



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:57 PM UTC

PDB ID : 1LL4 / pdb_00001ll4
Title : STRUCTURE OF C. IMMITIS CHITINASE 1 COMPLEXED WITH AL-
LOSAMIDIN
Authors : Bortone, K.; Monzingo, A.F.; Ernst, S.; Robertus, J.D.
Deposited on : 2002-04-26
Resolution : 2.80 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
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

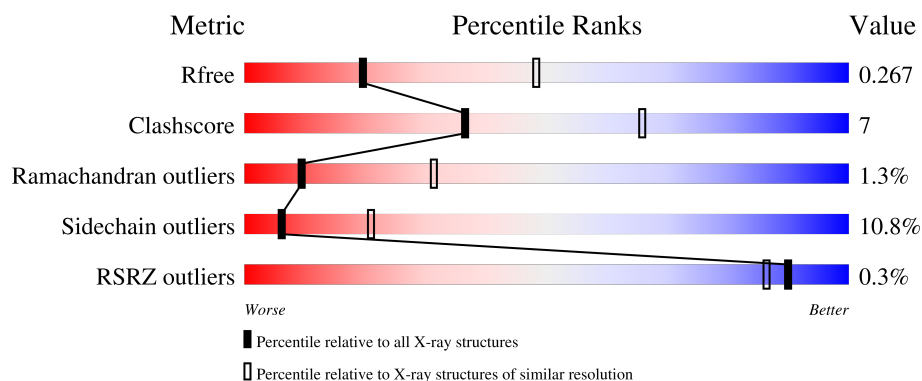
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	392	
1	B	392	
1	C	392	
1	D	392	
2	E	2	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	F	2	 100%
2	G	2	 100%
2	H	2	 100%

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 12604 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 CHITINASE 1.

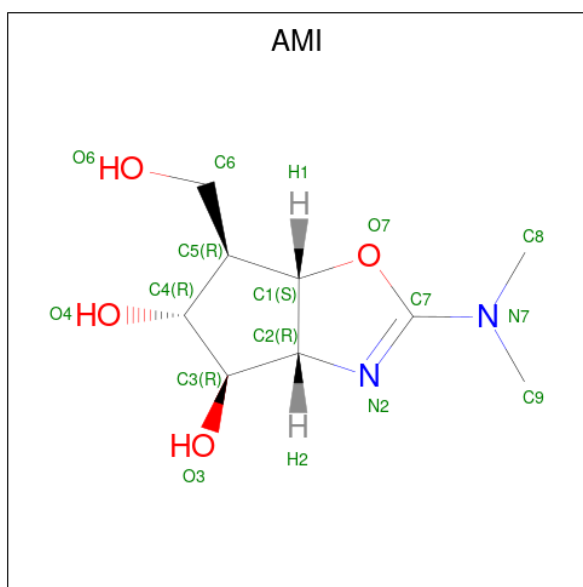
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	392	Total	C	N	O	S	0	0	0
			3083	1963	510	598	12			
1	B	392	Total	C	N	O	S	0	0	0
			3083	1963	510	598	12			
1	C	392	Total	C	N	O	S	0	0	0
			3083	1963	510	598	12			
1	D	392	Total	C	N	O	S	0	0	0
			3083	1963	510	598	12			

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



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

- Molecule 3 is ALLOSAMIZOLINE (CCD ID: AMI) (formula: C₉H₁₆N₂O₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			15	9	2	4		
3	B	1	Total	C	N	O	0	0
			15	9	2	4		
3	C	1	Total	C	N	O	0	0
			15	9	2	4		
3	D	1	Total	C	N	O	0	0
			15	9	2	4		

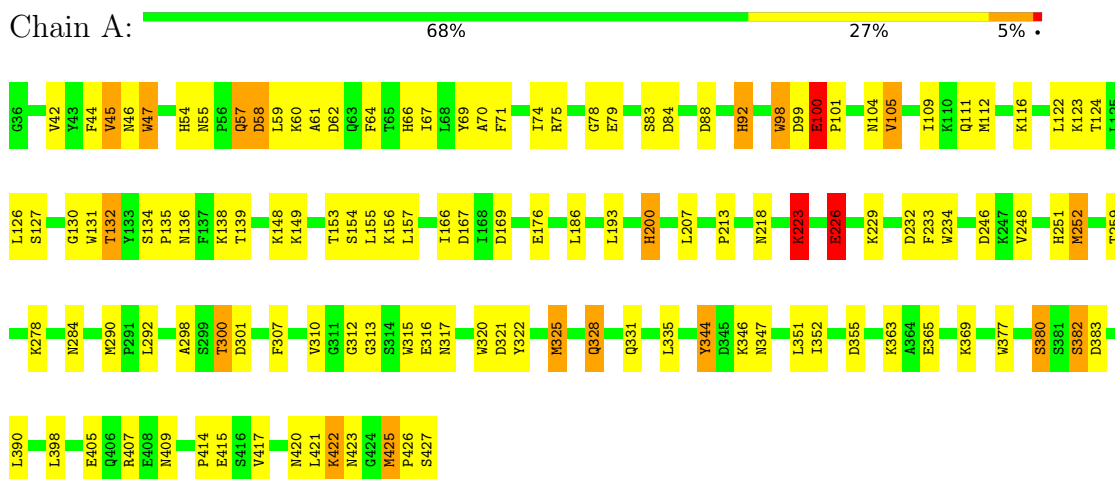
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	28	Total	O	0	0
			28	28		
4	B	22	Total	O	0	0
			22	22		
4	C	24	Total	O	0	0
			24	24		
4	D	26	Total	O	0	0
			26	26		

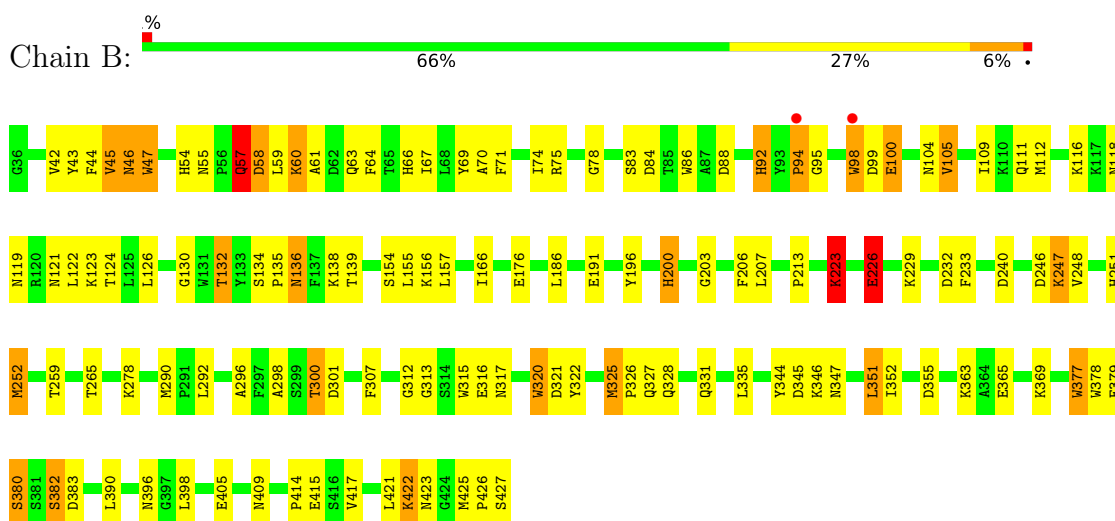
3 Residue-property plots

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: CHITINASE 1

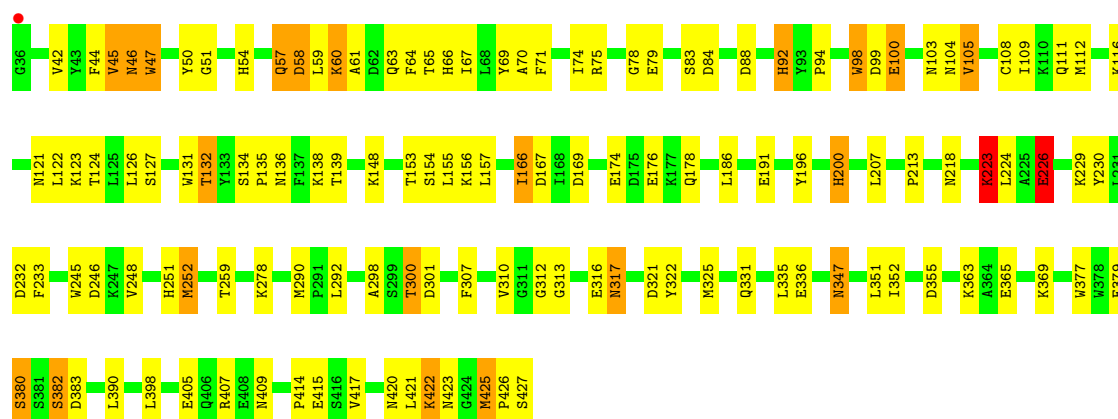


• Molecule 1: CHITINASE 1



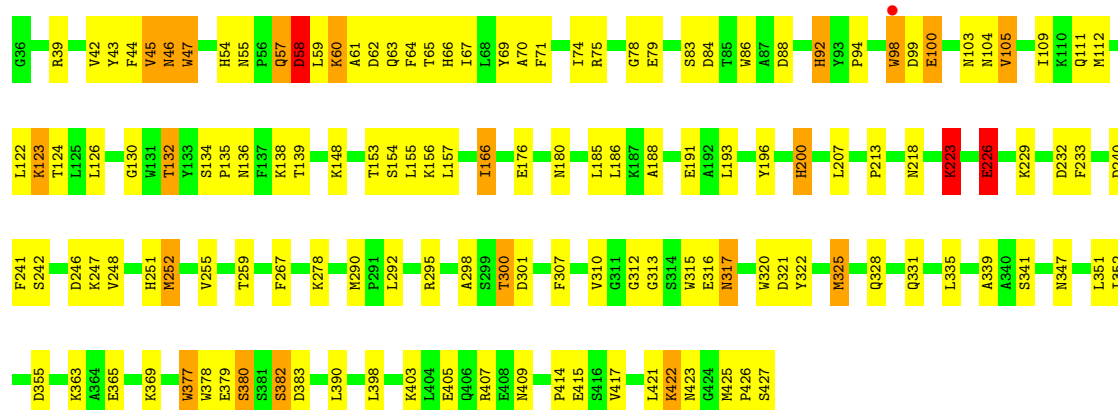
• Molecule 1: CHITINASE 1





• Molecule 1: CHITINASE 1

Chain D: 65% 29% 5% •



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

Chain E: 100%



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

Chain F: 100%



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

Chain G: 100%

MAA1
MAA2

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

Chain H:

100%

MAA1
MAA2

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	61.05Å 78.19Å 88.46Å 80.61° 82.27° 66.72°	Depositor
Resolution (Å)	5.00 – 2.80 5.00 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (5.00-2.80) 73.9 (5.00-2.80)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.44 (at 2.80Å)	Xtriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.197 , 0.258 0.205 , 0.267	Depositor DCC
R_{free} test set	1705 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	18.2	Xtriage
Anisotropy	0.585	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.95 , 133.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	12604	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.60% 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: NAA, AMI

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.97	7/3165 (0.2%)	1.75	60/4282 (1.4%)
1	B	0.98	7/3165 (0.2%)	1.78	70/4282 (1.6%)
1	C	0.97	8/3165 (0.3%)	1.76	69/4282 (1.6%)
1	D	0.97	7/3165 (0.2%)	1.78	70/4282 (1.6%)
All	All	0.97	29/12660 (0.2%)	1.77	269/17128 (1.6%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
All	All	0	2

All (29) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	54	HIS	CD2-NE2	-7.88	1.29	1.37
1	D	251	HIS	CD2-NE2	-7.53	1.29	1.37
1	C	200	HIS	CD2-NE2	-7.47	1.29	1.37
1	C	251	HIS	CD2-NE2	-7.28	1.29	1.37
1	C	54	HIS	CD2-NE2	-7.06	1.30	1.37
1	B	92	HIS	CD2-NE2	-6.89	1.30	1.37
1	D	54	HIS	CD2-NE2	-6.88	1.30	1.37
1	B	200	HIS	CD2-NE2	-6.65	1.30	1.37
1	B	54	HIS	CD2-NE2	-6.47	1.30	1.37
1	A	251	HIS	CD2-NE2	-6.42	1.30	1.37
1	D	200	HIS	CD2-NE2	-6.23	1.30	1.37
1	C	66	HIS	CD2-NE2	-6.23	1.31	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	66	HIS	CD2-NE2	-6.15	1.31	1.37
1	A	200	HIS	CD2-NE2	-6.13	1.31	1.37
1	B	251	HIS	CD2-NE2	-6.11	1.31	1.37
1	A	66	HIS	CD2-NE2	-6.10	1.31	1.37
1	A	251	HIS	CG-ND1	-5.82	1.31	1.38
1	D	92	HIS	CD2-NE2	-5.75	1.31	1.37
1	A	92	HIS	CD2-NE2	-5.65	1.31	1.37
1	B	265	THR	CA-CB	5.64	1.59	1.53
1	C	251	HIS	CG-ND1	-5.62	1.32	1.38
1	D	251	HIS	CG-ND1	-5.60	1.32	1.38
1	C	200	HIS	CG-ND1	-5.53	1.32	1.38
1	D	166	ILE	CA-CB	5.41	1.64	1.55
1	C	92	HIS	CD2-NE2	-5.33	1.31	1.37
1	C	166	ILE	CA-CB	5.25	1.64	1.55
1	B	200	HIS	CG-ND1	-5.18	1.32	1.38
1	A	200	HIS	CG-ND1	-5.13	1.32	1.38
1	B	66	HIS	CD2-NE2	-5.13	1.32	1.37

All (269) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	TRP	O-C-N	9.25	132.08	122.09
1	A	380	SER	N-CA-C	9.22	124.33	112.34
1	C	105	VAL	CB-CA-C	-8.79	98.59	110.98
1	D	98	TRP	O-C-N	8.79	131.58	122.09
1	D	246	ASP	CA-CB-CG	8.79	121.39	112.60
1	C	45	VAL	N-CA-CB	-8.72	100.47	111.46
1	A	105	VAL	CB-CA-C	-8.70	98.71	110.98
1	C	98	TRP	O-C-N	8.53	131.30	122.09
1	B	98	TRP	O-C-N	8.48	131.25	122.09
1	D	45	VAL	N-CA-CB	-8.48	100.78	111.46
1	C	138	LYS	N-CA-C	8.44	121.54	111.33
1	A	45	VAL	N-CA-CB	-8.40	100.87	111.46
1	D	138	LYS	N-CA-C	8.38	121.47	111.33
1	D	105	VAL	CB-CA-C	-8.33	99.23	110.98
1	B	138	LYS	N-CA-C	8.22	121.28	111.33
1	B	45	VAL	N-CA-CB	-8.22	101.11	111.46
1	B	105	VAL	CB-CA-C	-8.03	99.66	110.98
1	D	92	HIS	CB-CG-CD2	-8.02	120.78	131.20
1	A	138	LYS	N-CA-C	8.01	121.02	111.33
1	C	213	PRO	N-CA-C	7.96	122.99	110.50
1	A	92	HIS	CB-CG-CD2	-7.86	120.98	131.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	92	HIS	CB-CG-CD2	-7.84	121.01	131.20
1	A	88	ASP	N-CA-C	7.82	119.49	110.97
1	B	213	PRO	N-CA-C	7.79	122.73	110.50
1	C	75	ARG	NE-CZ-NH2	7.77	126.19	119.20
1	C	136	ASN	CA-CB-CG	7.68	120.28	112.60
1	D	301	ASP	N-CA-C	-7.53	101.98	112.45
1	D	213	PRO	N-CA-C	7.53	122.32	110.50
1	A	213	PRO	N-CA-C	7.51	122.14	110.80
1	C	132	THR	N-CA-CB	-7.47	99.14	110.12
1	D	88	ASP	N-CA-C	7.45	119.09	110.97
1	D	328	GLN	OE1-CD-NE2	-7.45	115.15	122.60
1	C	88	ASP	N-CA-C	7.41	119.05	110.97
1	C	92	HIS	CB-CG-CD2	-7.41	121.57	131.20
1	A	301	ASP	N-CA-C	-7.41	102.15	112.45
1	A	232	ASP	CA-CB-CG	-7.39	105.21	112.60
1	C	355	ASP	CA-CB-CG	7.32	119.92	112.60
1	A	246	ASP	CA-CB-CG	7.31	119.91	112.60
1	B	54	HIS	CB-CG-CD2	-7.29	121.72	131.20
1	D	132	THR	N-CA-CB	-7.28	99.42	110.12
1	B	246	ASP	CA-CB-CG	7.27	119.87	112.60
1	C	100	GLU	N-CA-C	7.26	125.85	109.81
1	B	136	ASN	CA-CB-CG	7.23	119.83	112.60
1	C	54	HIS	CB-CG-CD2	-7.18	121.86	131.20
1	D	57	GLN	OE1-CD-NE2	-7.18	115.42	122.60
1	B	100	GLU	N-CA-C	7.18	125.68	109.81
1	D	223	LYS	CG-CD-CE	-7.14	94.87	111.30
1	D	100	GLU	N-CA-C	7.12	125.54	109.81
1	B	104	ASN	N-CA-C	7.11	121.10	109.72
1	D	104	ASN	N-CA-C	7.10	121.08	109.72
1	B	409	ASN	CA-CB-CG	7.09	119.69	112.60
1	B	132	THR	N-CA-CB	-7.07	99.33	110.22
1	B	409	ASN	OD1-CG-ND2	-7.02	115.58	122.60
1	B	55	ASN	OD1-CG-ND2	-7.02	115.58	122.60
1	B	88	ASP	N-CA-C	7.02	118.62	110.97
1	A	54	HIS	CB-CG-CD2	-7.00	122.10	131.20
1	C	423	ASN	OD1-CG-ND2	-7.00	115.60	122.60
1	D	218	ASN	CA-CB-CG	-7.00	105.60	112.60
1	B	54	HIS	CB-CG-ND1	6.98	133.16	122.70
1	C	301	ASP	N-CA-C	-6.97	102.76	112.45
1	B	301	ASP	N-CA-C	-6.95	102.79	112.45
1	A	355	ASP	CA-CB-CG	6.94	119.54	112.60
1	A	100	GLU	N-CA-C	6.94	125.14	109.81

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	132	THR	N-CA-CB	-6.87	99.64	110.22
1	D	233	PHE	CA-CB-CG	6.82	120.62	113.80
1	D	136	ASN	CA-CB-CG	6.71	119.31	112.60
1	D	232	ASP	CA-CB-CG	-6.71	105.89	112.60
1	D	54	HIS	CB-CG-CD2	-6.67	122.53	131.20
1	C	380	SER	N-CA-C	6.63	124.92	110.80
1	A	104	ASN	N-CA-C	6.62	120.30	109.72
1	D	54	HIS	CB-CG-ND1	6.60	132.59	122.70
1	D	380	SER	N-CA-C	6.60	124.85	110.80
1	A	409	ASN	CA-CB-CG	6.58	119.18	112.60
1	C	246	ASP	CA-CB-CG	6.58	119.18	112.60
1	C	233	PHE	CA-CB-CG	6.56	120.36	113.80
1	D	92	HIS	CB-CG-ND1	6.53	132.49	122.70
1	D	409	ASN	CA-CB-CG	6.50	119.10	112.60
1	B	206	PHE	CA-CB-CG	-6.48	107.32	113.80
1	C	104	ASN	N-CA-C	6.46	120.06	109.72
1	C	54	HIS	CB-CG-ND1	6.46	132.39	122.70
1	A	54	HIS	CB-CG-ND1	6.43	132.34	122.70
1	B	328	GLN	OE1-CD-NE2	-6.43	116.17	122.60
1	D	252	MET	CG-SD-CE	-6.42	86.78	100.90
1	B	355	ASP	CA-CB-CG	6.39	118.99	112.60
1	A	44	PHE	N-CA-C	-6.38	98.50	108.90
1	D	317	ASN	OD1-CG-ND2	-6.37	116.23	122.60
1	B	380	SER	N-CA-C	6.35	124.33	110.80
1	A	423	ASN	OD1-CG-ND2	-6.29	116.31	122.60
1	A	233	PHE	CA-CB-CG	6.24	120.04	113.80
1	B	84	ASP	CA-CB-CG	6.23	118.83	112.60
1	C	321	ASP	CA-CB-CG	6.21	118.81	112.60
1	C	423	ASN	CB-CG-ND2	6.19	125.68	116.40
1	C	84	ASP	CA-CB-CG	6.18	118.78	112.60
1	C	83	SER	N-CA-C	6.17	119.91	112.38
1	D	60	LYS	CA-CB-CG	6.17	126.43	114.10
1	A	83	SER	N-CA-C	6.16	119.89	112.38
1	B	46	ASN	OD1-CG-ND2	-6.15	116.45	122.60
1	B	92	HIS	CB-CG-ND1	6.14	131.91	122.70
1	D	355	ASP	CA-CB-CG	6.13	118.73	112.60
1	D	409	ASN	OD1-CG-ND2	-6.13	116.47	122.60
1	D	63	GLN	OE1-CD-NE2	-6.11	116.49	122.60
1	B	83	SER	N-CA-C	6.11	119.83	112.38
1	D	75	ARG	NE-CZ-NH1	-6.10	115.40	121.50
1	C	75	ARG	NE-CZ-NH1	-6.09	115.41	121.50
1	B	232	ASP	CA-CB-CG	-6.09	106.51	112.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	57	GLN	OE1-CD-NE2	-6.07	116.53	122.60
1	C	218	ASN	CA-CB-CG	-6.07	106.53	112.60
1	B	58	ASP	CA-CB-CG	6.05	118.65	112.60
1	D	407	ARG	CA-CB-CG	-6.04	102.03	114.10
1	A	328	GLN	OE1-CD-NE2	-6.02	116.58	122.60
1	B	427	SER	N-CA-C	-6.01	94.16	111.00
1	A	223	LYS	CG-CD-CE	-6.00	97.49	111.30
1	D	136	ASN	N-CA-C	6.00	118.21	110.65
1	B	223	LYS	CG-CD-CE	-6.00	97.50	111.30
1	C	232	ASP	CA-CB-CG	-5.97	106.63	112.60
1	D	83	SER	N-CA-C	5.96	119.66	112.38
1	C	60	LYS	CA-CB-CG	5.95	126.00	114.10
1	B	233	PHE	CA-CB-CG	5.93	119.73	113.80
1	D	321	ASP	CA-CB-CG	5.93	118.53	112.60
1	B	78	GLY	N-CA-C	-5.91	106.37	114.64
1	A	78	GLY	N-CA-C	-5.90	106.39	114.64
1	C	409	ASN	CA-CB-CG	5.88	118.48	112.60
1	D	46	ASN	OD1-CG-ND2	-5.87	116.73	122.60
1	D	105	VAL	N-CA-CB	5.86	120.23	110.86
1	D	55	ASN	OD1-CG-ND2	-5.85	116.75	122.60
1	A	66	HIS	CB-CG-CD2	-5.85	123.60	131.20
1	B	118	ASN	OD1-CG-ND2	-5.84	116.76	122.60
1	A	55	ASN	OD1-CG-ND2	-5.82	116.78	122.60
1	A	136	ASN	CA-CB-CG	5.82	118.42	112.60
1	C	317	ASN	OD1-CG-ND2	-5.82	116.78	122.60
1	C	58	ASP	CA-CB-CG	5.81	118.41	112.60
1	D	328	GLN	CG-CD-NE2	5.81	125.12	116.40
1	D	423	ASN	OD1-CG-ND2	-5.81	116.79	122.60
1	C	226	GLU	CB-CG-CD	5.80	122.45	112.60
1	B	423	ASN	OD1-CG-ND2	-5.78	116.82	122.60
1	D	226	GLU	N-CA-C	-5.78	104.59	111.69
1	D	130	GLY	CA-C-O	-5.76	118.47	122.22
1	D	341	SER	CA-CB-OG	5.75	122.60	111.10
1	D	423	ASN	CB-CG-ND2	5.71	124.97	116.40
1	A	218	ASN	CA-CB-CG	-5.71	106.89	112.60
1	A	321	ASP	CA-CB-CG	5.70	118.30	112.60
1	C	136	ASN	N-CA-C	5.70	117.83	110.65
1	D	180	ASN	OD1-CG-ND2	-5.69	116.91	122.60
1	A	45	VAL	CB-CA-C	5.68	119.25	110.96
1	D	427	SER	N-CA-C	-5.66	95.15	111.00
1	B	75	ARG	NE-CZ-NH2	5.66	124.29	119.20
1	C	105	VAL	N-CA-CB	5.65	119.89	110.86

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	396	ASN	OD1-CG-ND2	-5.64	116.96	122.60
1	B	226	GLU	N-CA-C	-5.64	104.75	111.69
1	C	78	GLY	N-CA-C	-5.63	106.75	114.64
1	B	57	GLN	OE1-CD-NE2	-5.63	116.97	122.60
1	B	121	ASN	OD1-CG-ND2	-5.63	116.97	122.60
1	B	66	HIS	CB-CG-CD2	-5.61	123.91	131.20
1	A	420	ASN	CA-CB-CG	5.59	118.19	112.60
1	B	44	PHE	N-CA-C	-5.59	100.07	109.07
1	D	407	ARG	NE-CZ-NH2	-5.58	114.18	119.20
1	D	44	PHE	N-CA-C	-5.57	100.11	109.07
1	C	44	PHE	N-CA-C	-5.55	100.14	109.07
1	D	78	GLY	N-CA-C	-5.53	106.90	114.64
1	B	47	TRP	CE2-CD2-CG	-5.53	100.56	107.20
1	D	58	ASP	CA-CB-CG	5.53	118.13	112.60
1	B	105	VAL	N-CA-CB	5.52	119.69	110.86
1	C	427	SER	N-CA-C	-5.52	95.56	111.00
1	C	131	TRP	CE2-CD2-CG	-5.51	100.59	107.20
1	A	252	MET	CG-SD-CE	-5.50	88.80	100.90
1	B	136	ASN	N-CA-C	5.50	117.58	110.65
1	B	252	MET	CG-SD-CE	-5.50	88.80	100.90
1	C	409	ASN	OD1-CG-ND2	-5.49	117.11	122.60
1	C	379	GLU	CA-CB-CG	5.49	125.08	114.10
1	C	66	HIS	CB-CG-CD2	-5.48	124.07	131.20
1	B	60	LYS	CA-CB-CG	5.47	125.04	114.10
1	C	252	MET	CG-SD-CE	-5.46	88.88	100.90
1	D	315	TRP	CE2-CD2-CG	-5.46	100.65	107.20
1	C	45	VAL	CB-CA-C	5.46	118.93	110.96
1	A	75	ARG	NE-CZ-NH1	-5.45	116.05	121.50
1	B	130	GLY	CA-C-O	-5.44	118.69	122.22
1	D	47	TRP	CE2-CD2-CG	-5.44	100.67	107.20
1	A	75	ARG	NE-CZ-NH2	5.44	124.09	119.20
1	A	310	VAL	N-CA-C	-5.43	107.98	113.20
1	C	103	ASN	CA-CB-CG	-5.43	107.17	112.60
1	B	130	GLY	N-CA-C	-5.42	106.81	111.95
1	A	105	VAL	N-CA-CB	5.41	119.52	110.86
1	D	226	GLU	CB-CG-CD	5.41	121.79	112.60
1	D	103	ASN	CA-CB-CG	-5.40	107.20	112.60
1	B	226	GLU	CB-CG-CD	5.40	121.78	112.60
1	A	47	TRP	CE2-CD2-CG	-5.39	100.73	107.20
1	C	310	VAL	N-CA-C	-5.39	108.03	113.20
1	A	92	HIS	CB-CG-ND1	5.38	130.77	122.70
1	B	47	TRP	CG-CD2-CE3	5.37	139.27	133.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	315	TRP	CE2-CD2-CG	-5.37	100.76	107.20
1	C	347	ASN	OD1-CG-ND2	-5.36	117.24	122.60
1	A	58	ASP	CA-CB-CG	5.36	117.96	112.60
1	C	407	ARG	CA-CB-CG	-5.35	103.39	114.10
1	D	47	TRP	CG-CD2-CE3	5.35	139.25	133.90
1	D	84	ASP	CA-CB-CG	5.34	117.94	112.60
1	A	427	SER	N-CA-C	-5.34	96.05	111.00
1	D	45	VAL	CB-CA-C	5.34	118.75	110.96
1	D	75	ARG	NE-CZ-NH2	5.34	124.00	119.20
1	D	66	HIS	CB-CG-CD2	-5.32	124.29	131.20
1	A	75	ARG	CA-C-N	5.31	125.63	119.47
1	A	75	ARG	C-N-CA	5.31	125.63	119.47
1	A	409	ASN	OD1-CG-ND2	-5.31	117.29	122.60
1	B	327	GLN	OE1-CD-NE2	-5.31	117.29	122.60
1	A	226	GLU	N-CA-C	-5.30	105.17	111.69
1	B	251	HIS	CB-CG-CD2	-5.29	124.32	131.20
1	B	320	TRP	CE2-CD2-CG	-5.29	100.85	107.20
1	B	321	ASP	CA-CB-CG	5.29	117.89	112.60
1	C	46	ASN	OD1-CG-ND2	-5.26	117.34	122.60
1	A	130	GLY	CA-C-O	-5.25	118.81	122.22
1	B	409	ASN	CB-CG-ND2	5.25	124.27	116.40
1	A	284	ASN	CA-CB-CG	5.24	117.84	112.60
1	C	57	GLN	OE1-CD-NE2	-5.24	117.36	122.60
1	B	55	ASN	CB-CG-ND2	5.24	124.26	116.40
1	B	116	LYS	N-CA-C	5.24	116.99	111.28
1	A	136	ASN	N-CA-C	5.23	117.24	110.65
1	C	65	THR	N-CA-C	-5.23	107.57	114.31
1	C	63	GLN	CA-CB-CG	5.22	124.55	114.10
1	A	315	TRP	CE2-CD2-CG	-5.22	100.94	107.20
1	D	191	GLU	CA-CB-CG	-5.21	103.67	114.10
1	C	223	LYS	CG-CD-CE	-5.21	99.32	111.30
1	C	336	GLU	N-CA-C	5.20	116.95	111.28
1	A	325	MET	N-CA-C	-5.19	103.13	110.29
1	B	45	VAL	CB-CA-C	5.18	118.53	110.96
1	D	325	MET	N-CA-C	-5.18	103.14	110.29
1	C	245	TRP	CG-CD2-CE3	5.18	139.08	133.90
1	A	226	GLU	CB-CG-CD	5.17	121.40	112.60
1	B	98	TRP	CE2-CD2-CG	-5.17	101.00	107.20
1	D	377	TRP	CE2-CD2-CG	-5.16	101.00	107.20
1	A	116	LYS	N-CA-C	5.16	116.91	111.28
1	B	377	TRP	CE2-CD2-CG	-5.15	101.02	107.20
1	D	251	HIS	CB-CG-CD2	-5.15	124.51	131.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	86	TRP	CE2-CD2-CG	-5.15	101.02	107.20
1	B	63	GLN	CA-CB-CG	5.14	124.38	114.10
1	C	121	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	C	92	HIS	CB-CG-ND1	5.13	130.40	122.70
1	B	86	TRP	CE2-CD2-CG	-5.13	101.04	107.20
1	A	131	TRP	CE2-CD2-CG	-5.13	101.05	107.20
1	B	191	GLU	CA-CB-CG	-5.13	103.84	114.10
1	C	66	HIS	CB-CG-ND1	5.13	130.39	122.70
1	A	425	MET	CA-C-N	5.12	126.24	119.84
1	A	425	MET	C-N-CA	5.12	126.24	119.84
1	A	234	TRP	CE2-CD2-CG	-5.12	101.06	107.20
1	C	47	TRP	CG-CD2-CE3	5.11	139.01	133.90
1	B	200	HIS	CB-CG-CD2	-5.11	124.56	131.20
1	A	98	TRP	CE2-CD2-CG	-5.09	101.09	107.20
1	C	224	LEU	N-CA-C	5.09	117.22	111.11
1	B	66	HIS	CB-CG-ND1	5.09	130.33	122.70
1	B	325	MET	N-CA-C	-5.08	103.28	110.29
1	C	251	HIS	CB-CG-CD2	-5.08	124.59	131.20
1	C	425	MET	CA-C-N	5.08	126.19	119.84
1	C	425	MET	C-N-CA	5.08	126.19	119.84
1	B	247	LYS	CA-CB-CG	-5.08	103.95	114.10
1	D	130	GLY	N-CA-C	-5.08	107.13	111.95
1	C	191	GLU	CB-CG-CD	5.07	121.23	112.60
1	C	116	LYS	N-CA-C	5.07	116.81	111.28
1	C	191	GLU	CA-CB-CG	-5.07	103.96	114.10
1	D	132	THR	N-CA-C	5.06	116.80	111.28
1	C	420	ASN	CA-CB-CG	5.04	117.64	112.60
1	D	310	VAL	N-CA-C	-5.03	108.37	113.20
1	D	63	GLN	CA-CB-CG	5.03	124.15	114.10
1	C	407	ARG	NE-CZ-NH2	-5.02	114.68	119.20
1	D	47	TRP	CB-CG-CD1	-5.02	119.37	126.90
1	A	84	ASP	CA-CB-CG	5.01	117.61	112.60
1	D	98	TRP	CE2-CD2-CG	-5.01	101.19	107.20
1	B	345	ASP	CA-C-N	5.01	126.99	120.28
1	B	345	ASP	C-N-CA	5.01	126.99	120.28
1	C	47	TRP	CE2-CD2-CG	-5.00	101.20	107.20
1	A	407	ARG	CA-CB-CG	-5.00	104.10	114.10
1	C	245	TRP	CE2-CD2-CG	-5.00	101.20	107.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	344	TYR	Sidechain
1	C	230	TYR	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3083	0	2961	42	0
1	B	3083	0	2961	49	0
1	C	3083	0	2961	49	0
1	D	3083	0	2961	47	0
2	E	28	0	25	5	0
2	F	28	0	25	5	0
2	G	28	0	25	6	0
2	H	28	0	25	4	0
3	A	15	0	15	3	0
3	B	15	0	15	3	0
3	C	15	0	15	3	0
3	D	15	0	15	5	0
4	A	28	0	0	3	0
4	B	22	0	0	2	0
4	C	24	0	0	1	0
4	D	26	0	0	0	0
All	All	12604	0	12004	177	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 (177) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:THR:HG21	2:F:2:NAA:H81	1.26	1.18
1:A:132:THR:HG21	2:E:2:NAA:H81	1.41	1.02
1:B:132:THR:HG21	2:F:2:NAA:C8	1.91	1.00
1:C:132:THR:HG21	2:G:2:NAA:H81	1.43	0.99
1:C:132:THR:HG21	2:G:2:NAA:C8	1.99	0.92
1:D:132:THR:HG21	2:H:2:NAA:H81	1.51	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:THR:HG21	2:E:2:NAA:C8	2.06	0.85
1:A:71:PHE:HZ	3:A:503:AMI:H82	1.46	0.80
1:B:95:GLY:H	1:C:51:GLY:HA2	1.47	0.80
1:B:325:MET:HE1	1:B:352:ILE:HD12	1.64	0.78
1:B:47:TRP:CZ2	2:F:1:NAA:H4	2.22	0.74
1:C:47:TRP:CZ2	2:G:1:NAA:H4	2.23	0.73
1:B:132:THR:CG2	2:F:2:NAA:H81	2.14	0.73
1:D:325:MET:HE1	1:D:352:ILE:HD12	1.71	0.72
1:D:132:THR:HG21	2:H:2:NAA:C8	2.22	0.70
1:C:325:MET:HE1	1:C:352:ILE:HD12	1.75	0.69
1:A:71:PHE:CZ	3:A:503:AMI:H82	2.27	0.69
1:C:71:PHE:HZ	3:C:503:AMI:H82	1.59	0.68
1:A:98:TRP:HB2	4:A:1086:HOH:O	1.92	0.68
4:A:1029:HOH:O	2:E:1:NAA:H81	1.95	0.67
1:D:47:TRP:CZ2	2:H:1:NAA:H4	2.31	0.65
1:B:154:SER:HB3	1:B:166:ILE:HD13	1.79	0.65
1:B:92:HIS:NE2	1:B:98:TRP:HA	2.11	0.64
1:A:325:MET:HE1	1:A:352:ILE:HD12	1.81	0.63
1:A:47:TRP:CZ2	2:E:1:NAA:H4	2.34	0.63
1:A:132:THR:CG2	2:E:2:NAA:H81	2.24	0.63
1:C:154:SER:HB3	1:C:166:ILE:HD13	1.81	0.63
1:D:92:HIS:NE2	1:D:98:TRP:HA	2.14	0.62
1:A:92:HIS:NE2	1:A:98:TRP:HA	2.14	0.61
1:A:154:SER:HB3	1:A:166:ILE:HD13	1.83	0.60
1:C:92:HIS:NE2	1:C:98:TRP:HA	2.16	0.60
1:B:292:LEU:O	1:B:382:SER:HB2	2.02	0.60
1:C:69:TYR:HB2	1:C:112:MET:HE1	1.83	0.60
1:C:226:GLU:HA	1:C:229:LYS:HZ2	1.67	0.59
1:D:154:SER:HB3	1:D:166:ILE:HD13	1.85	0.59
1:B:226:GLU:HA	1:B:229:LYS:HZ3	1.68	0.59
1:C:42:VAL:HB	1:C:64:PHE:CE2	2.38	0.59
1:C:71:PHE:CZ	3:C:503:AMI:H82	2.37	0.59
1:A:69:TYR:HB2	1:A:112:MET:HE1	1.84	0.58
1:A:169:ASP:OD1	3:A:503:AMI:H83	2.04	0.58
1:B:94:PRO:HB3	1:C:50:TYR:HA	1.86	0.57
1:D:292:LEU:HD13	1:D:383:ASP:HB2	1.87	0.57
1:D:226:GLU:HA	1:D:229:LYS:HZ3	1.70	0.56
1:A:300:THR:HG23	1:A:307:PHE:HB3	1.87	0.56
1:D:69:TYR:HB2	1:D:112:MET:HE1	1.87	0.56
1:A:226:GLU:HA	1:A:229:LYS:HZ2	1.70	0.56
1:C:132:THR:CG2	2:G:2:NAA:H81	2.27	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:292:LEU:HD13	1:B:383:ASP:HB2	1.89	0.55
1:B:312:GLY:HA2	1:B:317:ASN:HD22	1.72	0.55
1:A:42:VAL:HB	1:A:64:PHE:CE2	2.42	0.55
1:C:292:LEU:O	1:C:382:SER:HB2	2.07	0.55
1:D:42:VAL:HB	1:D:64:PHE:CE2	2.42	0.54
1:B:95:GLY:H	1:C:51:GLY:CA	2.19	0.54
1:C:47:TRP:CH2	2:G:1:NAA:H4	2.43	0.54
1:A:292:LEU:HD13	1:A:383:ASP:HB2	1.89	0.54
1:B:95:GLY:CA	1:C:51:GLY:O	2.56	0.54
1:D:61:ALA:HB1	1:D:122:LEU:HD22	1.89	0.54
1:B:69:TYR:HB2	1:B:112:MET:HE1	1.90	0.54
1:A:61:ALA:HB1	1:A:122:LEU:HD22	1.89	0.53
1:B:95:GLY:HA2	1:C:51:GLY:O	2.08	0.53
1:C:300:THR:HG23	1:C:307:PHE:HB3	1.90	0.53
1:C:369:LYS:HE3	4:C:1092:HOH:O	2.09	0.53
1:D:312:GLY:HA2	1:D:317:ASN:HD22	1.73	0.53
1:B:61:ALA:HB1	1:B:122:LEU:HD22	1.90	0.53
1:B:42:VAL:HB	1:B:64:PHE:CE2	2.43	0.53
1:D:71:PHE:HZ	3:D:503:AMI:H82	1.71	0.53
1:C:414:PRO:O	1:C:422:LYS:HE2	2.09	0.52
1:B:92:HIS:CD2	1:B:98:TRP:HA	2.44	0.52
1:A:312:GLY:HA2	1:A:317:ASN:HD22	1.74	0.52
1:A:328:GLN:HB3	1:D:58:ASP:HB2	1.91	0.52
1:B:313:GLY:HA3	1:B:316:GLU:O	2.09	0.52
1:C:313:GLY:HA3	1:C:316:GLU:O	2.08	0.52
1:A:292:LEU:O	1:A:382:SER:HB2	2.10	0.52
1:C:312:GLY:HA2	1:C:317:ASN:HD22	1.74	0.52
1:B:119:ASN:HB3	4:B:1088:HOH:O	2.11	0.51
1:B:300:THR:HG23	1:B:307:PHE:HB3	1.92	0.51
1:C:292:LEU:HD13	1:C:383:ASP:HB2	1.92	0.51
1:A:79:GLU:OE1	1:B:247:LYS:HD3	2.11	0.51
1:C:176:GLU:CD	1:C:223:LYS:HZ1	2.19	0.50
1:D:313:GLY:HA3	1:D:316:GLU:O	2.11	0.50
1:D:365:GLU:O	1:D:369:LYS:HB2	2.10	0.50
1:C:61:ALA:HB1	1:C:122:LEU:HD22	1.93	0.50
1:D:42:VAL:HG23	1:D:377:TRP:HB2	1.94	0.49
1:B:43:TYR:CE2	3:B:503:AMI:H81	2.47	0.49
1:B:47:TRP:CH2	2:F:1:NAA:H4	2.47	0.49
1:C:79:GLU:HG3	1:C:153:THR:HG21	1.95	0.49
1:D:292:LEU:O	1:D:382:SER:HB2	2.12	0.49
1:A:79:GLU:HG3	1:A:153:THR:HG21	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:GLY:HA3	1:A:316:GLU:O	2.12	0.49
1:A:365:GLU:O	1:A:369:LYS:HB2	2.13	0.49
1:B:42:VAL:HG23	1:B:377:TRP:HB2	1.95	0.49
1:D:300:THR:HG23	1:D:307:PHE:HB3	1.95	0.48
1:D:92:HIS:CD2	1:D:98:TRP:HA	2.48	0.48
1:B:344:TYR:HE2	1:B:346:LYS:HD3	1.78	0.48
1:A:42:VAL:HG23	1:A:377:TRP:HB2	1.96	0.48
1:A:92:HIS:CD2	1:A:98:TRP:HA	2.49	0.47
1:C:42:VAL:HG23	1:C:377:TRP:HB2	1.96	0.47
1:C:169:ASP:OD1	3:C:503:AMI:H83	2.14	0.47
1:D:43:TYR:CE2	3:D:503:AMI:H81	2.49	0.47
1:D:240:ASP:OD1	3:D:503:AMI:H62	2.14	0.47
1:D:378:TRP:HE1	2:H:1:NAA:H83	1.79	0.47
1:D:134:SER:N	1:D:135:PRO:HD2	2.29	0.47
1:C:134:SER:N	1:C:135:PRO:HD2	2.30	0.47
1:A:200:HIS:HE1	1:A:415:GLU:OE1	1.98	0.47
1:A:176:GLU:CD	1:A:223:LYS:HZ1	2.22	0.47
1:D:155:LEU:HD21	1:D:196:TYR:HB2	1.97	0.47
1:A:313:GLY:HA2	1:A:320:TRP:CE2	2.51	0.46
1:B:365:GLU:O	1:B:369:LYS:HB2	2.14	0.46
1:B:176:GLU:CD	1:B:223:LYS:HZ1	2.23	0.46
1:B:200:HIS:HE1	1:B:415:GLU:OE1	1.98	0.46
1:C:365:GLU:O	1:C:369:LYS:HB2	2.15	0.46
1:D:71:PHE:CZ	3:D:503:AMI:H82	2.49	0.46
1:D:200:HIS:HE1	1:D:415:GLU:OE1	1.99	0.46
1:C:92:HIS:CD2	1:C:98:TRP:HA	2.51	0.46
1:A:155:LEU:HD13	1:A:193:LEU:HD12	1.98	0.45
1:D:298:ALA:O	1:D:307:PHE:HB2	2.17	0.45
1:A:290:MET:HG2	1:A:363:LYS:HD3	1.98	0.45
1:C:290:MET:HG2	1:C:363:LYS:HD3	1.98	0.45
1:B:94:PRO:HB3	1:C:50:TYR:C	2.41	0.45
1:A:57:GLN:HG3	1:A:111:GLN:HE21	1.82	0.45
1:C:132:THR:HG21	2:G:2:NAA:H83	1.93	0.45
1:C:322:TYR:CE2	1:C:390:LEU:HG	2.52	0.45
1:A:134:SER:N	1:A:135:PRO:HD2	2.32	0.45
1:B:134:SER:N	1:B:135:PRO:HD2	2.32	0.45
1:B:414:PRO:O	1:B:422:LYS:HE2	2.17	0.45
1:D:176:GLU:CD	1:D:223:LYS:HZ1	2.24	0.45
1:C:155:LEU:HD21	1:C:196:TYR:HB2	1.98	0.44
1:D:414:PRO:O	1:D:422:LYS:HE2	2.17	0.44
1:A:322:TYR:CE2	1:A:390:LEU:HG	2.52	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:PRO:O	1:A:422:LYS:HE2	2.17	0.44
1:C:69:TYR:OH	1:C:108:CYS:HB2	2.18	0.44
1:B:43:TYR:CE1	3:B:503:AMI:H91	2.53	0.44
1:B:67:ILE:O	1:B:124:THR:HA	2.18	0.44
1:A:344:TYR:HE2	1:A:346:LYS:HD3	1.83	0.43
1:C:57:GLN:HG3	1:C:111:GLN:HE21	1.83	0.43
1:B:203:GLY:HA3	4:B:1065:HOH:O	2.18	0.43
1:C:79:GLU:OE1	1:D:247:LYS:HD3	2.19	0.43
1:B:298:ALA:O	1:B:307:PHE:HB2	2.19	0.43
1:D:65:THR:O	1:D:123:LYS:HE3	2.19	0.43
1:D:79:GLU:HG3	1:D:153:THR:HG21	1.99	0.43
1:A:67:ILE:O	1:A:124:THR:HA	2.18	0.43
1:A:298:ALA:O	1:A:307:PHE:HB2	2.19	0.43
1:D:70:ALA:HA	1:D:71:PHE:HA	1.65	0.43
1:D:322:TYR:CE2	1:D:390:LEU:HG	2.53	0.43
1:D:242:SER:O	1:D:295:ARG:HD2	2.19	0.43
1:C:200:HIS:HE1	1:C:415:GLU:OE1	2.01	0.43
1:C:67:ILE:O	1:C:124:THR:HA	2.19	0.43
1:D:67:ILE:O	1:D:124:THR:HA	2.19	0.43
1:B:70:ALA:HA	1:B:71:PHE:HA	1.66	0.42
1:B:378:TRP:HA	1:B:379:GLU:HA	1.83	0.42
1:C:127:SER:HA	1:C:167:ASP:O	2.19	0.42
1:C:70:ALA:HA	1:C:71:PHE:HA	1.66	0.42
1:D:57:GLN:HG3	1:D:111:GLN:HE21	1.84	0.42
1:A:70:ALA:HA	1:A:71:PHE:HA	1.66	0.42
1:B:57:GLN:HG3	1:B:111:GLN:HE21	1.84	0.42
1:C:298:ALA:O	1:C:307:PHE:HB2	2.20	0.42
1:C:174:GLU:HG2	1:C:178:GLN:NE2	2.35	0.41
1:D:290:MET:HG2	1:D:363:LYS:HD3	2.02	0.41
1:B:313:GLY:HA2	1:B:320:TRP:CE2	2.55	0.41
1:D:313:GLY:HA2	1:D:320:TRP:CE2	2.55	0.41
1:A:127:SER:HA	1:A:167:ASP:O	2.20	0.41
1:D:39:ARG:HH11	1:D:39:ARG:HD3	1.69	0.41
1:D:378:TRP:HA	1:D:379:GLU:HA	1.84	0.41
1:A:223:LYS:HE3	4:A:1040:HOH:O	2.21	0.41
1:D:240:ASP:OD1	3:D:503:AMI:C6	2.68	0.41
1:D:241:PHE:CG	1:D:267:PHE:HB2	2.55	0.41
1:B:155:LEU:HD21	1:B:196:TYR:HB2	2.02	0.41
1:B:94:PRO:HB3	1:C:50:TYR:CA	2.51	0.41
1:B:95:GLY:N	1:C:51:GLY:HA2	2.27	0.41
1:D:255:VAL:CG2	1:D:339:ALA:HB3	2.51	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:TYR:CE2	1:B:390:LEU:HG	2.55	0.41
1:B:296:ALA:HA	1:B:351:LEU:O	2.20	0.40
1:D:185:LEU:O	1:D:188:ALA:HB3	2.21	0.40
1:B:240:ASP:OD1	3:B:503:AMI:H62	2.21	0.40
1:B:290:MET:HG2	1:B:363:LYS:HD3	2.04	0.40
1:D:155:LEU:HD13	1:D:193:LEU:HD12	2.03	0.40
1:A:100:GLU:HG3	1:A:101:PRO:HD2	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	390/392 (100%)	369 (95%)	16 (4%)	5 (1%)	9	31
1	B	390/392 (100%)	368 (94%)	17 (4%)	5 (1%)	9	31
1	C	390/392 (100%)	370 (95%)	15 (4%)	5 (1%)	9	31
1	D	390/392 (100%)	369 (95%)	16 (4%)	5 (1%)	9	31
All	All	1560/1568 (100%)	1476 (95%)	64 (4%)	20 (1%)	9	31

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	99	ASP
1	A	100	GLU
1	B	99	ASP
1	B	100	GLU
1	C	99	ASP
1	C	100	GLU
1	D	99	ASP
1	D	100	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	46	ASN
1	B	46	ASN
1	C	46	ASN
1	C	380	SER
1	D	46	ASN
1	D	380	SER
1	A	426	PRO
1	B	380	SER
1	B	426	PRO
1	D	426	PRO
1	A	380	SER
1	C	426	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	326/326 (100%)	291 (89%)	35 (11%)	6	21
1	B	326/326 (100%)	290 (89%)	36 (11%)	6	20
1	C	326/326 (100%)	292 (90%)	34 (10%)	7	22
1	D	326/326 (100%)	290 (89%)	36 (11%)	6	20
All	All	1304/1304 (100%)	1163 (89%)	141 (11%)	6	21

All (141) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	VAL
1	A	58	ASP
1	A	59	LEU
1	A	60	LYS
1	A	62	ASP
1	A	74	ILE
1	A	105	VAL
1	A	109	ILE
1	A	123	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	126	LEU
1	A	139	THR
1	A	148	LYS
1	A	149	LYS
1	A	156	LYS
1	A	157	LEU
1	A	186	LEU
1	A	207	LEU
1	A	223	LYS
1	A	226	GLU
1	A	248	VAL
1	A	252	MET
1	A	259	THR
1	A	278	LYS
1	A	300	THR
1	A	331	GLN
1	A	335	LEU
1	A	347	ASN
1	A	351	LEU
1	A	382	SER
1	A	398	LEU
1	A	405	GLU
1	A	417	VAL
1	A	421	LEU
1	A	422	LYS
1	A	425	MET
1	B	45	VAL
1	B	57	GLN
1	B	58	ASP
1	B	59	LEU
1	B	60	LYS
1	B	74	ILE
1	B	94	PRO
1	B	105	VAL
1	B	109	ILE
1	B	123	LYS
1	B	126	LEU
1	B	136	ASN
1	B	139	THR
1	B	156	LYS
1	B	157	LEU
1	B	186	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	207	LEU
1	B	223	LYS
1	B	226	GLU
1	B	248	VAL
1	B	252	MET
1	B	259	THR
1	B	278	LYS
1	B	300	THR
1	B	326	PRO
1	B	331	GLN
1	B	335	LEU
1	B	347	ASN
1	B	351	LEU
1	B	382	SER
1	B	398	LEU
1	B	405	GLU
1	B	417	VAL
1	B	421	LEU
1	B	422	LYS
1	B	425	MET
1	C	45	VAL
1	C	58	ASP
1	C	59	LEU
1	C	60	LYS
1	C	74	ILE
1	C	94	PRO
1	C	105	VAL
1	C	109	ILE
1	C	123	LYS
1	C	126	LEU
1	C	139	THR
1	C	148	LYS
1	C	156	LYS
1	C	157	LEU
1	C	186	LEU
1	C	207	LEU
1	C	223	LYS
1	C	226	GLU
1	C	248	VAL
1	C	252	MET
1	C	259	THR
1	C	278	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	300	THR
1	C	331	GLN
1	C	335	LEU
1	C	347	ASN
1	C	351	LEU
1	C	382	SER
1	C	398	LEU
1	C	405	GLU
1	C	417	VAL
1	C	421	LEU
1	C	422	LYS
1	C	425	MET
1	D	45	VAL
1	D	58	ASP
1	D	59	LEU
1	D	60	LYS
1	D	62	ASP
1	D	74	ILE
1	D	94	PRO
1	D	105	VAL
1	D	109	ILE
1	D	123	LYS
1	D	126	LEU
1	D	139	THR
1	D	148	LYS
1	D	156	LYS
1	D	157	LEU
1	D	186	LEU
1	D	207	LEU
1	D	223	LYS
1	D	226	GLU
1	D	248	VAL
1	D	252	MET
1	D	259	THR
1	D	278	LYS
1	D	300	THR
1	D	331	GLN
1	D	335	LEU
1	D	347	ASN
1	D	351	LEU
1	D	382	SER
1	D	398	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	403	LYS
1	D	405	GLU
1	D	417	VAL
1	D	421	LEU
1	D	422	LYS
1	D	425	MET

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	66	HIS
1	A	111	GLN
1	A	200	HIS
1	A	317	ASN
1	B	111	GLN
1	B	200	HIS
1	B	317	ASN
1	C	111	GLN
1	C	200	HIS
1	C	317	ASN
1	D	111	GLN
1	D	200	HIS
1	D	317	ASN
1	D	347	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

8 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	NAA	E	1	3,2	14,14,15	1.20	2 (14%)	17,19,21	1.51	5 (29%)
2	NAA	E	2	2	14,14,15	0.85	0	17,19,21	1.56	4 (23%)
2	NAA	F	1	3,2	14,14,15	0.97	0	17,19,21	1.62	4 (23%)
2	NAA	F	2	2	14,14,15	0.98	1 (7%)	17,19,21	1.91	4 (23%)
2	NAA	G	1	3,2	14,14,15	0.93	0	17,19,21	1.47	4 (23%)
2	NAA	G	2	2	14,14,15	0.95	1 (7%)	17,19,21	1.69	4 (23%)
2	NAA	H	1	3,2	14,14,15	1.11	0	17,19,21	1.53	4 (23%)
2	NAA	H	2	2	14,14,15	1.06	1 (7%)	17,19,21	1.65	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
2	NAA	E	1	3,2	-	2/6/23/26	0/1/1/1
2	NAA	E	2	2	-	2/6/23/26	0/1/1/1
2	NAA	F	1	3,2	-	2/6/23/26	0/1/1/1
2	NAA	F	2	2	-	2/6/23/26	0/1/1/1
2	NAA	G	1	3,2	-	2/6/23/26	0/1/1/1
2	NAA	G	2	2	-	2/6/23/26	0/1/1/1
2	NAA	H	1	3,2	-	2/6/23/26	0/1/1/1
2	NAA	H	2	2	-	2/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	NAA	O5-C1	-2.48	1.39	1.43
2	G	2	NAA	C1-C2	2.10	1.55	1.52
2	H	2	NAA	C2-N2	-2.06	1.42	1.46
2	F	2	NAA	C2-N2	-2.05	1.42	1.46
2	E	1	NAA	C4-C3	2.03	1.57	1.52

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1	NAA	C1-C2-N2	-3.91	104.28	110.43
2	F	2	NAA	C2-N2-C7	-3.84	117.76	122.90
2	H	1	NAA	C1-C2-N2	-3.67	104.65	110.43
2	F	2	NAA	C8-C7-N2	3.56	122.02	116.12
2	G	2	NAA	C2-N2-C7	-3.29	118.49	122.90
2	E	2	NAA	C6-C5-C4	3.26	121.03	113.02
2	G	1	NAA	C1-C2-N2	-3.26	105.30	110.43
2	H	2	NAA	C2-N2-C7	-3.22	118.58	122.90
2	G	1	NAA	O3-C3-C2	3.15	115.94	109.40
2	E	1	NAA	O3-C3-C2	3.15	115.94	109.40
2	G	2	NAA	O4-C4-C3	-2.99	103.32	110.38
2	E	1	NAA	C1-C2-N2	-2.97	105.75	110.43
2	F	1	NAA	O3-C3-C2	2.91	115.44	109.40
2	H	2	NAA	C6-C5-C4	2.87	120.08	113.02
2	F	2	NAA	O4-C4-C3	-2.87	103.61	110.38
2	F	2	NAA	C6-C5-C4	2.85	120.03	113.02
2	G	2	NAA	C6-C5-C4	2.81	119.91	113.02
2	G	2	NAA	C8-C7-N2	2.75	120.68	116.12
2	F	1	NAA	C6-C5-C4	2.72	119.69	113.02
2	H	1	NAA	O3-C3-C2	2.68	114.96	109.40
2	E	2	NAA	C2-N2-C7	-2.67	119.33	122.90
2	H	1	NAA	C6-C5-C4	2.57	119.32	113.02
2	H	2	NAA	C8-C7-N2	2.56	120.36	116.12
2	G	1	NAA	O5-C5-C6	-2.55	102.70	107.66
2	G	1	NAA	C6-C5-C4	2.53	119.23	113.02
2	H	2	NAA	O4-C4-C3	-2.47	104.54	110.38
2	E	2	NAA	C1-O5-C5	-2.43	108.93	112.19
2	F	1	NAA	O5-C5-C6	-2.37	103.04	107.66
2	E	2	NAA	O4-C4-C3	-2.32	104.91	110.38
2	E	1	NAA	O5-C5-C6	-2.30	103.18	107.66
2	E	1	NAA	C4-C3-C2	-2.27	107.69	111.02
2	H	1	NAA	O5-C5-C6	-2.25	103.28	107.66
2	E	1	NAA	C6-C5-C4	2.25	118.54	113.02

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	NAA	C8-C7-N2-C2
2	E	1	NAA	O7-C7-N2-C2
2	F	1	NAA	C8-C7-N2-C2
2	F	1	NAA	O7-C7-N2-C2
2	G	1	NAA	C8-C7-N2-C2

Continued on next page...

Continued from previous page...

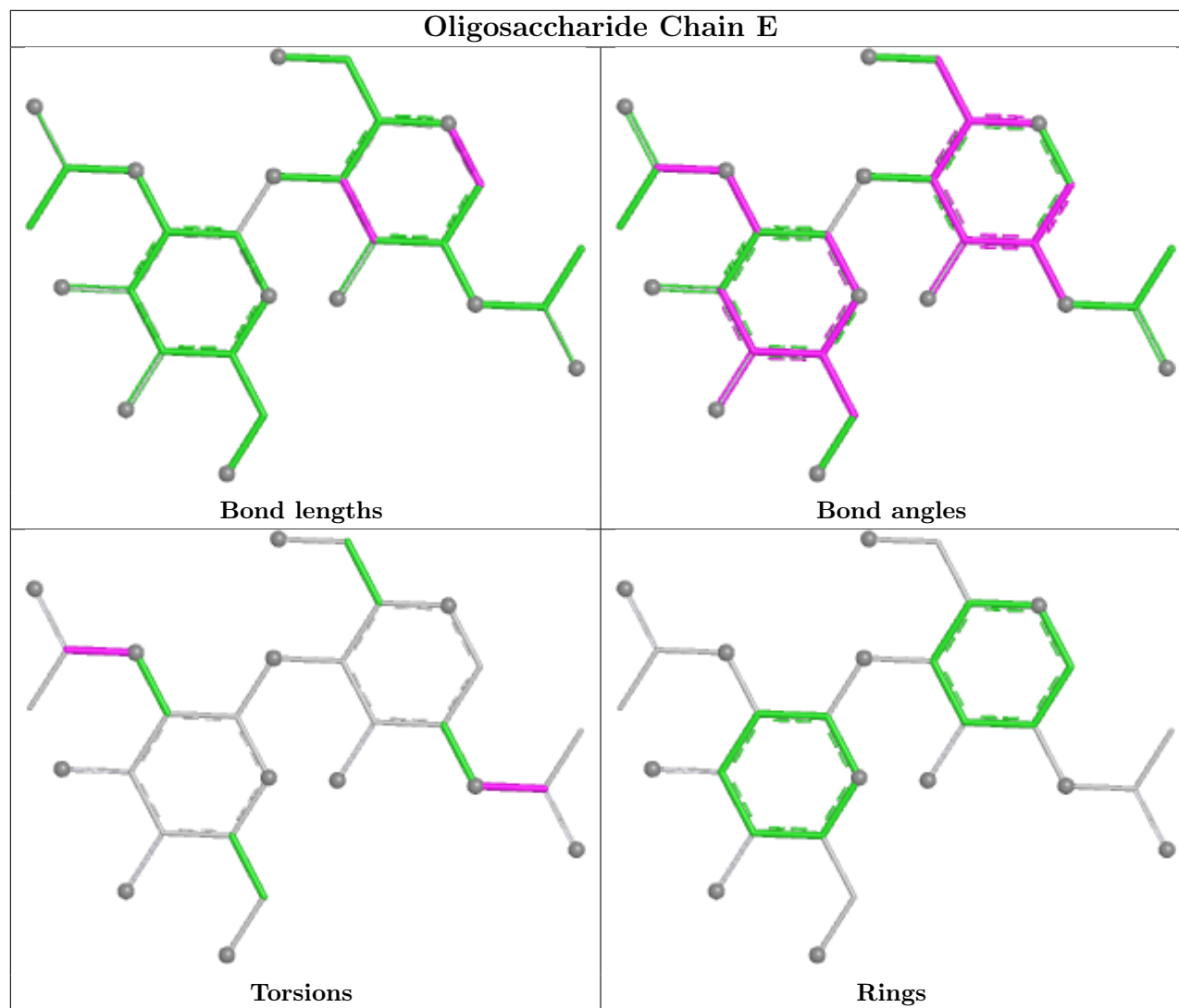
Mol	Chain	Res	Type	Atoms
2	G	1	NAA	O7-C7-N2-C2
2	H	1	NAA	C8-C7-N2-C2
2	H	1	NAA	O7-C7-N2-C2
2	E	2	NAA	C8-C7-N2-C2
2	E	2	NAA	O7-C7-N2-C2
2	F	2	NAA	C8-C7-N2-C2
2	F	2	NAA	O7-C7-N2-C2
2	G	2	NAA	C8-C7-N2-C2
2	G	2	NAA	O7-C7-N2-C2
2	H	2	NAA	C8-C7-N2-C2
2	H	2	NAA	O7-C7-N2-C2

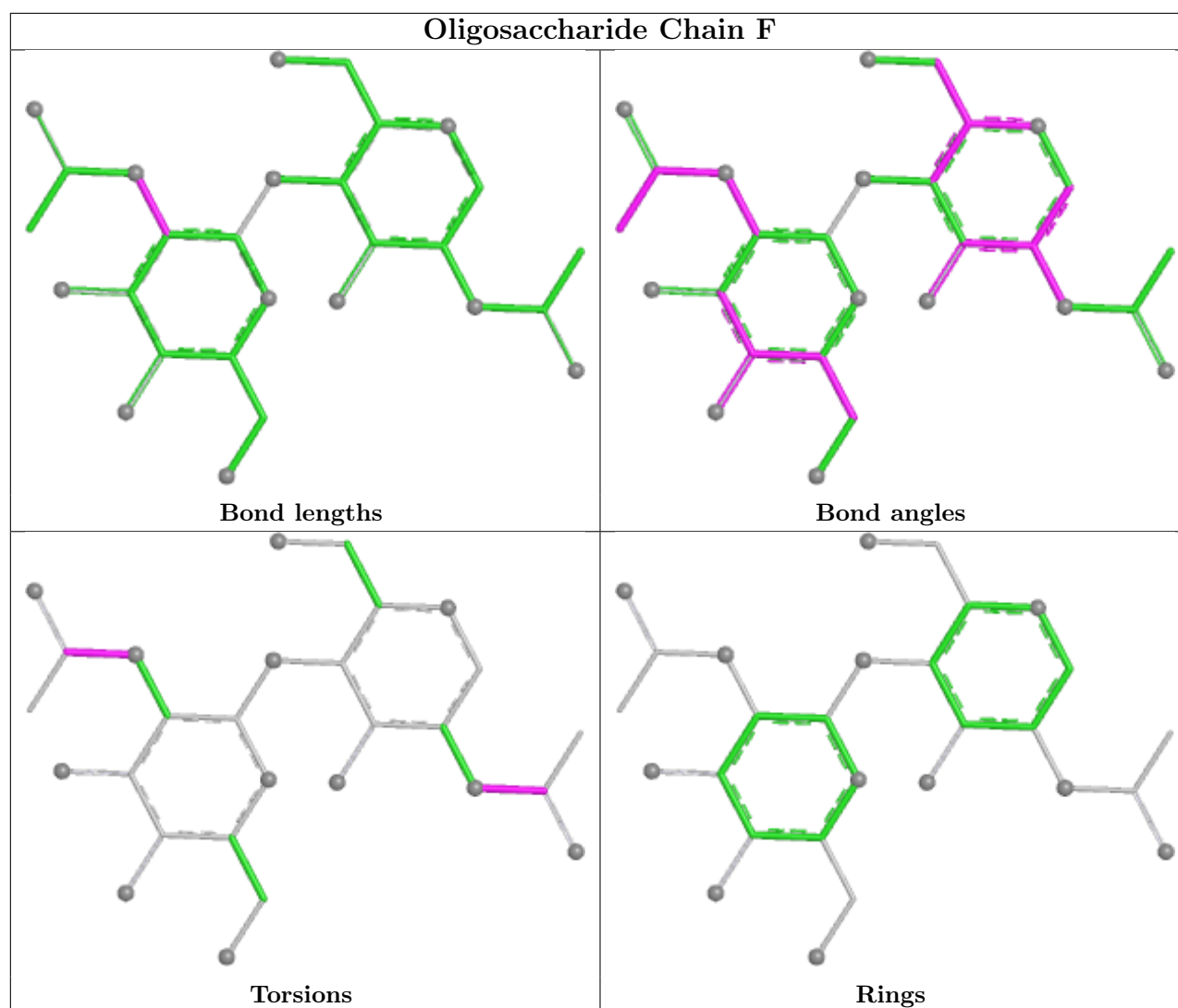
There are no ring outliers.

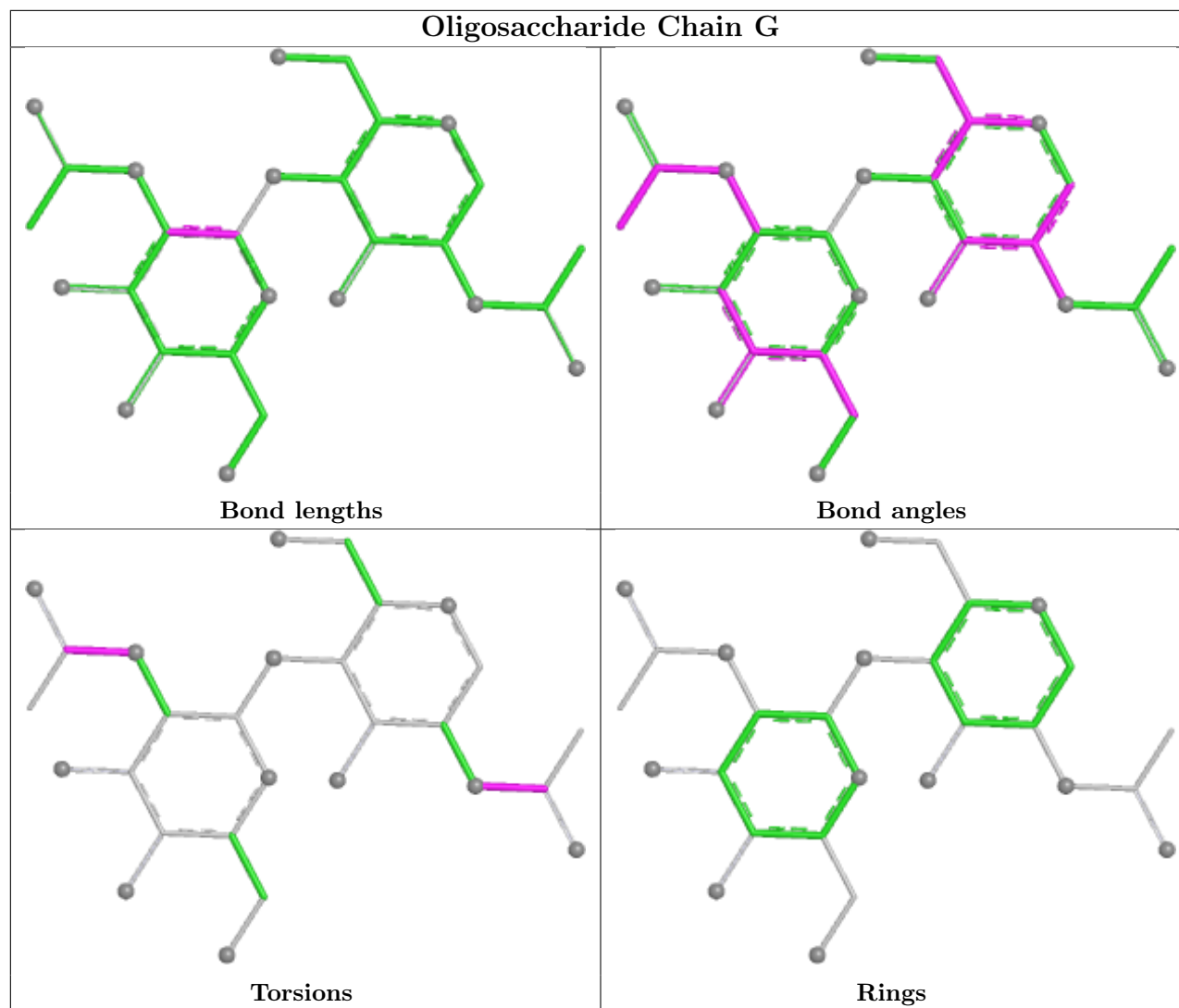
8 monomers are involved in 20 short contacts:

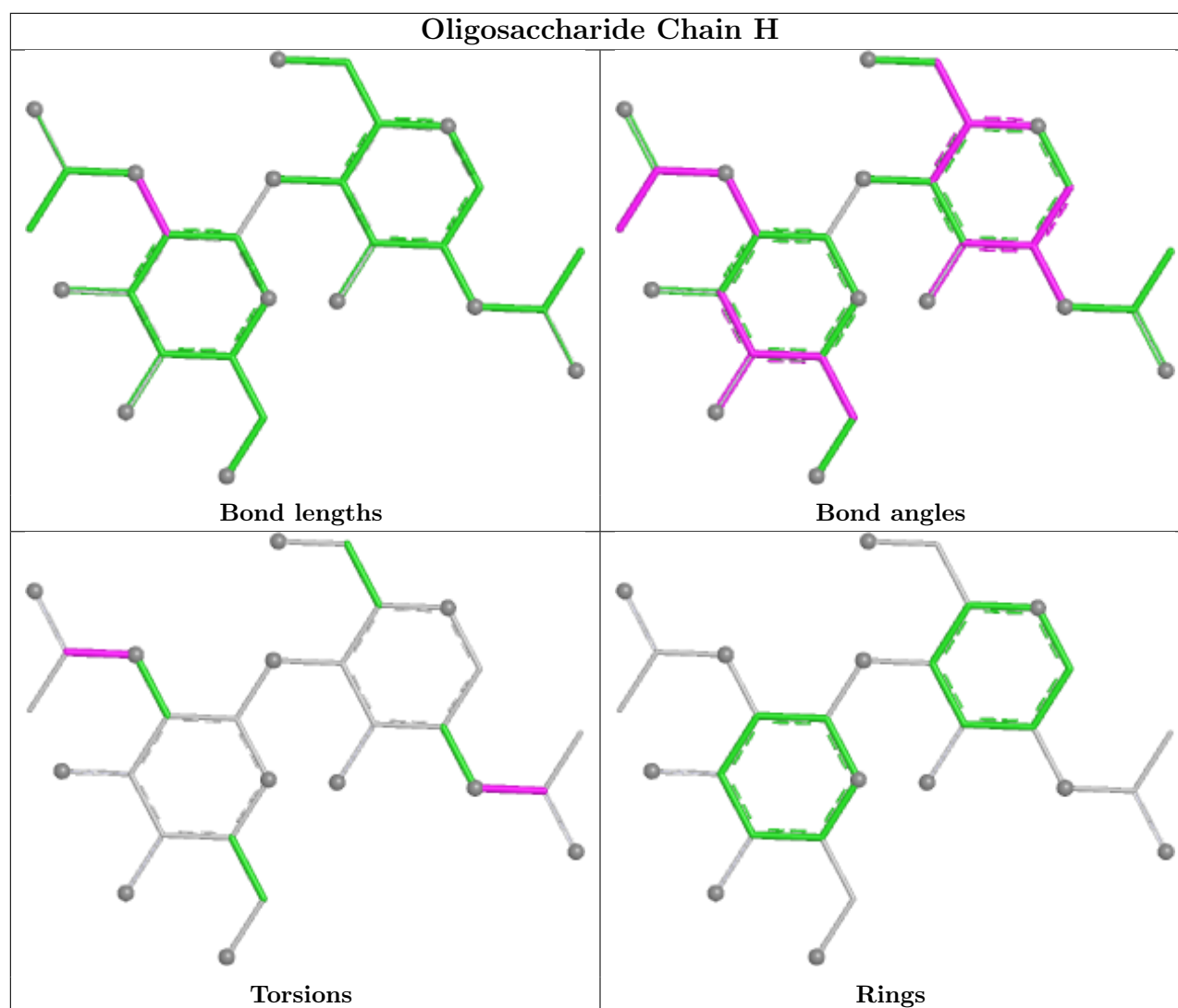
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	1	NAA	2	0
2	E	1	NAA	2	0
2	G	2	NAA	4	0
2	H	1	NAA	2	0
2	G	1	NAA	2	0
2	E	2	NAA	3	0
2	H	2	NAA	2	0
2	F	2	NAA	3	0

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](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	AMI	C	503	2	15,16,16	1.51	2 (13%)	15,24,24	3.30	5 (33%)
3	AMI	B	503	2	15,16,16	1.63	3 (20%)	15,24,24	2.66	5 (33%)
3	AMI	D	503	2	15,16,16	1.18	1 (6%)	15,24,24	3.55	5 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AMI	A	503	2	15,16,16	1.58	2 (13%)	15,24,24	2.84	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
3	AMI	C	503	2	-	4/6/34/34	0/2/2/2
3	AMI	B	503	2	-	4/6/34/34	0/2/2/2
3	AMI	D	503	2	-	4/6/34/34	0/2/2/2
3	AMI	A	503	2	-	4/6/34/34	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	503	AMI	C2-N2	-4.11	1.43	1.47
3	B	503	AMI	C2-N2	-4.08	1.43	1.47
3	A	503	AMI	C2-N2	-3.98	1.43	1.47
3	D	503	AMI	C2-N2	-2.70	1.45	1.47
3	B	503	AMI	O7-C7	2.28	1.37	1.34
3	B	503	AMI	C4-C3	-2.23	1.47	1.53
3	A	503	AMI	C4-C3	-2.13	1.47	1.53
3	C	503	AMI	C4-C3	-2.11	1.47	1.53

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	503	AMI	O7-C7-N2	-11.99	111.57	117.78
3	C	503	AMI	O7-C7-N2	-11.11	112.03	117.78
3	A	503	AMI	O7-C7-N2	-9.25	112.99	117.78
3	B	503	AMI	O7-C7-N2	-8.55	113.36	117.78
3	D	503	AMI	O7-C1-C2	-4.12	98.30	104.12
3	A	503	AMI	O3-C3-C2	-3.65	102.18	111.62
3	C	503	AMI	O3-C3-C2	-3.52	102.52	111.62
3	B	503	AMI	O3-C3-C2	-3.47	102.66	111.62
3	C	503	AMI	O7-C1-C2	-3.35	99.38	104.12
3	D	503	AMI	O3-C3-C2	-3.18	103.41	111.62
3	A	503	AMI	O7-C1-C2	-2.86	100.08	104.12
3	B	503	AMI	O7-C1-C2	-2.76	100.22	104.12
3	D	503	AMI	C1-O7-C7	2.75	112.05	108.67

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	503	AMI	O3-C3-C4	2.64	120.28	111.82
3	A	503	AMI	O3-C3-C4	2.61	120.17	111.82
3	D	503	AMI	O3-C3-C4	2.43	119.60	111.82
3	B	503	AMI	O3-C3-C4	2.33	119.27	111.82
3	B	503	AMI	C4-C3-C2	-2.19	99.97	102.80
3	C	503	AMI	C4-C3-C2	-2.07	100.13	102.80

There are no chirality outliers.

All (16) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	503	AMI	N2-C7-N7-C8
3	A	503	AMI	N2-C7-N7-C9
3	A	503	AMI	O7-C7-N7-C8
3	B	503	AMI	N2-C7-N7-C8
3	B	503	AMI	N2-C7-N7-C9
3	C	503	AMI	N2-C7-N7-C8
3	C	503	AMI	N2-C7-N7-C9
3	C	503	AMI	O7-C7-N7-C8
3	D	503	AMI	N2-C7-N7-C8
3	D	503	AMI	N2-C7-N7-C9
3	D	503	AMI	O7-C7-N7-C8
3	A	503	AMI	O7-C7-N7-C9
3	C	503	AMI	O7-C7-N7-C9
3	D	503	AMI	O7-C7-N7-C9
3	B	503	AMI	O7-C7-N7-C8
3	B	503	AMI	O7-C7-N7-C9

There are no ring outliers.

4 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	503	AMI	3	0
3	B	503	AMI	3	0
3	D	503	AMI	5	0
3	A	503	AMI	3	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	392/392 (100%)	-0.59	0 100 100	4, 16, 25, 30	0
1	B	392/392 (100%)	-0.50	2 (0%) 87 82	5, 18, 29, 40	0
1	C	392/392 (100%)	-0.56	1 (0%) 90 86	4, 16, 24, 37	0
1	D	392/392 (100%)	-0.54	1 (0%) 90 86	4, 17, 25, 36	0
All	All	1568/1568 (100%)	-0.55	4 (0%) 90 86	4, 17, 26, 40	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	36	GLY	3.8
1	B	98	TRP	3.1
1	B	94	PRO	3.1
1	D	98	TRP	2.3

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

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

6.3 Carbohydrates [i](#)

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

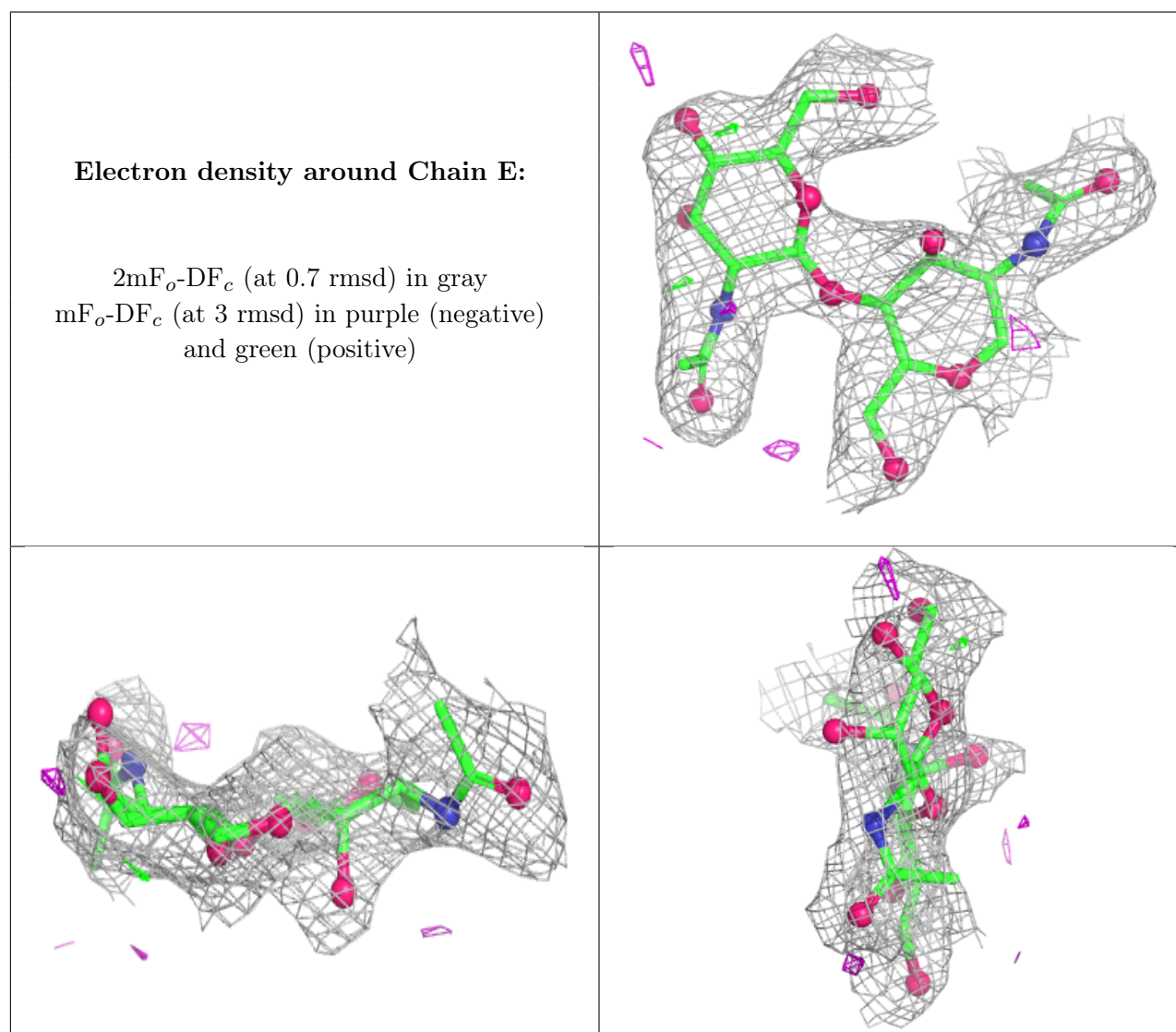
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAA	F	2	14/15	0.79	0.12	11,23,29,30	0
2	NAA	E	2	14/15	0.80	0.10	12,15,19,19	0
2	NAA	F	1	14/15	0.81	0.11	15,17,19,21	0

Continued on next page...

Continued from previous page...

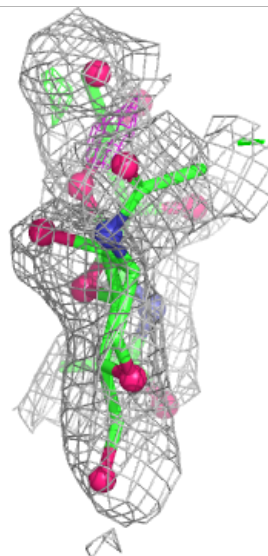
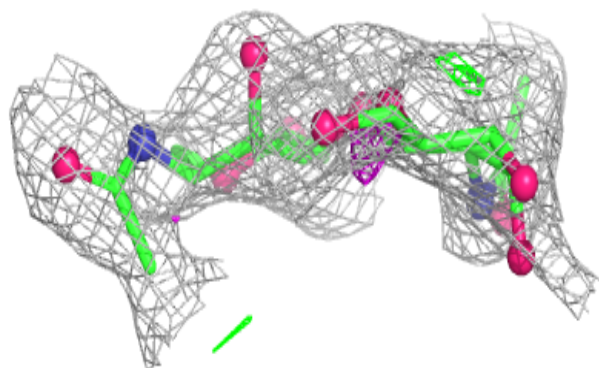
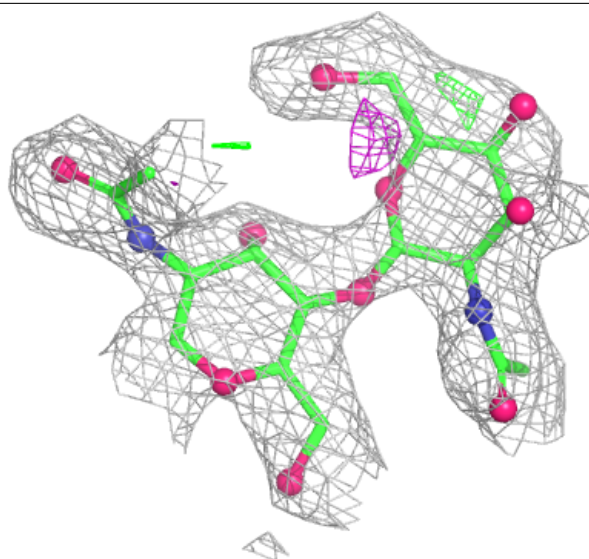
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAA	G	2	14/15	0.82	0.10	10,19,24,29	0
2	NAA	G	1	14/15	0.91	0.09	10,19,23,24	0
2	NAA	E	1	14/15	0.91	0.08	5,9,12,18	0
2	NAA	H	2	14/15	0.91	0.07	4,15,20,24	0
2	NAA	H	1	14/15	0.92	0.08	20,24,27,27	0

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.



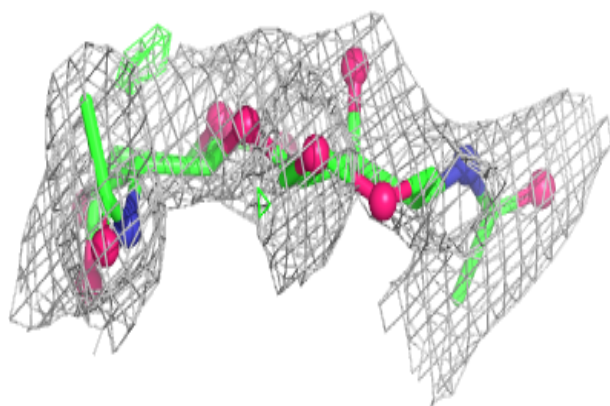
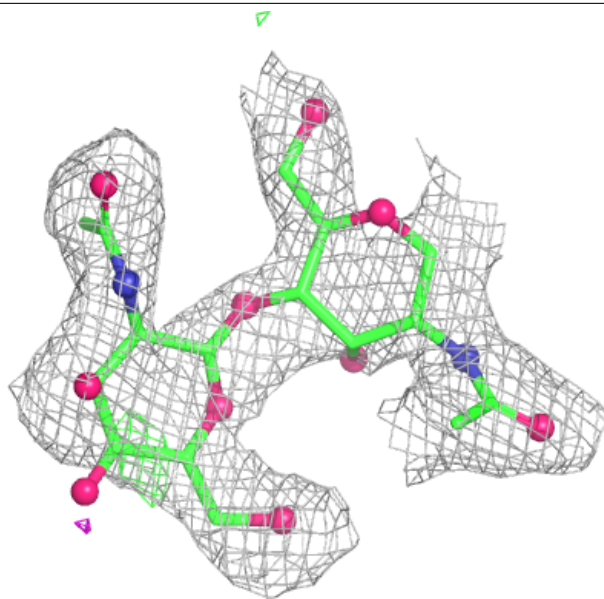
Electron density around Chain F:

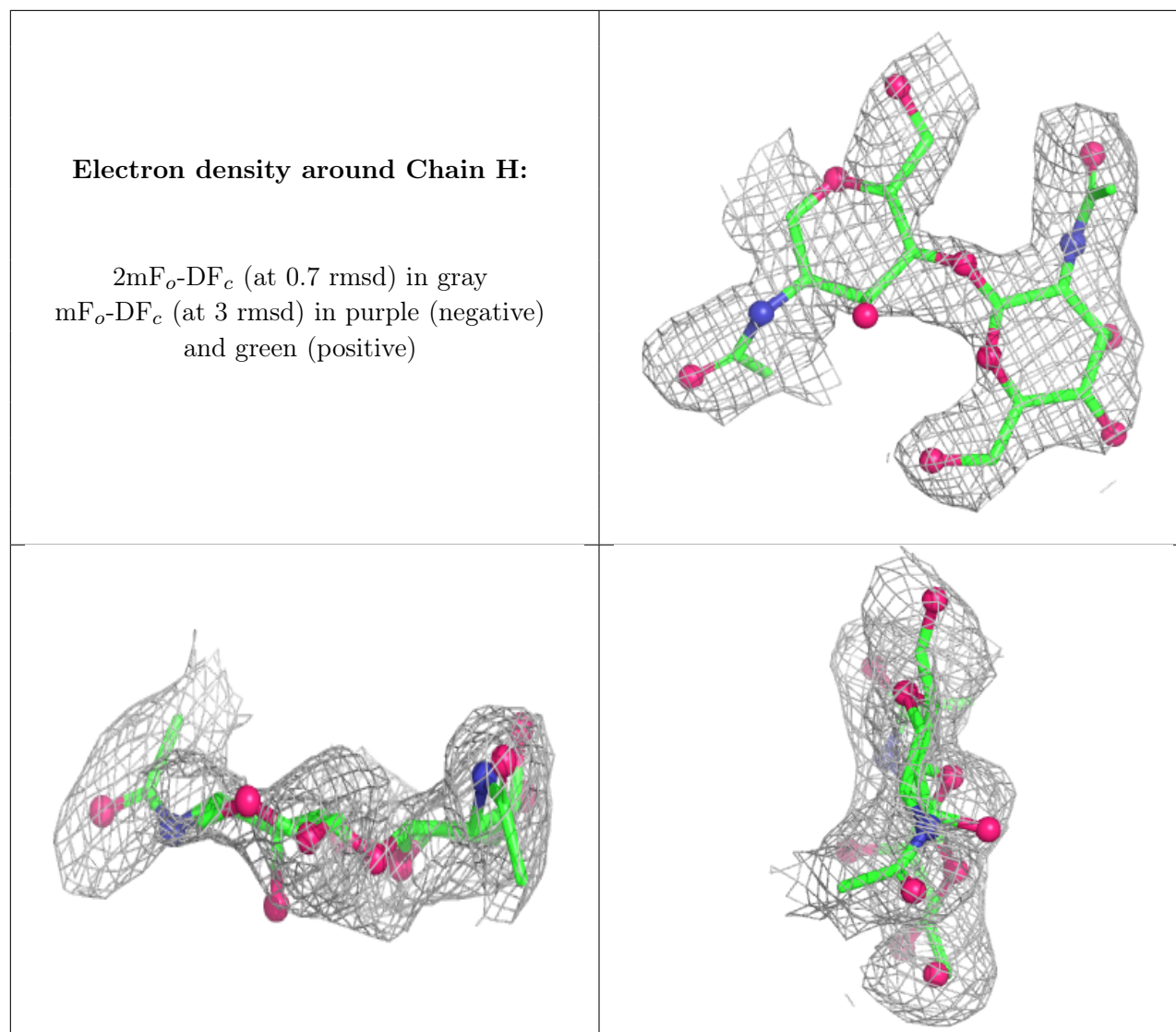
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain G:

$2mF_o-DF_c$ (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
3	AMI	D	503	15/15	0.92	0.08	16,21,23,23	0
3	AMI	C	503	15/15	0.93	0.06	13,16,20,21	0
3	AMI	A	503	15/15	0.94	0.07	10,16,25,29	0
3	AMI	B	503	15/15	0.94	0.07	15,18,21,24	0

6.5 Other polymers ⓘ

There are no such residues in this entry.