



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 27, 2025 – 06:12 PM JST

PDB ID : 8ZHZ
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	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.21
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.004 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

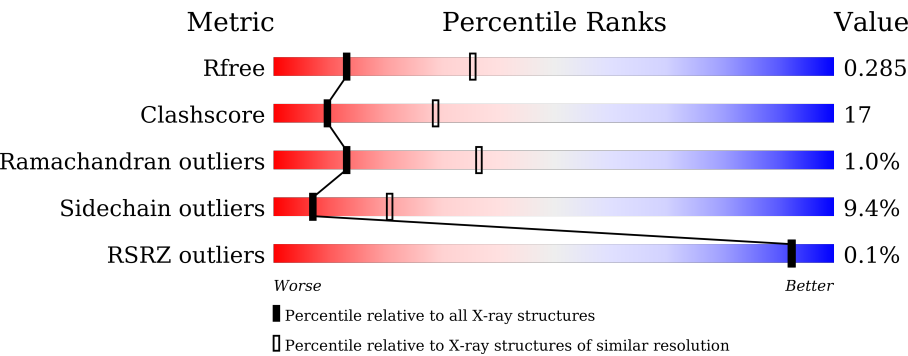
1 Overall quality at a glance i

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.



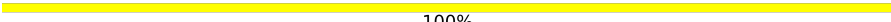
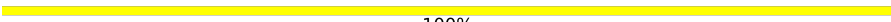

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	164625	3316 (2.90-2.86)
Clashscore	180529	3609 (2.90-2.86)
Ramachandran outliers	177936	3529 (2.90-2.86)
Sidechain outliers	177891	3532 (2.90-2.86)
RSRZ outliers	164620	3319 (2.90-2.86)

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	<div><div></div><div>55%26%.16%</div></div>
1	B	440	<div><div></div><div>49%30%.16%</div></div>
1	C	440	<div><div></div><div>47%30%.19%</div></div>
1	D	440	<div><div></div><div>53%26%5%16%</div></div>
1	E	440	<div><div></div><div>49%28%5%18%</div></div>
1	F	440	<div><div></div><div>55%26%.15%</div></div>

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Mol	Chain	Length	Quality of chain
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

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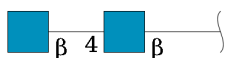
Chain	Residue	Modelled	Actual	Comment	Reference
B	76	GLY	-	linker	UNP J7JVS8
B	77	SER	-	linker	UNP J7JVS8
B	78	GLY	-	linker	UNP J7JVS8
B	79	GLY	-	linker	UNP J7JVS8
B	121	GLY	-	linker	UNP J7JVS8
B	122	GLY	-	linker	UNP J7JVS8
B	123	SER	-	linker	UNP J7JVS8
B	124	GLY	-	linker	UNP J7JVS8
B	125	GLY	-	linker	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

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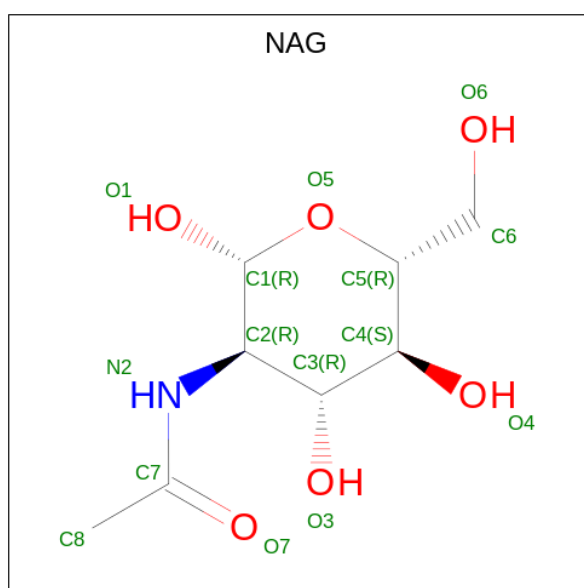
Chain	Residue	Modelled	Actual	Comment	Reference
D	440	HIS	-	expression tag	UNP J7JVS8
D	441	HIS	-	expression tag	UNP J7JVS8
D	442	HIS	-	expression tag	UNP J7JVS8
D	443	HIS	-	expression tag	UNP J7JVS8
D	444	HIS	-	expression tag	UNP J7JVS8
E	75	GLY	-	linker	UNP J7JVS8
E	76	GLY	-	linker	UNP J7JVS8
E	77	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 (three-letter code: 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		

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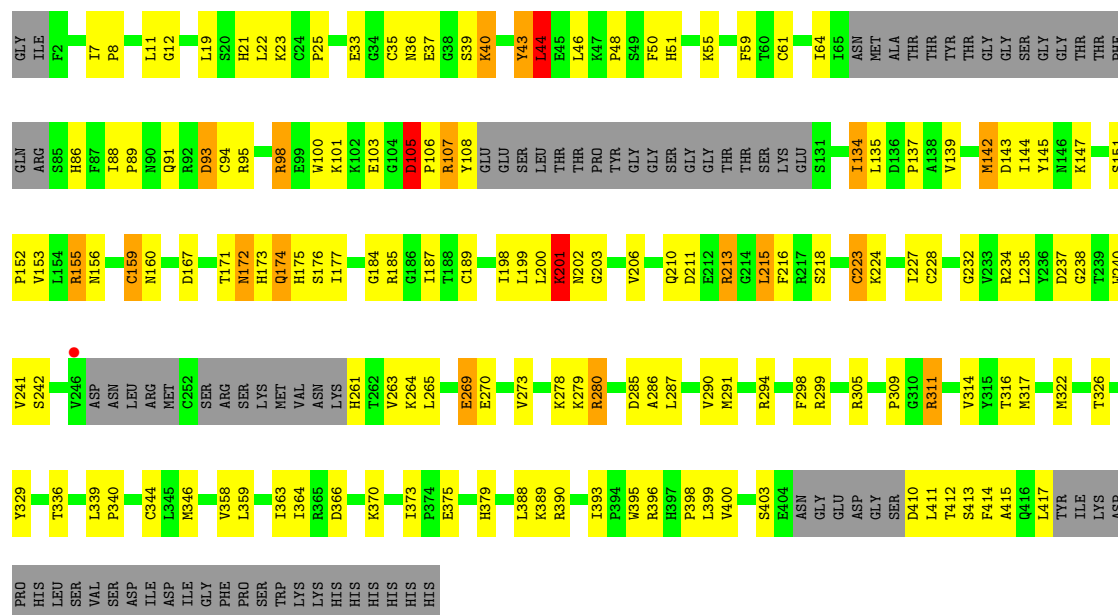
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	F	1	Total	C	N	O	0	0
			14	8	1	5		

PHE
PRO
SER
TRP
LYS
LYS
HIS
HIS
HIS
HIS
HIS

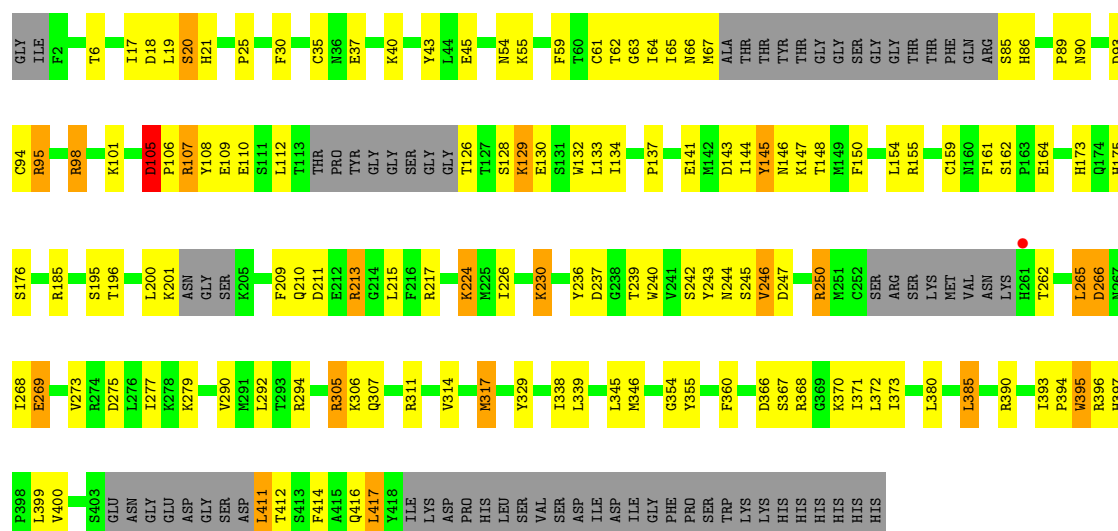
• Molecule 1: Glycoprotein

Chain C: 47% 30% 19%



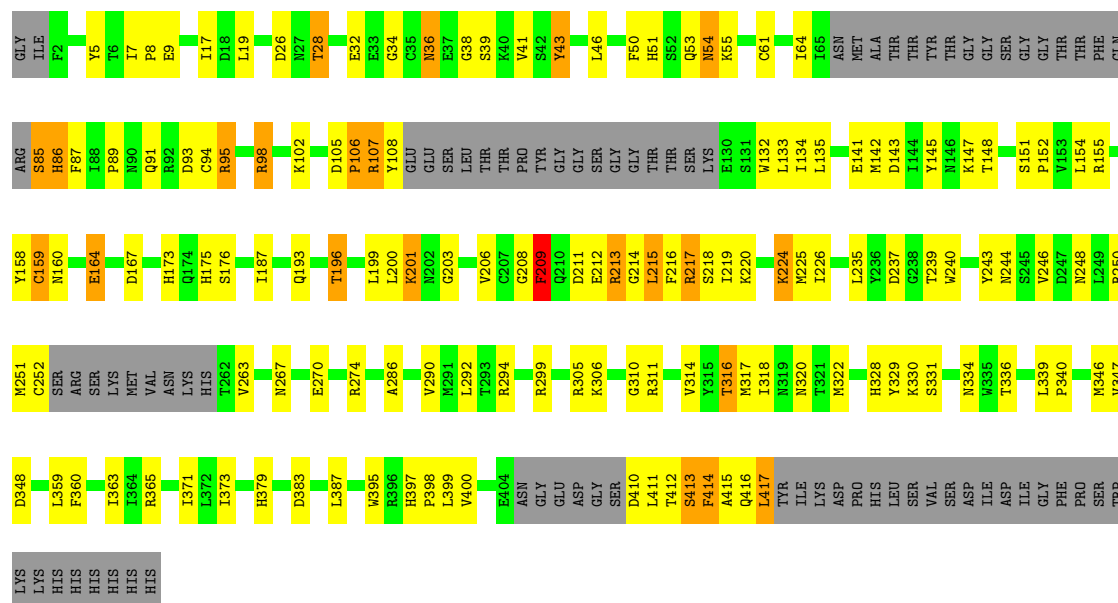
• Molecule 1: Glycoprotein

Chain D: 53% 26% 5% 16%

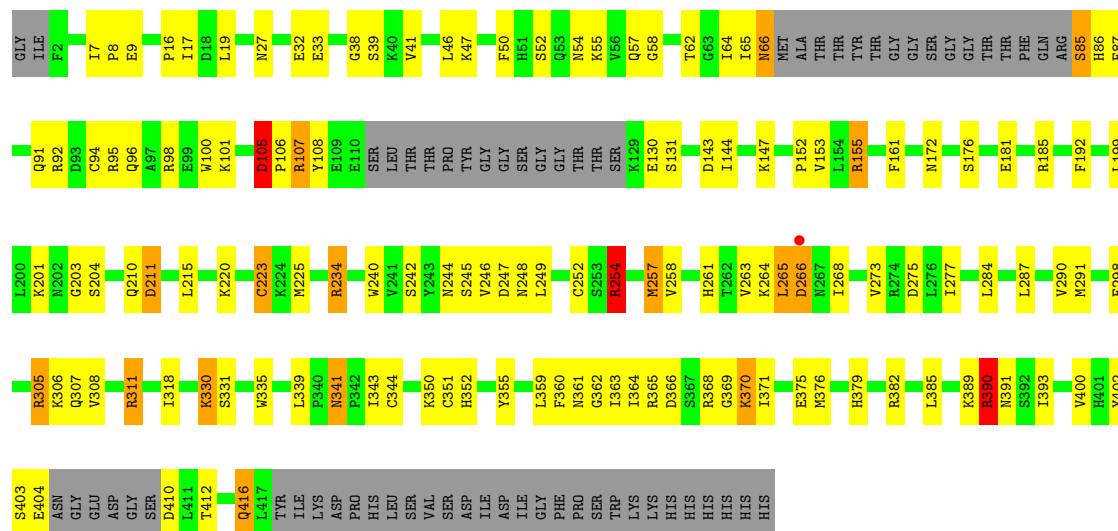


• Molecule 1: Glycoprotein

Chain E: 49% 28% 5% 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 (4.86%)	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 , 35.8	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	0.55	0/3057	0.83	12/4125 (0.3%)
1	B	0.56	0/3038	0.83	6/4099 (0.1%)
1	C	0.57	1/2925 (0.0%)	0.78	1/3951 (0.0%)
1	D	0.57	1/3051 (0.0%)	0.78	2/4119 (0.0%)
1	E	0.55	0/2979	0.83	6/4023 (0.1%)
1	F	0.59	0/3086	0.80	3/4166 (0.1%)
All	All	0.57	2/18136 (0.0%)	0.81	30/24483 (0.1%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	228	CYS	CB-SG	-6.39	1.71	1.82
1	D	105	ASP	C-N	5.51	1.44	1.34

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	66	ASN	N-CA-CB	8.58	126.05	110.60
1	A	415	ALA	N-CA-CB	-8.46	98.26	110.10
1	E	244	ASN	N-CA-CB	8.24	125.42	110.60
1	E	414	PHE	N-CA-C	-7.95	89.55	111.00
1	B	68	ALA	CB-CA-C	-7.38	99.02	110.10
1	B	151	SER	CB-CA-C	7.29	123.94	110.10
1	A	93	ASP	N-CA-C	-7.28	91.35	111.00
1	A	360	PHE	N-CA-CB	-6.79	98.37	110.60
1	A	360	PHE	N-CA-C	6.61	128.86	111.00
1	F	254	ARG	CB-CA-C	-6.57	97.26	110.40
1	E	243	TYR	CB-CA-C	6.55	123.50	110.40
1	A	92	ARG	CB-CA-C	-6.29	97.82	110.40
1	B	69	THR	N-CA-C	-6.14	94.43	111.00
1	A	265	LEU	CA-CB-CG	5.95	128.98	115.30
1	E	348	ASP	CB-CG-OD1	-5.93	112.96	118.30
1	D	360	PHE	N-CA-CB	-5.90	99.97	110.60
1	A	413	SER	CB-CA-C	-5.78	99.13	110.10
1	A	237	ASP	N-CA-C	-5.71	95.57	111.00
1	A	93	ASP	CB-CA-C	5.63	121.65	110.40
1	A	359	LEU	N-CA-C	-5.63	95.81	111.00
1	E	215	LEU	CB-CG-CD1	-5.50	101.65	111.00
1	F	257	MET	CG-SD-CE	5.49	108.98	100.20
1	E	215	LEU	CA-CB-CG	5.37	127.65	115.30
1	A	237	ASP	CB-CA-C	5.33	121.06	110.40
1	B	416	GLN	CA-CB-CG	5.25	124.95	113.40
1	B	85	SER	CB-CA-C	5.24	120.05	110.10
1	D	360	PHE	N-CA-C	5.14	124.88	111.00
1	A	413	SER	N-CA-C	5.13	124.86	111.00
1	C	44	LEU	CA-CB-CG	5.11	127.06	115.30
1	B	417	LEU	N-CA-C	-5.06	97.33	111.00

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

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Mol	Chain	Res	Type	Group
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

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	91	1
1	B	2971	0	2895	117	1
1	C	2858	0	2776	127	0
1	D	2982	0	2907	97	1
1	E	2911	0	2835	108	0
1	F	3016	0	2935	90	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	618	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 17.

All (618) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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
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	1.34	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:B:267:ASN:C	1:B:268:ILE:HD12	2.09	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:330:LYS:HD2	1:E:331:SER:N	2.04	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:E:317:MET:HE2	1:E:320:ASN:HA	1.75	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:D:394:PRO:O	1:D:395:TRP:C	2.33	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:66:ASN:HA	1:F:86:HIS:CE1	2.34	0.61
1:D:224:LYS:NZ	1:D:250:ARG:HB3	2.15	0.61
1:C:142:MET:O	1:C:142:MET:HG3	1.99	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: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
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:C:322:MET:CE	1:C:393:ILE:HD11	2.31	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:C:269:GLU:OE2	1:C:269:GLU:N	2.24	0.60
1:B:359:LEU:HD13	1:B:363:ILE:HG22	1.83	0.60
1:A:93:ASP:HB3	1:A:132:TRP:CZ2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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: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:110:GLU:CD	1:A:110:GLU:H	2.06	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
1:A:352:HIS:HB3	1:A:359:LEU:HD23	1.86	0.57
1:E:340:PRO:HG3	1:E:346:MET:HE3	1.86	0.57
1:F:265:LEU:HB3	1:F:268:ILE:HD12	1.85	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:F:264:LYS:HD3	1:F:264:LYS:C	2.24	0.57
1:B:93:ASP:HA	1:B:96:GLN:HB3	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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
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:E:211:ASP:CG	1:E:213:ARG:HG2	2.26	0.55
1:A:17:ILE:HG22	1:A:55:LYS:HG2	1.88	0.55
1:D:224:LYS:O	1:D:250:ARG:HG3	2.07	0.55
1:A:66:ASN:CG	1:A:86:HIS:HB2	2.27	0.55
1:B:216:PHE:HE1	1:B:218:SER:HB2	1.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:16:PRO:HG2	1:B:57:GLN:OE1	2.08	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: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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:E:286:ALA:O	1:E:290:VAL:HG23	2.11	0.51
1:D:67:MET:HB3	1:D:128:SER:HA	1.93	0.51
1:F:85:SER:N	1:F:412:THR:HG1	2.09	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: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:B:414:PHE:CD1	1:B:414:PHE:C	2.85	0.50
1:C:152:PRO:HB2	1:C:400:VAL:HG13	1.94	0.50
1:C:322:MET:HE3	1:C:393:ILE:HD11	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:107:ARG:C	1:D:107:ARG:HD2	2.32	0.50
1:E:134:ILE:HD12	1:E:134:ILE:N	2.26	0.50
1:C:344:CYS:SG	1:C:346:MET:HE2	2.52	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:C:184:GLY:O	1:C:187:ILE:HG13	2.12	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: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:F:341:ASN:C	1:F:341:ASN:OD1	2.50	0.49
1:C:173:HIS:HB2	1:C:399:LEU:HD22	1.95	0.49
1:B:151:SER:OG	1:B:153:VAL:HG22	2.13	0.49
1:C:269:GLU:H	1:C:269:GLU:CD	2.12	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:A:22:LEU:HD11	1:A:322:MET:HE2	1.94	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:370:LYS:HZ2	1:F:382:ARG:NH1	2.08	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
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:C:61:CYS:O	1:C:176:SER:HA	2.13	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
1:C:322:MET:HE1	1:C:393:ILE:HD11	1.96	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:C:340:PRO:HG3	1:C:346:MET:HE3	1.97	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:345:LEU:HD13	1:D:371:ILE:HG21	1.96	0.47
1:E:143:ASP:OD1	1:E:143:ASP:C	2.52	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:339:LEU:HD21	1:F:371:ILE:HB	1.96	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:A:341:ASN:C	1:A:341:ASN:OD1	2.53	0.47
1:C:37:GLU:O	1:C:201:LYS:N	2.44	0.47
1:C:317:MET:HB2	1:C:317:MET:HE2	1.55	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
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:237:ASP:C	1:E:239:THR:H	2.18	0.46
1:A:106:PRO:HB2	1:A:110:GLU:OE1	2.16	0.46
1:F:65:ILE:O	1:F:86:HIS:CE1	2.69	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:D:109:GLU:OE2	1:D:112:LEU:HD21	2.16	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:D:162:SER:OG	1:D:164:GLU:OE2	2.34	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: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:O	1:C:264:LYS:HD3	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:C:142:MET:HE3	1:C:185:ARG:HD2	1.98	0.44
1:E:106:PRO:O	1:E:107:ARG:C	2.55	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:142:MET:CE	1:B:149:MET:SD	3.06	0.44
1:F:403:SER:O	1:F:404:GLU:C	2.55	0.44
1:A:86:HIS:CD2	1:A:411:LEU:H	2.35	0.44
1:C:171:THR:C	1:C:173:HIS:H	2.21	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:D:6:THR:HG1	1:D:329:TYR:HD2	1.64	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:D:393:ILE:HG22	1:D:393:ILE:O	2.18	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:F:225:MET:HE1	1:F:257:MET:HB3	2.00	0.43
1:F:360:PHE:O	1:F:361:ASN:C	2.56	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:159:CYS:SG	1:E:160:ASN:N	2.91	0.43
1:E:412:THR:CG2	1:E:413:SER:N	2.82	0.43
1:B:66:ASN:ND2	1:B:67:MET:H	2.16	0.43
1:C:269:GLU:O	1:C:273:VAL:HG12	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:F:264:LYS:O	1:F:264:LYS:HD2	2.11	0.43
1:B:167:ASP:OD1	1:B:167:ASP:N	2.52	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: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:159:CYS:SG	1:C:160:ASN:N	2.91	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: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: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: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:D:146:ASN:C	1:D:148:THR:H	2.23	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: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: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
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:E:87:PHE:C	1:E:175:HIS:HB3	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:346:MET:HE2	1:B:349:GLY:O	2.19	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: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:C:216:PHE:CD1	1:C:216:PHE:C	2.94	0.41
1:F:306:LYS:HE3	1:F:308:VAL:HG23	2.03	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:168:PHE:CD2	1:B:177:ILE:HD11	2.56	0.41
1:C:89:PRO:HG2	1:C:177:ILE:HG12	2.02	0.41
1:E:413:SER:C	1:E:415:ALA:N	2.74	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:211:ASP:CG	1:C:215:LEU:HB3	2.40	0.41
1:D:200:LEU:HD11	1:D:210:GLN:HE21	1.85	0.41
1:D:416:GLN:O	1:D:417:LEU:C	2.59	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: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: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:B:43:TYR:CE2	1:B:195:SER:HB3	2.56	0.40
1:B:212:GLU:O	1:B:212:GLU:HG2	2.22	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:251:MET:H	1:B:251:MET:HG2	1.77	0.40
1:B:414:PHE:C	1:B:414:PHE:HD1	2.24	0.40
1:C:413:SER:C	1:C:415:ALA:H	2.24	0.40
1:D:250:ARG:C	1:D:250:ARG:HD3	2.41	0.40
1:F:62:THR:HG23	1:F:176:SER:OG	2.21	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

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the sym-

metry 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 [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	361/440 (82%)	333 (92%)	24 (7%)	4 (1%)	12	34
1	B	355/440 (81%)	329 (93%)	23 (6%)	3 (1%)	16	42
1	C	346/440 (79%)	318 (92%)	25 (7%)	3 (1%)	14	39
1	D	358/440 (81%)	323 (90%)	31 (9%)	4 (1%)	12	34
1	E	352/440 (80%)	325 (92%)	24 (7%)	3 (1%)	14	39
1	F	367/440 (83%)	331 (90%)	32 (9%)	4 (1%)	12	34
All	All	2139/2640 (81%)	1959 (92%)	159 (7%)	21 (1%)	13	36

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

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Mol	Chain	Res	Type
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%)	305 (91%)	31 (9%)	7	22
1	B	335/393 (85%)	306 (91%)	29 (9%)	8	24
1	C	320/393 (81%)	289 (90%)	31 (10%)	6	19
1	D	336/393 (86%)	303 (90%)	33 (10%)	6	19
1	E	327/393 (83%)	302 (92%)	25 (8%)	11	30
1	F	339/393 (86%)	301 (89%)	38 (11%)	5	14
All	All	1993/2358 (84%)	1806 (91%)	187 (9%)	7	21

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR
1	A	9	GLU
1	A	32	GLU
1	A	52	SER
1	A	61	CYS
1	A	66	ASN
1	A	87	PHE
1	A	90	ASN
1	A	91	GLN

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Mol	Chain	Res	Type
1	A	95	ARG
1	A	98	ARG
1	A	103	GLU
1	A	105	ASP
1	A	107	ARG
1	A	153	VAL
1	A	205	LYS
1	A	210	GLN
1	A	213	ARG
1	A	215	LEU
1	A	218	SER
1	A	234	ARG
1	A	237	ASP
1	A	264	LYS
1	A	265	LEU
1	A	270	GLU
1	A	311	ARG
1	A	331	SER
1	A	341	ASN
1	A	355	TYR
1	A	403	SER
1	A	410	ASP
1	B	6	THR
1	B	15	THR
1	B	20	SER
1	B	35	CYS
1	B	49	SER
1	B	54	ASN
1	B	67	MET
1	B	92	ARG
1	B	93	ASP
1	B	98	ARG
1	B	107	ARG
1	B	155	ARG
1	B	158	TYR
1	B	159	CYS
1	B	164	GLU
1	B	165	ASN
1	B	182	ASP
1	B	195	SER
1	B	209	PHE
1	B	215	LEU

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Mol	Chain	Res	Type
1	B	225	MET
1	B	230	LYS
1	B	234	ARG
1	B	252	CYS
1	B	266	ASP
1	B	305	ARG
1	B	307	GLN
1	B	368	ARG
1	B	414	PHE
1	C	39	SER
1	C	40	LYS
1	C	43	TYR
1	C	44	LEU
1	C	55	LYS
1	C	93	ASP
1	C	98	ARG
1	C	105	ASP
1	C	107	ARG
1	C	108	TYR
1	C	134	ILE
1	C	142	MET
1	C	155	ARG
1	C	159	CYS
1	C	189	CYS
1	C	201	LYS
1	C	213	ARG
1	C	215	LEU
1	C	223	CYS
1	C	227	ILE
1	C	237	ASP
1	C	261	HIS
1	C	263	VAL
1	C	265	LEU
1	C	269	GLU
1	C	270	GLU
1	C	278	LYS
1	C	280	ARG
1	C	311	ARG
1	C	316	THR
1	C	403	SER
1	D	20	SER
1	D	25	PRO

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Mol	Chain	Res	Type
1	D	54	ASN
1	D	98	ARG
1	D	107	ARG
1	D	108	TYR
1	D	126	THR
1	D	129	LYS
1	D	155	ARG
1	D	196	THR
1	D	201	LYS
1	D	213	ARG
1	D	224	LYS
1	D	230	LYS
1	D	236	TYR
1	D	243	TYR
1	D	244	ASN
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	305	ARG
1	D	317	MET
1	D	346	MET
1	D	355	TYR
1	D	367	SER
1	D	368	ARG
1	D	372	LEU
1	D	380	LEU
1	D	385	LEU
1	D	411	LEU
1	E	28	THR
1	E	43	TYR
1	E	54	ASN
1	E	85	SER
1	E	86	HIS
1	E	95	ARG
1	E	98	ARG
1	E	107	ARG
1	E	108	TYR
1	E	159	CYS
1	E	193	GLN

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Mol	Chain	Res	Type
1	E	196	THR
1	E	201	LYS
1	E	209	PHE
1	E	213	ARG
1	E	217	ARG
1	E	224	LYS
1	E	251	MET
1	E	252	CYS
1	E	263	VAL
1	E	267	ASN
1	E	294	ARG
1	E	316	THR
1	E	413	SER
1	E	417	LEU
1	F	33	GLU
1	F	39	SER
1	F	52	SER
1	F	85	SER
1	F	87	PHE
1	F	92	ARG
1	F	95	ARG
1	F	98	ARG
1	F	105	ASP
1	F	107	ARG
1	F	108	TYR
1	F	153	VAL
1	F	155	ARG
1	F	204	SER
1	F	211	ASP
1	F	220	LYS
1	F	223	CYS
1	F	234	ARG
1	F	244	ASN
1	F	245	SER
1	F	252	CYS
1	F	261	HIS
1	F	265	LEU
1	F	266	ASP
1	F	275	ASP
1	F	311	ARG
1	F	330	LYS
1	F	331	SER

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Mol	Chain	Res	Type
1	F	341	ASN
1	F	344	CYS
1	F	350	LYS
1	F	355	TYR
1	F	370	LYS
1	F	379	HIS
1	F	385	LEU
1	F	390	ARG
1	F	410	ASP
1	F	416	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	91	GLN
1	B	174	GLN
1	B	175	HIS
1	B	267	ASN
1	B	397	HIS
1	C	173	HIS
1	C	175	HIS
1	C	307	GLN
1	E	86	HIS
1	E	91	GLN
1	E	248	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 ⓘ

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	0.99	1 (7%)	17,19,21	0.85	0
2	NAG	G	2	2	14,14,15	0.41	0	17,19,21	0.85	1 (5%)
2	NAG	H	1	2,1	14,14,15	0.56	0	17,19,21	0.78	1 (5%)
2	NAG	H	2	2	14,14,15	0.68	1 (7%)	17,19,21	0.63	0
2	NAG	I	1	2,1	14,14,15	0.97	1 (7%)	17,19,21	0.75	0
2	NAG	I	2	2	14,14,15	0.93	1 (7%)	17,19,21	0.72	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	-	2/6/23/26	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	-3.46	1.38	1.43
2	G	1	NAG	O5-C1	-3.40	1.38	1.43
2	I	2	NAG	O5-C1	-3.31	1.38	1.43
2	H	2	NAG	C1-C2	2.33	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	2.20	115.17	112.19
2	I	2	NAG	C1-O5-C5	2.20	115.17	112.19
2	H	1	NAG	C1-O5-C5	2.19	115.15	112.19

There are no chirality outliers.

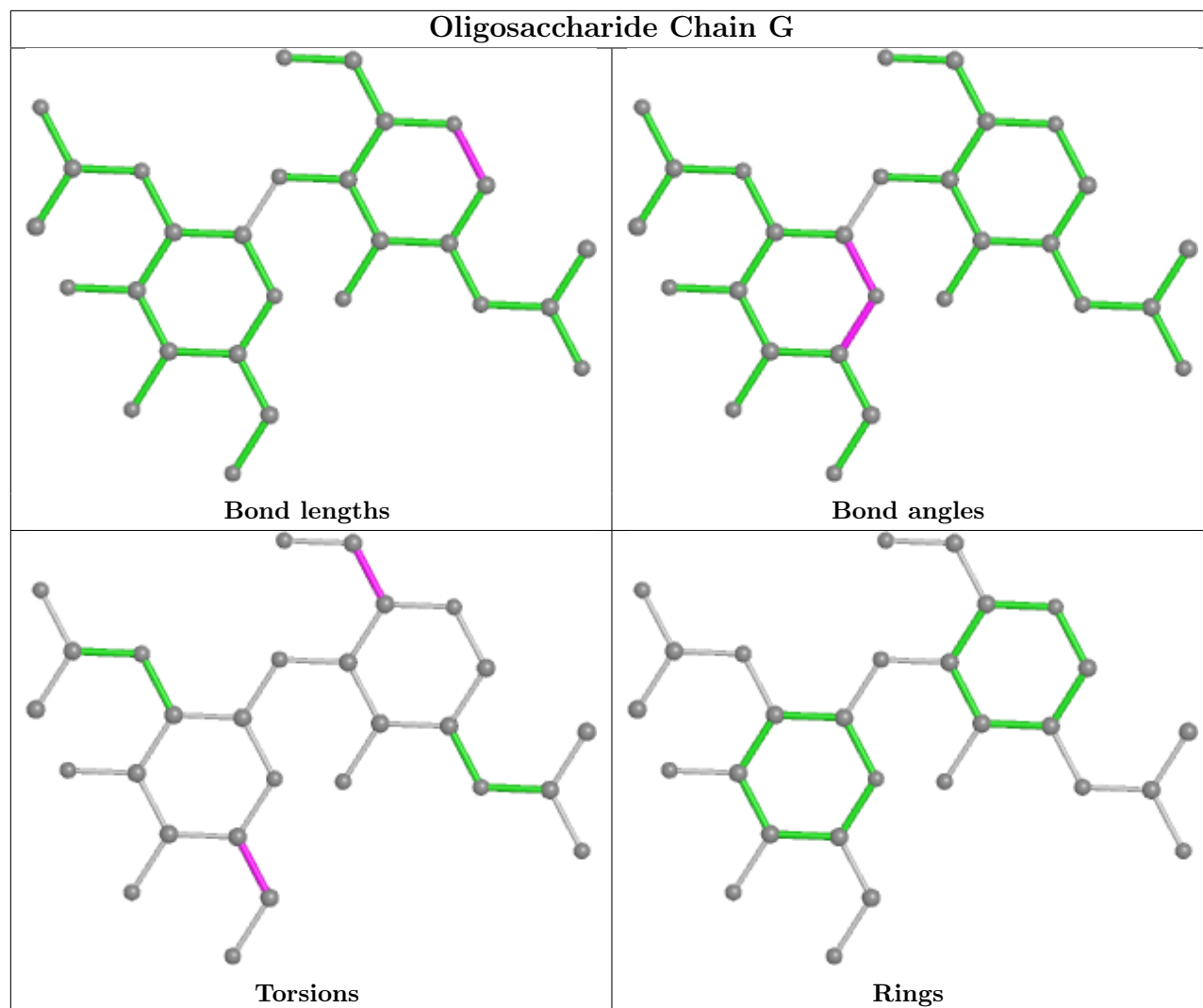
All (10) torsion outliers are listed below:

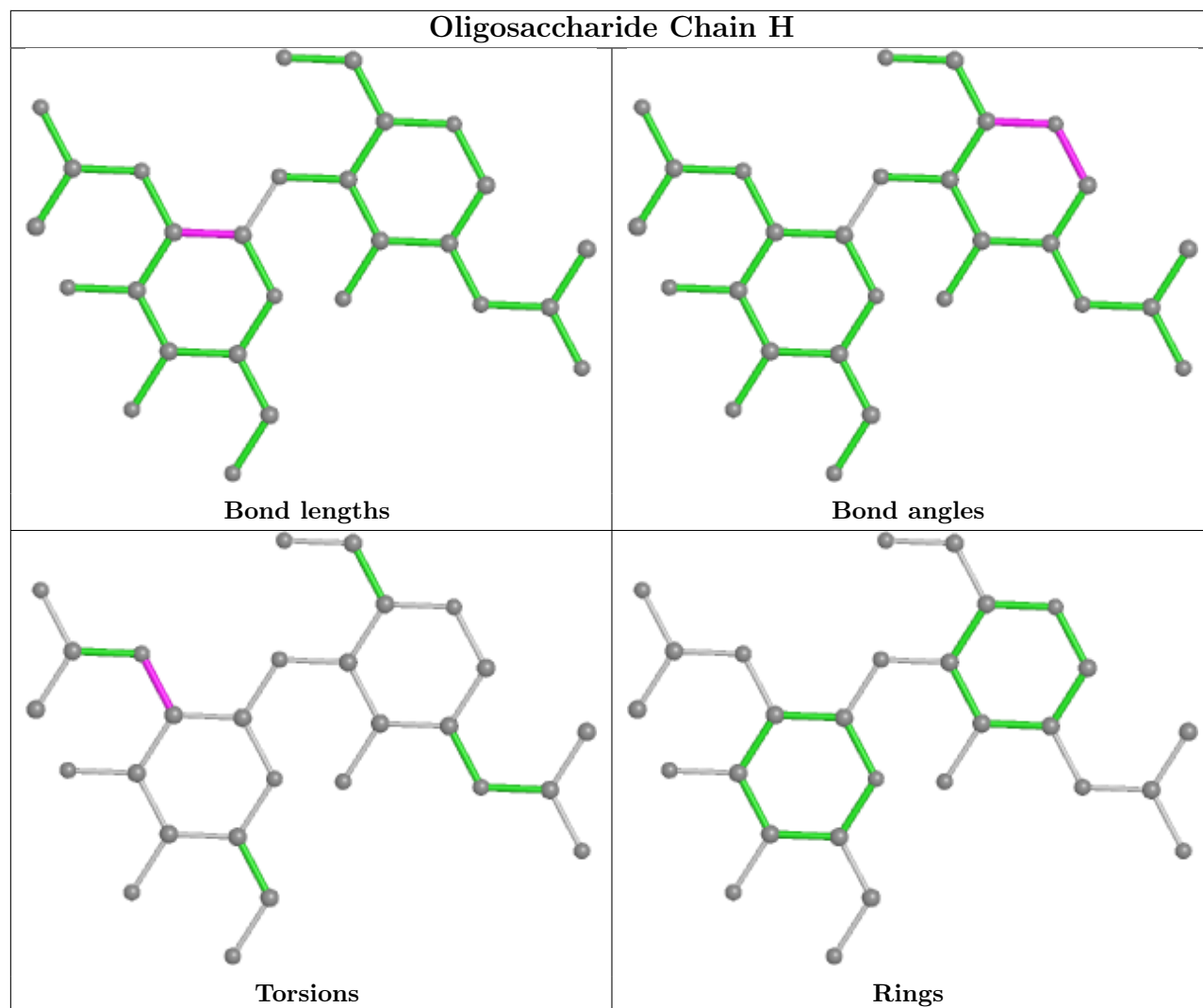
Mol	Chain	Res	Type	Atoms
2	I	2	NAG	O5-C5-C6-O6
2	I	1	NAG	C4-C5-C6-O6
2	G	1	NAG	C4-C5-C6-O6
2	G	2	NAG	O5-C5-C6-O6
2	I	2	NAG	C4-C5-C6-O6
2	I	1	NAG	O5-C5-C6-O6
2	G	2	NAG	C4-C5-C6-O6
2	G	1	NAG	O5-C5-C6-O6
2	H	2	NAG	C1-C2-N2-C7
2	H	2	NAG	C3-C2-N2-C7

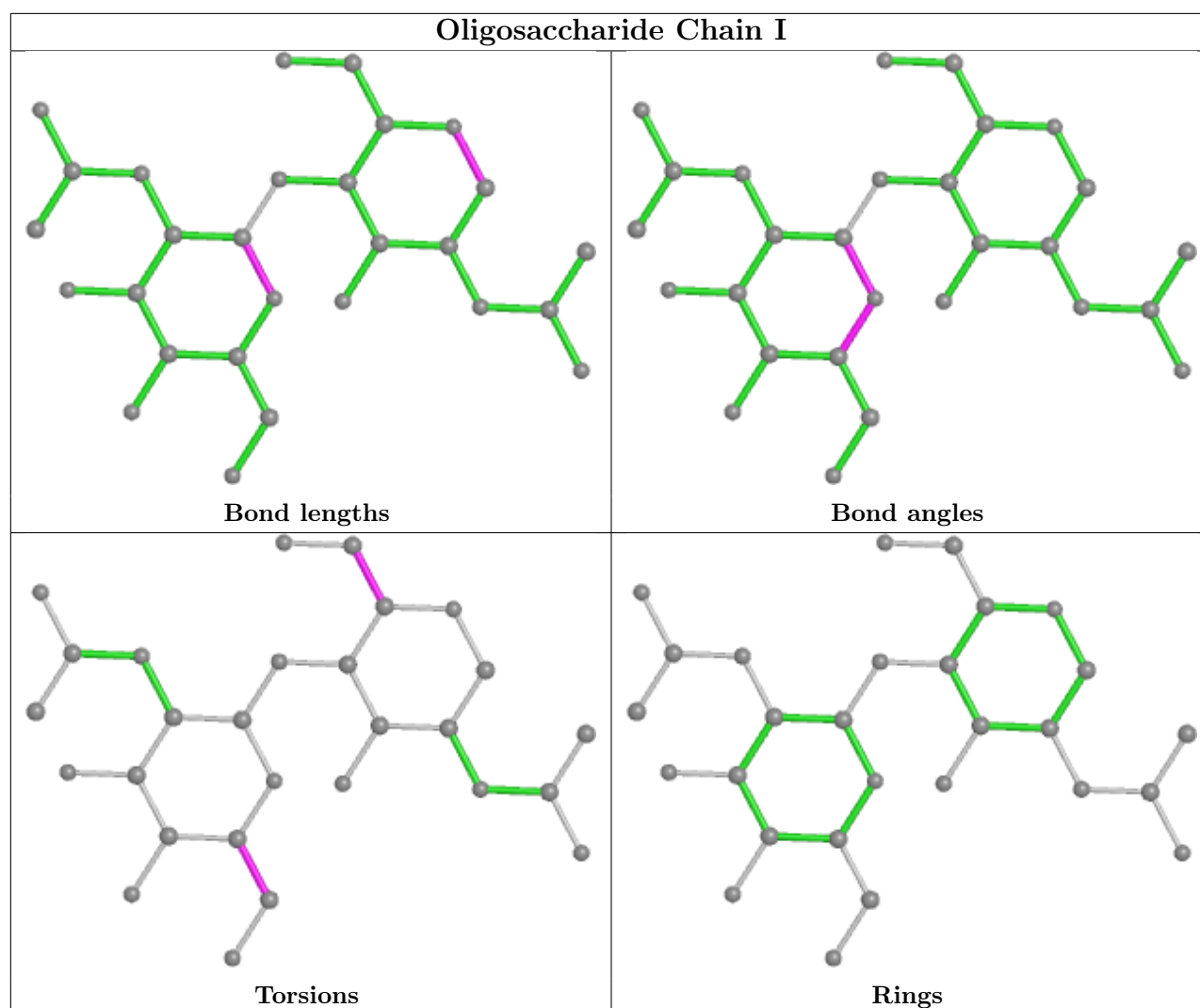
There are no ring outliers.

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	E	501	1	14,14,15	1.44	2 (14%)	17,19,21	0.88	1 (5%)
3	NAG	A	501	1	14,14,15	0.94	1 (7%)	17,19,21	1.13	1 (5%)
3	NAG	C	501	1	14,14,15	1.01	2 (14%)	17,19,21	1.11	1 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NAG	B	502	-	14,14,15	0.58	0	17,19,21	0.47	0
3	NAG	B	501	1	14,14,15	0.49	0	17,19,21	1.13	1 (5%)
3	NAG	F	501	1	14,14,15	0.85	1 (7%)	17,19,21	0.84	1 (5%)
3	NAG	D	501	1	14,14,15	0.64	0	17,19,21	0.62	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	E	501	1	-	2/6/23/26	0/1/1/1
3	NAG	A	501	1	-	0/6/23/26	0/1/1/1
3	NAG	C	501	1	-	2/6/23/26	0/1/1/1
3	NAG	B	502	-	-	1/6/23/26	0/1/1/1
3	NAG	B	501	1	-	1/6/23/26	0/1/1/1
3	NAG	F	501	1	-	2/6/23/26	0/1/1/1
3	NAG	D	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	4.86	1.51	1.43
3	F	501	NAG	O5-C1	2.95	1.48	1.43
3	A	501	NAG	O5-C1	2.94	1.48	1.43
3	C	501	NAG	C1-C2	2.51	1.56	1.52
3	C	501	NAG	O5-C1	2.44	1.47	1.43
3	E	501	NAG	C1-C2	2.03	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	4.20	117.88	112.19
3	C	501	NAG	C1-O5-C5	3.73	117.25	112.19
3	B	501	NAG	C1-O5-C5	3.70	117.21	112.19
3	F	501	NAG	C1-O5-C5	2.79	115.97	112.19
3	E	501	NAG	C1-O5-C5	2.70	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	C	501	NAG	C1-C2-N2-C7
3	E	501	NAG	O5-C5-C6-O6
3	D	501	NAG	C4-C5-C6-O6
3	F	501	NAG	C4-C5-C6-O6
3	E	501	NAG	C4-C5-C6-O6
3	B	501	NAG	O5-C5-C6-O6
3	B	502	NAG	C3-C2-N2-C7
3	C	501	NAG	C3-C2-N2-C7

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	E	501	NAG	1	0
3	C	501	NAG	1	0
3	F	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%)	-1.42	0	100 100	41, 61, 106, 127	0
1	B	369/440 (83%)	-1.38	0	100 100	38, 65, 118, 144	0
1	C	357/440 (81%)	-1.39	1 (0%)	90 89	40, 66, 111, 130	0
1	D	370/440 (84%)	-1.37	1 (0%)	90 89	38, 65, 122, 144	0
1	E	362/440 (82%)	-1.40	0	100 100	39, 67, 118, 154	0
1	F	375/440 (85%)	-1.46	1 (0%)	90 89	40, 62, 106, 132	0
All	All	2204/2640 (83%)	-1.40	3 (0%)	92 92	38, 64, 116, 154	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	261	HIS	2.4
1	F	266	ASP	2.1
1	C	246	VAL	2.1

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

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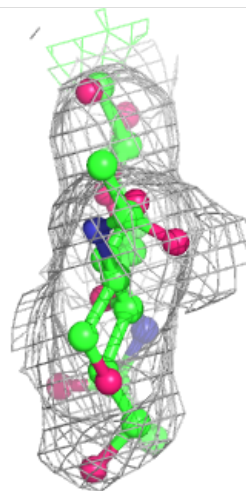
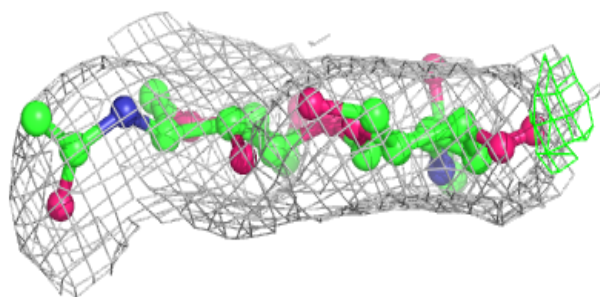
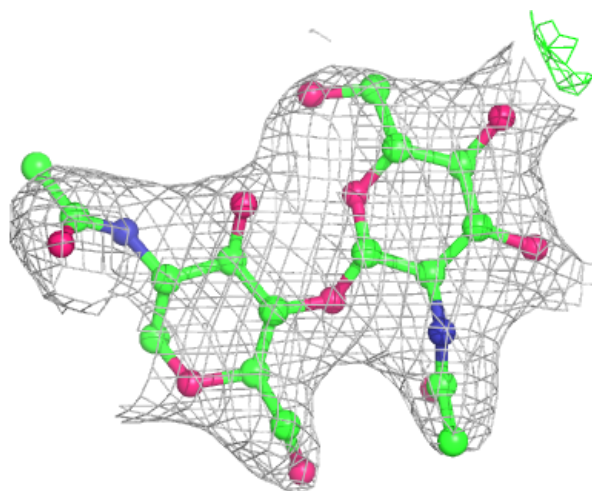
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	NAG	I	2	14/15	0.98	0.05	54,58,67,71	0
2	NAG	G	2	14/15	0.99	0.04	53,57,67,71	0
2	NAG	I	1	14/15	0.99	0.03	55,61,66,74	0
2	NAG	H	1	14/15	0.99	0.04	87,97,100,101	0
2	NAG	G	1	14/15	1.00	0.03	52,58,65,72	0

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

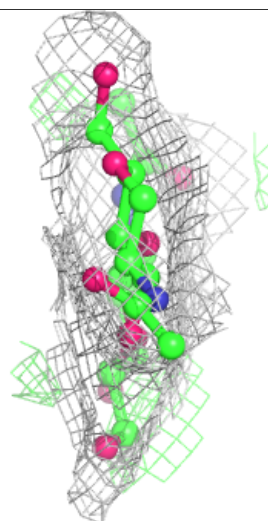
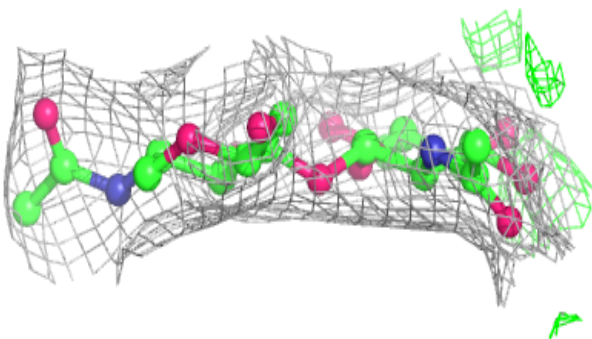
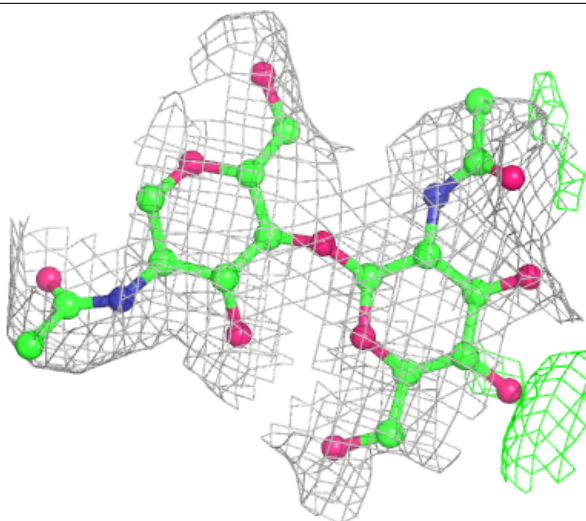
Electron density around Chain G:

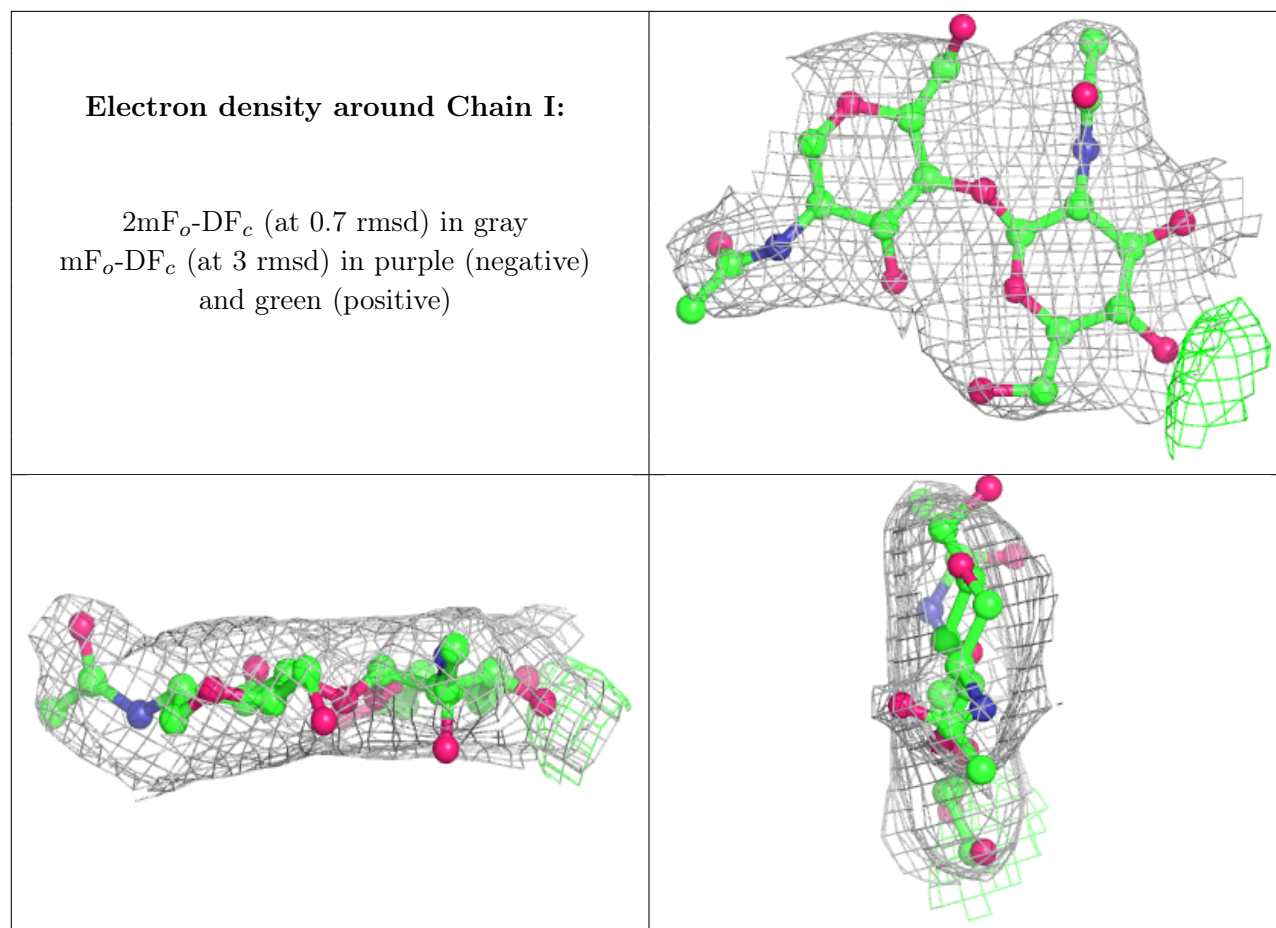
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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(\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.