



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 11:00 AM UTC

PDB ID : 8ZHZ / pdb_00008zhz
Title : Structure of Ikoma lyssavirus glycoprotein in pre-fusion state
Authors : Lu, G.W.; Yang, F.L.; Lin, S.; Yang, J.; Ye, F.
Deposited on : 2024-05-12
Resolution : 2.88 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

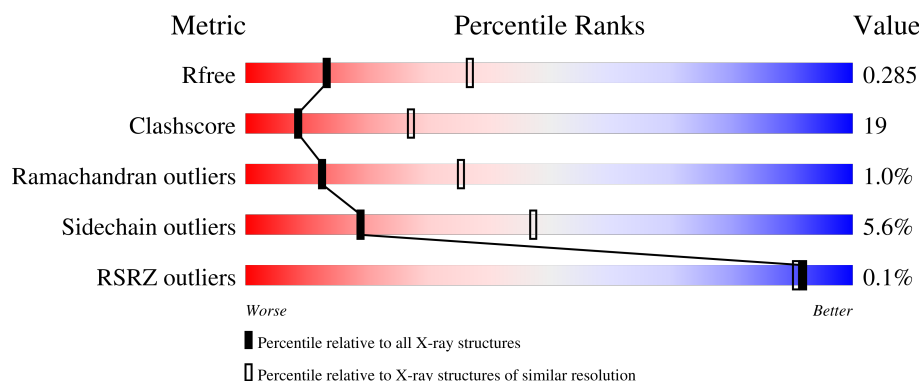
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.88 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	3557 (2.90-2.86)
Clashscore	190562	3801 (2.90-2.86)
Ramachandran outliers	187476	3699 (2.90-2.86)
Sidechain outliers	187428	3702 (2.90-2.86)
RSRZ outliers	180081	3558 (2.90-2.86)

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	440	
1	B	440	
1	C	440	
1	D	440	
1	E	440	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	F	440	55% 27% • • 15%
2	G	2	100%
2	H	2	100%
2	I	2	100%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 17908 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 Glycoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	371	Total	C	N	O	S	0	0	0
			2988	1891	519	553	25			
1	B	369	Total	C	N	O	S	0	0	0
			2971	1878	516	551	26			
1	C	357	Total	C	N	O	S	0	0	0
			2858	1814	492	528	24			
1	D	370	Total	C	N	O	S	0	0	0
			2982	1890	515	551	26			
1	E	362	Total	C	N	O	S	0	0	0
			2911	1844	504	538	25			
1	F	375	Total	C	N	O	S	0	0	0
			3016	1905	526	559	26			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	75	GLY	-	linker	UNP J7JVS8
A	76	GLY	-	linker	UNP J7JVS8
A	77	SER	-	linker	UNP J7JVS8
A	78	GLY	-	linker	UNP J7JVS8
A	79	GLY	-	linker	UNP J7JVS8
A	121	GLY	-	linker	UNP J7JVS8
A	122	GLY	-	linker	UNP J7JVS8
A	123	SER	-	linker	UNP J7JVS8
A	124	GLY	-	linker	UNP J7JVS8
A	125	GLY	-	linker	UNP J7JVS8
A	439	HIS	-	expression tag	UNP J7JVS8
A	440	HIS	-	expression tag	UNP J7JVS8
A	441	HIS	-	expression tag	UNP J7JVS8
A	442	HIS	-	expression tag	UNP J7JVS8
A	443	HIS	-	expression tag	UNP J7JVS8
A	444	HIS	-	expression tag	UNP J7JVS8
B	75	GLY	-	linker	UNP J7JVS8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	76	GLY	-	linker	UNP J7JVS8
B	77	SER	-	linker	UNP J7JVS8
B	78	GLY	-	linker	UNP J7JVS8
B	79	GLY	-	linker	UNP J7JVS8
B	121	GLY	-	linker	UNP J7JVS8
B	122	GLY	-	linker	UNP J7JVS8
B	123	SER	-	linker	UNP J7JVS8
B	124	GLY	-	linker	UNP J7JVS8
B	125	GLY	-	linker	UNP J7JVS8
B	439	HIS	-	expression tag	UNP J7JVS8
B	440	HIS	-	expression tag	UNP J7JVS8
B	441	HIS	-	expression tag	UNP J7JVS8
B	442	HIS	-	expression tag	UNP J7JVS8
B	443	HIS	-	expression tag	UNP J7JVS8
B	444	HIS	-	expression tag	UNP J7JVS8
C	75	GLY	-	linker	UNP J7JVS8
C	76	GLY	-	linker	UNP J7JVS8
C	77	SER	-	linker	UNP J7JVS8
C	78	GLY	-	linker	UNP J7JVS8
C	79	GLY	-	linker	UNP J7JVS8
C	121	GLY	-	linker	UNP J7JVS8
C	122	GLY	-	linker	UNP J7JVS8
C	123	SER	-	linker	UNP J7JVS8
C	124	GLY	-	linker	UNP J7JVS8
C	125	GLY	-	linker	UNP J7JVS8
C	439	HIS	-	expression tag	UNP J7JVS8
C	440	HIS	-	expression tag	UNP J7JVS8
C	441	HIS	-	expression tag	UNP J7JVS8
C	442	HIS	-	expression tag	UNP J7JVS8
C	443	HIS	-	expression tag	UNP J7JVS8
C	444	HIS	-	expression tag	UNP J7JVS8
D	75	GLY	-	linker	UNP J7JVS8
D	76	GLY	-	linker	UNP J7JVS8
D	77	SER	-	linker	UNP J7JVS8
D	78	GLY	-	linker	UNP J7JVS8
D	79	GLY	-	linker	UNP J7JVS8
D	121	GLY	-	linker	UNP J7JVS8
D	122	GLY	-	linker	UNP J7JVS8
D	123	SER	-	linker	UNP J7JVS8
D	124	GLY	-	linker	UNP J7JVS8
D	125	GLY	-	linker	UNP J7JVS8
D	439	HIS	-	expression tag	UNP J7JVS8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	440	HIS	-	expression tag	UNP J7JVS8
D	441	HIS	-	expression tag	UNP J7JVS8
D	442	HIS	-	expression tag	UNP J7JVS8
D	443	HIS	-	expression tag	UNP J7JVS8
D	444	HIS	-	expression tag	UNP J7JVS8
E	75	GLY	-	linker	UNP J7JVS8
E	76	GLY	-	linker	UNP J7JVS8
E	77	SER	-	linker	UNP J7JVS8
E	78	GLY	-	linker	UNP J7JVS8
E	79	GLY	-	linker	UNP J7JVS8
E	121	GLY	-	linker	UNP J7JVS8
E	122	GLY	-	linker	UNP J7JVS8
E	123	SER	-	linker	UNP J7JVS8
E	124	GLY	-	linker	UNP J7JVS8
E	125	GLY	-	linker	UNP J7JVS8
E	439	HIS	-	expression tag	UNP J7JVS8
E	440	HIS	-	expression tag	UNP J7JVS8
E	441	HIS	-	expression tag	UNP J7JVS8
E	442	HIS	-	expression tag	UNP J7JVS8
E	443	HIS	-	expression tag	UNP J7JVS8
E	444	HIS	-	expression tag	UNP J7JVS8
F	75	GLY	-	linker	UNP J7JVS8
F	76	GLY	-	linker	UNP J7JVS8
F	77	SER	-	linker	UNP J7JVS8
F	78	GLY	-	linker	UNP J7JVS8
F	79	GLY	-	linker	UNP J7JVS8
F	121	GLY	-	linker	UNP J7JVS8
F	122	GLY	-	linker	UNP J7JVS8
F	123	SER	-	linker	UNP J7JVS8
F	124	GLY	-	linker	UNP J7JVS8
F	125	GLY	-	linker	UNP J7JVS8
F	439	HIS	-	expression tag	UNP J7JVS8
F	440	HIS	-	expression tag	UNP J7JVS8
F	441	HIS	-	expression tag	UNP J7JVS8
F	442	HIS	-	expression tag	UNP J7JVS8
F	443	HIS	-	expression tag	UNP J7JVS8
F	444	HIS	-	expression tag	UNP J7JVS8

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



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

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



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

Continued on next page...

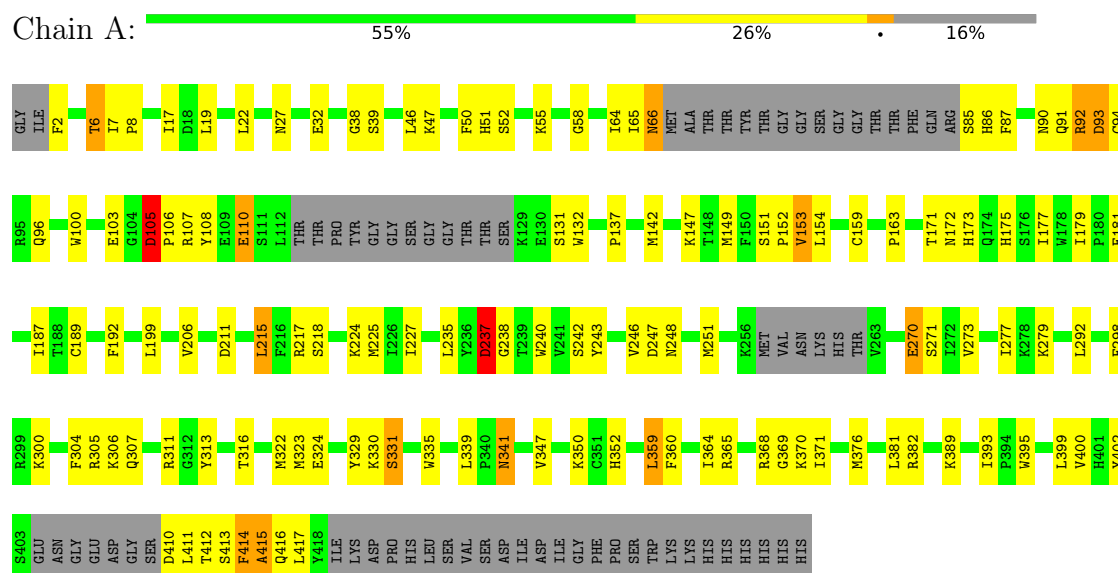
Continued from previous page...

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

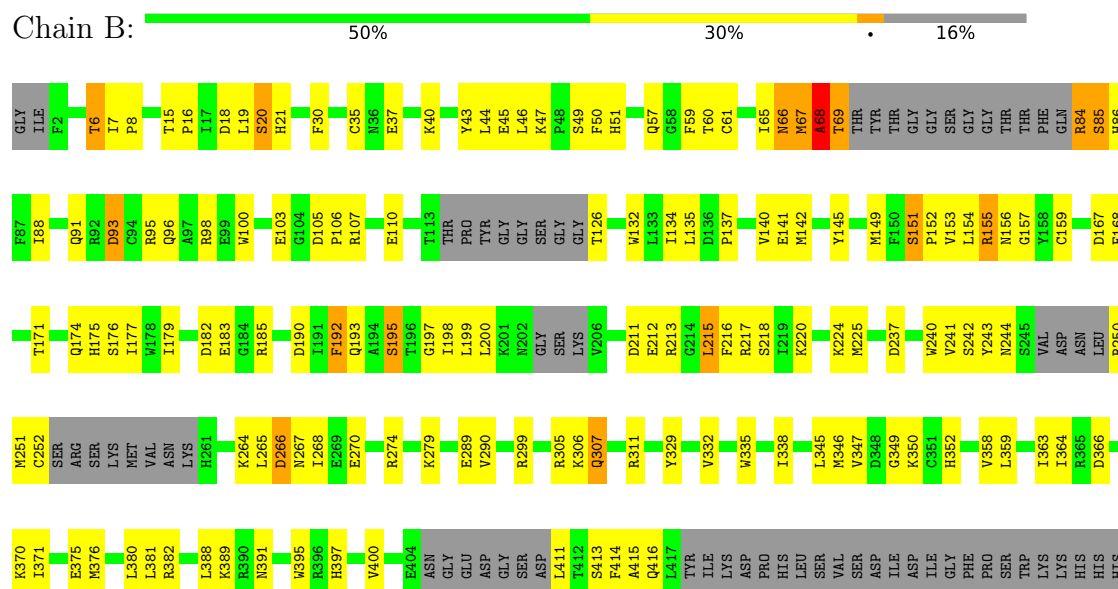
3 Residue-property plots

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: Glycoprotein



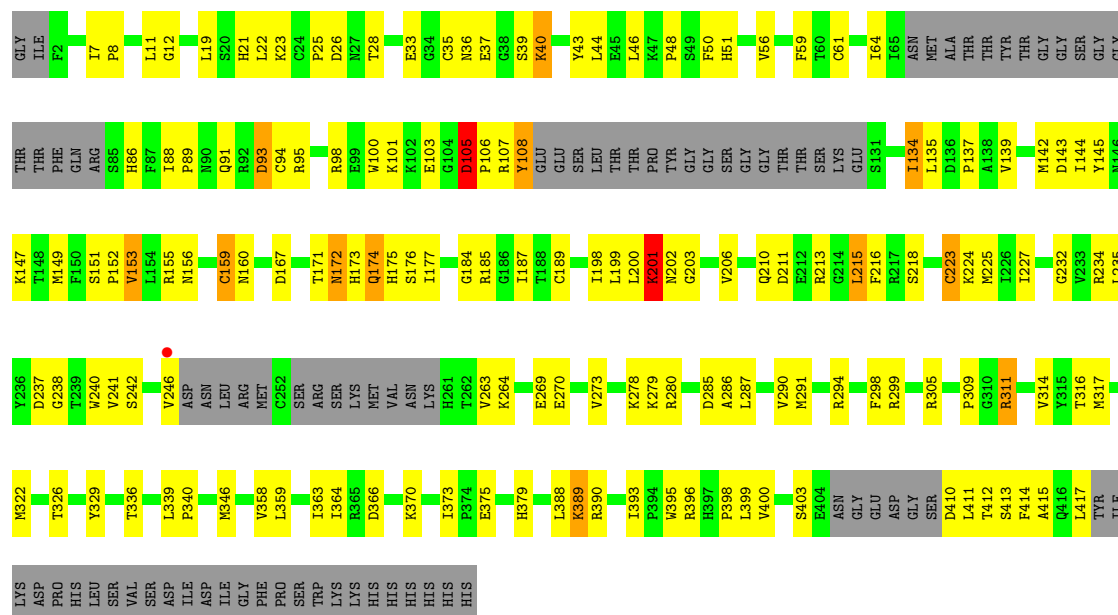
• Molecule 1: Glycoprotein



HIS
HIS
HIS

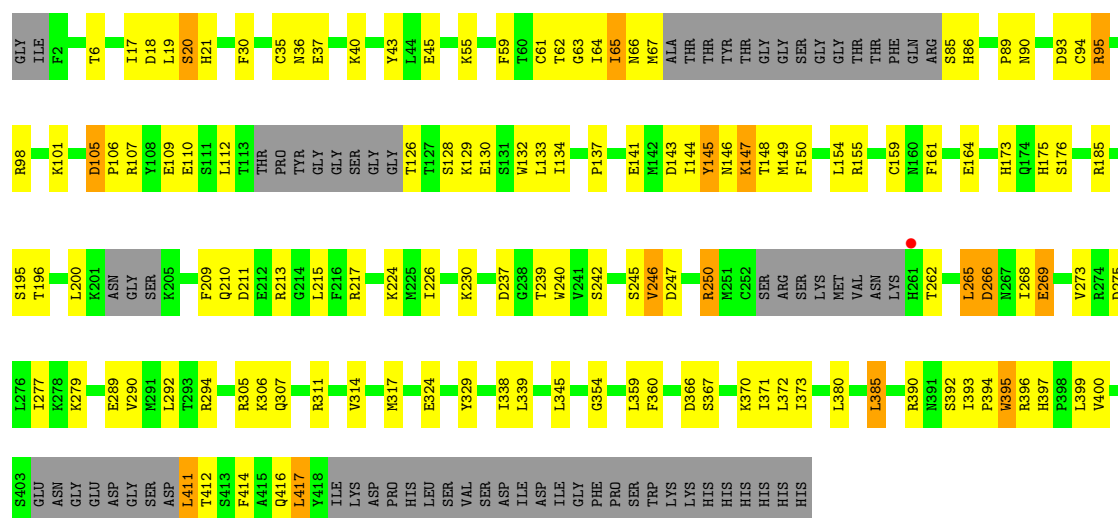
• Molecule 1: Glycoprotein

Chain C: 47% 31% • 19%



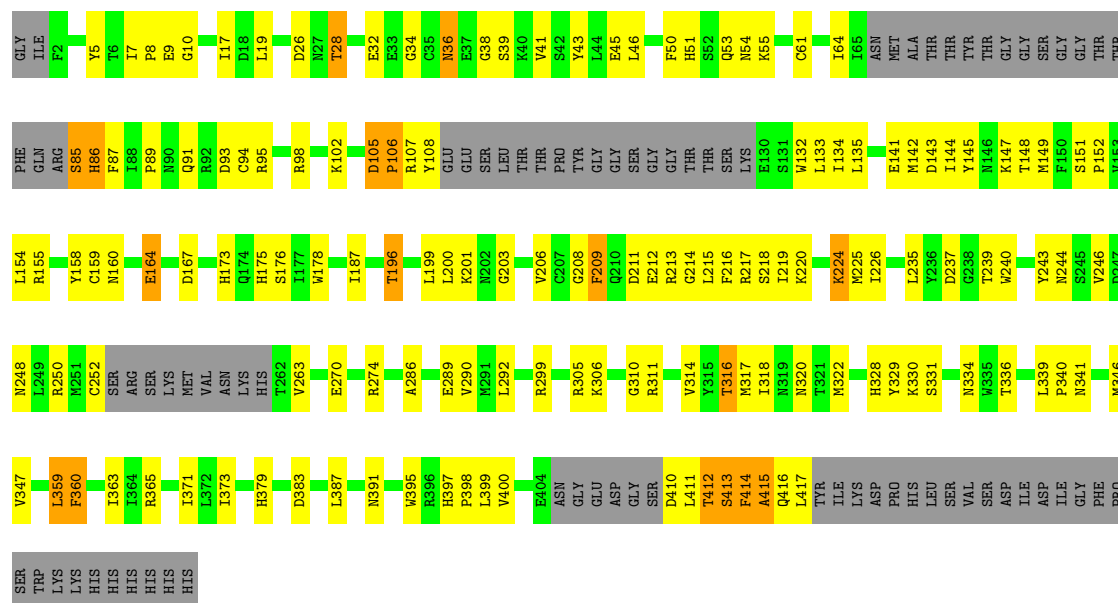
• Molecule 1: Glycoprotein

Chain D: 54% 27% • 16%

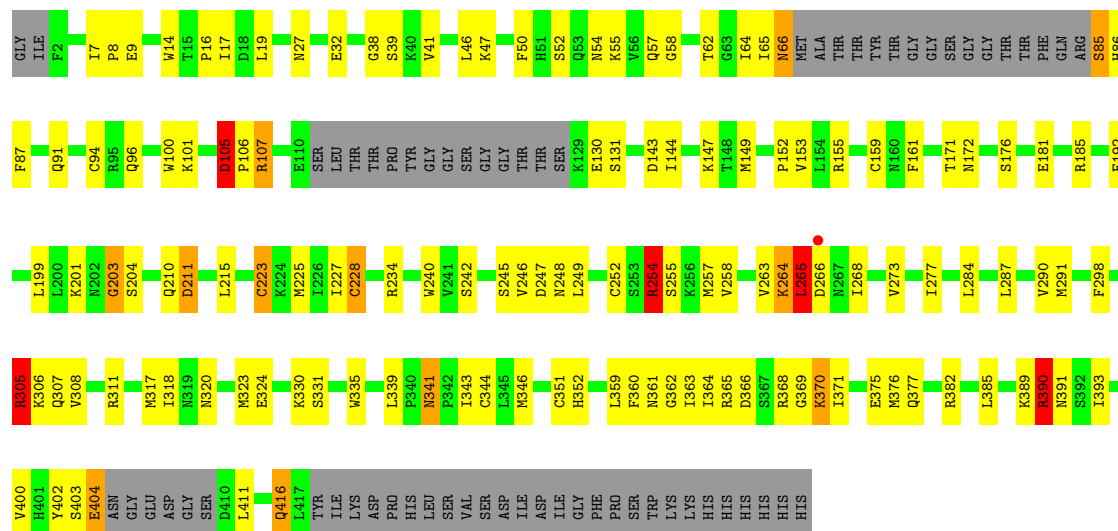


• Molecule 1: Glycoprotein

Chain E: 49% 30% • 18%



- Molecule 1: Glycoprotein



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



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



MAG1
MAG2

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

Chain I:

100%

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	122.92Å 90.75Å 151.31Å 90.00° 90.08° 90.00°	Depositor
Resolution (Å)	46.64 – 2.88 46.64 – 2.88	Depositor EDS
% Data completeness (in resolution range)	98.4 (46.64-2.88) 98.4 (46.64-2.88)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.50 (at 2.91Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.225 , 0.281 0.232 , 0.285	Depositor DCC
R_{free} test set	3613 reflections (4.78%)	wwPDB-VP
Wilson B-factor (Å ²)	65.3	Xtriage
Anisotropy	0.552	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.448 for h,-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	17908	wwPDB-VP
Average B, all atoms (Å ²)	71.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% 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: NAG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.52	0/3057	0.93	13/4125 (0.3%)
1	B	0.53	0/3038	0.83	9/4099 (0.2%)
1	C	0.55	0/2925	0.79	0/3951
1	D	0.53	0/3051	0.81	6/4119 (0.1%)
1	E	0.51	0/2979	0.88	7/4023 (0.2%)
1	F	0.55	0/3086	0.86	8/4166 (0.2%)
All	All	0.53	0/18136	0.85	43/24483 (0.2%)

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	B	0	3
1	C	0	1
1	D	0	3
1	E	0	3
1	F	0	2
All	All	0	12

There are no bond length outliers.

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	93	ASP	N-CA-C	-17.37	91.35	112.89
1	A	360	PHE	N-CA-C	15.00	128.86	110.41
1	F	255	SER	N-CA-C	-11.91	98.17	113.17
1	A	413	SER	N-CA-C	11.24	124.86	111.82
1	D	360	PHE	N-CA-C	11.13	124.88	110.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	237	ASP	N-CA-C	-10.59	95.57	110.50
1	E	415	ALA	N-CA-C	-10.48	99.55	114.12
1	E	360	PHE	N-CA-C	10.38	124.23	110.53
1	E	414	PHE	N-CA-C	-9.98	89.55	110.80
1	A	359	LEU	N-CA-C	-9.51	95.81	110.17
1	E	244	ASN	N-CA-CB	9.31	125.42	110.90
1	F	66	ASN	N-CA-CB	9.15	126.05	110.50
1	A	360	PHE	N-CA-CB	-8.77	98.37	110.38
1	A	415	ALA	N-CA-CB	-8.18	98.26	110.60
1	A	414	PHE	N-CA-C	-7.92	103.06	112.89
1	E	243	TYR	CB-CA-C	7.78	123.50	110.43
1	A	92	ARG	CB-CA-C	-7.54	97.82	110.56
1	D	360	PHE	N-CA-CB	-7.32	99.97	110.44
1	B	151	SER	CB-CA-C	6.99	123.94	110.17
1	E	359	LEU	N-CA-C	-6.91	99.09	109.94
1	F	254	ARG	CB-CA-C	-6.61	97.26	110.42
1	D	359	LEU	N-CA-C	-6.38	100.48	110.36
1	A	237	ASP	CB-CA-C	6.26	121.06	109.54
1	F	203	GLY	N-CA-C	-6.08	101.64	112.22
1	A	413	SER	CB-CA-C	-6.01	99.13	110.67
1	B	152	PRO	N-CA-C	-5.97	104.61	114.75
1	B	69	THR	N-CA-C	-5.92	94.43	111.00
1	F	264	LYS	N-CA-C	5.82	119.42	111.39
1	D	147	LYS	N-CA-C	-5.79	105.33	113.20
1	D	65	ILE	CA-C-N	-5.74	111.53	121.52
1	D	65	ILE	C-N-CA	-5.74	111.53	121.52
1	B	68	ALA	CB-CA-C	-5.73	99.02	110.42
1	B	416	GLN	CA-C-N	5.66	131.89	121.70
1	B	416	GLN	C-N-CA	5.66	131.89	121.70
1	A	93	ASP	CB-CA-C	5.58	121.65	109.99
1	F	265	LEU	N-CA-CB	-5.48	101.28	110.22
1	B	68	ALA	N-CA-C	-5.48	99.14	110.80
1	F	228	CYS	N-CA-C	-5.43	99.23	110.80
1	B	416	GLN	CA-CB-CG	5.43	124.95	114.10
1	E	10	GLY	N-CA-C	-5.09	101.10	113.18
1	F	265	LEU	N-CA-C	5.07	119.61	112.72
1	B	85	SER	CB-CA-C	5.06	120.05	110.95
1	A	415	ALA	N-CA-C	-5.03	101.39	109.39

There are no chirality outliers.

All (12) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	155	ARG	Sidechain
1	B	192	PHE	Peptide
1	B	84	ARG	Peptide
1	C	201	LYS	Peptide
1	D	145	TYR	Peptide
1	D	354	GLY	Peptide
1	D	95	ARG	Sidechain
1	E	164	GLU	Peptide
1	E	209	PHE	Peptide
1	E	305	ARG	Sidechain
1	F	305	ARG	Sidechain
1	F	390	ARG	Sidechain

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	2988	0	2913	98	1
1	B	2971	0	2895	128	1
1	C	2858	0	2776	136	0
1	D	2982	0	2907	100	1
1	E	2911	0	2835	115	0
1	F	3016	0	2935	100	1
2	G	28	0	25	0	0
2	H	28	0	25	0	0
2	I	28	0	25	0	0
3	A	14	0	13	0	0
3	B	28	0	26	0	0
3	C	14	0	13	1	0
3	D	14	0	13	0	0
3	E	14	0	13	1	0
3	F	14	0	13	1	0
All	All	17908	0	17427	665	2

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 19.

All (665) 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:F:264:LYS:O	1:F:264:LYS:HD3	1.58	1.02
1:B:217:ARG:NH1	1:B:237:ASP:OD2	1.96	0.99
1:A:92:ARG:O	1:A:92:ARG:HG2	1.61	0.97
1:A:330:LYS:HD2	1:A:331:SER:H	1.29	0.97
1:C:398:PRO:HB3	1:C:414:PHE:CE1	2.00	0.96
1:E:64:ILE:HG23	1:E:411:LEU:HD11	1.49	0.92
1:F:264:LYS:O	1:F:264:LYS:CD	2.18	0.91
1:E:105:ASP:HB2	1:E:106:PRO:HD3	1.53	0.90
1:E:217:ARG:HG2	1:E:235:LEU:HD22	1.54	0.89
1:F:254:ARG:HA	1:F:257:MET:SD	2.12	0.88
1:F:368:ARG:HD2	1:F:368:ARG:O	1.73	0.88
1:C:317:MET:HE2	1:C:322:MET:HE1	1.56	0.86
1:F:365:ARG:HG3	1:F:369:GLY:HA2	1.55	0.86
1:B:68:ALA:HB1	1:B:126:THR:HB	1.57	0.85
1:C:234:ARG:NH1	1:C:235:LEU:O	2.09	0.85
1:B:65:ILE:HB	1:B:85:SER:HB3	1.57	0.85
1:B:267:ASN:O	1:B:268:ILE:HD12	1.76	0.85
1:A:238:GLY:HA3	1:A:311:ARG:NH2	1.93	0.84
1:C:56:VAL:HG21	1:C:142:MET:HE3	1.59	0.84
1:C:322:MET:HE3	1:C:393:ILE:HD11	1.59	0.84
1:C:238:GLY:HA3	1:C:311:ARG:NH1	1.93	0.83
1:E:211:ASP:OD1	1:E:214:GLY:N	2.09	0.83
1:E:218:SER:HB3	1:E:220:LYS:HG3	1.61	0.83
1:C:105:ASP:N	1:C:105:ASP:OD1	2.10	0.82
1:D:317:MET:SD	1:D:393:ILE:HD11	2.20	0.82
1:A:330:LYS:HD2	1:A:331:SER:N	1.95	0.82
1:F:370:LYS:NZ	1:F:382:ARG:HH12	1.78	0.80
1:B:107:ARG:HH21	1:B:134:ILE:HB	1.47	0.80
1:A:105:ASP:OD1	1:A:106:PRO:HD2	1.81	0.80
1:C:305:ARG:NH1	1:C:375:GLU:OE2	2.15	0.79
1:E:413:SER:O	1:E:415:ALA:N	2.16	0.79
1:F:211:ASP:OD2	1:F:215:LEU:HB2	1.83	0.78
1:E:143:ASP:OD1	1:E:145:TYR:N	2.12	0.78
1:A:238:GLY:HA3	1:A:311:ARG:HH21	1.46	0.78
1:A:6:THR:HG21	1:A:306:LYS:O	1.83	0.78
1:B:68:ALA:O	1:B:69:THR:OG1	2.02	0.78
1:F:101:LYS:HD2	1:F:107:ARG:HH21	1.47	0.78
1:D:86:HIS:HB3	1:D:175:HIS:CG	2.18	0.77
1:C:211:ASP:HB2	1:C:213:ARG:HG2	1.68	0.76
1:B:267:ASN:C	1:B:268:ILE:HD12	2.09	0.76
1:C:215:LEU:HD21	1:C:309:PRO:HB2	1.65	0.76
1:E:7:ILE:HG13	1:E:8:PRO:HD2	1.67	0.76

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:265:LEU:HD12	1:F:265:LEU:H	1.52	0.75
1:E:46:LEU:HD11	1:E:240:TRP:HB3	1.67	0.75
1:A:365:ARG:HG3	1:A:369:GLY:HA2	1.68	0.75
1:F:370:LYS:HZ2	1:F:382:ARG:HH12	1.35	0.75
1:E:142:MET:HE3	1:E:147:LYS:HD2	1.68	0.74
1:E:173:HIS:HB3	1:E:176:SER:HB2	1.68	0.73
1:E:201:LYS:HD2	1:E:203:GLY:H	1.53	0.73
1:E:330:LYS:HD2	1:E:331:SER:N	2.04	0.72
1:D:394:PRO:O	1:D:395:TRP:C	2.33	0.72
1:C:363:ILE:HD13	1:C:373:ILE:HG12	1.70	0.72
1:D:164:GLU:N	1:D:164:GLU:OE2	2.22	0.72
1:C:201:LYS:HG2	1:C:203:GLY:H	1.54	0.71
1:E:199:LEU:HD11	1:E:206:VAL:HG12	1.72	0.71
1:E:135:LEU:HD13	1:E:398:PRO:HG2	1.73	0.70
1:F:19:LEU:HD21	1:F:393:ILE:HD13	1.73	0.70
1:A:19:LEU:HD21	1:A:393:ILE:HG13	1.74	0.70
1:F:144:ILE:O	1:F:147:LYS:NZ	2.18	0.69
1:D:107:ARG:HH22	1:D:134:ILE:H	1.41	0.69
1:E:64:ILE:HD13	1:E:86:HIS:HB3	1.75	0.69
1:D:6:THR:HG23	1:D:305:ARG:HH21	1.57	0.69
1:A:91:GLN:O	1:A:94:CYS:HB2	1.93	0.68
1:B:68:ALA:CB	1:B:126:THR:HB	2.23	0.68
1:C:147:LYS:HE2	1:C:187:ILE:HD13	1.74	0.68
1:C:287:LEU:O	1:C:291:MET:HG3	1.94	0.68
1:F:201:LYS:HG3	1:F:203:GLY:O	1.93	0.68
1:B:174:GLN:HE21	1:B:175:HIS:HE1	1.40	0.68
1:C:46:LEU:HD11	1:C:240:TRP:HB3	1.75	0.68
1:D:133:LEU:HD11	1:D:417:LEU:HD23	1.75	0.67
1:A:6:THR:HG23	1:A:329:TYR:CD1	2.30	0.67
1:A:199:LEU:HD11	1:A:206:VAL:HG21	1.75	0.67
1:C:86:HIS:HE1	1:C:411:LEU:HD23	1.59	0.67
1:A:381:LEU:HD12	1:B:265:LEU:HD13	1.75	0.67
1:A:370:LYS:NZ	1:A:382:ARG:HH12	1.93	0.67
1:B:155:ARG:NH1	1:B:156:ASN:OD1	2.27	0.66
1:B:6:THR:HG21	1:B:306:LYS:O	1.96	0.66
1:A:235:LEU:O	1:A:237:ASP:O	2.12	0.66
1:B:6:THR:HG23	1:B:329:TYR:CD1	2.31	0.66
1:C:86:HIS:CE1	1:C:411:LEU:HD23	2.30	0.65
1:B:299:ARG:HD2	1:B:388:LEU:HD12	1.77	0.65
1:A:224:LYS:HE2	1:A:248:ASN:HB2	1.78	0.65
1:C:91:GLN:NE2	1:C:95:ARG:HH21	1.96	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:101:LYS:HD3	1:C:134:ILE:HD13	1.78	0.64
1:D:65:ILE:HD12	1:D:130:GLU:HG2	1.78	0.64
1:E:224:LYS:HG2	1:E:250:ARG:CZ	2.27	0.64
1:D:306:LYS:HE3	1:D:311:ARG:O	1.97	0.64
1:D:273:VAL:O	1:D:277:ILE:HG13	1.97	0.64
1:C:37:GLU:HB2	1:C:201:LYS:HE2	1.79	0.64
1:E:318:ILE:HG21	3:E:501:NAG:H82	1.80	0.64
1:A:171:THR:HG21	1:A:399:LEU:HD13	1.80	0.63
1:C:398:PRO:HB3	1:C:414:PHE:CD1	2.32	0.63
1:D:65:ILE:HB	1:D:85:SER:HB2	1.80	0.63
1:C:7:ILE:HG13	1:C:8:PRO:HD2	1.80	0.63
1:C:145:TYR:N	1:C:145:TYR:HD1	1.97	0.63
1:B:224:LYS:NZ	1:B:244:ASN:OD1	2.29	0.63
1:C:22:LEU:HD21	1:C:322:MET:HG2	1.80	0.63
1:E:26:ASP:OD1	1:E:28:THR:OG1	2.17	0.63
1:D:215:LEU:HD22	1:D:217:ARG:HE	1.64	0.63
1:A:92:ARG:O	1:A:92:ARG:CG	2.35	0.63
1:D:217:ARG:NH1	1:D:237:ASP:OD2	2.32	0.63
1:A:107:ARG:HA	1:A:110:GLU:OE2	1.98	0.62
1:B:6:THR:HB	1:B:305:ARG:HH21	1.65	0.62
1:B:100:TRP:O	1:B:103:GLU:O	2.17	0.62
1:D:95:ARG:HH11	1:D:95:ARG:HG2	1.64	0.62
1:F:91:GLN:O	1:F:94:CYS:HB2	2.00	0.62
1:E:86:HIS:HD2	1:E:175:HIS:ND1	1.98	0.62
1:A:110:GLU:CD	1:A:110:GLU:H	2.06	0.62
1:E:399:LEU:HD11	1:E:414:PHE:CZ	2.34	0.62
1:E:86:HIS:ND1	1:E:411:LEU:HD12	2.14	0.62
1:F:264:LYS:HD3	1:F:264:LYS:C	2.24	0.62
1:C:234:ARG:NH1	1:C:238:GLY:HA2	2.15	0.62
1:A:64:ILE:HD13	1:A:85:SER:HB3	1.82	0.61
1:F:14:TRP:HB3	1:F:323:MET:HE3	1.82	0.61
1:F:66:ASN:HA	1:F:86:HIS:CE1	2.34	0.61
1:A:22:LEU:HD11	1:A:322:MET:HE2	1.81	0.61
1:D:224:LYS:NZ	1:D:250:ARG:HB3	2.15	0.61
1:A:96:GLN:OE1	1:A:100:TRP:NE1	2.33	0.61
1:A:100:TRP:CZ3	1:A:106:PRO:HG2	2.35	0.61
1:B:211:ASP:HB3	1:B:213:ARG:H	1.65	0.61
1:C:145:TYR:OH	1:C:225:MET:HE1	2.00	0.61
1:B:397:HIS:O	1:B:400:VAL:HG22	2.01	0.61
1:E:32:GLU:OE2	1:E:34:GLY:N	2.34	0.60
1:B:220:LYS:HE3	1:B:267:ASN:HD22	1.66	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:316:THR:HG23	1:E:317:MET:N	2.15	0.60
1:F:65:ILE:HD11	1:F:130:GLU:HA	1.83	0.60
1:A:189:CYS:HB2	1:E:164:GLU:HG2	1.82	0.60
1:E:347:VAL:HG21	1:E:360:PHE:HZ	1.66	0.60
1:B:6:THR:HG23	1:B:329:TYR:HD1	1.66	0.60
1:C:93:ASP:OD1	1:C:93:ASP:N	2.33	0.60
1:F:225:MET:HE1	1:F:257:MET:HB3	1.83	0.60
1:C:269:GLU:OE2	1:C:269:GLU:N	2.24	0.60
1:C:142:MET:O	1:C:142:MET:HG3	1.99	0.60
1:B:359:LEU:HD13	1:B:363:ILE:HG22	1.83	0.60
1:E:211:ASP:CG	1:E:213:ARG:HG2	2.26	0.60
1:A:93:ASP:HB3	1:A:132:TRP:CZ2	2.37	0.59
1:B:43:TYR:HE2	1:B:45:GLU:OE2	1.85	0.59
1:A:22:LEU:HD23	1:A:304:PHE:CZ	2.37	0.59
1:A:66:ASN:CG	1:A:86:HIS:HB2	2.27	0.59
1:B:183:GLU:OE2	1:B:183:GLU:N	2.25	0.59
1:F:223:CYS:HB3	1:F:234:ARG:HB3	1.84	0.59
1:B:43:TYR:CD2	1:B:241:VAL:HG23	2.37	0.59
1:A:225:MET:HE2	1:A:227:ILE:HG13	1.84	0.59
1:C:64:ILE:HG22	1:C:86:HIS:ND1	2.18	0.59
1:E:299:ARG:HG3	1:E:387:LEU:HB3	1.84	0.59
1:F:147:LYS:HB3	1:F:185:ARG:NH2	2.18	0.59
1:A:152:PRO:HB2	1:A:400:VAL:HG13	1.85	0.59
1:A:368:ARG:HD2	1:A:368:ARG:O	2.02	0.59
1:B:7:ILE:HG13	1:B:8:PRO:HD2	1.84	0.59
1:C:211:ASP:OD2	1:C:215:LEU:HB3	2.03	0.59
1:F:96:GLN:HE21	1:F:100:TRP:NE1	2.01	0.59
1:A:240:TRP:CH2	1:A:242:SER:HB3	2.38	0.58
1:E:46:LEU:CD1	1:E:240:TRP:HB3	2.33	0.58
1:A:171:THR:HG22	1:A:172:ASN:N	2.18	0.58
1:D:107:ARG:O	1:D:110:GLU:HG2	2.03	0.58
1:A:339:LEU:HD21	1:A:371:ILE:HB	1.84	0.58
1:B:91:GLN:NE2	1:B:95:ARG:HE	2.01	0.58
1:C:145:TYR:N	1:C:145:TYR:CD1	2.69	0.58
1:C:294:ARG:NH2	1:C:396:ARG:HD2	2.19	0.58
1:A:370:LYS:HE3	1:A:382:ARG:HH12	1.69	0.58
1:D:64:ILE:HG22	1:D:129:LYS:HD2	1.86	0.58
1:E:85:SER:N	1:E:411:LEU:HD13	2.19	0.58
1:C:33:GLU:OE1	1:C:33:GLU:N	2.37	0.58
1:D:107:ARG:HH12	1:D:134:ILE:HG12	1.69	0.58
1:F:246:VAL:O	1:F:248:ASN:N	2.37	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:352:HIS:HB3	1:A:359:LEU:HD23	1.86	0.57
1:F:265:LEU:HB3	1:F:268:ILE:HD12	1.85	0.57
1:E:340:PRO:HG3	1:E:346:MET:HE3	1.86	0.57
1:C:410:ASP:OD1	1:C:411:LEU:HD12	2.05	0.57
1:B:224:LYS:O	1:B:250:ARG:HG3	2.04	0.57
1:B:93:ASP:HA	1:B:96:GLN:HB3	1.85	0.57
1:C:322:MET:CE	1:C:393:ILE:HD11	2.31	0.57
1:E:17:ILE:HG22	1:E:55:LYS:HG2	1.87	0.57
1:A:199:LEU:HD22	1:A:243:TYR:HE2	1.69	0.57
1:B:137:PRO:HD2	1:B:395:TRP:CD1	2.39	0.57
1:D:245:SER:OG	1:D:246:VAL:HG23	2.04	0.57
1:C:199:LEU:HD11	1:C:206:VAL:HG12	1.86	0.57
1:E:155:ARG:HG3	1:E:155:ARG:HH11	1.69	0.57
1:E:246:VAL:O	1:E:248:ASN:ND2	2.37	0.57
1:D:390:ARG:HG3	1:E:292:LEU:HD22	1.87	0.57
1:B:151:SER:O	1:B:157:GLY:HA2	2.04	0.56
1:A:277:ILE:HD13	1:C:379:HIS:HA	1.87	0.56
1:B:185:ARG:HG3	1:B:185:ARG:HH11	1.69	0.56
1:C:322:MET:HE3	1:C:393:ILE:CD1	2.34	0.56
1:D:105:ASP:OD1	1:D:106:PRO:HD3	2.05	0.56
1:D:397:HIS:O	1:D:400:VAL:HG22	2.05	0.56
1:E:151:SER:N	1:E:154:LEU:HD12	2.21	0.56
1:D:292:LEU:HD13	1:F:390:ARG:HG3	1.88	0.56
1:C:137:PRO:HD2	1:C:395:TRP:CD1	2.41	0.56
1:C:142:MET:HE1	1:C:185:ARG:HD2	1.87	0.56
1:E:147:LYS:HE2	1:E:187:ILE:HD13	1.87	0.56
1:B:358:VAL:HG13	1:B:364:ILE:HG22	1.87	0.56
1:F:352:HIS:HB3	1:F:359:LEU:HD23	1.88	0.56
1:F:19:LEU:HD13	1:F:290:VAL:HG12	1.88	0.56
1:A:153:VAL:O	1:A:171:THR:HG23	2.05	0.56
1:B:60:THR:HG21	1:B:397:HIS:HE1	1.70	0.56
1:D:43:TYR:CZ	1:D:209:PHE:HZ	2.24	0.56
1:B:18:ASP:OD2	1:B:20:SER:OG	2.23	0.55
1:B:61:CYS:SG	1:B:132:TRP:HB3	2.46	0.55
1:C:22:LEU:HD21	1:C:322:MET:CG	2.36	0.55
1:A:370:LYS:CE	1:A:382:ARG:HH12	2.18	0.55
1:B:265:LEU:HA	1:B:268:ILE:HD13	1.87	0.55
1:A:335:TRP:CE2	1:A:376:MET:HG3	2.42	0.55
1:C:46:LEU:CD1	1:C:240:TRP:HB3	2.36	0.55
1:B:168:PHE:CG	1:B:177:ILE:HD11	2.41	0.55
1:D:90:ASN:HB3	1:D:93:ASP:OD2	2.07	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:225:MET:HE2	1:B:240:TRP:CD1	2.41	0.55
1:C:106:PRO:O	1:C:107:ARG:HG3	2.07	0.55
1:D:63:GLY:O	1:D:64:ILE:HD12	2.07	0.55
1:A:17:ILE:HG22	1:A:55:LYS:HG2	1.88	0.55
1:B:142:MET:HE1	1:B:185:ARG:HE	1.71	0.55
1:D:224:LYS:O	1:D:250:ARG:HG3	2.07	0.55
1:B:216:PHE:HE1	1:B:218:SER:HB2	1.72	0.55
1:B:414:PHE:CD1	1:B:414:PHE:C	2.85	0.55
1:D:107:ARG:C	1:D:107:ARG:HD2	2.32	0.55
1:D:294:ARG:HD3	1:D:396:ARG:NH1	2.22	0.54
1:E:5:TYR:OH	1:E:363:ILE:HD11	2.07	0.54
1:F:54:ASN:HB2	1:F:55:LYS:HD2	1.89	0.54
1:A:292:LEU:HD13	1:C:390:ARG:HG3	1.88	0.54
1:C:101:LYS:CD	1:C:134:ILE:HD13	2.38	0.54
1:E:330:LYS:HD2	1:E:331:SER:H	1.70	0.54
1:F:32:GLU:HG3	1:F:32:GLU:O	2.07	0.54
1:B:224:LYS:HD3	1:B:250:ARG:NH2	2.23	0.54
1:C:173:HIS:HD2	1:C:176:SER:OG	1.90	0.54
1:B:95:ARG:NH2	1:B:183:GLU:HG3	2.22	0.54
1:B:6:THR:HG22	1:B:305:ARG:HE	1.72	0.54
1:F:143:ASP:OD2	1:F:258:VAL:HG11	2.07	0.54
1:C:314:VAL:HG22	1:C:329:TYR:OH	2.07	0.54
1:F:265:LEU:H	1:F:265:LEU:CD1	2.16	0.54
1:F:341:ASN:C	1:F:341:ASN:OD1	2.50	0.54
1:B:16:PRO:HG2	1:B:57:GLN:OE1	2.08	0.53
1:C:269:GLU:H	1:C:269:GLU:CD	2.12	0.53
1:D:412:THR:HG21	1:D:414:PHE:CZ	2.42	0.53
1:F:62:THR:HG22	1:F:85:SER:OG	2.08	0.53
1:A:6:THR:HG22	1:A:305:ARG:HD2	1.90	0.53
1:E:379:HIS:HA	1:F:277:ILE:HD13	1.90	0.53
1:B:171:THR:OG1	1:B:176:SER:O	2.24	0.53
1:B:183:GLU:H	1:B:183:GLU:CD	2.12	0.53
1:E:201:LYS:HD2	1:E:203:GLY:N	2.21	0.53
1:F:7:ILE:HG13	1:F:8:PRO:HD2	1.91	0.53
1:C:142:MET:CE	1:C:185:ARG:HD2	2.38	0.53
1:D:294:ARG:HB3	1:D:394:PRO:HA	1.91	0.53
1:B:21:HIS:HD2	1:B:141:GLU:OE2	1.91	0.53
1:A:19:LEU:HD23	1:A:322:MET:HG3	1.90	0.53
1:F:9:GLU:OE2	1:F:330:LYS:NZ	2.33	0.52
1:A:189:CYS:HB2	1:E:164:GLU:CG	2.39	0.52
1:F:152:PRO:HB2	1:F:400:VAL:HG13	1.90	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:VAL:HG21	1:B:149:MET:HG2	1.89	0.52
1:B:366:ASP:OD2	1:B:370:LYS:HB3	2.09	0.52
1:C:151:SER:OG	1:C:153:VAL:HG12	2.09	0.52
1:D:30:PHE:HE1	1:D:268:ILE:HD11	1.74	0.52
1:C:398:PRO:HB3	1:C:414:PHE:CZ	2.43	0.52
1:E:235:LEU:HD12	1:E:235:LEU:H	1.75	0.52
1:D:246:VAL:HG12	1:D:247:ASP:OD1	2.09	0.52
1:E:347:VAL:HG21	1:E:360:PHE:CZ	2.45	0.52
1:A:86:HIS:NE2	1:A:410:ASP:HA	2.25	0.52
1:B:107:ARG:NH2	1:B:134:ILE:H	2.07	0.52
1:E:143:ASP:OD1	1:E:143:ASP:C	2.52	0.52
1:E:410:ASP:OD1	1:E:410:ASP:N	2.43	0.52
1:F:366:ASP:OD1	1:F:369:GLY:N	2.43	0.52
1:D:161:PHE:CD2	1:D:185:ARG:NH2	2.77	0.52
1:F:147:LYS:HB3	1:F:185:ARG:HH22	1.73	0.52
1:E:36:ASN:O	1:E:200:LEU:HD22	2.09	0.52
1:A:199:LEU:HD22	1:A:243:TYR:CE2	2.45	0.51
1:E:145:TYR:OH	1:E:225:MET:SD	2.64	0.51
1:F:403:SER:O	1:F:404:GLU:O	2.27	0.51
1:B:85:SER:O	1:B:86:HIS:HD2	1.93	0.51
1:D:412:THR:HG21	1:D:414:PHE:CE2	2.45	0.51
1:F:402:TYR:CE2	1:F:404:GLU:HB3	2.45	0.51
1:A:341:ASN:C	1:A:341:ASN:OD1	2.53	0.51
1:C:298:PHE:CD2	1:C:364:ILE:HG21	2.44	0.51
1:D:37:GLU:HA	1:D:200:LEU:HD22	1.93	0.51
1:F:389:LYS:HG2	1:F:391:ASN:OD1	2.10	0.51
1:B:37:GLU:HA	1:B:200:LEU:HD22	1.92	0.51
1:D:18:ASP:OD2	1:D:20:SER:OG	2.29	0.51
1:D:137:PRO:HG2	1:D:395:TRP:NE1	2.25	0.51
1:E:9:GLU:HB2	1:E:328:HIS:O	2.11	0.51
1:E:237:ASP:C	1:E:239:THR:H	2.18	0.51
1:F:101:LYS:HB2	1:F:107:ARG:HE	1.74	0.51
1:B:220:LYS:CE	1:B:267:ASN:HD22	2.24	0.51
1:F:298:PHE:CD2	1:F:364:ILE:HG21	2.44	0.51
1:A:110:GLU:HB3	1:A:131:SER:HB3	1.92	0.51
1:A:316:THR:HG22	1:A:323:MET:HB2	1.93	0.51
1:B:267:ASN:O	1:B:268:ILE:CD1	2.55	0.51
1:C:51:HIS:CE1	1:C:311:ARG:HD2	2.46	0.51
1:C:155:ARG:HG3	1:C:156:ASN:N	2.25	0.51
1:C:366:ASP:OD1	1:C:370:LYS:N	2.42	0.51
1:E:336:THR:HA	1:E:339:LEU:O	2.10	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:286:ALA:O	1:E:290:VAL:HG23	2.11	0.51
1:E:317:MET:HE1	1:E:391:ASN:HB3	1.92	0.51
1:A:225:MET:HE2	1:A:227:ILE:CG1	2.41	0.51
1:D:67:MET:HB3	1:D:128:SER:HA	1.93	0.51
1:B:332:VAL:HG11	1:B:338:ILE:HD11	1.91	0.51
1:C:216:PHE:HE1	1:C:218:SER:HB2	1.76	0.51
1:D:65:ILE:O	1:D:85:SER:N	2.44	0.51
1:E:215:LEU:HD23	1:E:216:PHE:O	2.11	0.51
1:A:7:ILE:HG13	1:A:8:PRO:HD2	1.93	0.50
1:C:107:ARG:HD2	1:C:107:ARG:O	2.11	0.50
1:E:135:LEU:HD21	1:E:417:LEU:HD13	1.92	0.50
1:A:6:THR:HG23	1:A:329:TYR:HD1	1.75	0.50
1:B:40:LYS:HG3	1:B:197:GLY:O	2.11	0.50
1:E:87:PHE:O	1:E:175:HIS:HB3	2.11	0.50
1:E:363:ILE:HG12	1:E:373:ILE:HG12	1.93	0.50
1:E:196:THR:HG23	1:E:212:GLU:HG2	1.92	0.50
1:A:173:HIS:HB2	1:A:402:TYR:CD2	2.46	0.50
1:B:43:TYR:CE2	1:B:45:GLU:OE2	2.65	0.50
1:D:215:LEU:CD2	1:D:217:ARG:HE	2.24	0.50
1:F:55:LYS:HZ3	1:F:324:GLU:CD	2.18	0.50
1:A:171:THR:HG22	1:A:172:ASN:H	1.77	0.50
1:A:238:GLY:HA3	1:A:311:ARG:CZ	2.42	0.50
1:B:98:ARG:HA	1:B:134:ILE:HG13	1.94	0.50
1:C:152:PRO:HB2	1:C:400:VAL:HG13	1.94	0.50
1:E:134:ILE:HD12	1:E:134:ILE:N	2.26	0.50
1:D:279:LYS:NZ	1:D:307:GLN:OE1	2.37	0.50
1:E:91:GLN:NE2	1:E:95:ARG:HE	2.09	0.50
1:F:305:ARG:NH1	1:F:375:GLU:OE2	2.45	0.50
1:C:64:ILE:HG22	1:C:86:HIS:HD1	1.77	0.49
1:D:17:ILE:HG22	1:D:55:LYS:HG2	1.93	0.49
1:A:58:GLY:HA2	1:A:181:GLU:HG2	1.93	0.49
1:B:142:MET:HE1	1:B:185:ARG:NE	2.27	0.49
1:C:184:GLY:O	1:C:187:ILE:HG13	2.12	0.49
1:E:317:MET:HE3	1:E:320:ASN:HA	1.94	0.49
1:F:105:ASP:HB3	1:F:106:PRO:HD2	1.94	0.49
1:C:89:PRO:HB2	1:C:94:CYS:SG	2.53	0.49
1:D:65:ILE:CD1	1:D:130:GLU:HG2	2.42	0.49
1:C:174:GLN:HG3	1:C:175:HIS:CE1	2.47	0.49
1:B:168:PHE:CB	1:B:177:ILE:HD11	2.42	0.49
1:E:199:LEU:HD11	1:E:206:VAL:CG1	2.40	0.49
1:E:106:PRO:O	1:E:107:ARG:C	2.55	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:67:MET:O	1:B:68:ALA:HB2	2.11	0.49
1:E:38:GLY:HA3	1:E:199:LEU:O	2.13	0.49
1:C:173:HIS:HB2	1:C:399:LEU:HD22	1.95	0.49
1:F:403:SER:O	1:F:404:GLU:C	2.55	0.49
1:B:151:SER:OG	1:B:153:VAL:HG22	2.13	0.49
1:B:346:MET:HE2	1:B:349:GLY:O	2.13	0.49
1:C:171:THR:C	1:C:173:HIS:H	2.21	0.49
1:D:224:LYS:HZ3	1:D:250:ARG:HB3	1.78	0.49
1:F:105:ASP:HB3	1:F:106:PRO:CD	2.43	0.49
1:B:47:LYS:NZ	1:B:190:ASP:OD1	2.46	0.48
1:B:105:ASP:O	1:B:107:ARG:N	2.38	0.48
1:E:383:ASP:OD1	1:F:284:LEU:HD11	2.13	0.48
1:D:43:TYR:CZ	1:D:195:SER:HB3	2.48	0.48
1:D:294:ARG:HD3	1:D:396:ARG:HH12	1.78	0.48
1:E:54:ASN:HB2	1:E:55:LYS:HD2	1.95	0.48
1:F:17:ILE:HG22	1:F:55:LYS:HG2	1.94	0.48
1:F:265:LEU:HB3	1:F:268:ILE:CD1	2.43	0.48
1:B:332:VAL:HG21	1:B:338:ILE:HD11	1.94	0.48
1:B:375:GLU:OE1	1:B:375:GLU:N	2.38	0.48
1:E:54:ASN:O	1:E:141:GLU:HA	2.14	0.48
1:B:30:PHE:CD2	1:B:220:LYS:HD3	2.49	0.48
1:B:85:SER:O	1:B:86:HIS:CD2	2.66	0.48
1:C:36:ASN:OD1	1:C:36:ASN:O	2.32	0.48
1:F:149:MET:HE3	1:F:159:CYS:SG	2.53	0.48
1:F:240:TRP:CH2	1:F:242:SER:HB3	2.49	0.48
1:A:27:ASN:ND2	1:A:307:GLN:HG3	2.29	0.48
1:C:106:PRO:O	1:C:107:ARG:NH1	2.46	0.48
1:C:234:ARG:HH12	1:C:238:GLY:HA2	1.77	0.48
1:D:107:ARG:O	1:D:107:ARG:HD2	2.13	0.48
1:F:360:PHE:O	1:F:361:ASN:C	2.56	0.48
1:B:51:HIS:CE1	1:B:311:ARG:HD2	2.49	0.48
1:C:211:ASP:CB	1:C:213:ARG:HG2	2.42	0.48
1:E:50:PHE:HA	1:E:53:GLN:HG3	1.96	0.48
1:E:314:VAL:HG22	1:E:329:TYR:OH	2.13	0.48
1:C:103:GLU:OE2	1:C:103:GLU:N	2.47	0.48
1:C:358:VAL:HG12	1:C:359:LEU:O	2.13	0.48
1:D:61:CYS:SG	1:D:132:TRP:HB3	2.54	0.48
1:D:144:ILE:HG13	1:D:145:TYR:CE1	2.49	0.48
1:E:270:GLU:OE1	1:E:274:ARG:HG3	2.13	0.48
1:B:43:TYR:CZ	1:B:195:SER:HB3	2.48	0.48
1:C:50:PHE:CZ	1:C:144:ILE:HD13	2.49	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:340:PRO:HG3	1:C:346:MET:HE3	1.96	0.48
1:F:58:GLY:HA2	1:F:181:GLU:HG2	1.95	0.48
1:F:390:ARG:HD2	1:F:390:ARG:HA	1.43	0.48
1:B:346:MET:HE3	1:B:350:LYS:C	2.39	0.47
1:C:61:CYS:O	1:C:176:SER:HA	2.13	0.47
1:E:149:MET:HE3	1:E:178:TRP:CZ3	2.49	0.47
1:E:225:MET:HG2	1:E:226:ILE:N	2.29	0.47
1:E:359:LEU:HD13	1:E:363:ILE:HG22	1.96	0.47
1:C:155:ARG:HA	1:C:172:ASN:HB3	1.96	0.47
1:C:412:THR:HG22	1:C:413:SER:N	2.29	0.47
1:D:61:CYS:O	1:D:176:SER:HA	2.14	0.47
1:E:152:PRO:HB2	1:E:400:VAL:HG13	1.95	0.47
3:C:501:NAG:O7	3:C:501:NAG:O3	2.23	0.47
1:E:211:ASP:OD2	1:E:215:LEU:HB3	2.15	0.47
1:D:143:ASP:OD2	1:D:146:ASN:HB2	2.14	0.47
1:E:41:VAL:HG21	1:E:199:LEU:HB2	1.96	0.47
1:B:168:PHE:CD2	1:B:177:ILE:CD1	2.98	0.47
1:B:389:LYS:HE3	1:B:391:ASN:OD1	2.15	0.47
1:D:43:TYR:HE2	1:D:45:GLU:HB3	1.80	0.47
1:D:146:ASN:C	1:D:148:THR:H	2.23	0.47
1:D:345:LEU:HD13	1:D:371:ILE:HG21	1.96	0.47
1:A:154:LEU:HD22	1:A:159:CYS:HB2	1.97	0.47
1:C:135:LEU:HD21	1:C:417:LEU:HD13	1.97	0.47
1:C:155:ARG:HB2	1:C:172:ASN:H	1.79	0.47
1:D:366:ASP:OD2	1:D:370:LYS:HB3	2.15	0.47
1:E:51:HIS:CE1	1:E:311:ARG:HD2	2.49	0.47
1:E:155:ARG:HG3	1:E:155:ARG:NH1	2.29	0.47
1:F:339:LEU:HD21	1:F:371:ILE:HB	1.96	0.47
1:F:376:MET:HE3	1:F:377:GLN:NE2	2.29	0.47
1:A:311:ARG:HE	1:A:311:ARG:HB3	1.64	0.47
1:D:21:HIS:HD2	1:D:141:GLU:OE2	1.97	0.47
1:D:161:PHE:CG	1:D:185:ARG:NH2	2.83	0.47
1:E:145:TYR:N	1:E:145:TYR:CD1	2.83	0.47
1:F:273:VAL:O	1:F:277:ILE:HG13	2.15	0.47
1:A:38:GLY:HA3	1:A:199:LEU:O	2.14	0.47
1:B:21:HIS:CD2	1:B:141:GLU:OE2	2.68	0.47
1:F:335:TRP:CE2	1:F:376:MET:HG3	2.50	0.47
1:A:163:PRO:HG3	1:E:158:TYR:HB3	1.97	0.47
1:C:37:GLU:O	1:C:201:LYS:N	2.44	0.47
1:C:336:THR:HA	1:C:339:LEU:O	2.15	0.47
1:D:19:LEU:HD22	1:D:290:VAL:CG1	2.45	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:248:ASN:HB3	1:F:249:LEU:HD22	1.96	0.47
1:A:177:ILE:HD11	1:A:179:ILE:HD11	1.96	0.46
1:A:298:PHE:CD2	1:A:364:ILE:HG21	2.50	0.46
1:B:61:CYS:O	1:B:176:SER:HA	2.15	0.46
1:B:168:PHE:HB2	1:B:177:ILE:HD11	1.97	0.46
1:B:84:ARG:O	1:B:411:LEU:HD13	2.15	0.46
1:F:27:ASN:ND2	1:F:307:GLN:HG3	2.30	0.46
1:B:155:ARG:HD3	1:B:156:ASN:OD1	2.14	0.46
1:D:101:LYS:HB2	1:D:107:ARG:HG2	1.96	0.46
1:E:87:PHE:C	1:E:175:HIS:HB3	2.39	0.46
1:A:106:PRO:HB2	1:A:110:GLU:OE1	2.16	0.46
1:C:216:PHE:CD1	1:C:216:PHE:C	2.94	0.46
1:F:65:ILE:O	1:F:86:HIS:CE1	2.69	0.46
1:F:318:ILE:HD12	1:F:323:MET:HE2	1.98	0.46
1:F:64:ILE:HB	1:F:131:SER:OG	2.15	0.46
1:B:46:LEU:HD13	1:B:50:PHE:CE2	2.51	0.46
1:B:88:ILE:HG13	1:B:174:GLN:O	2.16	0.46
1:E:208:GLY:HA2	1:E:219:ILE:HB	1.98	0.46
1:C:25:PRO:O	1:C:280:ARG:NH1	2.49	0.46
1:C:211:ASP:CG	1:C:215:LEU:HB3	2.40	0.46
1:D:109:GLU:OE2	1:D:112:LEU:HD21	2.16	0.46
1:D:416:GLN:O	1:D:417:LEU:C	2.59	0.46
1:F:171:THR:OG1	1:F:176:SER:O	2.29	0.46
1:A:47:LYS:HE3	1:A:192:PHE:O	2.16	0.45
1:C:234:ARG:NH1	1:C:238:GLY:CA	2.80	0.45
1:C:413:SER:C	1:C:415:ALA:H	2.24	0.45
1:D:107:ARG:HH12	1:D:134:ILE:CG1	2.28	0.45
1:E:64:ILE:HA	1:E:86:HIS:HB3	1.98	0.45
1:F:19:LEU:HD23	1:F:19:LEU:HA	1.47	0.45
1:A:335:TRP:CD1	1:A:376:MET:HG3	2.51	0.45
1:B:145:TYR:N	1:B:145:TYR:CD1	2.83	0.45
1:C:216:PHE:CE1	1:C:218:SER:HB2	2.52	0.45
1:A:17:ILE:HG21	1:A:324:GLU:OE1	2.16	0.45
1:A:46:LEU:HD13	1:A:50:PHE:CD2	2.52	0.45
1:B:381:LEU:HD23	1:B:381:LEU:HA	1.86	0.45
1:C:12:GLY:HA3	1:C:48:PRO:HB2	1.98	0.45
1:C:59:PHE:CG	1:C:98:ARG:HG3	2.52	0.45
1:A:414:PHE:H	1:A:414:PHE:HD1	1.64	0.45
1:D:250:ARG:HD3	1:D:250:ARG:C	2.41	0.45
1:E:43:TYR:CD2	1:E:209:PHE:HE2	2.35	0.45
1:A:273:VAL:O	1:A:277:ILE:HG13	2.16	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:264:LYS:O	1:B:265:LEU:HD23	2.17	0.45
1:B:266:ASP:O	1:B:268:ILE:N	2.48	0.45
1:B:414:PHE:C	1:B:414:PHE:HD1	2.24	0.45
1:D:217:ARG:NH1	1:D:239:THR:OG1	2.50	0.45
1:E:217:ARG:HD3	1:E:239:THR:HG21	1.99	0.45
1:C:43:TYR:CD2	1:C:241:VAL:HB	2.52	0.45
1:C:264:LYS:HD3	1:C:264:LYS:C	2.41	0.45
1:D:137:PRO:HD2	1:D:395:TRP:CE2	2.51	0.45
1:A:147:LYS:HE2	1:A:187:ILE:HD13	1.98	0.45
1:B:19:LEU:HD22	1:B:290:VAL:CG1	2.47	0.45
1:C:21:HIS:CE1	1:C:139:VAL:HG12	2.52	0.45
1:C:264:LYS:HD3	1:C:264:LYS:O	2.16	0.45
1:D:154:LEU:HD13	1:D:159:CYS:HB3	1.98	0.45
1:E:306:LYS:HE2	1:E:310:GLY:HA3	1.99	0.45
1:F:318:ILE:HG21	3:F:501:NAG:H82	1.99	0.45
1:C:279:LYS:HA	1:C:279:LYS:HD3	1.73	0.44
1:C:389:LYS:O	1:C:389:LYS:HG3	2.16	0.44
1:A:142:MET:HB2	1:A:149:MET:HG3	1.99	0.44
1:F:365:ARG:CG	1:F:369:GLY:HA2	2.39	0.44
1:B:270:GLU:OE2	1:B:274:ARG:NE	2.50	0.44
1:C:44:LEU:HD12	1:C:242:SER:HB3	1.98	0.44
1:A:105:ASP:CG	1:A:106:PRO:HD2	2.43	0.44
1:B:6:THR:CG2	1:B:305:ARG:HE	2.31	0.44
1:F:264:LYS:NZ	1:F:266:ASP:HB2	2.31	0.44
1:B:66:ASN:CG	1:B:67:MET:H	2.25	0.44
1:B:142:MET:CE	1:B:149:MET:SD	3.06	0.44
1:A:86:HIS:CD2	1:A:411:LEU:H	2.35	0.44
1:B:413:SER:C	1:B:415:ALA:H	2.26	0.44
1:C:322:MET:HE2	1:C:322:MET:HA	2.00	0.44
1:E:176:SER:CB	1:E:399:LEU:HD21	2.48	0.44
1:A:335:TRP:CD2	1:A:376:MET:HG3	2.51	0.44
1:D:143:ASP:HB3	1:D:146:ASN:O	2.17	0.44
1:B:335:TRP:CE2	1:B:376:MET:HG3	2.53	0.44
1:B:380:LEU:HB3	1:B:382:ARG:HG3	2.00	0.44
1:D:149:MET:HE1	1:D:185:ARG:HH21	1.83	0.44
1:D:224:LYS:HZ2	1:D:250:ARG:HB3	1.81	0.44
1:D:339:LEU:HD11	1:D:373:ILE:HD12	2.00	0.44
1:D:392:SER:C	1:D:394:PRO:HD3	2.43	0.44
1:E:339:LEU:C	1:E:341:ASN:H	2.26	0.44
1:F:66:ASN:CA	1:F:86:HIS:CE1	3.00	0.44
1:F:161:PHE:HE2	1:F:185:ARG:HD2	1.83	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:361:ASN:C	1:F:363:ILE:H	2.26	0.44
1:C:171:THR:O	1:C:173:HIS:N	2.51	0.44
1:E:86:HIS:CE1	1:E:411:LEU:HA	2.53	0.44
1:A:173:HIS:CE1	1:A:175:HIS:HB2	2.53	0.43
1:B:65:ILE:O	1:B:84:ARG:HA	2.18	0.43
1:E:19:LEU:HD23	1:E:322:MET:HG3	2.00	0.43
1:E:86:HIS:HD2	1:E:175:HIS:CE1	2.36	0.43
1:E:145:TYR:N	1:E:145:TYR:HD1	2.16	0.43
1:A:211:ASP:OD1	1:A:215:LEU:O	2.36	0.43
1:C:107:ARG:HG3	1:C:107:ARG:HH11	1.84	0.43
1:D:62:THR:OG1	1:D:176:SER:OG	2.24	0.43
1:D:143:ASP:O	1:D:146:ASN:O	2.36	0.43
1:E:224:LYS:HG2	1:E:250:ARG:NH2	2.33	0.43
1:F:47:LYS:HE3	1:F:192:PHE:O	2.18	0.43
1:F:96:GLN:NE2	1:F:100:TRP:HE1	2.15	0.43
1:B:192:PHE:O	1:B:193:GLN:HB3	2.18	0.43
1:C:40:LYS:HE3	1:C:40:LYS:HB2	1.66	0.43
1:E:98:ARG:NH1	1:E:102:LYS:HG3	2.33	0.43
1:A:217:ARG:HH11	1:A:237:ASP:HB3	1.82	0.43
1:C:59:PHE:CD2	1:C:98:ARG:HG3	2.53	0.43
1:C:201:LYS:HD2	1:C:202:ASN:HA	2.00	0.43
1:E:86:HIS:HE1	1:E:411:LEU:C	2.26	0.43
1:E:159:CYS:SG	1:E:160:ASN:N	2.91	0.43
1:B:66:ASN:ND2	1:B:67:MET:H	2.16	0.43
1:B:216:PHE:CD1	1:B:216:PHE:C	2.96	0.43
1:C:269:GLU:O	1:C:273:VAL:HG12	2.18	0.43
1:D:393:ILE:HG22	1:D:393:ILE:O	2.18	0.43
1:E:412:THR:CG2	1:E:413:SER:N	2.82	0.43
1:A:7:ILE:O	1:A:329:TYR:HA	2.19	0.43
1:A:411:LEU:HG	1:A:412:THR:H	1.84	0.43
1:C:213:ARG:HG3	1:C:215:LEU:HB2	2.00	0.43
1:D:265:LEU:O	1:D:266:ASP:OD1	2.36	0.43
1:D:385:LEU:HD12	1:D:385:LEU:HA	1.83	0.43
1:E:51:HIS:NE2	1:E:311:ARG:HD2	2.34	0.43
1:F:46:LEU:HD13	1:F:50:PHE:CD2	2.53	0.43
1:F:359:LEU:N	1:F:359:LEU:HD12	2.33	0.43
1:F:416:GLN:O	1:F:416:GLN:HG2	2.15	0.43
1:B:149:MET:HE2	1:B:149:MET:HB2	1.82	0.43
1:B:195:SER:OG	1:B:212:GLU:OE1	2.30	0.43
1:C:173:HIS:HB3	1:C:176:SER:HB2	1.99	0.43
1:E:413:SER:O	1:E:414:PHE:C	2.62	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:264:LYS:O	1:F:264:LYS:HD2	2.11	0.43
1:E:416:GLN:H	1:E:416:GLN:HG2	1.58	0.43
1:F:263:VAL:HB	1:F:265:LEU:HD11	2.01	0.43
1:B:154:LEU:HD13	1:B:159:CYS:HB3	2.01	0.43
1:C:108:TYR:CD1	1:C:108:TYR:C	2.97	0.43
1:E:218:SER:CB	1:E:220:LYS:HG3	2.42	0.43
1:E:379:HIS:HA	1:F:277:ILE:CD1	2.48	0.43
1:C:142:MET:HE2	1:C:149:MET:SD	2.59	0.43
1:C:159:CYS:SG	1:C:160:ASN:N	2.91	0.43
1:D:129:LYS:C	1:D:130:GLU:HG3	2.42	0.43
1:E:39:SER:O	1:E:41:VAL:HG23	2.19	0.43
1:A:151:SER:OG	1:A:153:VAL:HG22	2.19	0.42
1:C:51:HIS:NE2	1:C:311:ARG:HD2	2.34	0.42
1:C:108:TYR:C	1:C:108:TYR:HD1	2.27	0.42
1:C:144:ILE:O	1:C:147:LYS:NZ	2.47	0.42
1:C:223:CYS:SG	1:C:224:LYS:N	2.92	0.42
1:F:155:ARG:HA	1:F:172:ASN:OD1	2.18	0.42
1:B:44:LEU:N	1:B:242:SER:OG	2.33	0.42
1:D:6:THR:HG1	1:D:329:TYR:HD2	1.65	0.42
1:D:59:PHE:CD2	1:D:98:ARG:HG3	2.53	0.42
1:D:137:PRO:HD2	1:D:395:TRP:NE1	2.34	0.42
1:E:43:TYR:CD1	1:E:43:TYR:C	2.97	0.42
1:E:167:ASP:OD1	1:E:167:ASP:N	2.52	0.42
1:B:175:HIS:ND1	1:B:175:HIS:N	2.67	0.42
1:C:286:ALA:O	1:C:290:VAL:HG23	2.19	0.42
1:D:45:GLU:OE2	1:D:213:ARG:NH1	2.49	0.42
1:F:16:PRO:HG2	1:F:57:GLN:NE2	2.34	0.42
1:F:210:GLN:HA	1:F:215:LEU:O	2.19	0.42
1:D:40:LYS:HE3	1:D:40:LYS:HB2	1.87	0.42
1:D:147:LYS:HA	1:D:147:LYS:HD3	1.79	0.42
1:D:149:MET:HE1	1:D:185:ARG:NH2	2.34	0.42
1:D:399:LEU:HD21	1:D:414:PHE:CE2	2.54	0.42
1:F:38:GLY:HA3	1:F:199:LEU:O	2.19	0.42
1:F:227:ILE:O	1:F:228:CYS:C	2.62	0.42
1:F:341:ASN:OD1	1:F:343:ILE:HG13	2.19	0.42
1:B:60:THR:HG21	1:B:397:HIS:CE1	2.51	0.42
1:B:107:ARG:O	1:B:110:GLU:HB3	2.19	0.42
1:C:88:ILE:HD12	1:C:88:ILE:H	1.83	0.42
1:C:135:LEU:HD13	1:C:398:PRO:HG2	2.01	0.42
1:B:59:PHE:CD2	1:B:98:ARG:HG3	2.55	0.42
1:C:21:HIS:O	1:C:23:LYS:HG2	2.19	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:215:LEU:HD21	1:C:309:PRO:CB	2.44	0.42
1:D:89:PRO:HB2	1:D:94:CYS:SG	2.60	0.42
1:F:58:GLY:CA	1:F:181:GLU:HG2	2.50	0.42
1:C:232:GLY:HA3	1:C:240:TRP:NE1	2.34	0.42
1:F:361:ASN:O	1:F:363:ILE:N	2.52	0.42
1:A:300:LYS:HA	1:A:300:LYS:HD3	1.72	0.42
1:A:370:LYS:HE3	1:A:382:ARG:NH1	2.34	0.42
1:B:211:ASP:CB	1:B:213:ARG:H	2.33	0.42
1:C:234:ARG:HH12	1:C:238:GLY:N	2.17	0.42
1:C:412:THR:CG2	1:C:413:SER:N	2.82	0.42
1:E:397:HIS:CE1	1:E:399:LEU:HB2	2.55	0.42
1:A:370:LYS:HE3	1:A:382:ARG:HH22	1.85	0.42
1:B:299:ARG:NH1	1:C:285:ASP:OD1	2.45	0.42
1:C:198:ILE:HG13	1:C:210:GLN:HB3	2.02	0.42
1:F:65:ILE:O	1:F:86:HIS:NE2	2.53	0.42
1:A:2:PHE:CG	1:A:279:LYS:NZ	2.87	0.41
1:A:224:LYS:HE2	1:A:248:ASN:CB	2.49	0.41
1:B:347:VAL:HG11	1:B:352:HIS:CD2	2.55	0.41
1:D:211:ASP:HB3	1:D:213:ARG:H	1.85	0.41
1:E:89:PRO:HB2	1:E:94:CYS:SG	2.60	0.41
1:A:399:LEU:HD23	1:A:399:LEU:HA	1.74	0.41
1:C:26:ASP:OD1	1:C:28:THR:OG1	2.37	0.41
1:C:234:ARG:HH12	1:C:238:GLY:CA	2.32	0.41
1:E:87:PHE:HZ	1:E:132:TRP:HE1	1.67	0.41
1:C:100:TRP:CE3	1:C:106:PRO:HG3	2.55	0.41
1:C:167:ASP:OD1	1:C:167:ASP:N	2.53	0.41
1:D:226:ILE:HA	1:D:230:LYS:O	2.20	0.41
1:E:142:MET:HA	1:E:148:THR:O	2.20	0.41
1:E:365:ARG:NH2	1:E:371:ILE:HD11	2.35	0.41
1:F:41:VAL:HG21	1:F:199:LEU:HB2	2.00	0.41
1:B:345:LEU:HD13	1:B:371:ILE:HG21	2.02	0.41
1:F:306:LYS:HE3	1:F:308:VAL:HG23	2.03	0.41
1:A:270:GLU:O	1:A:271:SER:C	2.63	0.41
1:A:359:LEU:N	1:A:359:LEU:HD12	2.34	0.41
1:B:350:LYS:HA	1:B:350:LYS:HD2	1.76	0.41
1:E:61:CYS:HA	1:E:133:LEU:O	2.21	0.41
1:F:311:ARG:HE	1:F:311:ARG:HB3	1.66	0.41
1:B:7:ILE:HG13	1:B:8:PRO:CD	2.51	0.41
1:B:167:ASP:OD1	1:B:167:ASP:N	2.52	0.41
1:B:168:PHE:CD2	1:B:177:ILE:HD11	2.56	0.41
1:B:211:ASP:CG	1:B:215:LEU:HG	2.46	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:PRO:HG2	1:C:177:ILE:HG12	2.02	0.41
1:A:277:ILE:CD1	1:C:379:HIS:HA	2.49	0.41
1:A:412:THR:HG23	1:A:415:ALA:HB2	2.02	0.41
1:C:299:ARG:HD3	1:C:388:LEU:HD23	2.02	0.41
1:D:21:HIS:CD2	1:D:141:GLU:OE2	2.73	0.41
1:D:43:TYR:CE2	1:D:45:GLU:HB3	2.55	0.41
1:B:91:GLN:HG2	1:B:179:ILE:HD13	2.02	0.41
1:B:151:SER:HB3	1:B:154:LEU:HG	2.03	0.41
1:D:200:LEU:HD11	1:D:210:GLN:HE21	1.85	0.41
1:F:287:LEU:O	1:F:291:MET:HG3	2.21	0.41
1:A:246:VAL:O	1:A:247:ASP:HB2	2.21	0.41
1:A:251:MET:HE3	1:A:251:MET:HB3	1.79	0.41
1:B:135:LEU:HB2	1:B:397:HIS:HE2	1.86	0.41
1:B:242:SER:O	1:B:243:TYR:HB2	2.21	0.41
1:C:35:CYS:O	1:C:200:LEU:HD13	2.21	0.41
1:C:142:MET:SD	1:C:147:LYS:HD2	2.60	0.41
1:D:173:HIS:CD2	1:D:175:HIS:H	2.38	0.41
1:E:218:SER:O	1:E:235:LEU:HD23	2.20	0.41
1:C:388:LEU:HD23	1:C:388:LEU:HA	1.78	0.41
1:D:141:GLU:HB2	1:D:150:PHE:HB2	2.03	0.41
1:D:338:ILE:HD13	1:D:338:ILE:HG21	1.84	0.41
1:F:46:LEU:HD13	1:F:50:PHE:CE2	2.56	0.41
1:F:344:CYS:SG	1:F:346:MET:HE2	2.61	0.41
1:A:106:PRO:O	1:A:107:ARG:C	2.65	0.40
1:C:143:ASP:O	1:C:147:LYS:HA	2.20	0.40
1:D:66:ASN:ND2	1:D:411:LEU:HD23	2.36	0.40
1:E:93:ASP:HB3	1:E:132:TRP:CH2	2.57	0.40
1:E:334:ASN:OD1	1:E:336:THR:N	2.52	0.40
1:B:40:LYS:HA	1:B:198:ILE:HA	2.03	0.40
1:B:279:LYS:NZ	1:B:307:GLN:OE1	2.43	0.40
1:F:317:MET:HE3	1:F:320:ASN:HA	2.03	0.40
1:B:43:TYR:CE2	1:B:195:SER:HB3	2.56	0.40
1:C:11:LEU:HD12	1:C:326:THR:O	2.21	0.40
1:C:19:LEU:HD23	1:C:19:LEU:HA	1.78	0.40
1:D:35:CYS:O	1:D:200:LEU:HD13	2.22	0.40
1:D:269:GLU:O	1:D:273:VAL:HG23	2.21	0.40
1:D:314:VAL:HG22	1:D:329:TYR:OH	2.21	0.40
1:B:86:HIS:HB3	1:B:175:HIS:CD2	2.57	0.40
1:B:212:GLU:O	1:B:212:GLU:HG2	2.22	0.40
1:B:251:MET:H	1:B:251:MET:HG2	1.77	0.40
1:C:201:LYS:HD2	1:C:201:LYS:C	2.46	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:62:THR:HG23	1:F:176:SER:OG	2.21	0.40
1:F:246:VAL:C	1:F:248:ASN:H	2.29	0.40
1:A:51:HIS:O	1:A:313:TYR:OH	2.37	0.40
1:A:137:PRO:HD2	1:A:395:TRP:CD1	2.57	0.40
1:B:68:ALA:O	1:B:69:THR:CB	2.70	0.40
1:C:201:LYS:HG2	1:C:203:GLY:N	2.28	0.40
1:D:240:TRP:CH2	1:D:242:SER:HB3	2.57	0.40
1:E:45:GLU:CD	1:E:213:ARG:HH22	2.29	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:341:ASN:ND2	1:B:85:SER:OG[2_454]	2.07	0.13
1:D:130:GLU:OE1	1:F:351:CYS:N[2_555]	2.18	0.02

5.3 Torsion angles

5.3.1 Protein backbone

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	361/440 (82%)	333 (92%)	24 (7%)	4 (1%)	11	33
1	B	355/440 (81%)	329 (93%)	23 (6%)	3 (1%)	16	41
1	C	346/440 (79%)	318 (92%)	25 (7%)	3 (1%)	14	38
1	D	358/440 (81%)	323 (90%)	31 (9%)	4 (1%)	11	33
1	E	352/440 (80%)	325 (92%)	24 (7%)	3 (1%)	14	38
1	F	367/440 (83%)	331 (90%)	32 (9%)	4 (1%)	11	33
All	All	2139/2640 (81%)	1959 (92%)	159 (7%)	21 (1%)	12	35

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	68	ALA
1	C	172	ASN
1	D	105	ASP
1	E	106	PRO
1	F	105	ASP
1	F	247	ASP
1	A	108	TYR
1	A	389	LYS
1	C	174	GLN
1	A	65	ILE
1	A	105	ASP
1	B	106	PRO
1	D	395	TRP
1	E	36	ASN
1	F	254	ARG
1	F	362	GLY
1	C	105	ASP
1	D	246	VAL
1	B	66	ASN
1	E	395	TRP
1	D	417	LEU

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	336/393 (86%)	315 (94%)	21 (6%)	16	42
1	B	335/393 (85%)	320 (96%)	15 (4%)	24	55
1	C	320/393 (81%)	298 (93%)	22 (7%)	14	38
1	D	336/393 (86%)	318 (95%)	18 (5%)	20	49
1	E	327/393 (83%)	313 (96%)	14 (4%)	26	57
1	F	339/393 (86%)	317 (94%)	22 (6%)	15	41
All	All	1993/2358 (84%)	1881 (94%)	112 (6%)	19	47

All (112) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	32	GLU
1	A	39	SER
1	A	52	SER
1	A	66	ASN
1	A	87	PHE
1	A	90	ASN
1	A	103	GLU
1	A	105	ASP
1	A	110	GLU
1	A	153	VAL
1	A	215	LEU
1	A	218	SER
1	A	237	ASP
1	A	270	GLU
1	A	331	SER
1	A	341	ASN
1	A	347	VAL
1	A	350	LYS
1	A	416	GLN
1	A	417	LEU
1	B	6	THR
1	B	15	THR
1	B	20	SER
1	B	35	CYS
1	B	49	SER
1	B	67	MET
1	B	93	ASP
1	B	182	ASP
1	B	195	SER
1	B	199	LEU
1	B	215	LEU
1	B	252	CYS
1	B	266	ASP
1	B	289	GLU
1	B	307	GLN
1	C	39	SER
1	C	40	LYS
1	C	93	ASP
1	C	105	ASP
1	C	108	TYR
1	C	134	ILE
1	C	153	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	159	CYS
1	C	189	CYS
1	C	201	LYS
1	C	215	LEU
1	C	223	CYS
1	C	227	ILE
1	C	237	ASP
1	C	246	VAL
1	C	263	VAL
1	C	270	GLU
1	C	278	LYS
1	C	311	ARG
1	C	316	THR
1	C	389	LYS
1	C	403	SER
1	D	20	SER
1	D	36	ASN
1	D	126	THR
1	D	155	ARG
1	D	196	THR
1	D	250	ARG
1	D	262	THR
1	D	265	LEU
1	D	266	ASP
1	D	269	GLU
1	D	275	ASP
1	D	289	GLU
1	D	324	GLU
1	D	367	SER
1	D	372	LEU
1	D	380	LEU
1	D	385	LEU
1	D	411	LEU
1	E	28	THR
1	E	85	SER
1	E	86	HIS
1	E	105	ASP
1	E	108	TYR
1	E	144	ILE
1	E	196	THR
1	E	224	LYS
1	E	252	CYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	263	VAL
1	E	289	GLU
1	E	316	THR
1	E	412	THR
1	E	413	SER
1	F	39	SER
1	F	52	SER
1	F	85	SER
1	F	87	PHE
1	F	105	ASP
1	F	107	ARG
1	F	153	VAL
1	F	204	SER
1	F	211	ASP
1	F	223	CYS
1	F	245	SER
1	F	252	CYS
1	F	265	LEU
1	F	305	ARG
1	F	331	SER
1	F	341	ASN
1	F	370	LYS
1	F	385	LEU
1	F	390	ARG
1	F	404	GLU
1	F	411	LEU
1	F	416	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	352	HIS
1	A	377	GLN
1	B	174	GLN
1	B	175	HIS
1	B	193	GLN
1	B	267	ASN
1	B	320	ASN
1	B	377	GLN
1	C	173	HIS
1	C	175	HIS
1	C	307	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	53	GLN
1	D	328	HIS
1	E	86	HIS
1	E	91	GLN
1	F	53	GLN
1	F	96	GLN
1	F	267	ASN
1	F	352	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

6 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	G	1	2,1	14,14,15	0.95	1 (7%)	17,19,21	0.87	0
2	NAG	G	2	2	14,14,15	0.39	0	17,19,21	0.86	1 (5%)
2	NAG	H	1	2,1	14,14,15	0.58	0	17,19,21	0.80	1 (5%)
2	NAG	H	2	2	14,14,15	0.74	1 (7%)	17,19,21	0.64	0
2	NAG	I	1	2,1	14,14,15	0.92	1 (7%)	17,19,21	0.77	0
2	NAG	I	2	2	14,14,15	0.89	1 (7%)	17,19,21	0.73	1 (5%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the

Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns.
'-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	G	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	G	2	2	-	2/6/23/26	0/1/1/1
2	NAG	H	1	2,1	-	0/6/23/26	0/1/1/1
2	NAG	H	2	2	-	1/6/23/26	0/1/1/1
2	NAG	I	1	2,1	-	2/6/23/26	0/1/1/1
2	NAG	I	2	2	-	2/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	1	NAG	O5-C1	-3.28	1.38	1.43
2	G	1	NAG	O5-C1	-3.22	1.38	1.43
2	I	2	NAG	O5-C1	-3.14	1.38	1.43
2	H	2	NAG	C1-C2	2.55	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	2	NAG	C1-O5-C5	2.23	115.17	112.19
2	I	2	NAG	C1-O5-C5	2.23	115.17	112.19
2	H	1	NAG	C1-O5-C5	2.21	115.15	112.19

There are no chirality outliers.

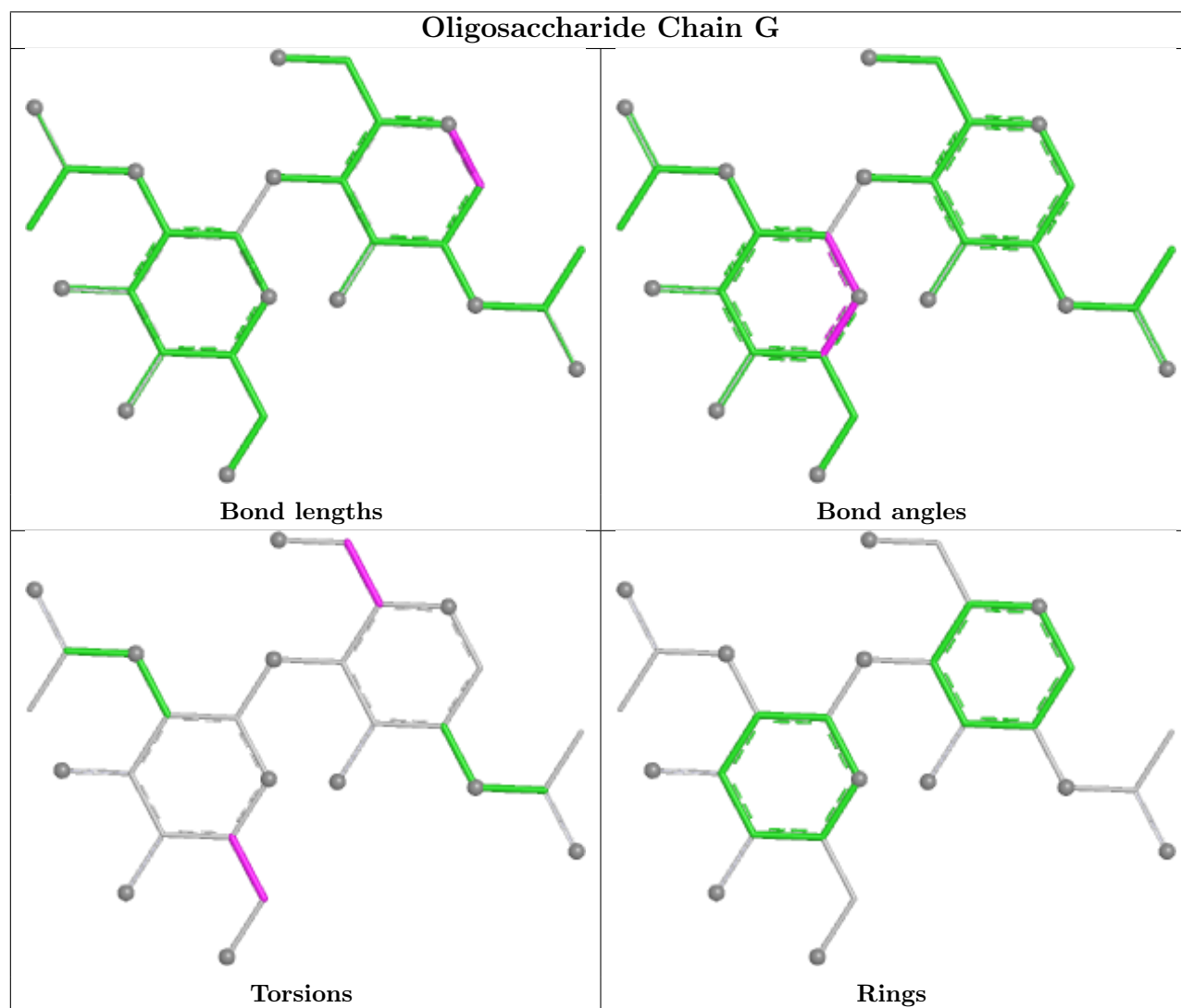
All (9) torsion outliers are listed below:

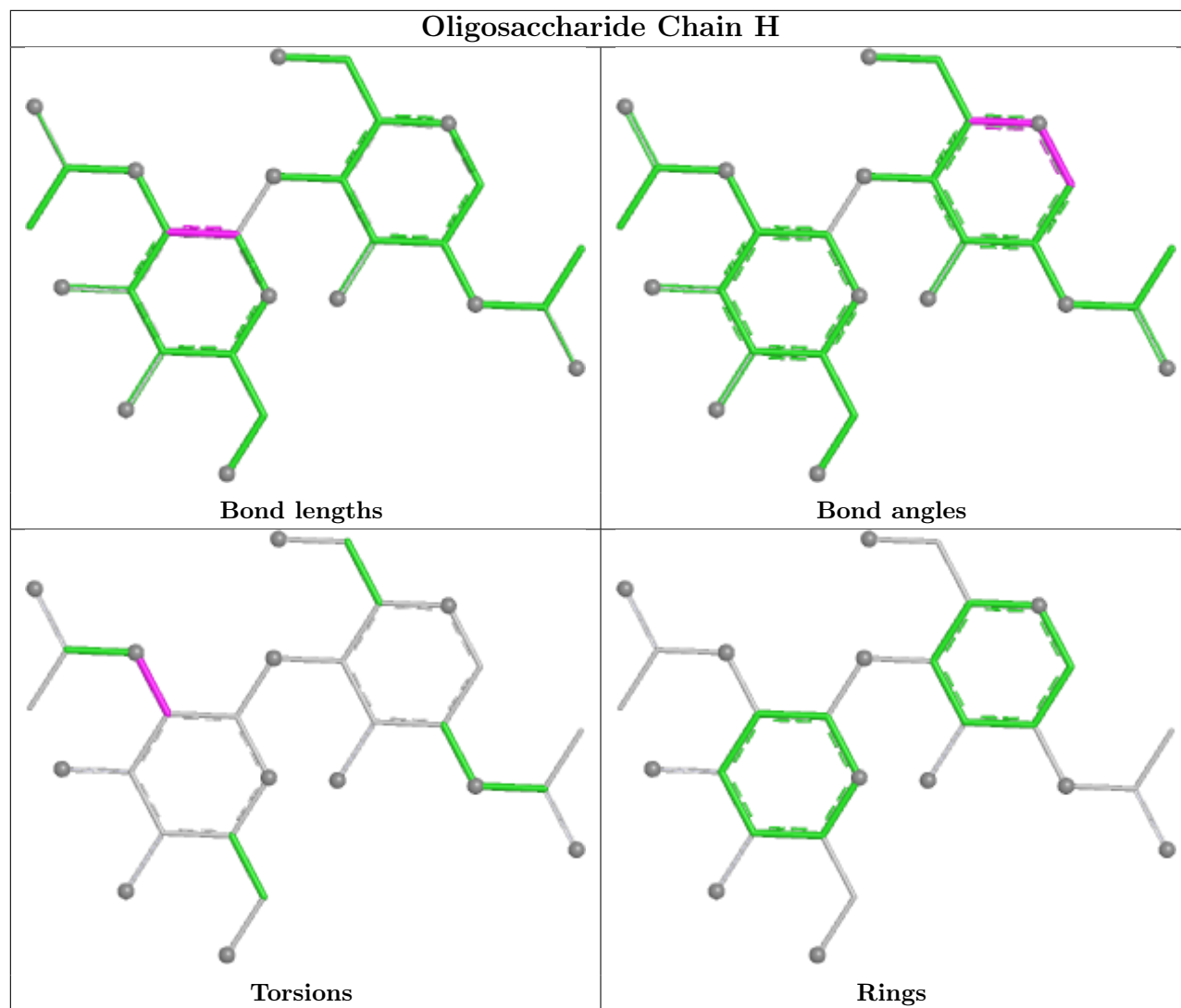
Mol	Chain	Res	Type	Atoms
2	I	2	NAG	O5-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	H	2	NAG	C3-C2-N2-C7

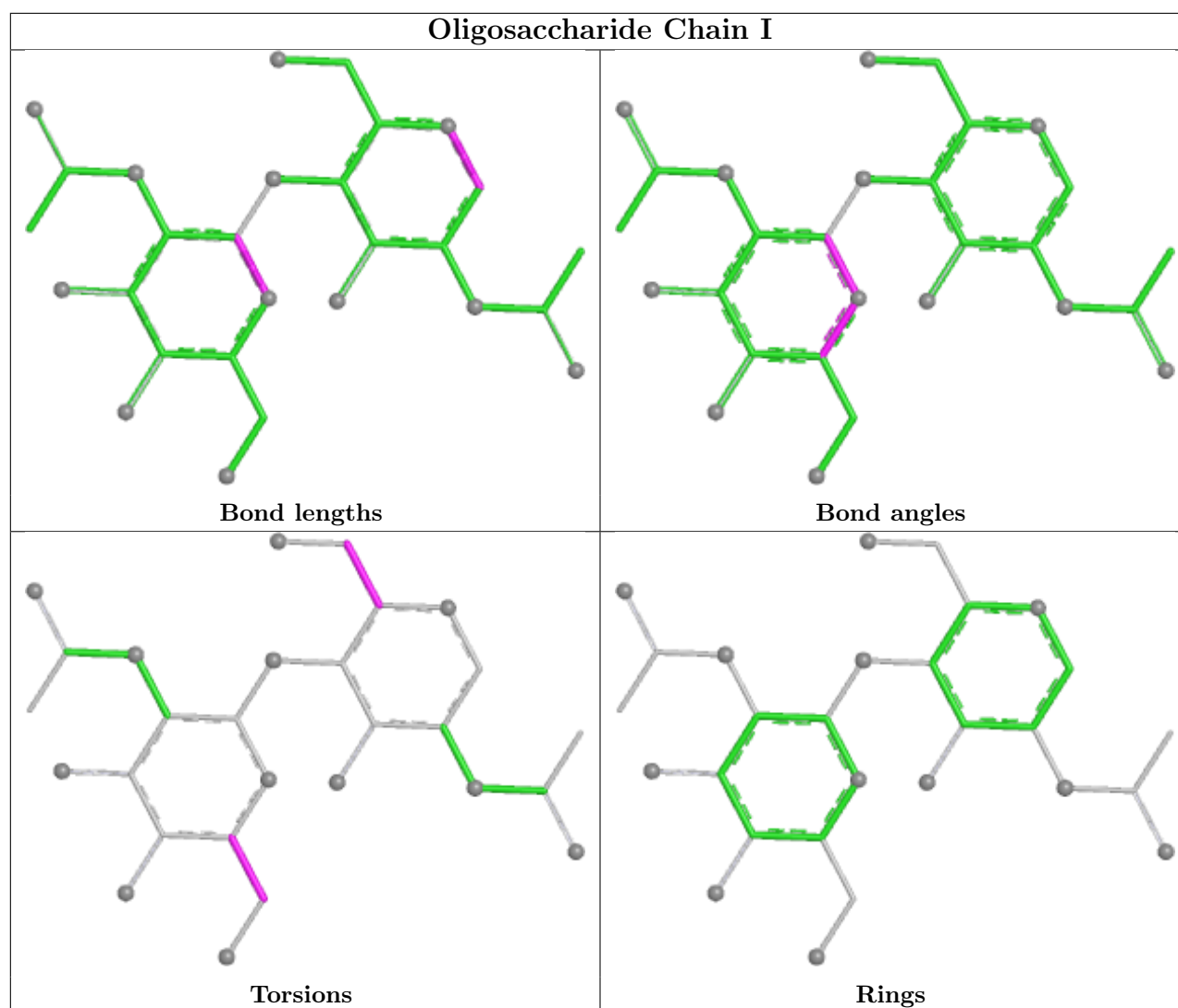
There are no ring outliers.

No monomer is involved in short contacts.

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](#)

7 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	F	501	1	14,14,15	0.82	1 (7%)	17,19,21	0.86	1 (5%)
3	NAG	B	501	1	14,14,15	0.49	0	17,19,21	1.15	1 (5%)
3	NAG	A	501	1	14,14,15	0.93	1 (7%)	17,19,21	1.15	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	D	501	1	14,14,15	0.65	0	17,19,21	0.65	0
3	NAG	B	502	-	14,14,15	0.59	0	17,19,21	0.49	0
3	NAG	C	501	1	14,14,15	1.04	2 (14%)	17,19,21	1.14	1 (5%)
3	NAG	E	501	1	14,14,15	1.41	2 (14%)	17,19,21	0.88	1 (5%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	F	501	1	-	2/6/23/26	0/1/1/1
3	NAG	B	501	1	-	1/6/23/26	0/1/1/1
3	NAG	A	501	1	-	0/6/23/26	0/1/1/1
3	NAG	D	501	1	-	2/6/23/26	0/1/1/1
3	NAG	B	502	-	-	1/6/23/26	0/1/1/1
3	NAG	C	501	1	-	2/6/23/26	0/1/1/1
3	NAG	E	501	1	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	501	NAG	O5-C1	4.63	1.51	1.43
3	F	501	NAG	O5-C1	2.82	1.48	1.43
3	A	501	NAG	O5-C1	2.81	1.48	1.43
3	C	501	NAG	C1-C2	2.75	1.56	1.52
3	C	501	NAG	O5-C1	2.33	1.47	1.43
3	E	501	NAG	C1-C2	2.22	1.55	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	NAG	C1-O5-C5	4.25	117.88	112.19
3	C	501	NAG	C1-O5-C5	3.78	117.25	112.19
3	B	501	NAG	C1-O5-C5	3.75	117.21	112.19
3	F	501	NAG	C1-O5-C5	2.82	115.97	112.19
3	E	501	NAG	C1-O5-C5	2.74	115.86	112.19

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	F	501	NAG	O5-C5-C6-O6
3	D	501	NAG	O5-C5-C6-O6
3	E	501	NAG	O5-C5-C6-O6
3	F	501	NAG	C4-C5-C6-O6
3	D	501	NAG	C4-C5-C6-O6
3	E	501	NAG	C4-C5-C6-O6
3	C	501	NAG	C3-C2-N2-C7
3	B	501	NAG	O5-C5-C6-O6
3	B	502	NAG	C1-C2-N2-C7
3	C	501	NAG	C1-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	501	NAG	1	0
3	C	501	NAG	1	0
3	E	501	NAG	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	371/440 (84%)	-1.26	0 100 100	41, 61, 106, 127	0
1	B	369/440 (83%)	-1.21	0 100 100	38, 65, 118, 144	0
1	C	357/440 (81%)	-1.22	1 (0%) 90 87	40, 66, 111, 130	0
1	D	370/440 (84%)	-1.20	1 (0%) 90 87	38, 65, 122, 144	0
1	E	362/440 (82%)	-1.23	0 100 100	39, 67, 118, 154	0
1	F	375/440 (85%)	-1.29	1 (0%) 90 87	40, 62, 106, 132	0
All	All	2204/2640 (83%)	-1.23	3 (0%) 92 90	38, 64, 116, 154	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	261	HIS	2.5
1	F	266	ASP	2.2
1	C	246	VAL	2.2

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.

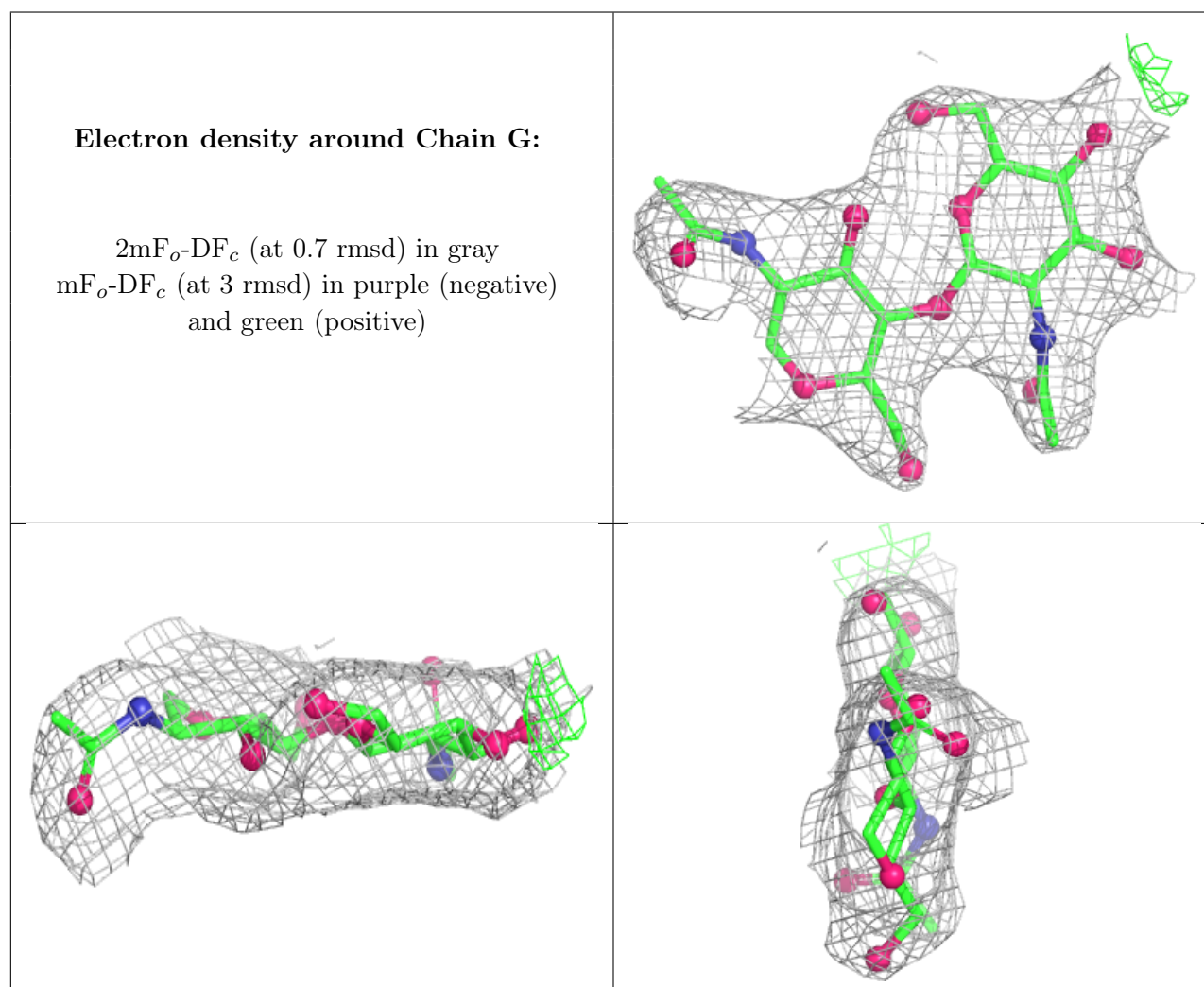
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	NAG	H	2	14/15	0.98	0.05	93,100,108,109	0

Continued on next page...

Continued from previous page...

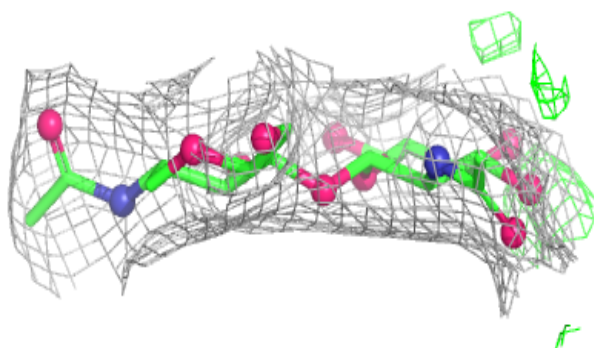
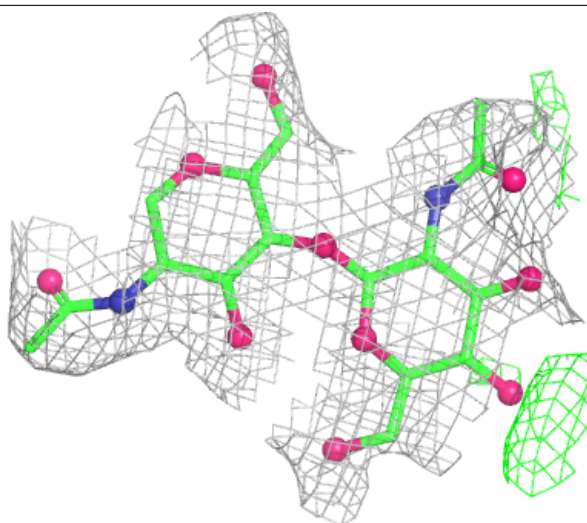
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	I	2	14/15	0.98	0.05	54,58,67,71	0
2	NAG	H	1	14/15	0.99	0.04	87,97,100,101	0
2	NAG	G	1	14/15	0.99	0.03	52,58,65,72	0
2	NAG	I	1	14/15	0.99	0.03	55,61,66,74	0
2	NAG	G	2	14/15	0.99	0.04	53,57,67,71	0

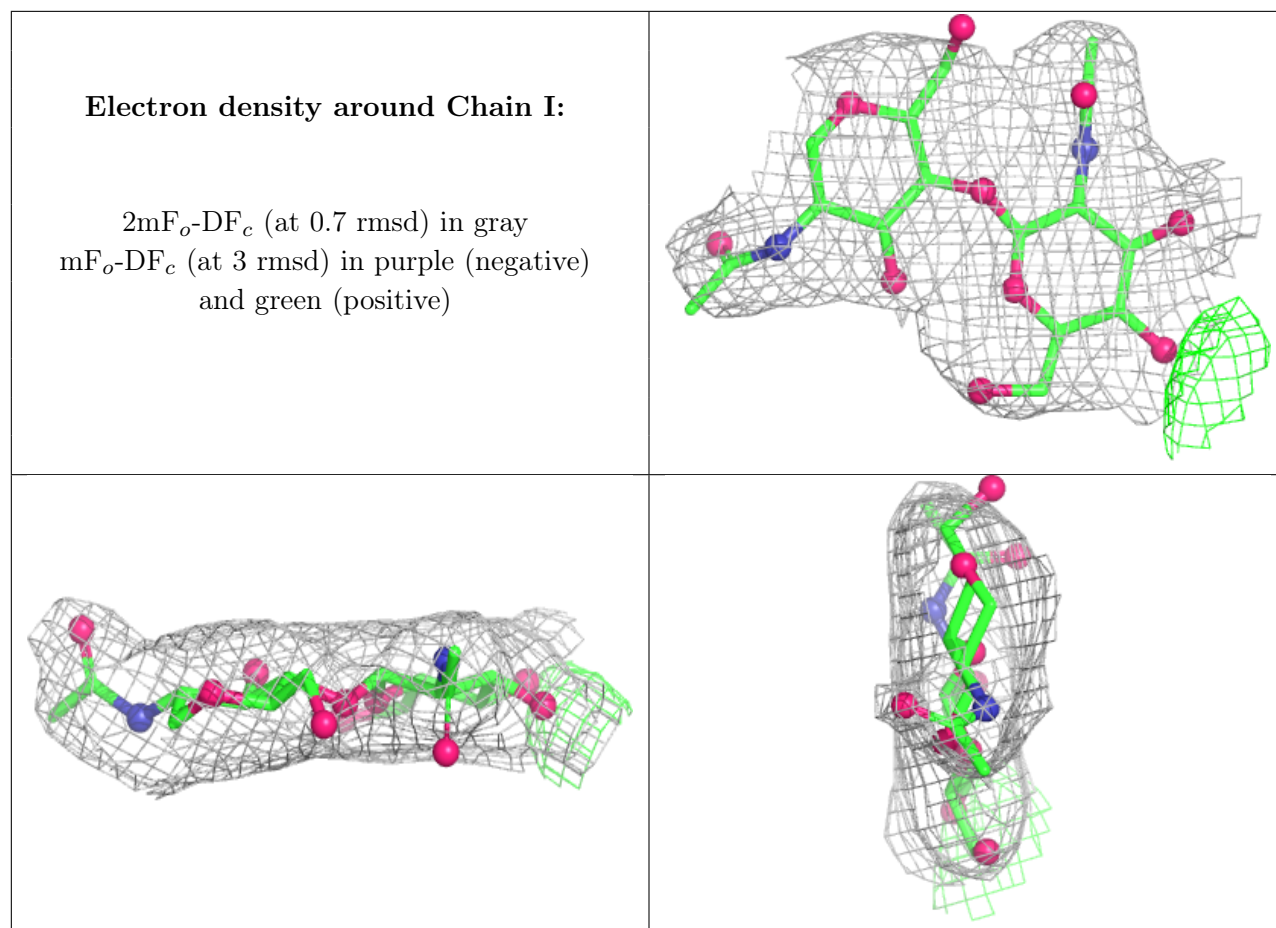
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.



Electron density around Chain H:

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





6.4 Ligands [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($\text{\AA}^2$)	Q<0.9
3	NAG	A	501	14/15	0.97	0.05	85,88,91,91	0
3	NAG	B	501	14/15	0.97	0.04	87,91,96,96	0
3	NAG	D	501	14/15	0.97	0.06	96,103,108,109	0
3	NAG	E	501	14/15	0.97	0.06	75,81,87,99	0
3	NAG	F	501	14/15	0.97	0.07	77,81,86,87	0
3	NAG	C	501	14/15	0.98	0.04	83,88,97,101	0
3	NAG	B	502	14/15	0.99	0.04	78,95,98,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.