



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:11 PM UTC

PDB ID : 3WJM / pdb_00003wjm
Title : Crystal structure of Bombyx mori Sp2/Sp3 heterohexamer
Authors : Yuan, Y.A.; Hou, Y.
Deposited on : 2013-10-11
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

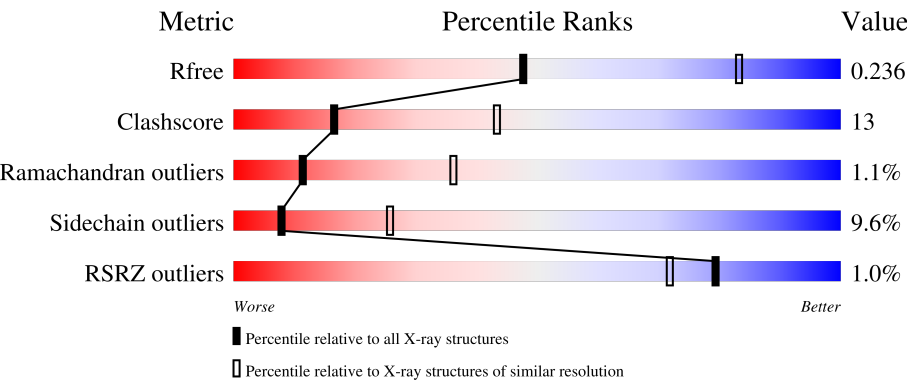
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	703	% 69% 23% • 5%
1	E	703	% 70% 21% • 5%
1	F	703	2% 65% 26% • 5%
2	B	696	% 64% 26% 6% • •
2	C	696	% 66% 25% 5% •

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Mol	Chain	Length	Quality of chain
2	D	696	66% 25% 5%
3	G	5	100%
4	H	5	40% 60%
5	I	6	100%
6	J	7	100%
7	K	6	67% 33%
8	L	5	20% 80%

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 34590 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.

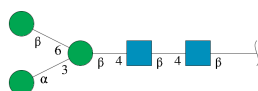
- Molecule 1 is a protein called Arylphorin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	670	Total	C	N	O	S	0	0	0
			5681	3734	892	1030	25			
1	E	669	Total	C	N	O	S	0	0	0
			5669	3725	891	1028	25			
1	F	669	Total	C	N	O	S	0	0	0
			5669	3725	891	1028	25			

- Molecule 2 is a protein called Silkworm storage protein.

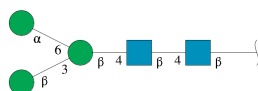
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	668	Total	C	N	O	S	0	0	0
			5669	3745	877	1021	26			
2	C	668	Total	C	N	O	S	0	0	0
			5669	3745	877	1021	26			
2	D	672	Total	C	N	O	S	0	0	0
			5703	3767	881	1029	26			

- Molecule 3 is an oligosaccharide called alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



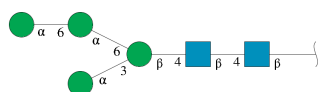
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	G	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 4 is an oligosaccharide called beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



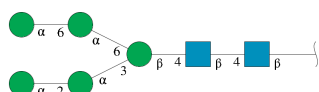
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	5	Total	C	N	O	0	0	0
			61	34	2	25			

- Molecule 5 is an oligosaccharide called alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



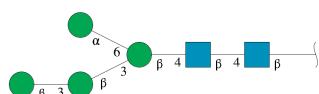
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	I	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 6 is an oligosaccharide called alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



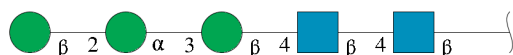
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
6	J	7	Total	C	N	O	0	0	0
			83	46	2	35			

- Molecule 7 is an oligosaccharide called beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
7	K	6	Total	C	N	O	0	0	0
			72	40	2	30			

- Molecule 8 is an oligosaccharide called beta-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
8	L	5	Total	C	N	O	0	0	0
			61	34	2	25			

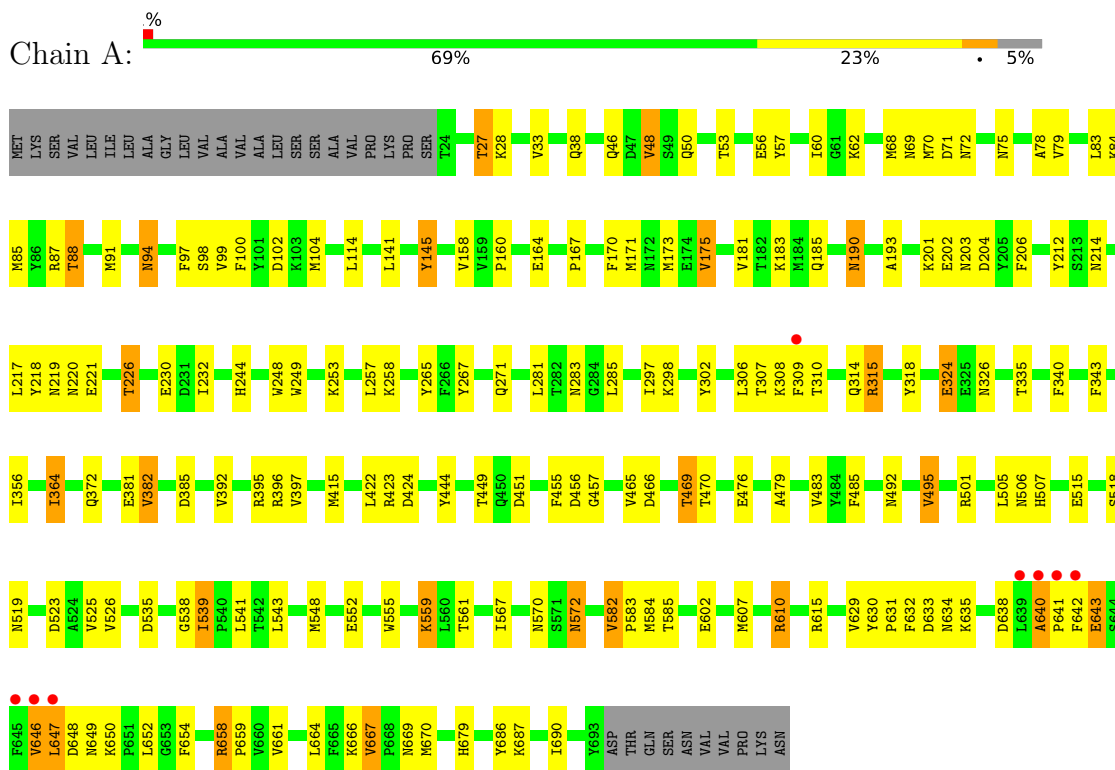
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	29	Total	O	0	0
			29	29		
9	B	14	Total	O	0	0
			14	14		
9	C	19	Total	O	0	0
			19	19		
9	D	27	Total	O	0	0
			27	27		
9	E	21	Total	O	0	0
			21	21		
9	F	10	Total	O	0	0
			10	10		

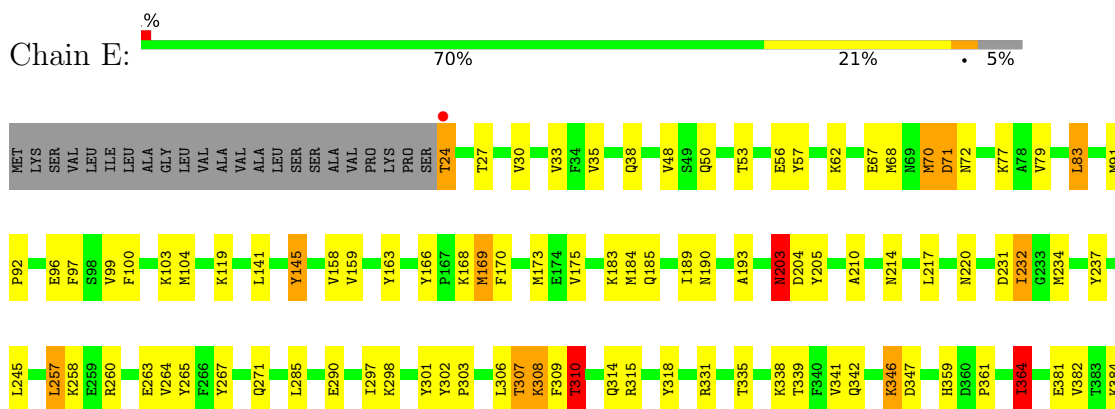
3 Residue-property plots

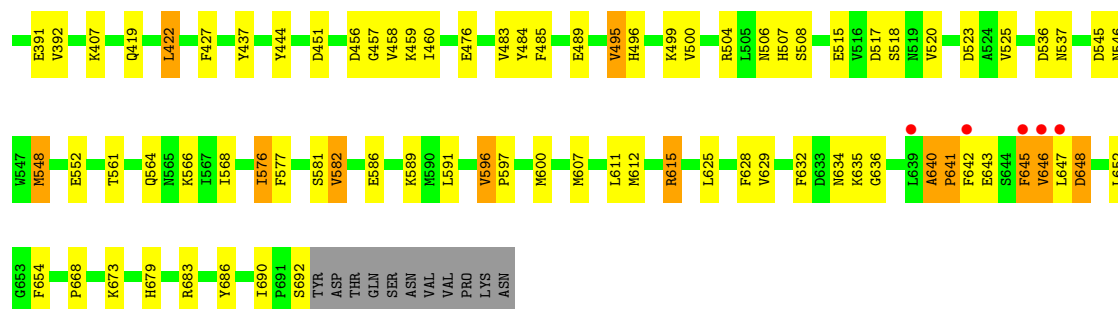
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Arylphorin

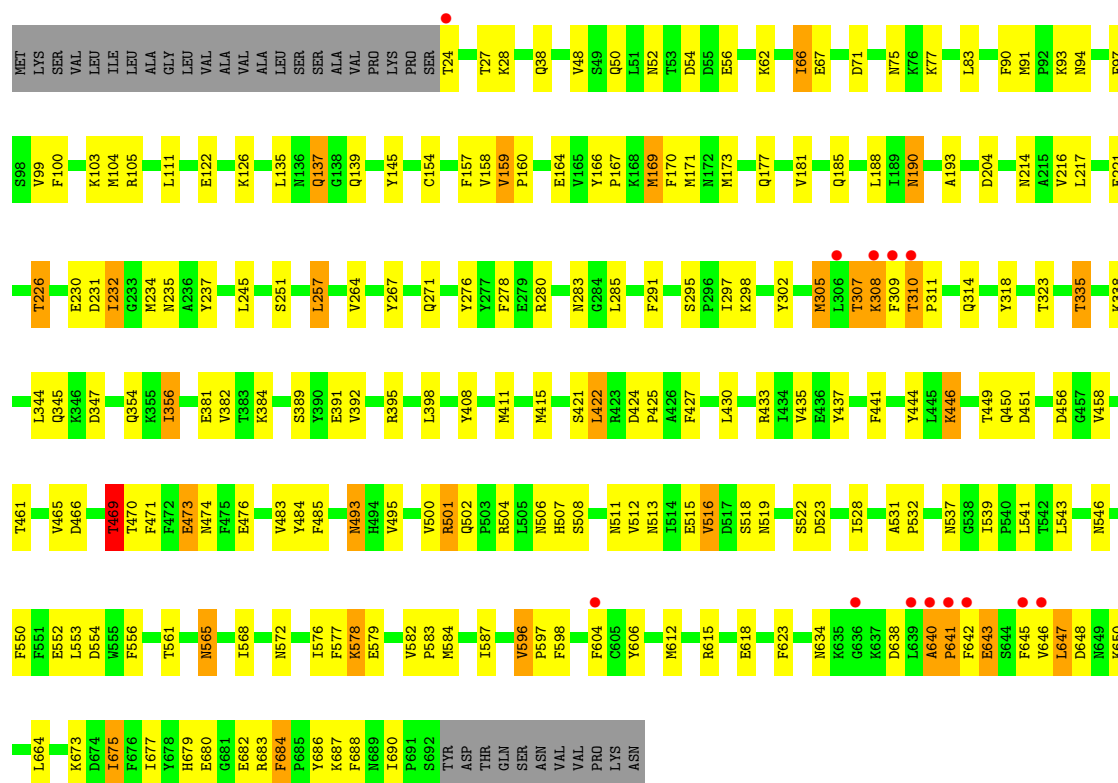


• Molecule 1: Arylphorin

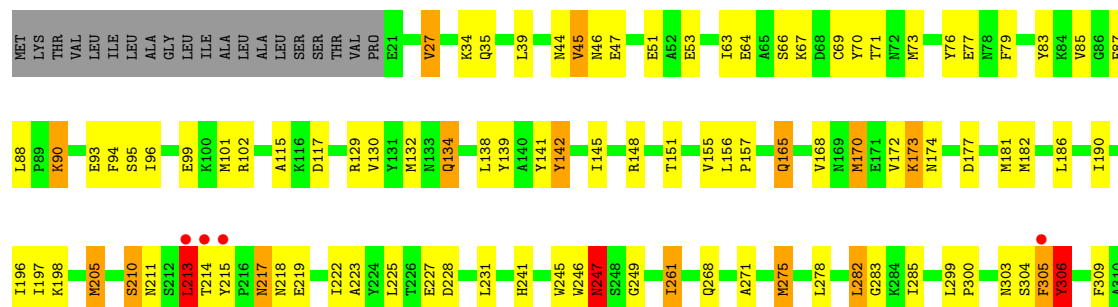


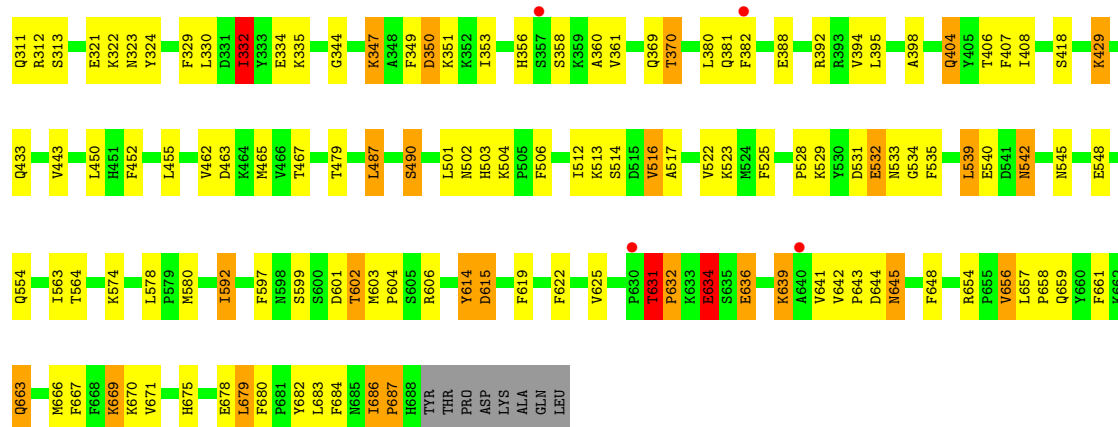


• Molecule 1: Arylphorin

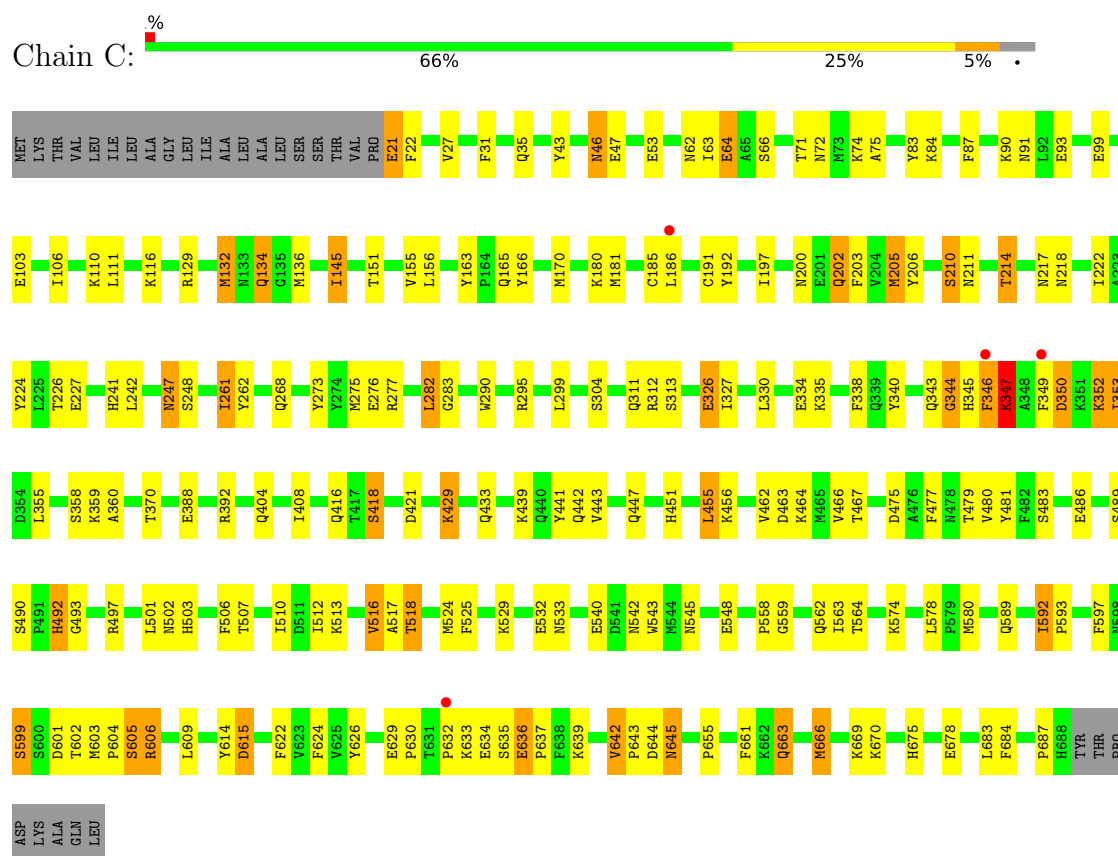


• Molecule 2: Silkworm storage protein

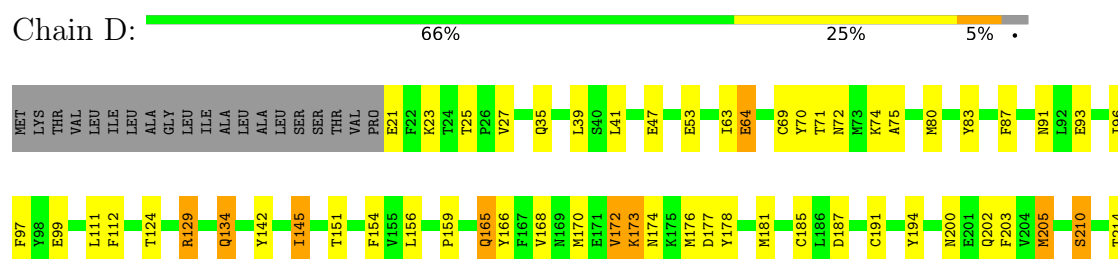


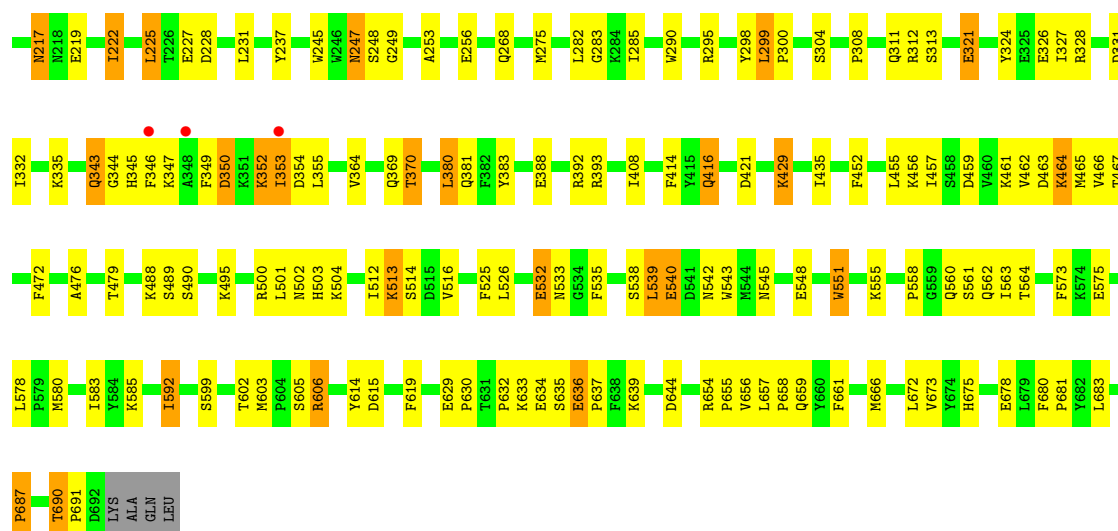


• Molecule 2: Silkworm storage protein



• Molecule 2: Silkworm storage protein





- Molecule 3: alpha-D-mannopyranose-(1-3)-[beta-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain G: 100%



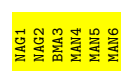
- Molecule 4: beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain H: 40%



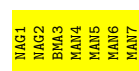
- Molecule 5: alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)-[alpha-D-mannopyranose-(1-3)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 100%

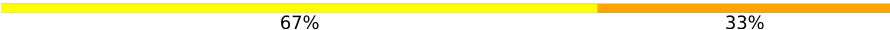


- Molecule 6: alpha-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)-alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 100%



- Molecule 7: beta-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-3)-[alpha-D-mannopyranose-(1-6)]beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K:  67% 33%



- Molecule 8: beta-D-mannopyranose-(1-2)-alpha-D-mannopyranose-(1-3)-beta-D-mannopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L:  20% 80%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	92.06Å 205.02Å 119.71Å 90.00° 103.00° 90.00°	Depositor
Resolution (Å)	48.37 – 2.80 48.37 – 2.80	Depositor EDS
% Data completeness (in resolution range)	96.5 (48.37-2.80) 96.4 (48.37-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.81 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.172 , 0.237 0.171 , 0.236	Depositor DCC
R_{free} test set	5121 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.238	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 37.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	34590	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.42% 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: MAN, BMA, 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	0.77	1/5863 (0.0%)	1.00	8/7934 (0.1%)
1	E	0.73	0/5850	0.98	12/7916 (0.2%)
1	F	0.72	0/5850	1.00	14/7916 (0.2%)
2	B	0.75	1/5865 (0.0%)	1.03	18/7945 (0.2%)
2	C	0.77	0/5865	1.02	12/7945 (0.2%)
2	D	0.78	0/5901	1.03	8/7996 (0.1%)
All	All	0.75	2/35194 (0.0%)	1.01	72/47652 (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
2	B	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	356	HIS	CG-ND1	6.81	1.45	1.38
1	A	315	ARG	C-O	-5.38	1.20	1.25

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	310	THR	N-CA-C	10.04	117.00	108.07
1	F	310	THR	N-CA-C	8.62	118.05	108.14
2	C	282	LEU	N-CA-C	7.53	122.64	113.38
1	F	295	SER	CA-C-N	-7.44	113.02	120.31
1	F	295	SER	C-N-CA	-7.44	113.02	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	282	LEU	N-CA-C	7.41	123.45	113.97
2	D	99	GLU	N-CA-C	7.35	119.08	111.14
2	B	654	ARG	N-CA-C	7.24	114.65	108.13
1	E	364	ILE	CB-CA-C	-6.77	101.67	112.16
2	B	631	THR	CA-C-N	6.63	128.13	119.84
2	B	631	THR	C-N-CA	6.63	128.13	119.84
1	A	658	ARG	CA-C-N	-6.49	113.95	120.31
1	A	658	ARG	C-N-CA	-6.49	113.95	120.31
1	E	690	ILE	CA-C-N	6.44	127.89	119.84
1	E	690	ILE	C-N-CA	6.44	127.89	119.84
2	C	614	TYR	N-CA-C	-6.41	104.34	111.71
2	C	615	ASP	N-CA-CB	-6.36	100.15	109.82
2	C	614	TYR	CA-C-N	6.33	129.59	120.79
2	C	614	TYR	C-N-CA	6.33	129.59	120.79
2	B	686	ILE	CA-C-N	6.31	127.72	119.84
2	B	686	ILE	C-N-CA	6.31	127.72	119.84
1	F	556	PHE	N-CA-C	6.12	117.54	108.60
1	E	315	ARG	CA-C-N	-5.96	114.61	120.52
1	E	315	ARG	C-N-CA	-5.96	114.61	120.52
1	E	346	LYS	N-CA-C	5.94	120.66	113.17
1	F	493	ASN	N-CA-C	5.88	119.67	111.90
1	F	684	PHE	CA-C-N	5.83	125.97	119.32
1	F	684	PHE	C-N-CA	5.83	125.97	119.32
2	D	408	ILE	CA-C-N	-5.83	114.60	120.31
2	D	408	ILE	C-N-CA	-5.83	114.60	120.31
2	D	457	ILE	CB-CA-C	-5.75	104.00	110.96
2	C	156	LEU	CA-C-N	-5.73	114.36	120.03
2	C	156	LEU	C-N-CA	-5.73	114.36	120.03
1	F	159	VAL	CA-C-N	-5.71	114.87	120.98
1	F	159	VAL	C-N-CA	-5.71	114.87	120.98
2	C	132	MET	N-CA-C	5.70	118.35	109.52
2	B	213	LEU	CA-CB-CG	5.68	136.20	116.30
1	A	226	THR	N-CA-C	5.66	118.18	111.33
2	B	636	GLU	N-CA-C	5.66	122.32	109.81
2	C	295	ARG	N-CA-C	5.54	117.12	111.14
1	F	690	ILE	CA-C-N	-5.53	112.93	119.84
1	F	690	ILE	C-N-CA	-5.53	112.93	119.84
2	B	634	GLU	CB-CA-C	-5.46	107.58	114.40
2	D	282	LEU	N-CA-C	5.45	119.91	112.88
2	B	332	ILE	CB-CA-C	-5.44	103.30	112.16
1	A	607	MET	CA-C-N	-5.38	114.25	119.90
1	A	607	MET	C-N-CA	-5.38	114.25	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	361	VAL	CB-CA-C	-5.36	105.02	111.88
2	B	99	GLU	N-CA-C	5.34	117.54	111.02
2	D	654	ARG	CA-C-N	5.31	125.31	119.90
2	D	654	ARG	C-N-CA	5.31	125.31	119.90
1	A	60	ILE	N-CA-C	-5.29	105.56	110.53
2	C	418	SER	N-CA-C	5.27	117.70	111.33
1	E	607	MET	CA-C-N	-5.26	114.50	119.76
1	E	607	MET	C-N-CA	-5.26	114.50	119.76
2	B	70	TYR	CA-C-N	5.24	127.30	120.28
2	B	70	TYR	C-N-CA	5.24	127.30	120.28
1	F	469	THR	CB-CA-C	-5.22	99.39	109.37
1	A	175	VAL	CB-CA-C	-5.21	105.11	112.14
1	E	546	ASN	N-CA-C	5.20	119.37	112.30
1	F	554	ASP	N-CA-C	5.19	116.95	108.55
2	D	295	ARG	N-CA-C	5.18	116.78	111.03
1	A	469	THR	CB-CA-C	5.15	117.76	110.24
2	C	163	TYR	CA-C-N	-5.15	113.62	119.28
2	C	163	TYR	C-N-CA	-5.15	113.62	119.28
1	E	285	LEU	N-CA-C	5.12	120.92	114.31
2	B	534	GLY	N-CA-C	-5.09	107.66	116.01
1	F	634	ASN	N-CA-C	-5.08	99.98	110.80
2	B	88	LEU	CA-C-N	5.05	125.33	119.92
2	B	88	LEU	C-N-CA	5.05	125.33	119.92
1	E	310	THR	CB-CA-C	-5.05	104.60	110.76
2	B	247	ASN	N-CA-CB	-5.03	101.98	110.49

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	246	TRP	Peptide
2	B	614	TYR	Peptide

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	5681	0	5434	132	0
1	E	5669	0	5425	130	0
1	F	5669	0	5425	160	0
2	B	5669	0	5390	204	0
2	C	5669	0	5392	150	0
2	D	5703	0	5419	156	0
3	G	61	0	52	0	0
4	H	61	0	52	3	0
5	I	72	0	61	0	0
6	J	83	0	70	0	0
7	K	72	0	61	1	0
8	L	61	0	52	0	0
9	A	29	0	0	0	0
9	B	14	0	0	0	0
9	C	19	0	0	1	0
9	D	27	0	0	0	0
9	E	21	0	0	0	0
9	F	10	0	0	1	0
All	All	34590	0	32833	866	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (866) 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)
2:B:631:THR:HB	2:B:632:PRO:CD	1.72	1.19
2:B:210:SER:HB2	2:B:214:THR:HG21	1.27	1.16
2:B:631:THR:CB	2:B:632:PRO:HD2	1.77	1.15
1:F:531:ALA:HB2	1:F:550:PHE:CD2	1.83	1.13
2:D:343:GLN:HA	2:D:343:GLN:HE21	1.15	1.11
2:B:95:SER:H	2:B:101:MET:CE	1.65	1.09
2:B:214:THR:HG23	2:B:215:TYR:HD2	1.14	1.08
1:F:531:ALA:HB2	1:F:550:PHE:CE2	1.95	1.01
2:B:631:THR:HB	2:B:632:PRO:HD2	1.01	1.00
2:B:332:ILE:HG12	2:C:335:LYS:HG2	1.42	1.00
2:B:663:GLN:HG2	2:B:666:MET:HE2	1.41	1.00
1:F:640:ALA:N	1:F:641:PRO:HD3	1.77	1.00
1:A:314:GLN:HE22	2:D:311:GLN:H	1.08	1.00
2:D:134:GLN:H	2:D:134:GLN:HE21	1.04	0.99
1:F:232:ILE:HD13	1:F:232:ILE:H	1.26	0.98
2:B:615:ASP:H	2:D:615:ASP:HB3	1.28	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:640:ALA:H	1:E:641:PRO:HD3	1.30	0.97
2:C:340:TYR:HB3	2:C:346:PHE:HD2	1.31	0.95
1:F:531:ALA:CB	1:F:550:PHE:CE2	2.50	0.94
2:B:283:GLY:HA2	2:B:532:GLU:HG2	1.48	0.94
2:C:134:GLN:H	2:C:134:GLN:HE21	1.10	0.94
2:D:283:GLY:HA2	2:D:532:GLU:HG2	1.50	0.94
2:B:502:ASN:HD22	2:B:503:HIS:H	1.09	0.93
2:B:210:SER:HB2	2:B:214:THR:CG2	1.98	0.93
1:E:506:ASN:HD22	1:E:507:HIS:H	1.15	0.93
2:B:211:ASN:O	2:B:214:THR:HG22	1.67	0.93
2:C:72:ASN:HD22	2:C:75:ALA:H	1.12	0.93
1:F:99:VAL:HG22	1:F:105:ARG:HG3	1.49	0.92
2:B:663:GLN:HG2	2:B:666:MET:CE	1.98	0.92
1:F:66:ILE:HD12	1:F:66:ILE:H	1.35	0.92
2:B:134:GLN:H	2:B:134:GLN:NE2	1.68	0.92
1:E:91:MET:SD	1:E:104:MET:HE3	2.09	0.91
2:D:134:GLN:H	2:D:134:GLN:NE2	1.67	0.91
1:E:50:GLN:HE22	1:E:485:PHE:H	1.19	0.91
2:B:182:MET:HE3	2:B:186:LEU:HG	1.52	0.91
2:C:165:GLN:HB3	2:C:479:THR:HG21	1.52	0.90
2:C:72:ASN:ND2	2:C:75:ALA:H	1.68	0.90
2:C:268:GLN:HE22	2:C:548:GLU:H	1.17	0.90
2:C:283:GLY:HA2	2:C:532:GLU:HG2	1.52	0.90
2:C:517:ALA:HB2	2:C:558:PRO:HD3	1.53	0.90
1:E:307:THR:HG22	1:E:310:THR:H	1.37	0.89
2:B:214:THR:HG23	2:B:215:TYR:CD2	2.06	0.89
2:B:134:GLN:H	2:B:134:GLN:HE21	0.89	0.88
2:B:247:ASN:ND2	2:B:249:GLY:H	1.72	0.88
2:B:210:SER:CB	2:B:214:THR:HG21	2.03	0.88
2:D:268:GLN:HE22	2:D:548:GLU:H	1.16	0.87
2:B:134:GLN:HE21	2:B:134:GLN:N	1.71	0.87
1:F:307:THR:HG22	1:F:310:THR:H	1.37	0.87
1:A:75:ASN:ND2	1:A:78:ALA:H	1.71	0.87
1:A:271:GLN:HE22	1:A:552:GLU:H	1.20	0.85
1:F:640:ALA:H	1:F:641:PRO:HD3	1.38	0.85
1:A:335:THR:OG1	2:B:335:LYS:HG2	1.75	0.85
2:C:615:ASP:OD1	1:F:618:GLU:HB3	1.75	0.85
2:C:134:GLN:HE21	2:C:134:GLN:N	1.75	0.84
1:F:190:ASN:HD22	1:F:193:ALA:H	1.24	0.84
1:A:212:TYR:HB3	1:A:226:THR:CG2	2.07	0.84
1:A:642:PHE:O	1:A:643:GLU:HG3	1.79	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:502:ASN:HD22	2:B:503:HIS:N	1.77	0.83
2:D:247:ASN:HD22	2:D:247:ASN:C	1.86	0.83
1:E:97:PHE:HA	1:E:104:MET:HE1	1.61	0.83
1:F:638:ASP:HB2	1:F:647:LEU:HA	1.59	0.82
2:C:181:MET:HE2	1:E:484:TYR:H	1.44	0.82
1:A:314:GLN:NE2	2:D:311:GLN:H	1.78	0.82
1:A:212:TYR:HB3	1:A:226:THR:HG21	1.60	0.82
1:E:97:PHE:HA	1:E:104:MET:CE	2.10	0.82
2:C:663:GLN:HB2	2:C:666:MET:HE2	1.63	0.81
1:E:545:ASP:O	1:E:548:MET:HE1	1.79	0.81
2:B:94:PHE:HA	2:B:101:MET:HE3	1.62	0.81
1:E:103:LYS:HG3	1:E:407:LYS:HB2	1.63	0.81
2:D:343:GLN:HA	2:D:343:GLN:NE2	1.93	0.80
1:A:298:LYS:HE2	1:E:318:TYR:OH	1.80	0.80
2:B:35:GLN:HE22	2:B:155:VAL:H	1.26	0.80
2:C:311:GLN:H	1:E:314:GLN:HE22	1.27	0.80
2:C:542:ASN:HD22	2:C:545:ASN:HD22	1.29	0.80
2:B:615:ASP:N	2:D:615:ASP:HB3	1.96	0.80
2:D:72:ASN:HD22	2:D:75:ALA:H	1.30	0.80
2:B:95:SER:N	2:B:101:MET:CE	2.45	0.80
2:D:573:PHE:HB3	2:D:605:SER:HB3	1.64	0.79
1:F:541:LEU:HD22	1:F:546:ASN:ND2	1.95	0.79
2:B:95:SER:H	2:B:101:MET:HE2	1.48	0.79
2:D:217:ASN:HD22	2:D:219:GLU:H	1.28	0.79
2:B:661:PHE:HA	2:B:666:MET:HE1	1.65	0.79
2:C:447:GLN:NE2	2:C:663:GLN:OE1	2.15	0.78
2:B:450:LEU:HB2	2:B:663:GLN:HE21	1.48	0.78
2:B:349:PHE:O	2:B:350:ASP:HB2	1.83	0.78
2:C:502:ASN:HD22	2:C:503:HIS:H	1.29	0.78
2:B:311:GLN:H	1:F:314:GLN:HE22	1.29	0.78
2:D:476:ALA:O	2:D:479:THR:HG22	1.84	0.78
1:E:271:GLN:HE22	1:E:552:GLU:H	1.29	0.78
1:F:137:GLN:H	1:F:137:GLN:CD	1.91	0.78
2:C:134:GLN:H	2:C:134:GLN:NE2	1.82	0.78
2:C:211:ASN:HB3	9:C:919:HOH:O	1.84	0.78
2:C:510:ILE:HD11	2:C:524:MET:HE2	1.66	0.77
1:A:638:ASP:HB2	1:A:647:LEU:HA	1.66	0.77
1:F:450:GLN:HG2	1:F:664:LEU:HD23	1.66	0.77
2:B:165:GLN:HG3	2:B:479:THR:CG2	2.15	0.76
2:C:166:TYR:CD1	2:C:416:GLN:HG3	2.20	0.76
1:E:91:MET:HE1	1:E:97:PHE:HD2	1.48	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:218:ASN:HB3	2:C:282:LEU:HD21	1.68	0.76
2:D:539:LEU:HG	2:D:656:VAL:HG11	1.66	0.76
1:F:450:GLN:HG2	1:F:664:LEU:CD2	2.16	0.76
2:D:35:GLN:HE21	2:D:39:LEU:HG	1.51	0.75
2:B:663:GLN:CG	2:B:666:MET:HE2	2.15	0.75
2:B:268:GLN:HE22	2:B:548:GLU:H	1.31	0.75
2:C:542:ASN:ND2	2:C:545:ASN:HD22	1.84	0.75
2:C:599:SER:HB3	2:C:639:LYS:HD2	1.69	0.75
1:E:640:ALA:N	1:E:641:PRO:HD3	2.01	0.75
1:A:190:ASN:ND2	1:A:193:ALA:H	1.85	0.75
1:E:67:GLU:CG	1:E:83:LEU:HD21	2.17	0.75
2:B:222:ILE:HD11	2:B:282:LEU:HD12	1.69	0.74
2:D:25:THR:HB	2:D:592:ILE:HG22	1.68	0.74
1:F:231:ASP:O	1:F:235:ASN:ND2	2.19	0.74
1:F:307:THR:HG22	1:F:309:PHE:H	1.53	0.74
2:C:132:MET:HE2	2:C:136:MET:HE3	1.69	0.73
1:A:48:VAL:CG1	1:A:141:LEU:HD11	2.19	0.73
1:F:640:ALA:N	1:F:641:PRO:CD	2.52	0.73
1:F:90:PHE:HD2	1:F:139:GLN:HE22	1.34	0.73
2:B:283:GLY:HA2	2:B:532:GLU:CG	2.19	0.73
2:B:615:ASP:OD1	2:D:614:TYR:HB2	1.88	0.72
1:E:307:THR:HG22	1:E:310:THR:N	2.03	0.72
1:A:75:ASN:HD22	1:A:78:ALA:H	1.36	0.72
1:F:474:ASN:HB3	1:F:501:ARG:HD3	1.69	0.72
1:A:298:LYS:HG2	1:A:318:TYR:CE2	2.24	0.71
2:C:507:THR:HG21	2:C:564:THR:CG2	2.21	0.71
2:C:202:GLN:HG3	2:C:493:GLY:HA2	1.72	0.71
1:E:460:ILE:HD11	1:E:629:VAL:HG23	1.73	0.71
2:B:311:GLN:H	1:F:314:GLN:NE2	1.88	0.71
1:E:525:VAL:HG23	1:E:632:PHE:HB2	1.71	0.71
1:A:48:VAL:HG11	1:A:141:LEU:HD11	1.72	0.71
2:C:507:THR:HG21	2:C:564:THR:HG23	1.72	0.70
1:F:232:ILE:HD13	1:F:232:ILE:N	2.06	0.70
1:F:506:ASN:HD22	1:F:507:HIS:H	1.37	0.70
2:D:23:LYS:HG2	2:D:575:GLU:OE1	1.90	0.70
2:C:340:TYR:HB3	2:C:346:PHE:CD2	2.22	0.70
1:E:234:MET:HE2	1:E:611:LEU:HD13	1.71	0.70
1:E:91:MET:HE1	1:E:97:PHE:CD2	2.26	0.70
1:A:506:ASN:HD22	1:A:507:HIS:H	1.38	0.70
2:C:202:GLN:HG3	2:C:493:GLY:CA	2.22	0.70
2:B:303:ASN:HB2	1:F:173:MET:HE1	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:349:PHE:H	2:C:343:GLN:HE22	1.39	0.70
2:D:247:ASN:C	2:D:247:ASN:ND2	2.46	0.70
1:E:506:ASN:ND2	1:E:507:HIS:H	1.88	0.69
1:F:311:PRO:O	1:F:411:MET:HE2	1.91	0.69
2:C:507:THR:CG2	2:C:564:THR:HG23	2.22	0.69
2:C:502:ASN:ND2	2:C:503:HIS:H	1.90	0.69
2:B:283:GLY:CA	2:B:532:GLU:HG2	2.22	0.69
1:A:470:THR:OG1	1:A:679:HIS:HD2	1.76	0.69
1:A:555:TRP:HH2	1:A:647:LEU:HD12	1.57	0.69
2:B:165:GLN:HG3	2:B:479:THR:HG22	1.73	0.69
2:B:210:SER:OG	2:B:227:GLU:OE2	2.10	0.69
2:C:21:GLU:OE1	2:C:21:GLU:HA	1.92	0.69
2:C:202:GLN:CG	2:C:493:GLY:HA2	2.23	0.69
2:C:512:ILE:HD12	2:C:563:ILE:HD12	1.75	0.69
1:A:307:THR:O	1:A:309:PHE:N	2.26	0.69
1:F:190:ASN:ND2	1:F:193:ALA:H	1.89	0.69
1:A:98:SER:O	1:A:104:MET:HE3	1.92	0.69
2:D:72:ASN:ND2	2:D:75:ALA:H	1.90	0.68
1:F:298:LYS:HG2	1:F:318:TYR:CE2	2.28	0.68
2:B:632:PRO:HB2	2:B:634:GLU:OE2	1.93	0.68
1:A:314:GLN:H	2:D:311:GLN:HE22	1.41	0.68
1:E:35:VAL:HG22	1:E:591:LEU:HD23	1.74	0.68
1:E:100:PHE:HD1	1:E:392:VAL:HG22	1.57	0.68
2:B:467:THR:OG1	2:B:675:HIS:HD2	1.77	0.68
2:D:299:LEU:HB3	2:D:311:GLN:HG2	1.76	0.68
1:F:271:GLN:HE22	1:F:552:GLU:H	1.38	0.68
1:F:476:GLU:HG2	1:F:501:ARG:HG2	1.75	0.67
1:F:232:ILE:H	1:F:232:ILE:CD1	1.94	0.67
1:F:465:VAL:HG21	1:F:675:ILE:HD11	1.76	0.67
2:B:645:ASN:H	2:B:645:ASN:ND2	1.91	0.67
2:B:615:ASP:H	2:D:615:ASP:CB	2.05	0.67
1:E:67:GLU:HG2	1:E:83:LEU:HD21	1.77	0.67
2:D:91:ASN:H	2:D:134:GLN:HE22	1.43	0.67
2:B:450:LEU:CB	2:B:663:GLN:HE21	2.08	0.67
2:D:178:TYR:HD2	2:D:181:MET:HE3	1.58	0.67
2:D:349:PHE:O	2:D:350:ASP:HB2	1.94	0.67
1:E:38:GLN:HE22	1:E:158:VAL:H	1.43	0.66
1:E:640:ALA:H	1:E:641:PRO:CD	2.06	0.66
2:D:134:GLN:HE21	2:D:134:GLN:N	1.84	0.66
2:D:247:ASN:HD22	2:D:248:SER:N	1.94	0.66
1:E:506:ASN:HD22	1:E:507:HIS:N	1.91	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:MET:HE1	1:A:97:PHE:HD2	1.61	0.66
2:C:429:LYS:O	2:C:433:GLN:HG2	1.94	0.66
2:C:467:THR:OG1	2:C:675:HIS:HD2	1.79	0.66
1:F:531:ALA:HB3	1:F:550:PHE:CE2	2.30	0.66
2:C:35:GLN:HE21	2:C:592:ILE:HD11	1.60	0.66
1:E:640:ALA:N	1:E:641:PRO:CD	2.59	0.66
1:E:361:PRO:O	1:E:364:ILE:HG13	1.95	0.66
1:A:50:GLN:HE22	1:A:485:PHE:H	1.42	0.66
2:B:523:LYS:HE2	2:B:548:GLU:OE2	1.95	0.66
1:F:66:ILE:HB	1:F:83:LEU:HD21	1.78	0.66
2:B:539:LEU:HD13	2:B:656:VAL:HG11	1.77	0.65
1:F:38:GLN:HE22	1:F:158:VAL:H	1.44	0.65
1:F:506:ASN:ND2	1:F:507:HIS:H	1.93	0.65
1:F:470:THR:OG1	1:F:679:HIS:HD2	1.78	0.65
2:C:516:VAL:CG1	2:C:518:THR:HG22	2.27	0.65
2:C:99:GLU:O	2:C:103:GLU:HG2	1.97	0.65
2:B:502:ASN:ND2	2:B:503:HIS:H	1.88	0.65
1:F:584:MET:HA	1:F:587:ILE:HD12	1.79	0.65
2:D:64:GLU:HA	2:D:80:MET:HE2	1.78	0.65
2:D:210:SER:OG	2:D:227:GLU:OE2	2.14	0.65
2:B:408:ILE:HG21	1:F:302:TYR:OH	1.97	0.65
2:D:166:TYR:CD1	2:D:416:GLN:HG3	2.32	0.64
2:D:185:CYS:HG	2:D:191:CYS:HG	1.46	0.64
2:D:346:PHE:HB3	2:D:353:ILE:HD11	1.79	0.64
2:C:516:VAL:HG12	2:C:518:THR:HG22	1.80	0.64
2:D:93:GLU:HG2	2:D:304:SER:HB2	1.78	0.64
1:E:628:PHE:HE1	1:E:654:PHE:CE2	2.15	0.64
1:A:190:ASN:C	1:A:190:ASN:HD22	2.06	0.64
1:A:526:VAL:HG22	1:A:629:VAL:HG22	1.80	0.64
2:B:96:ILE:HD13	2:B:139:TYR:CE2	2.33	0.64
2:C:347:LYS:HB3	2:C:352:LYS:HA	1.80	0.64
2:C:529:LYS:NZ	2:C:670:LYS:HE3	2.12	0.64
1:F:646:VAL:C	1:F:648:ASP:H	2.06	0.64
2:B:531:ASP:CG	2:B:533:ASN:HB2	2.24	0.63
2:B:181:MET:CE	1:F:483:VAL:HG13	2.29	0.63
2:C:181:MET:CE	1:E:484:TYR:H	2.09	0.63
2:C:35:GLN:HE22	2:C:155:VAL:H	1.46	0.63
2:D:35:GLN:NE2	2:D:39:LEU:HG	2.14	0.63
2:D:312:ARG:HH22	2:D:421:ASP:CG	2.07	0.63
2:C:529:LYS:HZ3	2:C:670:LYS:HE3	1.64	0.63
2:D:142:TYR:CD2	2:D:156:LEU:HD13	2.34	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:307:THR:CG2	1:F:309:PHE:H	2.11	0.63
1:E:96:GLU:O	1:E:104:MET:HE1	1.99	0.62
1:A:687:LYS:HA	1:A:690:ILE:CD1	2.29	0.62
2:B:66:SER:HB2	2:B:69:CYS:SG	2.40	0.62
1:E:163:TYR:CD1	1:E:232:ILE:HG23	2.35	0.62
2:D:231:LEU:HD13	2:D:603:MET:HE1	1.81	0.62
1:A:314:GLN:H	2:D:311:GLN:NE2	1.96	0.62
2:C:661:PHE:C	2:C:666:MET:HE1	2.25	0.62
1:F:469:THR:HG21	1:F:680:GLU:HG3	1.81	0.62
2:B:408:ILE:CG2	1:F:302:TYR:OH	2.47	0.62
2:C:344:GLY:HA2	2:C:355:LEU:HD12	1.81	0.62
1:F:221:GLU:HB3	1:F:285:LEU:HD21	1.82	0.62
2:C:480:VAL:HG12	1:E:184:MET:HE1	1.81	0.62
1:E:457:GLY:O	1:E:518:SER:HA	2.00	0.62
1:A:640:ALA:H	1:A:641:PRO:CD	2.13	0.62
1:F:307:THR:HG22	1:F:310:THR:N	2.14	0.62
1:F:173:MET:O	1:F:177:GLN:HG2	2.00	0.61
2:B:305:PHE:CD2	2:B:305:PHE:N	2.68	0.61
1:A:314:GLN:HE22	2:D:311:GLN:N	1.90	0.61
2:D:225:LEU:HD22	2:D:231:LEU:HD22	1.80	0.61
1:A:535:ASP:HB3	1:A:541:LEU:HD21	1.83	0.61
1:F:245:LEU:HD21	1:F:251:SER:HB3	1.83	0.61
1:E:50:GLN:NE2	1:E:485:PHE:H	1.96	0.61
2:B:213:LEU:HG	9:F:904:HOH:O	2.00	0.61
2:B:542:ASN:ND2	2:B:545:ASN:HD22	1.98	0.61
2:C:346:PHE:HE1	2:C:353:ILE:HB	1.65	0.61
2:D:459:ASP:OD1	2:D:461:LYS:HE3	2.00	0.61
2:B:165:GLN:HG3	2:B:479:THR:HG21	1.83	0.61
2:B:211:ASN:OD1	2:B:213:LEU:HB3	2.00	0.61
2:D:542:ASN:HD22	2:D:545:ASN:HD22	1.49	0.61
1:E:91:MET:SD	1:E:104:MET:CE	2.86	0.61
2:B:465:MET:HE1	2:B:671:VAL:HB	1.82	0.60
2:C:392:ARG:NH2	2:C:418:SER:OG	2.34	0.60
2:C:516:VAL:HG12	2:C:518:THR:CG2	2.31	0.60
1:F:347:ASP:OD1	1:F:444:TYR:HE2	1.84	0.60
2:B:358:SER:C	2:B:360:ALA:N	2.59	0.60
2:B:247:ASN:ND2	2:B:249:GLY:N	2.48	0.60
2:B:450:LEU:HB2	2:B:663:GLN:NE2	2.15	0.60
2:B:531:ASP:OD2	2:B:533:ASN:HB2	2.01	0.60
2:C:206:TYR:CE2	2:C:497:ARG:HD2	2.36	0.60
1:A:94:ASN:ND2	2:D:194:TYR:OH	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:GLU:HG2	1:A:423:ARG:NH1	2.17	0.60
2:C:185:CYS:HG	2:C:191:CYS:HG	1.47	0.60
2:B:173:LYS:HE2	2:B:177:ASP:OD2	2.02	0.60
2:D:465:MET:CE	2:D:673:VAL:HG22	2.32	0.60
2:B:93:GLU:HG2	2:B:304:SER:HB2	1.83	0.60
2:D:145:ILE:HG21	2:D:156:LEU:HD21	1.82	0.60
1:A:630:TYR:HB2	1:A:631:PRO:CD	2.32	0.60
2:C:210:SER:OG	2:C:227:GLU:OE2	2.20	0.60
2:D:551:TRP:C	2:D:551:TRP:CD1	2.80	0.59
2:B:217:ASN:HD21	2:B:219:GLU:HB2	1.66	0.59
2:B:358:SER:C	2:B:360:ALA:H	2.08	0.59
2:C:507:THR:CG2	2:C:564:THR:CG2	2.78	0.59
2:B:502:ASN:ND2	2:B:503:HIS:N	2.49	0.59
1:F:422:LEU:HD22	1:F:427:PHE:CE2	2.37	0.59
2:B:305:PHE:HA	1:F:177:GLN:HG3	1.85	0.59
2:B:392:ARG:NH2	2:B:418:SER:OG	2.35	0.59
2:C:247:ASN:N	2:C:247:ASN:HD22	1.99	0.59
1:A:642:PHE:C	1:A:643:GLU:HG3	2.27	0.59
1:E:257:LEU:HD11	1:E:264:VAL:HG21	1.84	0.59
1:E:260:ARG:HD3	1:E:263:GLU:OE1	2.03	0.59
2:B:217:ASN:C	2:B:217:ASN:HD22	2.10	0.59
1:F:446:LYS:H	1:F:446:LYS:HD3	1.68	0.59
2:B:217:ASN:HD22	2:B:219:GLU:H	1.51	0.59
1:E:307:THR:O	1:E:309:PHE:N	2.36	0.59
1:F:643:GLU:HB3	1:F:645:PHE:HB2	1.84	0.58
2:C:663:GLN:HB2	2:C:666:MET:CE	2.32	0.58
1:A:267:TYR:OH	1:A:552:GLU:OE1	2.19	0.58
2:D:247:ASN:ND2	2:D:249:GLY:H	2.00	0.58
2:B:217:ASN:ND2	2:B:219:GLU:H	2.00	0.58
2:B:463:ASP:HB2	2:B:506:PHE:HB2	1.85	0.58
2:D:268:GLN:NE2	2:D:548:GLU:H	1.96	0.58
2:C:502:ASN:HD22	2:C:503:HIS:N	1.97	0.58
2:B:95:SER:H	2:B:101:MET:HE3	1.62	0.58
2:B:145:ILE:HG23	2:B:151:THR:CG2	2.33	0.58
1:E:566:LYS:HD3	1:E:568:ILE:HD11	1.86	0.58
1:E:582:VAL:HG12	1:E:586:GLU:HB3	1.85	0.58
1:A:642:PHE:O	1:A:643:GLU:CG	2.51	0.57
2:C:290:TRP:HB3	2:C:327:ILE:HG12	1.86	0.57
1:F:50:GLN:HE22	1:F:485:PHE:H	1.52	0.57
2:C:93:GLU:HG2	2:C:304:SER:HB2	1.85	0.57
2:D:599:SER:HB3	2:D:639:LYS:HE3	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:97:PHE:HA	1:E:104:MET:HE2	1.86	0.57
2:B:332:ILE:CG1	2:C:335:LYS:HG2	2.27	0.57
2:B:388:GLU:O	2:B:392:ARG:HG3	2.05	0.57
2:C:525:PHE:CE2	2:C:548:GLU:HG3	2.39	0.57
2:D:178:TYR:CD2	2:D:181:MET:HE3	2.39	0.57
2:D:636:GLU:CD	2:D:636:GLU:H	2.12	0.57
1:F:283:ASN:OD1	1:F:615:ARG:NH2	2.38	0.57
2:D:465:MET:HE3	2:D:673:VAL:HG22	1.87	0.57
1:E:67:GLU:HG3	1:E:83:LEU:HD21	1.87	0.57
1:F:267:TYR:OH	1:F:552:GLU:OE1	2.23	0.57
2:D:283:GLY:HA2	2:D:532:GLU:CG	2.31	0.57
2:D:503:HIS:HD2	2:D:504:LYS:O	1.88	0.57
1:E:495:VAL:HG23	1:E:496:HIS:CD2	2.40	0.56
1:A:687:LYS:HA	1:A:690:ILE:HD12	1.87	0.56
2:B:429:LYS:O	2:B:433:GLN:HG2	2.06	0.56
2:D:344:GLY:HA2	2:D:355:LEU:HD12	1.85	0.56
1:A:160:PRO:HB3	1:A:584:MET:HG3	1.86	0.56
1:A:257:LEU:HG	1:A:257:LEU:O	2.04	0.56
2:B:304:SER:O	2:B:305:PHE:C	2.47	0.56
2:C:145:ILE:HG23	2:C:151:THR:HG22	1.85	0.56
2:D:388:GLU:O	2:D:392:ARG:HG3	2.05	0.56
1:E:347:ASP:OD1	1:E:444:TYR:HE2	1.89	0.56
1:E:615:ARG:HG2	1:E:679:HIS:CD2	2.41	0.56
1:E:646:VAL:C	1:E:648:ASP:H	2.13	0.56
1:F:24:THR:HG22	1:F:24:THR:O	2.05	0.56
1:F:104:MET:HE3	1:F:408:TYR:HA	1.87	0.56
1:F:170:PHE:HB3	1:F:232:ILE:HG22	1.86	0.56
2:B:663:GLN:HG2	2:B:666:MET:HE1	1.87	0.56
2:D:455:LEU:C	2:D:455:LEU:HD23	2.31	0.56
1:E:205:TYR:CE2	1:E:499:LYS:HE3	2.40	0.56
2:B:261:ILE:HG12	2:B:648:PHE:CE1	2.41	0.56
2:C:603:MET:HG2	2:C:604:PRO:HD2	1.88	0.56
2:D:177:ASP:O	2:D:181:MET:HG3	2.05	0.56
2:D:331:ASP:OD2	1:E:338:LYS:HE2	2.04	0.56
1:E:245:LEU:HB2	1:E:642:PHE:HE1	1.70	0.56
1:A:221:GLU:HB3	1:A:285:LEU:HD21	1.87	0.56
2:D:346:PHE:O	2:D:353:ILE:HG13	2.06	0.56
1:E:168:LYS:NZ	1:E:308:LYS:HE3	2.21	0.56
1:A:271:GLN:HE22	1:A:552:GLU:N	1.98	0.56
1:E:686:TYR:C	1:E:686:TYR:CD2	2.84	0.56
1:A:570:ASN:OD1	1:A:572:ASN:HB2	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:141:TYR:O	2:B:145:ILE:HD12	2.05	0.56
2:B:181:MET:HE2	1:F:484:TYR:H	1.71	0.56
2:D:222:ILE:O	2:D:222:ILE:CG2	2.54	0.55
1:F:398:LEU:HB2	1:F:415:MET:HE1	1.88	0.55
1:F:638:ASP:HB2	1:F:647:LEU:HD22	1.87	0.55
2:C:222:ILE:HG22	2:C:226:THR:HG23	1.88	0.55
2:C:349:PHE:O	2:C:350:ASP:HB2	2.05	0.55
1:A:98:SER:H	1:A:104:MET:CE	2.19	0.55
1:E:628:PHE:HE1	1:E:654:PHE:HE2	1.52	0.55
1:A:212:TYR:HB3	1:A:226:THR:HG22	1.86	0.55
1:A:244:HIS:HD2	1:A:642:PHE:CE1	2.25	0.55
1:A:283:ASN:OD1	1:A:615:ARG:NH2	2.39	0.55
2:D:661:PHE:CA	2:D:666:MET:HE1	2.37	0.55
2:B:170:MET:HE1	1:F:310:THR:N	2.22	0.55
2:B:522:VAL:HG22	2:B:625:VAL:HG22	1.89	0.55
1:F:686:TYR:CE2	1:F:687:LYS:HD2	2.41	0.55
1:A:98:SER:H	1:A:104:MET:HE3	1.71	0.55
1:A:145:TYR:OH	1:A:160:PRO:O	2.24	0.55
2:B:667:PHE:HE2	2:B:669:LYS:HG3	1.72	0.55
2:C:268:GLN:HE22	2:C:548:GLU:N	1.95	0.55
1:E:581:SER:HB2	1:E:600:MET:SD	2.47	0.55
1:F:422:LEU:N	1:F:422:LEU:HD23	2.22	0.55
1:F:541:LEU:HD13	1:F:546:ASN:HB3	1.88	0.55
1:A:46:GLN:CG	1:A:584:MET:HE1	2.37	0.54
2:D:551:TRP:CH2	2:D:644:ASP:HB2	2.42	0.54
2:D:513:LYS:NZ	2:D:560:GLN:HE21	2.06	0.54
1:F:111:LEU:HD22	1:F:135:LEU:HD12	1.89	0.54
2:C:661:PHE:HA	2:C:666:MET:HE1	1.88	0.54
2:D:678:GLU:HG3	2:D:691:PRO:HB3	1.89	0.54
1:F:291:PHE:HB2	1:F:297:ILE:HG22	1.90	0.54
1:F:395:ARG:NH2	1:F:421:SER:OG	2.41	0.54
2:C:203:PHE:HB3	2:C:205:MET:HE2	1.89	0.54
2:D:145:ILE:HG23	2:D:151:THR:HG22	1.90	0.54
2:D:285:ILE:HD12	2:D:429:LYS:HG2	1.89	0.54
2:B:275:MET:HE2	2:B:528:PRO:HD3	1.89	0.54
2:D:462:VAL:HG12	2:D:463:ASP:O	2.08	0.54
1:E:185:GLN:NE2	1:E:189:ILE:HD12	2.23	0.54
1:A:265:TYR:CE1	1:A:372:GLN:HB2	2.43	0.54
2:C:275:MET:CE	2:C:545:ASN:O	2.56	0.54
1:A:646:VAL:C	1:A:648:ASP:H	2.16	0.53
2:D:83:TYR:HA	2:D:87:PHE:CE1	2.43	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:190:ASN:HB3	1:E:193:ALA:HB3	1.90	0.53
1:A:75:ASN:ND2	1:A:78:ALA:N	2.50	0.53
2:B:67:LYS:HG2	2:B:76:TYR:CE2	2.43	0.53
2:D:47:GLU:O	2:D:129:ARG:NH2	2.41	0.53
1:F:166:TYR:HB3	1:F:169:MET:HG3	1.89	0.53
1:A:525:VAL:HG23	1:A:632:PHE:HB2	1.90	0.53
1:E:35:VAL:HG22	1:E:591:LEU:CD2	2.37	0.53
1:E:301:TYR:CD2	1:E:303:PRO:HD3	2.43	0.53
1:F:91:MET:HE1	1:F:97:PHE:HB2	1.89	0.53
2:C:663:GLN:CB	2:C:666:MET:HE2	2.36	0.53
1:E:190:ASN:C	1:E:190:ASN:HD22	2.17	0.53
2:C:346:PHE:CE1	2:C:353:ILE:HB	2.43	0.53
1:E:335:THR:OG1	1:F:338:LYS:HG2	2.08	0.53
1:F:465:VAL:HG21	1:F:675:ILE:CD1	2.39	0.53
2:C:224:TYR:OH	2:C:276:GLU:OE1	2.26	0.53
1:A:666:LYS:HA	1:A:670:MET:HE2	1.92	0.52
2:B:218:ASN:HB3	2:B:282:LEU:HD21	1.91	0.52
1:F:307:THR:HG22	1:F:309:PHE:N	2.23	0.52
2:C:624:PHE:CE1	2:C:626:TYR:CD2	2.98	0.52
2:B:174:ASN:ND2	1:F:308:LYS:HA	2.25	0.52
2:D:464:LYS:HD3	2:D:466:VAL:CG2	2.39	0.52
1:F:214:ASN:HA	1:F:217:LEU:O	2.08	0.52
1:A:190:ASN:HD22	1:A:193:ALA:H	1.55	0.52
2:C:83:TYR:HA	2:C:87:PHE:HE1	1.74	0.52
2:C:510:ILE:HD11	2:C:524:MET:CE	2.39	0.52
1:A:470:THR:OG1	1:A:679:HIS:CD2	2.61	0.52
1:A:476:GLU:HG2	1:A:501:ARG:HG3	1.91	0.52
2:C:502:ASN:ND2	2:C:503:HIS:N	2.58	0.52
2:B:303:ASN:HB2	1:F:173:MET:CE	2.39	0.52
1:F:100:PHE:HD1	1:F:392:VAL:HG22	1.74	0.52
2:B:531:ASP:OD1	2:B:533:ASN:HB2	2.10	0.52
2:B:533:ASN:HB3	2:B:535:PHE:HB2	1.91	0.52
1:E:459:LYS:HG3	1:E:668:PRO:HB3	1.92	0.52
1:F:506:ASN:HD22	1:F:507:HIS:N	2.06	0.52
1:F:93:LYS:O	1:F:94:ASN:HB2	2.09	0.52
1:A:505:LEU:O	1:A:610:ARG:HD3	2.10	0.51
2:B:271:ALA:O	2:B:275:MET:HE3	2.10	0.51
2:C:145:ILE:HG23	2:C:151:THR:CG2	2.40	0.51
1:E:57:TYR:CD1	1:E:57:TYR:C	2.88	0.51
1:E:70:MET:HG3	1:E:79:VAL:HG11	1.92	0.51
1:F:278:PHE:CE1	1:F:532:PRO:HG3	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:174:ASN:HD22	1:F:308:LYS:C	2.19	0.51
2:D:91:ASN:H	2:D:134:GLN:NE2	2.08	0.51
2:D:173:LYS:HA	2:D:176:MET:HE2	1.92	0.51
1:F:495:VAL:HG12	1:F:495:VAL:O	2.10	0.51
1:A:164:GLU:OE2	1:A:583:PRO:HA	2.11	0.51
2:D:222:ILE:O	2:D:222:ILE:HG22	2.09	0.51
2:D:290:TRP:HB3	2:D:327:ILE:HG12	1.92	0.51
2:D:343:GLN:NE2	2:D:343:GLN:CA	2.68	0.51
2:D:513:LYS:HZ2	2:D:560:GLN:HG2	1.76	0.51
1:F:91:MET:SD	1:F:104:MET:HE2	2.51	0.51
4:H:2:NAG:H61	4:H:3:BMA:C1	2.41	0.51
1:A:315:ARG:HH22	1:A:424:ASP:CG	2.17	0.51
2:B:615:ASP:HB2	2:D:615:ASP:HB3	1.92	0.51
1:A:173:MET:HE3	2:D:308:PRO:HD3	1.93	0.51
1:A:444:TYR:N	1:A:444:TYR:HD1	2.09	0.51
2:D:214:THR:HB	2:D:299:LEU:O	2.11	0.51
2:B:645:ASN:ND2	2:B:645:ASN:N	2.56	0.51
2:B:661:PHE:HA	2:B:666:MET:CE	2.37	0.51
2:C:312:ARG:NH2	2:C:421:ASP:OD2	2.43	0.51
2:D:349:PHE:O	2:D:350:ASP:CB	2.59	0.51
1:A:640:ALA:H	1:A:641:PRO:HD2	1.75	0.51
2:B:275:MET:HG2	2:B:619:PHE:CE1	2.45	0.51
1:F:94:ASN:H	1:F:137:GLN:HE22	1.58	0.51
2:B:217:ASN:HD22	2:B:219:GLU:N	2.09	0.50
2:B:245:TRP:HA	2:B:380:LEU:HG	1.93	0.50
2:C:47:GLU:O	2:C:129:ARG:NH2	2.44	0.50
2:C:330:LEU:O	2:C:334:GLU:HG3	2.10	0.50
2:C:533:ASN:HD21	1:F:214:ASN:HD22	1.58	0.50
2:C:578:LEU:HD12	2:C:593:PRO:HG3	1.94	0.50
1:F:648:ASP:C	1:F:650:LYS:H	2.19	0.50
2:C:475:ASP:OD1	2:C:477:PHE:HB3	2.10	0.50
1:F:190:ASN:ND2	1:F:193:ALA:N	2.60	0.50
1:A:181:VAL:O	1:A:185:GLN:HG3	2.12	0.50
1:A:217:LEU:HD21	1:A:302:TYR:HB3	1.93	0.50
1:E:615:ARG:HG2	1:E:679:HIS:HD2	1.74	0.50
2:B:222:ILE:HD11	2:B:282:LEU:CD1	2.39	0.50
2:B:663:GLN:H	2:B:666:MET:CE	2.25	0.50
1:E:234:MET:O	1:E:237:TYR:HB3	2.11	0.50
1:A:91:MET:HE1	1:A:97:PHE:CD2	2.45	0.49
2:D:176:MET:HG2	2:D:205:MET:HE3	1.94	0.49
2:D:533:ASN:OD1	2:D:535:PHE:HD1	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:278:PHE:HE1	1:F:532:PRO:HG3	1.76	0.49
2:B:44:ASN:HD22	2:B:487:LEU:HD21	1.76	0.49
2:C:180:LYS:HE3	2:C:481:TYR:O	2.12	0.49
2:B:321:GLU:HA	2:B:324:TYR:CE1	2.47	0.49
2:D:502:ASN:HD22	2:D:503:HIS:H	1.59	0.49
2:B:631:THR:HG21	2:B:645:ASN:OD1	2.13	0.49
2:C:304:SER:O	1:E:173:MET:HE1	2.12	0.49
2:C:678:GLU:OE1	2:C:683:LEU:HD13	2.12	0.49
2:D:203:PHE:HB3	2:D:205:MET:HE2	1.95	0.49
2:D:332:ILE:HG21	1:E:341:VAL:HB	1.95	0.49
1:F:458:VAL:HG22	1:F:518:SER:HB2	1.93	0.49
2:B:299:LEU:HD23	1:F:411:MET:SD	2.53	0.49
2:C:636:GLU:HB3	2:C:637:PRO:HD2	1.94	0.49
1:E:485:PHE:CD1	1:E:495:VAL:HG12	2.47	0.49
1:E:552:GLU:HG2	1:E:576:ILE:HD13	1.95	0.49
1:F:450:GLN:H	1:F:664:LEU:HD22	1.77	0.49
1:A:100:PHE:HD1	1:A:392:VAL:HG22	1.77	0.49
1:A:559:LYS:HD3	1:A:559:LYS:N	2.28	0.49
2:C:636:GLU:CD	2:C:636:GLU:H	2.19	0.49
2:D:217:ASN:ND2	2:D:219:GLU:H	2.04	0.49
1:E:307:THR:HG23	1:E:309:PHE:H	1.76	0.49
1:A:444:TYR:N	1:A:444:TYR:CD1	2.80	0.49
2:C:31:PHE:CE2	2:C:592:ILE:HD12	2.48	0.49
2:D:661:PHE:HA	2:D:666:MET:HE1	1.94	0.49
1:A:202:GLU:O	1:A:203:ASN:HB2	2.12	0.49
2:B:210:SER:HB2	2:B:214:THR:CB	2.43	0.49
2:B:631:THR:O	2:B:632:PRO:O	2.29	0.49
2:C:214:THR:HB	2:C:299:LEU:O	2.13	0.49
2:C:678:GLU:HB2	2:C:684:PHE:CE1	2.47	0.49
1:E:267:TYR:OH	1:E:552:GLU:OE1	2.29	0.49
1:F:159:VAL:CG1	1:F:160:PRO:HD2	2.43	0.49
1:A:84:LYS:HG3	1:A:87:ARG:NH2	2.28	0.49
1:A:648:ASP:C	1:A:650:LYS:H	2.21	0.49
1:F:469:THR:CG2	1:F:680:GLU:HG3	2.43	0.49
2:B:145:ILE:HG23	2:B:151:THR:HG22	1.95	0.48
2:B:151:THR:O	2:B:151:THR:HG22	2.13	0.48
1:F:52:ASN:OD1	1:F:54:ASP:HB2	2.13	0.48
2:B:332:ILE:HD11	2:C:338:PHE:CD1	2.48	0.48
1:F:430:LEU:O	1:F:433:ARG:HB3	2.14	0.48
1:A:173:MET:HE2	1:A:306:LEU:HG	1.94	0.48
1:E:234:MET:CE	1:E:611:LEU:HD13	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:577:PHE:CZ	1:F:612:MET:HG3	2.47	0.48
2:C:222:ILE:HG22	2:C:222:ILE:O	2.13	0.48
2:C:241:HIS:CE1	2:C:601:ASP:HB3	2.48	0.48
2:D:328:ARG:HD2	1:E:437:TYR:OH	2.13	0.48
1:F:67:GLU:HG2	1:F:83:LEU:HD13	1.95	0.48
1:A:214:ASN:O	1:E:537:ASN:ND2	2.36	0.48
2:B:168:VAL:HG13	2:B:172:VAL:HB	1.96	0.48
2:C:344:GLY:HA2	2:C:355:LEU:CD1	2.42	0.48
1:E:231:ASP:OD2	1:E:504:ARG:NH1	2.46	0.48
2:B:211:ASN:C	2:B:213:LEU:H	2.22	0.48
2:B:529:LYS:HE2	2:B:670:LYS:HG2	1.96	0.48
2:B:615:ASP:CA	2:D:615:ASP:HB3	2.43	0.48
2:D:151:THR:HA	2:D:154:PHE:HD2	1.78	0.48
1:A:48:VAL:HG13	1:A:141:LEU:HD11	1.92	0.48
2:B:142:TYR:OH	2:B:157:PRO:O	2.26	0.48
2:B:404:GLN:HE21	2:B:404:GLN:HA	1.78	0.48
2:C:192:TYR:HD1	2:C:197:ILE:CG2	2.26	0.48
2:D:145:ILE:CG1	2:D:151:THR:HG21	2.44	0.48
2:B:304:SER:O	2:B:306:TYR:HB2	2.13	0.48
1:F:159:VAL:HG12	1:F:160:PRO:HD2	1.96	0.48
2:C:326:GLU:O	2:C:330:LEU:HG	2.14	0.48
1:F:234:MET:O	1:F:237:TYR:HB3	2.13	0.48
1:A:506:ASN:HD22	1:A:507:HIS:N	2.08	0.47
1:F:643:GLU:HG3	1:F:645:PHE:HD1	1.79	0.47
1:A:167:PRO:HB2	1:A:171:MET:CE	2.44	0.47
1:A:326:ASN:ND2	1:A:397:VAL:HG13	2.29	0.47
2:B:304:SER:O	2:B:306:TYR:N	2.46	0.47
2:B:141:TYR:CZ	2:B:145:ILE:HD11	2.50	0.47
2:B:408:ILE:HG21	1:F:302:TYR:CZ	2.49	0.47
2:B:614:TYR:HE1	2:B:679:LEU:HD12	1.79	0.47
2:C:46:ASN:OD1	2:C:46:ASN:N	2.40	0.47
2:D:542:ASN:ND2	2:D:545:ASN:HD22	2.13	0.47
1:E:173:MET:CG	1:E:306:LEU:HG	2.44	0.47
1:E:517:ASP:OD1	1:E:564:GLN:HG2	2.14	0.47
1:F:638:ASP:CB	1:F:647:LEU:HA	2.39	0.47
2:C:483:SER:OG	2:C:486:GLU:HG3	2.14	0.47
1:A:492:ASN:HD22	1:A:492:ASN:N	2.11	0.47
2:B:285:ILE:HD12	2:B:429:LYS:HG3	1.97	0.47
2:D:298:TYR:CE2	2:D:300:PRO:HG3	2.49	0.47
2:D:335:LYS:HB3	1:F:335:THR:HG23	1.96	0.47
1:F:154:CYS:HA	1:F:157:PHE:HD1	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:457:GLY:O	1:A:518:SER:HA	2.15	0.47
1:A:667:VAL:HG13	1:A:669:ASN:OD1	2.15	0.47
2:B:39:LEU:HB3	2:B:580:MET:HE3	1.96	0.47
2:B:503:HIS:HD2	2:B:504:LYS:O	1.98	0.47
2:B:657:LEU:HB3	2:B:659:GLN:HE22	1.79	0.47
2:C:481:TYR:H	1:E:184:MET:HE2	1.80	0.47
2:D:168:VAL:CG1	2:D:172:VAL:HB	2.45	0.47
1:F:38:GLN:HE22	1:F:158:VAL:N	2.10	0.47
1:F:623:PHE:CD2	1:F:677:ILE:HD12	2.49	0.47
1:A:218:TYR:OH	1:E:536:ASP:HB3	2.15	0.47
2:B:680:PHE:HB2	2:B:683:LEU:HD12	1.96	0.47
2:C:451:HIS:ND1	2:C:663:GLN:NE2	2.61	0.47
1:A:658:ARG:HB2	1:A:659:PRO:HD2	1.97	0.47
2:B:96:ILE:HD11	2:B:102:ARG:HG3	1.96	0.47
2:B:96:ILE:HG13	2:B:96:ILE:O	2.15	0.47
2:C:642:VAL:O	2:C:644:ASP:N	2.47	0.47
2:D:151:THR:HA	2:D:154:PHE:CD2	2.50	0.47
2:D:636:GLU:CB	2:D:637:PRO:CD	2.92	0.47
1:E:38:GLN:HE22	1:E:158:VAL:N	2.09	0.47
2:C:451:HIS:HA	2:C:663:GLN:HG3	1.97	0.47
2:C:480:VAL:HA	1:E:184:MET:HE1	1.97	0.47
2:D:346:PHE:CB	2:D:353:ILE:HD11	2.45	0.47
1:E:646:VAL:HG21	1:E:652:LEU:HD21	1.96	0.47
1:A:686:TYR:C	1:A:686:TYR:CD2	2.92	0.46
2:C:43:TYR:CE1	2:C:580:MET:HE2	2.50	0.46
2:D:41:LEU:HD22	2:D:129:ARG:HG2	1.97	0.46
1:E:217:LEU:HD21	1:E:302:TYR:HB3	1.98	0.46
1:A:79:VAL:O	1:A:83:LEU:HG	2.14	0.46
1:A:219:ASN:O	1:A:220:ASN:HB3	2.15	0.46
2:B:222:ILE:HG22	2:B:222:ILE:O	2.15	0.46
2:C:455:LEU:C	2:C:455:LEU:HD12	2.40	0.46
1:F:347:ASP:OD1	1:F:444:TYR:CE2	2.66	0.46
2:C:312:ARG:HH22	2:C:421:ASP:CG	2.22	0.46
1:F:596:VAL:HG12	1:F:597:PRO:HD2	1.98	0.46
2:B:83:TYR:HB2	2:B:87:PHE:HE1	1.81	0.46
2:B:465:MET:HE1	2:B:671:VAL:CB	2.45	0.46
2:C:83:TYR:HA	2:C:87:PHE:CE1	2.51	0.46
2:C:206:TYR:CZ	2:C:497:ARG:HD2	2.51	0.46
2:B:501:LEU:HG	2:B:502:ASN:N	2.30	0.46
1:A:50:GLN:NE2	1:A:485:PHE:H	2.12	0.46
2:B:542:ASN:HD22	2:B:545:ASN:HD22	1.62	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:262:TYR:OH	2:C:388:GLU:OE1	2.26	0.46
2:D:185:CYS:SG	2:D:191:CYS:SG	3.02	0.46
1:F:231:ASP:OD1	1:F:504:ARG:HD2	2.14	0.46
1:E:339:THR:HG21	1:F:345:GLN:HE22	1.81	0.46
1:A:465:VAL:HG12	1:A:466:ASP:O	2.16	0.46
1:A:538:GLY:O	1:E:686:TYR:OH	2.29	0.46
2:B:44:ASN:O	2:B:46:ASN:N	2.49	0.46
1:F:682:GLU:HB2	1:F:688:PHE:CE1	2.51	0.46
1:A:615:ARG:HG3	1:A:679:HIS:CD2	2.51	0.46
2:B:145:ILE:HG23	2:B:151:THR:HG21	1.98	0.46
2:B:275:MET:HE1	2:B:545:ASN:O	2.16	0.46
2:C:180:LYS:HB3	1:E:184:MET:HE3	1.97	0.46
2:D:678:GLU:OE1	2:D:683:LEU:HD13	2.16	0.46
1:A:535:ASP:OD1	1:A:539:ILE:HD12	2.16	0.45
2:B:93:GLU:CG	2:B:304:SER:HB2	2.46	0.45
2:B:599:SER:HA	2:B:639:LYS:HD3	1.98	0.45
2:C:62:ASN:OD1	2:C:64:GLU:HG3	2.15	0.45
1:A:102:ASP:HB3	1:A:385:ASP:OD2	2.16	0.45
1:A:667:VAL:CG1	1:A:669:ASN:OD1	2.64	0.45
1:F:232:ILE:HD12	1:F:502:GLN:OE1	2.17	0.45
1:F:476:GLU:HA	1:F:500:VAL:O	2.15	0.45
1:F:578:LYS:HG2	1:F:606:TYR:HB2	1.98	0.45
2:B:44:ASN:C	2:B:46:ASN:H	2.24	0.45
2:C:35:GLN:NE2	2:C:155:VAL:HB	2.31	0.45
2:C:72:ASN:HD21	2:C:74:LYS:HB3	1.81	0.45
2:C:349:PHE:O	2:C:350:ASP:CB	2.64	0.45
1:E:643:GLU:HB3	1:E:645:PHE:HB2	1.97	0.45
2:B:95:SER:N	2:B:101:MET:HE1	2.31	0.45
2:D:690:THR:HA	2:D:691:PRO:HD3	1.63	0.45
1:E:568:ILE:HD12	1:E:568:ILE:N	2.31	0.45
1:F:167:PRO:O	1:F:171:MET:HE3	2.16	0.45
1:F:584:MET:HE2	1:F:584:MET:HB3	1.88	0.45
4:H:2:NAG:C6	4:H:3:BMA:C1	2.94	0.45
2:C:273:TYR:CE1	2:C:277:ARG:HD2	2.52	0.45
2:C:283:GLY:HA2	2:C:532:GLU:CG	2.34	0.45
2:C:542:ASN:HD22	2:C:545:ASN:ND2	2.05	0.45
1:E:307:THR:C	1:E:309:PHE:H	2.25	0.45
2:C:513:LYS:HA	2:C:559:GLY:O	2.17	0.45
2:D:275:MET:HE1	2:D:526:LEU:HG	1.99	0.45
1:E:183:LYS:NZ	1:E:489:GLU:OE1	2.50	0.45
1:F:181:VAL:O	1:F:185:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:190:ASN:ND2	1:A:190:ASN:C	2.74	0.45
2:B:347:LYS:HA	2:B:351:LYS:O	2.16	0.45
2:B:603:MET:HG2	2:B:604:PRO:HD2	1.99	0.45
2:D:247:ASN:HD22	2:D:249:GLY:H	1.63	0.45
1:E:507:HIS:HD2	1:E:508:SER:O	2.00	0.45
1:A:582:VAL:HG12	1:A:583:PRO:HD2	1.98	0.45
2:B:27:VAL:HG21	2:B:592:ILE:HG12	1.98	0.45
2:B:369:GLN:O	2:B:370:THR:C	2.60	0.45
2:B:467:THR:OG1	2:B:675:HIS:CD2	2.65	0.45
2:C:181:MET:HE1	1:E:483:VAL:HA	1.98	0.45
2:D:253:ALA:O	2:D:256:GLU:HG2	2.16	0.45
2:D:657:LEU:HB3	2:D:659:GLN:NE2	2.32	0.45
1:E:77:LYS:HD2	1:E:77:LYS:N	2.31	0.45
1:E:331:ARG:HD2	1:F:437:TYR:OH	2.16	0.45
1:A:38:GLN:NE2	1:A:158:VAL:HB	2.32	0.45
2:D:636:GLU:HB3	2:D:637:PRO:HD3	1.99	0.45
1:E:476:GLU:HA	1:E:500:VAL:O	2.17	0.45
2:D:467:THR:OG1	2:D:675:HIS:HD2	1.99	0.45
1:E:72:ASN:HA	1:E:119:LYS:HE2	1.99	0.45
1:A:27:THR:HG23	1:A:28:LYS:N	2.32	0.44
2:B:79:PHE:HZ	2:B:132:MET:HE1	1.82	0.44
2:C:455:LEU:HD12	2:C:456:LYS:N	2.32	0.44
1:A:395:ARG:HG2	1:A:415:MET:HE2	1.99	0.44
1:A:632:PHE:CG	1:A:632:PHE:O	2.71	0.44
2:B:35:GLN:HE22	2:B:155:VAL:N	2.03	0.44
2:B:95:SER:O	2:B:101:MET:HE2	2.16	0.44
2:B:101:MET:HE1	2:B:407:PHE:HE1	1.82	0.44
2:B:311:GLN:NE2	1:F:314:GLN:H	2.14	0.44
2:C:408:ILE:HG21	1:E:302:TYR:OH	2.17	0.44
2:D:202:GLN:OE1	2:D:495:LYS:HE3	2.18	0.44
2:D:343:GLN:HE21	2:D:343:GLN:CA	2.03	0.44
2:D:369:GLN:O	2:D:370:THR:C	2.60	0.44
1:E:141:LEU:O	1:E:145:TYR:HB2	2.17	0.44
1:F:541:LEU:HD13	1:F:546:ASN:CB	2.47	0.44
1:F:576:ILE:HG22	1:F:576:ILE:O	2.17	0.44
2:B:525:PHE:HB2	2:B:622:PHE:HB3	1.99	0.44
2:B:540:GLU:HG3	2:B:658:PRO:HD3	1.98	0.44
2:C:512:ILE:HD12	2:C:563:ILE:CD1	2.44	0.44
2:D:332:ILE:HG12	1:E:342:GLN:HG3	1.99	0.44
1:F:391:GLU:O	1:F:395:ARG:HG3	2.16	0.44
1:A:244:HIS:HD2	1:A:642:PHE:CZ	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:213:LEU:CD2	1:F:411:MET:HB2	2.48	0.44
2:B:312:ARG:HD3	2:B:395:LEU:O	2.18	0.44
2:D:452:PHE:CD1	2:D:452:PHE:C	2.95	0.44
2:D:512:ILE:HD11	2:D:561:SER:OG	2.17	0.44
1:E:173:MET:HG2	1:E:306:LEU:HG	1.99	0.44
1:E:458:VAL:HA	1:E:517:ASP:O	2.18	0.44
1:A:298:LYS:HE2	1:E:318:TYR:HH	1.78	0.44
2:B:322:LYS:NZ	2:B:398:ALA:O	2.50	0.44
2:D:112:PHE:HE1	2:D:124:THR:HG22	1.82	0.44
2:D:347:LYS:HE3	2:D:352:LYS:HE3	1.99	0.44
2:B:311:GLN:HE22	1:F:314:GLN:H	1.66	0.44
2:D:174:ASN:O	2:D:178:TYR:CD1	2.71	0.44
1:A:75:ASN:HD21	1:A:78:ALA:H	1.61	0.44
2:B:686:ILE:HA	2:B:687:PRO:HD2	1.70	0.44
2:C:106:ILE:HG22	2:C:110:LYS:HE3	1.99	0.44
1:E:203:ASN:HD22	1:E:204:ASP:H	1.66	0.44
1:F:122:GLU:O	1:F:126:LYS:HG3	2.18	0.44
1:F:226:THR:O	1:F:230:GLU:HB2	2.18	0.44
1:F:679:HIS:HE1	1:F:682:GLU:O	2.01	0.44
1:A:253:LYS:O	1:A:253:LYS:HG2	2.16	0.44
2:C:151:THR:HG22	2:C:151:THR:O	2.17	0.44
2:D:93:GLU:CG	2:D:304:SER:HB2	2.45	0.44
1:A:364:ILE:O	1:A:364:ILE:HD13	2.17	0.43
2:B:329:PHE:HA	2:B:332:ILE:CD1	2.48	0.43
1:E:173:MET:HE2	1:E:173:MET:HB3	1.70	0.43
1:A:214:ASN:HA	1:A:217:LEU:O	2.18	0.43
1:A:340:PHE:O	1:A:343:PHE:HB2	2.17	0.43
1:E:24:THR:HG23	1:E:24:THR:O	2.17	0.43
1:A:57:TYR:C	1:A:57:TYR:CD1	2.96	0.43
2:B:35:GLN:NE2	2:B:155:VAL:H	2.04	0.43
2:D:321:GLU:HA	2:D:324:TYR:CE1	2.53	0.43
1:F:640:ALA:H	1:F:641:PRO:CD	2.18	0.43
2:B:678:GLU:HB2	2:B:684:PHE:CE1	2.53	0.43
2:C:35:GLN:HE22	2:C:155:VAL:HB	1.83	0.43
2:C:525:PHE:HB2	2:C:622:PHE:HB3	2.01	0.43
2:D:275:MET:HE3	2:D:619:PHE:CD1	2.53	0.43
2:D:364:VAL:HG11	2:D:435:ILE:HG23	2.00	0.43
2:D:455:LEU:HD23	2:D:456:LYS:N	2.34	0.43
1:F:424:ASP:O	1:F:425:PRO:C	2.60	0.43
2:B:196:ILE:HG23	2:B:205:MET:HE3	2.01	0.43
2:B:241:HIS:CE1	2:B:601:ASP:HB3	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:278:LEU:CD2	2:B:532:GLU:HG3	2.49	0.43
2:C:629:GLU:HA	2:C:630:PRO:HD3	1.87	0.43
2:D:159:PRO:HD3	2:D:237:TYR:OH	2.19	0.43
1:E:170:PHE:O	1:E:232:ILE:HD11	2.18	0.43
1:F:458:VAL:HG22	1:F:518:SER:CB	2.48	0.43
1:F:466:ASP:OD2	1:F:511:ASN:HB2	2.19	0.43
2:B:181:MET:HE1	1:F:483:VAL:HA	2.00	0.43
2:D:170:MET:HE2	2:D:174:ASN:ND2	2.34	0.43
1:F:28:LYS:HD2	1:F:598:PHE:HD1	1.84	0.43
1:F:276:TYR:CE1	1:F:280:ARG:HD2	2.54	0.43
2:B:531:ASP:OD1	2:B:533:ASN:CB	2.66	0.43
2:D:383:TYR:CZ	1:E:359:HIS:HE1	2.36	0.43
1:F:528:ILE:HG22	1:F:553:LEU:HD12	2.00	0.43
1:A:173:MET:CE	2:D:308:PRO:HD3	2.48	0.43
1:A:183:LYS:HG2	1:A:483:VAL:HG13	2.01	0.43
1:A:455:PHE:CD2	1:A:630:TYR:HA	2.53	0.43
2:B:115:ALA:HB3	2:B:148:ARG:NH1	2.34	0.43
2:B:323:ASN:ND2	2:B:394:VAL:HG13	2.33	0.43
2:B:452:PHE:C	2:B:452:PHE:CD1	2.96	0.43
2:C:21:GLU:OE1	2:C:21:GLU:CA	2.66	0.43
2:C:501:LEU:O	2:C:606:ARG:HB2	2.19	0.43
1:E:577:PHE:CZ	1:E:612:MET:HG3	2.53	0.43
2:C:247:ASN:N	2:C:247:ASN:ND2	2.66	0.43
2:D:165:GLN:CD	2:D:165:GLN:H	2.27	0.43
1:E:71:ASP:OD1	1:E:71:ASP:N	2.40	0.43
1:F:543:LEU:HA	1:F:543:LEU:HD23	1.68	0.43
1:A:69:ASN:HB3	1:A:72:ASN:HD22	1.84	0.43
2:B:83:TYR:HB2	2:B:87:PHE:CE1	2.53	0.43
2:B:682:TYR:CD2	4:H:1:NAG:H62	2.53	0.43
2:C:574:LYS:O	2:C:605:SER:HB2	2.18	0.43
1:F:164:GLU:OE2	1:F:583:PRO:HA	2.19	0.43
1:A:298:LYS:HG2	1:A:318:TYR:HE2	1.78	0.42
2:B:329:PHE:O	2:B:332:ILE:HD12	2.19	0.42
2:D:501:LEU:O	2:D:606:ARG:HB2	2.19	0.42
2:D:543:TRP:CZ2	2:D:655:PRO:HD3	2.54	0.42
1:A:100:PHE:O	1:A:396:ARG:NH2	2.51	0.42
2:D:661:PHE:C	2:D:666:MET:HE1	2.44	0.42
1:F:28:LYS:HZ2	1:F:598:PHE:HE1	1.66	0.42
1:F:516:VAL:HB	1:F:565:ASN:HD21	1.84	0.42
1:A:630:TYR:HB2	1:A:631:PRO:HD2	2.01	0.42
1:A:640:ALA:N	1:A:641:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:170:MET:HE1	1:F:310:THR:CA	2.49	0.42
2:C:64:GLU:H	2:C:64:GLU:HG2	1.24	0.42
2:C:439:LYS:HD2	2:C:442:GLN:OE1	2.18	0.42
2:D:174:ASN:HB3	2:D:178:TYR:CE1	2.54	0.42
2:D:636:GLU:HB3	2:D:637:PRO:CD	2.49	0.42
1:E:643:GLU:C	1:E:645:PHE:H	2.26	0.42
2:C:492:HIS:HB2	2:C:493:GLY:H	1.65	0.42
1:A:171:MET:HE1	1:A:479:ALA:HB1	2.01	0.42
2:C:480:VAL:HG12	1:E:184:MET:CE	2.47	0.42
2:D:533:ASN:OD1	2:D:535:PHE:CD1	2.72	0.42
2:D:228:ASP:OD2	2:D:500:ARG:NH1	2.52	0.42
2:D:245:TRP:HA	2:D:380:LEU:HB2	2.02	0.42
1:E:185:GLN:CD	1:E:189:ILE:HD12	2.45	0.42
2:B:554:GLN:HG2	2:B:563:ILE:HD11	2.00	0.42
2:C:355:LEU:HD13	2:C:441:TYR:CD2	2.55	0.42
2:C:645:ASN:ND2	2:C:645:ASN:H	2.16	0.42
2:B:96:ILE:HD12	2:B:102:ARG:HA	2.02	0.42
2:B:117:ASP:OD2	2:B:117:ASP:C	2.63	0.42
2:D:580:MET:HA	2:D:583:ILE:HD12	2.00	0.42
2:B:329:PHE:HA	2:B:332:ILE:HD11	2.01	0.42
1:F:344:LEU:O	1:F:444:TYR:OH	2.32	0.42
1:A:85:MET:O	1:A:88:THR:HB	2.20	0.42
1:A:315:ARG:NH2	1:A:424:ASP:OD2	2.53	0.42
2:B:211:ASN:C	2:B:213:LEU:N	2.78	0.42
2:C:463:ASP:HB2	2:C:506:PHE:HB2	2.02	0.42
1:F:642:PHE:C	1:F:642:PHE:CD2	2.97	0.42
1:A:70:MET:HE2	1:A:70:MET:HB2	1.98	0.41
2:B:332:ILE:HG12	2:C:335:LYS:CG	2.30	0.41
2:C:543:TRP:CZ2	2:C:655:PRO:HD3	2.55	0.41
2:D:69:CYS:HB2	2:D:70:TYR:CE2	2.55	0.41
1:F:111:LEU:HD22	1:F:135:LEU:CD1	2.49	0.41
1:F:354:GLN:HB2	1:F:356:ILE:CD1	2.50	0.41
1:A:541:LEU:HD23	1:A:541:LEU:HA	1.80	0.41
2:D:352:LYS:HB2	2:D:352:LYS:NZ	2.34	0.41
2:D:472:PHE:HB3	2:D:500:ARG:HG3	2.01	0.41
2:B:90:LYS:HE3	2:B:130:VAL:O	2.20	0.41
2:D:332:ILE:HD13	1:E:338:LYS:HB3	2.02	0.41
2:D:344:GLY:O	2:D:355:LEU:HG	2.20	0.41
1:F:170:PHE:HD2	1:F:232:ILE:HG22	1.84	0.41
1:F:646:VAL:C	1:F:648:ASP:N	2.73	0.41
2:B:79:PHE:CZ	2:B:132:MET:HE1	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:223:ALA:O	2:B:227:GLU:HG3	2.21	0.41
2:B:349:PHE:O	2:B:350:ASP:CB	2.62	0.41
2:C:261:ILE:HD13	2:C:261:ILE:HA	1.88	0.41
2:D:629:GLU:HA	2:D:630:PRO:HD2	1.93	0.41
1:E:169:MET:HE3	1:E:419:GLN:NE2	2.35	0.41
1:E:265:TYR:OH	1:E:391:GLU:OE1	2.36	0.41
1:E:646:VAL:C	1:E:648:ASP:N	2.78	0.41
1:F:471:PHE:HE1	1:F:473:GLU:HB3	1.85	0.41
1:A:114:LEU:HD23	1:A:114:LEU:HA	1.82	0.41
1:A:248:TRP:O	1:A:382:VAL:HA	2.21	0.41
1:A:584:MET:HE2	1:A:584:MET:HB3	1.73	0.41
1:A:650:LYS:HD2	1:A:654:PHE:CE2	2.55	0.41
2:B:278:LEU:HD21	2:B:532:GLU:HG3	2.03	0.41
2:B:300:PRO:HG2	2:B:309:PHE:HB3	2.02	0.41
2:B:642:VAL:O	2:B:644:ASP:N	2.54	0.41
2:C:242:LEU:HD21	2:C:248:SER:HB3	2.02	0.41
1:E:67:GLU:HG2	1:E:83:LEU:CD2	2.48	0.41
2:C:90:LYS:O	2:C:91:ASN:HB2	2.21	0.41
2:D:97:PHE:O	2:D:393:ARG:NH2	2.54	0.41
2:D:514:SER:O	2:D:558:PRO:HA	2.21	0.41
2:D:540:GLU:OE2	2:D:658:PRO:HG2	2.20	0.41
2:D:680:PHE:HA	2:D:681:PRO:HD3	1.85	0.41
1:F:278:PHE:HE1	1:F:532:PRO:CG	2.34	0.41
1:F:507:HIS:HD2	1:F:508:SER:O	2.03	0.41
1:A:214:ASN:HB2	1:E:537:ASN:OD1	2.21	0.41
1:E:596:VAL:HA	1:E:597:PRO:HD3	1.95	0.41
1:E:634:ASN:HB3	1:E:635:LYS:H	1.78	0.41
1:A:201:LYS:HG3	1:A:206:PHE:CE2	2.55	0.41
1:A:634:ASN:HB3	1:A:635:LYS:H	1.76	0.41
2:B:574:LYS:HG2	2:B:602:THR:HG22	2.03	0.41
2:B:639:LYS:HD2	2:B:639:LYS:N	2.36	0.41
1:F:137:GLN:H	1:F:137:GLN:NE2	2.19	0.41
1:A:646:VAL:CG2	1:A:652:LEU:HD21	2.51	0.41
1:A:646:VAL:HG22	1:A:652:LEU:HD21	2.03	0.41
2:B:94:PHE:HA	2:B:101:MET:CE	2.42	0.41
2:B:138:LEU:HD23	2:B:138:LEU:HA	1.92	0.41
2:B:516:VAL:HG12	2:B:517:ALA:H	1.86	0.41
2:B:528:PRO:HA	2:B:619:PHE:HD1	1.85	0.41
2:C:145:ILE:HG13	2:C:151:THR:HG21	2.03	0.41
1:E:91:MET:HA	1:E:92:PRO:HD3	1.92	0.41
1:E:168:LYS:HE3	1:E:308:LYS:HE3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:257:LEU:HG	1:F:257:LEU:O	2.20	0.41
1:F:537:ASN:HB3	1:F:539:ILE:HD13	2.03	0.41
1:F:623:PHE:CE2	1:F:677:ILE:HD12	2.55	0.41
2:B:155:VAL:CG1	2:B:156:LEU:N	2.84	0.41
2:C:358:SER:C	2:C:360:ALA:N	2.73	0.41
2:D:63:ILE:HG23	2:D:80:MET:HE1	2.03	0.41
2:D:354:ASP:OD1	2:D:354:ASP:C	2.63	0.41
1:E:214:ASN:HA	1:E:217:LEU:O	2.21	0.41
1:F:170:PHE:CD2	1:F:232:ILE:HG22	2.55	0.41
1:F:267:TYR:O	1:F:271:GLN:HG2	2.20	0.41
7:K:4:BMA:O2	7:K:5:BMA:C1	2.69	0.41
2:B:227:GLU:O	2:B:228:ASP:C	2.63	0.40
1:F:305:MET:HE3	1:F:305:MET:HB3	1.73	0.40
1:A:248:TRP:CE3	1:A:249:TRP:HB2	2.56	0.40
2:B:330:LEU:O	2:B:334:GLU:HG3	2.20	0.40
2:C:222:ILE:O	2:C:222:ILE:CG2	2.69	0.40
1:F:217:LEU:HD21	1:F:302:TYR:HB3	2.04	0.40
2:B:45:VAL:HG11	2:B:138:LEU:HD11	2.03	0.40
2:B:170:MET:HE2	2:B:170:MET:HB3	1.61	0.40
2:D:145:ILE:HG23	2:D:151:THR:CG2	2.52	0.40
2:D:170:MET:CE	2:D:174:ASN:HD21	2.34	0.40
2:D:675:HIS:HE1	2:D:678:GLU:O	2.04	0.40
1:A:218:TYR:CZ	1:E:536:ASP:HB3	2.56	0.40
2:D:222:ILE:HD13	2:D:222:ILE:HG21	1.42	0.40
1:E:422:LEU:HD22	1:E:427:PHE:CE2	2.56	0.40
1:F:684:PHE:O	1:F:687:LYS:HB2	2.21	0.40
1:A:170:PHE:HB3	1:A:232:ILE:HG22	2.03	0.40
1:E:166:TYR:HB3	1:E:169:MET:HG3	2.03	0.40
1:E:175:VAL:HG21	1:E:210:ALA:HB2	2.04	0.40
1:E:307:THR:C	1:E:309:PHE:N	2.79	0.40

There are no symmetry-related clashes.

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	668/703 (95%)	629 (94%)	33 (5%)	6 (1%)	14	41
1	E	667/703 (95%)	628 (94%)	32 (5%)	7 (1%)	12	38
1	F	667/703 (95%)	630 (94%)	34 (5%)	3 (0%)	30	60
2	B	666/696 (96%)	619 (93%)	33 (5%)	14 (2%)	5	20
2	C	666/696 (96%)	633 (95%)	24 (4%)	9 (1%)	9	30
2	D	670/696 (96%)	637 (95%)	27 (4%)	6 (1%)	14	41
All	All	4004/4197 (95%)	3776 (94%)	183 (5%)	45 (1%)	11	36

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	308	LYS
2	B	247	ASN
2	B	632	PRO
2	B	636	GLU
2	B	687	PRO
2	C	347	LYS
2	C	350	ASP
2	C	632	PRO
2	C	687	PRO
2	D	350	ASP
2	D	632	PRO
2	D	687	PRO
1	E	308	LYS
2	B	45	VAL
2	B	350	ASP
2	B	382	PHE
2	B	615	ASP
2	C	344	GLY
2	D	488	LYS
1	E	203	ASN
1	F	308	LYS
1	F	641	PRO
1	A	94	ASN
1	A	647	LEU
2	D	635	SER
1	A	324	GLU
1	A	640	ALA

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Mol	Chain	Res	Type
2	B	306	TYR
2	C	635	SER
1	E	640	ALA
2	B	344	GLY
2	C	186	LEU
2	C	599	SER
2	D	321	GLU
1	E	220	ASN
1	E	636	GLY
1	E	641	PRO
1	E	647	LEU
1	F	640	ALA
2	B	631	THR
2	B	85	VAL
2	B	490	SER
2	C	643	PRO
1	A	495	VAL
2	B	643	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	610/638 (96%)	560 (92%)	50 (8%)	10	33
1	E	609/638 (96%)	558 (92%)	51 (8%)	10	32
1	F	609/638 (96%)	547 (90%)	62 (10%)	7	23
2	B	606/629 (96%)	541 (89%)	65 (11%)	6	21
2	C	606/629 (96%)	545 (90%)	61 (10%)	7	23
2	D	610/629 (97%)	549 (90%)	61 (10%)	7	24
All	All	3650/3801 (96%)	3300 (90%)	350 (10%)	8	26

All (350) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	27	THR
1	A	33	VAL
1	A	48	VAL
1	A	53	THR
1	A	56	GLU
1	A	62	LYS
1	A	68	MET
1	A	71	ASP
1	A	88	THR
1	A	99	VAL
1	A	145	TYR
1	A	175	VAL
1	A	190	ASN
1	A	204	ASP
1	A	258	LYS
1	A	281	LEU
1	A	297	ILE
1	A	310	THR
1	A	324	GLU
1	A	356	ILE
1	A	364	ILE
1	A	381	GLU
1	A	382	VAL
1	A	422	LEU
1	A	449	THR
1	A	451	ASP
1	A	456	ASP
1	A	469	THR
1	A	495	VAL
1	A	515	GLU
1	A	519	ASN
1	A	523	ASP
1	A	539	ILE
1	A	543	LEU
1	A	548	MET
1	A	559	LYS
1	A	561	THR
1	A	567	ILE
1	A	572	ASN
1	A	582	VAL
1	A	585	THR
1	A	602	GLU
1	A	610	ARG

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Mol	Chain	Res	Type
1	A	633	ASP
1	A	643	GLU
1	A	646	VAL
1	A	649	ASN
1	A	661	VAL
1	A	664	LEU
1	A	667	VAL
2	B	27	VAL
2	B	34	LYS
2	B	47	GLU
2	B	51	GLU
2	B	53	GLU
2	B	63	ILE
2	B	64	GLU
2	B	71	THR
2	B	73	MET
2	B	77	GLU
2	B	90	LYS
2	B	129	ARG
2	B	134	GLN
2	B	142	TYR
2	B	165	GLN
2	B	170	MET
2	B	173	LYS
2	B	190	ILE
2	B	197	ILE
2	B	198	LYS
2	B	205	MET
2	B	210	SER
2	B	213	LEU
2	B	217	ASN
2	B	225	LEU
2	B	231	LEU
2	B	261	ILE
2	B	275	MET
2	B	305	PHE
2	B	306	TYR
2	B	313	SER
2	B	332	ILE
2	B	347	LYS
2	B	353	ILE
2	B	370	THR

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Mol	Chain	Res	Type
2	B	381	GLN
2	B	404	GLN
2	B	406	THR
2	B	429	LYS
2	B	443	VAL
2	B	455	LEU
2	B	462	VAL
2	B	487	LEU
2	B	490	SER
2	B	512	ILE
2	B	513	LYS
2	B	514	SER
2	B	516	VAL
2	B	532	GLU
2	B	539	LEU
2	B	542	ASN
2	B	564	THR
2	B	578	LEU
2	B	592	ILE
2	B	597	PHE
2	B	602	THR
2	B	606	ARG
2	B	634	GLU
2	B	639	LYS
2	B	641	VAL
2	B	645	ASN
2	B	656	VAL
2	B	663	GLN
2	B	669	LYS
2	B	679	LEU
2	C	21	GLU
2	C	22	PHE
2	C	27	VAL
2	C	46	ASN
2	C	53	GLU
2	C	63	ILE
2	C	64	GLU
2	C	66	SER
2	C	71	THR
2	C	84	LYS
2	C	111	LEU
2	C	116	LYS

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Mol	Chain	Res	Type
2	C	134	GLN
2	C	145	ILE
2	C	170	MET
2	C	200	ASN
2	C	202	GLN
2	C	205	MET
2	C	210	SER
2	C	214	THR
2	C	217	ASN
2	C	247	ASN
2	C	261	ILE
2	C	313	SER
2	C	326	GLU
2	C	345	HIS
2	C	346	PHE
2	C	347	LYS
2	C	352	LYS
2	C	353	ILE
2	C	359	LYS
2	C	370	THR
2	C	404	GLN
2	C	429	LYS
2	C	443	VAL
2	C	455	LEU
2	C	462	VAL
2	C	464	LYS
2	C	466	VAL
2	C	489	SER
2	C	490	SER
2	C	492	HIS
2	C	516	VAL
2	C	518	THR
2	C	540	GLU
2	C	562	GLN
2	C	589	GLN
2	C	592	ILE
2	C	597	PHE
2	C	602	THR
2	C	605	SER
2	C	606	ARG
2	C	609	LEU
2	C	633	LYS

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Mol	Chain	Res	Type
2	C	634	GLU
2	C	636	GLU
2	C	642	VAL
2	C	645	ASN
2	C	663	GLN
2	C	666	MET
2	C	669	LYS
2	D	21	GLU
2	D	27	VAL
2	D	53	GLU
2	D	64	GLU
2	D	71	THR
2	D	74	LYS
2	D	96	ILE
2	D	111	LEU
2	D	129	ARG
2	D	134	GLN
2	D	145	ILE
2	D	165	GLN
2	D	172	VAL
2	D	173	LYS
2	D	187	ASP
2	D	200	ASN
2	D	205	MET
2	D	210	SER
2	D	217	ASN
2	D	222	ILE
2	D	225	LEU
2	D	247	ASN
2	D	299	LEU
2	D	313	SER
2	D	326	GLU
2	D	343	GLN
2	D	345	HIS
2	D	352	LYS
2	D	353	ILE
2	D	370	THR
2	D	380	LEU
2	D	381	GLN
2	D	414	PHE
2	D	416	GLN
2	D	429	LYS

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Mol	Chain	Res	Type
2	D	464	LYS
2	D	489	SER
2	D	490	SER
2	D	513	LYS
2	D	516	VAL
2	D	525	PHE
2	D	532	GLU
2	D	538	SER
2	D	539	LEU
2	D	540	GLU
2	D	551	TRP
2	D	555	LYS
2	D	562	GLN
2	D	563	ILE
2	D	564	THR
2	D	578	LEU
2	D	585	LYS
2	D	592	ILE
2	D	602	THR
2	D	606	ARG
2	D	633	LYS
2	D	634	GLU
2	D	636	GLU
2	D	672	LEU
2	D	687	PRO
2	D	690	THR
1	E	24	THR
1	E	27	THR
1	E	30	VAL
1	E	33	VAL
1	E	48	VAL
1	E	53	THR
1	E	56	GLU
1	E	62	LYS
1	E	68	MET
1	E	70	MET
1	E	71	ASP
1	E	83	LEU
1	E	99	VAL
1	E	145	TYR
1	E	159	VAL
1	E	169	MET

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Mol	Chain	Res	Type
1	E	203	ASN
1	E	232	ILE
1	E	257	LEU
1	E	258	LYS
1	E	290	GLU
1	E	297	ILE
1	E	298	LYS
1	E	307	THR
1	E	310	THR
1	E	346	LYS
1	E	364	ILE
1	E	381	GLU
1	E	382	VAL
1	E	384	LYS
1	E	422	LEU
1	E	451	ASP
1	E	456	ASP
1	E	495	VAL
1	E	515	GLU
1	E	520	VAL
1	E	523	ASP
1	E	548	MET
1	E	561	THR
1	E	576	ILE
1	E	582	VAL
1	E	589	LYS
1	E	596	VAL
1	E	615	ARG
1	E	625	LEU
1	E	645	PHE
1	E	646	VAL
1	E	648	ASP
1	E	673	LYS
1	E	683	ARG
1	E	692	SER
1	F	27	THR
1	F	48	VAL
1	F	56	GLU
1	F	62	LYS
1	F	66	ILE
1	F	71	ASP
1	F	75	ASN

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Mol	Chain	Res	Type
1	F	77	LYS
1	F	103	LYS
1	F	137	GLN
1	F	145	TYR
1	F	169	MET
1	F	188	LEU
1	F	190	ASN
1	F	204	ASP
1	F	216	VAL
1	F	226	THR
1	F	232	ILE
1	F	257	LEU
1	F	264	VAL
1	F	305	MET
1	F	307	THR
1	F	323	THR
1	F	335	THR
1	F	356	ILE
1	F	381	GLU
1	F	382	VAL
1	F	384	LYS
1	F	389	SER
1	F	422	LEU
1	F	435	VAL
1	F	441	PHE
1	F	446	LYS
1	F	449	THR
1	F	451	ASP
1	F	456	ASP
1	F	461	THR
1	F	469	THR
1	F	473	GLU
1	F	493	ASN
1	F	501	ARG
1	F	512	VAL
1	F	513	ASN
1	F	515	GLU
1	F	516	VAL
1	F	519	ASN
1	F	522	SER
1	F	523	ASP
1	F	561	THR

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Mol	Chain	Res	Type
1	F	565	ASN
1	F	568	ILE
1	F	572	ASN
1	F	578	LYS
1	F	579	GLU
1	F	582	VAL
1	F	596	VAL
1	F	604	PHE
1	F	643	GLU
1	F	647	LEU
1	F	673	LYS
1	F	675	ILE
1	F	683	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (124) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	38	GLN
1	A	50	GLN
1	A	72	ASN
1	A	75	ASN
1	A	94	ASN
1	A	172	ASN
1	A	190	ASN
1	A	244	HIS
1	A	271	GLN
1	A	314	GLN
1	A	342	GLN
1	A	345	GLN
1	A	359	HIS
1	A	429	GLN
1	A	492	ASN
1	A	493	ASN
1	A	506	ASN
1	A	507	HIS
1	A	513	ASN
1	A	679	HIS
2	B	35	GLN
2	B	134	GLN
2	B	217	ASN
2	B	232	ASN
2	B	247	ASN

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Mol	Chain	Res	Type
2	B	268	GLN
2	B	303	ASN
2	B	311	GLN
2	B	339	GLN
2	B	404	GLN
2	B	433	GLN
2	B	492	HIS
2	B	502	ASN
2	B	503	HIS
2	B	533	ASN
2	B	542	ASN
2	B	645	ASN
2	B	663	GLN
2	B	675	HIS
2	C	35	GLN
2	C	72	ASN
2	C	91	ASN
2	C	134	GLN
2	C	217	ASN
2	C	232	ASN
2	C	247	ASN
2	C	268	GLN
2	C	311	GLN
2	C	323	ASN
2	C	339	GLN
2	C	343	GLN
2	C	345	HIS
2	C	442	GLN
2	C	447	GLN
2	C	502	ASN
2	C	542	ASN
2	C	562	GLN
2	C	645	ASN
2	C	663	GLN
2	C	675	HIS
2	C	688	HIS
2	D	72	ASN
2	D	134	GLN
2	D	174	ASN
2	D	217	ASN
2	D	232	ASN
2	D	247	ASN

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Mol	Chain	Res	Type
2	D	268	GLN
2	D	311	GLN
2	D	339	GLN
2	D	343	GLN
2	D	381	GLN
2	D	447	GLN
2	D	451	HIS
2	D	471	HIS
2	D	502	ASN
2	D	503	HIS
2	D	519	ASN
2	D	542	ASN
2	D	560	GLN
2	D	675	HIS
1	E	38	GLN
1	E	50	GLN
1	E	69	ASN
1	E	72	ASN
1	E	203	ASN
1	E	235	ASN
1	E	271	GLN
1	E	314	GLN
1	E	342	GLN
1	E	348	HIS
1	E	359	HIS
1	E	369	ASN
1	E	372	GLN
1	E	374	ASN
1	E	450	GLN
1	E	506	ASN
1	E	507	HIS
1	E	513	ASN
1	E	679	HIS
1	F	38	GLN
1	F	50	GLN
1	F	113	HIS
1	F	134	HIS
1	F	137	GLN
1	F	139	GLN
1	F	177	GLN
1	F	190	ASN
1	F	200	HIS

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Mol	Chain	Res	Type
1	F	214	ASN
1	F	271	GLN
1	F	314	GLN
1	F	342	GLN
1	F	345	GLN
1	F	359	HIS
1	F	450	GLN
1	F	493	ASN
1	F	506	ASN
1	F	507	HIS
1	F	519	ASN
1	F	565	ASN
1	F	572	ASN
1	F	649	ASN
1	F	679	HIS

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 ⓘ

34 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	$\# Z > 2$
3	NAG	G	1	3,1	14,14,15	1.01	2 (14%)	17,19,21	1.89	5 (29%)
3	NAG	G	2	3	14,14,15	0.83	1 (7%)	17,19,21	2.15	6 (35%)
3	BMA	G	3	3	11,11,12	0.84	0	15,15,17	2.29	4 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	MAN	G	4	3	11,11,12	0.73	0	15,15,17	1.13	1 (6%)
3	BMA	G	5	3	11,11,12	1.02	1 (9%)	15,15,17	3.31	4 (26%)
4	NAG	H	1	2,4	14,14,15	0.75	1 (7%)	17,19,21	1.33	1 (5%)
4	NAG	H	2	4	14,14,15	0.64	0	17,19,21	1.45	2 (11%)
4	BMA	H	3	4	11,11,12	1.27	1 (9%)	15,15,17	1.37	3 (20%)
4	BMA	H	4	4	11,11,12	0.62	0	15,15,17	1.14	1 (6%)
4	MAN	H	5	4	11,11,12	0.69	0	15,15,17	1.13	1 (6%)
5	NAG	I	1	5,2	14,14,15	0.60	0	17,19,21	1.80	4 (23%)
5	NAG	I	2	5	14,14,15	0.78	1 (7%)	17,19,21	1.42	1 (5%)
5	BMA	I	3	5	11,11,12	0.67	0	15,15,17	1.98	5 (33%)
5	MAN	I	4	5	11,11,12	0.89	1 (9%)	15,15,17	1.86	3 (20%)
5	MAN	I	5	5	11,11,12	0.65	0	15,15,17	2.42	4 (26%)
5	MAN	I	6	5	11,11,12	0.74	0	15,15,17	1.79	3 (20%)
6	NAG	J	1	2,6	14,14,15	0.57	0	17,19,21	1.28	1 (5%)
6	NAG	J	2	6	14,14,15	0.87	1 (7%)	17,19,21	1.52	3 (17%)
6	BMA	J	3	6	11,11,12	0.47	0	15,15,17	1.67	3 (20%)
6	MAN	J	4	6	11,11,12	0.54	0	15,15,17	1.37	1 (6%)
6	MAN	J	5	6	11,11,12	0.79	0	15,15,17	1.29	3 (20%)
6	MAN	J	6	6	11,11,12	0.63	0	15,15,17	1.17	2 (13%)
6	MAN	J	7	6	11,11,12	0.67	0	15,15,17	2.45	3 (20%)
7	NAG	K	1	7,1	14,14,15	0.69	0	17,19,21	1.42	3 (17%)
7	NAG	K	2	7	14,14,15	0.54	0	17,19,21	1.09	1 (5%)
7	BMA	K	3	7	11,11,12	0.65	0	15,15,17	2.10	3 (20%)
7	BMA	K	4	7	11,11,12	0.68	0	15,15,17	2.26	4 (26%)
7	BMA	K	5	7	11,11,12	0.90	1 (9%)	15,15,17	2.10	2 (13%)
7	MAN	K	6	7	11,11,12	0.80	0	15,15,17	1.52	2 (13%)
8	NAG	L	1	8,1	14,14,15	0.52	0	17,19,21	1.72	4 (23%)
8	NAG	L	2	8	14,14,15	0.55	0	17,19,21	1.29	0
8	BMA	L	3	8	11,11,12	0.46	0	15,15,17	1.11	2 (13%)
8	MAN	L	4	8	11,11,12	0.78	1 (9%)	15,15,17	1.49	4 (26%)
8	BMA	L	5	8	11,11,12	0.67	0	15,15,17	2.32	3 (20%)

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	G	1	3,1	-	1/6/23/26	0/1/1/1
3	NAG	G	2	3	-	2/6/23/26	0/1/1/1
3	BMA	G	3	3	-	2/2/19/22	0/1/1/1
3	MAN	G	4	3	-	2/2/19/22	0/1/1/1
3	BMA	G	5	3	-	1/2/19/22	0/1/1/1
4	NAG	H	1	2,4	-	0/6/23/26	0/1/1/1
4	NAG	H	2	4	-	2/6/23/26	0/1/1/1
4	BMA	H	3	4	-	2/2/19/22	0/1/1/1
4	BMA	H	4	4	-	2/2/19/22	0/1/1/1
4	MAN	H	5	4	-	0/2/19/22	0/1/1/1
5	NAG	I	1	5,2	-	0/6/23/26	0/1/1/1
5	NAG	I	2	5	-	1/6/23/26	0/1/1/1
5	BMA	I	3	5	-	2/2/19/22	0/1/1/1
5	MAN	I	4	5	-	0/2/19/22	0/1/1/1
5	MAN	I	5	5	-	2/2/19/22	0/1/1/1
5	MAN	I	6	5	-	1/2/19/22	0/1/1/1
6	NAG	J	1	2,6	-	1/6/23/26	0/1/1/1
6	NAG	J	2	6	-	0/6/23/26	0/1/1/1
6	BMA	J	3	6	-	0/2/19/22	0/1/1/1
6	MAN	J	4	6	-	2/2/19/22	0/1/1/1
6	MAN	J	5	6	-	0/2/19/22	0/1/1/1
6	MAN	J	6	6	-	2/2/19/22	0/1/1/1
6	MAN	J	7	6	-	0/2/19/22	0/1/1/1
7	NAG	K	1	7,1	-	2/6/23/26	0/1/1/1
7	NAG	K	2	7	-	2/6/23/26	0/1/1/1
7	BMA	K	3	7	-	2/2/19/22	0/1/1/1
7	BMA	K	4	7	-	2/2/19/22	0/1/1/1
7	BMA	K	5	7	-	0/2/19/22	0/1/1/1
7	MAN	K	6	7	-	2/2/19/22	0/1/1/1
8	NAG	L	1	8,1	-	0/6/23/26	0/1/1/1
8	NAG	L	2	8	-	0/6/23/26	0/1/1/1
8	BMA	L	3	8	-	0/2/19/22	0/1/1/1
8	MAN	L	4	8	-	2/2/19/22	0/1/1/1
8	BMA	L	5	8	-	2/2/19/22	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	3	BMA	O5-C1	-3.72	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	1	NAG	O5-C1	-2.59	1.39	1.43
3	G	5	BMA	C2-C3	2.50	1.56	1.52
6	J	2	NAG	O5-C1	-2.25	1.39	1.43
4	H	1	NAG	O5-C1	-2.21	1.40	1.43
3	G	1	NAG	O5-C5	-2.20	1.39	1.43
8	L	4	MAN	C2-C3	2.15	1.55	1.52
5	I	4	MAN	C2-C3	2.14	1.55	1.52
5	I	2	NAG	O5-C1	-2.13	1.40	1.43
3	G	2	NAG	O3-C3	-2.06	1.37	1.43
7	K	5	BMA	C2-C3	2.01	1.55	1.52

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	5	BMA	C1-O5-C5	-9.13	99.95	112.19
6	J	7	MAN	C1-O5-C5	8.11	123.06	112.19
8	L	5	BMA	C1-O5-C5	7.51	122.25	112.19
3	G	3	BMA	O5-C5-C6	6.81	120.93	107.66
3	G	5	BMA	O5-C5-C6	6.79	120.87	107.66
7	K	4	BMA	C1-O5-C5	6.26	120.58	112.19
5	I	5	MAN	C1-O5-C5	6.13	120.41	112.19
7	K	5	BMA	C1-C2-C3	5.72	117.98	109.64
7	K	3	BMA	C1-O5-C5	5.66	119.78	112.19
5	I	1	NAG	C1-O5-C5	5.53	119.60	112.19
3	G	1	NAG	C2-N2-C7	-5.28	115.82	122.90
5	I	4	MAN	C1-C2-C3	5.04	116.98	109.64
5	I	6	MAN	C1-O5-C5	4.93	118.79	112.19
5	I	3	BMA	C1-C2-C3	4.84	116.69	109.64
6	J	4	MAN	C1-O5-C5	4.69	118.47	112.19
3	G	2	NAG	C3-C4-C5	-4.61	101.87	110.23
5	I	2	NAG	C1-O5-C5	4.59	118.33	112.19
7	K	5	BMA	C1-O5-C5	4.49	118.20	112.19
3	G	5	BMA	C3-C4-C5	-4.41	102.24	110.23
5	I	5	MAN	C1-C2-C3	4.40	116.05	109.64
4	H	1	NAG	C1-O5-C5	4.29	117.93	112.19
4	H	2	NAG	C1-O5-C5	4.25	117.88	112.19
8	L	1	NAG	C1-O5-C5	4.17	117.77	112.19
6	J	2	NAG	C2-N2-C7	-4.10	117.41	122.90
3	G	2	NAG	O3-C3-C2	-3.81	101.48	109.40
3	G	2	NAG	C1-C2-N2	-3.58	104.79	110.43
6	J	3	BMA	C1-C2-C3	3.56	114.83	109.64
7	K	1	NAG	C1-O5-C5	3.55	116.95	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	6	MAN	C1-C2-C3	3.53	114.78	109.64
7	K	6	MAN	C1-O5-C5	3.46	116.83	112.19
7	K	3	BMA	O3-C3-C2	3.46	117.11	110.05
7	K	4	BMA	C3-C4-C5	3.45	116.49	110.23
6	J	3	BMA	C1-O5-C5	3.40	116.74	112.19
3	G	4	MAN	C3-C4-C5	3.35	116.31	110.23
5	I	5	MAN	C3-C4-C5	3.33	116.26	110.23
5	I	4	MAN	C1-O5-C5	3.28	116.59	112.19
7	K	4	BMA	O5-C5-C4	3.28	118.80	110.83
7	K	6	MAN	C1-C2-C3	3.26	114.40	109.64
3	G	3	BMA	O6-C6-C5	3.17	122.13	111.33
8	L	1	NAG	C2-N2-C7	3.15	127.13	122.90
8	L	5	BMA	C1-C2-C3	3.08	114.13	109.64
5	I	3	BMA	C3-C4-C5	3.07	115.81	110.23
4	H	5	MAN	C1-O5-C5	3.04	116.26	112.19
7	K	1	NAG	C1-C2-N2	-3.00	105.71	110.43
3	G	2	NAG	O5-C5-C6	2.97	113.44	107.66
5	I	5	MAN	C2-C3-C4	2.96	116.07	110.86
5	I	3	BMA	C1-O5-C5	2.90	116.07	112.19
4	H	3	BMA	C3-C4-C5	2.88	115.46	110.23
6	J	6	MAN	C1-O5-C5	2.83	115.98	112.19
6	J	6	MAN	O5-C5-C6	2.69	112.90	107.66
8	L	4	MAN	C2-C3-C4	2.61	115.45	110.86
8	L	4	MAN	C1-C2-C3	2.59	113.42	109.64
8	L	4	MAN	C1-O5-C5	2.59	115.65	112.19
4	H	3	BMA	O3-C3-C2	2.54	115.24	110.05
4	H	4	BMA	C3-C4-C5	2.53	114.82	110.23
5	I	6	MAN	C2-C3-C4	2.49	115.24	110.86
3	G	5	BMA	C6-C5-C4	2.49	119.12	113.02
8	L	1	NAG	O7-C7-N2	2.48	126.37	121.98
7	K	4	BMA	O3-C3-C2	2.48	115.11	110.05
5	I	1	NAG	C1-C2-N2	-2.46	106.56	110.43
3	G	1	NAG	O6-C6-C5	-2.44	103.01	111.33
6	J	5	MAN	C1-C2-C3	2.38	113.12	109.64
6	J	3	BMA	O5-C1-C2	2.38	116.46	110.79
5	I	3	BMA	C2-C3-C4	2.36	115.01	110.86
3	G	3	BMA	C1-C2-C3	2.36	113.08	109.64
8	L	1	NAG	O7-C7-C8	-2.35	117.86	122.05
5	I	1	NAG	O4-C4-C5	-2.35	103.53	109.32
3	G	1	NAG	C3-C4-C5	-2.35	105.98	110.23
5	I	4	MAN	C2-C3-C4	2.34	114.98	110.86
6	J	7	MAN	C1-C2-C3	2.31	113.01	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	1	NAG	C1-O5-C5	2.28	115.24	112.19
8	L	5	BMA	O5-C1-C2	2.24	116.14	110.79
3	G	1	NAG	C8-C7-N2	2.24	119.83	116.12
6	J	2	NAG	O5-C1-C2	-2.20	107.88	111.29
7	K	1	NAG	C3-C4-C5	-2.16	106.31	110.23
6	J	5	MAN	O5-C5-C4	-2.15	105.60	110.83
5	I	3	BMA	O5-C1-C2	2.14	115.89	110.79
6	J	1	NAG	C3-C4-C5	-2.14	106.36	110.23
6	J	7	MAN	C3-C4-C5	-2.12	106.39	110.23
6	J	5	MAN	C1-O5-C5	2.10	115.01	112.19
7	K	3	BMA	O3-C3-C4	2.07	115.25	110.38
4	H	3	BMA	C1-O5-C5	-2.07	109.42	112.19
3	G	2	NAG	C6-C5-C4	2.06	118.09	113.02
8	L	3	BMA	O2-C2-C1	-2.06	104.52	109.22
5	I	1	NAG	O7-C7-C8	-2.05	118.40	122.05
4	H	2	NAG	C3-C4-C5	-2.04	106.53	110.23
7	K	2	NAG	O5-C5-C6	2.04	111.64	107.66
3	G	2	NAG	C1-O5-C5	-2.03	109.46	112.19
6	J	2	NAG	C1-O5-C5	2.03	114.91	112.19
8	L	4	MAN	O5-C5-C6	2.02	111.60	107.66
8	L	3	BMA	C3-C4-C5	2.01	113.88	110.23
3	G	3	BMA	O4-C4-C3	-2.00	105.66	110.38

There are no chirality outliers.

All (39) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	K	6	MAN	O5-C5-C6-O6
6	J	6	MAN	O5-C5-C6-O6
6	J	4	MAN	O5-C5-C6-O6
3	G	3	BMA	O5-C5-C6-O6
8	L	4	MAN	O5-C5-C6-O6
6	J	6	MAN	C4-C5-C6-O6
5	I	5	MAN	C4-C5-C6-O6
4	H	4	BMA	O5-C5-C6-O6
5	I	5	MAN	O5-C5-C6-O6
7	K	6	MAN	C4-C5-C6-O6
4	H	2	NAG	O5-C5-C6-O6
8	L	5	BMA	O5-C5-C6-O6
7	K	4	BMA	C4-C5-C6-O6
3	G	4	MAN	O5-C5-C6-O6
8	L	4	MAN	C4-C5-C6-O6

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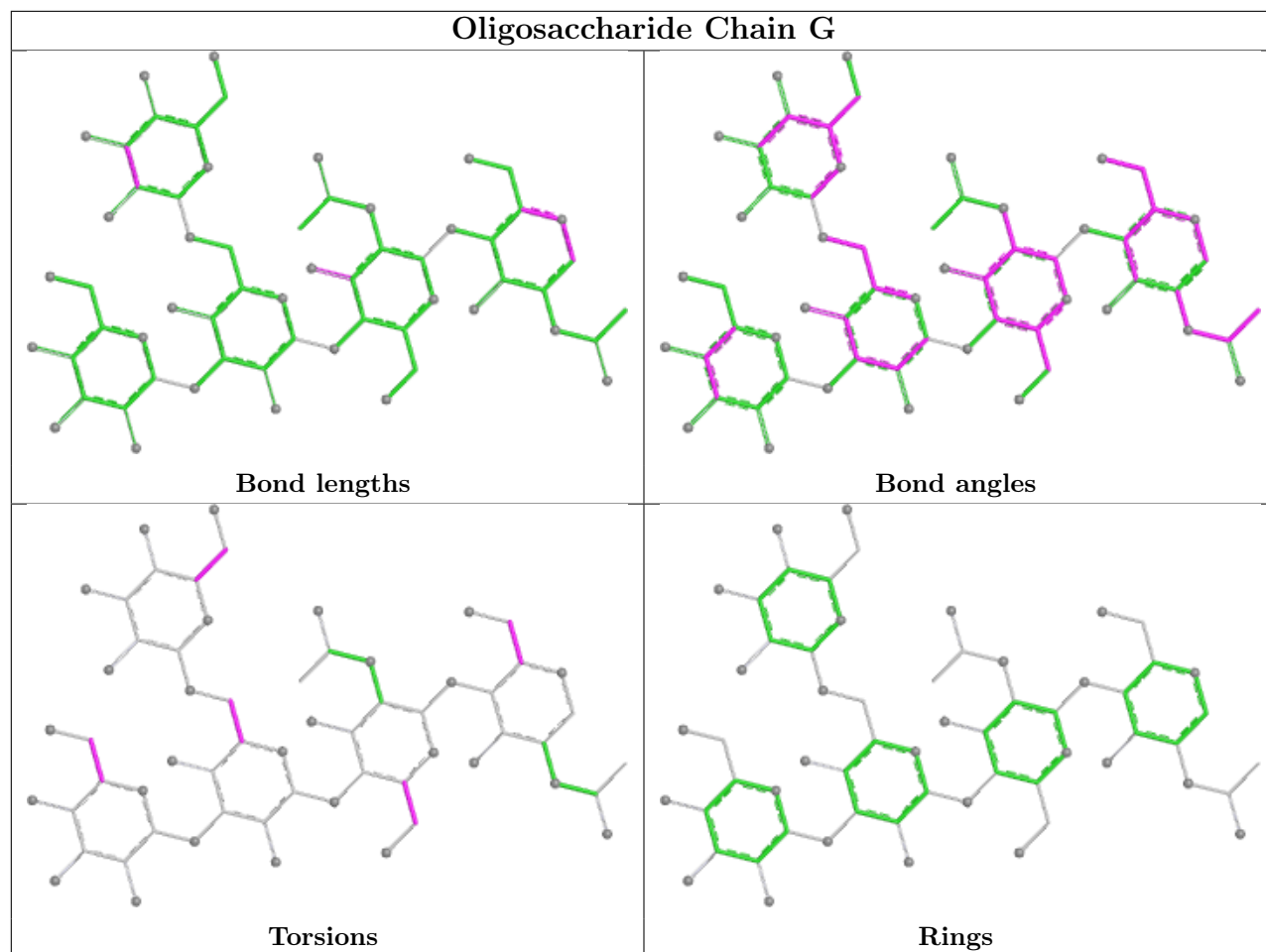
Mol	Chain	Res	Type	Atoms
8	L	5	BMA	C4-C5-C6-O6
6	J	4	MAN	C4-C5-C6-O6
3	G	3	BMA	C4-C5-C6-O6
4	H	2	NAG	C4-C5-C6-O6
5	I	3	BMA	C4-C5-C6-O6
5	I	3	BMA	O5-C5-C6-O6
3	G	2	NAG	C4-C5-C6-O6
3	G	2	NAG	O5-C5-C6-O6
7	K	3	BMA	O5-C5-C6-O6
7	K	3	BMA	C4-C5-C6-O6
7	K	4	BMA	O5-C5-C6-O6
7	K	2	NAG	O5-C5-C6-O6
3	G	5	BMA	O5-C5-C6-O6
4	H	4	BMA	C4-C5-C6-O6
5	I	6	MAN	O5-C5-C6-O6
3	G	4	MAN	C4-C5-C6-O6
4	H	3	BMA	O5-C5-C6-O6
3	G	1	NAG	C4-C5-C6-O6
4	H	3	BMA	C4-C5-C6-O6
5	I	2	NAG	C4-C5-C6-O6
6	J	1	NAG	C1-C2-N2-C7
7	K	1	NAG	O5-C5-C6-O6
7	K	1	NAG	C4-C5-C6-O6
7	K	2	NAG	C4-C5-C6-O6

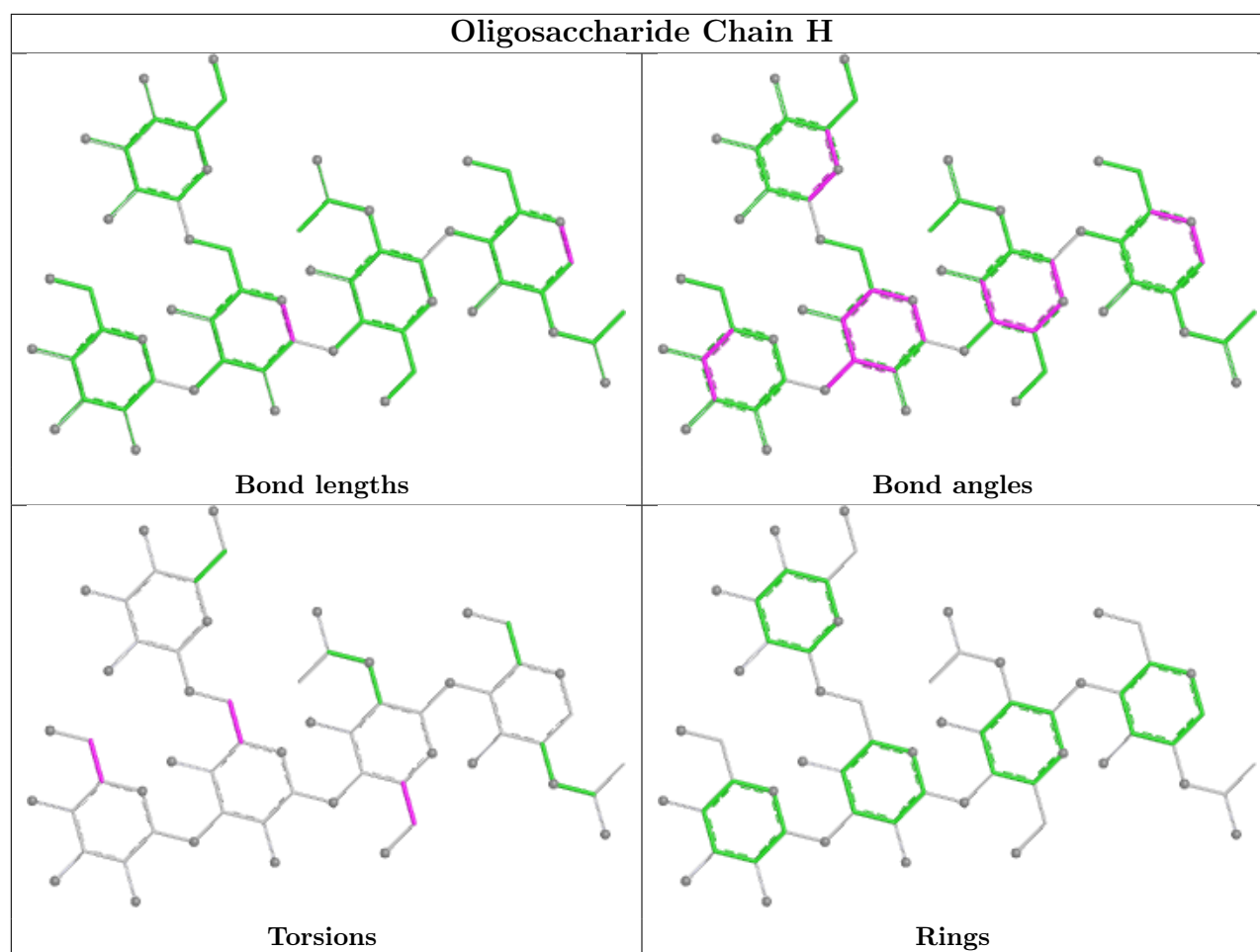
There are no ring outliers.

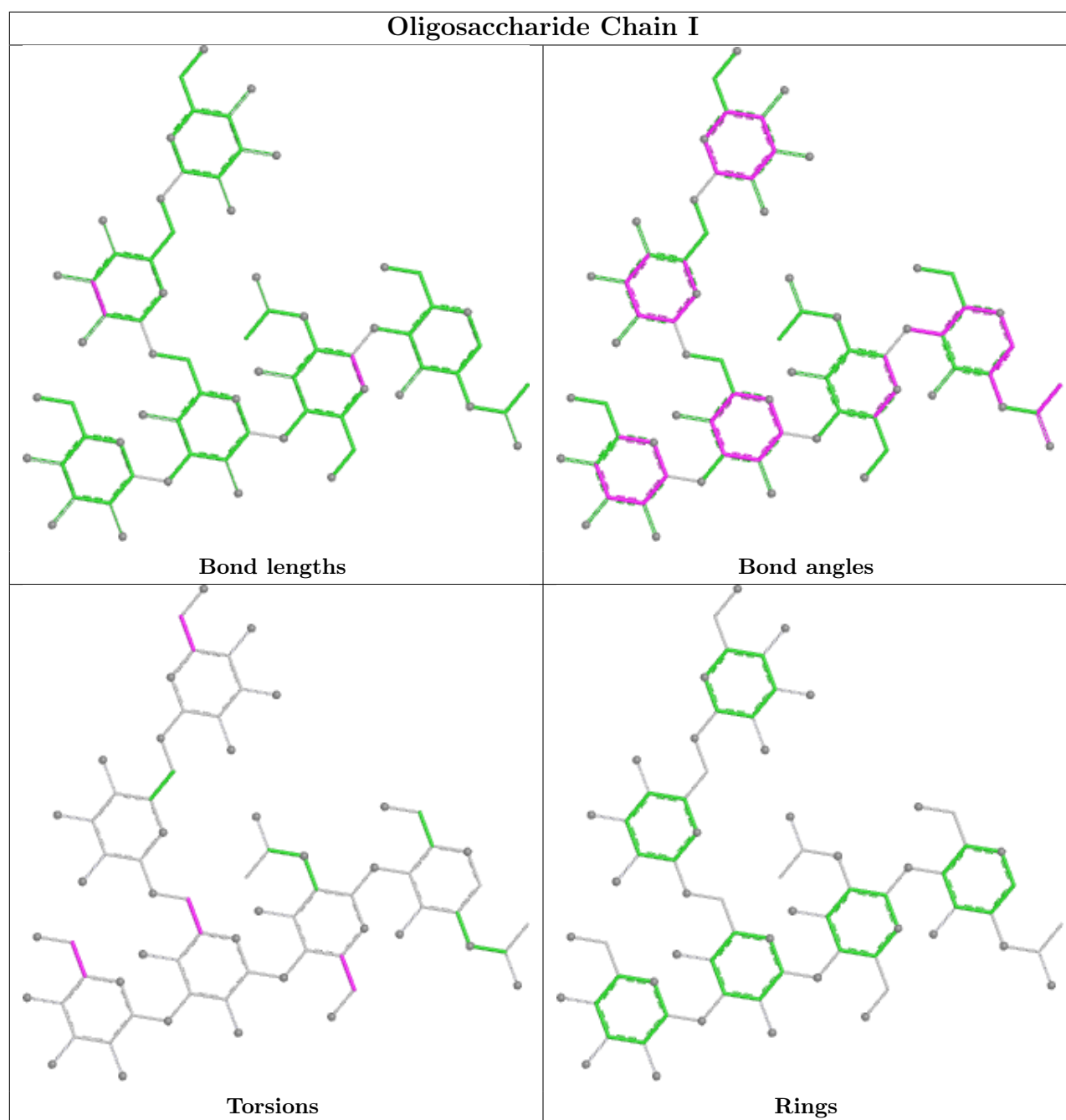
5 monomers are involved in 4 short contacts:

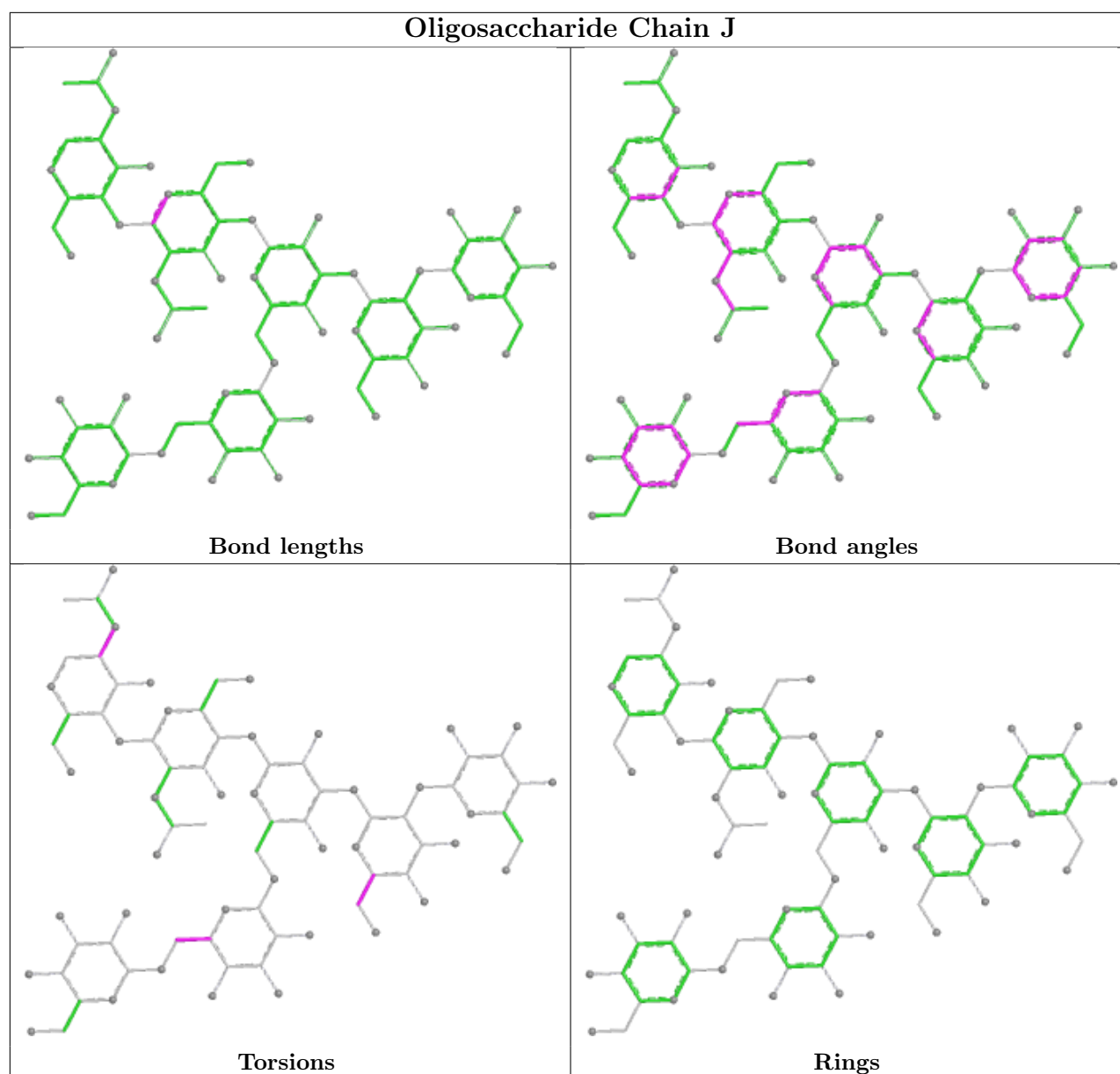
Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	K	5	BMA	1	0
7	K	4	BMA	1	0
4	H	3	BMA	2	0
4	H	1	NAG	1	0
4	H	2	NAG	2	0

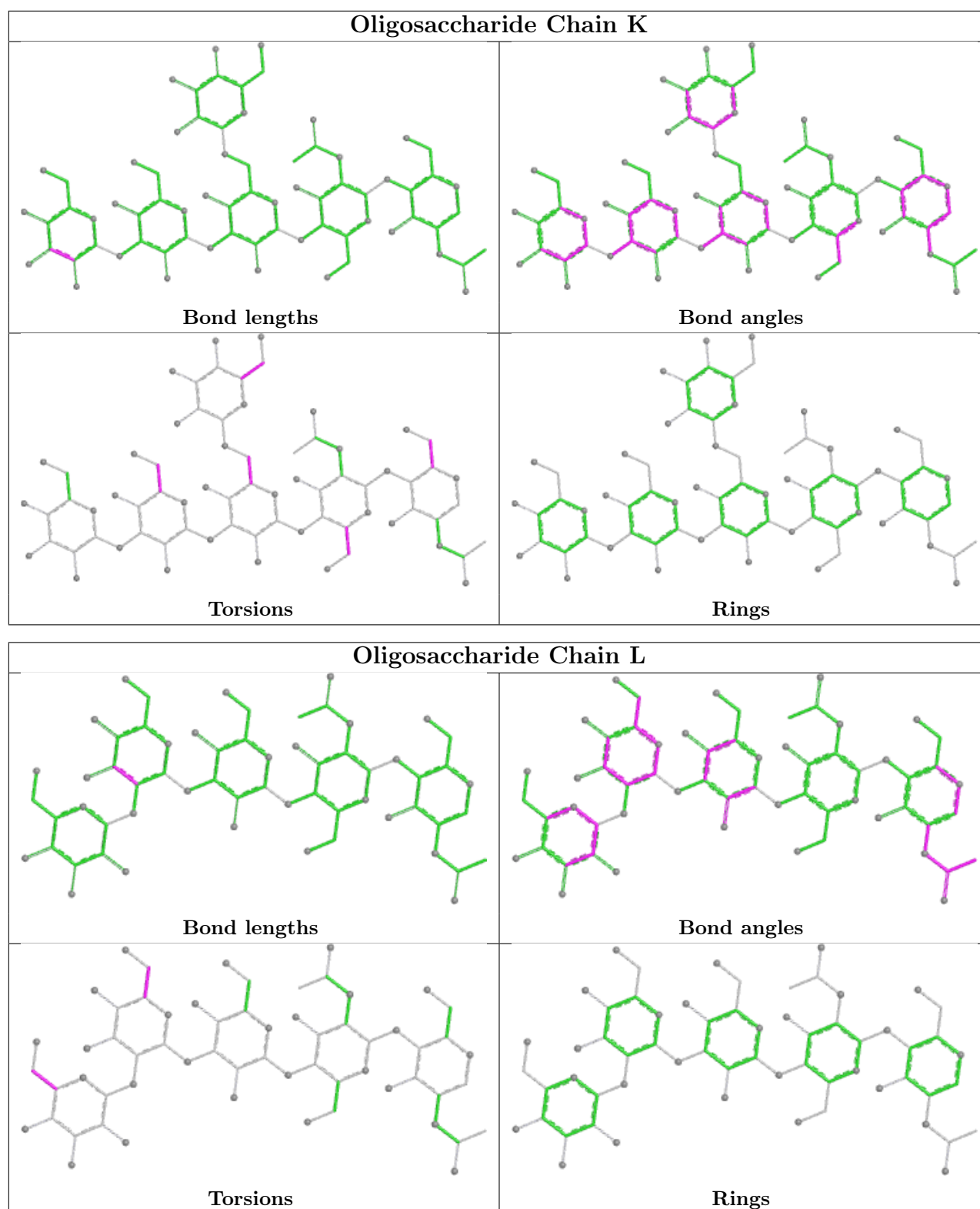
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.











5.6 Ligand geometry ⓘ

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	670/703 (95%)	-0.59	8 (1%) 76 68	20, 43, 85, 213	0
1	E	669/703 (95%)	-0.51	6 (0%) 81 74	24, 50, 91, 234	0
1	F	669/703 (95%)	-0.23	13 (1%) 66 57	27, 59, 102, 206	0
2	B	668/696 (95%)	-0.30	8 (1%) 76 68	25, 54, 92, 167	0
2	C	668/696 (95%)	-0.50	4 (0%) 85 80	24, 46, 86, 142	0
2	D	672/696 (96%)	-0.59	3 (0%) 88 84	20, 42, 82, 159	0
All	All	4016/4197 (95%)	-0.45	42 (1%) 79 72	20, 49, 92, 234	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	346	PHE	4.7
1	F	645	PHE	3.8
2	B	640	ALA	3.6
2	B	213	LEU	3.6
1	F	641	PRO	3.4
1	F	309	PHE	3.2
2	B	215	TYR	3.2
1	F	639	LEU	3.1
1	E	639	LEU	3.0
2	B	382	PHE	2.9
1	F	642	PHE	2.9
1	F	604	PHE	2.9
1	A	639	LEU	2.8
1	F	636	GLY	2.8
1	E	645	PHE	2.7
1	A	645	PHE	2.7
1	F	306	LEU	2.6
2	B	214	THR	2.6
2	C	186	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	642	PHE	2.5
1	E	647	LEU	2.5
1	A	640	ALA	2.4
1	E	24	THR	2.4
1	A	647	LEU	2.3
2	B	630	PRO	2.3
2	B	357	SER	2.3
2	B	305	PHE	2.2
1	F	640	ALA	2.2
1	F	646	VAL	2.2
2	D	348	ALA	2.2
2	C	632	PRO	2.2
2	C	346	PHE	2.2
2	D	353	ILE	2.1
1	A	641	PRO	2.1
1	F	308	LYS	2.1
1	E	642	PHE	2.1
2	C	349	PHE	2.1
1	A	309	PHE	2.1
1	F	310	THR	2.1
1	F	24	THR	2.0
1	A	646	VAL	2.0
1	E	646	VAL	2.0

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
8	BMA	L	5	11/12	0.39	0.13	110,121,124,125	0
7	BMA	K	5	11/12	0.55	0.12	103,108,112,114	0
6	MAN	J	7	11/12	0.55	0.11	98,111,114,115	0
4	MAN	H	5	11/12	0.58	0.12	91,97,100,100	0
5	MAN	I	5	11/12	0.59	0.10	102,112,115,115	0

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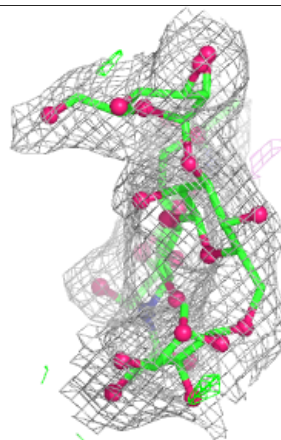
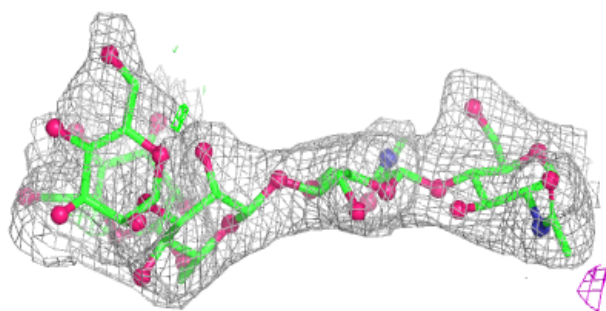
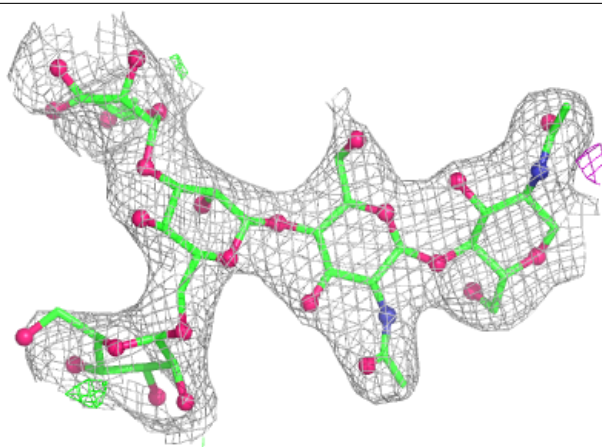
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	BMA	G	5	11/12	0.65	0.11	82,89,96,102	0
6	MAN	J	6	11/12	0.72	0.11	98,100,105,111	0
4	BMA	H	4	11/12	0.72	0.10	104,108,110,110	0
5	MAN	I	4	11/12	0.73	0.09	92,96,101,105	0
6	MAN	J	5	11/12	0.74	0.10	95,110,118,122	0
5	MAN	I	6	11/12	0.78	0.10	88,94,97,98	0
3	MAN	G	4	11/12	0.78	0.10	66,67,72,74	0
4	BMA	H	3	11/12	0.79	0.09	89,95,100,101	0
7	MAN	K	6	11/12	0.84	0.08	69,73,76,77	0
7	BMA	K	3	11/12	0.84	0.10	57,65,73,74	0
7	BMA	K	4	11/12	0.85	0.10	78,88,92,99	0
6	BMA	J	3	11/12	0.85	0.08	66,77,88,89	0
8	MAN	L	4	11/12	0.86	0.09	95,97,104,108	0
8	BMA	L	3	11/12	0.86	0.08	71,74,79,87	0
6	MAN	J	4	11/12	0.90	0.09	89,94,100,106	0
4	NAG	H	2	14/15	0.92	0.08	58,66,76,83	0
8	NAG	L	2	14/15	0.93	0.08	55,60,65,68	0
3	BMA	G	3	11/12	0.93	0.07	50,59,65,72	0
4	NAG	H	1	14/15	0.93	0.09	48,51,58,59	0
5	BMA	I	3	11/12	0.93	0.06	72,82,88,93	0
5	NAG	I	2	14/15	0.94	0.07	51,57,63,70	0
3	NAG	G	2	14/15	0.94	0.07	37,42,49,49	0
6	NAG	J	1	14/15	0.95	0.06	36,37,39,43	0
8	NAG	L	1	14/15	0.95	0.08	47,51,56,56	0
6	NAG	J	2	14/15	0.95	0.07	44,47,53,60	0
7	NAG	K	2	14/15	0.96	0.07	45,48,55,56	0
5	NAG	I	1	14/15	0.96	0.07	40,43,46,49	0
3	NAG	G	1	14/15	0.97	0.05	27,30,32,36	0
7	NAG	K	1	14/15	0.97	0.05	36,38,42,43	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.

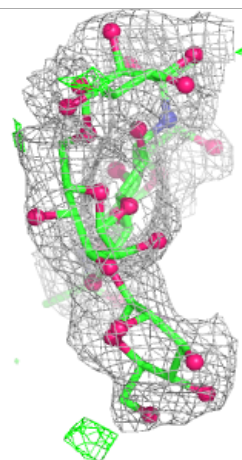
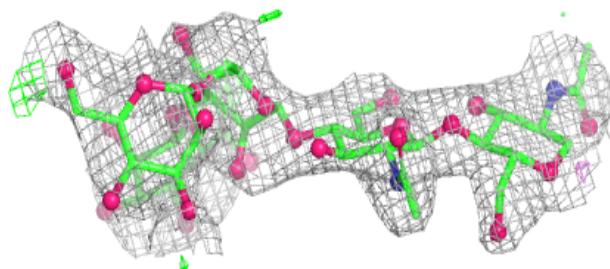
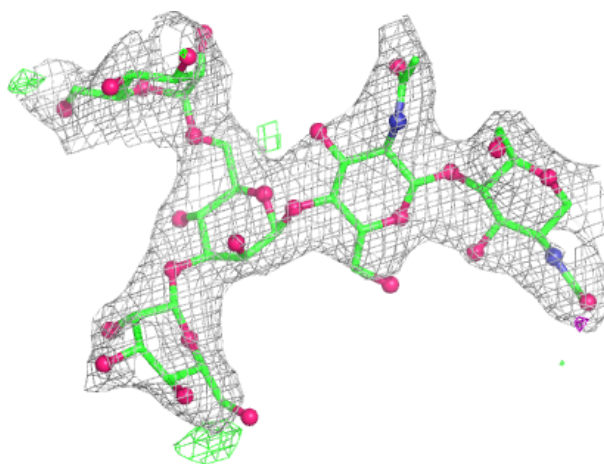
Electron density around Chain G:

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



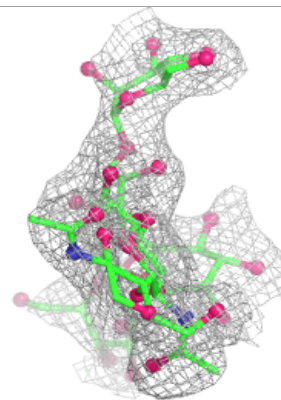
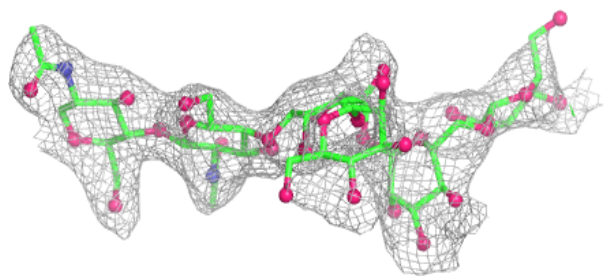
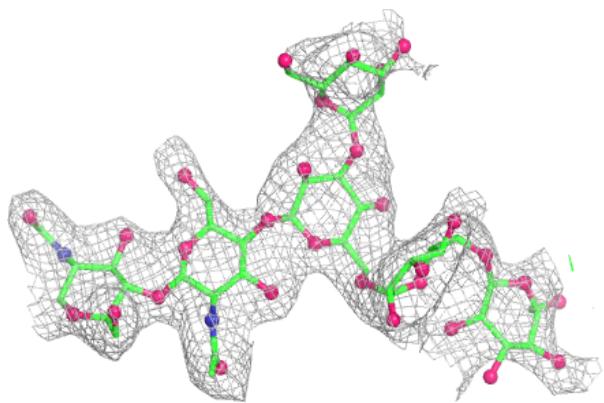
Electron density around Chain H:

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

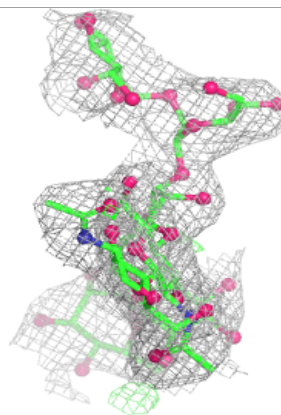
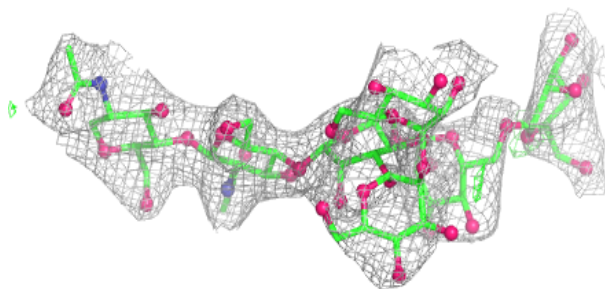
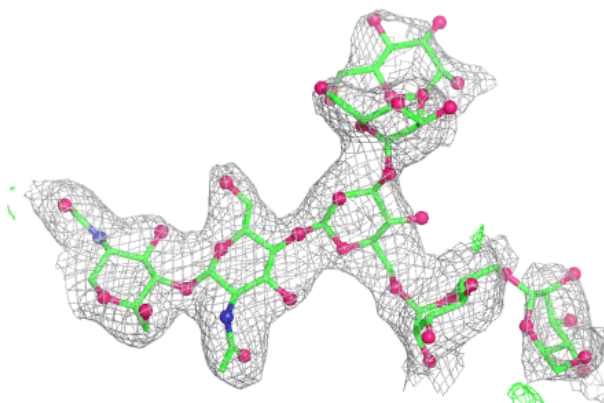


Electron density around Chain I:

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

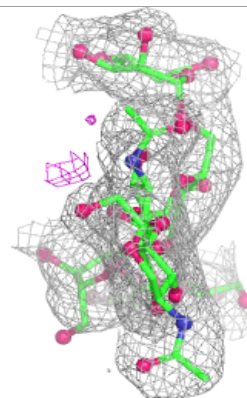
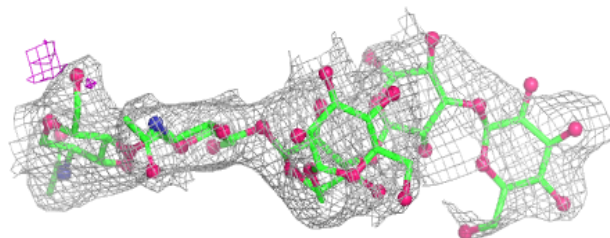
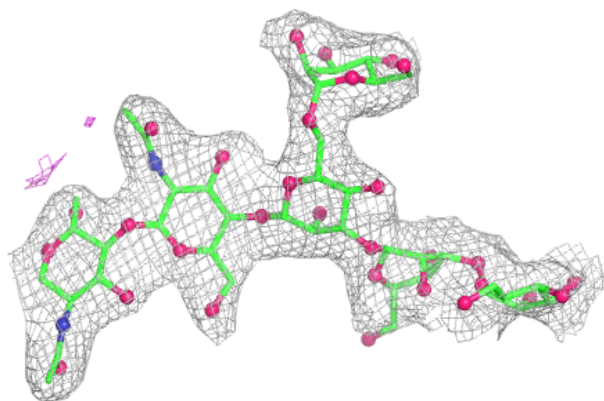
**Electron density around Chain J:**

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

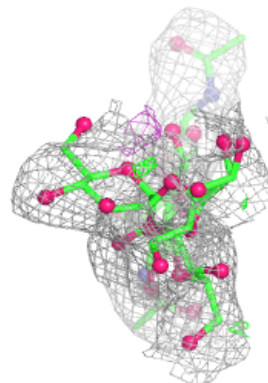
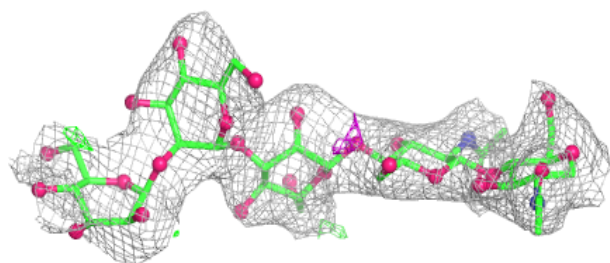
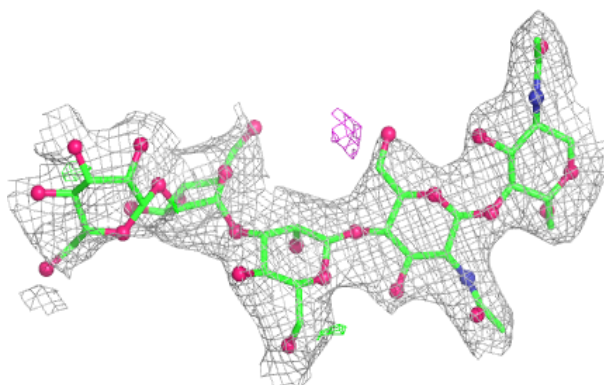


Electron density around Chain K:

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

**Electron density around Chain L:**

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



6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.