG13	1.95	0.49
1:A:203:LEU:HB3	1:A:213:MET:HE1	1.94	0.49
1:A:203:LEU:HB3	1:A:213:MET:HE3	1.93	0.49
1:A:310:ARG:HE	1:A:311:ASP:CG	2.20	0.49
1:A:320:GLU:HA	1:A:320:GLU:OE1	2.12	0.49
1:A:328:TYR:CD2	1:A:531:GLU:HB2	2.48	0.49
1:A:405:LYS:NZ	1:A:412:MET:O	2.43	0.49
1:A:127:THR:HG23	1:A:132:TYR:HE1	1.78	0.49
1:A:345:PHE:HZ	1:A:444:HIS:CG	2.30	0.49
1:A:572:TYR:CD2	1:A:573:PRO:N	2.81	0.49
1:A:24:ILE:HG13	1:A:200:ALA:HB2	1.94	0.49
1:A:18:ASN:C	1:A:20:PRO:HD3	2.38	0.48
1:A:572:TYR:HD2	1:A:573:PRO:HD3	1.78	0.48
1:A:150:LYS:HD2	1:A:158:MET:CE	2.42	0.48
1:A:169:THR:N	1:A:170:PRO:HD2	2.28	0.48
1:A:384:TRP:CZ3	1:A:385:ARG:HD3	2.48	0.48
7:A:610:IOD:I	8:A:717:HOH:O	2.90	0.48
1:A:171:PRO:HD3	8:A:716:HOH:O	2.13	0.48
1:A:365:TYR:CZ	1:A:576:PHE:CE2	3.02	0.48
1:A:16:ASP:HB3	8:A:900:HOH:O	2.13	0.48
1:A:21:TYR:CD1	1:A:294:GLN:CB	2.96	0.48
1:A:298:LYS:HE3	1:A:536:PHE:CE2	2.48	0.48
3:E:2:NAG:H5	3:E:2:NAG:N2	2.28	0.48
1:A:127:THR:HG23	1:A:132:TYR:CE1	2.48	0.48
1:A:348:ARG:NH1	4:A:605:HEM:HBA1	2.29	0.48
1:A:177:ARG:HA	8:A:774:HOH:O	2.14	0.47
1:A:423:GLN:O	1:A:425:THR:N	2.46	0.47
1:A:101:MET:SD	4:A:605:HEM:HMC2	2.54	0.47
1:A:338:ARG:HD2	8:A:859:HOH:O	2.15	0.47
1:A:377:HIS:O	1:A:429:HIS:CD2	2.67	0.47
1:A:113:PHE:C	1:A:115:PRO:HD3	2.39	0.47
1:A:142:ILE:HG23	8:A:651:HOH:O	2.15	0.47
1:A:545:GLN:N	1:A:545:GLN:NE2	2.56	0.47
1:A:229:PHE:CD2	7:A:613:IOD:I	3.38	0.47
1:A:237:CYS:SG	1:A:381:PHE:HB3	2.54	0.47
1:A:281:LYS:HD3	1:A:285:PRO:HA	1.96	0.47
1:A:230:ASN:OD1	1:A:231:ASN:N	2.47	0.47
1:A:260:ILE:O	1:A:264:THR:OG1	2.27	0.47
1:A:12:LEU:HB2	8:A:723:HOH:O	2.13	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:164:GLY:O	1:A:179:GLN:HA	2.14	0.47
1:A:354:VAL:HG11	1:A:376:LEU:HD11	1.97	0.47
1:A:478:LYS:HB2	1:A:478:LYS:HE3	1.56	0.47
4:A:605:HEM:ND	8:A:616:HOH:O	2.35	0.47
1:A:141:PRO:HB2	1:A:143:MET:HE3	1.91	0.47
1:A:544:LEU:C	1:A:546:LYS:N	2.73	0.47
1:A:85:TYR:CD2	1:A:411:LYS:HA	2.50	0.47
1:A:369:GLY:HA3	8:A:752:HOH:O	2.14	0.47
1:A:421:LEU:HD21	1:A:423:GLN:NE2	2.30	0.47
1:A:12:LEU:O	1:A:13:VAL:C	2.58	0.46
1:A:347:PHE:O	1:A:347:PHE:CD1	2.68	0.46
1:A:159:PRO:HB3	1:A:161:PHE:CE1	2.46	0.46
1:A:381:PHE:CZ	1:A:424:PRO:HD3	2.50	0.46
1:A:64:ARG:NH1	1:A:64:ARG:CG	2.73	0.46
1:A:432:ASP:OD1	1:A:434:ALA:N	2.47	0.46
1:A:468:GLN:OE1	1:A:474:LYS:HG3	2.16	0.46
1:A:199:LEU:O	1:A:200:ALA:C	2.59	0.46
1:A:202:ARG:HH21	1:A:231:ASN:ND2	2.13	0.46
1:A:494:ILE:C	1:A:494:ILE:CD1	2.89	0.46
1:A:561:LYS:HZ2	1:A:578:ASP:HB2	1.78	0.46
1:A:593:ARG:O	1:A:595:ASN:N	2.48	0.46
1:A:180:ILE:CG2	1:A:181:ASN:N	2.79	0.46
1:A:95:ASN:HA	1:A:569:ALA:HB2	1.98	0.46
1:A:99:LEU:HD23	1:A:566:ALA:HB1	1.97	0.46
1:A:229:PHE:HB2	7:A:613:IOD:I	2.86	0.45
1:A:19:SER:O	1:A:21:TYR:N	2.50	0.45
1:A:287:TRP:CB	1:A:292:LEU:HD11	2.45	0.45
1:A:476:LEU:HD21	1:A:498:ALA:HB1	1.97	0.45
1:A:275:ARG:HG2	1:A:275:ARG:NH1	2.32	0.45
1:A:53:ASP:C	1:A:55:LEU:N	2.75	0.45
1:A:240:ILE:HD12	1:A:381:PHE:O	2.17	0.45
1:A:517:ARG:CD	8:A:753:HOH:O	2.60	0.45
1:A:551:ARG:HD2	1:A:582:VAL:HG12	1.98	0.45
1:A:117:THR:HG22	1:A:164:GLY:HA2	1.98	0.45
1:A:14:LYS:HG3	1:A:15:CYS:N	2.32	0.45
1:A:349:PHE:HA	1:A:497:ASN:HD21	1.80	0.45
1:A:433:LEU:HD13	4:A:605:HEM:CMA	2.47	0.45
1:A:544:LEU:O	1:A:547:VAL:HG22	2.16	0.45
1:A:14:LYS:HA	1:A:14:LYS:HD2	1.82	0.45
1:A:365:TYR:CZ	1:A:576:PHE:HE2	2.34	0.45
1:A:384:TRP:C	1:A:386:ILE:N	2.75	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:441:CYS:SG	1:A:492:ILE:HG22	2.57	0.45
1:A:18:ASN:CG	1:A:20:PRO:HD3	2.42	0.44
1:A:203:LEU:HD21	1:A:252:GLY:HA2	1.98	0.44
1:A:104:GLY:C	4:A:605:HEM:HAC	2.41	0.44
1:A:36:LEU:CD1	8:A:709:HOH:O	2.65	0.44
1:A:117:THR:HG23	1:A:163:ALA:C	2.42	0.44
1:A:418:ARG:O	1:A:432:ASP:HB2	2.18	0.44
1:A:103:TRP:O	1:A:106:ILE:HB	2.18	0.44
1:A:167:CYS:CB	1:A:168:PRO:CD	2.93	0.44
1:A:362:ASP:O	1:A:363:GLU:C	2.61	0.44
1:A:562:VAL:O	1:A:577:VAL:HG22	2.17	0.44
1:A:362:ASP:HB3	1:A:368:TRP:HD1	1.83	0.44
1:A:166:VAL:HB	1:A:167:CYS:H	1.23	0.44
1:A:226:TYR:O	1:A:227:LEU:C	2.60	0.43
1:A:274:ASN:O	1:A:275:ARG:C	2.61	0.43
1:A:543:SER:O	1:A:546:LYS:HB2	2.18	0.43
1:A:348:ARG:HH11	1:A:437:ASN:ND2	2.15	0.43
1:A:387:ILE:HG12	1:A:388:LYS:HG3	2.00	0.43
1:A:502:VAL:HG13	1:A:507:VAL:O	2.19	0.43
1:A:220:TRP:HB2	8:A:712:HOH:O	2.18	0.43
1:A:345:PHE:CZ	1:A:444:HIS:HB2	2.53	0.43
1:A:46:TRP:CE2	1:A:340:SER:HB3	2.54	0.43
1:A:242:THR:O	1:A:245:ARG:CG	2.63	0.43
1:A:134:ILE:O	1:A:139:CYS:SG	2.76	0.43
1:A:260:ILE:HD11	1:A:386:ILE:CG1	2.31	0.43
1:A:475:ILE:O	1:A:479:LYS:HG3	2.19	0.43
1:A:557:THR:OG1	1:A:559:ILE:HG13	2.18	0.43
1:A:588:SER:N	1:A:589:PRO:CD	2.81	0.43
1:A:14:LYS:CG	1:A:15:CYS:N	2.80	0.43
1:A:189:ALA:O	1:A:190:SER:C	2.62	0.43
1:A:260:ILE:CD1	1:A:382:ASN:O	2.60	0.43
1:A:67:ARG:O	1:A:68:ASN:HB2	2.18	0.43
1:A:189:ALA:C	1:A:191:LEU:N	2.73	0.42
1:A:153:THR:O	1:A:153:THR:HG23	2.18	0.42
1:A:384:TRP:C	1:A:386:ILE:H	2.28	0.42
1:A:468:GLN:HE21	1:A:468:GLN:HB2	1.66	0.42
1:A:10:VAL:HG21	8:A:908:HOH:O	2.18	0.42
1:A:414:THR:O	1:A:414:THR:HG23	2.19	0.42
1:A:578:ASP:OD1	1:A:580:SER:N	2.52	0.42
1:A:134:ILE:O	1:A:134:ILE:HG22	2.20	0.42
1:A:345:PHE:CZ	1:A:444:HIS:CG	3.07	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:ASN:C	1:A:557:THR:CG2	2.93	0.42
1:A:106:ILE:O	1:A:107:VAL:C	2.61	0.42
1:A:8:ALA:O	1:A:10:VAL:N	2.46	0.42
1:A:526:ASP:OD1	1:A:526:ASP:C	2.61	0.42
2:D:2:NAG:H4	2:D:3:MAN:H2	1.61	0.42
1:A:450:ASN:OD1	1:A:460:GLN:HB3	2.18	0.42
1:A:545:GLN:HE21	1:A:545:GLN:CA	2.31	0.42
1:A:162:ARG:HE	1:A:162:ARG:HB3	1.63	0.42
1:A:169:THR:CB	1:A:170:PRO:CD	2.98	0.42
1:A:572:TYR:HD2	1:A:573:PRO:CD	2.32	0.42
1:A:22:ARG:NE	8:A:783:HOH:O	2.53	0.41
1:A:144:PHE:C	1:A:145:PRO:O	2.60	0.41
1:A:193:TYR:OH	1:A:297:ARG:HA	2.20	0.41
1:A:63:GLN:N	8:A:844:HOH:O	2.53	0.41
1:A:258:GLU:O	1:A:380:PHE:HA	2.20	0.41
1:A:276:LEU:HD11	1:A:587:LEU:HD21	2.00	0.41
1:A:184:THR:OG1	1:A:188:ASP:OD2	2.37	0.41
1:A:283:LEU:O	1:A:285:PRO:CD	2.68	0.41
1:A:333:ASN:O	1:A:333:ASN:ND2	2.54	0.41
1:A:450:ASN:CG	1:A:460:GLN:HB3	2.45	0.41
1:A:187:LEU:HD13	1:A:305:GLN:HG2	2.02	0.41
1:A:193:TYR:CZ	1:A:297:ARG:HA	2.55	0.41
1:A:213:MET:HG2	1:A:273:HIS:NE2	2.34	0.41
1:A:363:GLU:H	1:A:363:GLU:HG2	1.40	0.41
1:A:393:ASP:N	1:A:394:PRO:CD	2.75	0.41
1:A:236:PRO:HD2	1:A:248:CYS:SG	2.61	0.41
1:A:18:ASN:HB3	1:A:19:SER:H	1.27	0.41
1:A:73:PRO:HG3	1:A:483:LEU:O	2.20	0.41
1:A:144:PHE:CE2	1:A:150:LYS:HB2	2.56	0.41
1:A:212:LEU:H	1:A:212:LEU:HG	1.44	0.41
1:A:226:TYR:OH	1:A:391:GLY:HA2	2.20	0.41
1:A:270:LEU:HD13	8:A:620:HOH:O	2.21	0.41
1:A:352:MET:HE3	1:A:497:ASN:HB3	2.02	0.41
1:A:421:LEU:HG	1:A:422:PHE:N	2.35	0.41
1:A:152:LYS:H	1:A:152:LYS:HG2	1.63	0.41
1:A:364:ASN:HB3	8:A:864:HOH:O	2.20	0.41
1:A:564:LEU:HA	1:A:564:LEU:HD12	1.49	0.41
1:A:117:THR:HG23	1:A:164:GLY:CA	2.50	0.40
1:A:165:PHE:HA	1:A:179:GLN:HA	2.03	0.40
1:A:172:TYR:HD1	1:A:172:TYR:HA	1.27	0.40
1:A:203:LEU:HD12	1:A:203:LEU:HA	1.93	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:124:HIS:HA	8:A:711:HOH:O	2.20	0.40
1:A:188:ASP:C	1:A:188:ASP:OD1	2.64	0.40
1:A:206:LEU:H	1:A:206:LEU:HG	1.69	0.40
1:A:405:LYS:HG2	1:A:406:LEU:N	2.37	0.40
1:A:127:THR:CG2	1:A:128:GLN:N	2.82	0.40
1:A:306:ILE:O	1:A:310:ARG:CB	2.69	0.40
1:A:221:ASP:HB2	1:A:226:TYR:CE1	2.46	0.40
1:A:426:HIS:CD2	1:A:426:HIS:N	2.89	0.40
1:A:91:VAL:HG23	1:A:411:LYS:HD3	2.04	0.40
1:A:511:LEU:HD12	1:A:511:LEU:HA	1.97	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	592/595 (100%)	505 (85%)	66 (11%)	21 (4%)	3 4

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	167	CYS
1	A	168	PRO
1	A	169	THR
1	A	424	PRO
1	A	427	LYS
1	A	573	PRO
1	A	3	GLU
1	A	119	LEU
1	A	363	GLU
1	A	594	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	20	PRO
1	A	122	ASN
1	A	171	PRO
1	A	545	GLN
1	A	9	PRO
1	A	32	ARG
1	A	166	VAL
1	A	8	ALA
1	A	367	PRO
1	A	509	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	517/517 (100%)	425 (82%)	92 (18%)	2 3

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	SER
1	A	3	GLU
1	A	4	VAL
1	A	9	PRO
1	A	11	PRO
1	A	16	ASP
1	A	22	ARG
1	A	24	ILE
1	A	31	ARG
1	A	33	SER
1	A	34	PRO
1	A	36	LEU
1	A	52	GLU
1	A	57	LEU
1	A	62	THR
1	A	64	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	91	VAL
1	A	98	LEU
1	A	112	ASP
1	A	115	PRO
1	A	118	GLU
1	A	119	LEU
1	A	125	SER
1	A	126	LYS
1	A	127	THR
1	A	131	GLU
1	A	134	ILE
1	A	145	PRO
1	A	146	LYS
1	A	149	PRO
1	A	152	LYS
1	A	153	THR
1	A	159	PRO
1	A	161	PHE
1	A	162	ARG
1	A	169	THR
1	A	171	PRO
1	A	172	TYR
1	A	173	GLN
1	A	175	LEU
1	A	187	LEU
1	A	197	PRO
1	A	201	SER
1	A	203	LEU
1	A	206	LEU
1	A	208	SER
1	A	209	PRO
1	A	212	LEU
1	A	218	GLU
1	A	224	LEU
1	A	227	LEU
1	A	235	SER
1	A	240	ILE
1	A	245	ARG
1	A	261	LEU
1	A	276	LEU
1	A	279	GLU
1	A	281	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	282	LYS
1	A	283	LEU
1	A	285	PRO
1	A	292	LEU
1	A	317	LEU
1	A	329	GLN
1	A	333	ASN
1	A	352	MET
1	A	357	THR
1	A	360	ARG
1	A	363	GLU
1	A	376	LEU
1	A	387	ILE
1	A	394	PRO
1	A	402	LYS
1	A	424	PRO
1	A	427	LYS
1	A	431	PHE
1	A	461	PRO
1	A	464	LEU
1	A	475	ILE
1	A	480	LEU
1	A	486	THR
1	A	494	ILE
1	A	503	GLU
1	A	511	LEU
1	A	538	GLU
1	A	539	LYS
1	A	545	GLN
1	A	546	LYS
1	A	559	ILE
1	A	564	LEU
1	A	592	SER
1	A	593	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	18	ASN
1	A	147	ASN
1	A	222	HIS
1	A	273	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	423	GLN
1	A	429	HIS
1	A	460	GLN
1	A	468	GLN
1	A	497	ASN
1	A	545	GLN
1	A	558	HIS
1	A	568	GLN
1	A	574	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	SEP	A	198	1	8,9,10	1.67	3 (37%)	7,12,14	3.61	3 (42%)

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	SEP	A	198	1	-	0/6/8/10	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	198	SEP	P-O1P	2.80	1.59	1.50
1	A	198	SEP	O-C	2.13	1.28	1.20
1	A	198	SEP	CA-N	-2.00	1.42	1.48

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	198	SEP	O3P-P-OG	7.17	125.35	106.67
1	A	198	SEP	O2P-P-OG	-5.02	93.57	106.67
1	A	198	SEP	O3P-P-O1P	-2.89	99.57	110.83

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	198	SEP	1	0

5.5 Carbohydrates [i](#)

10 monosaccharides are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	B	1	2,1	14,14,15	1.42	3 (21%)	17,19,21	1.97	3 (17%)
2	NAG	B	2	2	14,14,15	1.80	3 (21%)	17,19,21	2.32	6 (35%)
2	MAN	B	3	2	11,11,12	0.90	1 (9%)	15,15,17	2.02	2 (13%)
3	NAG	C	1	1,3	14,14,15	1.28	2 (14%)	17,19,21	2.55	7 (41%)
3	NAG	C	2	3	14,14,15	0.94	1 (7%)	17,19,21	1.03	1 (5%)
2	NAG	D	1	2,1	14,14,15	1.15	1 (7%)	17,19,21	1.75	4 (23%)
2	NAG	D	2	2	14,14,15	0.70	0	17,19,21	1.27	2 (11%)
2	MAN	D	3	2	11,11,12	0.77	0	15,15,17	0.74	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	E	1	1,3	14,14,15	1.29	1 (7%)	17,19,21	1.97	4 (23%)
3	NAG	E	2	3	14,14,15	1.26	1 (7%)	17,19,21	0.90	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	B	1	2,1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	2	2	-	0/6/23/26	0/1/1/1
2	MAN	B	3	2	-	1/2/19/22	0/1/1/1
3	NAG	C	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	C	2	3	-	2/6/23/26	0/1/1/1
2	NAG	D	1	2,1	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	D	2	2	-	2/6/23/26	0/1/1/1
2	MAN	D	3	2	-	2/2/19/22	1/1/1/1
3	NAG	E	1	1,3	-	0/6/23/26	0/1/1/1
3	NAG	E	2	3	-	3/6/23/26	0/1/1/1

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2	NAG	C1-C2	3.95	1.57	1.52
3	E	2	NAG	C1-C2	3.83	1.57	1.52
2	D	1	NAG	C1-C2	3.26	1.56	1.52
2	B	2	NAG	C8-C7	3.09	1.57	1.50
3	C	2	NAG	C1-C2	2.60	1.55	1.52
3	C	1	NAG	O5-C1	2.48	1.47	1.43
3	C	1	NAG	O5-C5	2.38	1.48	1.43
2	B	1	NAG	O5-C1	2.32	1.47	1.43
2	B	1	NAG	C4-C3	2.31	1.58	1.52
3	E	1	NAG	C4-C5	2.25	1.57	1.53
2	B	3	MAN	C2-C3	2.19	1.55	1.52
2	B	2	NAG	C4-C5	2.15	1.57	1.53
2	B	1	NAG	O4-C4	2.11	1.48	1.43

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	3	MAN	C1-C2-C3	6.75	119.47	109.64

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1	NAG	C4-C3-C2	-6.25	101.86	111.02
3	C	1	NAG	C1-C2-N2	6.20	120.21	110.43
2	B	1	NAG	C1-C2-N2	-5.52	101.73	110.43
2	B	2	NAG	C2-N2-C7	-4.92	116.31	122.90
2	B	2	NAG	C1-C2-N2	4.51	117.55	110.43
3	E	1	NAG	C1-C2-N2	-4.49	103.36	110.43
3	E	1	NAG	C2-N2-C7	-4.30	117.13	122.90
2	D	1	NAG	C2-N2-C7	-3.91	117.66	122.90
2	B	2	NAG	C6-C5-C4	-3.90	103.43	113.02
2	B	1	NAG	C3-C4-C5	-3.90	103.15	110.23
3	E	1	NAG	C4-C3-C2	3.04	115.47	111.02
2	B	3	MAN	C2-C3-C4	2.93	116.02	110.86
2	D	1	NAG	C3-C4-C5	-2.79	105.18	110.23
2	D	2	NAG	C4-C3-C2	-2.78	106.95	111.02
2	B	1	NAG	C1-O5-C5	2.74	115.85	112.19
2	B	2	NAG	C8-C7-N2	2.58	120.40	116.12
2	D	1	NAG	C8-C7-N2	2.53	120.31	116.12
2	D	2	NAG	C2-N2-C7	-2.50	119.55	122.90
3	C	1	NAG	C8-C7-N2	2.48	120.22	116.12
2	B	2	NAG	O7-C7-C8	-2.35	117.87	122.05
3	C	2	NAG	C1-C2-N2	-2.30	106.81	110.43
3	C	1	NAG	O5-C1-C2	-2.26	107.80	111.29
3	C	1	NAG	O7-C7-C8	-2.23	118.09	122.05
3	C	1	NAG	C3-C4-C5	-2.21	106.22	110.23
2	B	2	NAG	C4-C3-C2	2.21	114.26	111.02
3	E	1	NAG	O5-C1-C2	-2.19	107.90	111.29
3	C	1	NAG	C2-N2-C7	-2.15	120.02	122.90
2	D	1	NAG	C6-C5-C4	2.14	118.27	113.02

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1	NAG	C1
2	D	1	NAG	C1

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	E	2	NAG	C1-C2-N2-C7
2	D	3	MAN	O5-C5-C6-O6
2	D	3	MAN	C4-C5-C6-O6
2	D	2	NAG	O5-C5-C6-O6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	D	2	NAG	C4-C5-C6-O6
3	C	2	NAG	O5-C5-C6-O6
3	E	2	NAG	O5-C5-C6-O6
3	E	2	NAG	C3-C2-N2-C7
2	B	3	MAN	O5-C5-C6-O6
3	C	2	NAG	C4-C5-C6-O6

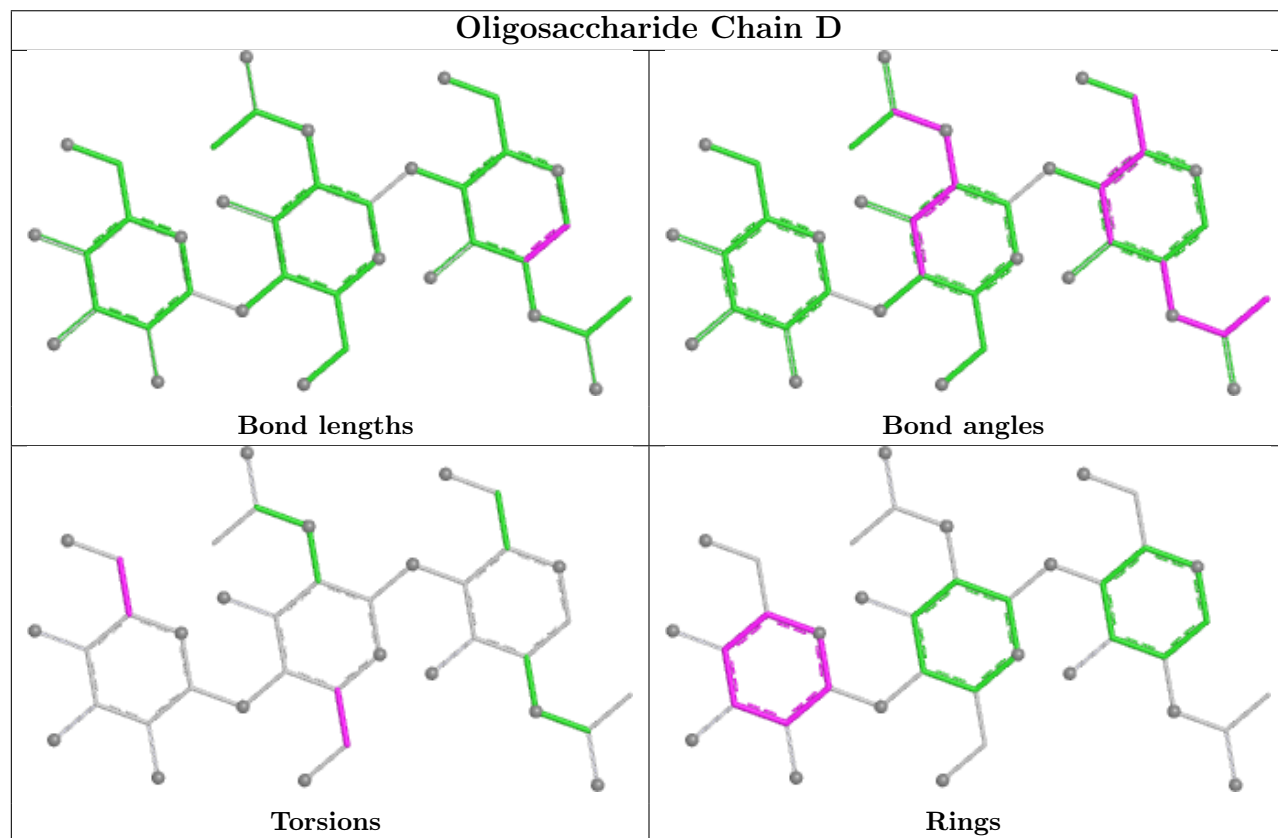
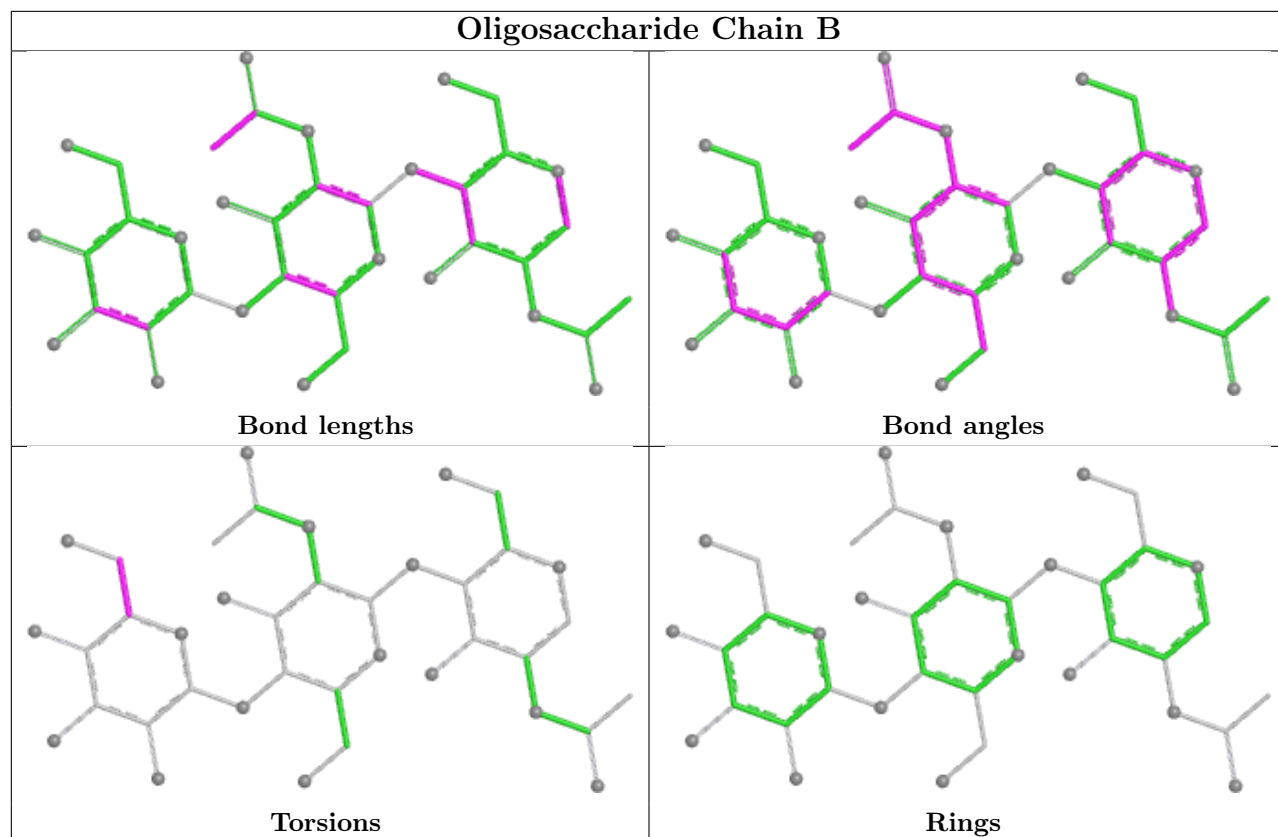
All (1) ring outliers are listed below:

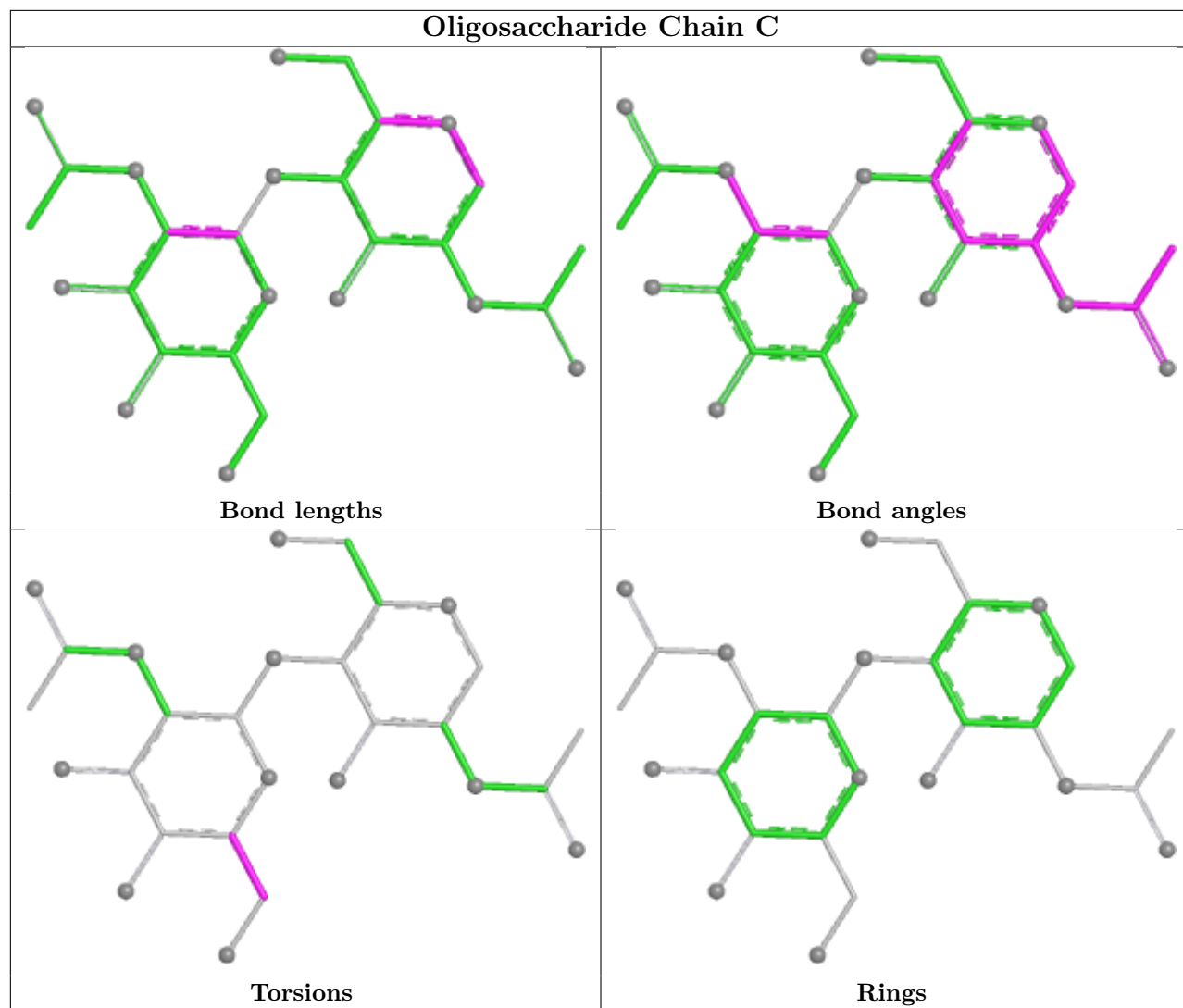
Mol	Chain	Res	Type	Atoms
2	D	3	MAN	C1-C2-C3-C4-C5-O5

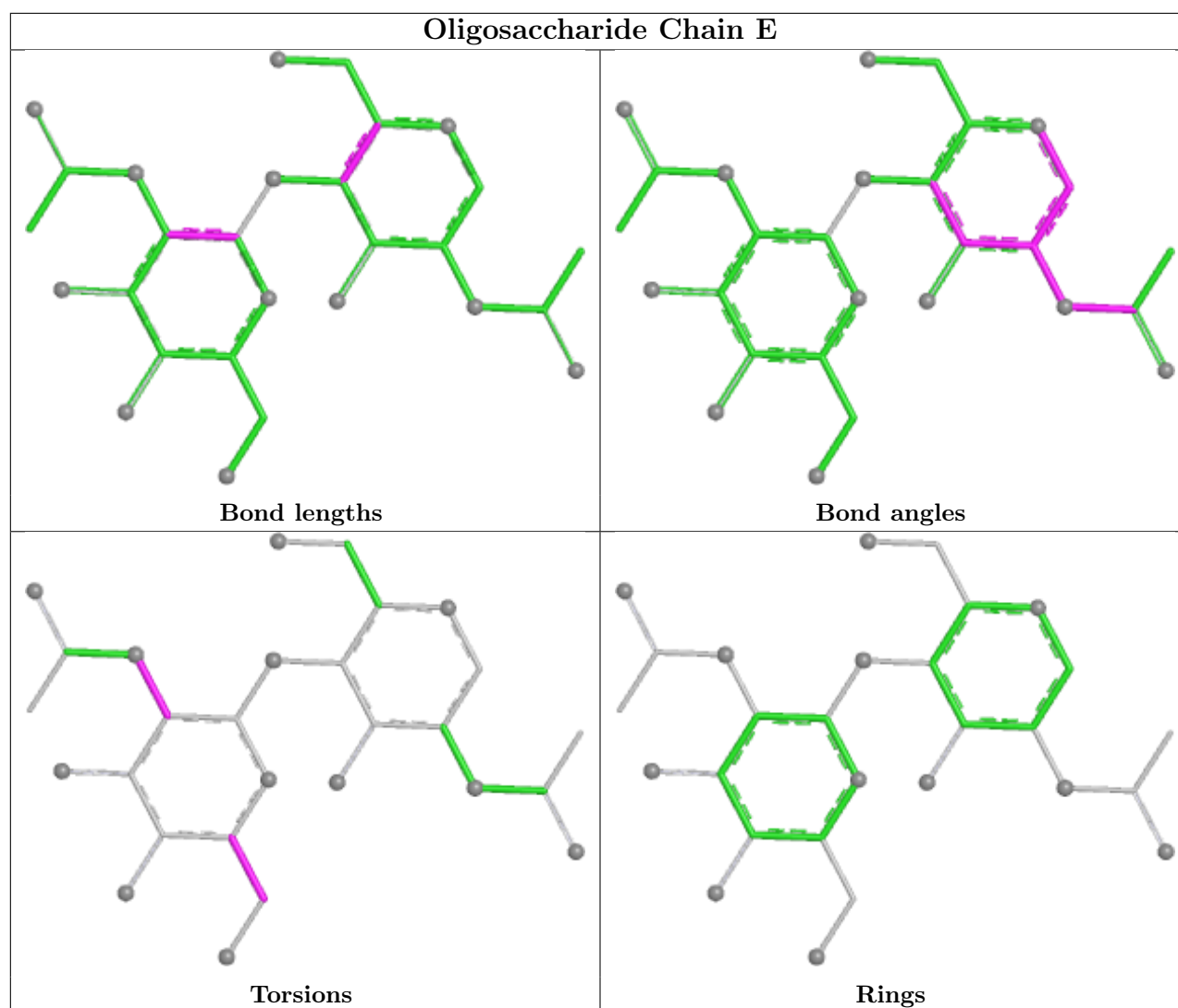
6 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3	MAN	2	0
3	C	1	NAG	1	0
2	D	2	NAG	1	0
3	E	2	NAG	2	0
2	B	1	NAG	6	0
3	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](#)

Of 10 ligands modelled in this entry, 8 are monoatomic - leaving 2 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	$\# Z > 2$
4	HEM	A	605	1	50,50,50	3.56	25 (50%)	67,82,82	2.20	24 (35%)
6	SCN	A	615	-	1,2,2	1.31	0	0,1,1	-	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	HEM	A	605	1	-	5/14/54/54	-

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	605	HEM	FE-NC	16.78	2.50	1.95
4	A	605	HEM	C3D-C2D	6.77	1.51	1.36
4	A	605	HEM	CAB-C3B	5.48	1.62	1.47
4	A	605	HEM	CMA-C3A	5.16	1.61	1.50
4	A	605	HEM	FE-ND	4.83	2.09	1.94
4	A	605	HEM	C1A-C2A	4.45	1.53	1.44
4	A	605	HEM	CMB-C2B	4.20	1.59	1.50
4	A	605	HEM	C1C-NC	-4.17	1.31	1.39
4	A	605	HEM	C1A-NA	-3.78	1.32	1.39
4	A	605	HEM	CMC-C2C	3.72	1.58	1.50
4	A	605	HEM	CAC-C3C	3.66	1.57	1.47
4	A	605	HEM	CAD-C3D	3.24	1.59	1.51
4	A	605	HEM	CHD-C1D	2.93	1.45	1.39
4	A	605	HEM	C4C-NC	-2.91	1.34	1.39
4	A	605	HEM	CHC-C1C	-2.89	1.32	1.38
4	A	605	HEM	C4A-C3A	2.87	1.49	1.43
4	A	605	HEM	CBD-CGD	2.81	1.57	1.50
4	A	605	HEM	CHA-C1A	-2.80	1.33	1.39
4	A	605	HEM	CHC-C4B	-2.76	1.32	1.39
4	A	605	HEM	C4B-NB	2.73	1.44	1.38
4	A	605	HEM	C1B-C2B	2.63	1.49	1.44
4	A	605	HEM	CMD-C2D	2.59	1.56	1.50
4	A	605	HEM	O2A-CGA	-2.41	1.22	1.30
4	A	605	HEM	CHB-C4A	2.27	1.44	1.39
4	A	605	HEM	FE-NB	-2.04	1.88	1.94

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	605	HEM	CHA-C4D-ND	5.30	130.92	124.37
4	A	605	HEM	C3B-C4B-NB	5.11	113.14	109.47
4	A	605	HEM	CBD-CAD-C3D	-4.85	99.13	112.53
4	A	605	HEM	CHC-C1C-NC	4.34	129.17	124.45

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	605	HEM	CHD-C1D-ND	4.09	128.82	124.42
4	A	605	HEM	CHA-C4D-C3D	-3.85	118.13	125.23
4	A	605	HEM	CHD-C4C-NC	-3.84	120.27	124.45
4	A	605	HEM	CHC-C4B-NB	3.76	128.47	124.42
4	A	605	HEM	CHD-C1D-C2D	-3.46	119.57	125.03
4	A	605	HEM	CAA-C2A-C1A	3.39	131.56	124.94
4	A	605	HEM	CHC-C4B-C3B	-3.35	118.39	125.07
4	A	605	HEM	CHC-C1C-C2C	-3.18	118.88	125.49
4	A	605	HEM	CMA-C3A-C4A	3.11	130.15	125.42
4	A	605	HEM	CMB-C2B-C1B	2.95	129.65	125.03
4	A	605	HEM	CAD-C3D-C4D	2.88	129.72	124.70
4	A	605	HEM	O1D-CGD-CBD	-2.60	114.85	123.09
4	A	605	HEM	C4B-C3B-C2B	-2.56	104.93	107.28
4	A	605	HEM	CMB-C2B-C3B	-2.53	122.30	128.43
4	A	605	HEM	CAA-CBA-CGA	-2.49	107.07	113.67
4	A	605	HEM	C4C-CHD-C1D	-2.43	120.86	126.02
4	A	605	HEM	O2D-CGD-CBD	2.32	121.32	114.00
4	A	605	HEM	C4C-C3C-C2C	-2.24	104.87	106.81
4	A	605	HEM	C3B-C2B-C1B	2.19	108.06	106.41
4	A	605	HEM	CAA-C2A-C3A	-2.08	122.41	127.07

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	605	HEM	C1A-C2A-CAA-CBA
4	A	605	HEM	C3A-C2A-CAA-CBA
4	A	605	HEM	C2A-CAA-CBA-CGA
4	A	605	HEM	CAD-CBD-CGD-O1D
4	A	605	HEM	CAD-CBD-CGD-O2D

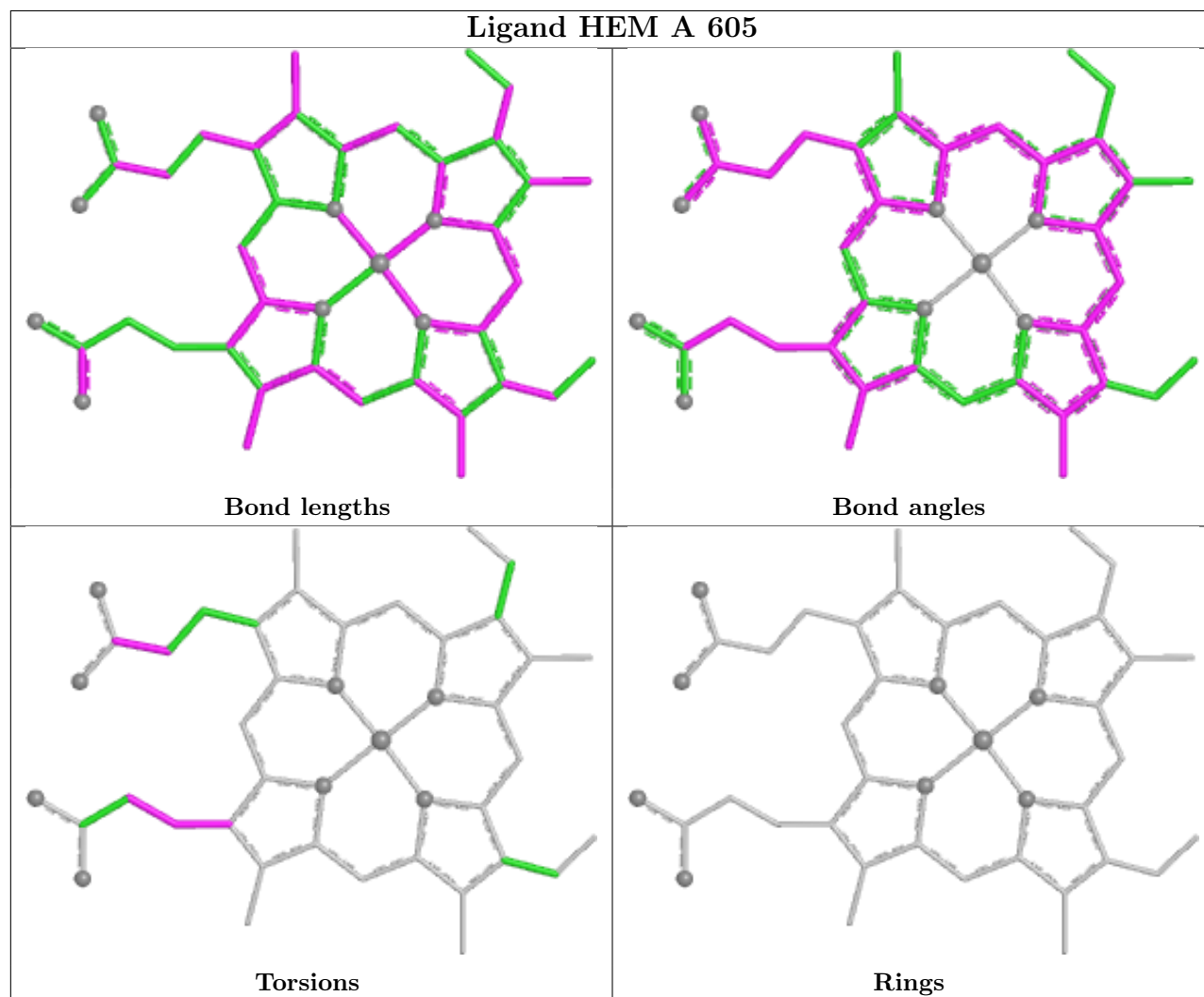
There are no ring outliers.

1 monomer is involved in 32 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	605	HEM	32	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier.

Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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	594/595 (99%)	0.88	63 (10%) 11 9	28, 47, 86, 100	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	9	PRO	5.1
1	A	229	PHE	4.5
1	A	127	THR	4.2
1	A	172	TYR	4.1
1	A	18	ASN	4.0
1	A	4	VAL	3.9
1	A	362	ASP	3.6
1	A	2	TRP	3.5
1	A	532	ASN	3.2
1	A	246	VAL	3.0
1	A	170	PRO	3.0
1	A	340	SER	3.0
1	A	26	GLY	3.0
1	A	569	ALA	2.9
1	A	20	PRO	2.9
1	A	207	SER	2.8
1	A	8	ALA	2.8
1	A	160	PHE	2.8
1	A	33	SER	2.8
1	A	12	LEU	2.7
1	A	10	VAL	2.7
1	A	361	LEU	2.7
1	A	337	PRO	2.7
1	A	541	ARG	2.6
1	A	7	GLY	2.6
1	A	171	PRO	2.6
1	A	274	ASN	2.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	583	ASP	2.5
1	A	129	CYS	2.5
1	A	529	TRP	2.5
1	A	124	HIS	2.5
1	A	13	VAL	2.5
1	A	119	LEU	2.5
1	A	592	SER	2.5
1	A	153	THR	2.4
1	A	254	PHE	2.4
1	A	214	ALA	2.4
1	A	292	LEU	2.4
1	A	247	PRO	2.3
1	A	283	LEU	2.3
1	A	540	GLN	2.3
1	A	21	TYR	2.3
1	A	570	ASN	2.3
1	A	125	SER	2.3
1	A	168	PRO	2.2
1	A	582	VAL	2.2
1	A	93	ASP	2.2
1	A	538	GLU	2.2
1	A	192	VAL	2.1
1	A	120	GLY	2.1
1	A	175	LEU	2.1
1	A	537	THR	2.1
1	A	568	GLN	2.1
1	A	591	ALA	2.1
1	A	169	THR	2.1
1	A	11	PRO	2.1
1	A	173	GLN	2.1
1	A	215	VAL	2.1
1	A	572	TYR	2.1
1	A	1	SER	2.1
1	A	510	LEU	2.1
1	A	595	ASN	2.0
1	A	287	TRP	2.0

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

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($\text{\AA}^2$)	Q<0.9
1	SEP	A	198	10/11	0.94	0.12	31,48,50,50	0

6.3 Carbohydrates

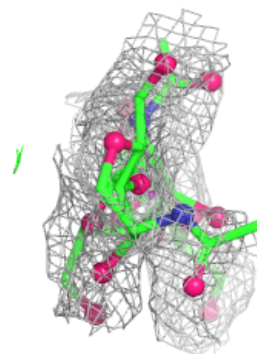
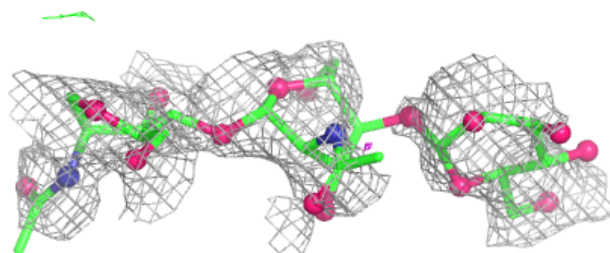
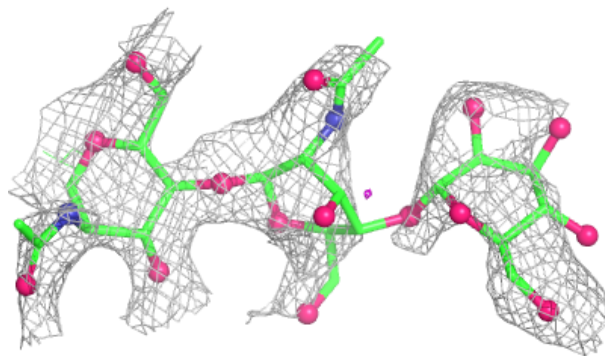
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	MAN	B	3	11/12	0.36	0.15	94,95,96,96	0
3	NAG	E	2	14/15	0.44	0.16	86,89,91,91	0
3	NAG	C	2	14/15	0.59	0.18	80,82,83,84	0
2	NAG	B	2	14/15	0.62	0.14	83,87,89,91	0
2	MAN	D	3	11/12	0.66	0.15	78,80,81,82	0
3	NAG	E	1	14/15	0.68	0.15	71,74,77,82	0
2	NAG	B	1	14/15	0.69	0.14	68,70,74,78	0
2	NAG	D	2	14/15	0.69	0.12	64,66,70,74	0
3	NAG	C	1	14/15	0.76	0.15	72,73,75,77	0
2	NAG	D	1	14/15	0.84	0.12	56,57,58,62	0

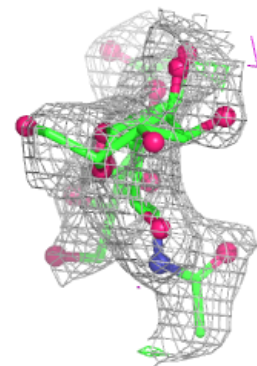
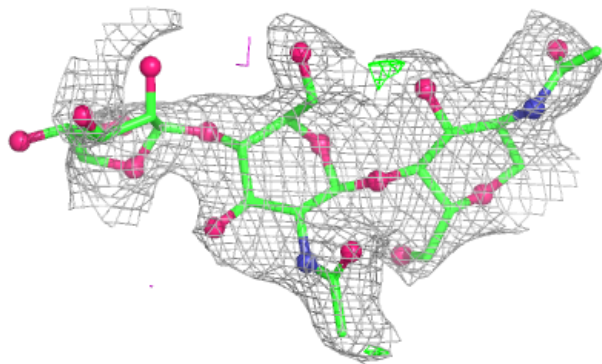
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain B:

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

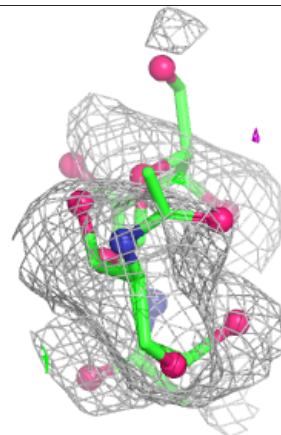
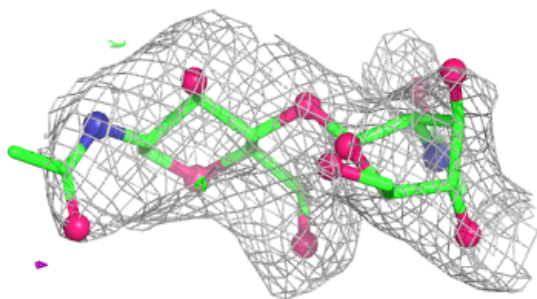
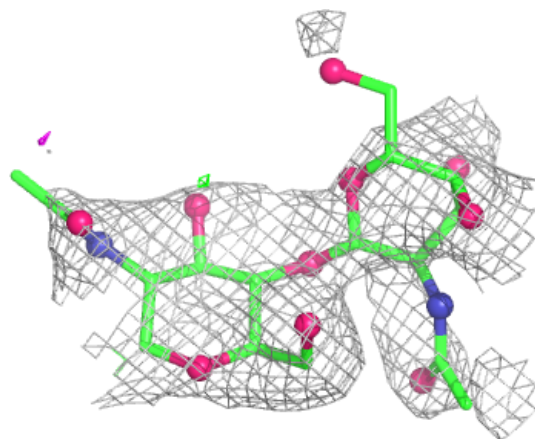
**Electron density around Chain D:**

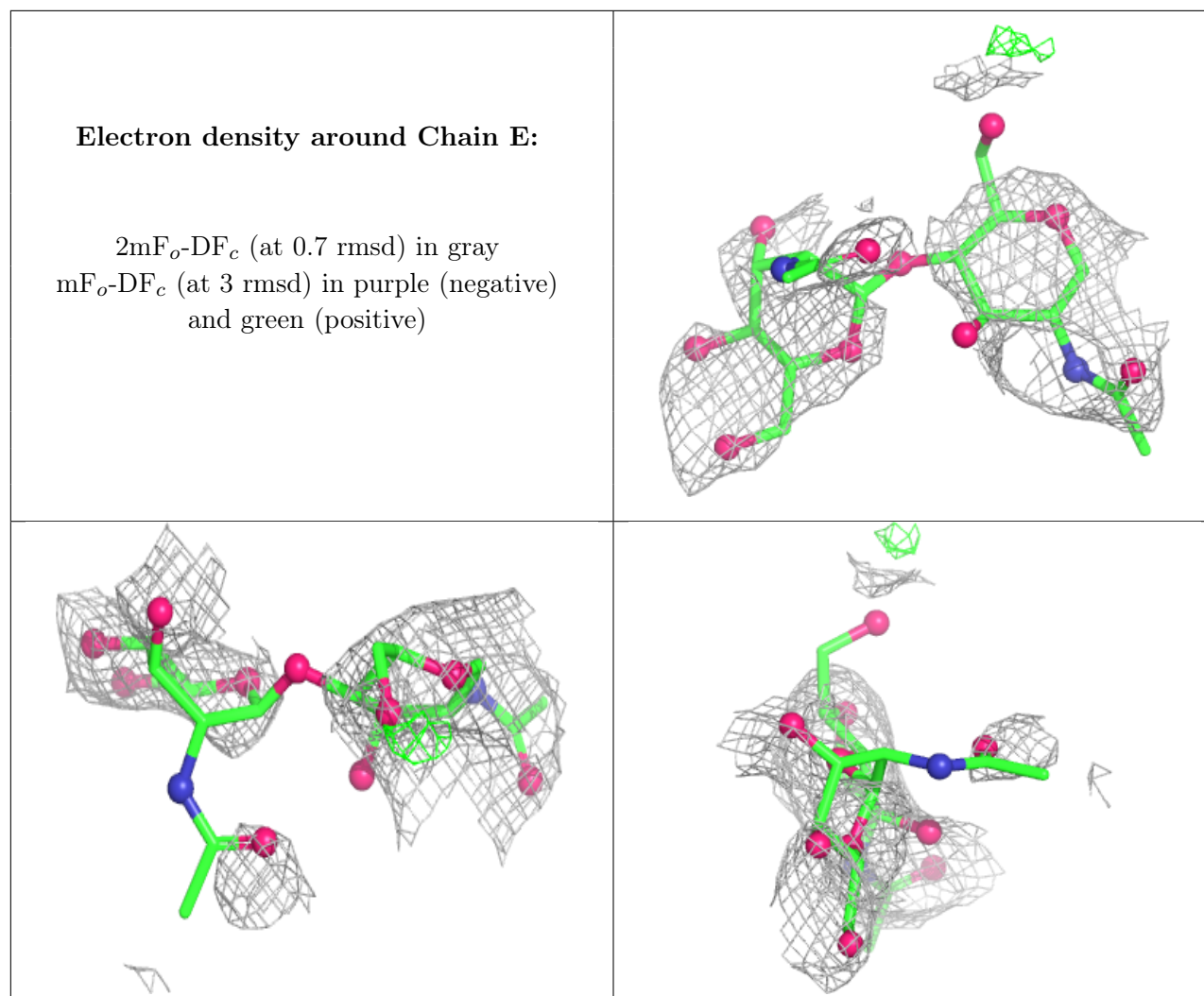
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain C:

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





6.4 Ligands ⓘ

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.

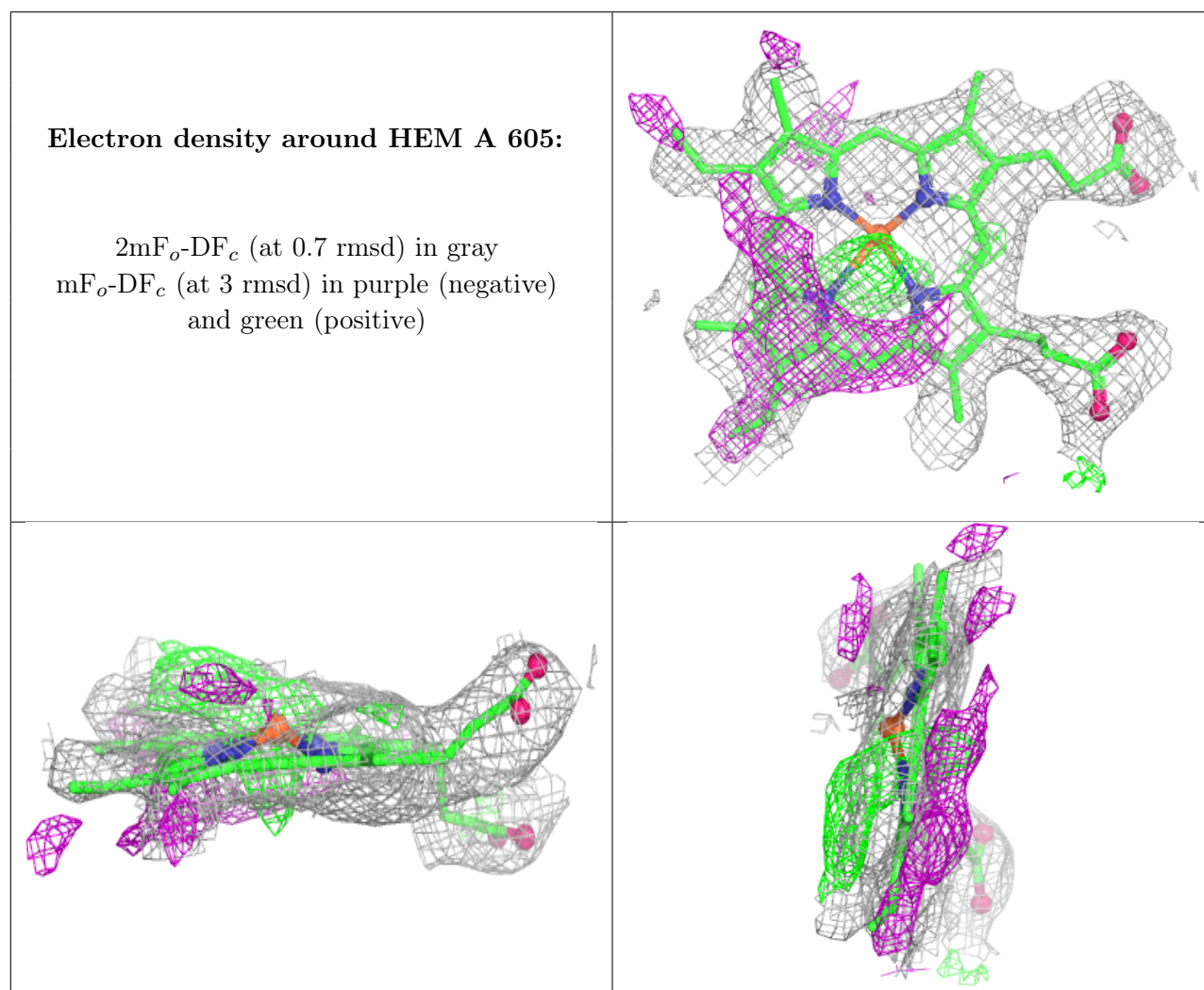
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	HEM	A	605	43/43	0.82	0.17	22,27,34,38	0
7	IOD	A	614	1/1	0.92	0.22	54,54,54,54	0
5	CA	A	606	1/1	0.95	0.05	44,44,44,44	0
7	IOD	A	613	1/1	0.96	0.10	85,85,85,85	0
7	IOD	A	612	1/1	0.96	0.06	75,75,75,75	0
7	IOD	A	611	1/1	0.97	0.04	57,57,57,57	0
6	SCN	A	615	3/3	0.97	0.14	17,17,21,25	0
7	IOD	A	609	1/1	0.97	0.04	60,60,60,60	0
7	IOD	A	610	1/1	0.97	0.04	56,56,56,56	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	IOD	A	608	1/1	0.99	0.05	43,43,43,43	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.